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DEVELOPMENT OF PHASE 1 IHLW MODELS FOR PCT RESPONSE AND ONE-PERCENT CRYSTAL FRACTION TEMPERATURE (T1%), VSL-05R5780-1, REV. 0

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

P.O. Box 550
Richland, Washington 99352

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Final Report

Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature ($T_{1\%}$)

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Rev. 0

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Completeness of Testing:

This report describes the results of work and testing specified by the above-listed Test Specifications, Test Plans, and Test Exceptions. The work and any associated testing followed established quality assurance requirements and were conducted as authorized. The descriptions provided in this report are an accurate account of both the conduct of the work and the data collected. Results required by the Test Plans are reported. Also reported are any unusual or anomalous occurrences that are different from the starting hypotheses. The test results and this report have been reviewed and verified.

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VSL Program Director/Principal Investigator

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ACED	Algorithms for the Construction of Experimental Designs (commercial software used to select a mixture experiment design from a set of candidate points)
AES	Atomic Emission Spectroscopy
ANL	Argonne National Laboratory
CUA	Catholic University of America
CVS	Composition Variation Study
DCP	Direct Current Plasma
DOE	United States Department of Energy
DWPF	Defense Waste Processing Facility
EA	Environmental Assessment
EDS	Energy Dispersive X-Ray Spectroscopy
EGCR	Experimental Glass Composition Region
EPA	United States Environmental Protection Agency
HLW	High Level Waste
HWVP	Hanford Waste Vitrification Plant
ID	Identification
IHLW	Immobilized High Level Waste
ILAW	Immobilized Low Activity Waste
LAW	Low Activity Waste
LM	Linear Mixture
LOF	Lack-of-Fit
LRM	Low Activity Waste Reference Material
MIXSOFT	commercial software used to design mixture and other constrained region experiments
NCAW	Neutralized Current Acid Waste
NQA	Nuclear Quality Assurance
PCT	Product Consistency Test
PI	Prediction Interval
PNNL	Pacific Northwest National Laboratory
PNWD	Battelle—Pacific Northwest Division
PQM	Partial Quadratic Mixture
PvM	Predicted versus Measured
QA	Quality Assurance
QARD	Quality Assurance Requirements and Descriptions Document
QGCR	Qualified Glass Composition Region
R^2	This statistic is referred to as *R-squared*, and is the proportion of variation in values of a response variable over a model development dataset that is accounted for by a fitted model. The R^2 statistic takes a value between 0 and 1.
R_A^2	This statistic is referred to as *adjusted R-squared*, and is the proportion of variation in values of a response variable over a model development

	dataset that is accounted for by a fitted model after adjusting for the number of fitted coefficients in the model. The R_A^2 statistic takes a value between 0 and 1, and $R_A^2 \leq R^2$.
R_P^2	This statistic is referred to as *predicted R-squared*, and is the proportion of variation in values of a response variable over a model development dataset that is accounted for by a fitted model, where each data point is in-turn left out of the fitting process and thus not used to obtain the predicted value of the response variable for that data point. Generally $R_P^2 \leq R_A^2 \leq R^2 \leq 1$, although R_P^2 can take negative values in cases where there are one or more highly influential data points in the model development dataset.
R_V^2	This statistic is referred to as validation *R-squared*, and is the proportion of variation in values of a response variable over a model validation dataset that is accounted for by a fitted model. Generally $R_V^2 \leq R_P^2 \leq R_A^2 \leq R^2 \leq 1$, although R_V^2 can take negative values and can take values larger than R_P^2, R_A^2, or R^2.
RCRA	Resource Conservation and Recovery Act
RMSE	Root-Mean-Squared-Error
RPD	Relative Percent Difference
RPP	River Protection Project
RSD	Relative Standard Deviation
SD	Standard Deviation
SEM	Scanning Electron Microscopy
SUCI	Simultaneous Upper Confidence Interval
$T_{1\%}$	One-Percent Crystal Fraction Temperature
T_L	Liquidus Temperature
THERMO	Thermal Hydration Energy Reaction Model
TCLP	Toxicity Characteristic Leaching Procedure
TF COUP	Tank Farm Contractor Operations and Utilization Plan
TWRS	Tank Waste Remediation System
UCI	Upper Confidence Interval
ULS	Unweighted Least Squares
VSL	Vitreous State Laboratory
WAPS	Waste Acceptance Product Specification
WASRD	Waste Acceptance System Requirements Document
WLS	Weighted Least Squares
WTP	Hanford Tank Waste Treatment and Immobilization Plant
WTPSP	Waste Treatment Plant Support Project
WVDP	West Valley Demonstration Project
WVNS	West Valley Nuclear Services
XRF	X-ray Fluorescence Spectrometry

SUMMARY OF TESTING

A) Objectives

This report is one in a series of reports that presents the results from the High Level Waste (HLW) glass formulation development and testing work performed at the Vitreous State Laboratory (VSL) of the Catholic University of America (CUA) and the development of IHLW property-composition models performed jointly by Battelle-Pacific Northwest Division (PNWD) and VSL for the River Protection Project-Waste Treatment and Immobilization Plant (RPP-WTP). Specifically, this report presents results of glass testing and model development at VSL and PNWD for Phase 1 IHLW Product Consistency Test (PCT) and one-percent crystal fraction temperature ($T_{1\%}$) models. The models presented in this report will be augmented and refined during Phase 2 of the IHLW model development work. The Phase 2 IHLW PCT and $T_{1\%}$ models will be used to support qualification of the IHLW products. Completion of the test objectives is addressed in the table below.

Test Objective	Objective Met	Discussion
Develop property-composition models and supporting data that relate IHLW performance on the PCT to IHLW composition and are suitable for predicting the PCT performance of IHLW glasses to be produced in the WTP.	Yes	The PCT models developed are described in Section 5. The supporting data are described in Section 4. The test matrices and experimental methods are described in Sections 2 and 3, respectively. Two models are recommended to predict each of the PCT responses (i.e., B, Na, and Li): a 19-term full linear mixture model, and an 8-term reduced linear mixture model. The full models are intended as baselines, but both the full models and reduced models are recommended to be applied and their performances compared during IHLW glass formulation and waste form qualification work.
Develop models for liquids temperature (T_L) suitable for predicting the primary liquidus phase in RPP-WTP glasses. This phase is expected to be spinel for AZ-101, AZ-102, and AY-102/C-106 wastes, and thorium-containing phases for AY-101/C-104 wastes.	Yes	As directed by WTP, instead of models used to predict T_L, models were developed for prediction of $T_{1\%}$ (see Section B below), which are described in Section 6. The supporting data are described in Section 4. The test matrices and experimental methods are described in Sections 2 and 3, respectively. The models developed are for predicting $T_{!\%}$ *only* in glasses with spinel as the primary crystalline phase. Upcoming Phase 2 modeling efforts will address AY-101/C-104 glasses, which are expected to exhibit thorium-containing liquidus phases. Two models are recommended to predict (spinel) $T_{1\%}$: a 13-term reduced linear mixture model and a 19-term full linear mixture model. The reduced model is preferred as the primary Phase 1 model, but again, both models are recommended to be applied and their performances compared during IHLW glass formulation and waste form qualification work.

Other objectives in the Test Specification and Test Plans for this work relate to the development of models for other properties. Property-composition models have been developed to predict the Toxicity Characteristic Leaching Procedure (TCLP) performance of IHLW glasses. The TCLP models and associated data are the subjects of a separate report that will be used to support a petition to delist IHLW glasses. Models to predict viscosity and electrical conductivity of glass melts have also been developed and reported previously. Section 1 of this report provides further discussion of these test objectives and references to the corresponding reports.

B) Test Exceptions

One of the initial test objectives was to develop models for predicting the liquidus temperature (T_L) of the primary liquidus phase in HLW glasses, which addresses a WTP process requirement to avoid formation and subsequent settling of crystals in the melter. However, in practice, all HLW glasses are in fact produced below the liquidus temperature because of the presence of noble metals in the wastes. In addition, a strict application of the liquidus temperature for phases other than noble metals also is overly restrictive on waste loading. In view of these considerations, the WTP has instead adopted an operational definition of the original liquidus temperature requirement: the glass melt must contain less than 1% by volume of crystalline phases at 950°C. Accordingly, WTP R&T directed the change from modeling T_L to modeling $T_{1\%}$, which was documented in a Test Exception (24590-WTP-TEF-RT-03-078, Rev. 0).

C) Results and Performance Against Success Criteria

The data in this work were based on a Combined Matrix of glasses that was composed of 102 HLW glasses (including 57 glasses from the Initial Matrix to focus on AZ-101, AZ-102, and AY-102/C-106 wastes, and 45 glasses from the Augmentation Matrix to include AY-101/C-104 wastes).

The measured PCT results varied from 0.104 g/l (excluding one extreme outlier) to 4.418 g/l for boron, 0.378 g/l to 3.252 g/l for lithium, and 0.076 g/l to 2.802 g/l for sodium. These can be compared with the PCT release values for the DWPF-EA glass: 16.695 g/l for boron, 9.565 g/l for lithium, and 13.346 g/l for sodium. Thus, all the matrix glasses outperformed the DWPF-EA glass, which was expected because the benchmark values from the DWPF-EA glass were used as PCT constraints to design the matrices. The PCT data collected are seen to follow the expected general trends as functions of the glass composition: glass formers including B_2O_3 and SiO_2 typically reduce PCT releases while glass modifiers such as Na_2O and Li_2O have the opposite effect.

The PCT data were fitted to linear mixture (LM) models and partial quadratic mixture (PQM) models. A number of regression statistics were then computed to assess the performance of the fitted models. Validation of the models was performed in two ways. The primary validation method involved data-splitting, in which a subset of the data was left out of model regression and the ability of the resulting model to predict the responses for the omitted data was

then assessed. The second validation method assessed the ability of the fitted models to predict the responses for a set of 574 glasses from earlier independent studies. The data set for the 574 glasses was divided into subsets based on the closeness of glass compositions to the compositional region defined by the Combined Matrix.

Based on the modeling data, statistics, and model validations, fitted models were selected from among those investigated as the recommended IHLW Phase 1 models. For each of the responses of PCT-boron, -lithium, and -sodium, two models were recommended: (i) a 19-term full LM model, and (ii) an 8-term reduced LM model. The 19-term full LM models were intended as baselines for comparisons with the performance of the reduced LM models. It is recommended that both the full LM models and reduced LM models be applied and their performances compared during IHLW glass formulation and waste form qualification work. Finally, an example was provided to illustrate how to predict PCT releases and estimate model prediction uncertainty for a given HLW glass composition.

Of the 102 Combined Matrix glasses, $T_{1\%}$ values could be estimated for 97, spinel being the dominant crystalline phase for 91 of those 97 glasses. After exclusion of one outlier, the $T_{1\%}$ values range from 741 °C to 1248 °C, with a median of 946.1 °C (compared with the WTP process requirement of $T_{1\%} \leq 950$°C) suggesting a fairly symmetric distribution of $T_{1\%}$ values in the range of interest. Gross compositional trends of the estimated $T_{1\%}$ values were less evident than was the case for the PCT data and no simple correlations between compositions and $T_{1\%}$ could be identified.

Data for 90 of the Combined Matrix glasses were fitted to LM models and PQM models to predict $T_{1\%}$ with spinel as the primary crystalline phase. Validation of the models followed closely that used for the PCT models. That is, two validation methods were used, with the primary method using data-splitting and the secondary method using an independent data set. However, because relatively few data have been published on volume % crystal fractions, data for only 39 glasses were available for the secondary validation, including many HLW glasses developed for WTP studies. These glasses were also divided into validation data subsets according to the closeness of their compositions to the matrix compositional space.

Based on the modeling data, statistics, and model validations, fitted $T_{1\%}$ models were selected as the recommended IHLW Phase 1 models. Two models again were recommended, including a 13-term reduced LM model as the primary Phase 1 model, with a 19-term full LM model as a baseline for comparison to the reduced LM model. The reduced LM containing more terms than the PCT reduced LM model (13 vs. 8) likely is a reflection of the more complex relationship that exists between crystal formation and composition. It is also recommended that both these IHLW $T_{1\%}$ models be applied and their performances compared during future IHLW glass formulation and waste form qualification to predict $T_{1\%}$ with spinel as the dominant crystalline phase. Finally, an example was provided to illustrate how to predict $T_{1\%}$ and estimate model prediction uncertainty for a given HLW glass composition.

D) Quality Requirements

The portions of this work performed at VSL were conducted under a quality assurance (QA) program compliant with NQA-1 (1989) and NQA-2a (1990) subpart 2.7 and DOE/RW-0333P, Rev. 13, "Quality Assurance and Requirements and Description" (QARD). This program is supplemented by a Quality Assurance Project Plan for RPP-WTP work performed at VSL. Test and procedure requirements by which the testing activities are planned and controlled are also defined in this plan. The program is supported by VSL standard operating procedures that were used for this work.

The QA requirements for the PNWD work were met through the Quality Assurance Project Plan for the PNWD Waste Treatment Plant Support Project (WTPSP). The WTPSP implementing procedures comply with the requirements of NQA-1, NQA-2a Part 2.7, and QARD, Rev. 13.

The following specific areas are subject to QARD: glass preparation, glass compositional analysis, PCT testing, and PCT model development. All work in these areas was performed according to VSL and PNWD QA programs and implementing procedures that are compliant with QARD.

E) R&T Test Conditions

The compositions of the Combined Matrix glasses were developed by applying statistical experimental design methods to optimally cover compositional regions defined by various constraints. These constraints were developed by considering a variety of inputs including waste compositions and glass properties.

The 102 Combined Matrix glasses were fabricated and characterized with respect to composition, PCT responses, and crystal formation (volume %) vs. heat-treatment temperature. Regression of the volume % crystal fraction data provided estimates of $T_{1\%}$. All data are reported herein. In addition, glasses from previous work (some of which were in support of the WTP) were selected to provide independent data for model validation. PCT- and $T_{1\%}$-glass composition models were developed by regression of the Combined Matrix glasses and validated by a combination of data-splitting using the regression set as well as by independent validation using the validation set. Based on the performance of the models that were investigated, recommended models were selected.

Crucible melts of the glasses (about 420 g) were prepared by melting mixtures of reagent grade or higher purity chemicals in platinum-gold crucibles at 1150°C for 120 minutes. Mixing of the batched chemicals was accomplished by dry blending while mixing of the melt was accomplished mechanically using a platinum stirrer. Samples of the resulting glasses were then analyzed by XRF on solid samples. The PCT (at 90°C for seven days) was performed on all of the glasses and the leachates were analyzed by Direct Current Plasma-Atomic Emission Spectroscopy. The Combined Matrix glasses were heat treated isothermally between 650°C and 1200°C (after a pre-melt temperature of 1200°C) at selected temperatures for 70+ hours. The

heat-treated samples were examined by Scanning Electron Microscopy and Energy Dispersive X-ray Spectroscopy to identify the crystalline phases and to estimate their volume fraction.

F) Simulant Use

Waste simulants were not used in this work. All of the glasses were prepared from reagent grade chemicals in combinations designed to achieve the target compositions in the statistically-designed test matrices.

G) Discrepancies and Follow-On Tests

Follow-on tests are planned as part of the Phase 2 model development effort, which will provide the final WTP models for the IHLW PCT and $T_{1\%}$ responses. In particular, Phase 2 efforts will include the development of models to predict $T_{1\%}$ for RPP-WTP IHLW glasses (e.g., for AY-101/C-104 wastes) that are expected to exhibit thorium-containing phases as the primary crystalline phases.

SECTION 1
INTRODUCTION

The United States Department of Energy's (DOE's) Hanford site in the state of Washington is the current storage location of about 50 million gallons of high level mixed waste. This waste is stored in underground tanks at the Hanford site. The Hanford Tank Waste Treatment and Immobilization Plant (WTP) will provide DOE with a means for treating this waste by vitrification for subsequent disposal. The tank waste will be partitioned into low and high activity fractions, which will then be vitrified respectively into Immobilized Low Activity Waste (ILAW) and Immobilized High Level Waste (IHLW) products. The ILAW product will be disposed of in an engineered facility on the Hanford site while the IHLW product will be directed to the national deep geological disposal facility for high level nuclear waste. The ILAW and IHLW products must meet a variety of requirements with respect to protection of the environment before they can be accepted for disposal.

This report is one in a series of reports that present the results from High Level Waste (HLW) glass formulation development and testing work, which was performed at the Vitreous State Laboratory (VSL) of the Catholic University of America (CUA), and the results from development of IHLW property-composition models, which was performed jointly by Battelle–Pacific Northwest Division (PNWD) and VSL for the WTP. Specifically, this report presents results of glass testing and development of Phase 1 IHLW models for two glass properties: models that relate Product Consistency Test (PCT) responses (i.e., releases of boron, lithium, and sodium) to glass composition, and models that relate $T_{1\%}$, which is the temperature at which the volume fraction of crystals in equilibrium with glass melt equals 1%, to glass composition. The models reported herein will be used to support qualification of the IHLW products for disposal. These models will be augmented and refined during Phase 2 of model development, which is planned for 2005 through 2007.

This report is responsive to the Test Specifications [1, 2], Test Plans [3, 4] and Test Exception [5] for HLW property-composition modeling. The objective of the work described in these documents is to develop property-composition models to support HLW waste form qualification and processing. It is intended that the models will provide the basis to define the Qualified Glass Composition Regions (QGCRs), operating ranges and target glass compositions for HLW processing at the WTP.

1.1 Test Objectives

The objectives of the HLW glass property-composition modeling work as given in the Test Plans [3, 4] are listed below along with the strategy to address them.

- *Develop property-composition models and supporting data that relate IHLW performance on the PCT to IHLW composition and are suitable for predicting the PCT performance of IHLW glasses to be produced in the WTP.*

  Development of the Phase 1 PCT property-composition model is presented in this report. The data used in developing the model have previously been reported [6].

- *Develop models for liquidus temperature (T_L) suitable for predicting the primary liquidus phase in RPP-WTP glasses. This phase is expected to be spinel for AZ-101, AZ-102, and AY-102/C-106 wastes, and thorium-containing phases for AY-101/C-104 wastes.*

  As directed by the Test Exception [5], instead of liquidus temperature (T_L) models, models to predict one-percent crystal fraction temperatures ($T_{1\%}$) have been developed and are presented herein. The change to modeling $T_{1\%}$ instead of T_L was made because WTP is adopting an operational definition of liquidus temperature and corresponding limit. Specifically, the amount of crystalline phases that are present in equilibrium with the glass melt at 950°C must be less than 1 volume %. The less-conservative operational definition is adopted in recognition of the fact that all HLW glasses are, in actuality, produced below the liquidus temperature of the glass melt as a result of the presence of sparingly soluble species such as noble metals in the wastes. A strict application of the liquidus temperature criterion (for phases other than noble metals) is also overly restrictive on waste loading. Preliminary information on the $T_{1\%}$ data and models has been reported previously [7].

  As will be seen subsequently, the difference in compositions between (i) AZ-101, AZ-102, and AY-106/C-106 wastes and (ii) AY-101/C-104 wastes was addressed by the development of two test matrices of glass compositions, each focusing on the expected characteristic compositions of the two groups.

- *Develop property-composition models and supporting data that relate IHLW performance in the TCLP to IHLW composition and are suitable for predicting the TCLP performance of IHLW glasses to be produced in the WTP.*

  Toxicity Characteristic Leaching Procedure (TCLP) data have been collected on 118 HLW glasses (including replicates) and the data used to support the development of a TCLP cadmium release model. The data and the developed model have been reported [8].

- *Develop property-composition models that relate viscosity and electrical conductivity of glass melts to IHLW composition and are suitable for predicting the properties of IHLW glasses to be produced in the WTP*.

  Viscosity and electrical conductivity data have been collected on 102 HLW glasses (including replicates) and part of the data (60 glasses) were used in the investigation of model forms and development of viscosity and conductivity models. These data and models have been reported previously [9].

- *Develop property-composition models that relate density of IHLW glasses to composition in order to predict overall volumes of IHLW that would be produced from a given waste feed.*

The density property-composition model may be developed and reported at a later date if so directed by WTP R&T.

1.2 Test Overview

The development of PCT and $T_{1\%}$ property-composition models was a multi-step process that involved:

(i) The development of constraints on IHLW components describing the IHLW experimental glass composition regions (EGCRs) of interest (These constraints were developed at the Vitreous State Laboratory (VSL) of The Catholic University of America (CUA) based on inputs from the WTP Project. Because the initial focus was on developing TCLP models, which had the earliest WTP need date, IHLW components and constraints were included that were relevant to modeling TCLP releases. However, the same IHLW composition region and test matrices also formed the basis for PCT and $T_{1\%}$ model development.)

(ii) Statistical design of the test matrices by Battelle–Pacific Northwest Division (PNWD) to adequately explore the EGCRs. (As noted in (i), these test matrices were initially developed for modeling TCLP releases, but were also developed for modeling PCT and $T_{1\%}$ responses.)

(iii) Fabrication of the test glasses in the test matrices at VSL

(iv) PCT and $T_{1\%}$ measurements of the fabricated glasses at VSL

(v) Investigation and recommendation of initial mathematical model forms at VSL

(vi) Detailed statistical analyses of the PCT and $T_{1\%}$ data performed by PNWD to develop the PCT and $T_{1\%}$ models that are reported herein.

The Phase 1 property-composition data and models discussed in this report will be supplemented in future Phase 2 efforts.

Development of the design constraints for the test matrices, which is described in Section 2, required a variety of considerations and inputs including waste compositions. As stated above, the target waste groups for this work are from the source tanks AZ-101, AZ-102, AY-102/C-106, and AY-101/C-104. Based on earlier HLW glass formulation studies [10], the primary crystalline phase for AZ-101, AZ-102, and AY-102/C-106 wastes is expected to be spinel, while thorium- and zirconium-containing phases likely will dominate for AY-101/C-104 waste. Consequently, two sets of constraints have been developed to address the different EGCRs of interest. Statistical experimental design based on the developed constraints, which is

also described in Section 2, resulted in two test matrices: (i) a matrix that contained 57 HLW test glasses, which was termed the *Initial Matrix*, focused on AZ-101, AZ-102, and AY-102/C-106 wastes, and (ii) a matrix with 45 HLW test glasses, which was termed the *Augmentation Matrix* that encompassed AY-101/C-104 wastes as well as the other three wastes. The two test matrices consisting of 102 glasses total, was termed the *Combined Matrix*.

After generation of the test matrices, the 102 test glasses were fabricated (on ≈ 400 g scale) using reagent-grade chemicals in platinum alloy crucibles and then were tested at VSL. Among the tests performed were PCT and crystal fraction determination. The collected data underwent preliminary evaluation and initial analyses at VSL, as well as subsequent assessments by the WTP Project and PNWD. The results formed the basis for the development at PNWD of PCT-composition models and $T_{1\%}$-composition models, together with the associated statistical uncertainty expressions. Fabrication and testing of the 102 matrix glasses are described in Section 3. Section 4 presents and summarizes the PCT and $T_{1\%}$ test data. Sections 5 and 6 respectively describe the development and validation of the PCT and $T_{1\%}$ models; they also discuss the corresponding uncertainly expressions.

SECTION 2
DEVELOPMENT OF TEST MATRICES

In order to develop property-composition models, adequate property-composition data covering the EGCRs of interest are required. This section describes the development and generation of two test matrices to support the collection of the necessary data on the relevant properties. The design and development of both matrices have been reported previously [11, 12]; Section 2.1 summarizes the assumptions and considerations used to develop the EGCRs and design the test matrices. Section 2.2 discusses the resulting matrix glasses. Section 2.3 describes the glasses selected for validation of the property-composition models.

2.1 Development of EGCRs and Test Matrices

The data used to develop property-composition models were collected to cover two regions of simulated HLW glass compositions (i.e., EGCRs). The two EGCRs were developed using information about Hanford HLW compositions, previous WTP glass formulation work, and glass science knowledge and experience. Two EGCRs were developed to focus the modeling efforts on the different waste compositions expected of the initial WTP feed tanks. The first EGCR focused on wastes from AZ-101, AZ-102, and C-106/AY-102 (with blended LAW pretreatment products). The second EGCR expanded the first EGCR to include HLW glasses for C-104/AY-101 wastes, which contain considerable amounts of thorium and zirconium, and increased concentrations of LAW Sr/TRU pretreatment products. Thus the first EGCR is a subregion of the second EGCR. The Initial Matrix explored the first EGCR, while the Augmentation Matrix focused on new portions of the larger second EGCR. Together the Initial and Augmentation Matrices, referred to as the Combined Matrix as mentioned previously, explore the second EGCR. Henceforth, the second EGCR will be referred to as the EGCR, because property-composition models were developed using Combined Matrix data covering that EGCR.

Additionally, it should be noted that the Combined Matrix was developed chiefly to support the development of TCLP property-composition models, which have the earliest WTP need date. The TCLP models are intended to support delisting of the IHLW products that no longer meet the criteria which cause HLW to be listed as hazardous. The use of matrix glasses to support modeling of other properties, including PCT and $T_{1\%}$, was considered a secondary objective. The property-composition databases for PCT and $T_{1\%}$ therefore will require further augmentation during Phase 2 of model development. The phased approach employed in model development allows continual incorporation of new information and data on waste compositions and process knowledge, thus refining and improving the models.

Design of the EGCR involved inputs and considerations of many different kinds; they are summarized in the following sections.

2.1.1 Waste Composition Inputs

The following sources of waste compositions were considered in developing the constraints defining the EGCR, which was to be covered by the Combined Matrix:

- Tank Farm Contractor Operations and Utilization Plan (TF COUP), Rev. 3A [13]
- TF COUP, Rev 2 [14]
- Waste compositions estimates and flow-sheet impacts for HLW streams provided by the WTP [15]
- Data on WTP actual waste samples
- VSL assessments performed during Part B1 work [10]
- LAW Sr/TRU pretreatment product compositions [16]
- For the Augmentation Matrix, additional information on waste composition was provided by WTP guidance [17].

2.1.2 HLW Glass Composition Constraints

The following bases were used in identifying glass components and constraints to define the EGCR, which was to be covered by the Combined Matrix:

- Ongoing WTP glass formulation work
- Current WTP working compositions
- Part B1 WTP glass formulation work [10]
- Division of constituents:
    - Major oxides that significantly affect glass properties were treated as design variables.
    - Minor constituents were treated as design constants.
    - RCRA constituents, which were the subjects of TCLP studies, were treated as design variables, either individually or in a grouped variable denoted “spike”.
    - Radioactive constituents (U and Th) were not included in the Initial Matrix but were treated as design variables for the Augmentation Matrix.

2.1.3 RCRA Constituents and Constraints

As stated above, the test matrices were designed primarily to support development of a TCLP property-composition model, which was intended to support delisting of the IHLW products. Special considerations were therefore given in selecting RCRA constituents to be treated as design variables and the ranges of these variables to explore. The following bases were used:

- Expected amounts of RCRA constituents in HLW glass products based on waste data and glass formulations
- Part B1 TCLP data [10]
- Part B1 TCLP models [18] and subsequent work
- Delisting limits found in the Delisting Data Quality Objective [19]
- For each RCRA constituent, an assessment of "importance" was made based on the likelihood of challenging the delisting limit for that constituent. The assessment for each RCRA element was based on the expected: amount in waste, amount in glass, rate of TCLP release, and range of matrix TCLP durability vs. delisting limit. This assessment yielded three groups of RCRA elements listed in increasing order of their likelihood of exceeding their respective limits:

    1. Low: Pb, Ag, As, Ba, Cr, Cu, V, Zn
    2. Medium: Ni, Tl, Sb, Se
    3. High: Cd

- Based on the assessment above, Cd, Ni, Tl, Sb, and Se were treated as individual variables in defining the EGCR and developing the test matrices. Zn is present as part of the glass forming additives and ZnO was included as part of the "Constant" group in the Initial Matrix. For the Augmentation Matrix, ZnO was included as a design variable in order to address potential process variations during feed make-up.
- During design of the Augmentation Matrix, the WTP Project directed that Cr contents be spanned up to the waste loading limit for a chromium-limited glass (WTP Contract Specification 1), which is 0.5 wt%. One approach would be to fix the amount of Cr in the "Spike" component (discussed subsequently) to a maximum of 0.5 wt%. However, because of the very strong effect of Cr on spinel liquidus temperature, the spinel liquidus temperature constraint (see Section 2.1.5) would then have the effect of suppressing the concentrations of all of the other "Spike" constituents. It was decided that Cr would be treated as a separate varied design variable.
- The remaining RCRA constituents (7 for the Initial Matrix and 6 for the Augmentation Matrix) were treated as *spikes* in a single grouped component (denoted as "Spike") used in defining the EGCR.

2.1.4 Waste Loading Constraints

Waste loading constraints were developed based on the following considerations. In defining these constraints for the Combined Matrix, several iterations were made based on assessments of distributions of glass component and predicted glass property values for vertices of the EGCR.

- Requirements of the WTP Contract Specification 1.2.2.1.6, "Product Loading" [20]
- Based on glass formulation work, the relevant waste loading constraints found in the WTP Contract Specification 1.2.2.1.6 (only one of them needs to be met) were:
  - $Al_2O_3 + Fe_2O_3 + ZrO_2 \geq 21.0$ wt%
  - $Fe_2O_3 \geq 12.5$ wt%
  - $ThO_2 \geq 4.0$ wt% for the Augmentation Matrix (ThO_2 was not included in the Initial Matrix)
- For the Augmentation Matrix, the requirements above were addressed in a combined constraint of $Al_2O_3 + Fe_2O_3 + ZrO_2 + 3ThO_2 \geq 19.0$ wt%, which has the effect of increasing $Al_2O_3 + Fe_2O_3 + ZrO_2$ when ThO_2 is low and vice versa. To eliminate glasses with undesirable properties, related upper-limit constraints were also imposed:
  - $Al_2O_3 + Fe_2O_3 + ZrO_2 + 3ThO_2 \leq 34.0$ wt%
  - $Al_2O_3 + Fe_2O_3 + ZrO_2 \leq 26.0$ wt%.

2.1.5 HLW Glass Property Constraints

The bases for glass property constraints used to define the EGCR and to develop the test matrices are as follows:

- Part B1 data and property-composition models [10, 18]
- Viscosity and electrical conductivity constraints were based on processing limits (see below).
- PCT constraints were based on the Defense Waste Processing Facility Environmental Assessment (DWPF EA) glass limits [21].
- The spinel liquidus temperature constraint was an upper bound to limit crystallization.
- A limit on TCLP releases was imposed to ensure reasonably realistic maximum TCLP matrix dissolution rates. The limit was based on a TCLP normalized boron release model, which was derived from an analysis of Part B1 data [10].

- For the Augmentation Matrix, the zircon liquidus temperature was an upper bound to limit crystallization. The model described by Rao et al. [22] was used to implement the constraint. This model was relatively simple to implement and performed reasonably well for WTP glasses.

2.1.6 Experimental Design Approach for the Test Matrices

A layered design approach [23, 24] was chosen to generate the Initial Matrix [11], with glass compositions on one inner layer and one outer layer. It was also decided that the matrix should include a center glass composition and several replicate data points. The layered design approach provides for collecting data on a larger glass compositional region (the outer layer) as well as a smaller glass compositional region (the inner layer). Models must be able to predict glass properties sufficiently well to qualify as large a compositional region as possible, and to discriminate between glasses with acceptable and unacceptable properties. Hence, some data over a larger compositional region covering a wider range of property values are needed. However, data over a smaller, more realistic compositional region are also needed for property models to be accurate over such regions. Layered designs are an excellent choice for this type of problem.

For the Augmentation Matrix, a layered approach was also well-suited for its design, because the objectives involved: (1) covering the glass compositional region likely to be associated with C-104/AY-101 wastes, and (2) spanning the wider transition region between the C-104/AY-101 region and the region covered by the Initial Matrix. In the design of the Augmentation Matrix [12], these objectives were addressed by a layered design with an outer layer and an inner layer, respectively. The layers of the compositional region for the Augmentation Matrix, however, were not the same as those used for the Initial Matrix. As with the Initial Matrix, the Augmentation Matrix includes a center glass, glasses from the inner and outer layers of the new EGCR, and several replicate glass formulations.

The EGCR constraints for the Initial Matrix and the Augmentation Matrix, based on the previously discussed considerations, are listed in Tables 2.1 to 2.6. Table 2.1 lists the components (15 for the Initial Matrix and, with the addition of ThO_2, UO_2, Cr_2O_3, and ZnO, 19 for the Augmentation Matrix) selected to be varied in the matrices, as well as the component limits for the inner and outer layers of the design. Along with the variable components, there is a group of constant components (denoted as "Constant") that total 4.2 wt% for the Initial Matrix and 2.2 wt% for the Augmentation Matrix. The "Constant" components are present in constant amounts for every glass in the respective matrices. Further, one of the design components is a "Spike" component, which consists of a group of several RCRA constituents. Note that the makeup of the "Spike" component is also different for the two matrices, with the Initial Matrix "Spike" consisting of 7 components and the Augmentation Matrix "Spike" consisting of 6 components (Cr_2O_3 was removed and included as a separate design variable). Tables 2.2 and 2.3 provide the compositions of the "Spike" and "Constant" components, respectively, for both the Initial Matrix and the Augmentation Matrix. Table 2.4 lists the waste loading constraints. Table 2.5 provides the selected glass property constraints, while Table 2.6 lists the coefficients and

lower and upper limits used to implement the glass property constraints. Note that the values for the lower and upper limits found in Table 2.6 include contribution of oxide components from "Constant" to the respective glass properties. Note also that some of the constraints were subsequently found to be unnecessary (i.e., not triggered) because other constraints were found to be more restrictive. For example, the imposed PCT constraints are unnecessary in that all glasses in the constrained glass composition region, and hence the test matrices, have predicted PCT responses below the defined limits.

2.2 Test Matrices and Glass Compositions

Both the Initial and the Augmentation Matrices were generated using the MIXSOFT [25] and ACED [26] software packages. The process steps used in developing the two matrices, however, were somewhat different. Both development efforts have been described in detail previously [11, 12]. For the Initial Matrix, a total of 57 glasses were generated, including 1 center-point glass, 26 outer-layer glasses, 24 inner-layer glasses, and 6 replicates (one of which was a replicate of the center point composition). Tables 2.7 and 2.8 present the compositions of the 57 glasses in the Initial Matrix, which are designated as the HLW02- series. The Augmentation Matrix contains 45 glasses (designated as the HLW03- series): 1 center point, 20 outer-layer, 20 inner-layer, and 4 replicates (one of the four replicates was a replicate of a glass from the Initial Matrix). Tables 2.7 and 2.8 also summarize the Augmentation Matrix glass compositions. Figure 2.1 provides a 3-dimensional graphical distribution of the major glass components Na_2O, SiO_2, and Fe_2O_3 in the glasses of the Initial Matrix, while Figure 2.2 shows the distribution of the components Na_2O, LiO_2 and, ThO_2 in the Augmentation Matrix (ThO_2 was not part of the Initial Matrix design).

After the Combined Matrix was generated, the compositions of the test glasses were revised, per WTP direction, to include alternate oxide forms (i.e., different oxidation states for the metals) for selected components. The adoption of the revised oxide forms was to ensure consistency in reporting. Table 2.9 lists the "original oxides" used in developing the test matrices as well as the "revised" oxides, with the affected oxides shown in boldface. The compositions of the 102 Combined Matrix test glasses have been converted from the original oxide forms to the revised oxide forms and are given in Tables 2.10 and 2.11. The changes in compositions are relatively minor and involve primarily the components with the revised oxidation states. However, it should be noted that all modeling efforts were performed with glass compositions that are based on revised oxides (see Sections 5 and 6).

2.3 Glasses for Model Validation

The approach used to validate the PCT and $T_{1\%}$ models developed are discussed in detail in the following sections. Two approaches were used to validate models for both properties. The primary approach involved splitting the Combined Matrix data points into modeling and validation partitions. The secondary approach utilized existing glasses that were not part of the Combined Matrix. This section provides a brief summary of the glasses that were selected for the secondary validation approach.

2.3.1 Glasses for Validating PCT-Composition Model

A number of waste glass property-composition databases exist from earlier studies and they are the source of data used in this work for validating the PCT models. These data sets, which have been used previously to support development of interim property-composition models [27], are summarized in Table 2.12 and described in the following paragraphs. Validation glass compositions and PCT data are provided in Appendix A.

TWRS Part A and RPP-WTP Part B1 HLW Glass Formulations [10, 28]

These studies included the results of HLW glass formulation development with Tank Waste Remediation System (TWRS) simulants during TWRS Part A and during Part B1 of the WTP Project. Both studies were conducted at VSL. The Part A glasses were formulated based on the HLW Envelope D composition specifications provided by the TWRS contract. The Part B1 work built on the Part A results and employed two approaches in formulating HLW glasses, including a matrix of glass compositions designed statistically.

Hanford Composition Variation Study (CVS) 1 and 2 [29]

These studies were performed at Pacific Northwest National Laboratory (PNNL) for the Hanford HLW program and included 146 glasses from five statistically designed experimental phases. The design strategy involved defining a glass compositional region expected to contain glasses that might be made from the neutralized current acid waste (NCAW) and expected to be processed by the previously planned Hanford Waste Vitrification Plant (HWVP). Specific compositions were selected for study so as to appropriately cover the defined region.

Defense Waste Processing Facility (DWPF) PCT Modeling [30]

This study was used to develop the Thermodynamic Hydration Energy Reaction Model (THERMO) to predict glass PCT releases based on estimated glass hydration free energy. The THERMO is used in DWPF to assess product consistency and quality. The glasses examined in this study were fabricated under a variety of laboratory and pilot-scale conditions by various researchers and vendors.

West Valley Demonstration Project (WVDP) Support [31]

Two studies were conducted as part of glass-composition variability testing under the PNNL West Valley Support Program to support the establishment of a glass-composition control strategy by West Valley Nuclear Services (WVNS). Results of PCT releases for 20 glasses were available.

West Valley Composition Variation Study (CVS) [32]

The PCT method was used to evaluate 44 West Valley glasses to support WVDP. These glasses were fabricated as sets of CVS glasses by the West Valley Support Task at PNNL and were initially tested with a modified Materials Characterization Center-3 test method. They were retested with the PCT method after Waste Acceptance Product Specifications (WAPS) [33] included the PCT in an acceptance specification.

West Valley Composition Waste Form Qualification Report [34]

West Valley Nuclear Services (WVNS) developed a data set consisting 58 glass compositions. The data were used to develop PCT release models for use in WVDP for high level nuclear waste glasses. The glasses were selected to evenly cover a glass compositional region centered on the WVDP target glass composition with the boundary taken to be three times the expected process variation. Only nine components known to influence PCT releases were varied in these glasses. Out of the 58 glasses, 10 glasses of the alkali series were from the WVDP Support study (see above) and thus were included only once in the validation database.

RPP-WTP LAW Glass Formulation [35]

This study was performed at VSL to develop LAW glass formulations in support of the Part B1 phase of the RPP-WTP privatization project. An iterative approach was adopted in developing glass formulations such that glasses were formulated, prepared, and characterized to obtain the required property-composition information, followed by analyses of the results and revision of the glass compositions to optimize the important glass properties. No statistically designed glasses were included.

The studies described above together included PCT and other data on 576 glasses. However, many of these glasses have compositions that are outside the constraints used to define the EGCR of interest corresponding to the Combined Matrix. For example, the WTP LAW glasses may contain up to 24 wt% of Na_2O [35], compared with design maximum of 15 wt% (Table 2.1). The validation glasses were therefore divided into subsets based on whether they met the constraints that defined the test matrices and applied in model validation accordingly. The approach used in validation of PCT models is described more fully in Section 5.1.

2.3.2 Glasses for Validating $T_{1\%}$-Composition Model

In contrast to the relatively large data set available for validating the PCT model, there are only limited data suitable for $T_{1\%}$ model validation. Published data on volume % crystal vs. temperature are scarce. Additionally, the WTP Project has only recently chosen $T_{1\%}$ as the appropriate property to be modeled [5], which is a less conservative approach compared to previous operations at WVDP and DWPF. The validation data set was taken from the literature and included a total of 39 glasses, including 11 WTP-TL glasses, which belonged to a matrix statistically designed to develop and evaluate liquidus-temperature (T_L) and $T_{1\%}$ models for WTP

HLW glass melts [36]. The other 28 literature glasses were also used in the same study [36]. Compositions of the 39 validation glasses (in revised oxides) are given in Table 2.13. It can be seen that the validation glasses do not contain UO_3 or ThO_2; they also have lower maximum values of ZnO and ZrO_2, with much narrower concentration ranges for the TCLP-relevant elements. In general, however, the upper and lower bounds of most major glass components found in the validation set are comparable to those of the Combined Matrix (with the validation glasses spanning a region somewhat wider than that of the Combined Matrix). Data from the 39 validation glasses therefore allowed for a reasonable evaluation of the prediction performance of the $T_{1\%}$ models developed.

The validation data were converted from weight percent crystals to volume percent crystals using the density data provided [36]. The volume percent versus temperature data were then regressed to determine the $T_{1\%}$ values. These data are presented and discussed in Section 6.1.3.

SECTION 3
EXPERIMENTAL PROCEDURES

After completion of the statistical design of the Initial Matrix (57 glasses, including replicates) and the Augmentation Matrix (45 glasses, including replicates), these glasses were fabricated at VSL on a crucible scale (about 420 grams). The resulting glasses were divided into smaller portions for different testing, including PCT and $T_{1\%}$ determination. The experimental procedures employed in preparing and characterizing the 102 IHLW Combined Matrix glasses are summarized in this section.

3.1 Glass Batching and Preparation

All HLW test glasses were fabricated at VSL using reagent grade chemicals and solutions of known purity. The Technical Procedure *Crucible Melts* [37] describes the details of crucible preparation of HLW glasses. The following section summarizes the procedural steps.

3.1.1 Batching of Starting Materials

Glass preparation began with a batching sheet that provided information on the required starting materials. The information included the chemicals needed, identification of the chemicals according to the vendors and catalog numbers, the associated purity, together with the amount required to melt a given amount of glass. Chemicals were weighed and batched according to the batching sheets.

Calculation of the required amounts of starting materials in the batching sheets made use of not only purity information, but also volatility characteristics of the chemicals. Specifically, thallium (III) oxide is relatively volatile, with a boiling point of only 875 °C, and substantial loss is expected at the glass-melting temperature of over 1000°C. Previous glass formulation work at VSL has accumulated a data base of thallium-containing glasses [10, 28], which suggested that thallium loss may vary with concentration and glass composition. On the average, however, those data showed that only 54 % of the starting thallium (III) oxide was retained in glass. Consequently, thallium (III) oxide was "over-batched" by a factor of 1.85 in the batching sheets. Another component, selenium (IV) oxide, which melts at about 350°C and sublimes at high temperatures, was also over-batched in the HLW glasses by a factor of 2.29.

In batching recipes for preparing these HLW glasses, up to 41 components might be needed. It was possible to take advantage of the fact that many of those components were present in the HLW glasses in constant concentrations. Glass frits, which consisted of 16 (for the Initial Matrix) or 13 (for the Augmentation Matrix) components that were prepared with reagent grade chemicals, were therefore prepared and employed as a starting material in the batching for the HLW matrix glasses in order to reduce the number of components required.

After the starting materials were weighed and batched, a blender was used to mix and homogenize the starting materials before they were loaded into platinum/gold crucibles that were engraved with individual identification numbers. A pre-weighed noble metal solution (which consisted of ruthenium (Ru), rhodium (Rh), and palladium (Pd) in nitric acid) was then added and blended with the chemicals. Addition of the noble metals as a solution instead of as a solid (typically less than 0.5 g of oxide was required) was found to aid in the dispersion of noble metals in the glasses.

3.1.2 Glass Melting

Glass melting was performed in a random order with the exact sequence of melts determined by assigning a random number to each HLW glass and then placing the glasses in ascending order according to the associated random number. After the melt order had been determined and the batching completed, the loaded platinum/gold crucible was placed inside a Deltech DT-28 (or DT-29) furnace, the heating of which was controlled by a Eurotherm 2404 temperature controller. The melting temperature was 1150°C, at which the melt was kept for 2 hours. Mixing of the melt was accomplished mechanically using a platinum stirrer, beginning 20 minutes after the furnace temperature reached 1150°C and continuing for the next 90 minutes. The molten glass was poured at the end of 120 minutes onto a graphite plate to cool before recovery.

3.2 Analyses of Glass Composition

Compositions of the prepared HLW glasses were analyzed with x-ray fluorescence (XRF) spectroscopy. Powdered glass samples were analyzed with an ARL 9400 wavelength dispersive XRF spectrometer, which was calibrated over a range of glass compositions using standard reference materials traceable to NIST, as well as waste glasses such as Argonne National Laboratory–Low Activity Waste Reference Material (ANL-LRM) and DWPF-EA glass.

Appendix B presents the XRF analysis results for 102 HLW Combined Matrix glasses. Note, however, that the batched (target) compositions were used for modeling since they were derived from simple weighing of pure chemicals, which are believed to provide the best compositional data. Since target glass compositions are used in modeling, the principal role of the composition analysis is one of confirmation.

3.3 Product Consistency Test

The PCT data for the matrix glasses were collected at VSL from tests performed at 90°C for 7 days according to ASTM C1285 [38], as required in Specification 1 of the WTP contract [20]. Samples of crushed glasses (4 g, 100-200 mesh, or 75-149 μm) were placed in 40 ml of test solution (de-ionized water) inside 304L stainless steel vessels. All tests were conducted in

triplicate, and in parallel with the DWPA-EA standard glass included in each test set. The leachates were sampled after 7 days, when 1 ml of sampled leachate was mixed with 20 ml of 1M HNO_3 and the resulting solution analyzed by direct current plasma atomic emission spectroscopy (DCP-AES). Another 3 ml of the sampled leachate was used for pH measurement.

In addition to the leachate concentrations themselves, it is convenient and conventional to also consider the *normalized* leachate concentrations. The normalization is performed by dividing the concentration measured in the leachate for any given component by its fraction in the glass. Target mass fractions in glass are used in this work. Thus, the *normalized* concentration r_i of element i is calculated from the elemental concentrations c_i measured in the leachate (in ppm) as:

$$r_i = \frac{c_i}{f_i} \ , \tag{3.1}$$

where f_i is the target mass fraction of element i in the glass. The normalized mass loss is then obtained from:

$$L_i = \frac{r_i}{(S/V)} \ , \tag{3.2}$$

where S/V is the ratio of the glass surface area to the volume of the leachant, which for the standard PCT is 2000 m^{-1}. Assuming this value of S/V, if r_i is expressed in g/l, one need only divide by two to obtain L_i in g/m^2 (because 1 g/l = 1000 g/m^3). Except where indicated, the present work is performed in terms of the normalized concentration in g/l (i.e., r_i).

By reference, Specification 1 of the WTP contract requires that the normalized mass losses of B, Na, and Li in PCT be below the respective values for the DWPF-EA glass. The nominal values for normalized leachate concentrations from the DWPF-EA glass are 16.695, 13.346, and 9.565 g/l for B, Na, and Li, respectively [21].

3.4 Determination of One-Percent Crystal Fraction Temperature ($T_{1\%}$)

Glass samples (about 3 to 5 grams each) were heat-treated in a platinum, platinum-gold, or platinum-rhodium crucible at a pre-melt temperature of 1200°C for 1 hour to destroy any pre-existing nuclei, followed by heat treatment for 70 to 72 hours at prescribed temperatures between 650°C and 1200°C. At the end of the heat-treatment period, the glass samples were quenched by contacting the crucible with cold water. This quenching freezes in the phase assemblage in equilibrium with the melt at the heat-treatment temperature. The sample was then prepared for Scanning Electron Microscopy/Energy Dispersive X-ray Spectroscopy (SEM/EDS, Scanning Electron Microscopes JEOL Model JSM-35C, equipped with Noran Vantage Integrated EDS or Model JSM-5910LV, equipped with Oxford Instruments INCAEnergy 300 system) examination to determine the volume fraction of crystalline phases and for identification of the dominant crystalline phases. For each glass, a sufficient number of heat treatments were

performed to obtain non-zero vol% data for at least three temperatures in order to reasonably constrain the $T_{1\%}$ value. Effort was also made to bracket the $T_{1\%}$ temperature so that it could be obtained by interpolation rather than extrapolation, which was the case for 90 of the 97 glasses for which $T_{1\%}$ values could be determined (see Section 4 for a discussion of the $T_{1\%}$ data).

The crystalline phases found in the heat-treated glasses were characterized by SEM/EDS and the volume percents were obtained as the average of 4 to 10 viewing area counts from glass sub-samples collected at different locations in the crucible (e.g., near the bottom, center, side of the crucible, etc.). The selection of the glass fragments and viewing areas were intended to provide a representative measure of the overall crystal fraction in the sample.

The $T_{1\%}$ value for each glass was obtained by linear regression of the heat-treatment temperature (°C) as the dependent variable versus crystal fraction (vol%) as the independent variable. The choice of vol% (which has the larger measurement error) as the independent variable, rather than the temperature (which has the smaller measurement error), is contrary to the selection that would normally be made for regression. However, as discussed in Section 6.1.1, there are significant advantages to using this "inverse regression" approach in the present application. The differences in the $T_{1\%}$ values estimated using either choice of independent variable were generally small with respect to the standard deviations obtained for the replicates (see Section 6.1.1 and Table 6.3).

SECTION 4
PROCUCT CONSISTENCY TEST (PCT) AND ONE-PERCENT CRYSTAL FRACTION TEMPERATURE ($T_{1\%}$) RESULTS

Product Consistency Test (PCT) and one-percent crystal fraction temperature ($T_{1\%}$) results collected for the 102 matrix glasses are presented in this section. In addition, general compositional trends observed in the PCT and $T_{1\%}$ response data are discussed. Quantitative statistical modeling of the collected data is discussed in Sections 5 and 6.

4.1 Product Consistency Test (PCT) Results

The data for PCT releases of boron, lithium, and sodium for the 57 Initial Matrix glasses and 45 Augmentation Matrix glasses are listed, respectively, in Tables 4.1 and 4.2. Normalized PCT releases were calculated using target mass fractions of boron, lithium, and sodium in glass. Figures 4.1 and 4.2 show, respectively, the PCT boron and sodium releases for all 102 glasses. There is no discernable difference in the data between the Initial Matrix glasses and the Augmentation Matrix glasses. (The Augmentation Matrix member HLW03-13 has an uncommonly low PCT boron release and was excluded from model development. See Section 5.1 for a discussion of data selection in developing PCT models.) This is not surprising since the same PCT constraints were used in the design of both matrices, which were to be compliant with IHLW performance requirements (Table 2.6). In fact, the PCT constraints were not triggered for most of the designs (i.e., the PCT constraints were not necessary to limit the matrix glass compositions in the designs), and the resulting PCT normalized boron release values are in general relatively low, with the observed maximum being 4.418 g/l (for HLW02-57). This can be compared with the nominal PCT normalized boron release of 16.695 g/l for the reference glass DWPF-EA. For sodium and lithium, the maximum PCT normalized releases observed for the matrix glasses are 2.802 g/l and 3.252 g/l, respectively, compared with the corresponding nominal values of 13.346 g/l and 9.565 g/l for the DWPF-EA glass. Thus, all of the matrix glasses outperformed the reference glass DWPF-EA in PCT, often by considerable margins. Previous WTP HLW glass formulation work has repeatedly shown that PCT is not a particularly constraining requirement and that the vast majority of actively designed HLW glasses consistently surpass the performance limits set by the reference glass DWPF-EA [21]. However, for the purpose of model development, it may be desirable to include IHLW glasses that span a wider range of PCT performance. Figure 4.3 shows the distribution of normalized PCT releases for boron, lithium, and sodium for all matrix glasses.

Ten pairs of replicate compositions were designed into the Combined Matrix. The glasses were then fabricated and tested in the same way as the other matrix glasses in random order. These replicate pairs are identified in Tables 4.1 and 4.2, which also give the associated PCT data. These data are addressed statistically in Section 5. It can be seen, however, that the agreement between the replicates is reasonably good for lithium and sodium (and silicon, the data for which are not shown), but is significantly worse for boron. A detailed review of the fabrication and testing processes revealed nothing that might account for the observed difference.

One possibility under investigation is phase separation (e.g., leading to the formation of some amount of a more leachable boron-rich phase, depending on the precise cooling history).

The principles that control leaching of glasses in water are relatively well known. The important mechanisms are hydration, diffusion of alkali ions and their exchange with hydrogen ions, hydrolysis of the glass network, and formation of modified layers at the glass surface [39, 40]. Glass compositions have a profound effect in determining the relative importance of these mechanisms. However, with over 40 design component oxides in the matrix glasses and with many of these components being varied simultaneously in the matrix design, it is possible only to identify general trends between the PCT results and glass compositions.

Although both boron and silicon are considered structurally as network formers in borosilicate glasses, boron is significantly more soluble than silicon during PCT leaching. In addition, boron forms few secondary phases that precipitate from the leaching solution. These factors suggest that boron concentration in the leachate will be a good indicator of the extent of reaction of the glass with the leachant. In many attempts to explain the leaching results of borosilicate glasses, boron oxide content and its fraction in the glass network are two of the most important parameters (see, for example, reference [41]). Figure 4.4 shows the considerably higher solubility of boron than silicon for the Combined Matrix glasses. It also shows that, as leaching increased, sodium and lithium dissolution behavior deviates from being congruent with boron release. This general relation between PCT releases of sodium and boron is common and has been observed previously in the testing of WTP IHLW (and ILAW) glass formulations [10].

The properties of the leaching solution, such as temperature and pH, are also important in determining the rate and mechanism of leaching in borosilicate glasses. Release of alkali ions from the glass matrix rapidly increases the leachate pH, which in turn increases the rate of hydrolysis of the silicate network. One study has classified the interaction of glasses containing high alkali contents with basic solution as the most reactive (the least reactive being silica in neutral to acidic solution), with the results often being total dissolution [40]. De-ionized water is the leachant used in PCT and the leachate pH is another good indicator of extent of leaching. The data in Table 4.1 show that the pH values range from 9.38 to 11.85 in the leachates for the Initial Matrix glasses, which show little difference from those for the Augmentation Matrix glasses (9.17 to 11.75, see Table 4.2). Figure 4.5 shows the relationship between leachate pH and the amounts of alkali oxides in the matrix glasses, while Figure 4.6 relates the normalized PCT boron and sodium releases to the leachate pH. Both plots show the expected trends—increasing pH with increasing alkali contents (i.e., $Li_2O+Na_2O+K_2O$) in Figure 4.5 and increasing PCT releases (of boron and sodium) with increasing pH in Figure 4.6—with Figure 4.5 exhibiting a much more uniform increase.

The extent of PCT leaching can also be correlated with the compositions of the glasses in terms of glass network formers and modifiers. The PCT releases from glass generally increase with increasing modifier contents but with decreasing glass former contents. Alkalis are the most effective network modifiers in disrupting the glass network structure. The general effects of alkalis on PCT releases are shown in Figures 4.7 (boron) and 4.8 (sodium). While there are fair amounts of scatter in the displayed data, the overall trend clearly shows the increased PCT releases with higher alkalis contents. Figure 4.9, which correlates PCT boron release with one

ratio of glass modifiers to glass formers (i.e., $(Li_2O + Na_2O + K_2O + MgO + CaO + SrO)/(Al_2O_3 + B_2O_3 + Fe_2O_3 + SiO_2 + ZrO_2)$), also shows the expected trend, but again with considerable scatter in the data. Statistical modeling of these results with respect to glass compositions is described in Section 5.

4.2 One-Percent Crystal Fraction Temperature ($T_{1\%}$) Results

Heat treatment of the matrix glasses was conducted between 650°C and 1200°C, at regular temperature intervals of 50°C (measurements were also performed on some glasses at 875°C). The measured crystal vol% data are tabulated in Table 4.3. Regression of these data provided estimates of $T_{1\%}$ for the matrix glasses, which are given in Table 4.4 together with identification of the dominant crystalline phases. The typical relationship observed between crystal vol% and heat treatment temperature is relatively simple and can be adequately described by a linear relationship. One example is given in Figure 4.10, which shows the heat treatment results of HLW02-01 and its replicate, HLW02-52. In a few cases, the temperature dependence of vol% is non-linear. For example, the data for the replicate pair HLW02-04 and HLW02-54 show an abrupt slope change at about 850°C, characteristic of the appearance of a second phase (Figure 4.11). It is, however, still straightforward to estimate $T_{1\%}$ based on the linear trend defined by spinel crystallization. Section 6 provides further discussion on data regression to estimate $T_{1\%}$, assesses data obtained for the replicate test pairs, and discusses the selection of data for modeling.

Overall, $T_{1\%}$ was estimated for 97 of the 102 Combined Matrix glasses; the other 5 glasses in the matrix did not result in enough crystallization data even at low heat-treatment temperatures to allow estimation of $T_{1\%}$. Of the 97 $T_{1\%}$ values, the 15 highest estimates belong to the Augmentation glasses, a reflection of the expanded constraint for spinel liquidus temperature (from 1050°C to 1150°C). Further, the median of the estimated $T_{1\%}$ values after excluding one outlier is 946.1°C (average = 945.6°C), which can be compared with the WTP processing requirement of $T_{1\%} \leq 950$°C. Figure 4.12 shows the distribution of the estimated $T_{1\%}$ for the Combined Matrix. The dominant crystal phase in 54 (out of 57) Initial Matrix glasses was spinel, with only one glass (HLW02-14) exhibiting a non-spinel (zircon) principal crystalline phase. For the other two Initial Matrix glasses, only noble metals were detected in one and a trace amount of spinel was found in the other. In contrast, heat treatment of the Augmentation Matrix glasses resulted in more frequent observation of non-spinel crystal phases, which include zircon, zirconia, and thoria. Nevertheless, the prevalent crystal phase found in the Augmentation Matrix glasses was also spinel. It is likely that individual models will be required for each crystalline phase, and therefore the $T_{1\%}$ model developed in this work focused only on spinel.

Previous HLW glass formulation work for AZ-101, AZ-102, and C-106/AY-102 wastes has identified spinel crystallization as the primary constraint that prevented attainment of higher waste loadings [10]. The iron contents in these wastes were comparatively high such that extensive use of additive components to effectively suppress spinel formation was required. These components included Li_2O, Na_2O, and B_2O_3 [10]. Attempts have been made to qualitatively correlate the estimated $T_{1\%}$ values with glass compositions, as was performed for the PCT data above. Any trends observed of the $T_{1\%}$ data, however, are not as noticeable as those

observed for PCT. Figure 4.13 provides one such example, which relates the $T_{1\%}$ data to the molar ratio of Fe_2O_3 to (alkali oxides + B_2O_3). Data for outliers and glasses with non-spinel primary crystalline phase are not included in Figure 4.13. While glasses with higher iron concentrations generally do tend to have higher $T_{1\%}$ values, the data show a good deal of scatter and the trend is not as obvious as those found for PCT data. Many other similar attempts did not result in better correlations. For instance, adding chromium and nickel, two components known to greatly promote spinel formation, did not significantly reduce the scatter in data (see Figure 4.13). This suggests that $T_{1\%}$-composition modeling may be more complicated than PCT-composition modeling in the sense that additional modeling terms may be required.

Recent IHLW glass formulation efforts have developed performance and process compliant glasses with increased waste loadings of up to 14 wt% Fe_2O_3 [42], compared with a maximum of 12.56 wt% in earlier work [43]. The Combined Matrix includes seven glasses with 14.00 wt% Fe_2O_3 (two other glasses have > 13.90 wt%) as the design maximum. It is of interest to note that, of these seven glasses, about half (four) have an estimated $T_{1\%}$ of ≤ 950°C, indicating that even higher waste loading may be achievable for IHLW glasses.

SECTION 5
MODELS RELATING PCT BORON, LITHIUM, AND SODIUM RELEASES TO HLW GLASS COMPOSITION

This section documents the development and validation of property-composition models and corresponding uncertainty expressions for predicting the PCT-Boron, PCT-Lithium, and PCT-Sodium releases from high level waste (HLW) glasses. Specification 4.8.1.2 of the Waste Acceptance System Requirements Document (WASRD), Rev. 4 [44] requires that HLW glasses have PCT normalized releases of boron, lithium, and sodium lower than the corresponding releases from the DWPF-EA glass [21]. The property-composition models and corresponding uncertainty expressions for PCT-Boron, PCT-Lithium, and PCT-Sodium releases from HLW glasses presented in this section were developed and validated using composition and PCT release data collected on simulated HLW glasses. The simulated HLW glasses used for model development and model validation are discussed in Sections 2.2 and 2.3.

Section 5.1 summarizes the data used to develop and validate the PCT-composition models. Section 5.2 presents the model forms for PCT-Boron, PCT-Lithium, and PCT-Sodium releases that were investigated. Sections 5.3, 5.4, and 5.5 summarize the results for the selected PCT-Boron, PCT-Lithium, and PCT-Sodium model forms, respectively. Using the selected models and corresponding uncertainty equations for each of PCT-Boron, PCT-Lithium, and PCT-Sodium, Section 5.6 illustrates the calculation of PCT release predictions and the uncertainties in those predictions. Section 5.7 briefly discusses the consequences of lack-of-fit and prediction uncertainties in the recommended PCT-Boron, PCT-Lithium, and PCT-Sodium models. Appendix C discusses the statistical methods and summary statistics used to develop, evaluate, and validate the several model forms investigated, as well as statistical equations for quantifying the uncertainties in PCT release predictions made with the selected models.

5.1 PCT Release Data Used for Model Development and Validation

The data used for developing PCT-Boron, PCT-Lithium, and PCT-Sodium release models are discussed in Section 5.1.1. The two approaches and data used for validating the models are discussed in Sections 5.1.2 and 5.1.3.

5.1.1 Model Development Data for PCT Releases

The data available for developing property-composition models for PCT-Boron, PCT-Lithium, and PCT-Sodium releases consist of composition and PCT release data from two matrices of simulated HLW glasses. The two matrices were developed using information about Hanford HLW compositions, previous WTP glass formulation work, glass science knowledge and experience, and statistical experimental design methods. The first matrix, referred to as the *Initial Matrix*, consists of 57 HLW glass compositions selected by statistical experimental design methods. The second matrix, referred to as the *Augmentation Matrix*, consists of 45 simulated

HLW glasses selected by statistical experimental design methods to optimally augment the Initial Matrix. Both matrices together are referred to as the *Combined Matrix* for Phase 1 IHLW property model development. Layered experimental designs [23, 24] were used to obtain both the Initial Matrix and the Augmentation Matrix. In both cases, the layered designs involved an outer layer, an inner layer, and a center composition. Details of the experimental design methods and development of the Initial Matrix and Augmentation Matrix are given respectively by Piepel et al. [11] and Cooley et al. [12]. The glasses of the Combined Matrix were used to develop the composition-property models for IHLW PCT and $T_{1\%}$ in this report, as well as the TCLP Cd release models [8]. Further details of the Phase 1 IHLW modeling data are given in Section 2 of this report.

Table 5.1 lists the normalized glass compositions for the 57 Initial Matrix glasses and the 45 Augmentation Matrix glasses in the oxide forms used for PCT model development. The glass compositions in Table 5.1 are the normalized weight percents (wt%) of the 19 components varied in each of the IHLW design matrices. These are the same 19 components involved in $T_{1\%}$ model development, namely Al_2O_3, B_2O_3, CdO, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, Sb_2O_3, SeO_2, SiO_2, SrO, ThO_2, Tl_2O, UO_3, ZnO, ZrO_2, and Spike. The compositions listed in Table 5.1 are normalized so that they sum to 100% over the 19 components varied in the Combined Matrix. In contrast, Table 2.10 (and Table 2.7, based on the original oxides) lists the 19-component unnormalized mass fraction compositions of the Combined Matrix glasses. The compositions in Table 2.10 are unnormalized in the sense that they sum to 100% over the complete list of 56 oxides included in the dataset, but do not sum to 100% over the 19 components of the Combined Matrix. For model development purposes, the 19-component normalized wt% compositions of the Combined Matrix were converted to mass fractions so that each composition summed to 1.0. The Layer column of Table 5.1 indicates the design layer containing each of the Combined Matrix glasses.

Table 5.2 contains columns of unnormalized (given in ppm units) and normalized (given in g/m^2 units) versions of the as-measured PCT-Boron, PCT-Lithium, and PCT-Sodium releases for the 102 glasses of the Combined Matrix. The normalized releases were calculated as described previously in Section 4.

Five of the 102 IHLW Combined Matrix glasses were not used to develop the PCT models. The five glasses dropped were outliers in PCT release space, either based on the release value for a single element or on the combination of two elemental releases. The five glasses dropped from the model development set were HLW02-22, HLW03-13, HLW03-17, HLW03-43, and HLW03-36. Specific reasons for dropping these five glasses are given below:

- HLW02-22 and HLW03-17 were outliers in PCT-Lithium vs. PCT-Sodium space.
- HLW03-13 was very low in PCT-Boron release.
- HLW03-43 and HLW03-36 were outliers in PCT-Boron vs. PCT-Sodium space.

Tables 5.1 and 5.2 include a column identifying these five glasses as having been excluded from PCT model development. Note that these five glasses were used for $T_{1\%}$ model development, but that different glasses were excluded from the $T_{1\%}$ model development as discussed in Section 6.1.1.

Table 5.3 lists the replicate pairs of glasses in the IHLW PCT modeling dataset, the corresponding PCT-Boron, PCT-Lithium, and PCT-Sodium normalized releases in g/l, and pairwise as well as pooled estimates of percent relative standard deviations (%RSDs) based on the replicate pairs. A pooled %RSD combines the separate pairwise %RSDs so that a more accurate, combined estimate of the %RSD is obtained. This pooled %RSD includes variations due to fabrication of glasses, performance of the PCT, and chemical analyses of the leachates. Table 5.3 also contains pairwise standard deviations (SDs) and pooled estimates of standard deviations that account for variations in the natural logarithms of normalized PCT releases in ln(g/l) due to fabrication of glasses, performance of the PCT, and chemical analyses of the leachates. Note that the %RSD values are in close agreement with the corresponding SD values in Table 5.3. This is a consequence addressed by Equation (5.7) in Section 5.2.2.

The magnitude of the pooled %RSDs in Table 5.3 for PCT-Lithium and PCT-Sodium are very similar to the approximately 10 %RSD values reported in Table F.5 of Hrma et al. [29]. However, the pooled %RSD for PCT-Boron in Table 5.3 is noticeably larger than 10%. The results from Table F.5 of Hrma et al. [29] were based on replicate pairs of the same glasses fabricated and tested several times over several years. Hence, the approximately 10% RSD values for PCT-Boron, PCT-Lithium, and PCT-Sodium reported by Hrma et al. [29] include an additional source of variation not included in the replicate data of Table 5.3. This suggests that the PCT-Boron data for the IHLW Combined Matrix in Table 5.2 were subject to more experimental, testing, and measurement uncertainty than in other past glass composition variation studies. It is not clear why the uncertainty in the PCT-Boron releases for this data set is larger, but as discussed in Section 4.1, phase separation could be a possible cause.

5.1.2 Primary Model Validation Approach and Data

The primary model validation approach for PCT modeling was based on splitting the Combined Matrix data points remaining for model development into five modeling/validation partitions. Of the 102 IHLW Combined Matrix glasses, 20 were intended to be replicates (10 replicate pairs). One pair (HLW02-46 and HLW03-42) is actually a near replicate pair, having very slight differences for some component values. The differences could be due to round off or renormalization because one of these glasses is from the Initial Matrix and the other is from the Augmentation Matrix. This pair was treated as a true replicate pair for model development and evaluation. Of the 97 glasses remaining for PCT modeling after dropping the 5 glasses mentioned previously, 18 were intended to be replicates. As mentioned in Section 5.1.1, one of the 5 glasses dropped from PCT modeling was HLW03-43. This glass, along with HLW03-06, formed a replicate pair. Although HLW03-06 was among the 97 glasses that remained for PCT modeling, dropping HLW03-43 meant that only 9 replicate pairs remained out of the initial 10. These 18 glasses (9 replicate pairs) were included in each of the five modeling splits. This was done so that replicate pairs would not be split between modeling and validation subsets, which would otherwise negate the intent to have validation glasses different than model development glasses. The remaining 79 glasses were divided into the five modeling/validation splits as follows:

- The remaining 97 – 18 = 79 data points (glasses) were ordered from smallest to largest according to their values of normalized PCT-Boron, PCT-Lithium, or PCT-Sodium release (g/l) depending on which PCT model was being validated. The 79 ordered data points were numbered 1, 2, 3, 4, 5, 1, 2, 3, 4, 5, etc. All of the 1's formed the first model validation set, while all of the remaining points formed the first model development dataset. Similarly, all of the 2's, 3's, 4's, and 5's respectively formed the second, third, fourth, and fifth model validation sets. In each case, the remaining non-2's, non-3's, non-4's, and non-5's formed, respectively, the second, third, fourth, and fifth model development datasets. Accordingly, four of these splits contained 16 glasses for validation and 63 glasses for modeling, and one of the splits contained 15 glasses for validation and 64 glasses for modeling.

- The 18 'replicate' glasses were added to each of the modeling splits yielding 4 splits with 81 glasses for modeling and 16 glasses for validation, and one split with 82 glasses for modeling and 15 glasses for validation. The last three columns of Table 5.2 specify the validation subsets for the five modeling/validation splits for the primary validation approach for PCT-Boron, PCT-Lithium, and PCT-Sodium model development.

Data splitting was chosen as the primary validation approach because even though there was a large amount of other PCT-composition data available for model validation purposes (see Section 5.1.3), the number that satisfied all of the constraints defining the IHLW composition region and meeting quality assurance (QA) requirements were somewhat limited.

5.1.3 Secondary Model Validation Approach and Data

There were 574 glasses, not included in the IHLW Combined Matrix, available for validation of the IHLW PCT models (see Section 2 for details). However, the majority of these validation glasses had compositions outside the constraints that defined the EGCR of interest for WTP IHLW property-composition model development. Thus, subsets of the validation glasses were formed. The complete set of validation glasses (all 574 glasses) is referred to as the V1 validation set. Note that 75 of the validation glasses had no reported PCT-Lithium release. Thus, there were only 499 V1 glasses for validating PCT-Lithium models. The glasses that satisfy all single-component constraints (within reasonable tolerance) are referred to as the V2a validation set. There were 115 glasses in the V2a validation set. The V2a glasses were further screened to remove glasses having any non-matrix components (components that were not varied in the IHLW design matrix) with wt% value greater than 1 wt%. Such screening by non-matrix components with wt% values greater than 1 wt% is consistent with compositions of glasses in the IHLW Combined Matrix where non-matrix components were bounded from above by 0.50 wt%. Only 15 of the 115 V2a glasses remained after the screening by non-matrix components. This set of 15 glasses is referred to as the V2b validation set. The glasses that satisfy all single- and multi-component constraints (within reasonable tolerance) are referred to as the V3a validation set. There were 38 glasses in the V3a validation set. The glasses in the V3a validation set were also screened to remove glasses with greater than 1 wt% for any one or more of the non-matrix components. The screened set contained only 13 glasses and is referred to as the V3b validation set. Note that of the non-matrix components, MgO, K_2O, CaO, P_2O_5, and TiO_2

exceeded the 1 wt% limit more frequently than other components, thus having the biggest impact on screening from the V2a to V2b and from the V3a to V3b validation sets. Validation glasses contained as much as 8 wt% MgO, 8.75 wt% K_2O, or 10 wt% CaO.

Thus, glasses in the V3b validation subset satisfy all single- and multi-component constraints that define the IHLW glass composition region (so the V3b glasses are within the IHLW EGCR), and satisfy the additional requirement that non-matrix components have wt% values less than 1 wt%. This makes the V3b subset the most reliable data set for validating the IHLW PCT models. The other validation subsets (V2a, V2b, and V3a), and the complete V1 validation dataset, contain glasses with compositions that are different from the IHLW modeling data in at least one respect. Either they: (i) violate one or more multi-component constraints, (ii) violate one or more single-component constraints, or (iii) include non-matrix components having wt% values greater than 1 wt%. This means that applying the IHLW PCT models to validation sets other than V3b results in an extrapolation of the models. Such extrapolations often result in less accurate property predictions than would result if the models were applied to compositions within the glass composition region of interest.

The compositions for the 574 validation glasses are given in Table A.1, of Appendix A, listed as weight percents summing to 100%. The corresponding PCT release data (unnormalized and normalized) are given in Table A.2 of Appendix A. Table A.2 also contains columns that indicate which validation glasses were included in the validation subsets V2a, V2b, V3a, and V3b described above. Note that the validation compositions listed in Table A.1 were converted into the same compositional forms employed by the Combined Matrix used for PCT model development. That is, the same 19 components were used from the validation data compositions. Validation compositions were normalized to sum to 1 for computational purposes during software applications that generated the IHLW PCT models.

Use of these 574 validation glasses was considered a secondary model validation approach because the glasses were not part of the IHLW experimental design work discussed by Cooley et al. [12]. The data-splitting approach discussed in Section 5.1.2 is considered the primary validation approach because the data used by that approach are from the IHLW Combined Matrix and satisfy the full QA requirements. The separate validation dataset and subsets thereof are used as a secondary validation approach because most of these glasses are not within the IHLW glass composition region, and some of them do not satisfy the full QARD [45] requirements.

5.2 PCT Release Model Forms

Ideally, a property-composition model for PCT would utilize known mechanisms of PCT release as a function of glass composition and other aspects of the PCT. However, no such mechanisms are known, so that mechanistic and semi-empirical model forms are not available. Hence, several empirical model forms with parameters to be estimated from model development data were considered. These model forms are from the general class of *mixture experiment models* [46]. Section 5.2.1 discusses mixture experiments and the two general forms of mixture

experiment models used in this work. Section 5.2.2 discusses the choice between modeling unnormalized and normalized PCT releases and transformations thereof.

5.2.1 Mixture Experiment Model Forms

Linear mixture (LM) and partial quadratic mixture (PQM) model forms introduced in Section C.1.1 of Appendix C were chosen for use in modeling PCT-Boron, PCT-Lithium, and PCT-Sodium releases. For modeling PCT-Boron, PCT-Lithium, and PCT-Sodium, the specific LM model form is given by

$$ln(r_B),\ ln(r_{Li}),\text{ or } ln(r_{Na}) = \sum_{i=1}^{q} b_i x_i + \varepsilon\ , \tag{5.1}$$

while the specific PQM model form is given by

$$ln(r_B),\ ln(r_{Li}),\text{ or } ln(r_B) = \sum_{i=1}^{q} b_i x_i + \text{Selected}\left\{\sum_{i=1}^{q} b_{ii} x_i^2 + \sum_{i<j}^{q-1}\sum^{q} b_{ij} x_i x_j\right\} + \varepsilon\ . \tag{5.2}$$

In Equations (5.1) and (5.2): $ln(r_B)$ denotes the natural logarithm of the normalized PCT-Boron release (in g/l); $ln(r_{Li})$ denotes the natural logarithm of the normalized PCT-Lithium release (in g/l); $ln(r_{Na})$ denotes the natural logarithm of the normalized PCT-Sodium release (in g/l); the x_i (i = 1, 2, …, q) are normalized mass fractions of q glass oxide or halide components such that $\sum_{i=1}^{q} x_i = 1$; the b_i (i = 1, 2, …, q), the b_{ii} (selected), and the b_{ij} (selected) are coefficients to be estimated from data; and ε is a random error for each data point. Many statistical methods exist for the case where the ε are independent (i.e., not correlated) and normally distributed with mean 0 and standard deviation σ. In Equation (5.2), "Selected" means that only some of the terms in curly brackets are included in the model. The subset is selected using standard stepwise regression or related methods [47]. PQM models are discussed in more detail and illustrated by Piepel et al. [48].

Normalization and the natural log transformation of the PCT release values are discussed further in the next section.

5.2.2 Normalization and Transformation of PCT Release Values

A transformation to "normalized" concentrations is widely employed in the data analysis and modeling of leaching data [18]. The normalized PCT-Boron (r_B), PCT-Lithium (r_{Li}), and PCT-Sodium releases (r_{Na}) were calculated according to the following formulas. For PCT-Boron,

$$r_B\ (\text{g/l}) = \frac{c_B\ (\text{mg/l})}{[1000\ (\text{mg/g})]\left[w_{B_2O_3}\ (\text{g } B_2O_3/\text{g glass})\right][0.3106(\text{g B/g } B_2O_3)]}\ , \tag{5.3}$$

where c_B is the non-normalized boron release (concentration) from the 7-day PCT, and w_{B2O3} is the unnormalized mass fraction of B_2O_3 in the glass. This is calculated as

$$w_{B2O3} = W_{B2O3}/100\ , \tag{5.4}$$

where W_{B2O3} is the wt% of B_2O_3 in the glass. Similarly,

$$r_{Li}\ (\text{g/l}) = \frac{c_{Li}\ (\text{mg/l})}{[1000\ (\text{mg/g})]\left[w_{Li_2O}\ (\text{g } Li_2O/\text{g glass})\right][0.4646\ (\text{g Li/g } Li_2O)]}\ , \tag{5.5}$$

and

$$r_{Na}\ (\text{g/l}) = \frac{c_{Na}\ (\text{mg/l})}{[1000\ (\text{mg/g})]\left[w_{Na_2O}\ (\text{g } Na_2O/\text{g glass})\right][0.7419\ (\text{g Na/g } Na_2O)]}\ . \tag{5.6}$$

As seen in Equations (5.3), (5.5), and (5.6), normalizing involves dividing the measured leachate concentration for a given element by the corresponding mass fraction of that element in the glass. Mechanistically, this crudely takes into account the fact that, for a given amount of glass reacted, the concentration of a specific element in the leachate should be proportional to the mass fraction of the element in the glass. This is an approximation for a number of reasons, including the fact that the mass fraction of the element in question *affects* the amount of glass reacted, and not necessarily all of the constituents in the reacted glass are released to the solution. Nevertheless, factoring out this dependence by normalization is often empirically observed to improve model fits to leaching data and to further reduce the need for non-linear composition terms in the model.

In describing preliminary modeling work for IHLW PCT releases, Perez-Cardenas et al. [6] found little difference in predictive performance for models based on normalized PCT elemental releases versus unnormalized PCT releases. Because contract specifications [20] are stated in terms of normalized PCT releases, Perez-Cardenas et al. focused on normalized releases for their preliminary model investigations. Likewise, the model development work summarized in this report was conducted based on PCT normalized elemental releases.

In modeling PCT elemental releases (unnormalized or normalized), it is advantageous to transform the PCT release concentrations in the leachate to the natural logarithm of the concentrations. The advantages of this transformation include:

- The PCT-Boron unnormalized releases for the subset of the 97 Combined Matrix glasses used for modeling range from 1.62 to 192.10 ppm, while the normalized releases range from 0.104 to 4.418 g/l The PCT-Lithium unnormalized releases range from 3.543 to

77.210 ppm, while the normalized releases range from 0.378 to 3.252 g/l. The PCT-Sodium unnormalized releases range from 4.777 to 285.500 ppm, while the normalized releases range from 0.144 to 2.802 g/l. These ranges generally involve more than an order-of-magnitude difference. In such cases, typically the uncertainty in making glasses, performing the PCT, and analyzing the leachate leads to smaller absolute uncertainties for smaller releases and larger absolute uncertainties for larger releases. Hence, the unweighted least squares (ULS) regression assumption of equal variances for all response variable values (see Section C.2 of Appendix C) is violated. After a logarithmic transformation, variances of response values tend to be approximately equal as required for ULS regression.

- A logarithmic transformation tends to linearize the compositional dependence of leach test data and reduce the need for non-linear terms in the model form.

- A natural logarithm transformation is preferred over a common logarithm (or other base logarithm) transformation because of the approximate relationship

$$\text{SD}\,[\ln(y)] \cong \text{RSD}\,(y) \tag{5.7}$$

where SD denotes standard deviation, and RSD denotes relative standard deviation (i.e., the standard deviation divided by the mean). The relationship in Equation (5.7) is very useful, in that uncertainties of the natural logarithm of the response variable y can be interpreted as RSDs of the untransformed response variable y.

For these reasons, the natural logarithmic transformation was employed for all PCT release model forms.

In summary, natural logarithmic transformations of PCT normalized releases (g/l) were used as the response in modeling PCT-Boron, PCT-Lithium, and PCT-Sodium releases.

5.3 Property-Composition Model Results for PCT-Boron Release

This section discusses the results of fitting several different models using natural logarithms of IHLW PCT normalized boron release (g/l) as the response variable. Section 5.3.1 discusses the assessment of whether there is any difference (i.e., bias) in PCT-Boron data for the Initial Matrix and the Augmentation Matrix glasses. Section 5.3.2 presents the results of modeling PCT-Boron based on compositions involving all 19 components from the IHLW design matrix. In this case, the full LM model, as well as the full LM model augmented with selected quadratic terms (i.e., PQM models), were considered. Section 5.3.3 presents the results of modeling PCT-Boron using LM and PQM models based on a reduced set of mixture components. Finally, Section 5.3.4 presents the recommended PCT-Boron models.

5.3.1 Preliminary Modeling of IHLW PCT-Boron Data to Compare Initial Matrix and Augmentation Matrix Subsets of Data

The modeling data for IHLW PCT-Boron consist of results for the Initial Matrix and the Augmentation Matrix, as discussed in Section 5.1.1. The glasses in these two matrices were fabricated and melted at different times, and the PCT was performed and leachates analyzed at different times. Because the modeling data were collected in two "blocks", it was prudent before performing substantial modeling work to assess whether there were any "block effects" associated with collecting the two subsets of data at different times. The results of that assessment are briefly summarized in this section.

Two variants of the LM model in Equation (5.1) were used to assess whether there were any block effects in the PCT-Boron data between the Initial Matrix and Augmentation Matrix subsets of glasses. These two LM model variants are listed in Equations (C.6) and (C.7) of Appendix C. Both of these models were fitted to the PCT-Boron modeling data (97 glasses), and the statistical significance of the block-effect coefficients was assessed as discussed in Section C.1.2 of Appendix C. No statistically significant block effects were identified, which means it was acceptable to proceed with the IHLW PCT-Boron modeling using the data for the Combined Matrix and ignoring whether data points were from the Initial Matrix or Augmentation Matrix.

5.3.2 Results for Full LM and PQM Models for IHLW PCT-Boron

Initially, a full LM model in the 19 components was fit to the PCT-Boron modeling data (97 glasses) with the response being the natural logarithm of normalized PCT-Boron releases. This model form was a reasonable starting point based on the preliminary data and model assessment work by Perez-Cardenas et al. [6]. The full LM model offered marginal performance, so it was decided that PQM models based on the full LM model should be investigated. PQM models are discussed in detail by Piepel et al. [48].

The MAXR selection routine (see Section C.4.2 of Appendix C) was used to select quadratic terms (squared and two-component crossproduct terms) to include with the 19 linear terms in the hope of obtaining a better fitting model by including important nonlinear blending effects of the glass components. Identifying components having nonlinear blending effects on PCT can be important even if a full PQM model is ultimately not used for modeling PCT release. Such components may be forced to remain in reduced LM models so that quadratic terms involving these components can be considered when developing reduced PQM models. The MAXR selection was run multiple times so as to generate "full PQM" models containing the 19 linear terms plus anywhere from one to eight quadratic terms.

Table 5.4 contains IHLW PCT-Boron model and performance summaries using both the modeling and validation datasets for the full LM model. Summary statistics for the five splits described in Section 5.1.2 are labeled DS# to represent the five modeling/validation "data splits" of the modeling data. The split labeled DS1 is the 82/15 split; the splits labeled DS2, DS3, DS4, and DS5 are the 81/16 splits. The last column of the data splitting section of Table 5.4 shows the averages for the different statistics over the five splits. Table 5.2 includes a column that indicates

which glasses were in each of the five internal validation splits for the PCT-Boron model development. The variance-covariance matrix associated with the model coefficients for the full LM model for PCT-Boron is given in Table D.1 of Appendix D.

5.3.3 Results for Reduced LM and PQM Models for IHLW PCT-Boron

Model reduction was the next model development approach investigated, wherein LM models for PCT-Boron involving less than the 19 components were considered. In this case, the sequential F-test model reduction approach (see Section C.4.1 of Appendix C) was used to conduct model reduction. These F-tests compare full models to reduced models obtained by excluding in turn each of the 19 terms in the full LM model discussed in the previous section. If all linear terms are significant, no model reduction occurs. Otherwise, the least significant linear term is identified. The term identified is dropped from the model, and the remaining components are renormalized. The sequence of F-tests continues until a model is obtained that does not include non-significant terms, based on a specified significance level.

Reduced LM Model for IHLW PCT-Boron

The sequential F-test approach was used to reduce the full PCT-Boron LM model. A significance level of 0.05 was used as the stopping criterion for the sequence of F-tests. Another option available with the F-test approach is to force certain terms to remain in the model during the model reduction process. For PCT-Boron, no terms were forced into the reduced LM model. The reduced LM model obtained for PCT-Boron using the F-test approach contained linear terms for 8 components: Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, and ZrO_2. Summary statistics for the reduced LM model for PCT-Boron (see Table 5.5) indicate that it performs as well or better than the full LM model (see Table 5.4) for both the modeling and validation datasets. The variance-covariance matrix associated with the model coefficients for the reduced LM model for PCT-Boron is given in Table D.2 of Appendix D.

Reduced PQM Models for IHLW PCT-Boron

Adding selected quadratic terms to the reduced LM model was also investigated, thus yielding what are referred to here as "reduced PQM models". The MAXR selection algorithm was used to select quadratic terms (squared and crossproduct terms) from among all possible quadratic terms formed using the terms of the reduced LM model. Different reduced PQM models were obtained depending on the number of quadratic terms specified to be added. Reduced PQM models generated using the MAXR selection option with up to 16 terms (the 8 linear terms from the reduced LM model plus up to 8 quadratic terms) were considered. Performance results for all of the reduced PCT-Boron PQM models considered, as well as the full and reduced PCT-Boron LM models described previously, applied to the IHLW PCT model development data (97 glasses) are given in Table 5.6.

The reduced PQM models being considered for PCT-Boron were also applied to the five modeling/validation splits formed using the modeling data, as described previously. The

averages from the data-splitting validation results are also given in Table 5.6 for the reduced models considered.

5.3.4 Recommended IHLW PCT-Boron Models

Based on the results of the PCT-Boron model development work for:

- the modeling data
- the separate validation dataset and subsets thereof
- the modeling data-splitting results

it was decided to recommend the 19-term full LM model as a baseline model, as well as the 8-term reduced LM model as the preferred model.

Although the PQM models formed by augmenting the reduced LM models with quadratic terms had statistically significant improvements over the reduced LM model for the modeling data and data-splitting investigations, these improvements were not evident for the separate validation data. It is not clear how much the lack of improved prediction performance by PQM models for the separate validation data was due to the limited nature of that data within the compositional region of interest and other factors (e.g., lab-to-lab and long-term variations). However, for conservatism it was decided to recommend as the preferred model the reduced LM model for PCT-Boron release. It was also decided to provide the model coefficients and summary statistics for the full LM model for PCT-Boron as a baseline for comparison with (and justification of) the reduced LM model, particularly when these models are applied to future data. Similar recommendations are made for PCT-Lithium and PCT-Sodium models, see Sections 5.4.4 and 5.5.4, respectively.

Recommended Full LM Model for IHLW PCT-Boron

Table 5.4 gives the coefficients of the 19-term full LM model for ln(PCT-Boron), as well as performance statistics for the modeling data, the validation dataset and its subsets, and the data-split modeling data. The value of $R^2 = 0.751$ indicates that the full LM model accounts for approximately 75% of the variation in $ln(r_B)$ values in the modeling dataset. While this is a reasonably large number, a larger value would be preferable. $R^2_A = 0.694$ is fairly close to R^2, but the magnitude of the difference does indicate that the model could be improved by removing unneeded components. The value for $R^2_P = 0.567$ is sufficiently below the R^2 and R^2_A values to indicate that there may be some influential data points in the modeling dataset. In any case, $R^2_P = 0.567$ provides a more conservative estimate than do R^2 and R^2_A of the fraction of variation in $ln(r_B)$ values for future datasets over the same glass composition region that might be accounted for by this full LM model. Over the five data splits of the modeling data, the average R^2_V was also 0.567. The R^2 validation values for the complete validation dataset, V1, and subsets V2a, V2b, V3a and V3b, range from 0.348 to 0.621. These fractions of variation in $ln(r_B)$ values accounted for by the full LM model are, in most cases, less than indicated by R^2_P and the average R^2_V over the data splits. However, as mentioned in Section 5.1.3, most of the validation glasses are outside the HLW glass composition region of interest defined previously in Tables 2.1

through 2.6. The validation subsets V2b and V3b contain glasses that are "close" to or within the IHLW composition region of interest. The V2b glasses satisfy the single-component constraints used to define the glass composition region, the V3b glass satisfy both single- and multi-component constraints used to define the glass composition region. Glasses from both V2b and V3b subsets were also screened to exclude glasses having non-matrix components present in more than 1 wt% (see Section 5.1.3). The R^2 validation values for these two subsets are larger (0.500 and 0.621, respectively) than those from the other validation sets, but the R^2 validation values are, in general, lower than desired. It is not clear whether this poor prediction performance for the validation data is because of something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the full LM model for PCT-Boron.

Per Equation (5.7), the RMSE = SD[ln(r_B)] in Table 5.4 can be interpreted as the RSD in fabricating simulated HLW glasses and measuring r_B if the model does not have statistically significant LOF. However, RMSE = 0.3834 for the full PCT-Boron LM model is much larger than the historical replicate RSDs in fabricating simulated HLW glasses and measuring PCT-Boron (e.g., ~0.10 in Appendix F of Hrma et al. [29] as discussed near the end of Section 5.1.1). Analysis of replicate PCT-Boron data summarized in Table 5.3 indicates a replicate RSD of ~0.35 (over the 9 replicate pairs) which is similar to the RMSE value. This suggests the model LOF may not be statistically significant. This indication is confirmed by the model LOF test for the PCT-Boron full LM model (see Section C.3 of Appendix C) which is statistically non-significant, having p-value of 0.4666. However, it may be that the full LM model for PCT-Boron does have some LOF that was not detected by the statistical LOF test because of the relatively large uncertainty in the replicate PCT-Boron data.

Figures 5.1 through 5.4 show various regression diagnostic plots for the ln(PCT-Boron) full LM model applied to the 97 glasses of the modeling dataset. Figures 5.1 and 5.2 generally indicate that the assumption of normally distributed errors in the PCT-Boron data is reasonable (see Section C.2 of Appendix C). Figures 5.3 and 5.4 show well-distributed prediction errors for the modeling dataset, although the scatter about the ideal prediction line in Figure 5.4 is larger than would be preferred. It is unclear how much of this scatter is due to model LOF and how much is due to the uncertainties inherent in the PCT-Boron data. Figure 5.3 shows some indication that outer layer glasses had larger uncertainty than inner layer or center glasses.

Figure 5.5 is a component response trace plot produced using the full LM model for ln(PCT-Boron). As discussed in Section C.4.1 of Appendix C, this plot displays how ln(PCT-Boron) changes as components are decreased and increased from their values in a reference composition, keeping all other components in the same relative proportions. Figure 5.5 shows that some components such as SrO, Fe_2O_3, and ZnO have nearly horizontal traces, thus indicating that these components may have non-significant effects on PCT-Boron release. In fact, these components, along with several other components, were dropped from the model as part of the model reduction process that led to the PCT-Boron reduced LM model. Figures 5.6 through 5.10 show *predicted versus measured plots* when the full LM model for IHLW PCT-Boron is applied to the validation dataset and various subsets thereof.

Recommended Reduced LM Model for IHLW PCT-Boron

Table 5.5 gives the coefficients of the 8-term reduced LM model for ln(PCT-Boron), as well as performance statistics for the modeling data, the validation dataset and its subsets, and data-split modeling data. The model evaluation statistics $R^2 = 0.722$, $R^2_A = 0.700$, $R^2_P = 0.667$, and RMSE = 0.3791 are very similar to the corresponding statistics for the 19-term full LM model. The differences between R^2 and R^2_A and between R^2_A and R^2_P are less for the reduced LM model than for the full LM model. This suggests that the model reduction was beneficial and that the reduced LM model is less affected by influential data points than is the full LM model. Over the five data splits of the modeling data, the average R^2_V was 0.693, which is similar to the R^2_P value. The R^2 validation values for the complete validation dataset, V1, and subsets V2a, V2b, V3a and V3b, range from 0.342 to 0.600. These fractions of variation in $ln(r_B)$ values accounted for by the reduced LM model are consistently less than indicated by R^2_P and the average R^2_V over the data splits. But again, most of the validation glasses are outside the HLW glass composition region of interest defined previously in Tables 2.1 through 2.6. The validation subsets V2b and V3b contain glasses that are "close" to or within the IHLW composition region of interest. The V2b glasses satisfy the single-component constraints used to define the glass composition region, the V3b glass satisfy both single- and multi-component constraints used to define the glass composition region. Glasses from both V2b and V3b subsets were also screened to exclude glasses having non-matrix components present in more than 1 wt% (see Section 5.1.3). The R^2 validation values for these two subsets are larger (0.563 and 0.600, respectively) than those from the other validation sets, but the R^2 validation values are, in general, lower than desired. As with the full LM model for PCT-Boron, it is not clear whether the poor prediction performance for these subsets of the validation dataset is due to something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the reduced LM model for PCT-Boron.

Per Equation (5.7), the RMSE = SD[ln(r_B)] in Table 5.5 can be interpreted as the RSD in fabricating simulated HLW glasses and measuring r_B if the model does not have statistically significant LOF. The RMSE value for the reduced LM model was 0.3791 which, like the RMSE value for the full LM model for PCT-Boron, is larger than the historical replicate RSDs in fabricating simulated HLW glasses and measuring PCT-Boron (e.g., ~0.10 in Appendix F of Hrma et al. [29] as discussed near the end of Section 5.1.1). Analysis of replicate PCT-Boron data summarized in Table 5.3 indicates a replicate RSD of ~0.35 (over the 9 replicate pairs) which is similar to the RMSE value. This suggests the model LOF may not be statistically significant. This indication is confirmed by the model LOF test for the PCT-Boron reduced LM model (see Section C.3 of Appendix C) which is statistically non-significant, having p-value of 0.4878. However, it may be that the reduced LM model for PCT-Boron does have some LOF that was not detected by the statistical LOF test because of the relatively large uncertainty in the replicate PCT-Boron data.

Figures 5.11 through 5.14 show various regression diagnostic plots for the ln(PCT-Boron) reduced LM model applied to the 97 glasses of the modeling dataset. Figures 5.11 and 5.12 generally indicate that the assumption of normally distributed errors in the PCT-Boron data is reasonable (see Section C.2 of Appendix C). Figures 5.13 and 5.14 show

well-distributed prediction errors for the modeling dataset, although the scatter about the ideal prediction line in Figure 5.14 is larger than would be preferred. It is unclear how much of this scatter is due to any LOF of the reduced LM model, and how much is due to the uncertainties inherent in the PCT-Boron data. Also, the reduced LM model shows a possible tendency to under-predict PCT-Boron normalized releases above about 0.5 ln(g/l) = 1.65 g/l.

Figure 5.15 is a component response trace plot produced using the reduced LM model for ln(PCT-Boron). As discussed in Section C.4.1 of Appendix C, this plot displays how ln(PCT-Boron) changes as components are decreased and increased from their values in a reference composition, keeping all other components in the same relative proportions. Figure 5.15 shows that each of the component traces has relatively steep slope, reinforcing the idea that the 8 components remaining in the reduced LM model have significant effects on PCT-Boron release. Figures 5.16 through 5.20 show predicted versus measured plots from applying the reduced LM model to the validation dataset and various subsets thereof. These predicted versus measured plots provide visual evidence that predictive performance for the reduced LM model should be very comparable to that of the full LM model for PCT-Boron.

In conclusion, the recommended IHLW Phase 1 models for PCT-Boron are the 19-term full LM model in Table 5.4 (as a baseline model) and the 8-term reduced LM model in Table 5.5 (as the preferred model). It is recommended that both these IHLW PCT-Boron models be applied and their performances compared during future IHLW glass formulation and waste form qualification work.

5.4 Property-Composition Model Results for PCT-Lithium Release

This section discusses the results of fitting several different models using natural logarithms of IHLW PCT normalized lithium release (g/l) as the response variable. Section 5.4.1 discusses the assessment of whether there is any difference (i.e., bias) in PCT-Lithium data for the Initial Matrix and the Augmentation Matrix glasses. Section 5.4.2 presents the results of modeling PCT-Lithium based on compositions involving all 19 components from the IHLW design matrix. As with the PCT-Boron modeling, the full LM model, as well as the full LM model augmented with selected quadratic terms (i.e., PQM models) were considered for PCT-Lithium modeling. Section 5.4.3 presents the results of modeling PCT-Lithium using LM and PQM models based on a reduced set of mixture components. Finally, Section 5.4.4 presents the recommended PCT-Lithium models.

5.4.1 Preliminary Modeling of IHLW PCT-Lithium Data to Compare Initial Matrix and Augmentation Matrix Subsets of Data

The modeling data for IHLW PCT-Lithium consist of results for the Initial Matrix and the Augmentation Matrix, as discussed in Section 5.1.1. The glasses in these two matrices were fabricated and melted at different times, and the PCT was performed and leachates analyzed at different times. Because the modeling data were collected in two “blocks”, it was prudent before performing substantial modeling work to assess whether there are any “block effects” associated

with collecting the two subsets of data at different times. The results of that assessment are briefly summarized in this section.

Two variants of the LM model in Equation (5.1) were used to assess whether there were any block effects in the PCT-Lithium data between the Initial Matrix and Augmentation Matrix subsets of glasses. These two LM model variants are listed in Equations (C.6) and (C.7) of Appendix C. Both of these models were fitted to the PCT-Lithium modeling data (97 glasses), and the statistical significance of the block-effect coefficients was assessed as discussed in Section C.1.2 of Appendix C. No statistically significant block effects were identified, which means it was acceptable to proceed with the IHLW PCT-Lithium modeling using the data for the Combined Matrix and ignoring whether data points were from the Initial Matrix or Augmentation Matrix.

5.4.2 Results for Full LM and PQM Models for IHLW PCT-Lithium

As with the IHLW PCT-Boron model development, a full LM model was the first model form considered for IHLW PCT-Lithium modeling. The full LM model included the same 19 components involved in the PCT-Boron modeling, and used the same 97 of 102 glass compositions from the IHLW Combined Matrix. The PCT-Lithium full LM model performed somewhat worse than the PCT-Boron full LM model for the modeling data. Again, full PQM models were investigated for IHLW PCT-Lithium, using the MAXR selection method to select quadratic terms to augment the linear terms of the full LM model for PCT-Lithium. Full PQM models were generated that contained the 19 linear terms of the full LM model plus anywhere form one to eight quadratic terms.

Model evaluation and validation performance results for the full LM model for PCT-Lithium are listed in Table 5.7. Included in Table 5.7 are validation results for the complete validation set, as well as various validation subsets. The validation set and subsets are the same as were used for the PCT-Boron models, as discussed in Section 5.1.3. The same five modeling/validation splits formed from the modeling data and described previously in Section 5.1.2 were used to conduct data-splitting model validation for the full LM model for PCT-Lithium. Again, the split labeled DS1 in Table 5.7 is the 82/15 split; the splits labeled DS2, DS3, DS4, and DS5 are the 81/16 splits The last column of the data splitting section of Table 5.7 shows the averages for the different statistics over the five modeling/validation splits. The variance-covariance matrix associated with the model coefficients for the full LM model for PCT-Lithium is given in Table D.3 of Appendix D.

5.4.3 Results for Reduced LM and PQM Models for IHLW PCT-Lithium

As with the PCT-Boron modeling, reduced LM and PQM models for PCT-Lithium were also pursued with the goal of improving the predictive performance for validation data by dropping unnecessary terms. The iterative F-test approach (see Section C.4.1 of Appendix C) was again used to identify non-significant linear terms in the full LM model and normalize them out. Again, a significance level of 0.05 was used for the F-tests. As with the PCT-Boron model

reduction, an initial reduction of the full PCT-Lithium LM model was conducted where no terms were forced into the reduced PCT-Lithium LM model. However, this initial model reduction attempt resulted in a 6-term reduced LM model involving Al_2O_3, B_2O_3, Li_2O, Na_2O, SiO_2, and ZrO_2. The two terms missing in this initial reduced PCT-Lithium LM model compared to the 8-term reduced LM model for PCT-Boron are MnO and ThO_2. These two terms were two of the final three terms dropped during the initial reduction process. As is subsequently discussed in Section 5.5.3, the sequential F-test reduction algorithm resulted in a reduced LM model for PCT-Sodium that contained the same 8 terms as the reduced LM model for PCT-Boron. Furthermore, for both PCT-Boron and PCT-Sodium, the model reduction algorithm yielded the same 8-term reduced model form without forcing any terms into the reduced LM model. Having the same reduced LM model form for all three PCT releases would be an advantage, or at least a convenience. Thus, the sequential F-test reduction algorithm was re-run for PCT-Lithium, this time forcing MnO and ThO_2 into the reduced LM model. The result of this second model reduction run was a reduced LM model for PCT-Lithium containing the same 8 terms included in the reduced PCT-Boron and PCT-Sodium models; Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, and ZrO_2. Summary statistics for the reduced LM model for PCT-Lithium (see Table 5.8) indicate that it performs as well or better than the full LM model (see Table 5.7) for both the modeling and validation datasets. The variance-covariance matrix associated with the model coefficients for the reduced LM model for PCT-Lithium is given in Table D.4 of Appendix D.

Reduced PQM models were also developed for PCT-Lithium using the MAXR selection algorithm. Reduced PQM models with up to 16 terms (the 8 linear terms from the reduced LM model for PCT-Lithium plus up to 8 quadratic terms) were considered. Performance results for all of the reduced PCT-Lithium PQM models considered, as well as the full and reduced PCT-Lithium LM models described previously, applied to the IHLW PCT model development data (97 glasses) are given in Table 5.9. The reduced LM and PQM models for PCT-Lithium were applied to the five modeling/validation splits formed using the modeling data that were described previously. The averages from the data-splitting validation results are also given in Table 5.9 for the reduced PCT-Sodium models considered.

5.4.4 Recommended IHLW PCT-Lithium Models

Based on the results of the PCT-Lithium model development work for:

- the modeling data
- the separate validation dataset and subsets thereof
- the modeling data-splitting results

it was decided to recommend the 19-term full LM model as a baseline model, as well as the 8-term reduced LM model as the preferred model. Again, the full LM model is intended to serve as a baseline for comparisons with the performance of the reduced LM model applied to future datasets.

Recommended Full LM Model for IHLW PCT-Lithium

Table 5.7 gives the coefficients of the 19-term full LM model for ln(PCT-Lithium), as well as performance statistics for the modeling data, the validation dataset and its subsets, and data-split modeling data.

The value of $R^2 = 0.666$ indicates that the full LM model accounts for over 66% of the variation in $ln(r_{Li})$ values in the modeling dataset. This is a marginal value, a larger value would clearly be preferable. $R^2_A = 0.589$ is sufficiently below the R^2 value, suggesting that the full LM model probably contains unneeded model terms. The value for $R^2_P = 0.422$ is far enough from the R^2 and R^2_A values to indicate that there may be some points in the modeling dataset that are influential in determining the full LM model. Again, $R^2_P = 0.422$ provides a more conservative estimate of the fraction of variation in $ln(r_{Li})$ values for future datasets over the same glass composition region that might be accounted for by this full LM model. Over the five data splits of the modeling data, the average R^2_V was 0.446, which is similar to the R^2_P value. The R^2 validation values for the complete validation dataset, V1, and the V2a subset are 0.401 and 0.415, respectively. The R^2 validation value for the V3a subset is 0.145, which is dramatically lower than the other R^2 validation values. However, the V3a glasses do not satisfy the additional screening requirement imposed on the V3b glass compositions that non-matrix components be less than 1 wt%. Unlike the V3a subset, the fractions of variation in $ln(r_{Li})$ values accounted for by the full LM model, as represented by the R^2 validation values for V1 and V2a, are similar to the fractions indicated by R^2_P and the average R^2_V over the data splits. The R^2 validation values are higher for the V2b and V3b subsets, 0.575 and 0.640, respectively. These R^2 values are somewhat higher than the R^2_P and the average R^2_V over the data splits for the full LM model. Although all of these R^2 validation values are lower than desired, it is encouraging that the values are highest for the V2b and V3b subsets. Recall from Section 5.1.3 that most of the validation glasses have compositions outside the IHLW glass composition region of interest but that the glasses in the V2b and V3b validation subsets have compositions that are within the IHLW glass composition region or are very similar to such compositions. It is not clear whether the poor prediction performance for these subsets of the validation dataset is due to something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the full LM model for PCT-Lithium, particularly when extrapolating the model beyond the IHLW glass composition region.

Per Equation (5.7), the RMSE = SD[ln(r_{Li})] in Table 5.7 can be interpreted as the RSD in fabricating simulated HLW glasses and measuring r_{Li} if the model does not have statistically significant LOF. However, RMSE = 0.3058 for the full PCT-Lithium LM model is larger than the historical replicate RSDs in fabricating simulated HLW glasses and measuring PCT-Lithium (e.g., ~0.10 in Appendix F of Hrma et al. [29] as discussed near the end of Section 5.1.1). Analysis of replicate PCT-Lithium data summarized in Table 5.3 indicates a replicate RSD of ~0.11 (over the 9 replicate pairs) which is considerably lower than the RMSE value. This indicates the full LM model for PCT-Lithium may have a statistically significant lack of fit. This indication is confirmed by the model LOF test for the PCT-Lithium full LM model (see Section C.3 of Appendix C) which is statistically significant, having p-value of 0.0007. The consequences of model LOF and prediction uncertainties are discussed further in Section 5.7.

Figures 5.21 through 5.24 show various regression diagnostic plots for the ln(PCT-Lithium) full LM model applied to the 97 IHLW design matrix glasses used for model development. Figures 5.21 and 5.22 generally indicate that the assumption of normally distributed errors is reasonable when the PCT-Lithium full LM model is applied to the modeling data (see Section C.2 of Appendix C). Figures 5.23 and 5.24 show well-distributed prediction errors for the modeling dataset, except for a possible tendency to under-predict PCT-Sodium normalized releases above about 0.25 ln(g/l) = 1.28 g/l.

Figure 5.25 is a component response trace plot produced using the full LM model for ln(PCT-Lithium). As discussed in Section C.4.1 of Appendix C, this plot displays how ln(PCT-Lithium) changes as components are decreased and increased from their values in a reference composition, keeping all other components in the same relative proportions. Figures 5.26 through 5.30 show predicted versus measured plots from applying the full LM model to the validation dataset and various subsets thereof.

Recommended Reduced LM Model for IHLW PCT-Lithium

Table 5.8 gives the coefficients of the 8-term reduced LM model for ln(PCT-Lithium), as well as performance statistics for the modeling data, the validation dataset and its subsets, and data-split modeling data. The modeling evaluation statistics R^2 = 0.641, R^2_A = 0.612, R^2_P = 0.571, and RMSE = 0.2968 are similar to or better than the corresponding statistics for the 19-term full LM model. The limited drop in values from R^2 to R^2_A suggests that model reduction was effective in eliminating unneeded terms from the full LM model. The drop is slightly greater from R^2_A to R^2_P suggesting that the modeling dataset may contain some influential data points. R^2_P = 0.571 provides a more conservative estimate of the fraction of variation in $ln(r_{Li})$ values for future datasets over the same glass composition region that might be accounted for by this reduced LM model. Over the five data splits of the modeling data, the average R^2_V was 0.578, which is very close to the R^2_P value. The R^2 validation values for the complete V1 validation dataset and the V2a and V3a subsets range from 0.303 to 0.377. But again, the R2 validation values are higher for the V2b and V3b subset, 0.586 and 0.637, respectively. These fractions of variation in $ln(r_{Li})$ values accounted for by the reduced LM model are slightly higher than indicated by R^2_P and the average R^2_V over the data splits. These measures of model performance seem to be consistent with the nature of the compositions contained in the validation sets. As discussed in Section 5.1.3, the majority of the glasses in the complete V1 validation dataset have compositions that are outside the HLW glass composition region of interest (defined previously in Tables 2.1 through 2.6). Glasses in the other validation subsets have compositions that are either inside the IHLW glass composition region or are similar to such compositions. Differences in glass composition may not completely explain the drop in model performance for the V1, V2a, and V3a validation sets. It is not clear whether this poorer prediction performance for the complete validation dataset and certain subsets thereof is because of something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the reduced LM model for PCT-Lithium.

Per Equation (5.7), the RMSE = SD[$ln(r_{Li})$] in Table 5.8 can be interpreted as the RSD in fabricating simulated HLW glasses and measuring r_{Li} if the model does not have statistically significant LOF. As with the other PCT models presented in this report, RMSE = 0.2968 for the reduced PCT-Lithium LM model is larger than the historical replicate RSDs in fabricating simulated HLW glasses and measuring PCT-Lithium (e.g., ~0.10 in Appendix F of Hrma et al. [29] as discussed near the end of Section 5.1.1). Analysis of replicate PCT-Lithium data summarized in Table 5.3 indicates a replicate RSD of ~0.11 (over the 9 replicate pairs) which is considerably lower than the RMSE value. This indicates the reduced LM model for PCT-Lithium may have a statistically significant lack of fit. This indication is confirmed by the model LOF test for the PCT-Lithium reduced LM model (see Section C.3 of Appendix C) which is statistically significant, having p-value of 0.0010. The consequences of model LOF and prediction uncertainties are discussed further in Section 5.7.

Figures 5.31 through 5.34 show various regression diagnostic plots for the ln(PCT-Lithium) reduced LM model applied to the 97 IHLW design matrix glasses used for model development. Figures 5.31 and 5.32 generally indicate that the assumption of normally distributed errors is reasonable when the PCT-Lithium reduced LM model is applied to the modeling data (see Section C.2 of Appendix C). Figures 5.33 and 5.34 show well-distributed prediction errors for the modeling dataset, except for a possible tendency (as with the full LM model) to under-predict PCT-Lithium normalized releases above about 0.25 ln(g/l) = 1.28 g/l.

Figure 5.35 is a component response trace plot produced using the reduced LM model for ln(PCT-Lithium). As discussed in Section C.4.1 of Appendix C, this plot displays how ln(PCT-Lithium) changes as components are decreased and increased from their values in a reference composition, keeping all other components in the same relative proportions. Figures 5.36 through 5.40 show predicted versus measured plots from applying the reduced LM model to the validation dataset and various subsets thereof.

In conclusion, the recommended IHLW Phase 1 models for PCT-Lithium are the 19-term full LM model in Table 5.7 (as a baseline model) and the 8-term reduced LM model in Table 5.8 (as the preferred model). It is recommended that both these IHLW PCT-Lithium models be applied and their performances compared during future IHLW glass formulation and waste form qualification work.

5.5 Property-Composition Model Results for PCT-Sodium Release

This section discusses the results of fitting several different models using natural logarithms of IHLW PCT normalized sodium release (g/l) as the response variable. Section 5.5.1 discusses the assessment of whether there is any difference (i.e., bias) in PCT-Sodium data for the Initial Matrix and the Augmentation Matrix glasses. Section 5.5.2 presents the results of modeling PCT-Sodium based on compositions involving all 19 components from the IHLW design matrix. As with the PCT-Boron and PCT-Lithium modeling, the full LM model and the full LM model augmented with selected quadratic terms (i.e., PQM models) were considered for PCT-Sodium modeling. Section 5.5.3 presents the results of modeling PCT-Sodium using LM

and PQM models based on a reduced set of mixture components. Finally, Section 5.5.4 presents the recommended PCT-Sodium models.

5.5.1 Preliminary Modeling of IHLW PCT-Sodium Data to Compare Initial Matrix and Augmentation Matrix Subsets of Data

The modeling data for IHLW PCT-Sodium consist of results for the Initial Matrix and the Augmentation Matrix, as discussed in Section 5.1.1. The glasses in these two matrices were fabricated and melted at different times, and the PCT was performed and leachates analyzed at different times. Because the modeling data were collected in two "blocks", it was prudent before performing substantial modeling work to assess whether there are any "block effects" associated with collecting the two subsets of data at different times. The results of that assessment are briefly summarized in this section.

Two variants of the LM model in Equation (5.1) were used to assess whether there were any block effects in the PCT-Sodium data between the Initial Matrix and Augmentation Matrix subsets of glasses. These two LM model variants are listed in Equations (C.6) and (C.7) of Appendix C. Both of these models were fitted to the PCT- Sodium modeling data (97 glasses), and the statistical significance of the block-effect coefficients was assessed as discussed in Section C.1.2 of Appendix C. No statistically significant block effects were identified, which means it was acceptable to proceed with the IHLW PCT- Sodium modeling using the data for the Combined Matrix and ignoring whether data points were from the Initial Matrix or Augmentation Matrix.

5.5.2 Results for Full LM and PQM Models for IHLW PCT-Sodium

As with the IHLW PCT-Boron and PCT-Lithium model development, a full LM model was the first model form considered for IHLW PCT-Sodium modeling. The full LM model included the same 19 components involved in the PCT-Boron and PCT-Lithium modeling, and used the same 97 of 102 glass compositions from the IHLW Combined Matrix. The PCT-Sodium full LM model performed slightly better than the PCT-Boron and PCT-Lithium full LM models for the modeling data. But again, full PQM models were investigated for IHLW PCT-Sodium, using the MAXR selection method to select quadratic terms to augment the linear terms of the full LM model for PCT-Sodium. Full PQM models were generated that contained the 19 linear terms of the full LM model plus anywhere form one to eight quadratic terms.

Model evaluation and validation performance results for the full LM model for PCT-Sodium are listed in Table 5.10. Included in Table 5.10 are validation results for the complete validation set, as well as various validation subsets. The validation set and subsets are the same as were used for the PCT-Boron and PCT-Lithium models, as discussed in Section 5.1.3. The same five modeling/validation splits formed from the modeling data and described previously in Section 5.1.2 were used to conduct data-splitting model validation for the full LM model for PCT-Sodium. Again, the split labeled DS1 in Table 5.10 is the 82/15 split; the splits labeled DS2, DS3, DS4, and DS5 are the 81/16 splits The last column of the data splitting

section of Table 5.10 shows the averages for the different statistics over the five modeling/validation splits. The variance-covariance matrix associated with the model coefficients for the full LM model for PCT-Sodium is given in Table D.5 of Appendix D

5.5.3 Results for Reduced LM and PQM Models for IHLW PCT-Sodium

As with the PCT-Boron and PCT-Lithium modeling, reduced LM and PQM models for PCT-Sodium were also pursued with the goal of improving the predictive performance for validation data by dropping unnecessary terms. The iterative F-test approach (see Section C.4.1 of Appendix C) was again used to identify non-significant linear terms in the full LM model and normalize them out. Again, a significance level of 0.05 was used for the F-tests. As with the PCT-Boron model reduction, no terms were forced into the reduced PCT-Sodium LM model. The reduced LM model for PCT-Sodium contains the same 8 terms included in the reduced PCT-Boron and PCT-Lithium models; Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, and ZrO_2. Summary statistics for the reduced LM model for PCT-Sodium (see Table 5.11) indicate that it performs as well or better than the full LM model (see Table 5.10) for both the modeling and validation datasets. The variance-covariance matrix associated with the model coefficients for the reduced LM model for PCT-Sodium is given in Table D.6 of Appendix D.

Reduced PQM models were also developed for PCT-Sodium using the MAXR selection algorithm. Reduced PQM models with up to 16 terms (the 8 linear terms from the reduced LM model for PCT-Sodium plus up to 8 quadratic terms) were considered. Performance results for all of the reduced PCT-Sodium PQM models considered, as well as the full and reduced PCT-Sodium LM models described previously, applied to the IHLW PCT model development data (97 glasses) are given in Table 5.12. The reduced LM and PQM models for PCT-Sodium were applied to the five modeling/validation splits formed using the modeling data that were described previously. The averages from the data-splitting validation results are also given in Table 5.12 for the reduced PCT-Sodium models considered.

5.5.4 Recommended IHLW PCT-Sodium Models

Based on the results of the PCT-Sodium model development work for:

- the modeling data
- the separate validation dataset and subsets thereof
- the modeling data-splitting results

it was decided to recommend the 19-term full LM model as a baseline model, as well as the 8-term reduced LM model as the preferred model. Again, the full LM model is intended to serve as a baseline for comparisons with the performance of the reduced LM model applied to future datasets.

Recommended Full LM Model for IHLW PCT-Sodium

Table 5.10 gives the coefficients of the 19-term full LM model for ln(PCT-Sodium), as well as performance statistics for the modeling data, the validation dataset and its subsets, and data-split modeling data.

The value of $R^2 = 0.865$ indicates that the full LM model accounts for over 86% of the variation in $ln(r_{Na})$ values in the modeling dataset. While this is a reasonably large number and is noticeably higher than the R^2 values for the full PCT-Boron and PCT-Lithium LM models, a larger value would still be preferable. $R^2_A = 0.833$ is relatively close to R^2, indicating that the full LM model is not overly hindered by unneeded components. The value for $R^2_P = 0.775$ is far enough below the R^2 and R^2_A values to indicate that there may be some points in the modeling dataset that are influential in determining the full LM model. Again, $R^2_P = 0.775$ provides a more conservative estimate of the fraction of variation in $ln(r_{Na})$ values for future datasets over the same glass composition region that might be accounted for by this full LM model. Over the five data splits of the modeling data, the average R^2_V was 0.784, which is similar to the R^2_P value. The R^2 validation values for the complete validation dataset, V1, and subsets V2a, and V3a, range from 0.289 to 0.561. These fractions of variation in $ln(r_{Na})$ values accounted for by the full LM model are noticeably less than indicated by R^2_P and the average R^2_V over the data splits. However, R^2 validation values for the V2b and V3b subsets are 0.712 and 0.766, respectively. These R^2 values are comparable to the R^2_P and the average R^2_V over the data splits for the full LM model. Such validation results may be understandable based on the nature of the glass compositions included in the different validation sets. Recall from Section 5.1.3 that most of the validation glasses have compositions outside the IHLW glass composition region of interest but that the glasses in the V2b and V3b validation subsets have compositions that are within the IHLW glass composition region or are very similar to such compositions. It is not clear whether the poor prediction performance for these subsets of the validation dataset is due to something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the reduced LM model for PCT-Sodium, particularly when extrapolating the model beyond the IHLW glass composition region.

Per Equation (5.7), the RMSE = SD[ln(r_{Na})] in Table 5.10 can be interpreted as the RSD in fabricating simulated HLW glasses and measuring r_{Na} if the model does not have statistically significant LOF. However, RMSE = 0.2548 for the full PCT-Sodium LM model is larger than the historical replicate RSDs in fabricating simulated HLW glasses and measuring PCT-Sodium (e.g., ~0.10 in Appendix F of Hrma et al. [29] as discussed near the end of Section 5.1.1). Analysis of replicate PCT-Sodium data summarized in Table 5.3 indicates a replicate RSD of ~0.09 (over the 9 replicate pairs) which is considerably lower than the RMSE value. This indicates the full LM model for PCT-Sodium may have a statistically significant lack of fit. This indication is confirmed by the model LOF test for the PCT-Sodium full LM model (see Section C.3 of Appendix C) which is statistically significant, having p-value of 0.0010. The consequences of model LOF and prediction uncertainties are discussed further in Section 5.7.

Figures 5.41 through 5.44 show various regression diagnostic plots for the ln(PCT-Sodium) full LM model applied to the 97 IHLW design matrix glasses used for model

development. Figures 5.41 and 5.42 generally indicate that the assumption of normally distributed errors is reasonable when the PCT-Sodium full LM model is applied to the modeling data (see Section C.2 of Appendix C). Figures 5.43 and 5.44 show well-distributed prediction errors for the modeling dataset, except for a possible tendency to under-predict PCT-Sodium normalized releases above about 0.5 ln(g/l) = 1.65 g/l.

Figure 5.45 is a component response trace plot produced using the full LM model for ln(PCT-Sodium). As discussed in Section C.4.1 of Appendix C, this plot displays how ln(PCT-Sodium) changes as components are decreased and increased from their values in a reference composition, keeping all other components in the same relative proportions. Figures 5.46 through 5.50 show predicted versus measured plots from applying the full LM model to the validation dataset and various subsets thereof.

Recommended Reduced LM Model for IHLW PCT-Sodium

Table 5.11 gives the coefficients of the 8-term reduced LM model for ln(PCT-Sodium), as well as performance statistics for the modeling data, the validation dataset and its subsets, and data-split modeling data. The modeling evaluation statistics R^2 = 0.843, R^2_A = 0.830, R^2_P = 0.813, and RMSE = 0.2572 are very comparable to the corresponding statistics for the 19-term full LM model. The limited drop in values from R^2 to R^2_A and from R^2_A to R^2_P suggests that model reduction was effective in eliminating unneeded terms from the full LM model, and that the modeling dataset probably does not contain any highly influential data points. R^2_P = 0.813 provides a more conservative estimate of the fraction of variation in $ln(r_{Na})$ values for future datasets over the same glass composition region that might be accounted for by this reduced LM model. Over the five data splits of the modeling data, the average R^2_V was 0.820, which is slightly higher than the R^2_P value. The R^2 validation values for the complete V1 validation dataset and the V2a and V3a subsets range from 0.290 to 0.592. But again, the R2 validation values are higher for the V2b and V3b subset, 0.695 and 0.728, respectively. These fractions of variation in $ln(r_{Na})$ values accounted for by the reduced LM model are noticeably less than indicated by R^2_P and the average R^2_V over the data splits. Such drops in model performance may be understandable for the complete V1 validation dataset for which a majority of the glasses are outside the HLW glass composition region of interest defined previously in Tables 2.1 through 2.6. Differences in glass composition may not completely explain the drop in model performance for the validation subsets, particularly V2b and V3b, which contain glasses that are within the HLW glass composition region or are similar to such glasses. It is not clear whether this poorer prediction performance for the validation dataset and subsets thereof is because of something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the reduced LM model for PCT-Sodium.

Per Equation (5.7), the RMSE = SD[$ln(r_{Na})$] in Table 5.11 can be interpreted as the RSD in fabricating simulated HLW glasses and measuring r_{Na} if the model does not have statistically significant LOF. As with the other PCT models, RMSE = 0.2572 for the reduced PCT-Sodium LM model is larger than the historical replicate RSDs in fabricating simulated HLW glasses and measuring PCT-Sodium (e.g., ~0.10 in Appendix F of Hrma et al. [29] as discussed near the end of Section 5.1.1). Analysis of replicate PCT-Sodium data summarized in Table 5.3 indicates a

replicate RSD of ~0.09 (over the 9 replicate pairs) which is considerably lower than the RMSE value. This indicates the reduced LM model for PCT-Sodium may have a statistically significant lack of fit. This indication is confirmed by the model LOF test for the PCT-Sodium reduced LM model (see Section C.3 of Appendix C) which is statistically significant, having p-value of 0.0009. The consequences of model LOF and prediction uncertainties are discussed further in Section 5.7.

Figures 5.51 through 5.54 show various regression diagnostic plots for the ln(PCT-Sodium) reduced LM model applied to the 97 IHLW design matrix glasses used for model development. Figures 5.51 and 5.52 generally indicate that the assumption of normally distributed errors is reasonable when the PCT-Sodium reduced LM model is applied to the modeling data (see Section C.2 of Appendix C). Figures 5.53 and 5.54 show well-distributed prediction errors for the modeling dataset, except for a possible tendency (although less of a tendency than for the full LM model) to under-predict PCT-Sodium normalized releases above about 0.5 ln(g/l) = 1.65 g/l.

Figure 5.55 is a component response trace plot produced using the reduced LM model for ln(PCT-Sodium). As discussed in Section C.4.1 of Appendix C, this plot displays how ln(PCT-Sodium) changes as components are decreased and increased from their values in a reference composition, keeping all other components in the same relative proportions. Figures 5.56 through 5.60 show predicted versus measured plots from applying the reduced LM model to the validation dataset and various subsets thereof.

In conclusion, the recommended IHLW Phase 1 models for PCT-Sodium are the 19-term full LM model in Table 5.10 (as a baseline model) and the 8-term reduced LM model in Table 5.11 (as the preferred model). It is recommended that both these IHLW PCT-Sodium models be applied and their performances compared during future IHLW glass formulation and waste form qualification work.

5.6 Example Illustrating Model Predictions and Statistical Intervals

This section contains examples to illustrate the use of both the full and reduced LM models for PCT-Boron, PCT-Lithium, and PCT-Sodium to obtain predicted PCT releases for a specific HLW glass composition. This section also describes how corresponding 95% UCIs and 95% SUCIs are calculated.

The glass composition used in this example is that of HLW03-06, which is one of the glasses in the IHLW Combined Matrix. The composition of HLW03-06 for PCT modeling is given in Table 5.1 in normalized weight percent format. In order to apply the PCT models to this composition, the weight percentages must be converted to normalized mass fractions (that sum to 1.0) over the linear components contained in the different models. Table 5.13 contains the composition for HLW03-06 prepared for use in the different IHLW models for PCT-Boron, PCT-Lithium, and PCT-Sodium.

For each of the different PCT models, predicted ln(PCT releases) are obtained by multiplying the composition in the format needed for the specific models by the coefficients for the different models (see Tables 5.4, 5.5, 5.7, 5.8, 5.10, and 5.11), then summing the results. That is, the predicted values are calculated by

$$\hat{y}(\boldsymbol{a}) = \boldsymbol{a}^T\boldsymbol{b}\,,$$

where $\boldsymbol{a}$ is the composition of HLW03-06 formatted to match the terms in a given model (from Table 5.13), T represents a matrix transpose (or vector transpose in this case), and $\boldsymbol{b}$ is the vector of model coefficients for a given model. The predicted ln(PCT release) values from each of the six IHLW PCT models are listed in the second column of Table 5.14. The predicted ln(PCT releases) in ln(g/l) units are easily converted to the usual PCT release units of g/l by exponentiation. The third column of Table 5.14 contains the predicted PCT releases in g/l units. However, as discussed in Section C.6 of Appendix C, these back-transformed PCT release predictions in g/l units should be considered estimates of the true median of the distribution of PCT releases that would result if the PCT were repeated multiple times using samples of the HLW03-06 glass, not estimates of the true mean.

Equation (C.13) can be used to calculate a 95% UCI for the true mean of ln(PCT releases) from the HLW03-06 glass composition for each of the IHLW PCT models. In the notation of Equation (C.13):

- $100(1-\alpha)\% = 95\%$, so that $\alpha = 0.05$.
- The vector $\boldsymbol{a}$ is the composition of HLW03-06 formatted to match the terms in a given model.
- The matrix $\boldsymbol{A}$ is the design matrix of normalized linear components formatted to match the terms in a given model.

To obtain an 95% UCI in ln(PCT release) units of ln(g/l), the quantity $t_{1-\alpha,n-p}RMSE\sqrt{\boldsymbol{a}^T(\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{a}}$ is added to the predicted PCT release $\hat{y}(\boldsymbol{a})$ described above, as indicated by Equation (C.13). The $MSE[(\boldsymbol{A}^T\boldsymbol{A})^{-1}]$ portion of this expression is the variance-covariance matrix for the estimated model coefficients, as discussed near the end of Section C.6 of Appendix C. The variance-covariance matrices for the different PCT models are listed in Appendix D. The quantity *MSE* is the mean squared error from regression, *RMSE* is the square root of *MSE*.

The 95% UCI values for the true mean ln(PCT release) in units of ln(g/l) for the HLW03-06 composition based on the different IHLW PCT models are given in the fourth column of Table 5.14. Exponentiating the resulting 95% UCIs on the mean in ln(g/l) units yields 95% UCIs for the median in g/l units. For example, the full LM model for PCT-Boron has −1.0755 ln(g/l) as the upper limit of the 95% UCI on the true mean ln(PCT-Boron release) for HLW03-06, whereas $e^{-1.0755} = 0.3411$ g/l is the upper limit of the 95% UCI on the true median

PCT-Boron release. The fifth column of Table 5.14 contains 95% UCIs for the true median PCT releases from the HLW03-06 glass composition based on the different IHLW PCT models. Note that the 95% UCI values in g/l units for the different IHLW PCT models are well below the PCT release limits for DWPF-EA glass [i.e., 8.348 g/m^2 (= 16.695 g/l) for PCT-Boron, 4.783 g/m^2 (= 9.565 g/l) for PCT-Lithium, and 6.673 g/m^2 (= 13.346 g/l) for PCT-Sodium].

As discussed in Appendix C, there are times when a SUCI may be preferred rather than an UCI. This is particularly true when the regression model (composition-property model) is to be used a large number of times for various glass compositions from a specified composition region. Equation (C.15) can be used, in much the same way as how Equation (C.13) is used to obtain UCIs, to calculate a 95% SUCI for the true mean of ln(PCT release) for glasses having a specified composition. The 95% SUCI values for the true mean ln(PCT release) in units of ln(g/l) for the HLW03-06 composition based on the IHLW PCT models are given in the sixth column of Table 5.14. Exponentiating the resulting 95% SUCIs for the mean in ln(g/l) units yields 95% SUCIs for the median in g/l. The seventh column of Table 5.14 contains 95% SUCIs for the true median PCT release from the HLW03-06 glass composition based on the IHLW PCT models. Note that the 95% SUCI values in g/l for the different IHLW PCT models are well below the PCT release limits for EA glass mentioned above.

5.7 Consequences of LOFs and Prediction Uncertainties in PCT-Boron, PCT-Lithium, and PCT-Sodium Models

The consequences of LOFs and prediction uncertainties of PCT-Boron, PCT-Lithium, and PCT-Sodium models on the ability to demonstrate compliance with WASRD 4.8.1.2 [44] is addressed as part of work documented in a separate PNWD report that addresses compliance requirements for immobilized waste [49]. That work shows that HLW glasses expected to be produced in the RPP-WTP HLW vitrification plant will have PCT-Boron, PCT-Lithium, and PCT-Sodium releases sufficiently below the EA glass limits (mentioned in the previous section), even after accounting for composition and model uncertainties. However, if in the future there should be a need to reduce uncertainties in models for PCT-Boron, PCT-Lithium, and PCT-Sodium releases from HLW glasses, there are two possible paths to explore.

The first path is to investigate why the PCT-Boron normalized releases in this study appear to have larger uncertainties (from glass fabrication, PCT testing, and chemical analysis of leachate) than those for lithium and sodium. Reducing the uncertainty of individual PCT-Boron normalized releases would directly reduce the uncertainties in models developed from the data, at least for PCT-Boron.

As a second path, “local” rather than “global” modeling approaches could be used to obtain models with smaller prediction uncertainties. One type of local modeling approach would be to develop models over smaller, local regions of HLW glass composition space. Past experience has shown that LM models (versus PQM models, say) may perform better and have smaller prediction uncertainty for less expansive glass composition regions. Another type of local modeling approach would be to use so-called non-parametric regression methods such as local linear (or polynomial) regression, neural networks, or others. Such modeling methods are

not restricted by requiring the same global model form to apply over all subregions of the glass composition space of interest. However, the non-parametric regression methods have the disadvantage of requiring larger data sets with more evenly distributed data than does the global, parametric modeling approach.

SECTION 6
MODELS RELATING ONE-PERCENT CRYSTAL FRACTION TEMPERATURE ($T_{1\%}$) TO HLW GLASS COMPOSITION

This section documents the development and validation of property-composition models and corresponding uncertainty expressions for predicting the temperature at which the equilibrium crystal fraction is 1 volume percent (vol%) of the molten high level waste (HLW) glass ($T_{1\%}$). For operation of the WTP HLW vitrification facility, the processing constraint is $T_{1\%} \leq 950°C$ for all crystalline phases [10]. This constraint will be implemented using $T_{1\%}$ property-composition models and corresponding uncertainty expressions. The $T_{1\%}$ models and uncertainty expressions presented in this section were developed and validated using composition and $T_{1\%}$ data collected on simulated HLW glasses. The simulated HLW glasses used for model development and model validation are discussed briefly in Section 6.1 (because they have already been described in detail in Section 2). It will be seen that, because of the compositional space defined for the test glasses, the primary crystalline phase under consideration is chiefly spinel, with other phases (e.g., zirconia and thorium-containing phases) being of minor importance. Consequently, the primary use of the $T_{1\%}$-composition models described herein is to predict the temperature at which spinel crystal fraction in equilibrium with the HLW glass melt is 1 vol%. The models will therefore need to be supplemented, during Phase 2 of model development, to address non-spinel phases, which may become the dominant crystalline phases for some composition sub-regions.

Section 6.1 summarizes the data used to develop and validate the $T_{1\%}$-composition models. Section 6.2 presents the model forms for $T_{1\%}$ that were investigated. Section 6.3 summarizes the results for two selected $T_{1\%}$ model forms. Using the selected models and corresponding uncertainty equations for $T_{1\%}$, Section 6.4 illustrates the calculation of $T_{1\%}$ predictions and the uncertainties in those predictions. Section 6.5 briefly discusses the consequences of lack-of-fit and prediction uncertainties in the recommended $T_{1\%}$ models. Appendix C discusses the statistical methods and summary statistics used to develop, evaluate, and validate the several model forms investigated, as well as statistical equations for quantifying the uncertainties in $T_{1\%}$ predictions made with the selected models.

6.1 $T_{1\%}$ Data Used for Model Development and Validation

The data used for developing $T_{1\%}$-composition models are discussed in Section 6.1.1. The two approaches and data used for validating the models are discussed in Sections 6.1.2 and 6.1.3.

6.1.1 Model Development Data for $T_{1\%}$

The data available for developing property-composition models for $T_{1\%}$ consist of composition and $T_{1\%}$ (with spinel as the primary crystalline phase) data from two matrices of simulated HLW glasses. The two matrices were developed using information about Hanford

HLW compositions, previous WTP glass formulation work, glass science knowledge and experience, and statistical experimental design methods. The first matrix, referred to as the *Initial Matrix*, consists of 57 HLW glass compositions selected by statistical experimental design methods. The second matrix, referred to as the *Augmentation Matrix*, consists of 45 simulated HLW glasses selected by statistical experimental design methods to optimally augment the Initial Matrix. Both matrices together are referred to as the *Combined Matrix* for Phase 1 IHLW property model development. Layered experimental designs [23, 24] were used to obtain both the Initial Matrix and the Augmentation Matrix. In both cases, the layered designs involved an outer layer, an inner layer, and a center composition. Details of the experimental design methods and development of the Initial Matrix and Augmentation Matrix are given respectively by Piepel et al. [11] and Cooley et al. [12]. The glasses of the Combined Matrix were used to develop the composition-property models for IHLW PCT and $T_{1\%}$ in this report, as well as the TCLP Cd release models [8]. Further details of the Phase 1 IHLW modeling data are given in Section 2 of this report.

Table 5.1 lists the normalized glass compositions for the 57 Initial Matrix glasses and the 45 Augmentation Matrix glasses in the oxide forms used for $T_{1\%}$ model development. The glass compositions in Table 5.1 are the normalized weight percents (wt%) of the 19 components varied in each of the IHLW design matrices. These are the same 19 components involved in PCT model development, namely Al_2O_3, B_2O_3, CdO, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, Sb_2O_3, SeO_2, SiO_2, SrO, ThO_2, Tl_2O, UO_3, ZnO, ZrO_2, and Spike. The compositions listed in Table 5.1 are normalized so that they sum to 100% over the 19 components varied in the Combined Matrix. In contrast, Table 2.10 (and Table 2.7, with the original oxides) lists the 19-component unnormalized mass fraction compositions of the Combined Matrix glasses. The compositions in Table 2.10 are unnormalized in the sense that they sum to 100% over the complete list of 56 oxides included in the dataset, but do not sum to 100% over the 19 components of the Combined Matrix. For model development purposes, the 19-component normalized wt% compositions of the Combined Matrix were converted to mass fractions so that each composition summed to 1.0. The Layer column of Table 5.1 indicates the design layer containing each of the Combined Matrix glasses.

Table 6.1 contains data relating temperature to equilibrium crystal fraction (vol %) for each of the 102 glasses of the Combined Matrix. The modeling proceeded in two steps.

Step 1: For each glass, the temperature and volume %-crystallinity data were used to fit a separate regression equation of the form

$$T = a_0 + a_1 X \ , \tag{6.1}$$

where X is the volume % crystallinity at a given temperature T, and a_0 and a_1 are the fitted intercept and slope of the T vs. X model for that glass. Equations of the form (6.1) were fit for each glass using unweighted least squares (ULS) regression. Substituting X = 1 vol% into the fitted equation for a given glass yields an estimate of $T_{1\%}$ for that glass. Using statistical regression theory and equations, the standard deviation of the $T_{1\%}$ value, denoted $SD(T_{1\%})$, can also be calculated.

In Equation (6.1), temperature (T) was used as the response variable, and vol% crystals (X) was used as the explanatory variable. This assignment of variables is considered an *inverse regression* approach. In the *classical regression* approach, the explanatory variable should have no uncertainty, or uncertainty that is small relative to the uncertainty in the response variable. Hence, with the classical approach, T would be the explanatory variable and X would be the response variable. However, the classical approach presents problems for calculating the uncertainty of $T_{1\%}$ values. Also, statistical research [50] has shown that if the number of data points is small, it is better to use the inverse regression approach.

Equations involving matrix algebra can be used to calculate the $SD(T_{1\%})$ values mentioned above. However, because simple linear regression is used to relate temperature to volume %-crystallinity in Equation (6.1), a simpler equation can be used to calculate the $SD(T_{1\%})$ values. This equation is

$$SD(T_{1\%}) = \sqrt{MSE * \left(\frac{1}{n} + \frac{(v_0 - \bar{v})^2}{\sum_{i=1}^{n} (v_i - \bar{v})^2} \right)} \quad , \tag{6.2}$$

where n is the number of temperature versus volume %-crystallinity data points used in the simple linear regression to calculate the slope, intercept, estimated $T_{1\%}$ value and $SD(T_{1\%})$ for a particular glass; v_0 is the 1 volume %-crystallinity limit for this work; v_i is the i^{th} volume %-crystallinity value among the n data points; $\bar{v}$ is the mean volume %-crystallinity value for the n data points; and MSE is the mean squared error for the simple linear regression involving the n data points, and is calculated using

$$MSE = \frac{SSE}{n-2} = \frac{\sum_{i=1}^{n} (T_i - \hat{T}_i)^2}{n-2} \, , \tag{6.3}$$

where T_i is the measured temperature for the i^{th} data point among the n data points used in the simple linear regression, and $\hat{T}_i$ is the predicted temperature corresponding to the i^{th} volume %-crystallinity value among the n data points. Appendix E contains an example that illustrates the use of Equation 6.1 through 6.3 to calculate estimated $T_{1\%}$ values and their corresponding standard deviations.

Step 2: Using the set of modeling glass compositions and estimated $T_{1\%}$ values, $T_{1\%}$-composition models were developed using ULS regression. Model development using weighted least squares (WLS) regression was also considered because of the almost

two orders of magnitude span in the SD($T_{1\%}$) values. For WLS regression, the weight for the i^{th} data point was given by

$$w_i = \frac{1}{\left[SD_i\left(T_{1\%}\right)\right]^2} \tag{6.4}$$

so that $T_{1\%}$ values with larger uncertainty receive a lower weight and $T_{1\%}$ values with smaller uncertainties receive a larger weight. However, use of WLS regression did not consistently produce the kind of improvements that were desired in terms of model performance for modeling and validation data, and reduced uncertainty in predictions. Thus, models were developed using ULS rather than WLS regression.

Starting with the 102 glasses in the IHLW Combined Matrix, 12 glasses were removed from the modeling dataset before conducting any model development (i.e., Step 2 above) regressions:

- 5 glasses had undetermined $T_{1\%}$ values: HLW02-05, HLW02-21, HLW03-09, HLW03-11, and HLW03-44.
- 6 glasses had non-spinel primary phases: HLW02-14, HLW03-08, HLW03-33, HLW03-34, HLW03-35, and HLW03-36.
- 1 glass was removed because it had an unusually low $T_{1\%}$ value: HLW02-10.

This left 90 glasses for use in developing property-composition models for $T_{1\%}$. Table 6.1 lists the heat-treatment temperatures and corresponding volume %-crystallinity values for all 102 test matrix glasses where available. Five additional glasses were identified as outliers based on regression runs during early stages of the model development process, and were removed form the model development dataset. Four of these five outlying glasses (HLW03-01, HLW03-31, HLW03-32, and HLW03-10) had standardized residuals greater than 2.5 in absolute value from an initial regression based on a linear mixture model (see Section C.1 of Appendix C) involving all 19 components of the IHLW Combined Matrix and the 90 glasses remaining after dropping the 12 glasses mentioned above. The fifth outlying glass (HLW02-47) had a standardized residual of –2.12 for the initial regression, but was identified as a clear outlier in subsequent regressions, particularly model-reduction regressions. Thus, the $T_{1\%}$ models presented in this report (Section 6.3) were developed using 85 IHLW glass compositions and their corresponding $T_{1\%}$ crystallinity values calculated using Equation (6.1). Table 6.1 contains a column indicating the 85 data points that were included in the $T_{1\%}$ model development, as does Tables 5.1, the table of IHLW glass compositions.

Table 6.2 lists the intercept and slope [a_0 and a_1 from Equation (6.1)] for each of the IHLW Combined Matrix glasses, as well as the estimated $T_{1\%}$ value obtained using Equation (6.1), the standard deviation of the estimated $T_{1\%}$ value, and the number of data points involved in the application of Equation (6.1) for each glass. Figure 6.1 is a histogram of the estimated $T_{1\%}$ values obtained using Equation (6.1) for the 85 glasses used for $T_{1\%}$ model development. This histogram shows that the estimated $T_{1\%}$ values are well distributed about the $T_{1\%}$ processability limit of 950ºC (marked with a vertical red line), and that the distribution includes glasses with

estimated $T_{1\%}$ values below, close to, and above the specified property limit. Such a distribution is desirable because models generated using a given dataset are typically more accurate within the range of response values used for model development than they are when extrapolated beyond the range of responses used for model development. Thus, models developed using data that are well distributed around a specified property limit are generally better able to discern between glasses that satisfy the property limit versus those that do not.

Table 6.3 lists the replicate pairs of glasses in the IHLW $T_{1\%}$ modeling dataset, the corresponding estimated $T_{1\%}$ values, and pairwise as well as pooled estimates of standard deviations (SDs) based on the replicate pairs. A pooled SD combines the separate pairwise SDs so that a more accurate, combined estimate of the SD is obtained. This pooled SD includes variations due to batching and melting the glasses, measuring melt temperatures and %-crystallinity, and applying Equation (6.1) to obtain estimated $T_{1\%}$ values.

6.1.2 Primary Model Validation Approach and Data

The primary model validation approach for $T_{1\%}$ modeling, like that used for PCT modeling (see Section 5.1.2), was based on splitting the Combined Matrix data points remaining for model development into five modeling/validation partitions. Of the 102 IHLW Combined Matrix glasses, 20 were intended to be replicates (10 replicate pairs). One pair (HLW02-46 and HLW03-42) is actually a near-replicate pair, having very slight differences for some component values. The differences could be due to round off or renormalization since one of these glasses is from the Initial Matrix and the other is from the Augmentation Matrix. This pair was treated as a true replicate pair for model development and evaluation. Of the 85 glasses remaining for $T_{1\%}$ modeling after dropping the 17 glasses mentioned previously, 18 were intended to be replicates. As mentioned in Section 6.1.1, HLW03-11 and HLW03-44 were among the 17 glasses dropped from $T_{1\%}$ modeling. These two glasses formed a replicate pair, so dropping these two glasses meant that only 9 replicate pairs remained out of the initial 10. These 18 glasses (9 replicate pairs) were included in each of the five modeling splits. This was done so that replicate pairs would not be split between modeling and validation subsets, which would otherwise negate the intent to have validation glasses different than model development glasses. The remaining 67 glasses were divided to finish forming the five modeling/validation splits as follows.

- The remaining 85 – 18 = 67 data points (glasses) were ordered from smallest to largest according to their predicted $T_{1\%}$ values [based on use of Equation (6.1)]. The 67 ordered data points were numbered 1, 2, 3, 4, 5, 1, 2, 3, 4, 5, etc. All of the 1's formed the first model validation set, while all of the remaining points formed the first model development dataset. Similarly, all of the 2's, 3's, 4's, and 5's respectively formed the second, third, fourth, and fifth model validation sets. In each case, the remaining non-2's, non-3's, non-4's, and non-5's formed, respectively, the second, third, fourth, and fifth model development datasets. Accordingly, two of these splits contained 14 glasses for validation and 53 glasses for modeling, and three of the splits contained 13 glasses for validation and 54 glasses for modeling.

- The 18 'replicate' glasses were added to each of the modeling splits yielding two splits with 71 glasses for modeling and 14 glasses for validation, and three splits with 72 glasses for modeling and 13 glasses for validation. The last column of Table 6.2 specifies the validation subsets for the five modeling/validation splits for the primary validation approach for $T_{1\%}$ model development.

Data splitting was chosen as the primary validation approach because there was a limited amount of other temperature vs. vol%-crystallinity data available for model validation purposes (see Section 6.1.3). Furthermore, not all of the separate validation glasses had compositions that satisfied all of the constraints defining the IHLW composition region and meeting quality assurance (QA) requirements.

6.1.3 Secondary Model Validation Approach and Data

There were 39 glasses, not included in the IHLW Combined Matrix, available for validation of the IHLW spinel $T_{1\%}$ models (see Section 2 for details). The full compositions for the 39 validation glasses are given in wt% values in Table 2.13. One of these glasses (SPA-18) had a composition that summed to only 0.9121 over the 19 components of the IHLW Combined Matrix. Therefore, this glass was dropped from the $T_{1\%}$ model validation. Additionally, many of the remaining 38 validation glasses had compositions outside the constraints that defined the EGCR of interest for WTP IHLW property-composition model development. Thus, subsets of the validation glasses were formed. The complete set of validation glasses (all 38 glasses used for the validation analysis) is referred to as the V1 validation set. The glasses that satisfy all single-component constraints (see Table 6.6 within reasonable tolerance are referred to as the V2 validation set. There were 27 glasses in the V2 validation set. The glasses that satisfy all single- and multi-component constraints (see Table 6.6) within reasonable tolerance are referred to as the V3 validation set. There were 20 glasses in the V3 validation set. Thus, the V3 glasses are within the IHLW glass composition region. The other validation sets (V1 and V2) contain glasses with compositions that are different from the IHLW modeling data in at least one respect. Either they: (i) violate one or more single-component constraints, or (ii) violate one or more multi-component constraints. This means that applying the IHLW $T_{1\%}$ models to validation sets other than the V3 set results in extrapolation of the models. Such extrapolations often result in less accurate property predictions than would result if the models were applied to compositions within the glass composition region of interest. Note that although similar labels (V1, V2, V3) were used to represent the $T_{1\%}$ model validation subsets as were used to represent the PCT model validation subsets, the subsets themselves were not the same set of glasses.

The compositions for the 39 available validation glasses for $T_{1\%}$ are given in Table 6.4 listed as normalized (over the 19 components varied in the Combined Matrix) weight percents summing to 100%. Table 6.5 contains data relating temperature to volume %-crystallinity of spinel for each of the 39 available validation glasses. Table 6.6 lists the intercept and slope [a_0 and a_1 from Equation (6.1)] for each of the 39 available validation glasses, as well as the estimated spinel $T_{1\%}$ value obtained using Equation (6.1), the standard deviation of the estimated $T_{1\%}$ values, and the number of data points involved in the fitting of Equation (6.1) for each validation glass. Tables 6.4 and 6.6 include columns to identify the 38 glasses actually used for

the $T_{1\%}$ model validation (i.e., the V1 set). Table 6.6 also includes a column that identifies the glasses in the V2 and V3 validation subsets. Note that the validation compositions listed in Table 6.4 were converted into the same compositional forms employed by the Combined Matrix used for spinel $T_{1\%}$ model development. That is, the same 19 components were used from the validation data compositions. Validation compositions were normalized to sum to 1 (i.e., mass fractions rather than wt%) for computational purposes during software applications that generated the IHLW $T_{1\%}$ models. Figure 6.2 is a histogram of the estimated $T_{1\%}$ values obtained using Equation (6.1) for the 38 glasses actually used for $T_{1\%}$ model validation. This histogram shows that the estimated $T_{1\%}$ values for the validation data are well distributed about the processability limit of 950ºC (marked with a vertical red line), and that the distribution includes glasses with estimated $T_{1\%}$ values below, close to, and above the specified property limit.

Use of these 38 validation glasses was considered a secondary model validation approach because the glasses were not part of the IHLW experimental design work discussed by Cooley et al. [12]. The data-splitting approach discussed in Section 6.1.2 is considered the primary validation approach because the data used by that approach are from the IHLW Combined Matrix and satisfy the full QA requirements. The separate validation dataset and subsets thereof are used as a secondary validation approach because many of these glasses are not within the IHLW glass composition region.

6.2 $T_{1\%}$ Model Forms

Ideally, a property-composition model for $T_{1\%}$ would utilize known mechanisms of crystal formation as a function of glass composition. However, there is insufficient information available to support such fundamental models for the complex systems with the large numbers of components of interest here. Hence, several empirical model forms with parameters to be estimated from model development data were considered. These model forms are from the general class of *mixture experiment models* [46]. Two different mixture experiment model forms were investigated as part of the $T_{1\%}$ model development process. The first was the linear mixture (LM) model form, and the second was the partial quadratic mixture (PQM) model form. These two model forms are discussed in Section C.1.1 of Appendix C, and are the same model forms used in modeling PCT-Boron, PCT-Lithium, and PCT-Sodium releases, as discussed in Section 4. For modeling $T_{1\%}$, the specific LM model form is given by

$$T_{1\%} = \sum_{i=1}^{q} b_i x_i + \varepsilon \ , \tag{6.5}$$

while the specific PQM model form is given by

$$T_{1\%} = \sum_{i=1}^{q} b_i x_i + \text{Selected} \left\{ \sum_{i=1}^{q} b_{ii} x_i^2 + \sum_{i<}^{q-1} \sum_{j}^{q} b_{ij} x_i x_j \right\} + \varepsilon \ . \tag{6.6}$$

In Equations (6.5) and (6.6): $T_{1\%}$ represents the estimated $T_{1\%}$ values in °C, obtained by using Equation (6.1); x_i (i = 1, 2, …, q) are normalized mass fractions of q glass oxide or halide components such that $\sum_{i=1}^{q} x_i = 1$; b_i (i = 1, 2, …, q), b_{ii} (selected), and b_{ij} (selected) are coefficients to be estimated from data; and ε is a random error for each data point. Many statistical methods exist for the case where the ε are independent (i.e., not correlated) and normally distributed with mean 0 and standard deviation σ. In Equation (6.6), "Selected" means that only some of the terms in curly brackets are included in the model. The subset is selected using standard stepwise regression or related methods [47]. PQM models are discussed in more detail and illustrated by Piepel et al. [48].

6.3 Property-Composition Model Results for $T_{1\%}$ LM Models

This section discusses the results of fitting several different models using $T_{1\%}$ values (in ºC) as the response variable. Section 6.3.1 discusses the assessment of whether there is any difference (i.e., bias) in $T_{1\%}$ data for the Initial Matrix and the Augmentation Matrix glasses. Section 6.3.2 presents the results of modeling $T_{1\%}$ based on compositions involving all 19 components from the IHLW Combined Matrix. In this case, the full LM model, as well as the full LM model augmented with selected quadratic terms (i.e., PQM models), were considered. Section 6.3.3 presents the results of modeling $T_{1\%}$ using LM and PQM models based on a reduced set of mixture components. Finally, Section 6.3.4 presents the recommended $T_{1\%}$ models.

6.3.1 Preliminary Modeling of IHLW $T_{1\%}$ Data to Compare Initial Matrix and Augmentation Matrix Subsets of Data

The modeling data for IHLW $T_{1\%}$ consist of results for the Initial Matrix and the Augmentation Matrix, as discussed in Section 6.1.1. The glasses in these two matrices were fabricated and melted at different times, and the %-crystallinity determinations were performed at different times. Because the modeling data were collected in two "blocks", it was prudent before performing substantial modeling work to assess whether there were any "block effects" associated with collecting the two subsets of data at different times. The results of that assessment are briefly summarized in this section.

Two variants of the LM model in Equation (6.5) were used to assess whether there were any block effects in the $T_{1\%}$ data between the Initial Matrix and Augmentation Matrix subsets of glasses. These two LM model variants are listed in Equations (C.6) and (C.7) of Appendix C. Both of these models were fitted to the $T_{1\%}$ modeling data (85 glasses), and the statistical significance of the block-effect coefficients was assessed as discussed in Section C.1.2 of Appendix C. No statistically significant block effects were identified, which means it was acceptable to proceed with the IHLW $T_{1\%}$ modeling using the data for the Combined Matrix and ignoring whether data points were from the Initial Matrix or Augmentation Matrix.

6.3.2 Results for Full LM and PQM Models for IHLW $T_{1\%}$

Initially, a full LM model in the 19 components was fit to the $T_{1\%}$ modeling data (85 glasses) using WLS regression with the response being the $T_{1\%}$ values in ºC. WLS regression is discussed in Appendix C, particularly in Section C.2. The full LM model form was a reasonable starting point based on the preliminary data and model assessment work by Gan et al. [7]. As mentioned in Section 6.1.1, WLS regression was considered an appropriate approach to use based on the range of the standard deviations associated with the estimated $T_{1\%}$ values. These standard deviations are denoted $SD(T_{1\%})$, and took on values ranging over two orders of magnitude. The weights used for this initial WLS regression were the reciprocals of predicted $T_{1\%}$ variance as shown in Equation (6.4). Use of WLS regression with reduced LM model forms (to be discussed subsequently) was also investigated. However, as mentioned in Section 6.1.1, the WLS regressions did not provide substantial improvements over ULS regression. Therefore, subsequent $T_{1\%}$ model development was conducted using ULS regression methods. Consequently, the $T_{1\%}$ models discussed and recommended in this report are based on ULS regression.

A full LM model for $T_{1\%}$ was generated using ULS regression. This full LM model offered reasonable performance, but it was decided that PQM models based on the full LM model should also be investigated. PQM models are discussed in detail by Piepel et al. [48]. The MAXR selection routine (see Section C.4.2 of Appendix C) was used to select quadratic terms (squared and two-component crossproduct terms) to include with the 19 linear terms in the hope of obtaining an even better fitting $T_{1\%}$ model by including important nonlinear blending effects of the glass components. Identifying components having nonlinear blending effects on $T_{1\%}$ values can be important even if a full PQM model (i.e., a full LM model with PQM model terms added) is ultimately not used. Such components may be forced to remain in reduced LM models so that quadratic terms involving these components can be considered when developing reduced PQM models. The MAXR selection was run multiple times so as to generate "full PQM" models containing the 19 linear terms plus anywhere from one to eight quadratic terms.

Ultimately, it was decided to recommend LM models rather than PQM models for $T_{1\%}$. Table 6.7 contains IHLW $T_{1\%}$ model and performance summaries, based on both the modeling and validation datasets, for the full LM model. Summary statistics for the five splits described in Section 6.1.2 are labeled DS# to represent the five modeling/validation "data splits" of the modeling data. The splits labeled DS1 and DS2 are the 71/14 splits; the splits labeled DS3, DS4, and DS5 are the 72/13 splits. The last column of the data splitting section of Table 6.7 shows the averages for the different statistics over the five splits. Table 6.2 includes a column that indicates which glasses were in each of the five internal validation splits for the $T_{1\%}$ model development. The variance-covariance matrix associated with the model coefficients for the $T_{1\%}$ full LM model is given in Table D.7 of Appendix D.

6.3.3 Results for Reduced LM and PQM Models for IHLW $T_{1\%}$

Model reduction was another model development approach investigated, wherein LM models for $T_{1\%}$ involving less than the 19 variable components of the IHLW Combined Matrix were considered. In this case, the sequential F-test model reduction approach (see Section C.4.1 of Appendix C) was used to conduct model reduction. These F-tests compare full models to reduced models obtained by excluding in turn each of the 19 terms in the full LM model generated using ULS discussed in the previous section. If all linear terms are significant, no model reduction occurs. Otherwise, the least significant linear term is identified. The term identified is dropped from the model, and the remaining components are renormalized. The sequence of F-tests continues until a model is obtained that does not include non-significant terms, based on a specified significance level. The sequential F-test approach can be run based on either WLS or ULS.

Reduced LM Model for IHLW $T_{1\%}$

The sequential F-test approach (based on ULS regression) was used to reduce the $T_{1\%}$ full LM model. A significance level of 0.05 was used as the stopping criterion for the sequence of F-tests. An option available with the F-test approach is to force specified terms to remain in the model during the model reduction process. For $T_{1\%}$ model reduction, no terms were forced into the reduced LM model. Another option available with the F-test approach is to force specified terms to be excluded from the reduced LM model. An initial application of the sequential F-test reduction algorithm resulted in a reduced LM model involving 14 components: Al_2O_3, B_2O_3, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, SeO_2, SiO_2, SrO, ThO_2, ZnO, and ZrO_2. Note that no terms were forced into or out of the model for this initial model reduction attempt. In this 14-component LM model, the coefficients for Cr_2O_3, NiO, and SeO_2 were quite large. These large coefficients do not necessarily indicate a problem. Because the mass fractions of these components are small compared to other components, large coefficients are needed to represent component contributions to the model's prediction of $T_{1\%}$. Because Cr_2O_3 and NiO are key oxides in spinel, these two components should remain in any $T_{1\%}$-composition models developed with spinel as the primary crystalline phase, but SeO_2 could potentially be dropped. A scatterplot matrix of the compositions of the glasses used in model development did not indicate any obvious collinearities that would provide justification for the SeO_2 effect being spurious. However, there is no glass science knowledge or experience indicating SeO_2 has any impact on spinel crystallinity. Thus, the sequential F-test model reduction algorithm was re-run with SeO_2 being forced out of the model. The result of this second model reduction run was a 13-component LM model. The 13-component model included Al_2O_3, B_2O_3, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, SiO_2, SrO, ThO_2, ZnO, and ZrO_2. Note that the SeO_2 term could have been eliminated from the reduced LM model by using a tighter significance level in the sequential F-test algorithm, for example 0.01 rather than 0.05. The lack of extremely high statistical significance lends further support to the subject matter knowledge for excluding SeO_2. Summary statistics for the $T_{1\%}$ reduced LM model given in Table 6.8 indicate that it performs as well or better than the full LM model (see Table 6.7) for both the modeling and validation datasets. The variance-covariance matrix associated with the model coefficients for the reduced LM model for spinel $T_{1\%}$ is given in Table D.8 of Appendix D.

Reduced PQM Models for IHLW $T_{1\%}$

Adding selected quadratic terms to the reduced LM model was also investigated, thus yielding what are referred to here as "reduced PQM models". The MAXR selection algorithm was used to select quadratic terms (squared and crossproduct terms) from among all possible quadratic terms formed using the 13 terms of the reduced LM model. Different reduced PQM models were obtained depending on the number of quadratic terms specified for addition. Reduced PQM models generated using the MAXR selection option with up to 21 terms (the 13 linear terms from the reduced LM model plus up to 8 quadratic terms) were considered. Performance results for (1) all of the $T_{1\%}$ reduced PQM models considered, and (2) the $T_{1\%}$ full and reduced LM models described previously, applied to the IHLW $T_{1\%}$ model development data (85 glasses), are given in Table 6.9.

The reduced PQM models being considered for $T_{1\%}$ were also applied to the five modeling/validation splits formed using the modeling data, as described previously. The averages from the data-splitting validation results are also given in Table 6.9 for the reduced models considered.

6.3.4 Recommended IHLW $T_{1\%}$ Models

Based on the results of the $T_{1\%}$ model development work for:

- the modeling data;
- the separate validation dataset and subsets thereof;
- the modeling data-splitting results;

it was decided to recommend both the 19-term full LM model as a baseline model, as well as the 13-term reduced LM model as the preferred model for $T_{1\%}$ with spinel as the dominant crystalline phase.

Although the PQM models formed by augmenting the reduced LM models with quadratic terms had statistically significant improvements over the reduced LM model for the modeling data and data-splitting investigations, these improvements were not evident for the separate validation data. In fact, the validation statistics are generally worse for the reduced PQM models than for the full or reduced LM models (see Table 6.9). It is not clear how much the lack of improved prediction performance by PQM models for the separate validation data was due to the limited nature of that data within the compositional region of interest and other factors (e.g., lab-to-lab and long-term variations). However, for conservatism it was decided to recommend the reduced LM model as the primary $T_{1\%}$ model. It was also decided to provide the model coefficients and summary statistics for the $T_{1\%}$ full LM model as a baseline for comparison with (and justification of) the reduced LM model, particularly when these models are applied to future data.

Recommended Full LM Model for IHLW $T_{1\%}$

Table 6.7 gives the coefficients of the $T_{1\%}$ 19-term full LM model, as well as performance statistics for the modeling data, the validation dataset and its subsets, and the data-split modeling data. The value of $R^2 = 0.912$ indicates that the full LM model accounts for approximately 91% of the variation in $T_{1\%}$ values in the modeling dataset. While this value indicates that the full LM model provides a very reasonable fit to the modeling data, a larger value would still be preferable. $R^2_A = 0.888$ is fairly close to R^2, indicating that the model is probably not overly hampered by unneeded components. The value for $R^2_P = 0.853$ is sufficiently close to the R^2 and R^2_A values to indicate that the model is probably not adversely affected by influential data points in the modeling dataset (after the removal of outliers, as discussed previously in Section 6.1.1. In any case, $R^2_P = 0.853$ provides a more conservative estimate than do R^2 and R^2_A of the fraction of variation in $T_{1\%}$ values for future datasets over the same glass composition region that might be accounted for by this full LM model. Over the five data splits of the modeling data, the average R^2_V was 0.828. The R^2 validation values for the complete validation dataset, V1, and subsets V2 and V3, are noticeably lower than the different R-squared values calculated from the modeling data. The R^2 values from the validation sets range from 0.583 to 0.661. These fractions of variation in $T_{1\%}$ values accounted for by the full LM model are considerably lower than indicated by R^2_P and the average R^2_V over the data splits. However, as mentioned in Section 6.1.3, many of the validation glasses are outside the HLW glass composition region of interest defined previously in Tables 2.1 through 2.6. The validation subsets V2 and V3 contain glasses that are "close" to or within the IHLW composition region of interest. The V2 glasses satisfy the single-component constraints used to define the IHLW glass composition region, the V3 glass satisfy both single- and multi-component constraints used to define the glass composition region. It is not clear whether this poor prediction performance for the validation data is because of something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the full LM model for $T_{1\%}$.

The SD($T_{1\%}$) values in Table 6.3 represent the standard deviation in forming melts of simulated HLW glasses and determining $T_{1\%}$ values for those glass melts, based on the assumption that the fitted model of the form given in Equation (6.1) does not have statistically significant LOF. The pooled SD($T_{1\%}$) over the 9 replicate pairs of glasses used in the $T_{1\%}$ model development was 26.062 (see Table 6.3) which is comparable to RMSE = 31.8791 from the $T_{1\%}$ full LM model. This suggests the full LM model does not have a statistically significant LOF, which was confirmed by the formal LOF test with a non-significant p-value of 0.2377 (see Table 6.4). However, the statistical non-significance of the model LOF could be due to the relatively large pooled SD of ~26°C for $T_{1\%}$ values.

Figures 6.3 through 6.6 show various regression diagnostic plots for the $T_{1\%}$ full LM model applied to the 85 glasses of the modeling dataset. Figures 6.3 and 6.4 generally indicate that the assumption of normally distributed errors in the $T_{1\%}$ data is reasonable (see Section C.2 of Appendix C). Figures 6.5 and 6.6 show well-distributed prediction errors for the modeling dataset. Figure 6.7 is a component trace plot associated with the components of the full LM model. Components with nearly horizontal traces and short traces may have nonsignificant effects on $T_{1\%}$ when spinel is the primary crystalline phase. Figures 6.8 through 6.10 show

predicted versus measured plots when the full LM model for IHLW $T_{1\%}$ is applied to the validation dataset and various subsets thereof.

Recommended Reduced LM Model for IHLW $T_{1\%}$

Table 6.8 gives the coefficients of the 13-term reduced LM model for $T_{1\%}$ prediction, as well as performance statistics for the modeling data, the validation dataset and its subsets, and data-split modeling data. The model evaluation statistics $R^2 = 0.901$, $R^2_A = 0.884$, $R^2_P = 0.860$, and RMSE = 32.3888 are very similar to the corresponding statistics for the 19-term full LM model. The differences between R^2 and R^2_A and between R^2_A and R^2_P are slightly less for the reduced LM model than for the full LM model. This suggests that the model reduction was beneficial and that the reduced LM model is even less affected by influential data points than is the full LM model. Over the five data splits of the modeling data, the average R^2_V was 0.856, which is very similar to the R^2_P value. The R^2 validation values for the complete validation dataset, V1, and subsets V2 and V3, range from 0.558 to 0.649. As with the full LM model, these fractions of variation in $T_{1\%}$ values accounted for by the reduced LM model are noticeably less than indicated by R^2_P and the average R^2_V over the data splits. But again, many of the validation glasses are outside the HLW glass composition region of interest defined previously in Tables 2.1 through 2.6. The validation subsets V2 and V3 contain glasses that are "close" to or within the IHLW composition region of interest. The V2 glasses satisfy the single-component constraints used to define the glass composition region, the V3 glasses satisfy both single- and multi-component constraints used to define the glass composition region. As with the full LM model for $T_{1\%}$, it is not clear whether the poor prediction performance for these validation datasets is due to something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the reduced LM model for $T_{1\%}$.

The SD($T_{1\%}$) values in Table 6.3 represent the standard deviation in preparing simulated HLW glasses and determining $T_{1\%}$ values for those glasses, based on the assumption that the fitted model of the form in Equation (6.1) does not have statistically significant LOF. The pooled SD($T_{1\%}$) over the 9 replicate pairs of glasses used in the $T_{1\%}$ model development was 26.062 (see Table Y.3) which is comparable to RMSE = 32.3888 from the $T_{1\%}$ reduced LM model. This suggests the reduced LM model does not have a statistically significant LOF, which was confirmed by the formal LOF test with a non-significant p-value of 0.2214 (see Table 6.5). However, the statistical non-significance of the model LOF could be due to the relatively large pooled SD of ~26°C for $T_{1\%}$ values.

Figures 6.11 through 6.14 show various regression diagnostic plots for the $T_{1\%}$ reduced LM model applied to the 85 glasses of the modeling dataset. Figures 6.11 and 6.12 generally indicate that the assumption of normally distributed errors in the $T_{1\%}$ data is reasonable (see Section C.2 of Appendix C). Figures 6.13 and 6.14 show well-distributed prediction errors for the modeling dataset. Figures 6.15 through 6.17 show predicted versus measured plots from applying the reduced LM model to the validation dataset and subsets thereof. These predicted versus measured plots provide visual evidence that predictive performance for the reduced LM model should be very comparable to that of the full LM model for $T_{1\%}$.

In conclusion, the primary recommended IHLW Phase 1 model for $T_{1\%}$ prediction with spinel as the primary crystalline phase is the 13-term reduced LM model in Table 6.8. The 19-term full LM model in Table 6.7 is recommended as a baseline for comparison to the reduced LM model. It is recommended that both these IHLW $T_{1\%}$ models be applied and their performances compared during future IHLW glass formulation and waste form qualification work.

6.4 Example Illustrating Model Predictions and Statistical Intervals

This section contains examples to illustrate the use of both the full and reduced LM models for $T_{1\%}$ to obtain predicted $T_{1\%}$ values for a specific HLW glass composition. This section also describes how corresponding statistical intervals are calculated to quantify the uncertainty in model predicted values of $T_{1\%}$.

The glass composition used in this example is HLW03-06, which is one of the glasses in the IHLW Combined Matrix. This same glass composition was used in the PCT examples presented in Section 5.6. The composition of HLW03-06 for $T_{1\%}$ modeling is given in Table 5.1 in normalized weight percent format. In order to apply the $T_{1\%}$ models to this composition, the weight percentages must be converted to normalized mass fractions (that sum to 1.0) over the linear components contained in the different models. Table 6.10 contains the composition for HLW03-06 prepared for use in the two IHLW $T_{1\%}$ models recommended in Section 6.3.4.

For the $T_{1\%}$ full and reduced LM models, predicted $T_{1\%}$ values are obtained by multiplying the composition in the format needed for the specific models by the coefficients for the different models (see Tables 6.7 and 6.8), then summing the results. That is, the predicted values are calculated by

$$\hat{y}(\boldsymbol{a}) = \boldsymbol{a}^T\boldsymbol{b}\,, \tag{6.7}$$

where $\boldsymbol{a}$ is the composition of HLW03-06 formatted to match the terms in a given model (from Table 6.10), T represents a matrix transpose (or vector transpose in this case), and $\boldsymbol{b}$ is the vector of model coefficients for a given model. The predicted $T_{1\%}$ values (ºC) from each of the two recommended models are listed in the second column of Table 6.11.

The predicted $T_{1\%}$ values in Table 6.11 can be considered as estimates of the true mean of the distribution of $T_{1\%}$ values that would result if the process for making $T_{1\%}$ determinations (see Step 1 described in Section 6.1.1) were repeated multiple times for the HLW03-06 glass. Then, Equation (C.13a) can be used to calculate a CL% upper confidence internal (CL% UCI) for the true mean $T_{1\%}$ value for the HLW03-06 glass composition for each of the IHLW $T_{1\%}$ models. A CL% UCI is of interest because the processing constraint is $T_{1\%} \le 950$°C. For the illustrations to follow, we consider CL% = 90%. In the notation of Equation (C.13a):

- CL% = 100(1−α)% = 90%, so that $\alpha = 0.10$.

- The vector $\boldsymbol{a}$ is the composition of HLW03-06 formatted to match the terms in a given model.

- The matrix $\boldsymbol{A}$ is the design matrix of normalized linear components formatted to match the terms in a given model.

To obtain an 90% UCI in ºC, the quantity $t_{1-\alpha,n-p} RMSE \sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{a}}$ is added to the predicted $T_{1\%}$ value $\hat{y}(\boldsymbol{a})$ described above, as indicated by Equation (C.13a). The $MSE[(\boldsymbol{A}^T \boldsymbol{A})^{-1}]$ portion of this expression is the variance-covariance matrix for the estimated model coefficients, as discussed near the end of Section C.6 of Appendix C. The variance-covariance matrices for the recommended $T_{1\%}$ models are listed in Appendix D. The quantity *MSE* is the mean squared error from regression, while *RMSE* is the root mean squared error (i.e., the square root of *MSE*).

The 90% UCI values for the true mean $T_{1\%}$ value for the HLW03-06 composition based on the two IHLW $T_{1\%}$ models are given in the third column of Table 6.11. Note that the 90% UCI values are somewhat above and hence fail the $T_{1\%}$ processing limit of 950°C. As discussed in Section 6.1.1, it is desirable for the modeling data set to contain glasses with property values below, close to, and above the property limit. In this case, HLW03-06 has a $T_{1\%}$ value close to the limiting value.

As discussed in Appendix C, there are times when a CL% simultaneous upper confidence interval (SUCI) may be preferred rather than an CL% UCI. This is particularly true when the regression model (composition-property model) is to be used a large number of times for various glass compositions within a specified composition region. For this illustration, CL% = 90% SUCIs are illustrated. Equation (C.15a) can be used (in much the same way as how Equation (C.13a) is used to obtain UCIs) to calculate a 90% SUCI for the true mean $T_{1\%}$ value for each of any number of glass compositions in the model validity region. Then, the resulting SUCIs for those glass compositions simultaneously have 90% confidence for containing their true mean values. The 90% SUCI values for the true mean $T_{1\%}$ (in ºC) for the HLW03-06 composition based on the IHLW $T_{1\%}$ models are given in the fourth column of Table 6.11. Note that the 90% SUCIs are larger than the corresponding 90% UCIs, because of the simultaneous confidence protection for multiple uses of the same model.

6.5 Consequences of Prediction Uncertainties in $T_{1\%}$ Models

As discussed in Section 6.3.4, the recommended full and reduced LM models for $T_{1\%}$ did not have statistically significant LOFs, which may be a result of the relatively large uncertainty in estimating $T_{1\%}$ values. The consequences of $T_{1\%}$ model prediction uncertainties on the ability to demonstrate meeting the 950°C processing limit [10] will be addressed as part of work that will be documented in a future PNWD report that will quantify variations and uncertainties in compositions and properties (such as $T_{1\%}$) of IHLW and ILAW [51]. Should uncertainties in the

$T_{1\%}$ full and reduced LM models for HLW glasses be too large and negatively affect glass formulation and the ability to meet the 950°C limit, there are two possible paths to explore.

The first path would be to investigate reducing the uncertainty of individual $T_{1\%}$ determinations (as represented in Table 6.3) since that would directly reduce the uncertainties in models developed from the data. One way to reduce uncertainties in $T_{1\%}$ determinations is to reduce the uncertainty with which temperatures and/or volume %-crystallinity are measured. Alternately, averaging multiple measurements can effectively reduce the inherent measurement uncertainties. Other ways to reduce uncertainties in $T_{1\%}$ determinations is to (1) obtain more volume %-crystallinity versus temperature data points for each glass, and/or (2) obtain data points with a roughly equal distribution of volume %-crystallinity values above and below 1%.

As a second path, "local" rather than "global" modeling approaches could be used to obtain models with smaller prediction uncertainties. One type of local modeling approach would be to develop models over smaller, local regions of HLW glass composition space. Past experience has shown that LM models (versus PQM models, say) may perform better and have smaller prediction uncertainty for less expansive glass compositions regions. Another type of local modeling approach would be to use so-called non-parametric regression methods such as local linear (or polynomial) regression, neural networks, or others. Such modeling methods are not restricted by requiring the same global model form to apply over all subregions of the glass composition space of interest. However, the non-parametric regression methods have the disadvantage of requiring larger data sets with more evenly distributed data than does the global, parametric modeling approach.

SECTION 7
SUMMARY AND CONCLUSIONS

Two test matrices have been designed statistically based on various compositional, glass properties, and other constraints to support development of IHLW property-composition models. Data have been collected and analyzed in this work to develop models that relate the PCT responses (for boron, lithium, and sodium) and one-percent crystal fraction temperature ($T_{1\%}$) to the compositions of WTP HLW glasses. This work constitutes Phase 1 of that modeling effort, which will continue with Phase 2. The Phase 2 model development work will employ the results presented herein as the basis to produce the final WTP models.

The test matrices (collectively referred to as the Combined Matrix) were designed with the primary objective of supporting the development of a TCLP-composition model, which had the earliest WTP need date and has been reported previously [8]. Development of models covering other glass properties also made use of these two matrices [9]. The Initial Matrix was composed of 57 glasses and the Augmentation Matrix 45. The 102 Combined matrix glasses were fabricated and characterized with respect to composition, PCT releases, and $T_{1\%}$. PCT-composition models and $T_{1\%}$-composition models were developed by regression of the collected data and validated by two approaches. The primary validation approach involved data-splitting using the regression set, while the secondary approach made use of independent data sets with glass compositions that partially overlap with the Combined Matrix glasses. Based on the performance of the models that were investigated, recommended models were selected.

The measured PCT results varied from 0.104 g/l (excluding one extreme outlier) to 4.418 g/l for boron, 0.378 g/l to 3.252 g/l for lithium, and 0.076 g/l to 2.802 g/l for sodium. These can be compared with the PCT release values for the DWPF-EA glass: 16.695 g/l for boron, 9.565 g/l for lithium, and 13.346 g/l for sodium. Thus, all of the matrix glasses outperformed the DWPF-EA glass, as was expected since the benchmark values from the DWPF-EA glass were used as PCT constraints to design the matrices. It may be desirable for modeling purpose during Phase 2, however, to include HLW glasses that span a much wider range of PCT responses. The PCT data collected have been shown to follow the expected general trends as functions of glass composition: glass formers including Al_2O_3 and SiO_2 typically reduce PCT releases while glass modifiers such as Na_2O and Li_2O have the opposite effect.

The PCT data were fitted to linear mixture (LM) models and partial quadratic mixture (PQM) models. A number of regression statistics were then computed to assess the performance of the fitted models. Validation of the models was performed in two ways. The primary validation method involved data-splitting, in which a subset of the data was left out of model regression and the ability of the resulting model to predict the responses for the omitted data was then assessed. The second validation method assessed the ability of the fitted models to predict the responses for a set of 574 glasses from earlier independent studies. The data set for the 574 glasses was divided into subsets based on the closeness of glass compositions to the compositional region defined by the Combined Matrix.

Based on the modeling data, statistics, and model validations, recommended IHLW Phase 1 models were selected from the fitted models. For each of the PCT responses (boron, lithium, and sodium), two models were recommended: (i) a 19-term full LM model, and (ii) an 8-term reduced LM model. The 19-term full LM models were intended as baselines for comparisons with the performance of the reduced LM models. It is recommended that both the full LM models and reduced LM models be applied and their performances compared during IHLW glass formulation and waste form qualification work. Finally, an example was provided to illustrate how to predict PCT releases for a HLW glass composition.

For the development of $T_{1\%}$-composition models, isothermal heat-treatment data were collected and regressed to provide estimates of $T_{1\%}$ for the matrix glasses. Of the 102 glasses from the Combined Matrix, $T_{1\%}$ values could be estimated for 97, spinel being the dominant crystalline phase for 91 of those 97 glasses. After exclusion of one outlier, the $T_{1\%}$ values range from 741 °C to 1248 °C, with a median of 946.1 °C (compared with the WTP process requirement of $T_{1\%} \leq 950$°C), suggesting a relatively uniform distribution of $T_{1\%}$ values in the range of interest. Gross compositional trends of the estimated $T_{1\%}$ values were less apparent than for the PCT data and no simple correlations between compositions and $T_{1\%}$ could be identified.

Data for 90 matrix glasses were fitted to LM models and PQM models to predict $T_{1\%}$ with spinel as the primary crystalline phase. Validation of the models followed closely that used for the PCT models. That is, two validation methods were used, with the primary method using data-splitting and the secondary method using an independent data set. However, since relatively few data have been published on volume% crystal fractions, data for only 39 glasses are available for the secondary validation, including many HLW glasses developed for WTP studies. These glasses were also divided into validation data subsets according to the closeness of their compositions to the matrix compositional space.

Based on the modeling data, statistics, and model validations, recommended IHLW Phase 1 models were selected from the fitted models. Two models again were recommended for predicting $T_{1\%}$, including a 13-term reduced LM model as the primary Phase 1 model, with a 19-term full LM model as a baseline for comparison to the reduced LM model. The reduced LM consists of more terms than the PCT reduced LM model (13 vs. 8) likely is a reflection of the more complex relationship that exists between crystal formation and composition. It is also recommended that both these IHLW $T_{1\%}$ models be applied and their performances compared during future IHLW glass formulation and waste form qualification to predict $T_{1\%}$ with spinel as the dominant crystalline phase. Finally, an example was provided to illustrate application of the model.

SECTION 8
QUALITY ASSURANCE

The VSL portion of this work was conducted under a quality assurance program compliant with NQA-1 (1989) and NQA-2a (1990) subpart 2.7, and the *Quality Assurance Requirements and Description* (QARD) Document (DOE/RW-0333P, Rev. 13) [45]. This program is supplemented by a Quality Assurance Project Plan for RPP-WTP work performed at VSL [52]. Test and procedure requirements by which the testing activities are planned and controlled are also defined in that plan. The program is supported by VSL standard operating procedures that were used for this work [53].

The QA requirements for PNWD work were met through the Quality Assurance Project Plan [54] for the PNWD Waste Treatment Plant Support (WTPSP). The WTPSP implementing procedures [55] comply with the requirements of NQA-1, NQA-2a subpart 2.7, and QARD, Rev. 13.

The following specific areas of this work are subject to the QARD: glass preparation, glass compositional analysis, PCT testing, and PCT model development. All work in these areas was performed according to VSL and PNWD QA programs and implementing procedures that are compliant with QARD.

Although not directly relevant to the applications described in the present report, it is noted that the glass preparation in this work also was subject to the requirements in *Quality Assurance Project Plan for Test Programs Generating Environmental Regulatory Data*, PL-24590-QA00001, Rev. 0 (WTP QAPjP) [56]. Under this document appropriate applications are defined of the following additional documents:

- *EPA Requirements for Quality Assurance Project Plans for Environmental Data Operation*s, EPA QA/R-5
- *Test Methods for Evaluating Solid Waste—Physical/Chemical Methods*, SW-846, 3rd edition [57].

SECTION 9
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Table 2.1. Components and Constraints for IHLW Initial and Augmentation Test Matrices.

Glass Components	Initial Matrix				Augmentation Matrix			
	Inner Layer (wt%)		Outer Layer (wt%)		Inner Layer (wt%)		Outer Layer (wt%)	
Al_2O_3	5.5	7.5	4	8.5	3	5	2	8.5
B_2O_3	8	13	5	14	7	12	5	14
Fe_2O_3	10	12	8	14	5	10	2	14
Li_2O	2.5	5	2	6	2.5	5	2	6
MnO	1.5	3.5	0	5	1.5	4.5	0	7
Na_2O	9	15	4	15	7	12	4	15
SiO_2	41	49	38	53	41	49	36	53
SrO	1.5	3.5	0	5	1.5	4.5	0	10
ThO_2	*not included in initial matrix*				3	4.5	0	6
UO_2	*not included in initial matrix*				2	4	0	6
ZrO_2	1.5	4.5	0	6	6	9	0	10
ZnO	*included in "Constant"*				1	3	0	4
CdO	0.5	1	0.05	1.5	0.1	0.3	0.05	1.6
Cr_2O_3	*included in "Spike"*				0.08	0.2	0.02	0.5
NiO	0.3	0.8	0.1	1	0.3	0.5	0.1	1
Tl_2O_3	0.05	0.15	0.02	0.2	0.05	0.15	0.02	0.33
Sb_2O_3	0.05	0.15	0.02	0.2	0.05	0.15	0.02	0.3
SeO_2	0.05	0.15	0.02	0.2	0.05	0.15	0.02	0.2
"Spike"	0.15	1.5	0.3	1	0.26	0.87	0.13	1.3
"Constant"	4.2		4.2		2.2		2.2	

Table 2.2 Composition of "Spike" Components for IHLW Initial and Augmentation Test Matrices.

Components	Initial Matrix		Augmentation Matrix	
	Relative %	**Maximum wt% in Glass**	**Relative %**	**Maximum wt% in Glass**
Ag_2O	13.3	0.2	15.4	0.2
PbO	26.7	0.4	30.8	0.4
V_2O_5	6.7	0.1	7.7	0.1
As_2O_3	13.3	0.2	15.4	0.2
BaO	20.0	0.3	23.1	0.3
Cr_2O_3	13.3	0.2	*not included in "Spike" (See Table 2.1)*	
CuO	6.7	0.1	7.7	0.1
Subtotal	100	1.5	100	1.3

Table 2.3. Composition of "Constant" Components for IHLW Initial and Augmentation Test Matrices.

Components	Initial Matrix		Augmentation Matrix	
	Relative %	**Wt% in Glass**	**Relative %**	**Wt% in Glass**
Bi_2O_3	0.24	0.01	0.46	0.01
CaO	11.9	0.5	22.7	0.50
CeO_2	1.2	0.05	2.3	0.05
Cl	4.8	0.2	9.1	0.20
CoO	0.24	0.01	0.46	0.01
Cs_2O	0.24	0.01	0.46	0.01
F	1.2	0.05	2.3	0.05
K_2O	1.4	0.06	2.7	0.06
La_2O_3	7.1	0.3	13.6	0.30
MgO	2.9	0.12	5.5	0.12
P_2O_5	11.9	0.5	22.7	0.50
PdO	2.9	0.12	5.5	0.12
Rh_2O_3	1.2	0.05	2.3	0.05
RuO_2	1.9	0.08	3.6	0.08
SO_3	2.4	0.1	4.5	0.10
TeO_2	0.24	0.01	0.46	0.01
TiO_2	0.71	0.03	1.4	0.03
ZnO	47.6	2.0	*not included in "Constant" (see Table 2.1)*	
Subtotal	100	4.2	100	2.20

Table 2.4. Waste Loading Constraints for IHLW Initial and Augmentation Test Matrices.

Parameter	Initial Matrix		Augmentation Matrix	
	Lower Limit (wt%)	**Upper Limit (wt%)**	**Lower Limit (wt%)**	**Upper Limit (wt%)**
$Al_2O_3+Fe_2O_3+ZrO_2$	18	22.5	*none*	26
$Al_2O_3+Fe_2O_3+ZrO_2+3ThO_2$	*none*	*none*	19[(a)]	34

[(a)] Constraint unnecessary for the inner layer.

Table 2.5. Glass Property Constraints for IHLW Initial and Augmentation Test Matrices.

Property	Initial Matrix		Augmentation Matrix	
	Lower Limit	**Upper Limit**	**Lower Limit**	**Upper Limit**
Viscosity at 1150 °C (η_{1150})	10 P	100 P	10 P	100 P
Conductivity at 1150 °C (σ_{1150})	0.2 S/cm	0.6 S/cm (inner layer) 0.7 S/cm (outer layer)	0.2 S/cm	0.6 S/cm (inner layer) 0.7 S/cm (outer layer)
7-day Normalized B PCT (r_B^{PCT})	*none*	16.695 g/l	*none*	16.695 g/l
7-day Normalized Na PCT (r_{Na}^{PCT})	*none*	13.346 g/l	*none*	13.346 g/l
7-day Normalized Li PCT (r_{Li}^{PCT})	*none*	9.565 g/l	*none*	9.565 g/l
TCLP Normalized B	*none*	0.3 g/l	*none*	0.3 g/l
Liquidus Temperature of Cr-bearing Spinels (T_{LS})	*none*	1050 °C	*none*	1150 °C
Liquidus Temperature of Zircon (T_{LZ})	*none*	*none*	*none*	1150 °C
Composition Constraint to Limit Thorium Crystallization: $2Li_2O+Na_2O-3.75ThO_2$	*none*	*none*	0.0 wt%	*none*

Table 2.6. Model-Based[a, b] Glass Property Constraints for IHLW Initial and Augmentation Matrices.

Property	η_{1150}	σ_{1150}	r_B^{PCT}	r_{Na}^{PCT}	r_{Li}^{PCT}	TCLP B	Spinel T_{LS}	Zircon T_{LZ}
Modeled Response	$\ln(\eta_{1150})$	$\ln(\sigma_{1150})$	$\ln(r_B^{PCT})$	$\ln(r_{Na}^{PCT})$	$\ln(r_{Li}^{PCT})$	ln(TCLP B)	$1000/T_{LS}$	$1000/T_{LS}$
Unit	ln(poise)	ln(S/cm)	ln(g/l)	ln(g/l)	ln(g/l)	ln(g/l)	1000/K	°C
Component	***Constraint Model Coefficients and Constraint Lower & Upper Limits***							
Al_2O_3	0.18657	–0.01728	–0.05722	–0.06358	–0.05649	0.177471	–0.008872(I) –0.010035(A)	19.33(A)
B_2O_3	–0.02217	0.023548	0.12314	0.07598	0.10705	0.020751	0.004608(I) 0.003834(A)	6.02(A)
Fe_2O_3	0.0390715	–0.01971	–0.0049	–0.01541	–0.02529	–0.142703	–0.008202(I) –0.009954(A)	22.54(A)
Li_2O	–0.290011	0.206174	0.2443	0.18435	0.29065	0.154931	0.154931(I) 0.014920(A)	–16.20(A)
MnO	—[c]	—	0.11568	0.08245	0.14456	—	–0.003258(I) 0.001536(A)	16.31(A)
Na_2O	–0.044155	0.114266	0.23097	0.22255	0.21421	0.105911	0.012308(I) 0.011639(A)	–28.45(A)
SiO_2	0.1485	–0.01638	–0.00802	–0.01545	0.01268	–0.136931	0.000257(I) –0.001100(A)	9.99(A)
SrO	—	—	—	—	—	–0.023195	—	16.31(A)
ThO_2	—	—	—		—	–0.09344(A)	—	16.31(A)
UO_2	—	—	0.07011(A)	0.06703(A)	0.13294(A)	–0.07421(A)	–0.002953(A)	16.31(A)
ZrO_2	0.09522	–0.07185	–0.01614	–0.0411	–0.06408	–0.15205	–0.006011(I) –0.006041(A)	54.68(A)
ZnO	0.05186(A)	–0.01459(A)	—	—	—	—	–0.046261(A)	16.31(A)
Cr_2O_3	—	—	—	—	—	—	–0.111396(A)	16.31(A)
NiO	—	—	0.1300	0.157237	0.031708	—	–0.038605(I) –0.047065(A)	16.31(A)
Spike	—	—	—	—	—	—	–0.0119967(I)	—
CdO, Sb_2O_3, SeO_2, Tl_2O_3	—	—	—	—	—	—	—	—
Lower Limit	5.498(I)[e] 5.60181(A)	0.157185(I)[e] 0.128005(A)	(d)	(d)	(d)	(d)	0.03355(I) –0.234627(A)	(d)
Upper Limit	7.80045(I) 7.904176(A)	1.25578(I, IL) 1.4099(I, OL) 1.22657(A,IL) 1.38073(A,OL)	6.94232(I)[f] 7.032582(A)[f]	7.77179(I)[f] 5.881264(A)[f]	6.95212(I)[f] 7.02258(A)[e]	–5.25536(I)[f] –5.255706(A)[e]	(d)	1079.06(A)

[a] Property-composition model intercepts and the part due to "Constant" are incorporated into the lower and/or upper limits.
[b] All values are used for both Initial and Augmentation Matrices, unless otherwise stated: (I)=for Initial Matrix only, (A)=for Augmentation Matrix only, (IL)=Inner Layer, (OL)=Outer Layer. Values are listed as used in constraints development and without rounding.
[c] — indicates the component is expected to have a minor effect on the property and is not included in the model used to form the constraint.
[d] No limits were imposed for these properties.
[e] Constraints unnecessary (i.e., not triggered) for the inner layer.
[f] Constraints unnecessary (i.e., not triggered) for both the inner and outer layers.

Table 2.7. Target Glass Compositions (wt%) for the Initial and Augmentation Test Matrices.

Glass ID[(a)]	Point Type[(b)]	Melt Order	Al_2O_3	B_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	SiO_2	SrO	ThO_2	UO_2	ZrO_2	Cr_2O_3	NiO	ZnO	CdO	Tl_2O_3	Sb_2O_3	SeO_2	Spike	Constant
HLW02-01	1a.Center	I-29	6.172	9.928	10.899	3.996	2.385	10.958	43.616	2.444	0.000	0.000	2.974	0.108	0.518	2.000	0.771	0.110	0.110	0.110	0.702	2.200
HLW02-02	1a.Outer01	I-25	4.000	14.000	14.000	6.000	0.000	4.000	50.460	0.000	0.000	0.000	0.000	0.200	0.100	2.000	1.500	0.020	0.200	0.020	1.301	2.200
HLW02-03	1a.Outer02	I-12	4.000	14.000	8.000	2.000	0.000	15.000	38.000	4.380	0.000	0.000	6.000	0.200	1.000	2.000	1.500	0.200	0.020	0.200	1.301	2.200
HLW02-04	1a.Outer03	I-46	4.000	5.000	14.000	2.000	0.518	15.000	52.932	0.000	0.000	0.000	0.000	0.020	0.100	2.000	1.500	0.200	0.200	0.200	0.130	2.200
HLW02-05	1a.Outer04	I-53	4.000	5.000	8.000	6.000	0.000	13.788	52.653	0.000	0.000	0.000	6.000	0.020	0.100	2.000	0.050	0.020	0.020	0.020	0.130	2.200
HLW02-06	1a.Outer05	I-45	8.500	5.000	8.000	4.739	5.000	15.000	40.491	0.000	0.000	0.000	6.000	0.020	1.000	2.000	1.500	0.200	0.020	0.200	0.130	2.200
HLW02-07	1a.Outer06	I-43	8.500	5.000	8.000	6.000	0.000	11.705	53.000	0.000	0.000	0.000	1.525	0.200	0.100	2.000	0.050	0.200	0.200	0.020	1.301	2.200
HLW02-08	1a.Outer07	I-56	4.000	14.000	9.205	3.310	5.000	15.000	38.745	0.000	0.000	0.000	6.000	0.020	0.100	2.000	0.050	0.020	0.200	0.020	0.130	2.200
HLW02-09	1a.Outer08	I-21	8.500	11.589	14.000	2.271	0.000	15.000	38.000	5.000	0.000	0.000	0.000	0.020	1.000	2.000	0.050	0.020	0.200	0.020	0.130	2.200
HLW02-10	1a.Outer09	I-42	8.500	14.000	8.000	6.000	0.000	10.513	38.000	2.797	0.000	0.000	6.000	0.020	0.100	2.000	1.500	0.020	0.020	0.200	0.130	2.200
HLW02-11	1a.Outer10	I-32	4.000	14.000	8.000	6.000	0.000	10.857	45.144	0.000	0.000	0.000	6.000	0.020	1.000	2.000	0.050	0.200	0.200	0.200	0.130	2.200
HLW02-12	1a.Outer11	I-44	4.000	5.000	11.386	6.000	5.000	12.761	41.414	0.000	0.000	0.000	6.000	0.200	1.000	2.000	1.500	0.020	0.020	0.200	1.301	2.200
HLW02-13	1a.Outer12	I-39	4.000	5.000	14.000	6.000	5.000	10.427	43.121	5.000	0.000	0.000	1.182	0.200	0.100	2.000	0.050	0.200	0.020	0.200	1.301	2.200
HLW02-14	1a.Outer13	I-41	4.000	5.000	8.000	6.000	2.490	4.140	53.000	5.000	0.000	0.000	6.000	0.020	0.100	2.000	1.500	0.200	0.200	0.020	0.130	2.200
HLW02-15	1a.Outer14	I-18	8.500	14.000	14.000	2.000	4.689	12.541	38.000	0.000	0.000	0.000	0.000	0.200	0.100	2.000	0.050	0.200	0.020	0.200	1.301	2.200
HLW02-16	1a.Outer15	I-51	8.500	5.000	8.000	6.000	5.000	9.654	39.126	5.000	0.000	0.000	6.000	0.200	0.100	2.000	1.500	0.020	0.200	0.200	1.301	2.200
HLW02-17	1a.Outer16	I-19	8.500	5.000	13.843	6.000	0.000	7.690	52.958	0.000	0.000	0.000	0.000	0.020	0.100	2.000	1.500	0.020	0.020	0.020	0.130	2.200
HLW02-18	1a.Outer17	I-8	4.000	5.000	11.130	2.014	0.000	15.000	49.867	0.000	0.000	0.000	6.000	0.200	1.000	2.000	0.050	0.020	0.200	0.020	1.301	2.200
HLW02-19	1a.Outer18	I-57	4.000	14.000	10.781	2.000	5.000	8.849	38.000	5.000	0.000	0.000	6.000	0.020	0.100	2.000	1.500	0.020	0.200	0.200	0.130	2.200
HLW02-20	1a.Outer19	I-30	4.000	14.000	14.000	2.000	0.000	6.453	51.734	3.253	0.000	0.000	0.000	0.020	0.100	2.000	0.050	0.020	0.020	0.020	0.130	2.200
HLW02-21	1a.Outer20	I-24	8.500	14.000	8.000	2.000	0.000	15.000	46.440	0.000	0.000	0.000	1.500	0.020	0.100	2.000	0.050	0.020	0.020	0.020	0.130	2.200
HLW02-22	1a.Outer21	I-36	8.500	14.000	9.500	6.000	0.000	4.000	53.000	0.080	0.000	0.000	0.000	0.020	0.100	2.000	0.050	0.020	0.200	0.200	0.130	2.200
HLW02-23	1a.Outer22	I-15	8.500	14.000	8.000	6.000	5.000	5.590	39.320	5.000	0.000	0.000	1.500	0.020	1.000	2.000	1.500	0.200	0.020	0.020	0.130	2.200
HLW02-24	1a.Outer23	I-31	8.500	5.000	8.000	2.000	5.000	12.198	47.062	5.000	0.000	0.000	1.500	0.153	0.100	2.000	0.050	0.020	0.020	0.200	0.998	2.200
HLW02-25	1a.Outer24	I-34	8.500	14.000	9.500	2.000	0.355	6.883	47.392	5.000	0.000	0.000	0.000	0.020	0.100	2.000	1.500	0.200	0.200	0.020	0.130	2.200
HLW02-26	1a.Outer25	I-5	4.000	5.000	12.500	2.000	4.960	15.000	38.000	5.000	0.000	0.000	6.000	0.200	0.100	2.000	1.500	0.200	0.020	0.020	1.301	2.200
HLW02-27	1a.Outer26	I-23	4.000	14.000	12.500	6.000	3.365	4.274	39.941	5.000	0.000	0.000	6.000	0.020	0.100	2.000	0.050	0.200	0.020	0.200	0.130	2.200
HLW02-28	1a.Inner01	I-49	7.500	8.000	10.450	2.500	1.500	15.000	41.000	3.500	0.000	0.000	4.500	0.040	0.300	2.000	1.000	0.150	0.050	0.050	0.260	2.200
HLW02-29	1a.Inner02	I-6	7.500	13.000	10.000	3.750	1.500	9.000	41.000	3.500	0.000	0.000	4.500	0.133	0.300	2.000	0.500	0.050	0.050	0.150	0.867	2.200
HLW02-30	1a.Inner03	I-22	5.500	9.722	10.000	5.000	3.500	11.229	41.000	3.500	0.000	0.000	4.500	0.040	0.300	2.000	1.000	0.050	0.150	0.050	0.260	2.200
HLW02-31	1a.Inner04	I-20	5.500	13.000	10.000	2.500	1.500	14.981	41.000	1.500	0.000	0.000	4.369	0.040	0.300	2.000	0.500	0.150	0.050	0.150	0.260	2.200
HLW02-32	1a.Inner05	I-9	7.500	8.000	10.000	5.000	1.500	10.733	46.118	3.500	0.000	0.000	1.500	0.040	0.300	2.000	1.000	0.050	0.150	0.150	0.260	2.200
HLW02-33	1a.Inner06	I-17	6.341	8.000	12.000	2.500	3.500	15.000	41.000	3.500	0.000	0.000	2.009	0.040	0.800	2.000	0.500	0.050	0.150	0.150	0.260	2.200
HLW02-34	1a.Inner07	I-26	5.500	13.000	12.000	3.957	1.500	10.893	41.000	3.500	0.000	0.000	1.500	0.133	0.800	2.000	1.000	0.050	0.050	0.050	0.867	2.200
HLW02-35	1a.Inner08	I-35	6.489	13.000	12.000	5.000	3.500	9.161	41.000	1.500	0.000	0.000	1.500	0.133	0.800	2.000	0.500	0.150	0.150	0.050	0.867	2.200
HLW02-36	1a.Inner09	I-48	5.500	8.669	12.000	2.500	1.500	15.000	45.082	1.500	0.000	0.000	1.500	0.133	0.300	2.000	1.000	0.050	0.050	0.150	0.867	2.200
HLW02-37	1a.Inner10	I-3	6.762	13.000	10.000	2.500	3.500	11.188	41.000	1.500	0.000	0.000	4.500	0.040	0.800	2.000	0.500	0.050	0.150	0.050	0.260	2.200
HLW02-38	1a.Inner11	I-4	6.894	13.000	12.000	4.256	1.500	9.000	41.000	3.500	0.000	0.000	1.500	0.133	0.800	2.000	1.000	0.050	0.150	0.150	0.867	2.200
HLW02-39	1a.Inner12	I-40	7.500	8.992	10.000	2.500	1.500	11.059	49.000	1.500	0.000	0.000	1.500	0.040	0.800	2.000	1.000	0.050	0.050	0.050	0.260	2.200
HLW02-40	1a.Inner13	I-33	7.500	9.834	10.000	2.632	1.500	9.684	49.000	1.500	0.000	0.000	1.500	0.133	0.300	2.000	1.000	0.150	0.150	0.050	0.867	2.200

Table 2.7. Target Glass Compositions (wt%) for the Initial and Augmentation Test Matrices (continued).

Glass ID[(a)]	Point Type[(b)]	Melt Order	Al_2O_3	B_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	SiO_2	SrO	ThO_2	UO_2	ZrO_2	Cr_2O_3	NiO	ZnO	CdO	Tl_2O_3	Sb_2O_3	SeO_2	Spike	Constant
HLW02-41	1a.Inner14	I-14	6.500	13.000	10.000	2.500	1.500	9.000	48.950	1.500	0.000	0.000	1.500	0.040	0.300	2.000	0.500	0.150	0.050	0.050	0.260	2.200
HLW02-42	1a.Inner15	I-55	5.500	13.000	10.000	5.000	1.500	9.000	44.450	3.500	0.000	0.000	2.500	0.040	0.300	2.000	0.500	0.150	0.050	0.050	0.260	2.200
HLW02-43	1a.Inner16	I-38	6.500	13.000	10.000	2.500	3.500	12.450	41.000	3.500	0.000	0.000	1.500	0.040	0.300	2.000	1.000	0.050	0.150	0.050	0.260	2.200
HLW02-44	1a.Inner17	I-2	5.500	9.071	10.000	2.500	3.500	15.000	43.680	1.500	0.000	0.000	2.500	0.133	0.300	2.000	1.000	0.050	0.150	0.050	0.867	2.200
HLW02-45	1a.Inner18	I-11	5.500	8.000	11.000	2.500	3.500	9.619	48.831	3.500	0.000	0.000	1.500	0.040	0.300	2.000	1.000	0.050	0.050	0.150	0.260	2.200
HLW02-46	1a.Inner19	I-13	5.500	9.149	10.000	3.701	3.500	9.000	49.000	1.500	0.000	0.000	2.500	0.040	0.800	2.000	0.500	0.150	0.050	0.150	0.260	2.200
HLW02-47	1a.Inner20	I-27	5.500	9.807	10.000	2.500	3.500	9.444	49.000	1.500	0.000	0.000	2.500	0.133	0.300	2.000	0.500	0.150	0.050	0.050	0.867	2.200
HLW02-48	1a.Inner21	I-10	6.000	8.000	12.000	3.340	1.500	15.000	41.000	1.711	0.000	0.000	4.500	0.133	0.800	2.000	0.500	0.150	0.150	0.150	0.867	2.200
HLW02-49	1a.Inner22	I-54	7.500	8.740	12.000	5.000	3.500	9.000	44.211	1.500	0.000	0.000	3.000	0.040	0.300	2.000	0.500	0.150	0.050	0.050	0.260	2.200
HLW02-50	1a.Inner23	I-28	6.000	13.000	12.000	2.500	1.500	9.820	43.530	1.500	0.000	0.000	4.500	0.040	0.300	2.000	0.500	0.150	0.150	0.050	0.260	2.200
HLW02-51	1a.Inner24	I-7	7.500	8.000	10.500	4.589	1.500	9.000	45.162	3.500	0.000	0.000	4.500	0.040	0.300	2.000	0.500	0.150	0.150	0.150	0.260	2.200
HLW02-52	RepHLW02-01	I-50	6.172	9.928	10.899	3.996	2.385	10.958	43.616	2.444	0.000	0.000	2.974	0.108	0.518	2.000	0.771	0.110	0.110	0.110	0.702	2.200
HLW02-53	RepHLW02-17	I-52	8.500	5.000	13.843	6.000	0.000	7.690	52.958	0.000	0.000	0.000	0.000	0.020	0.100	2.000	1.500	0.020	0.020	0.020	0.130	2.200
HLW02-54	RepHLW02-4	I-1	4.000	5.000	14.000	2.000	0.518	15.000	52.932	0.000	0.000	0.000	0.000	0.020	0.100	2.000	1.500	0.200	0.200	0.200	0.130	2.200
HLW02-55	RepHLW02-42	I-16	5.500	13.000	10.000	5.000	1.500	9.000	44.450	3.500	0.000	0.000	2.500	0.040	0.300	2.000	0.500	0.150	0.050	0.050	0.260	2.200
HLW02-56	RepHLW02-44	I-37	5.500	9.071	10.000	2.500	3.500	15.000	43.680	1.500	0.000	0.000	2.500	0.133	0.300	2.000	1.000	0.050	0.150	0.050	0.867	2.200
HLW02-57	RepHLW02-8	I-47	4.000	14.000	9.205	3.310	5.000	15.000	38.745	0.000	0.000	0.000	6.000	0.020	0.100	2.000	0.050	0.020	0.200	0.020	0.130	2.200
HLW03-01	1b.Outer01	A-4	8.335	13.728	13.728	5.883	6.078	3.922	35.301	0.000	2.764	0.000	2.983	0.020	0.098	3.059	0.050	0.330	0.020	0.200	1.300	2.200
HLW03-02	1b.Outer02	A-28	1.951	13.659	13.659	2.472	6.830	11.175	35.124	0.000	0.000	0.000	9.086	0.488	0.976	0.000	1.600	0.330	0.300	0.020	0.130	2.200
HLW03-03	1b.Outer03	A-26	1.953	4.883	13.674	2.677	6.837	10.753	35.161	9.767	0.000	0.000	6.403	0.488	0.977	1.946	1.600	0.330	0.020	0.200	0.130	2.200
HLW03-04	1b.Outer04	A-9	1.961	4.903	13.728	5.883	3.172	4.458	42.575	9.806	0.000	5.883	2.942	0.490	0.098	0.000	0.050	0.330	0.020	0.200	1.300	2.200
HLW03-05	1b.Outer05	A-2	8.176	4.809	1.924	1.924	6.733	14.428	47.840	0.000	3.812	0.000	0.000	0.481	0.096	3.847	1.600	0.330	0.300	0.200	1.300	2.200
HLW03-06	1b.Outer06	A-35	8.344	4.908	1.963	5.890	6.872	3.927	52.030	5.091	1.416	0.000	4.095	0.491	0.982	0.000	1.600	0.020	0.020	0.020	0.130	2.200
HLW03-07	1b.Outer07	A-25	4.979	4.979	13.940	4.767	6.970	11.735	39.967	0.000	0.000	5.974	0.000	0.498	0.100	3.473	0.050	0.020	0.020	0.200	0.130	2.200
HLW03-08	1b.Outer08	A-31	8.033	4.834	1.934	5.152	6.768	14.503	34.807	0.000	4.413	0.000	9.669	0.483	0.097	3.867	1.600	0.020	0.300	0.020	1.300	2.200
HLW03-09	1b.Outer09	A-11	7.666	13.692	3.485	1.979	0.000	14.845	52.453	0.000	2.551	0.000	0.000	0.020	0.099	0.000	0.050	0.330	0.300	0.200	0.130	2.200
HLW03-10	1b.Outer10	A-45	8.377	4.928	9.991	5.913	6.899	12.863	35.481	0.000	2.628	1.047	7.257	0.020	0.986	0.000	0.050	0.020	0.020	0.020	1.300	2.200
HLW03-11	1b.Outer11	A-38	1.991	4.979	9.572	1.991	0.000	14.936	52.772	0.000	5.045	5.974	0.000	0.020	0.100	0.000	0.050	0.020	0.020	0.200	0.130	2.200
HLW03-12	1b.Outer12	A-34	1.989	4.973	1.989	5.026	6.963	3.979	44.433	9.947	3.742	5.968	3.695	0.497	0.099	3.979	0.050	0.020	0.300	0.020	0.130	2.200
HLW03-13	1b.Outer13	A-13	8.463	4.979	8.664	5.227	6.970	3.983	35.845	9.957	3.850	5.974	0.849	0.498	0.996	1.125	0.050	0.020	0.020	0.200	0.130	2.200
HLW03-14	1b.Outer14	A-27	1.989	4.972	9.045	2.503	6.961	10.423	35.798	9.944	4.114	0.000	6.510	0.020	0.994	3.978	0.050	0.330	0.020	0.020	0.130	2.200
HLW03-15	1b.Outer15	A-1	1.951	13.659	13.659	1.951	1.348	5.247	51.710	0.000	2.440	0.000	0.000	0.020	0.098	3.336	1.600	0.330	0.300	0.020	0.130	2.200
HLW03-16	1b.Outer16	A-30	1.962	4.904	7.935	2.873	6.866	3.924	44.407	9.809	2.578	5.885	1.005	0.020	0.981	2.782	0.050	0.020	0.300	0.200	1.300	2.200
HLW03-17	1b.Outer17	A-29	8.377	13.798	1.971	1.971	6.899	4.474	46.224	0.000	2.244	4.530	1.644	0.020	0.294	3.942	0.050	0.020	0.020	0.020	1.300	2.200
HLW03-18	1b.Outer18	A-14	1.989	4.972	13.921	5.921	0.000	10.531	52.472	0.000	5.966	0.000	0.000	0.497	0.980	0.000	0.050	0.330	0.020	0.020	0.130	2.200
HLW03-19	1b.Outer19	A-37	1.963	4.908	9.634	5.890	0.197	10.142	52.030	0.000	5.846	0.000	0.000	0.491	0.982	3.927	1.600	0.020	0.020	0.020	0.130	2.200
HLW03-20	1b.Outer20	A-22	1.924	4.809	13.466	5.771	0.000	10.100	50.697	0.145	5.771	0.406	0.000	0.019	0.962	0.000	1.600	0.330	0.300	0.200	1.300	2.200
HLW03-21	1b.Inner01	A-44	4.964	6.949	4.964	2.482	4.467	10.841	48.644	1.489	2.978	1.985	5.956	0.079	0.298	0.993	0.300	0.050	0.050	0.050	0.260	2.200
HLW03-22	1b.Inner02	A-36	4.927	6.898	9.776	2.464	1.478	11.826	40.405	4.435	2.956	3.942	5.913	0.079	0.296	0.985	0.300	0.050	0.050	0.150	0.870	2.200
HLW03-23	1b.Inner03	A-10	4.969	11.925	7.751	2.484	1.491	11.925	40.744	1.491	2.981	3.975	5.963	0.199	0.298	0.994	0.100	0.050	0.050	0.150	0.260	2.200

Table 2.7. Target Glass Compositions (wt%) for the Initial and Augmentation Test Matrices (continued).

Glass ID[(a)]	Point Type[(b)]	Melt Order	Al_2O_3	B_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	SiO_2	SrO	ThO_2	UO_2	ZrO_2	Cr_2O_3	NiO	ZnO	CdO	Tl_2O_3	Sb_2O_3	SeO_2	Spike	Constant
HLW03-24	1b.Inner04	A-3	2.978	6.949	4.964	4.964	4.467	8.160	48.644	1.489	2.978	1.985	5.956	0.079	0.496	2.978	0.300	0.050	0.050	0.050	0.260	2.200
HLW03-25	1b.Inner05	A-39	2.960	11.838	4.933	2.466	1.480	11.838	42.143	4.439	2.960	1.973	5.919	0.079	0.493	2.960	0.100	0.150	0.050	0.150	0.870	2.200
HLW03-26	1b.Inner06	A-17	4.933	6.906	4.933	4.933	1.480	10.457	40.447	4.439	4.439	3.946	5.919	0.197	0.493	2.960	0.100	0.050	0.150	0.150	0.870	2.200
HLW03-27	1b.Inner07	A-24	4.933	6.906	9.372	4.045	1.480	11.838	40.447	1.480	4.439	1.973	5.919	0.197	0.493	2.960	0.100	0.050	0.150	0.150	0.870	2.200
HLW03-28	1b.Inner08	A-5	3.633	11.925	9.938	4.969	1.491	10.499	40.744	1.491	2.981	1.988	5.963	0.080	0.497	0.994	0.100	0.050	0.150	0.050	0.260	2.200
HLW03-29	1b.Inner09	A-41	2.978	6.949	4.964	4.964	3.526	11.913	40.702	1.489	4.467	3.971	7.692	0.199	0.298	2.978	0.300	0.050	0.050	0.050	0.260	2.200
HLW03-30	1b.Inner10	A-6	2.975	11.901	4.959	4.959	4.463	6.942	43.252	1.488	4.463	1.983	8.238	0.079	0.298	0.992	0.100	0.150	0.150	0.150	0.260	2.200
HLW03-31	1b.Inner11	A-43	4.959	6.942	4.959	4.959	4.463	8.543	45.109	1.488	2.975	1.983	8.925	0.198	0.496	0.992	0.100	0.150	0.150	0.150	0.260	2.200
HLW03-32	1b.Inner12	A-40	4.933	6.906	4.933	4.933	2.932	9.123	40.447	1.480	4.439	3.946	8.879	0.079	0.493	2.960	0.100	0.150	0.150	0.050	0.870	2.200
HLW03-33	1b.Inner13	A-15	4.969	11.925	9.938	3.905	1.491	6.956	40.744	1.491	2.981	3.195	5.963	0.199	0.452	2.981	0.100	0.050	0.150	0.050	0.260	2.200
HLW03-34	1b.Inner14	A-23	2.960	6.906	9.865	2.466	1.480	9.553	48.339	1.480	3.863	1.973	5.919	0.197	0.493	0.987	0.100	0.150	0.050	0.150	0.870	2.200
HLW03-35	1b.Inner15	A-20	4.969	10.409	4.969	2.484	4.472	6.956	48.694	1.491	3.180	1.988	5.963	0.080	0.497	1.040	0.100	0.150	0.050	0.050	0.260	2.200
HLW03-36	1b.Inner16	A-8	4.927	6.898	9.520	2.696	1.478	7.971	48.289	1.478	3.563	1.971	5.913	0.197	0.493	0.985	0.300	0.050	0.150	0.050	0.870	2.200
HLW03-37	1b.Inner17	A-21	2.960	11.838	7.240	4.871	1.480	6.906	40.447	1.480	4.439	3.946	7.343	0.079	0.493	2.960	0.100	0.150	0.050	0.150	0.870	2.200
HLW03-38	1b.Inner18	A-12	4.927	6.898	9.855	2.464	1.478	9.642	43.263	1.478	3.885	3.942	7.069	0.197	0.296	0.985	0.300	0.050	0.050	0.150	0.870	2.200
HLW03-39	1b.Inner19	A-16	2.950	6.884	8.513	4.856	1.475	6.884	48.188	1.475	4.425	1.967	7.087	0.197	0.295	0.983	0.300	0.150	0.150	0.150	0.870	2.200
HLW03-40	1b.Inner20	A-7	4.953	6.935	9.412	4.892	1.486	6.935	43.060	3.287	4.458	3.963	5.944	0.079	0.495	0.991	0.300	0.050	0.150	0.150	0.260	2.200
HLW03-41	1b.Center	A-18	3.895	8.747	6.951	3.716	2.703	9.109	43.134	2.710	3.664	2.867	6.779	0.140	0.396	1.923	0.200	0.100	0.100	0.100	0.565	2.200
HLW03-42	RepHLW02-46	A-19	5.500	9.149	10.000	3.701	3.500	9.000	49.000	1.500	0.000	0.000	2.500	0.040	0.800	1.999	0.500	0.150	0.050	0.150	0.260	2.200
HLW03-43	RepHLW03-06	A-42	8.344	4.908	1.963	5.890	6.872	3.927	52.030	5.091	1.416	0.000	4.095	0.491	0.982	0.000	1.600	0.020	0.020	0.020	0.130	2.200
HLW03-44	RepHLW03-11	A-33	1.991	4.979	9.572	1.991	0.000	14.936	52.772	0.000	5.045	5.974	0.000	0.020	0.100	0.000	0.050	0.020	0.020	0.200	0.130	2.200
HLW03-45	RepHLW03-26	A-32	4.933	6.906	4.933	4.933	1.480	10.457	40.447	4.439	4.439	3.946	5.919	0.197	0.493	2.960	0.100	0.050	0.150	0.150	0.870	2.200

(a) Glass IDs HLW02-01 to HLW02-57 identify the initial test matrix of IHLW glasses, while Glass IDs HLW03-01 to HLW03-45 identify the augmentation test matrix.

(b) The "Point Type" notation generally begins with either 1a [denoting the initial (Phase 1a) test matrix] or 1b [denoting the augmentation (Phase 1b) test matrix]. After a separating dot, the notation continues with "Center", "Outer", or "Inner", denoting whether the glass was a center point, outer-layer point, or inner-layer point. The "Center", "Outer", or "Inner" designation is with respect to Phase 1a or Phase 1b. The "XX" following "Outer" and "Inner" denotes the number of each outer-layer or inner-layer point with respect to Phase 1a or Phase 1b. Replicate points are denoted by "RepHLW02-xx" and "RepHLW03-xx", where the "xx" represents a specific Glass ID number for a replicated glass.

Table 2.8. Composition Expansions of Spike and Constant Components for the Initial and Augmentation Test Matrices in Table 2.7.

Glass ID[a]	Spike Components (wt%) [b]						Constant Components (wt%) [c]															
	Ag_2O	PbO	V_2O_5	As_2O_3	BaO	CuO	Bi_2O_3	CaO	CeO_2	Cl	CoO	Cs_2O	F	K_2O	La_2O_3	MgO	P_2O_5	PdO	Rh_2O_3	RuO_2	SO_3	TeO_2	TiO_2
HLW02-01	0.108	0.216	0.054	0.108	0.162	0.054	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-02	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-03	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-04	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-05	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-06	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-07	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-08	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-09	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-10	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-11	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-12	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-13	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-14	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-15	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-16	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-17	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-18	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-19	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-20	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-21	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-22	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-23	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-24	0.154	0.307	0.077	0.154	0.230	0.077	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-25	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-26	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-27	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-28	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-29	0.133	0.267	0.067	0.133	0.200	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-30	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-31	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-32	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-33	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-34	0.133	0.267	0.067	0.133	0.200	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-35	0.133	0.267	0.067	0.133	0.200	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-36	0.133	0.267	0.067	0.133	0.200	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03

Table 2.8. Composition Expansions of Spike and Constant Components for the Initial and Augmentation Test Matrices in Table 2.7 (continued).

Glass ID[a]	Spike Components (wt%) [b]						Constant Components (wt%) [c]															
	Ag_2O	PbO	V_2O_5	As_2O_3	BaO	CuO	Bi_2O_3	CaO	CeO_2	Cl	CoO	Cs_2O	F	K_2O	La_2O_3	MgO	P_2O_5	PdO	Rh_2O_3	RuO_2	SO_3	TeO_2	TiO_2
HLW02-37	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-38	0.133	0.267	0.067	0.133	0.200	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-39	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-40	0.133	0.267	0.067	0.133	0.200	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-41	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-42	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.1	0.01	0.03
HLW02-43	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-44	0.133	0.267	0.067	0.133	0.200	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-45	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-46	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-47	0.133	0.267	0.067	0.133	0.200	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-48	0.133	0.267	0.067	0.133	0.200	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-49	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-50	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-51	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-52	0.108	0.216	0.054	0.108	0.162	0.054	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-53	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-54	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-55	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-56	0.133	0.267	0.067	0.133	0.200	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW02-57	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-01	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-02	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-03	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-04	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-05	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-06	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-07	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-08	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-09	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-10	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-11	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-12	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-13	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-14	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-15	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03

Table 2.8. Composition Expansions of Spike and Constant Components for the Initial and Augmentation Test Matrices in Table 2.7 (continued).

Glass ID[a]	Spike Components (wt%) [b]						Constant Components (wt%) [c]															
	Ag_2O	PbO	V_2O_5	As_2O_3	BaO	CuO	Bi_2O_3	CaO	CeO_2	Cl	CoO	Cs_2O	F	K_2O	La_2O_3	MgO	P_2O_5	PdO	Rh_2O_3	RuO_2	SO_3	TeO_2	TiO_2
HLW03-16	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-17	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-18	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-19	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-20	0.200	0.400	0.100	0.200	0.300	0.100	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-21	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-22	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-23	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-24	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-25	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-26	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-27	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-28	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-29	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-30	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-31	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-32	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-33	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-34	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-35	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-36	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-37	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-38	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-39	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-40	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-41	0.087	0.174	0.044	0.087	0.130	0.044	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-42	0.040	0.080	0.020	0.040	0.060	0.020	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-43	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-44	0.020	0.040	0.010	0.020	0.030	0.010	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03
HLW03-45	0.134	0.268	0.067	0.134	0.201	0.067	0.01	0.50	0.05	0.20	0.01	0.01	0.05	0.06	0.30	0.12	0.50	0.12	0.05	0.08	0.10	0.01	0.03

[a] Glass IDs HLW02-01 to HLW02-57 comprise the initial test matrix of IHLW glasses. Glass IDs HLW03-01 to HLW03-45 comprise the augmentation matrix of IHLW glasses.

[b] Spike component wt% values are rounded to 3 decimal places for each glass and may not equal the wt% value listed in the Spike column of Table 2.7.

[c] The sum of the Constant component wt% values sum to 2.20 wt% for each glass, as shown in Table 2.7.

Table 2.9. Original and Revised Oxide Forms for IHLW Glass Compositions.

Original Oxide Forms			Revised Oxide Forms		
Main	**Spike**	**Constant**	**Main**	**Spike**	**Constant**
Al_2O_3	Ag_2O	Bi_2O_3	Al_2O_3	Ag_2O	Bi_2O_3
B_2O_3	PbO	CaO	B_2O_3	PbO	CaO
Fe_2O_3	V_2O_5	**CeO_2**	Fe_2O_3	V_2O_5	**Ce_2O_3**
Li_2O	**As_2O_3**	Cl	Li_2O	**As_2O_5**	Cl
MnO	BaO	CoO	MnO	BaO	CoO
Na_2O	CuO	Cs_2O	Na_2O	CuO	Cs_2O
SiO_2		F	SiO_2		F
SrO		K_2O	SrO		K_2O
ThO_2		La_2O_3	ThO_2		La_2O_3
UO_2		MgO	**UO_3**		MgO
ZrO_2		P_2O_5	ZrO_2		P_2O_5
Cr_2O_3		PdO	Cr_2O_3		PdO
NiO		Rh_2O_3	NiO		Rh_2O_3
ZnO		RuO_2	ZnO		RuO_2
CdO		SO_3	CdO		SO_3
Tl_2O_3		TeO_2	**Tl_2O**		TeO_2
Sb_2O_3		TiO_2	Sb_2O_3		TiO_2
SeO_2			SeO_2		

Table 2.10. Target Glass Compositions Expressed in Revised Oxides (wt%) for the Combined Test Matrix.

Glass ID[a]	Point Type[b]	Melt Order	Al_2O_3	B_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	SiO_2	SrO	ThO_2	UO_3	ZrO_2	Cr_2O_3	NiO	ZnO	CdO	Tl_2O	Sb_2O_3	SeO_2	Spike	Constant[c]
HLW02-01	1a.Center	I-29	6.171	9.927	10.898	3.996	2.385	10.957	43.612	2.444	0.000	0.000	2.974	0.108	0.518	2.000	0.771	0.102	0.110	0.110	0.721	2.197
HLW02-02	1a.Outer01	I-25	3.999	13.996	13.996	5.998	0.000	3.999	50.445	0.000	0.000	0.000	0.000	0.200	0.100	1.999	1.500	0.019	0.200	0.020	1.333	2.197
HLW02-03	1a.Outer02	I-12	3.999	13.998	7.999	2.000	0.000	14.997	37.993	4.379	0.000	0.000	5.999	0.200	1.000	2.000	1.500	0.186	0.020	0.200	1.333	2.197
HLW02-04	1a.Outer03	I-46	4.001	5.001	14.002	2.000	0.518	15.002	52.939	0.000	0.000	0.000	0.000	0.020	0.100	2.000	1.500	0.186	0.200	0.200	0.133	2.198
HLW02-05	1a.Outer04	I-53	4.000	5.000	8.000	6.000	0.000	13.788	52.653	0.000	0.000	0.000	6.000	0.020	0.100	2.000	0.050	0.019	0.020	0.020	0.133	2.198
HLW02-06	1a.Outer05	I-45	8.501	5.001	8.001	4.740	5.001	15.002	40.496	0.000	0.000	0.000	6.001	0.020	1.000	2.000	1.500	0.186	0.020	0.200	0.133	2.198
HLW02-07	1a.Outer06	I-43	8.499	4.999	7.999	5.999	0.000	11.703	52.991	0.000	0.000	0.000	1.525	0.200	0.100	2.000	0.050	0.186	0.200	0.020	1.333	2.197
HLW02-08	1a.Outer07	I-56	4.000	14.000	9.205	3.310	5.000	15.000	38.745	0.000	0.000	0.000	6.000	0.020	0.100	2.000	0.050	0.019	0.200	0.020	0.133	2.198
HLW02-09	1a.Outer08	I-21	8.500	11.589	14.000	2.271	0.000	15.000	38.000	5.000	0.000	0.000	0.000	0.020	1.000	2.000	0.050	0.019	0.200	0.020	0.133	2.198
HLW02-10	1a.Outer09	I-42	8.500	14.000	8.000	6.000	0.000	10.513	38.000	2.797	0.000	0.000	6.000	0.020	0.100	2.000	1.500	0.019	0.020	0.200	0.133	2.198
HLW02-11	1a.Outer10	I-32	4.000	14.002	8.001	6.001	0.000	10.858	45.149	0.000	0.000	0.000	6.001	0.020	1.000	2.000	0.050	0.186	0.200	0.200	0.133	2.198
HLW02-12	1a.Outer11	I-44	3.999	4.998	11.382	5.998	4.998	12.757	41.401	0.000	0.000	0.000	5.998	0.200	1.000	1.999	1.500	0.019	0.020	0.200	1.333	2.197
HLW02-13	1a.Outer12	I-39	3.999	4.999	13.998	5.999	4.999	10.425	43.114	4.999	0.000	0.000	1.182	0.200	0.100	2.000	0.050	0.186	0.020	0.200	1.333	2.197
HLW02-14	1a.Outer13	I-41	4.001	5.001	8.001	6.001	2.490	4.141	53.007	5.001	0.000	0.000	6.001	0.020	0.100	2.000	1.500	0.186	0.200	0.020	0.133	2.198
HLW02-15	1a.Outer14	I-18	8.499	13.998	13.998	2.000	4.688	12.539	37.993	0.000	0.000	0.000	0.000	0.200	0.100	2.000	0.050	0.186	0.020	0.200	1.333	2.197
HLW02-16	1a.Outer15	I-51	8.497	4.999	7.998	5.998	4.999	9.651	39.114	4.999	0.000	0.000	5.998	0.200	0.100	1.999	1.500	0.019	0.200	0.200	1.333	2.197
HLW02-17	1a.Outer16	I-19	8.500	5.000	13.843	6.000	0.000	7.690	52.958	0.000	0.000	0.000	0.000	0.020	0.100	2.000	1.500	0.019	0.020	0.020	0.133	2.198
HLW02-18	1a.Outer17	I-8	3.999	4.998	11.127	2.013	0.000	14.995	49.852	0.000	0.000	0.000	5.998	0.200	1.000	1.999	0.050	0.019	0.200	0.020	1.333	2.197
HLW02-19	1a.Outer18	I-57	4.000	14.000	10.781	2.000	5.000	8.849	38.000	5.000	0.000	0.000	6.000	0.020	0.100	2.000	1.500	0.019	0.200	0.200	0.133	2.198
HLW02-20	1a.Outer19	I-30	4.000	14.000	14.000	2.000	0.000	6.453	51.734	3.253	0.000	0.000	0.000	0.020	0.100	2.000	0.050	0.019	0.020	0.020	0.133	2.198
HLW02-21	1a.Outer20	I-24	8.500	14.000	8.000	2.000	0.000	15.000	46.440	0.000	0.000	0.000	1.500	0.020	0.100	2.000	0.050	0.019	0.020	0.020	0.133	2.198
HLW02-22	1a.Outer21	I-36	8.500	14.000	9.500	6.000	0.000	4.000	53.000	0.080	0.000	0.000	0.000	0.020	0.100	2.000	0.050	0.019	0.200	0.200	0.133	2.198
HLW02-23	1a.Outer22	I-15	8.501	14.002	8.001	6.001	5.001	5.591	39.325	5.001	0.000	0.000	1.500	0.020	1.000	2.000	1.500	0.186	0.020	0.020	0.133	2.198
HLW02-24	1a.Outer23	I-31	8.498	4.999	7.998	2.000	4.999	12.195	47.052	4.999	0.000	0.000	1.500	0.153	0.100	2.000	0.050	0.019	0.020	0.200	1.023	2.197
HLW02-25	1a.Outer24	I-34	8.501	14.002	9.501	2.000	0.355	6.884	47.398	5.001	0.000	0.000	0.000	0.020	0.100	2.000	1.500	0.186	0.200	0.020	0.133	2.198
HLW02-26	1a.Outer25	I-5	3.999	4.999	12.498	2.000	4.959	14.997	37.993	4.999	0.000	0.000	5.999	0.200	0.100	2.000	1.500	0.186	0.020	0.020	1.333	2.197
HLW02-27	1a.Outer26	I-23	4.001	14.002	12.502	6.001	3.365	4.275	39.946	5.001	0.000	0.000	6.001	0.020	0.100	2.000	0.050	0.186	0.020	0.200	0.133	2.198
HLW02-28	1a.Inner01	I-49	7.500	8.001	10.451	2.500	1.500	15.001	41.003	3.500	0.000	0.000	4.500	0.040	0.300	2.000	1.000	0.140	0.050	0.050	0.266	2.198
HLW02-29	1a.Inner02	I-6	7.499	12.998	9.998	3.749	1.500	8.999	40.994	3.499	0.000	0.000	4.499	0.133	0.300	2.000	0.500	0.046	0.050	0.150	0.889	2.197
HLW02-30	1a.Inner03	I-22	5.500	9.722	10.000	5.000	3.500	11.229	40.999	3.500	0.000	0.000	4.500	0.040	0.300	2.000	1.000	0.046	0.150	0.050	0.266	2.198
HLW02-31	1a.Inner04	I-20	5.500	13.001	10.001	2.500	1.500	14.982	41.003	1.500	0.000	0.000	4.369	0.040	0.300	2.000	0.500	0.140	0.050	0.150	0.266	2.198
HLW02-32	1a.Inner05	I-9	7.500	8.000	10.000	5.000	1.500	10.733	46.117	3.500	0.000	0.000	1.500	0.040	0.300	2.000	1.000	0.046	0.150	0.150	0.266	2.198
HLW02-33	1a.Inner06	I-17	6.341	8.000	12.000	2.500	3.500	15.000	41.000	3.500	0.000	0.000	2.009	0.040	0.800	2.000	0.500	0.046	0.150	0.150	0.266	2.198
HLW02-34	1a.Inner07	I-26	5.499	12.998	11.998	3.956	1.500	10.891	40.994	3.499	0.000	0.000	1.500	0.133	0.800	2.000	1.000	0.046	0.050	0.050	0.889	2.197
HLW02-35	1a.Inner08	I-35	6.488	12.999	11.999	5.000	3.500	9.160	40.996	1.500	0.000	0.000	1.500	0.133	0.800	2.000	0.500	0.139	0.150	0.050	0.889	2.197
HLW02-36	1a.Inner09	I-48	5.499	8.668	11.998	2.500	1.500	14.997	45.074	1.500	0.000	0.000	1.500	0.133	0.300	2.000	1.000	0.046	0.050	0.150	0.889	2.197
HLW02-37	1a.Inner10	I-3	6.762	13.000	10.000	2.500	3.500	11.188	41.000	1.500	0.000	0.000	4.500	0.040	0.800	2.000	0.500	0.046	0.150	0.050	0.266	2.198
HLW02-38	1a.Inner11	I-4	6.893	12.998	11.998	4.255	1.500	8.999	40.994	3.499	0.000	0.000	1.500	0.133	0.800	2.000	1.000	0.046	0.150	0.150	0.889	2.197
HLW02-39	1a.Inner12	I-40	7.500	8.992	10.000	2.500	1.500	11.059	48.999	1.500	0.000	0.000	1.500	0.040	0.800	2.000	1.000	0.046	0.050	0.050	0.266	2.198
HLW02-40	1a.Inner13	I-33	7.499	9.833	9.999	2.632	1.500	9.683	48.996	1.500	0.000	0.000	1.500	0.133	0.300	2.000	1.000	0.139	0.150	0.050	0.889	2.197

Table 2.10. Target Glass Compositions Expressed in Revised Oxides (wt%) for the Combined Test Matrix (continued).

Glass ID[a]	Point Type[b]	Melt Order	Al_2O_3	B_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	SiO_2	SrO	ThO_2	UO_3	ZrO_2	Cr_2O_3	NiO	ZnO	CdO	Tl_2O	Sb_2O_3	SeO_2	Spike	Constant[c]
HLW02-41	1a.Inner14	I-14	6.500	13.001	10.001	2.500	1.500	9.001	48.953	1.500	0.000	0.000	1.500	0.040	0.300	2.000	0.500	0.140	0.050	0.050	0.266	2.198
HLW02-42	1a.Inner15	I-55	5.500	13.001	10.001	5.000	1.500	9.001	44.453	3.500	0.000	0.000	2.500	0.040	0.300	2.000	0.500	0.140	0.050	0.050	0.266	2.198
HLW02-43	1a.Inner16	I-38	6.500	13.000	10.000	2.500	3.500	12.450	41.000	3.500	0.000	0.000	1.500	0.040	0.300	2.000	1.000	0.046	0.150	0.050	0.266	2.198
HLW02-44	1a.Inner17	I-2	5.499	9.069	9.998	2.500	3.499	14.997	43.673	1.500	0.000	0.000	2.500	0.133	0.300	2.000	1.000	0.046	0.150	0.050	0.889	2.197
HLW02-45	1a.Inner18	I-11	5.500	8.000	11.000	2.500	3.500	9.619	48.831	3.500	0.000	0.000	1.500	0.040	0.300	2.000	1.000	0.046	0.050	0.150	0.266	2.198
HLW02-46	1a.Inner19	I-13	5.500	9.150	10.001	3.701	3.500	9.001	49.003	1.500	0.000	0.000	2.500	0.040	0.800	2.000	0.500	0.140	0.050	0.150	0.266	2.198
HLW02-47	1a.Inner20	I-27	5.499	9.806	9.999	2.500	3.500	9.443	48.995	1.500	0.000	0.000	2.500	0.133	0.300	2.000	0.500	0.139	0.050	0.050	0.889	2.197
HLW02-48	1a.Inner21	I-10	5.999	7.999	11.999	3.340	1.500	14.999	40.996	1.711	0.000	0.000	4.500	0.133	0.800	2.000	0.500	0.139	0.150	0.150	0.889	2.197
HLW02-49	1a.Inner22	I-54	7.500	8.740	12.001	5.000	3.500	9.000	44.213	1.500	0.000	0.000	3.000	0.040	0.300	2.000	0.500	0.139	0.050	0.050	0.266	2.198
HLW02-50	1a.Inner23	I-28	6.000	13.001	12.001	2.500	1.500	9.821	43.533	1.500	0.000	0.000	4.500	0.040	0.300	2.000	0.500	0.140	0.150	0.050	0.266	2.198
HLW02-51	1a.Inner24	I-7	7.500	8.000	10.501	4.589	1.500	9.000	45.164	3.500	0.000	0.000	4.500	0.040	0.300	2.000	0.500	0.139	0.150	0.150	0.266	2.198
HLW02-52	RepHLW02-01	I-50	6.171	9.927	10.898	3.996	2.385	10.957	43.612	2.444	0.000	0.000	2.974	0.108	0.518	2.000	0.771	0.102	0.110	0.110	0.719	2.197
HLW02-53	RepHLW02-17	I-52	8.500	5.000	13.843	6.000	0.000	7.690	52.958	0.000	0.000	0.000	0.000	0.020	0.100	2.000	1.500	0.019	0.020	0.020	0.133	2.198
HLW02-54	RepHLW02-4	I-1	4.001	5.001	14.002	2.000	0.518	15.002	52.939	0.000	0.000	0.000	0.000	0.020	0.100	2.000	1.500	0.186	0.200	0.200	0.133	2.198
HLW02-55	RepHLW02-42	I-16	5.500	13.001	10.001	5.000	1.500	9.001	44.453	3.500	0.000	0.000	2.500	0.040	0.300	2.000	0.500	0.140	0.050	0.050	0.266	2.198
HLW02-56	RepHLW02-44	I-37	5.499	9.069	9.998	2.500	3.499	14.997	43.673	1.500	0.000	0.000	2.500	0.133	0.300	2.000	1.000	0.046	0.150	0.050	0.889	2.197
HLW02-57	RepHLW02-8	I-47	4.000	14.000	9.205	3.310	5.000	15.000	38.745	0.000	0.000	0.000	6.000	0.020	0.100	2.000	0.050	0.019	0.200	0.020	0.133	2.198
HLW03-01	1b.Outer01	A-4	8.335	13.727	13.727	5.883	6.078	3.922	35.299	0.000	2.764	0.000	2.983	0.020	0.098	3.059	0.050	0.307	0.020	0.200	1.332	2.198
HLW03-02	1b.Outer02	A-28	1.951	13.662	13.662	2.473	6.832	11.177	35.132	0.000	0.000	0.000	9.088	0.488	0.976	0.000	1.600	0.307	0.300	0.020	0.133	2.198
HLW03-03	1b.Outer03	A-26	1.953	4.884	13.677	2.678	6.839	10.755	35.169	9.769	0.000	0.000	6.404	0.488	0.977	1.946	1.600	0.307	0.020	0.200	0.133	2.198
HLW03-04	1b.Outer04	A-9	1.954	4.886	13.680	5.862	3.161	4.442	42.425	9.771	0.000	6.210	2.932	0.488	0.098	0.000	0.050	0.306	0.020	0.199	1.328	2.190
HLW03-05	1b.Outer05	A-2	8.175	4.809	1.924	1.924	6.733	14.427	47.837	0.000	3.812	0.000	0.000	0.481	0.096	3.847	1.600	0.307	0.300	0.200	1.332	2.198
HLW03-06	1b.Outer06	A-35	8.344	4.908	1.963	5.890	6.872	3.927	52.031	5.091	1.416	0.000	4.095	0.491	0.982	0.000	1.600	0.019	0.020	0.020	0.133	2.198
HLW03-07	1b.Outer07	A-25	4.961	4.961	13.891	4.750	6.945	11.693	39.825	0.000	0.000	6.306	0.000	0.496	0.100	3.461	0.050	0.019	0.020	0.199	0.133	2.190
HLW03-08	1b.Outer08	A-31	8.031	4.833	1.933	5.151	6.766	14.499	34.797	0.000	4.412	0.000	9.666	0.483	0.097	3.866	1.600	0.019	0.300	0.020	1.332	2.197
HLW03-09	1b.Outer09	A-11	7.668	13.695	3.486	1.979	0.000	14.848	52.465	0.000	2.552	0.000	0.000	0.020	0.099	0.000	0.050	0.307	0.300	0.200	0.133	2.198
HLW03-10	1b.Outer10	A-45	8.369	4.924	9.982	5.908	6.893	12.851	35.449	0.000	2.626	1.108	7.250	0.020	0.985	0.000	0.050	0.019	0.020	0.020	1.331	2.196
HLW03-11	1b.Outer11	A-38	1.984	4.961	9.538	1.984	0.000	14.883	52.586	0.000	5.027	6.306	0.000	0.020	0.100	0.000	0.050	0.019	0.020	0.199	0.133	2.190
HLW03-12	1b.Outer12	A-34	1.982	4.956	1.982	5.008	6.939	3.965	44.277	9.912	3.729	6.299	3.682	0.495	0.099	3.965	0.050	0.019	0.299	0.020	0.133	2.190
HLW03-13	1b.Outer13	A-13	8.433	4.961	8.633	5.209	6.945	3.969	35.719	9.922	3.836	6.306	0.846	0.496	0.992	1.121	0.050	0.019	0.020	0.199	0.133	2.190
HLW03-14	1b.Outer14	A-27	1.989	4.973	9.047	2.504	6.962	10.425	35.806	9.946	4.115	0.000	6.511	0.020	0.994	3.979	0.050	0.307	0.020	0.020	0.133	2.198
HLW03-15	1b.Outer15	A-1	1.951	13.662	13.662	1.951	1.348	5.248	51.722	0.000	2.441	0.000	0.000	0.020	0.098	3.337	1.600	0.307	0.300	0.020	0.133	2.198
HLW03-16	1b.Outer16	A-30	1.955	4.886	7.905	2.862	6.840	3.909	44.240	9.772	2.568	6.210	1.001	0.020	0.977	2.772	0.050	0.019	0.299	0.199	1.327	2.189
HLW03-17	1b.Outer17	A-29	8.352	13.757	1.965	1.965	6.879	4.461	46.088	0.000	2.237	4.784	1.639	0.020	0.293	3.930	0.050	0.019	0.020	0.020	1.328	2.191
HLW03-18	1b.Outer18	A-14	1.989	4.973	13.924	5.922	0.000	10.533	52.484	0.000	5.967	0.000	0.000	0.497	0.980	0.000	0.050	0.307	0.020	0.020	0.133	2.198
HLW03-19	1b.Outer19	A-37	1.963	4.908	9.634	5.890	0.197	10.142	52.030	0.000	5.846	0.000	0.000	0.491	0.982	3.927	1.600	0.019	0.020	0.020	0.133	2.198
HLW03-20	1b.Outer20	A-22	1.923	4.808	13.462	5.769	0.000	10.097	50.681	0.145	5.769	0.430	0.000	0.019	0.962	0.000	1.600	0.307	0.300	0.200	1.332	2.197
HLW03-21	1b.Inner01	A-44	4.958	6.941	4.958	2.479	4.462	10.828	48.587	1.487	2.975	2.100	5.949	0.079	0.298	0.992	0.300	0.046	0.050	0.050	0.266	2.195
HLW03-22	1b.Inner02	A-36	4.915	6.881	9.752	2.458	1.474	11.797	40.305	4.424	2.949	4.165	5.898	0.079	0.295	0.983	0.299	0.046	0.050	0.150	0.889	2.192
HLW03-23	1b.Inner03	A-10	4.957	11.897	7.733	2.478	1.487	11.897	40.648	1.487	2.974	4.201	5.949	0.199	0.297	0.992	0.100	0.046	0.050	0.150	0.266	2.193

Table 2.10. Target Glass Compositions Expressed in Revised Oxides (wt%) for the Combined Test Matrix (continued).

Glass ID[(a)]	Point Type[(b)]	Melt Order	Al_2O_3	B_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	SiO_2	SrO	ThO_2	UO_3	ZrO_2	Cr_2O_3	NiO	ZnO	CdO	Tl_2O	Sb_2O_3	SeO_2	Spike	Constant[(c)]
HLW03-24	1b.Inner04	A-3	2.975	6.941	4.958	4.958	4.462	8.151	48.588	1.487	2.975	2.100	5.949	0.079	0.495	2.975	0.300	0.046	0.050	0.050	0.266	2.195
HLW03-25	1b.Inner05	A-39	2.956	11.823	4.927	2.463	1.478	11.823	42.090	4.433	2.956	2.087	5.912	0.079	0.492	2.956	0.100	0.139	0.050	0.150	0.890	2.195
HLW03-26	1b.Inner06	A-17	4.921	6.889	4.921	4.921	1.476	10.431	40.346	4.428	4.428	4.169	5.904	0.197	0.492	2.953	0.100	0.046	0.150	0.150	0.889	2.192
HLW03-27	1b.Inner07	A-24	4.926	6.897	9.359	4.040	1.478	11.822	40.393	1.478	4.433	2.087	5.911	0.197	0.492	2.956	0.100	0.046	0.150	0.150	0.890	2.195
HLW03-28	1b.Inner08	A-5	3.629	11.911	9.926	4.963	1.489	10.486	40.695	1.489	2.977	2.103	5.956	0.080	0.496	0.993	0.100	0.046	0.150	0.050	0.266	2.195
HLW03-29	1b.Inner09	A-41	2.971	6.933	4.952	4.952	3.518	11.885	40.606	1.485	4.456	4.196	7.674	0.199	0.297	2.971	0.299	0.046	0.050	0.050	0.266	2.193
HLW03-30	1b.Inner10	A-6	2.972	11.888	4.953	4.953	4.458	6.934	43.203	1.486	4.458	2.098	8.229	0.079	0.298	0.991	0.100	0.139	0.150	0.150	0.266	2.195
HLW03-31	1b.Inner11	A-43	4.953	6.934	4.953	4.953	4.458	8.533	45.058	1.486	2.972	2.098	8.915	0.198	0.495	0.991	0.100	0.139	0.150	0.150	0.266	2.195
HLW03-32	1b.Inner12	A-40	4.921	6.889	4.921	4.921	2.925	9.101	40.348	1.476	4.428	4.170	8.857	0.079	0.492	2.953	0.100	0.139	0.150	0.050	0.889	2.192
HLW03-33	1b.Inner13	A-15	4.960	11.902	9.919	3.898	1.488	6.943	40.667	1.488	2.975	3.378	5.952	0.199	0.451	2.975	0.100	0.046	0.150	0.050	0.266	2.194
HLW03-34	1b.Inner14	A-23	2.956	6.897	9.853	2.463	1.478	9.541	48.278	1.478	3.858	2.087	5.912	0.197	0.492	0.986	0.100	0.139	0.050	0.150	0.890	2.195
HLW03-35	1b.Inner15	A-20	4.963	10.397	4.963	2.481	4.467	6.948	48.639	1.489	3.176	2.103	5.956	0.080	0.496	1.039	0.100	0.139	0.050	0.050	0.266	2.195
HLW03-36	1b.Inner16	A-8	4.921	6.889	9.507	2.692	1.476	7.961	48.226	1.476	3.558	2.085	5.905	0.197	0.492	0.984	0.300	0.046	0.150	0.050	0.890	2.195
HLW03-37	1b.Inner17	A-21	2.953	11.809	7.222	4.859	1.476	6.889	40.348	1.476	4.428	4.170	7.325	0.079	0.492	2.953	0.100	0.139	0.050	0.150	0.889	2.192
HLW03-38	1b.Inner18	A-12	4.915	6.881	9.831	2.458	1.474	9.618	43.156	1.474	3.875	4.165	7.051	0.197	0.295	0.983	0.299	0.046	0.050	0.150	0.889	2.192
HLW03-39	1b.Inner19	A-16	2.946	6.875	8.502	4.850	1.473	6.875	48.128	1.473	4.420	2.081	7.078	0.197	0.295	0.982	0.300	0.139	0.150	0.150	0.890	2.195
HLW03-40	1b.Inner20	A-7	4.941	6.919	9.390	4.881	1.483	6.919	42.959	3.279	4.448	4.188	5.930	0.079	0.494	0.989	0.299	0.046	0.150	0.150	0.266	2.193
HLW03-41	1b.Center	A-18	3.888	8.732	6.939	3.710	2.698	9.093	43.059	2.705	3.658	3.032	6.767	0.140	0.395	1.920	0.200	0.093	0.100	0.100	0.578	2.194
HLW03-42	RepHLW02-46	A-19	5.500	9.150	10.001	3.701	3.500	9.001	49.004	1.500	0.000	0.000	2.500	0.040	0.800	1.999	0.500	0.140	0.050	0.150	0.266	2.198
HLW03-43	RepHLW03-06	A-42	8.344	4.908	1.963	5.890	6.872	3.927	52.031	5.091	1.416	0.000	4.095	0.491	0.982	0.000	1.600	0.019	0.020	0.020	0.133	2.198
HLW03-44	RepHLW03-11	A-33	1.984	4.961	9.538	1.984	0.000	14.883	52.586	0.000	5.027	6.306	0.000	0.020	0.100	0.000	0.050	0.019	0.020	0.199	0.133	2.190
HLW03-45	RepHLW03-26	A-32	4.921	6.889	4.921	4.921	1.476	10.431	40.346	4.428	4.428	4.169	5.904	0.197	0.492	2.953	0.100	0.046	0.150	0.150	0.889	2.192

(a) Glass IDs HLW02-01 to HLW02-57 identify the initial test matrix of IHLW glasses, while Glass IDs HLW03-01 to HLW03-45 identify the augmentation test matrix of IHLW glasses.

(b) The "Point Type" notation generally begins with either 1a [denoting the initial (Phase 1a) test matrix] or 1b [denoting the augmentation (Phase 1b) test matrix]. After a separating dot, the notation continues with "Center", "Outer", or "Inner", denoting whether the glass was a center point, outer-layer point, or inner-layer point. The "Center", "Outer", or "Inner" designation is with respect to Phase 1a or Phase 1b. The "XX" following "Outer" and "Inner" denotes the number of each outer-layer or inner-layer point with respect to Phase 1a or Phase 1b. Replicate points are denoted by "RepHLW02-xx" and "RepHLW03-xx", where the "xx" represents a specific Glass ID number for a replicated glass.

(c) Note that the values in the Constant column are no longer exactly constant because of the change in oxides forms used to express glass composition.

Table 2.11. Composition Expansions in Revised Oxides of Spike and Constant Components for the Combined Test Matrix in Table 2.10.

Glass ID[a]	Spike Components (wt%) [b]						Constant Components (wt%) [c]															
	Ag_2O	PbO	V_2O_5	As_2O_5	BaO	CuO	Bi_2O_3	CaO	Ce_2O_3	Cl	CoO	Cs_2O	F	K_2O	La_2O_3	MgO	P_2O_5	PdO	Rh_2O_3	RuO_2	SO_3	TeO_2	TiO_2
HLW02-01	0.110	0.216	0.054	0.125	0.162	0.054	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-02	0.200	0.400	0.100	0.233	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-03	0.200	0.400	0.100	0.233	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-04	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-05	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-06	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-07	0.200	0.400	0.100	0.233	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-08	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-09	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-10	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-11	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-12	0.200	0.400	0.100	0.233	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-13	0.200	0.400	0.100	0.233	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-14	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-15	0.200	0.400	0.100	0.233	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-16	0.200	0.400	0.100	0.233	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-17	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-18	0.200	0.400	0.100	0.233	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-19	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-20	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-21	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-22	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-23	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-24	0.153	0.307	0.077	0.178	0.230	0.077	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-25	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-26	0.200	0.400	0.100	0.233	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-27	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-28	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-29	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-30	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-31	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-32	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-33	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-34	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-35	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-36	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030

Table 2.11. Composition Expansions in Revised Oxides of Spike and Constant Components for the Combined Test Matrix in Table 2.10 (continued).

Glass ID[a]	Spike Components (wt%) [b]						Constant Components (wt%) [c]															
	Ag_2O	PbO	V_2O_5	As_2O_5	BaO	CuO	Bi_2O_3	CaO	Ce_2O_3	Cl	CoO	Cs_2O	F	K_2O	La_2O_3	MgO	P_2O_5	PdO	Rh_2O_3	RuO_2	SO_3	TeO_2	TiO_2
HLW02-37	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-38	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-39	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-40	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-41	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-42	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-43	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-44	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-45	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-46	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-47	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-48	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-49	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-50	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-51	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-52	0.108	0.216	0.054	0.125	0.162	0.054	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-53	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-54	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-55	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-56	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW02-57	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-01	0.200	0.400	0.100	0.232	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-02	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-03	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-04	0.199	0.399	0.100	0.232	0.299	0.100	0.010	0.498	0.048	0.199	0.010	0.010	0.050	0.060	0.299	0.120	0.498	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-05	0.200	0.400	0.100	0.232	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-06	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-07	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.498	0.048	0.199	0.010	0.010	0.050	0.060	0.299	0.120	0.498	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-08	0.200	0.400	0.100	0.232	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-09	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-10	0.200	0.400	0.100	0.232	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-11	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.498	0.048	0.199	0.010	0.010	0.050	0.060	0.299	0.120	0.498	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-12	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.498	0.048	0.199	0.010	0.010	0.050	0.060	0.299	0.120	0.498	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-13	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.498	0.048	0.199	0.010	0.010	0.050	0.060	0.299	0.120	0.498	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-14	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-15	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030

Table 2.11. Composition Expansions in Revised Oxides of Spike and Constant Components for the Combined Test Matrix in Table 2.10 (continued).

Glass ID[a]	Spike Components (wt%) [b]						Constant Components (wt%) [c]															
	Ag_2O	PbO	V_2O_5	As_2O_5	BaO	CuO	Bi_2O_3	CaO	Ce_2O_3	Cl	CoO	Cs_2O	F	K_2O	La_2O_3	MgO	P_2O_5	PdO	Rh_2O_3	RuO_2	SO_3	TeO_2	TiO_2
HLW03-16	0.199	0.398	0.100	0.231	0.299	0.100	0.010	0.498	0.047	0.199	0.010	0.010	0.050	0.060	0.299	0.120	0.498	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-17	0.199	0.399	0.100	0.232	0.299	0.100	0.010	0.499	0.048	0.199	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-18	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-19	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-20	0.200	0.400	0.100	0.232	0.300	0.100	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-21	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-22	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-23	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-24	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-25	0.134	0.267	0.067	0.155	0.201	0.067	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-26	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.499	0.048	0.199	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-27	0.134	0.267	0.067	0.155	0.201	0.067	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-28	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-29	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-30	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-31	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-32	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-33	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-34	0.134	0.267	0.067	0.155	0.201	0.067	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-35	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-36	0.134	0.267	0.067	0.155	0.201	0.067	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-37	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-38	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-39	0.134	0.267	0.067	0.155	0.201	0.067	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-40	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-41	0.087	0.173	0.043	0.101	0.130	0.043	0.010	0.499	0.048	0.200	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-42	0.040	0.080	0.020	0.046	0.060	0.020	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-43	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.500	0.048	0.200	0.010	0.010	0.050	0.060	0.300	0.120	0.500	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-44	0.020	0.040	0.010	0.023	0.030	0.010	0.010	0.498	0.048	0.199	0.010	0.010	0.050	0.060	0.299	0.120	0.498	0.120	0.050	0.080	0.100	0.010	0.030
HLW03-45	0.133	0.267	0.067	0.155	0.200	0.067	0.010	0.499	0.048	0.199	0.010	0.010	0.050	0.060	0.299	0.120	0.499	0.120	0.050	0.080	0.100	0.010	0.030

[a] Glass IDs HLW02-01 to HLW02-57 identify the initial test matrix of IHLW glasses. Glass IDs HLW03-01 to HLW03-45 identify the augmentation matrix of IHLW glasses.

[b] Spike component wt% values are rounded to 3 decimal places for each glass and may not equal the wt% value listed in the Spike column of Table 2.10.

[c] The sum of the Constant component wt% values for each glass equals the wt% value listed in the Constant column shown in Table 2.10. Note that the values are no longer exactly constant due to the revision in oxide forms.

Table 2.12 Summary of Data Sets for Validation of PCT Models.

Study	Description	Number of Glasses	Reference
WTP HLW Glass Formulations at VSL	TWRS Part A (based on contract Envelope D waste specification) and WTP Part B1 (based on inventory and actual waste data) Studies	75	[28, 10]
HWVP CVS at PNNL	Five statistically designed experimental phases. Compositions based on glasses to be made from NCAW and processed by HWVP	146	[29]
DWPF PCT Modeling at SRTC	Data used to develop THERMO	177	[30]
WVDP Support at PNNL	Support development of glass-composition control strategy at VWNS	20	[31]
WVDP CVS at PNNL	Glasses fabricated as sets of CVS glasses	44	[32]
WVDP WQR at WVNS	Glasses and data support development of PCT release models. Compositions based on WVDP target glass, with boundary equal to 3× expected process variation	46	[33]
WTP LAW Glass Formulations at VSL	Glasses and data developed for LAW	66	[34]

Table 2.13. Composition of Glasses for Validation of $T_{1\%}$ Models (wt%).

Glass ID	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2
MS-7a	8.00	7.00	0.00	0.30	11.50	4.54	0.50	15.30	0.95	0.00	0.00	45.31	0.00	0.00	0.00	0.00	0.00	6.00
MS-7d	8.00	7.00	0.00	0.30	11.50	4.54	0.50	15.30	0.95	0.00	0.00	45.31	0.00	0.00	0.00	0.00	0.00	6.00
MS-7e	8.00	7.00	0.00	0.30	11.50	4.54	0.50	15.30	0.95	0.00	0.00	45.31	0.00	0.00	0.00	0.00	0.00	6.00
MS7-H-Al	11.00	6.77	0.00	0.29	11.13	4.39	0.48	14.80	0.92	0.00	0.00	43.83	0.00	0.00	0.00	0.00	0.00	5.80
MS7-L-Al	5.00	7.23	0.00	0.31	11.81	4.69	0.52	15.81	0.98	0.00	0.00	46.82	0.00	0.00	0.00	0.00	0.00	6.20
MS7-H-Cr	7.90	7.00	0.00	0.50	11.49	4.53	0.50	15.28	0.95	0.00	0.00	45.26	0.00	0.00	0.00	0.00	0.00	5.99
MS7-L-Cr	8.02	7.01	0.00	0.10	11.52	4.55	0.50	15.33	0.95	0.00	0.00	45.40	0.00	0.00	0.00	0.00	0.00	6.01
MS7-L-Fe	8.32	7.28	0.00	0.31	8.00	4.72	0.52	15.91	0.99	0.00	0.00	47.10	0.00	0.00	0.00	0.00	0.00	6.24
MS7-H-Li	7.88	6.89	0.00	0.30	11.32	6.00	0.49	15.07	0.94	0.00	0.00	44.62	0.00	0.00	0.00	0.00	0.00	5.91
MS7-L-Li	8.13	7.11	0.00	0.30	11.69	3.00	0.51	15.55	0.97	0.00	0.00	46.04	0.00	0.00	0.00	0.00	0.00	6.10
MS7-H-Mg	7.81	6.83	0.00	0.29	11.22	4.43	0.49	14.93	0.93	0.00	0.00	44.22	0.00	0.00	0.00	0.00	0.00	5.86
MS7-L-Mg	8.05	7.04	0.00	0.30	11.57	4.57	0.50	15.39	0.96	0.00	0.00	45.58	0.00	0.00	0.00	0.00	0.00	6.04
MS7-H-Na	7.74	6.78	0.00	0.29	11.13	4.40	0.48	18.00	0.92	0.00	0.00	43.87	0.00	0.00	0.00	0.00	0.00	5.81
MS7-L-Na	8.31	7.27	0.00	0.31	11.95	4.72	0.52	12.00	0.99	0.00	0.00	47.08	0.00	0.00	0.00	0.00	0.00	6.23
MS7-H-Ni	7.93	6.94	0.00	0.30	11.40	4.50	0.50	15.17	1.80	0.00	0.00	44.92	0.00	0.00	0.00	0.00	0.00	5.95
MS7-L-Ni	8.05	7.05	0.00	0.30	11.58	4.57	0.50	15.40	0.30	0.00	0.00	45.61	0.00	0.00	0.00	0.00	0.00	6.04
SP-Al-1[(a)]	4.00	7.30	0.73	0.23	13.04	3.13	0.38	16.41	0.54	0.09	0.09	48.01	0.03	0.00	0.00	0.00	0.04	1.93
SP-Cr-1-o	8.02	7.02	0.70	0.00	12.53	3.01	0.36	15.77	0.52	0.09	0.09	46.10	0.03	0.00	0.00	0.00	0.04	1.85
SP-Cr-1-r	8.02	7.02	0.70	0.00	12.53	3.01	0.36	15.77	0.52	0.09	0.09	46.10	0.03	0.00	0.00	0.00	0.04	1.85
SP-Li-3-o	8.00	7.00	0.70	0.22	12.50	3.00	0.36	15.73	0.52	0.09	0.09	46.00	0.03	0.00	0.00	0.00	0.04	1.85
SP-Li-3-r	8.00	7.00	0.70	0.22	12.50	3.00	0.36	15.73	0.52	0.09	0.09	46.00	0.03	0.00	0.00	0.00	0.04	1.85
SP-Mg-1	7.97	6.97	0.69	0.22	12.45	2.99	0.36	15.67	0.52	0.09	0.09	45.81	0.03	0.00	0.00	0.00	0.04	1.84
SP-Mn-1	8.03	7.03	0.70	0.22	12.55	3.01	0.00	15.79	0.52	0.09	0.09	46.17	0.03	0.00	0.00	0.00	0.04	1.85
SP-Mn-3	7.71	6.74	0.67	0.21	12.04	2.89	4.00	15.16	0.50	0.09	0.09	44.31	0.03	0.00	0.00	0.00	0.04	1.78
SP-Na-1	8.73	7.64	0.76	0.24	13.65	3.28	0.39	8.00	0.57	0.10	0.10	50.21	0.03	0.00	0.00	0.00	0.04	2.02
SP-Na-3	7.59	6.65	0.66	0.21	11.87	2.85	0.34	20.00	0.49	0.08	0.09	43.66	0.03	0.00	0.00	0.00	0.04	1.75
SPA-18	6.00	8.18	0.00	0.30	14.00	3.79	1.00	15.89	0.50	0.03	0.06	35.54	1.42	0.00	0.00	0.00	0.99	3.00
SPA-38	8.00	7.00	0.70	0.22	12.50	3.00	0.36	15.73	0.52	0.08	0.09	46.01	0.03	0.00	0.00	0.00	0.04	1.85
WTP-TL-16	11.00	15.00	1.00	0.50	13.00	6.00	5.00	4.00	0.00	0.07	0.12	40.06	0.00	0.00	0.00	0.00	2.50	0.00
WTP-TL-17	11.00	15.00	0.00	0.50	6.56	0.00	0.00	15.00	1.00	0.07	0.12	38.00	8.50	0.00	0.00	0.00	2.50	0.00
WTP-TL-19	2.00	15.00	1.00	0.50	3.00	0.00	5.00	15.00	1.00	0.07	0.12	49.56	0.00	0.00	0.00	0.00	0.00	6.00
WTP-TL-20	2.00	4.00	1.00	0.50	13.00	6.00	0.00	4.00	1.00	0.07	0.12	49.56	8.50	0.00	0.00	0.00	2.50	6.00
WTP-TL-21	2.00	4.00	1.00	0.50	13.00	0.02	5.00	15.00	0.00	0.07	0.12	52.99	2.04	0.00	0.00	0.00	2.50	0.00
WTP-TL-23	8.75	6.75	0.75	0.38	7.93	4.50	3.75	6.75	0.75	0.07	0.12	49.25	6.38	0.00	0.00	0.00	0.62	1.50
WTP-TL-24	4.25	6.75	0.25	0.12	10.50	1.50	3.75	11.18	0.75	0.07	0.12	49.25	6.38	0.00	0.00	0.00	1.88	1.50
WTP-TL-27	8.75	12.25	0.25	0.12	10.50	4.50	3.75	6.75	0.25	0.07	0.12	42.44	2.12	0.00	0.00	0.00	1.88	4.50
WTP-TL-28	4.25	6.75	0.25	0.12	10.50	4.50	3.75	6.75	0.25	0.07	0.12	48.18	6.38	0.00	0.00	0.00	1.88	4.50
WTP-TL-29	4.25	12.25	0.75	0.38	10.50	1.50	3.75	6.75	0.25	0.07	0.12	49.25	5.20	0.00	0.00	0.00	0.62	2.61
WTP-TL-30	8.75	12.25	0.25	0.38	5.50	4.50	1.58	6.75	0.75	0.07	0.12	48.85	2.12	0.00	0.00	0.00	1.88	4.50

Table 2.13. Composition of Glasses for Validation of $T_{1\%}$ Models (wt%) (continued).

Glass ID	Ag_2O	As_2O_5	BaO	Bi_2O_3	CaO	Ce_2O_3	Cl	CoO	Cs_2O	CuO	F	K_2O	La_2O_3	MgO	MoO_3	Nd_2O_3	P_2O_5	PbO	PdO	Pr_2O_3
MS-7a	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.60	0.00	0.00	0.00	0.00	0.00	0.00
MS-7d	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.60	0.00	0.00	0.00	0.00	0.00	0.00
MS-7e	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.60	0.00	0.00	0.00	0.00	0.00	0.00
MS7-H-Al	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.58	0.00	0.00	0.00	0.00	0.00	0.00
MS7-L-Al	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.62	0.00	0.00	0.00	0.00	0.00	0.00
MS7-H-Cr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.60	0.00	0.00	0.00	0.00	0.00	0.00
MS7-L-Cr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.60	0.00	0.00	0.00	0.00	0.00	0.00
MS7-L-Fe	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.62	0.00	0.00	0.00	0.00	0.00	0.00
MS7-H-Li	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.59	0.00	0.00	0.00	0.00	0.00	0.00
MS7-L-Li	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.00	0.00	0.00	0.00
MS7-H-Mg	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.00	0.00	0.00	0.00	0.00	0.00	0.00
MS7-L-Mg	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MS7-H-Na	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.58	0.00	0.00	0.00	0.00	0.00	0.00
MS7-L-Na	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.62	0.00	0.00	0.00	0.00	0.00	0.00
MS7-H-Ni	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.59	0.00	0.00	0.00	0.00	0.00	0.00
MS7-L-Ni	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.60	0.00	0.00	0.00	0.00	0.00	0.00
SP-Al-1[(a)]	0.07	0.00	0.32	0.00	1.04	0.07	0.01	0.09	0.00	0.03	0.06	0.29	0.28	0.63	0.01	0.19	0.48	0.18	0.00	0.00
SP-Cr-1-o	0.07	0.00	0.30	0.00	1.00	0.07	0.01	0.08	0.00	0.03	0.06	0.28	0.27	0.60	0.01	0.18	0.47	0.17	0.00	0.00
SP-Cr-1-r	0.07	0.00	0.30	0.00	1.00	0.07	0.01	0.08	0.00	0.03	0.06	0.28	0.27	0.60	0.01	0.18	0.47	0.17	0.00	0.00
SP-Li-3-o	0.07	0.00	0.30	0.00	1.00	0.07	0.01	0.08	0.00	0.03	0.06	0.28	0.27	0.60	0.01	0.18	0.46	0.17	0.00	0.00
SP-Li-3-r	0.07	0.00	0.30	0.00	1.00	0.07	0.01	0.08	0.00	0.03	0.06	0.28	0.27	0.60	0.01	0.18	0.46	0.17	0.00	0.00
SP-Mg-1	0.07	0.00	0.30	0.00	1.00	0.07	0.01	0.08	0.00	0.03	0.06	0.28	0.27	1.00	0.01	0.18	0.46	0.17	0.00	0.00
SP-Mn-1	0.07	0.00	0.30	0.00	1.00	0.07	0.01	0.08	0.00	0.03	0.06	0.28	0.27	0.60	0.01	0.18	0.47	0.17	0.00	0.00
SP-Mn-3	0.07	0.00	0.29	0.00	0.96	0.06	0.01	0.08	0.00	0.03	0.06	0.27	0.26	0.58	0.01	0.18	0.45	0.17	0.00	0.00
SP-Na-1	0.08	0.00	0.33	0.00	1.09	0.07	0.01	0.09	0.00	0.03	0.07	0.31	0.30	0.66	0.01	0.20	0.51	0.19	0.00	0.00
SP-Na-3	0.07	0.00	0.29	0.00	0.95	0.06	0.01	0.08	0.00	0.03	0.06	0.27	0.26	0.57	0.01	0.17	0.44	0.16	0.00	0.00
SPA-18	0.04	0.06	0.07	0.00	2.00	0.44	0.01	0.01	0.00	0.02	1.50	3.89	0.26	0.00	0.01	0.08	0.50	0.29	0.00	0.00
SPA-38	0.07	0.00	0.30	0.00	1.00	0.07	0.01	0.08	0.00	0.03	0.06	0.28	0.27	0.60	0.01	0.18	0.46	0.17	0.00	0.00
WTP-TL-16	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01
WTP-TL-17	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01
WTP-TL-19	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01
WTP-TL-20	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01
WTP-TL-21	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01
WTP-TL-23	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01
WTP-TL-24	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01
WTP-TL-27	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01
WTP-TL-28	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01
WTP-TL-29	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01
WTP-TL-30	0.08	0.08	0.01	0.00	0.38	0.00	0.05	0.00	0.00	0.03	0.03	0.02	0.28	0.38	0.01	0.15	0.05	0.12	0.00	0.01

Table 2.13. Composition of Glasses for Validation of $T_{1\%}$ Models (wt%) (continued).

Glass ID	Rb_2O	Rh_2O_3	RuO_2	Sm_2O_3	SO_3	TeO_2	TiO_2	V_2O_5	WO_3	Y_2O_3	Total	$T_{1\%}$ (°C)
MS-7a	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	913.2
MS-7d	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	883.5
MS-7e	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	909.8
MS7-H-Al	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	1053.1
MS7-L-Al	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	892.6
MS7-H-Cr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	998.4
MS7-L-Cr	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	930.1
MS7-L-Fe	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	893.7
MS7-H-Li	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	931.8
MS7-L-Li	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	1009.6
MS7-H-Mg	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	1050.0
MS7-L-Mg	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	971.3
MS7-H-Na	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	896.7
MS7-L-Na	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	1082.6
MS7-H-Ni	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	1109.4
MS7-L-Ni	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	100.00	815.0
SP-Al-1[(a)]	0.00	0.03	0.03	0.00	0.20	0.00	0.03	0.00	0.00	0.00	100.00	671.8
SP-Cr-1-o	0.00	0.03	0.03	0.00	0.19	0.00	0.03	0.00	0.00	0.00	100.00	694.9
SP-Cr-1-r	0.00	0.03	0.03	0.00	0.19	0.00	0.03	0.00	0.00	0.00	100.00	787.7
SP-Li-3-o	0.00	0.03	0.03	0.00	0.19	0.00	0.03	0.00	0.00	0.00	100.00	853.9
SP-Li-3-r	0.00	0.03	0.03	0.00	0.19	0.00	0.03	0.00	0.00	0.00	100.00	794.7
SP-Mg-1	0.00	0.03	0.03	0.00	0.19	0.00	0.03	0.00	0.00	0.00	100.00	902.9
SP-Mn-1	0.00	0.03	0.03	0.00	0.19	0.00	0.03	0.00	0.00	0.00	100.00	930.5
SP-Mn-3	0.00	0.03	0.03	0.00	0.18	0.00	0.03	0.00	0.00	0.00	100.00	958.7
SP-Na-1	0.00	0.03	0.03	0.00	0.21	0.00	0.03	0.00	0.00	0.00	100.00	1118.3
SP-Na-3	0.00	0.03	0.03	0.00	0.18	0.00	0.03	0.00	0.00	0.00	100.00	813.0
SPA-18	0.00	0.00	0.00	0.00	0.09	0.01	0.00	0.03	0.00	0.00	100.00	874.7
SPA-38	0.00	0.03	0.03	0.00	0.19	0.00	0.03	0.00	0.00	0.00	100.00	852.4
WTP-TL-16	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	1183.2
WTP-TL-17	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	800.2
WTP-TL-19	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	870.1
WTP-TL-20	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	1109.3
WTP-TL-21	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	740.5
WTP-TL-23	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	954.6
WTP-TL-24	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	880.9
WTP-TL-27	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	1043.0
WTP-TL-28	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	969.1
WTP-TL-29	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	996.1
WTP-TL-30	0.01	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	100.00	1039.1

[(a)] Values of Sb_2O_3 used for the SP- series of glasses in validation were incorrect due to an error in renormalization. They do not, however, affect the validation results or statistics.

Table 4.1. PCT Release Data (Leachate Concentration in ppm and Normalized Release in g/l) for the IHLW Initial Matrix.

Glass ID[(a)]	Retained for Model Development	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/l)	PCT-Li (g/l)	PCT-Na (g/l)	Leachate pH
HLW02-01[(1)]	Yes	21.580	12.720	51.060	0.700	0.686	0.628	10.64
HLW02-02	Yes	39.350	22.260	11.810	0.906	0.798	0.398	9.86
HLW02-03	Yes	123.300	19.880	224.200	2.836	2.140	2.014	10.68
HLW02-04[(2)]	Yes	8.913	6.730	97.650	0.574	0.724	0.878	10.84
HLW02-05	Yes	11.340	23.700	103.800	0.730	0.850	1.014	11.46
HLW02-06	Yes	6.167	15.440	110.800	0.398	0.702	0.996	11.54
HLW02-07	Yes	7.795	18.710	54.280	0.502	0.672	0.626	11.18
HLW02-08[(3)]	Yes	153.500	41.200	251.700	3.530	2.680	2.262	10.97
HLW02-09	Yes	23.260	6.140	80.670	0.646	0.582	0.724	10.74
HLW02-10	Yes	40.640	23.210	57.820	0.934	0.832	0.742	10.82
HLW02-11	Yes	99.010	47.040	103.700	2.278	1.688	1.288	10.64
HLW02-12	Yes	50.760	64.600	210.700	3.268	2.318	2.226	11.84
HLW02-13	Yes	54.240	69.930	205.400	3.492	2.508	2.656	11.85
HLW02-14	Yes	1.620	10.670	5.787	0.104	0.382	0.188	10.51
HLW02-15	Yes	55.180	9.717	85.220	1.270	1.046	0.916	9.95
HLW02-16	Yes	11.470	20.810	49.660	0.738	0.746	0.694	11.23
HLW02-17[(4)]	Yes	8.470	20.240	19.400	0.546	0.726	0.340	10.66
HLW02-18	Yes	9.360	5.303	80.290	0.602	0.566	0.722	10.86
HLW02-19	Yes	27.610	5.480	33.770	0.636	0.590	0.514	9.84
HLW02-20	Yes	21.530	5.717	14.670	0.496	0.616	0.306	9.38
HLW02-21	Yes	63.100	10.460	102.800	1.452	1.126	0.924	10.33
HLW02-22	*No*	23.890	17.270	2.257	0.550	0.620	0.076	9.84
HLW02-23	Yes	29.920	18.730	24.990	0.688	0.672	0.602	10.38
HLW02-24	Yes	4.900	4.027	46.970	0.316	0.434	0.520	10.84
HLW02-25	Yes	13.770	3.543	7.317	0.316	0.382	0.144	9.43
HLW02-26	Yes	19.250	8.577	121.700	1.240	0.924	1.094	11.43
HLW02-27	Yes	25.920	15.460	13.330	0.596	0.554	0.420	10.14
HLW02-28	Yes	14.910	5.413	66.330	0.600	0.466	0.596	11.06
HLW02-29	Yes	33.080	10.450	37.970	0.820	0.600	0.568	9.85
HLW02-30	Yes	66.440	41.240	134.100	2.200	1.776	1.610	11.31
HLW02-31	Yes	53.250	12.510	58.850	1.318	1.078	0.530	10.53
HLW02-32	Yes	14.060	15.420	48.390	0.566	0.664	0.608	10.88
HLW02-33	Yes	24.940	8.553	95.340	1.004	0.736	0.856	11.16
HLW02-34	Yes	47.390	17.270	70.940	1.174	0.940	0.878	10.46
HLW02-35	Yes	49.600	23.910	62.290	1.228	1.030	0.916	10.47
HLW02-36	Yes	15.970	7.027	85.590	0.594	0.606	0.770	10.77
HLW02-37	Yes	22.020	5.990	36.900	0.546	0.516	0.444	9.97
HLW02-38	Yes	25.640	13.620	38.030	0.636	0.688	0.570	10.14
HLW02-39	Yes	7.930	6.183	31.910	0.284	0.532	0.388	10.14
HLW02-40	Yes	8.447	6.797	23.200	0.276	0.556	0.322	9.96
HLW02-41	Yes	19.340	7.677	23.620	0.480	0.660	0.354	9.84
HLW02-42[(5)]	Yes	43.600	22.060	54.970	1.080	0.950	0.824	10.33
HLW02-43	Yes	42.650	9.747	77.980	1.056	0.840	0.844	10.42
HLW02-44[(6)]	Yes	22.780	8.683	94.940	0.808	0.748	0.854	10.84
HLW02-45	Yes	15.790	7.353	35.330	0.636	0.634	0.496	10.25
HLW02-46[(7)]	Yes	15.240	10.860	30.170	0.536	0.632	0.452	10.14
HLW02-47	Yes	14.790	6.377	23.700	0.486	0.550	0.338	9.93
HLW02-48	Yes	21.540	13.250	111.400	0.866	0.854	1.002	11.26
HLW02-49	Yes	16.040	15.850	38.640	0.590	0.682	0.578	10.66
HLW02-50	Yes	21.540	7.873	30.430	0.534	0.678	0.418	9.95
HLW02-51	Yes	6.473	12.110	26.770	0.260	0.568	0.400	10.48
HLW02-52[(1)]	Yes	18.140	12.510	51.790	0.588	0.674	0.638	10.57
HLW02-53[(4)]	Yes	5.337	21.730	21.470	0.344	0.780	0.376	10.64
HLW02-54[(2)]	Yes	25.950	6.553	104.400	1.672	0.706	0.938	10.64
HLW02-55[(5)]	Yes	33.480	20.070	47.770	0.830	0.864	0.716	10.35
HLW02-56[(6)]	Yes	21.000	6.720	81.370	0.746	0.578	0.732	10.93
HLW02-57[(3)]	Yes	192.100	50.000	285.500	4.418	3.252	2.566	11.07

[(a)]Superscripted numbers identify pairs of replicates, with (7) being an "inter-matrix" replicate pair.

Table 4.2. PCT Release Data (Leachate Concentration in ppm and Normalized Release in g/l) for the IHLW Augmentation Matrix.

Glass ID[(a)]	Retained for Model Development	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/l)	PCT-Li (g/l)	PCT-Na (g/l)	Leachate pH
HLW03-01	Yes	41.110	20.230	16.780	0.964	0.740	0.576	9.93
HLW03-02	Yes	53.890	10.870	71.470	1.270	0.946	0.862	10.05
HLW03-03	Yes	20.560	17.330	119.600	1.356	1.394	1.500	11.54
HLW03-04	Yes	8.377	26.900	26.600	0.550	0.984	0.804	11.17
HLW03-05	Yes	8.290	4.237	70.160	0.556	0.474	0.656	10.78
HLW03-06[(8)]	Yes	4.590	10.350	4.777	0.302	0.378	0.164	10.43
HLW03-07	Yes	44.710	41.510	181.800	2.892	1.874	2.088	11.48
HLW03-08	Yes	19.320	24.920	162.500	1.286	1.042	1.510	11.75
HLW03-09	Yes	106.600	16.610	161.100	2.506	1.806	1.462	10.16
HLW03-10	Yes	13.550	27.990	112.500	0.886	1.018	1.178	11.57
HLW03-11[(9)]	Yes	21.750	8.963	133.200	1.406	0.970	1.202	10.65
HLW03-12	Yes	12.860	17.790	21.740	0.832	0.762	0.736	10.67
HLW03-13	*No*	0.310	14.390	13.510	0.020	0.592	0.458	10.97
HLW03-14	Yes	23.480	15.670	101.400	1.520	1.348	1.312	11.36
HLW03-15	Yes	23.860	5.630	13.740	0.562	0.622	0.352	9.33
HLW03-16	Yes	10.100	10.510	22.470	0.664	0.788	0.772	10.16
HLW03-17	*No*	17.780	6.370	3.200	0.414	0.696	0.096	9.17
HLW03-18	Yes	53.920	73.430	197.900	3.492	2.670	2.534	11.25
HLW03-19	Yes	43.670	58.220	172.400	2.864	2.128	2.292	11.35
HLW03-20	Yes	59.420	77.210	209.900	3.978	2.880	2.802	11.35
HLW03-21	Yes	8.693	5.370	27.900	0.402	0.466	0.346	10.23
HLW03-22	Yes	12.880	7.650	58.510	0.602	0.668	0.666	10.84
HLW03-23	Yes	30.730	8.475	52.510	0.830	0.734	0.594	10.18
HLW03-24	Yes	15.260	15.550	31.770	0.708	0.674	0.524	10.45
HLW03-25	Yes	72.950	17.090	129.300	1.984	1.492	1.472	10.32
HLW03-26[(10)]	Yes	28.100	18.980	63.470	1.310	0.828	0.818	11.16
HLW03-27	Yes	22.620	15.790	75.600	1.054	0.840	0.860	11.12
HLW03-28	Yes	60.520	29.310	87.180	1.634	1.270	1.120	10.76
HLW03-29	Yes	23.600	21.470	85.440	1.094	0.930	0.966	11.23
HLW03-30	Yes	33.960	16.860	25.230	0.918	0.732	0.490	10.16
HLW03-31	Yes	23.740	14.060	26.310	1.102	0.610	0.416	10.66
HLW03-32	Yes	10.710	15.110	37.190	0.500	0.660	0.550	11.14
HLW03-33	Yes	20.740	10.690	17.830	0.560	0.590	0.346	9.89
HLW03-34	Yes	14.200	8.927	33.490	0.662	0.780	0.472	10.24
HLW03-35	Yes	12.630	7.173	11.680	0.390	0.622	0.226	9.64
HLW03-36	*No*	27.000	8.313	14.200	1.260	0.664	0.240	10.04
HLW03-37	Yes	63.260	42.450	48.840	1.720	1.876	0.954	10.58
HLW03-38	Yes	11.890	7.633	28.270	0.556	0.666	0.396	10.38
HLW03-39	Yes	9.740	14.660	15.140	0.456	0.650	0.296	10.35
HLW03-40	Yes	8.530	13.380	19.040	0.396	0.588	0.370	10.48
HLW03-41	Yes	13.510	9.680	31.340	0.498	0.560	0.464	10.34
HLW03-42[(7)]	Yes	10.630	8.100	22.810	0.374	0.472	0.342	10.14
HLW03-43[(8)]	*No*	20.230	10.430	4.413	1.328	0.382	0.152	10.42
HLW03-44[(9)]	Yes	12.320	8.910	125.600	0.796	0.964	1.134	10.75
HLW03-45[(10)]	Yes	14.530	17.240	60.120	0.678	0.752	0.774	11.34

[(a)] Superscripted numbers identify pairs of replicates, with (7) being an “inter-matrix” replicate pair.

Table 4.3. Temperature and Volume %-Crystallinity Data for IHLW Phase 1 Combined Matrix Glasses.

Glass ID	Temperature in °C												
	650	700	750	800	850[(b)]	875	900[(b)]	950[(b)]	1000[(b)]	1050	1100	1150	1200
HLW02-01	NA[(a)]	NA	3	NA	1.88	NA	NA	0.27, 0.5	NA	NA	NA	NA	NA
HLW02-02	NA	NA	NA	NA	1.1	NA	1.1	0.5	NA	NA	NA	NA	NA
HLW02-03	NA	NA	1.8	NA	0.7	NA	NA	0.2	NA	NA	NA	NA	NA
HLW02-04	NA	NA	23.4	14.2	0.1, 0.7	NA	NA	NA	NA	NA	NA	NA	NA
HLW02-05	NA	NA	0.1	NA	0.1	NA	0.1	0.1	NA	NA	NA	NA	NA
HLW02-06	NA	NA	NA	NA	5.1	NA	3.2	2.8, 2.4	NA	0.8	NA	NA	NA
HLW02-07	NA	NA	1	NA	0.8	NA	0.5	0.4	NA	NA	NA	NA	NA
HLW02-08	NA	NA	1.2	NA	0.6	NA	NA	0.1	NA	NA	NA	NA	NA
HLW02-09	NA	NA	NA	NA	2.9	NA	4.4, 3.5	1.2	0.2	NA	NA	NA	NA
HLW02-10	NA	0.4	0.6	NA	0.1	NA	0.1	0.1	NA	NA	NA	NA	NA
HLW02-11	NA	1.8	1.2	NA	1	NA	NA	0.1	NA	NA	NA	NA	NA
HLW02-12	NA	NA	NA	NA	4.4	NA	3.3	NA	NA	1	NA	NA	NA
HLW02-13	NA	NA	NA	NA	5.6	4.3	0.2	NA	1.0	0.3	NA	NA	NA
HLW02-14	NA	NA	NA	NA	1.7	NA	NA	1.4, 1.1	0.2	NA	NA	NA	NA
HLW02-15	NA	NA	NA	NA	3.7	NA	3.1	2.7	NA	0.9	NA	NA	NA
HLW02-16	NA	NA	NA	NA	4	NA	3.6	3.1, 1.3	0.7	NA	NA	NA	NA
HLW02-17	NA	NA	NA	NA	NA	NA	2.07	0.9, 1.2	0.2	0.4	NA	NA	NA
HLW02-18	NA	NA	2.2	NA	1.8	NA	NA	1	NA	NA	NA	NA	NA
HLW02-19	NA	NA	NA	NA	1.6, 2.4	NA	1.2	0.8, 0.6	NA	NA	NA	NA	NA
HLW02-20	NA	NA	NA	NA	6.4	NA	1.65	0.8, 2.1	NA	NA	NA	NA	NA
HLW02-21	NA	NA	0.2	0.2	NA	NA	0.2	NA	NA	NA	NA	NA	NA
HLW02-22	NA	NA	NA	NA	1.6	NA	0.7	1.5	NA	0.2	NA	NA	NA
HLW02-23	NA	NA	NA	NA	2.4	NA	1.7	1.1, 0.8	NA	NA	NA	NA	NA
HLW02-24	NA	NA	NA	NA	2.3	NA	1.24	0.61	NA	NA	NA	NA	NA
HLW02-25	NA	NA	NA	NA	2	NA	0.5	1.0	NA	NA	NA	NA	NA
HLW02-26	NA	NA	NA	NA	3.9	NA	2.47	0.9, 1.6	0.8	NA	NA	NA	NA
HLW02-27	NA	NA	NA	NA	2.5	NA	1.28	1.5	0.5	0.2	NA	NA	NA
HLW02-28	NA	NA	NA	NA	1.9	NA	1.1	0.9	0.1	NA	NA	NA	NA
HLW02-29	NA	NA	NA	NA	3.5	NA	1.86	0.7,0.6,0.8	NA	0.2	NA	NA	NA
HLW02-30	NA	NA	2.3	NA	1.1	NA	NA	0.8	NA	NA	NA	NA	NA
HLW02-31	NA	1.2	1.3	NA	0.99	NA	NA	0.2	NA	NA	NA	NA	NA
HLW02-32	NA	1.1	NA	1.4	0.27	NA	0.4	0.4	NA	NA	NA	NA	NA
HLW02-33	NA	NA	NA	NA	5.8	NA	2.74	0.14,1.5,1.7	NA	NA	NA	NA	NA
HLW02-34	NA	NA	NA	NA	6.2	NA	2.46	0.11,0.6,1.5	NA	NA	NA	NA	NA
HLW02-35	NA	NA	NA	NA	7.2	NA	NA	1.7,2.3	0.8	NA	NA	NA	NA
HLW02-36	NA	NA	1.9	NA	1.4	NA	0.3, 0.6	0.8	NA	NA	NA	NA	NA
HLW02-37	NA	NA	NA	NA	2.9	NA	2.1	0.8	NA	0.6	NA	NA	NA
HLW02-38	NA	NA	NA	NA	2.7	NA	1.25	1.61, 1.5	NA	0.2	NA	NA	NA

[(a)] NA indicates that no data were collected for specified temperatures.
[(b)] More than one set of data were collected for selected glasses at these temperatures. All data were used in regression.

Table 4.3. Temperature and Volume %-Crystallinity Data for IHLW Phase 1 Combined Matrix Glasses (continued).

Glass ID	Temperature in °C												
	650	700	750	800	850[b]	875	900[b]	950[b]	1000[b]	1050	1100	1150	1200
HLW02-39	NA[a]	NA	NA	NA	2.5	NA	1.79	1.95, 1.6	NA	0.2	NA	NA	NA
HLW02-40	NA	NA	4	NA	1.95	NA	NA	1.6	0.4	NA	NA	NA	NA
HLW02-41	NA	NA	NA	NA	2.4	NA	1.04	0.6, 0.6	NA	0.1	NA	NA	NA
HLW02-42	NA	2.1	1.1	NA	0.66	NA	0.3	0.5	NA	NA	NA	NA	NA
HLW02-43	NA	NA	NA	NA	2.6	NA	0.58	0.31, 0.9	NA	NA	NA	NA	NA
HLW02-44	NA	NA	1.3	1.1	0.8	NA	0.57	NA	NA	NA	NA	NA	NA
HLW02-45	NA	NA	NA	NA	2.4	NA	0.95	0.8	NA	NA	NA	NA	NA
HLW02-46	NA	NA	NA	NA	2.9	NA	1.6	1.07, 0.9	NA	0.2	NA	NA	NA
HLW02-47	4.5	4.9	NA	2.4	0.8	NA	NA	NA	NA	NA	NA	NA	NA
HLW02-48	NA	NA	2.7	NA	1.5	NA	NA	1.4	0.7	NA	NA	NA	NA
HLW02-49	NA	NA	NA	NA	3.68	NA	1.73	2.1,0.9,2.4	NA	0.8	NA	NA	NA
HLW02-50	NA	NA	NA	NA	5.3	NA	1.96	1.52, 0.8	NA	0.9	NA	NA	NA
HLW02-51	NA	NA	NA	NA	2	1.2	0.8	0.8	NA	NA	NA	NA	NA
HLW02-52	NA	NA	2.5	NA	1.3	NA	2.1	1.2	NA	0.4	NA	NA	NA
HLW02-53	NA	NA	NA	NA	2.1	NA	1.4, 1.4	1.0, 0.8	0.4, 0.9	NA	NA	NA	NA
HLW02-54	NA	NA	NA	NA	2.6	NA	1.1	0.1	NA	NA	NA	NA	NA
HLW02-55	NA	1.9	1.1	NA	1.4	NA	NA	0.2	NA	NA	NA	NA	NA
HLW02-56	NA	1.4	0.9	NA	1	NA	0.4	0.5	NA	NA	NA	NA	NA
HLW02-57	NA	1.3	0.9	NA	0.3	NA	NA	NA	NA	NA	NA	NA	NA
HLW03-01	NA	NA	13	NA	10	NA	NA	1.4	NA	2.2	1.1	0.7	NA
HLW03-02	NA	NA	NA	NA	7.3	NA	NA	4.6, 2.9	NA	2	3.3	3.3	4
HLW03-03	NA	NA	NA	NA	NA	NA	NA	2.6, 2.8	NA	2.5	NA	2	0.05
HLW03-04	NA	NA	NA	8.3	2.4, 2.8	NA	NA	0.6	NA	0.4	NA	NA	NA
HLW03-05	NA	NA	NA	NA	2.1	NA	1.2	0.5	NA	NA	NA	NA	NA
HLW03-06	NA	NA	NA	NA	NA	NA	2.0, 1.9	1.0, 0.9	0.9	NA	NA	NA	NA
HLW03-07	NA	NA	9.9	NA	6.2	NA	NA	6	NA	4.2	NA	2.9	1
HLW03-08	NA	NA	NA	NA	NA	NA	NA	12.2	NA	6.6	7.3	9.8	4.2
HLW03-09	0.2	NA	0.1	NA	0.2	NA	NA	0.1	NA	NA	NA	NA	NA
HLW03-10	NA	NA	10.3	NA	12.5	NA	NA	8.7	NA	3.7	2.9	3.5	1.4
HLW03-11	0.4	NA	0.4	NA	0.3	NA	NA	0.2	NA	NA	NA	NA	NA
HLW03-12	NA	NA	1.2	NA	0.7	NA	0.8	0.6	NA	NA	NA	NA	NA
HLW03-13	NA	NA	NA	NA	7.9	NA	NA	5.3	NA	5	NA	3.5	0.6
HLW03-14	NA	NA	NA	NA	4.6	NA	NA	3.5, 2.9	1.5	2.2	0.5	NA	NA
HLW03-15	NA	NA	NA	NA	NA	NA	NA	2.7	NA	0.9	0.3	NA	NA
HLW03-16	NA	NA	4.6	NA	2.8, 2.8	NA	NA	1.9	NA	0.9	NA	NA	NA
HLW03-17	NA	NA	NA	NA	5.7	NA	NA	2.4, 1.7	NA	0.5	NA	NA	NA
HLW03-18	NA	NA	NA	NA	2.4	NA	NA	0.5, 0.7	NA	0.5	NA	NA	NA
HLW03-19	NA	NA	NA	NA	1.5	NA	NA	0.8	NA	0.6	NA	NA	NA

[a] NA indicates that no data were collected for specified temperatures.
[b] More than one set of data were collected for selected glasses at these temperatures. All data were used in regression.

Table 4.3. Temperature and Volume %-Crystallinity Data for IHLW Phase 1 Combined Matrix Glasses (continued).

Glass ID	Temperature in °C												
	650	700	750	800	850[b]	875	900[b]	950[b]	1000[b]	1050	1100	1150	1200
HLW03-20	NA[a]	NA	NA	NA	1	NA	1	0.3	NA	NA	NA	NA	NA
HLW03-21	NA	NA	NA	2	1	NA	0.3	0.2	NA	NA	NA	NA	NA
HLW03-22	NA	NA	4.4	NA	2.3	NA	0.6	0.5	NA	NA	NA	NA	NA
HLW03-23	NA	NA	1.5	1.3	0.9, 0.6	NA	NA	0.4	NA	NA	NA	NA	NA
HLW03-24	NA	NA	2.3	1.6	0,6, 0.4	NA	NA	NA	NA	NA	NA	NA	NA
HLW03-25	NA	NA	1.6	0.2	0.2	NA	NA	0.1	NA	NA	NA	NA	NA
HLW03-26	NA	NA	1.2	1	0.8	NA	0.4	0.3	NA	NA	NA	NA	NA
HLW03-27	NA	NA	NA	NA	1.7	NA	NA	1.6	NA	0.6	NA	NA	NA
HLW03-28	NA	NA	1.4	1.3	1.0, 0.5	NA	NA	0.2	NA	NA	NA	NA	NA
HLW03-29	NA	NA	1.4	1.7	0.7	NA	NA	0.4	NA	NA	NA	NA	NA
HLW03-30	NA	NA	1	0.9	0.6	NA	NA	0.2	NA	NA	NA	NA	NA
HLW03-31	NA	NA	2.6	NA	2.4	NA	NA	1.6	1.8	0.7	NA	0.9	NA
HLW03-32	NA	NA	5	NA	4.6	NA	3.6	1.6	NA	2	1.5	NA	NA
HLW03-33	NA	NA	5.5	NA	2.7	NA	NA	3.9	NA	1.8	NA	1.1	NA
HLW03-34	NA	NA	NA	3	1.7	NA	NA	1	NA	0.3	NA	NA	NA
HLW03-35	NA	NA	NA	NA	NA	NA	NA	6.2	NA	3	2.4	0.4	NA
HLW03-36	NA	NA	NA	NA	10	NA	NA	6.1	NA	3.4	NA	3.5	0.1
HLW03-37	NA	NA	NA	NA	1.9	NA	0.9	0.3	NA	NA	NA	NA	NA
HLW03-38	NA	NA	6.5	NA	3.8	NA	NA	2.5	NA	1.4	2	NA	NA
HLW03-39	NA	NA	2.8	NA	1.8	NA	NA	0.4	NA	NA	NA	NA	NA
HLW03-40	NA	NA	5.6	NA	2.5	NA	NA	1.3	NA	0.4	NA	NA	NA
HLW03-41	NA	NA	NA	1.5	0.8	NA	NA	0.4	NA	NA	NA	NA	NA
HLW03-42	NA	NA	NA	NA	3	NA	NA	1.2, 1.1	NA	0.3	NA	NA	NA
HLW03-43	NA	NA	NA	NA	1.8	NA	1.6	0.6	0.9	NA	NA	NA	NA
HLW03-44	0.3	NA	NA	NA	0.1	NA	NA	0.1	NA	NA	NA	NA	NA
HLW03-45	NA	NA	NA	1.3	1.3	NA	0.3	NA	NA	NA	NA	NA	NA

[a] NA indicates that no data were collected for specified temperatures.
[b] More than one set of data were collected for selected glasses at these temperatures. All data were used in regression.

Table 4.4. Estimated One-Percent Crystal Fraction Temperature ($T_{1\%}$) and Observed Crystal Phases for the IHLW Combined Matrix Glasses.

Glass ID	$T_{1\%}$ (°C)	Crystals
HLW02-01	905.81	Spinel
HLW02-02	887.50	Spinel
HLW02-03	838.06	Spinel
HLW02-04	848.84	Spinel
HLW02-05	NA[(a)]	Noble metal
HLW02-06	1026.68	Spinel
HLW02-07	764.29	Spinel
HLW02-08	783.52	Spinel
HLW02-09	957.93	Spinel
HLW02-10	554.25	Spinel
HLW02-11	816.30	Spinel
HLW02-12	1046.95	Spinel
HLW02-13	967.86	Spinel
HLW02-14	945.83	$ZrSiO_4$+ Spinel
HLW02-15	1049.43	Spinel
HLW02-16	982.77	Spinel+ZrO_2
HLW02-17	966.86	Spinel
HLW02-18	957.14	Spinel
HLW02-19	920.31	Spinel
HLW02-20	941.39	Spinel
HLW02-21	NA	Spinel
HLW02-22	937.50	Spinel
HLW02-23	945.83	Spinel
HLW02-24	922.20	Spinel
HLW02-25	907.14	Spinel
HLW02-26	969.52	Spinel
HLW02-27	966.09	Spinel+$ZrSiO_4$
HLW02-28	925.00	Spinel
HLW02-29	954.99	Spinel
HLW02-30	897.62	Spinel
HLW02-31	796.75	Spinel
HLW02-32	800.72	Spinel
HLW02-33	947.44	Spinel
HLW02-34	940.84	Spinel
HLW02-35	980.48	Spinel
HLW02-36	870.00	Spinel
HLW02-37	980.24	Spinel
HLW02-38	973.96	Spinel
HLW02-39	989.64	Spinel
HLW02-40	957.74	Spinel
HLW02-41	936.04	Spinel
HLW02-42	821.16	Spinel
HLW02-43	916.31	Spinel
HLW02-44	813.52	Spinel
HLW02-45	919.64	Spinel
HLW02-46	963.27	Spinel
HLW02-47	847.01	Spinel
HLW02-48	960.16	Spinel
HLW02-49	987.31	Spinel
HLW02-50	974.59	Spinel
HLW02-51	906.25	Spinel
HLW02-52	959.26	Spinel
HLW02-53	949.28	Spinel
HLW02-54	910.53	Spinel
HLW02-55	832.35	Spinel
HLW02-56	794.17	Spinel
HLW02-57	741.45	Spinel
HLW03-01	1073.77	Spinel
HLW03-02	1156.98	Spinel +ZrO_2
HLW03-03	1144.65	Spinel
HLW03-04	946.39	Spinel
HLW03-05	916.58	Spinel
HLW03-06	962.54	Spinel
HLW03-07	1213.18	Spinel
HLW03-08	1247.81	ZrO2
HLW03-09	NA	Noble Metal
HLW03-10	1189.72	Spinel+ZrO_2 (ThO_2)
HLW03-11	NA	ThO_2+ Noble metal
HLW03-12	810.84	Spinel
HLW03-13	1214.74	Spinel + ThO_2 (UO_2)
HLW03-14	1069.21	Spinel+ZrO_2
HLW03-15	1051.60	Spinel + ThO_2
HLW03-16	1020.83	Spinel
HLW03-17	1005.09	Spinel
HLW03-18	951.86	Spinel
HLW03-19	943.28	Spinel
HLW03-20	875.00	Spinel
HLW03-21	865.78	Spinel
HLW03-22	905.75	Spinel
HLW03-23	830.99	Spinel
HLW03-24	824.50	Spinel
HLW03-25	796.45	Spinel
HLW03-26	797.30	Spinel + ThO_2
HLW03-27	994.59	Spinel + ThO_2
HLW03-28	824.16	Spinel
HLW03-29	843.58	Spinel
HLW03-30	760.97	Spinel
HLW03-31	1071.95	Spinel+ZrO_2
HLW03-32	1087.32	Spinel+ZrO_2
HLW03-33	1109.02	$ZrSiO_4$+ThO_2+Spinel
HLW03-34	958.35	ThO2+Spinel
HLW03-35	1132.78	$ZrSiO_4$+ThO_2+ZrO_2
HLW03-36	1174.25	$ZrSiO_4$ (ThO2)+Spinel
HLW03-37	902.04	Spinel
HLW03-38	1087.13	Spinel+ZrO_2
HLW03-39	905.05	Spinel
HLW03-40	978.83	Spinel+ThO_2
HLW03-41	853.76	Spinel
HLW03-42	977.69	Spinel
HLW03-43	946.51	Spinel
HLW03-44	NA	Noble Metal
HLW03-45	847.50	Spinel +ThO_2

[(a)] NA=Not Available ($T_{1\%}$ could not be estimated for 5 glasses).

Table 5.1. Compositions of IHLW Phase 1 Combined Matrix Glasses, 19 Normalized[(a)] Components Wt%.

Glass ID	Layer[(b)]	Retained for PCT Model Development	Retained for $T_{1\%}$ Model Development	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
HLW02-01	1a.Center	Yes	Yes	6.310	10.150	0.788	0.110	11.143	4.085	2.438	11.203	0.530	0.112	0.112	44.592	2.499	0.000	0.105	0.000	2.045	3.041	0.735
HLW02-02	1a.Outer	Yes	Yes	4.089	14.310	1.533	0.204	14.310	6.133	0.000	4.089	0.102	0.204	0.020	51.578	0.000	0.000	0.019	0.000	2.044	0.000	1.363
HLW02-03	1a.Outer	Yes	Yes	4.089	14.312	1.533	0.204	8.178	2.045	0.000	15.334	1.022	0.020	0.204	38.847	4.478	0.000	0.190	0.000	2.045	6.134	1.363
HLW02-04	1a.Outer	Yes	Yes	4.090	5.113	1.534	0.020	14.317	2.045	0.530	15.339	0.102	0.205	0.205	54.129	0.000	0.000	0.190	0.000	2.045	0.000	0.136
HLW02-05	1a.Outer	Yes	No	4.090	5.112	0.051	0.020	8.180	6.135	0.000	14.098	0.102	0.020	0.020	53.836	0.000	0.000	0.019	0.000	2.045	6.135	0.136
HLW02-06	1a.Outer	Yes	Yes	8.692	5.113	1.534	0.020	8.181	4.846	5.113	15.339	1.023	0.020	0.205	41.407	0.000	0.000	0.190	0.000	2.045	6.136	0.136
HLW02-07	1a.Outer	Yes	Yes	8.689	5.111	0.051	0.204	8.178	6.134	0.000	11.966	0.102	0.204	0.020	54.182	0.000	0.000	0.190	0.000	2.045	1.559	1.363
HLW02-08	1a.Outer	Yes	Yes	4.090	14.315	0.051	0.020	9.412	3.384	5.112	15.337	0.102	0.204	0.020	39.616	0.000	0.000	0.019	0.000	2.045	6.135	0.136
HLW02-09	1a.Outer	Yes	Yes	8.691	11.849	0.051	0.020	14.315	2.322	0.000	15.337	1.022	0.204	0.020	38.854	5.112	0.000	0.019	0.000	2.045	0.000	0.136
HLW02-10	1a.Outer	Yes	No	8.691	14.315	1.534	0.020	8.180	6.135	0.000	10.749	0.102	0.020	0.204	38.854	2.860	0.000	0.019	0.000	2.045	6.135	0.136
HLW02-11	1a.Outer	Yes	Yes	4.090	14.316	0.051	0.020	8.181	6.136	0.000	11.102	1.023	0.205	0.205	46.164	0.000	0.000	0.190	0.000	2.045	6.136	0.136
HLW02-12	1a.Outer	Yes	Yes	4.089	5.111	1.533	0.204	11.638	6.133	5.111	13.044	1.022	0.020	0.204	42.331	0.000	0.000	0.019	0.000	2.044	6.133	1.363
HLW02-13	1a.Outer	Yes	Yes	4.089	5.111	0.051	0.204	14.312	6.134	5.111	10.659	0.102	0.020	0.204	44.082	5.111	0.000	0.190	0.000	2.045	1.208	1.363
HLW02-14	1a.Outer	Yes	No	4.090	5.113	1.534	0.020	8.181	6.136	2.546	4.234	0.102	0.205	0.020	54.198	5.113	0.000	0.190	0.000	2.045	6.136	0.136
HLW02-15	1a.Outer	Yes	Yes	8.689	14.312	0.051	0.204	14.312	2.045	4.794	12.821	0.102	0.020	0.204	38.847	0.000	0.000	0.190	0.000	2.045	0.000	1.363
HLW02-16	1a.Outer	Yes	Yes	8.688	5.111	1.533	0.204	8.177	6.133	5.111	9.868	0.102	0.204	0.204	39.993	5.111	0.000	0.019	0.000	2.044	6.133	1.363
HLW02-17	1a.Outer	Yes	Yes	8.691	5.112	1.534	0.020	14.154	6.135	0.000	7.863	0.102	0.020	0.020	54.148	0.000	0.000	0.019	0.000	2.045	0.000	0.136
HLW02-18	1a.Outer	Yes	Yes	4.089	5.111	0.051	0.204	11.377	2.059	0.000	15.332	1.022	0.204	0.020	50.972	0.000	0.000	0.019	0.000	2.044	6.133	1.363
HLW02-19	1a.Outer	Yes	Yes	4.090	14.315	1.534	0.020	11.023	2.045	5.112	9.048	0.102	0.204	0.204	38.854	5.112	0.000	0.019	0.000	2.045	6.135	0.136
HLW02-20	1a.Outer	Yes	Yes	4.090	14.315	0.051	0.020	14.315	2.045	0.000	6.598	0.102	0.020	0.020	52.897	3.326	0.000	0.019	0.000	2.045	0.000	0.136
HLW02-21	1a.Outer	Yes	No	8.691	14.315	0.051	0.020	8.180	2.045	0.000	15.337	0.102	0.020	0.020	47.484	0.000	0.000	0.019	0.000	2.045	1.534	0.136
HLW02-22	1a.Outer	No	Yes	8.691	14.315	0.051	0.020	9.714	6.135	0.000	4.090	0.102	0.204	0.204	54.191	0.082	0.000	0.019	0.000	2.045	0.000	0.136
HLW02-23	1a.Outer	Yes	Yes	8.692	14.317	1.534	0.020	8.181	6.136	5.113	5.716	1.023	0.020	0.020	40.209	5.113	0.000	0.190	0.000	2.045	1.534	0.136
HLW02-24	1a.Outer	Yes	Yes	8.689	5.111	0.051	0.156	8.178	2.044	5.111	12.469	0.102	0.020	0.204	48.108	5.111	0.000	0.019	0.000	2.044	1.533	1.046
HLW02-25	1a.Outer	Yes	Yes	8.692	14.317	1.534	0.020	9.715	2.045	0.363	7.039	0.102	0.205	0.020	48.464	5.113	0.000	0.190	0.000	2.045	0.000	0.136
HLW02-26	1a.Outer	Yes	Yes	4.089	5.111	1.533	0.204	12.779	2.045	5.071	15.334	0.102	0.020	0.020	38.847	5.111	0.000	0.190	0.000	2.045	6.134	1.363
HLW02-27	1a.Outer	Yes	Yes	4.090	14.317	0.051	0.020	12.783	6.136	3.441	4.371	0.102	0.020	0.205	40.844	5.113	0.000	0.190	0.000	2.045	6.136	0.136
HLW02-28	1a.Inner	Yes	Yes	7.669	8.180	1.023	0.041	10.686	2.556	1.534	15.338	0.307	0.051	0.051	41.924	3.579	0.000	0.143	0.000	2.045	4.601	0.272
HLW02-29	1a.Inner	Yes	Yes	7.667	13.290	0.511	0.136	10.223	3.834	1.533	9.201	0.307	0.051	0.153	41.914	3.578	0.000	0.048	0.000	2.045	4.600	0.909
HLW02-30	1a.Inner	Yes	Yes	5.624	9.940	1.022	0.041	10.225	5.112	3.579	11.481	0.307	0.153	0.051	41.921	3.579	0.000	0.048	0.000	2.045	4.601	0.272
HLW02-31	1a.Inner	Yes	Yes	5.624	13.293	0.511	0.041	10.225	2.556	1.534	15.319	0.307	0.051	0.153	41.924	1.534	0.000	0.143	0.000	2.045	4.467	0.272
HLW02-32	1a.Inner	Yes	Yes	7.668	8.180	1.022	0.041	10.225	5.112	1.534	10.974	0.307	0.153	0.153	47.154	3.579	0.000	0.048	0.000	2.045	1.534	0.272
HLW02-33	1a.Inner	Yes	Yes	6.483	8.180	0.511	0.041	12.270	2.556	3.579	15.337	0.818	0.153	0.153	41.921	3.579	0.000	0.048	0.000	2.045	2.054	0.272
HLW02-34	1a.Inner	Yes	Yes	5.623	13.290	1.022	0.136	12.268	4.045	1.533	11.136	0.818	0.051	0.051	41.914	3.578	0.000	0.048	0.000	2.045	1.533	0.909
HLW02-35	1a.Inner	Yes	Yes	6.634	13.291	0.511	0.136	12.268	5.112	3.578	9.366	0.818	0.153	0.051	41.917	1.534	0.000	0.143	0.000	2.045	1.534	0.909

(a) Normalized to sum to 100% over the 19 components listed in this table.
(b) Indicates the design layer containing each of the compositions (see Section 5.1.1). In the case of replicate glasses, this column lists the layer for one glass composition from each replicate pair, and lists the Glass ID of the glass for which the other composition from the replicate pair is a replicate.

Table 5.1. Compositions of IHLW Phase 1 Combined Matrix Glasses, 19 Normalized[(a)] Components Wt% (continued).

Glass ID	Layer[(b)]	Retained for PCT Model Development	Retained for $T_{1\%}$ Model Development	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
HLW02-36	1a.Inner	Yes	Yes	5.623	8.862	1.022	0.136	12.267	2.556	1.533	15.334	0.307	0.051	0.153	46.087	1.533	0.000	0.048	0.000	2.045	1.533	0.909
HLW02-37	1a.Inner	Yes	Yes	6.914	13.292	0.511	0.041	10.225	2.556	3.579	11.439	0.818	0.153	0.051	41.921	1.534	0.000	0.048	0.000	2.045	4.601	0.272
HLW02-38	1a.Inner	Yes	Yes	7.048	13.290	1.022	0.136	12.268	4.351	1.533	9.201	0.818	0.153	0.153	41.914	3.578	0.000	0.048	0.000	2.045	1.533	0.909
HLW02-39	1a.Inner	Yes	Yes	7.668	9.194	1.022	0.041	10.225	2.556	1.534	11.307	0.818	0.051	0.051	50.100	1.534	0.000	0.048	0.000	2.045	1.534	0.272
HLW02-40	1a.Inner	Yes	Yes	7.668	10.054	1.022	0.136	10.224	2.691	1.534	9.901	0.307	0.153	0.051	50.096	1.534	0.000	0.143	0.000	2.045	1.534	0.909
HLW02-41	1a.Inner	Yes	Yes	6.647	13.293	0.511	0.041	10.225	2.556	1.534	9.203	0.307	0.051	0.051	50.053	1.534	0.000	0.143	0.000	2.045	1.534	0.272
HLW02-42	1a.Inner	Yes	Yes	5.624	13.293	0.511	0.041	10.225	5.113	1.534	9.203	0.307	0.051	0.051	45.452	3.579	0.000	0.143	0.000	2.045	2.556	0.272
HLW02-43	1a.Inner	Yes	Yes	6.646	13.292	1.022	0.041	10.225	2.556	3.579	12.730	0.307	0.153	0.051	41.921	3.579	0.000	0.048	0.000	2.045	1.534	0.272
HLW02-44	1a.Inner	Yes	Yes	5.623	9.273	1.022	0.136	10.223	2.556	3.578	15.334	0.307	0.153	0.051	44.654	1.533	0.000	0.048	0.000	2.045	2.556	0.909
HLW02-45	1a.Inner	Yes	Yes	5.624	8.180	1.022	0.041	11.247	2.556	3.579	9.835	0.307	0.051	0.153	49.928	3.579	0.000	0.048	0.000	2.045	1.534	0.272
HLW02-46	1a.Inner	Yes	Yes	5.624	9.355	0.511	0.041	10.225	3.784	3.579	9.203	0.818	0.051	0.153	50.105	1.534	0.000	0.143	0.000	2.045	2.556	0.272
HLW02-47	1a.Inner	Yes	No	5.623	10.026	0.511	0.136	10.224	2.556	3.578	9.655	0.307	0.051	0.051	50.096	1.534	0.000	0.143	0.000	2.045	2.556	0.909
HLW02-48	1a.Inner	Yes	Yes	6.134	8.179	0.511	0.136	12.268	3.415	1.534	15.335	0.818	0.153	0.153	41.917	1.749	0.000	0.143	0.000	2.045	4.601	0.909
HLW02-49	1a.Inner	Yes	Yes	7.669	8.937	0.511	0.041	12.270	5.113	3.579	9.203	0.307	0.051	0.051	45.207	1.534	0.000	0.143	0.000	2.045	3.068	0.272
HLW02-50	1a.Inner	Yes	Yes	6.135	13.293	0.511	0.041	12.271	2.556	1.534	10.041	0.307	0.153	0.051	44.511	1.534	0.000	0.143	0.000	2.045	4.601	0.272
HLW02-51	1a.Inner	Yes	Yes	7.669	8.180	0.511	0.041	10.737	4.692	1.534	9.203	0.307	0.153	0.153	46.180	3.579	0.000	0.143	0.000	2.045	4.601	0.272
HLW02-52	RepHLW02-01	Yes	Yes	6.310	10.150	0.788	0.110	11.143	4.085	2.438	11.203	0.530	0.112	0.112	44.592	2.499	0.000	0.105	0.000	2.045	3.041	0.735
HLW02-53	RepHLW02-17	Yes	Yes	8.691	5.112	1.534	0.020	14.154	6.135	0.000	7.863	0.102	0.020	0.020	54.148	0.000	0.000	0.019	0.000	2.045	0.000	0.136
HLW02-54	RepHLW02-4	Yes	Yes	4.090	5.113	1.534	0.020	14.317	2.045	0.530	15.339	0.102	0.205	0.205	54.129	0.000	0.000	0.190	0.000	2.045	0.000	0.136
HLW02-55	RepHLW02-42	Yes	Yes	5.624	13.293	0.511	0.041	10.225	5.113	1.534	9.203	0.307	0.051	0.051	45.452	3.579	0.000	0.143	0.000	2.045	2.556	0.272
HLW02-56	RepHLW02-44	Yes	Yes	5.623	9.273	1.022	0.136	10.223	2.556	3.578	15.334	0.307	0.153	0.051	44.654	1.533	0.000	0.048	0.000	2.045	2.556	0.909
HLW02-57	RepHLW02-8	Yes	Yes	4.090	14.315	0.051	0.020	9.412	3.384	5.112	15.337	0.102	0.204	0.020	39.616	0.000	0.000	0.019	0.000	2.045	6.135	0.136
HLW03-01	1b.Outer	Yes	No	8.522	14.036	0.051	0.020	14.036	6.015	6.214	4.010	0.100	0.020	0.204	36.092	0.000	2.826	0.314	0.000	3.128	3.050	1.362
HLW03-02	1b.Outer	Yes	Yes	1.995	13.969	1.636	0.499	13.969	2.528	6.985	11.429	0.998	0.307	0.020	35.922	0.000	0.000	0.314	0.000	0.000	9.292	0.136
HLW03-03	1b.Outer	Yes	Yes	1.997	4.994	1.636	0.499	13.985	2.738	6.992	10.997	0.999	0.020	0.205	35.960	9.989	0.000	0.314	0.000	1.990	6.548	0.136
HLW03-04	1b.Outer	Yes	Yes	1.998	4.995	0.051	0.499	13.986	5.993	3.232	4.542	0.100	0.020	0.204	43.374	9.990	0.000	0.313	6.349	0.000	2.997	1.358
HLW03-05	1b.Outer	Yes	Yes	8.359	4.917	1.636	0.492	1.967	1.967	6.884	14.751	0.098	0.307	0.204	48.912	0.000	3.897	0.314	0.000	3.933	0.000	1.362
HLW03-06	1b.Outer	Yes	Yes	8.532	5.018	1.636	0.502	2.007	6.022	7.027	4.015	1.004	0.020	0.020	53.200	5.205	1.448	0.019	0.000	0.000	4.187	0.136
HLW03-07	1b.Outer	Yes	Yes	5.072	5.072	0.051	0.507	14.202	4.856	7.101	11.955	0.102	0.020	0.204	40.717	0.000	0.000	0.019	6.447	3.538	0.000	0.136
HLW03-08	1b.Outer	Yes	No	8.211	4.941	1.635	0.494	1.977	5.266	6.918	14.825	0.099	0.307	0.020	35.579	0.000	4.511	0.019	0.000	3.953	9.883	1.362
HLW03-09	1b.Outer	Yes	No	7.840	14.003	0.051	0.020	3.564	2.024	0.000	15.182	0.101	0.307	0.205	53.644	0.000	2.609	0.314	0.000	0.000	0.000	0.136
HLW03-10	1b.Outer	Yes	No	8.557	5.034	0.051	0.020	10.206	6.040	7.048	13.140	1.007	0.020	0.020	36.245	0.000	2.685	0.019	1.133	0.000	7.413	1.361
HLW03-11	1b.Outer	Yes	No	2.028	5.073	0.051	0.020	9.752	2.028	0.000	15.217	0.102	0.020	0.204	53.763	0.000	5.140	0.019	6.447	0.000	0.000	0.136
HLW03-12	1b.Outer	Yes	Yes	2.026	5.066	0.051	0.506	2.026	5.120	7.094	4.054	0.101	0.306	0.020	45.268	10.134	3.812	0.019	6.440	4.054	3.764	0.136
HLW03-13	1b.Outer	No	Yes	8.622	5.073	0.051	0.507	8.827	5.325	7.101	4.058	1.015	0.020	0.204	36.518	10.144	3.922	0.019	6.447	1.146	0.865	0.136

(a) Normalized to sum to 100% over the 19 components listed in this table.
(b) Indicates the design layer containing each of the compositions (see Section 5.1.1). In the case of replicate glasses, this column lists the layer for one glass composition from each replicate pair, and lists the Glass ID of the glass for which the other composition from the replicate pair is a replicate.

Table 5.1. Compositions of IHLW Phase 1 Combined Matrix Glasses, 19 Normalized[(a)] Components Wt% (continued).

Glass ID	Layer[(b)]	Retained for PCT Model Development	Retained for $T_{1\%}$ Model Development	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
HLW03-14	1b.Outer	Yes	Yes	2.034	5.085	0.051	0.020	9.250	2.560	7.119	10.660	1.017	0.020	0.020	36.610	10.170	4.207	0.314	0.000	4.068	6.658	0.136
HLW03-15	1b.Outer	Yes	Yes	1.995	13.969	1.636	0.020	13.969	1.995	1.379	5.366	0.100	0.307	0.020	52.885	0.000	2.495	0.314	0.000	3.412	0.000	0.136
HLW03-16	1b.Outer	Yes	Yes	1.998	4.995	0.051	0.020	8.082	2.926	6.993	3.997	0.999	0.306	0.204	45.230	9.991	2.626	0.019	6.349	2.834	1.024	1.357
HLW03-17	1b.Outer	No	Yes	8.540	14.066	0.051	0.020	2.009	2.009	7.033	4.561	0.300	0.020	0.020	47.121	0.000	2.288	0.019	4.891	4.018	1.676	1.358
HLW03-18	1b.Outer	Yes	Yes	2.034	5.085	0.051	0.508	14.237	6.056	0.000	10.770	1.002	0.020	0.020	53.664	0.000	6.102	0.314	0.000	0.000	0.000	0.136
HLW03-19	1b.Outer	Yes	Yes	2.007	5.018	1.636	0.502	9.851	6.022	0.201	10.370	1.004	0.020	0.020	53.200	0.000	5.977	0.019	0.000	4.015	0.000	0.136
HLW03-20	1b.Outer	Yes	Yes	1.967	4.916	1.635	0.019	13.764	5.899	0.000	10.324	0.983	0.307	0.204	51.820	0.148	5.899	0.314	0.440	0.000	0.000	1.362
HLW03-21	1b.Inner	Yes	Yes	5.069	7.097	0.306	0.081	5.069	2.535	4.562	11.071	0.304	0.051	0.051	49.678	1.521	3.041	0.047	2.147	1.014	6.083	0.272
HLW03-22	1b.Inner	Yes	Yes	5.025	7.035	0.306	0.081	9.970	2.513	1.507	12.061	0.302	0.051	0.153	41.208	4.523	3.015	0.047	4.259	1.005	6.031	0.909
HLW03-23	1b.Inner	Yes	Yes	5.068	12.164	0.102	0.203	7.906	2.534	1.521	12.164	0.304	0.051	0.153	41.559	1.521	3.041	0.047	4.295	1.014	6.082	0.272
HLW03-24	1b.Inner	Yes	Yes	3.041	7.097	0.306	0.081	5.070	5.070	4.562	8.334	0.507	0.051	0.051	49.679	1.521	3.041	0.047	2.147	3.041	6.083	0.272
HLW03-25	1b.Inner	Yes	Yes	3.023	12.088	0.102	0.081	5.037	2.518	1.511	12.088	0.503	0.051	0.153	43.034	4.533	3.023	0.142	2.134	3.023	6.044	0.910
HLW03-26	1b.Inner	Yes	Yes	5.031	7.043	0.102	0.201	5.031	5.031	1.509	10.665	0.503	0.153	0.153	41.250	4.527	4.527	0.047	4.263	3.019	6.036	0.909
HLW03-27	1b.Inner	Yes	Yes	5.037	7.052	0.102	0.201	9.569	4.130	1.511	12.087	0.503	0.153	0.153	41.299	1.511	4.533	0.047	2.134	3.022	6.044	0.910
HLW03-28	1b.Inner	Yes	Yes	3.710	12.178	0.102	0.082	10.149	5.074	1.523	10.722	0.508	0.153	0.051	41.608	1.523	3.044	0.047	2.150	1.015	6.089	0.272
HLW03-29	1b.Inner	Yes	Yes	3.038	7.088	0.306	0.203	5.063	5.063	3.597	12.151	0.304	0.051	0.051	41.516	1.519	4.556	0.047	4.290	3.038	7.846	0.272
HLW03-30	1b.Inner	Yes	Yes	3.038	12.154	0.102	0.081	5.065	5.065	4.558	7.090	0.304	0.153	0.153	44.173	1.520	4.558	0.142	2.145	1.013	8.413	0.272
HLW03-31	1b.Inner	Yes	No	5.065	7.090	0.102	0.202	5.065	5.065	4.558	8.725	0.507	0.153	0.153	46.070	1.520	3.038	0.142	2.145	1.013	9.115	0.272
HLW03-32	1b.Inner	Yes	No	5.031	7.044	0.102	0.081	5.031	5.031	2.990	9.305	0.503	0.153	0.051	41.252	1.509	4.527	0.142	4.263	3.019	9.056	0.909
HLW03-33	1b.Inner	Yes	No	5.071	12.169	0.102	0.203	10.142	3.985	1.522	7.099	0.461	0.153	0.051	41.579	1.522	3.042	0.047	3.454	3.042	6.085	0.272
HLW03-34	1b.Inner	Yes	No	3.023	7.052	0.102	0.201	10.074	2.518	1.511	9.755	0.503	0.051	0.153	49.362	1.511	3.945	0.142	2.134	1.008	6.044	0.910
HLW03-35	1b.Inner	Yes	No	5.075	10.631	0.102	0.082	5.075	2.537	4.567	7.104	0.508	0.051	0.051	49.731	1.523	3.248	0.142	2.151	1.062	6.090	0.272
HLW03-36	1b.Inner	No	No	5.031	7.044	0.306	0.201	9.721	2.753	1.509	8.139	0.503	0.153	0.051	49.308	1.509	3.638	0.047	2.132	1.006	6.038	0.910
HLW03-37	1b.Inner	Yes	Yes	3.019	12.074	0.102	0.081	7.384	4.968	1.509	7.044	0.503	0.051	0.153	41.253	1.509	4.527	0.142	4.263	3.019	7.489	0.909
HLW03-38	1b.Inner	Yes	Yes	5.025	7.035	0.306	0.201	10.051	2.513	1.507	9.834	0.302	0.051	0.153	44.123	1.507	3.962	0.047	4.259	1.005	7.210	0.909
HLW03-39	1b.Inner	Yes	Yes	3.012	7.030	0.306	0.201	8.693	4.959	1.506	7.030	0.301	0.153	0.153	49.209	1.506	4.519	0.142	2.128	1.004	7.237	0.910
HLW03-40	1b.Inner	Yes	Yes	5.052	7.074	0.306	0.081	9.600	4.990	1.516	7.074	0.505	0.153	0.153	43.922	3.353	4.547	0.047	4.282	1.011	6.063	0.272
HLW03-41	1b.Center	Yes	Yes	3.975	8.928	0.204	0.143	7.095	3.793	2.759	9.297	0.404	0.102	0.102	44.025	2.766	3.740	0.095	3.100	1.963	6.919	0.591
HLW03-42	RepHLW02-46	Yes	Yes	5.624	9.355	0.511	0.041	10.226	3.784	3.579	9.203	0.818	0.051	0.153	50.105	1.534	0.000	0.143	0.000	2.044	2.556	0.272
HLW03-43	RepHLW03-06	No	Yes	8.532	5.018	1.636	0.502	2.007	6.022	7.027	4.015	1.004	0.020	0.020	53.200	5.205	1.448	0.019	0.000	0.000	4.187	0.136
HLW03-44	RepHLW03-11	Yes	No	2.028	5.073	0.051	0.020	9.752	2.028	0.000	15.217	0.102	0.020	0.204	53.763	0.000	5.140	0.019	6.447	0.000	0.000	0.136
HLW03-45	RepHLW03-26	Yes	Yes	5.031	7.043	0.102	0.201	5.031	5.031	1.509	10.665	0.503	0.153	0.153	41.250	4.527	4.527	0.047	4.263	3.019	6.036	0.909

(a) Normalized to sum to 100% over the 19 components listed in this table.
(b) Indicates the design layer containing each of the compositions (see Section 5.1.1). In the case of replicate glasses, this column lists the layer for one glass composition from each replicate pair, and lists the Glass ID of the glass for which the other composition from the replicate pair is a replicate.

Table 5.2. PCT Release Data for IHLW Phase 1 Combined Matrix Glasses.

Glass ID	Retained for PCT Model Development	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/l)	PCT-Li (g/l)	PCT-Na (g/l)	PCT-B Data Splitting Validation Set	PCT-Li Data Splitting Validation Set	PCT-Na Data Splitting Validation Set
HLW02-01	Yes	21.580	12.720	51.060	0.700	0.686	0.628	NA-Rep[a]	NA-Rep	NA-Rep
HLW02-02	Yes	39.350	22.260	11.810	0.906	0.798	0.398	3	3	5
HLW02-03	Yes	123.300	19.880	224.200	2.836	2.140	2.014	3	1	3
HLW02-04	Yes	8.913	6.730	97.650	0.574	0.724	0.878	NA-Rep	NA-Rep	NA-Rep
HLW02-05	Yes	11.340	23.700	103.800	0.730	0.850	1.014	5	4	4
HLW02-06	Yes	6.167	15.440	110.800	0.398	0.702	0.996	1	2	1
HLW02-07	Yes	7.795	18.710	54.280	0.502	0.672	0.626	3	2	2
HLW02-08	Yes	153.500	41.200	251.700	3.530	2.680	2.262	NA-Rep	NA-Rep	NA-Rep
HLW02-09	Yes	23.260	6.140	80.670	0.646	0.582	0.724	5	5	2
HLW02-10	Yes	40.640	23.210	57.820	0.934	0.832	0.742	1	2	5
HLW02-11	Yes	99.010	47.040	103.700	2.278	1.688	1.288	5	2	5
HLW02-12	Yes	50.760	64.600	210.700	3.268	2.318	2.226	5	5	1
HLW02-13	Yes	54.240	69.930	205.400	3.492	2.508	2.656	3	4	3
HLW02-14	Yes	1.620	10.670	5.787	0.104	0.382	0.188	5	3	3
HLW02-15	Yes	55.180	9.717	85.220	1.270	1.046	0.916	5	4	5
HLW02-16	Yes	11.470	20.810	49.660	0.738	0.746	0.694	4	2	4
HLW02-17	Yes	8.470	20.240	19.400	0.546	0.726	0.340	NA-Rep	NA-Rep	NA-Rep
HLW02-18	Yes	9.360	5.303	80.290	0.602	0.566	0.722	4	2	3
HLW02-19	Yes	27.610	5.480	33.770	0.636	0.590	0.514	1	2	5
HLW02-20	Yes	21.530	5.717	14.670	0.496	0.616	0.306	1	3	5
HLW02-21	Yes	63.100	10.460	102.800	1.452	1.126	0.924	1	2	4
HLW02-22	No	23.890	17.270	2.257	0.550	0.620	0.076	NA-Dropped[b]	NA-Dropped	NA-Dropped
HLW02-23	Yes	29.920	18.730	24.990	0.688	0.672	0.602	2	3	4
HLW02-24	Yes	4.900	4.027	46.970	0.316	0.434	0.520	4	2	4
HLW02-25	Yes	13.770	3.543	7.317	0.316	0.382	0.144	5	4	5
HLW02-26	Yes	19.250	8.577	121.700	1.240	0.924	1.094	2	2	3
HLW02-27	Yes	25.920	15.460	13.330	0.596	0.554	0.420	2	5	1
HLW02-28	Yes	14.910	5.413	66.330	0.600	0.466	0.596	1	5	5
HLW02-29	Yes	33.080	10.450	37.970	0.820	0.600	0.568	3	1	5
HLW02-30	Yes	66.440	41.240	134.100	2.200	1.776	1.610	1	1	4
HLW02-31	Yes	53.250	12.510	58.850	1.318	1.078	0.530	3	3	2
HLW02-32	Yes	14.060	15.420	48.390	0.566	0.664	0.608	5	1	3
HLW02-33	Yes	24.940	8.553	95.340	1.004	0.736	0.856	4	4	5
HLW02-34	Yes	47.390	17.270	70.940	1.174	0.940	0.878	4	5	2

Table 5.2. PCT Release Data for IHLW Phase 1 Combined Matrix Glasses (continued).

Glass ID	Retained for PCT Model Development	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/l)	PCT-Li (g/l)	PCT-Na (g/l)	PCT-B Data Splitting Validation Set	PCT-Li Data Splitting Validation Set	PCT-Na Data Splitting Validation Set
HLW02-35	Yes	49.600	23.910	62.290	1.228	1.030	0.916	3	1	1
HLW02-36	Yes	15.970	7.027	85.590	0.594	0.606	0.770	3	5	4
HLW02-37	Yes	22.020	5.990	36.900	0.546	0.516	0.444	1	3	5
HLW02-38	Yes	25.640	13.620	38.030	0.636	0.688	0.570	2	3	4
HLW02-39	Yes	7.930	6.183	31.910	0.284	0.532	0.388	2	2	2
HLW02-40	Yes	8.447	6.797	23.200	0.276	0.556	0.322	3	4	4
HLW02-41	Yes	19.340	7.677	23.620	0.480	0.660	0.354	3	2	4
HLW02-42	Yes	43.600	22.060	54.970	1.080	0.950	0.824	NA-Rep	NA-Rep	NA-Rep
HLW02-43	Yes	42.650	9.747	77.980	1.056	0.840	0.844	2	5	1
HLW02-44	Yes	22.780	8.683	94.940	0.808	0.748	0.854	NA-Rep	NA-Rep	NA-Rep
HLW02-45	Yes	15.790	7.353	35.330	0.636	0.634	0.496	3	5	1
HLW02-46	Yes	15.240	10.860	30.170	0.536	0.632	0.452	NA-Rep	NA-Rep	NA-Rep
HLW02-47	Yes	14.790	6.377	23.700	0.486	0.550	0.338	2	1	3
HLW02-48	Yes	21.540	13.250	111.400	0.866	0.854	1.002	5	3	5
HLW02-49	Yes	16.040	15.850	38.640	0.590	0.682	0.578	4	4	2
HLW02-50	Yes	21.540	7.873	30.430	0.534	0.678	0.418	2	5	2
HLW02-51	Yes	6.473	12.110	26.770	0.260	0.568	0.400	4	1	4
HLW02-52	Yes	18.140	12.510	51.790	0.588	0.674	0.638	NA-Rep	NA-Rep	NA-Rep
HLW02-53	Yes	5.337	21.730	21.470	0.344	0.780	0.376	NA-Rep	NA-Rep	NA-Rep
HLW02-54	Yes	25.950	6.553	104.400	1.672	0.706	0.938	NA-Rep	NA-Rep	NA-Rep
HLW02-55	Yes	33.480	20.070	47.770	0.830	0.864	0.716	NA-Rep	NA-Rep	NA-Rep
HLW02-56	Yes	21.000	6.720	81.370	0.746	0.578	0.732	NA-Rep	NA-Rep	NA-Rep
HLW02-57	Yes	192.100	50.000	285.500	4.418	3.252	2.566	NA-Rep	NA-Rep	NA-Rep
HLW03-01	Yes	41.110	20.230	16.780	0.964	0.740	0.576	5	3	3
HLW03-02	Yes	53.890	10.870	71.470	1.270	0.946	0.862	1	4	3
HLW03-03	Yes	20.560	17.330	119.600	1.356	1.394	1.500	2	4	1
HLW03-04	Yes	8.377	26.900	26.600	0.550	0.984	0.804	5	3	2
HLW03-05	Yes	8.290	4.237	70.160	0.556	0.474	0.656	3	4	1
HLW03-06	Yes	4.590	10.350	4.777	0.302	0.378	0.164	1	5	4
HLW03-07	Yes	44.710	41.510	181.800	2.892	1.874	2.088	1	4	2
HLW03-08	Yes	19.320	24.920	162.500	1.286	1.042	1.510	4	5	5
HLW03-09	Yes	106.600	16.610	161.100	2.506	1.806	1.462	4	5	3
HLW03-10	Yes	13.550	27.990	112.500	0.886	1.018	1.178	4	2	1
HLW03-11	Yes	21.750	8.963	133.200	1.406	0.970	1.202	NA-Rep	NA-Rep	NA-Rep

Table 5.2. PCT Release Data for IHLW Phase 1 Combined Matrix Glasses (continued).

Glass ID	Retained for PCT Model Development	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/l)	PCT-Li (g/l)	PCT-Na (g/l)	PCT-B Data Splitting Validation Set	PCT-Li Data Splitting Validation Set	PCT-Na Data Splitting Validation Set
HLW03-12	Yes	12.860	17.790	21.740	0.832	0.762	0.736	1	1	1
HLW03-13	No	0.310	14.390	13.510	0.020	0.592	0.458	NA-Dropped	NA-Dropped	NA-Dropped
HLW03-14	Yes	23.480	15.670	101.400	1.520	1.348	1.312	5	5	4
HLW03-15	Yes	23.860	5.630	13.740	0.562	0.622	0.352	1	1	5
HLW03-16	Yes	10.100	10.510	22.470	0.664	0.788	0.772	3	4	3
HLW03-17	No	17.780	6.370	3.200	0.414	0.696	0.096	NA-Dropped	NA-Dropped	NA-Dropped
HLW03-18	Yes	53.920	73.430	197.900	3.492	2.670	2.534	4	3	4
HLW03-19	Yes	43.670	58.220	172.400	2.864	2.128	2.292	2	2	5
HLW03-20	Yes	59.420	77.210	209.900	3.978	2.880	2.802	2	2	2
HLW03-21	Yes	8.693	5.370	27.900	0.402	0.466	0.346	5	1	1
HLW03-22	Yes	12.880	7.650	58.510	0.602	0.668	0.666	5	4	5
HLW03-23	Yes	30.730	8.475	52.510	0.830	0.734	0.594	2	5	1
HLW03-24	Yes	15.260	15.550	31.770	0.708	0.674	0.524	1	1	3
HLW03-25	Yes	72.950	17.090	129.300	1.984	1.492	1.472	2	3	2
HLW03-26	Yes	28.100	18.980	63.470	1.310	0.828	0.818	NA-Rep	NA-Rep	NA-Rep
HLW03-27	Yes	22.620	15.790	75.600	1.054	0.840	0.860	3	1	4
HLW03-28	Yes	60.520	29.310	87.180	1.634	1.270	1.120	4	1	2
HLW03-29	Yes	23.600	21.470	85.440	1.094	0.930	0.966	1	1	2
HLW03-30	Yes	33.960	16.860	25.230	0.918	0.732	0.490	2	1	2
HLW03-31	Yes	23.740	14.060	26.310	1.102	0.610	0.416	5	4	3
HLW03-32	Yes	10.710	15.110	37.190	0.500	0.660	0.550	4	3	1
HLW03-33	Yes	20.740	10.690	17.830	0.560	0.590	0.346	2	3	2
HLW03-34	Yes	14.200	8.927	33.490	0.662	0.780	0.472	4	5	3
HLW03-35	Yes	12.630	7.173	11.680	0.390	0.622	0.226	3	2	2
HLW03-36	No	27.000	8.313	14.200	1.260	0.664	0.240	NA-Dropped	NA-Dropped	NA-Dropped
HLW03-37	Yes	63.260	42.450	48.840	1.720	1.876	0.954	3	3	3
HLW03-38	Yes	11.890	7.633	28.270	0.556	0.666	0.396	4	5	1
HLW03-39	Yes	9.740	14.660	15.140	0.456	0.650	0.296	4	4	1
HLW03-40	Yes	8.530	13.380	19.040	0.396	0.588	0.370	2	4	3
HLW03-41	Yes	13.510	9.680	31.340	0.498	0.560	0.464	5	3	4
HLW03-42	Yes	10.630	8.100	22.810	0.374	0.472	0.342	NA-Rep	NA-Rep	NA-Rep
HLW03-43	No	20.230	10.430	4.413	1.328	0.382	0.152	NA-Drop-Rep	NA-Drop-Rep	NA-Drop-Rep
HLW03-44	Yes	12.320	8.910	125.600	0.796	0.964	1.134	NA-Rep	NA-Rep	NA-Rep
HLW03-45	Yes	14.530	17.240	60.120	0.678	0.752	0.774	NA-Rep	NA-Rep	NA-Rep

(a) NA-Rep indicates glasses that were not included in any of the validation splits because they were replicates.

(b) NA-Dropped indicates glasses that were not included in any of the validation splits because they were dropped from the PCT modeling.

Table 5.3. PCT Release Data and Standard Deviations for Replicates Among IHLW Phase 1 Combined Matrix Glasses.

Glass IDs of Replicate Pairs	Retained for PCT Model Development	PCT-Boron		PCT-Lithium		PCT-Sodium	
		g/l	ln(g/l)	g/l	ln(g/l)	g/l	ln(g/l)
HLW02-52	Yes	0.588	-0.531	0.674	-0.395	0.638	-0.449
HLW02-01	Yes	0.700	-0.357	0.686	-0.377	0.628	-0.465
		%RSD=12.30	**SD=0.1233**	**%RSD=1.25**	**SD=0.0125**	**%RSD=1.12**	**SD=0.0112**
HLW02-53	Yes	0.344	-1.067	0.780	-0.248	0.376	-0.978
HLW02-17	Yes	0.546	-0.605	0.726	-0.320	0.340	-1.079
		%RSD=32.10	**SD=0.3267**	**%RSD=5.07**	**SD=0.0507**	**%RSD=7.11**	**SD=0.0712**
HLW02-54	Yes	1.672	0.514	0.706	-0.348	0.938	-0.064
HLW02-04	Yes	0.574	-0.555	0.724	-0.323	0.878	-0.130
		%RSD=69.14	**SD=0.756**	**%RSD=1.78**	**SD=0.0178**	**%RSD=4.67**	**SD=0.0467**
HLW02-55	Yes	0.830	-0.186	0.864	-0.146	0.716	-0.334
HLW02-42	Yes	1.080	0.077	0.950	-0.051	0.824	-0.194
		%RSD=18.51	**SD=0.1862**	**%RSD=6.70**	**SD=0.0671**	**%RSD=9.92**	**SD=0.0993**
HLW02-56	Yes	0.746	-0.293	0.578	-0.548	0.732	-0.312
HLW02-44	Yes	0.808	-0.213	0.748	-0.290	0.854	-0.158
		%RSD=5.64	**SD=0.0565**	**%RSD=18.13**	**SD=0.1823**	**%RSD=10.88**	**SD=0.1090**
HLW02-57	Yes	4.418	1.486	3.252	1.179	2.566	0.942
HLW02-08	Yes	3.530	1.261	2.680	0.986	2.262	0.816
		%RSD=15.80	**SD=0.1587**	**%RSD=13.64**	**SD=0.1368**	**%RSD=8.90**	**SD=0.0892**
HLW03-42	Yes	0.374	-0.983	0.472	-0.751	0.342	-1.073
HLW02-46	Yes	0.536	-0.624	0.632	-0.459	0.452	-0.794
		%RSD=25.18	**SD=0.2545**	**%RSD=20.50**	**SD=0.2064**	**%RSD=19.59**	**SD=0.1972**
HLW03-43	No	1.328	0.284	0.382	-0.962	0.152	-1.884
HLW03-06	No	0.302	-1.197	0.378	-0.973	0.164	-1.808
		%RSD=89.02	**SD=1.0472**	**%RSD=0.74**	**SD=0.0074**	**%RSD=5.37**	**SD=0.0537**
HLW03-44	Yes	0.796	-0.228	0.964	-0.037	1.134	0.126
HLW03-11	Yes	1.406	0.341	0.970	-0.030	1.202	0.184
		%RSD=39.18	**SD=0.4023**	**%RSD=0.44**	**SD=0.0044**	**%RSD=4.12**	**SD=0.0412**
HLW03-45	Yes	0.678	-0.389	0.752	-0.285	0.774	-0.256
HLW03-26	Yes	1.310	0.270	0.828	-0.189	0.818	-0.201
		%RSD=44.96	**SD=0.4657**	**%RSD=6.80**	**SD=0.0681**	**%RSD=3.91**	**SD=0.0391**
Pooled Over All 10 Replicate Pairs		**%RSD=43.24**	**SD=0.4792**	**%RSD=10.28**	**SD=0.1034**	**%RSD=9.03**	**SD=0.0906**
Pooled Over 9 Replicate Pairs Used In PCT Model Development		**%RSD=34.60**	**SD=0.3651**	**%RSD=10.84**	**SD=0.1089**	**%RSD=9.34**	**SD=0.0938**

Table 5.4. IHLW PCT-Boron 19-Term Full LM Model and Performance Summary.

ln(PCT-Boron) Full LM Model Term	Coefficient Estimate	Coefficient Standard Deviation
Al_2O_3	-20.4797	2.3504
B_2O_3	7.8844	1.2438
CdO	-8.3278	8.1380
Cr_2O_3	50.7509	34.0197
Fe_2O_3	-1.6451	1.5563
Li_2O	24.4745	3.1481
MnO	4.8773	2.1694
Na_2O	14.2904	1.4431
NiO	-6.6058	12.9858
Sb_2O_3	-20.6043	48.3055
SeO_2	85.1006	62.0009
SiO_2	-4.0989	0.5455
SrO	-0.6733	1.9006
ThO_2	8.6192	3.1705
Tl_2O	-24.7861	52.0067
UO_3	-7.8305	3.4626
ZnO	-2.5245	4.5279
ZrO_2	-11.6246	1.8156
Spike	5.5227	9.5650

Statistic from Modeling Data	Value
R^2	0.751
R^2_A	0.694
R^2_P	0.567
RMSE	0.3834
LOF p-value	0.4666
N	97

Statistics from Data Splitting						
Statistic	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.777	0.740	0.773	0.744	0.755	0.758
R^2_A	0.713	0.665	0.707	0.669	0.684	0.688
R^2_P	0.571	0.478	0.562	0.511	0.486	0.522
RMSE	0.3793	0.4004	0.3768	0.3995	0.3766	0.3865
R^2_V	0.320	0.710	0.464	0.718	0.623	0.567

	R^2 for Validation					RMSE for Validation					Number of Points				
Validation Set	V1	V2a	V2b	V3a	V3b	V1	V2a	V2b	V3a	V3b	V1	V2a	V2b	V3a	V3b
VSL Validation	0.141	0.486	0.500	0.631	0.621	0.8223	0.4130	0.4309	0.3732	0.4007	75	18	15	15	13
Hanford CVS	0.219	0.130	NA	NA	NA	1.3249	1.0865	NA	NA	NA	146	23	0	0	0
DWPF PCT Model	0.485	0.405	NA	(a)	NA	1.0222	0.4269	NA	0.1869	NA	177	45	0	3	0
WVDP Sets	0.755	0.167	NA	(a)	NA	0.5420	0.4370	NA	0.4337	NA	110	29	0	20	0
RPP-WTP LAW	(a)	NA	NA	NA	NA	0.4665	NA	NA	NA	NA	66	0	0	0	0
All	0.448	0.414	0.500	0.348	0.621	0.9768	0.6183	0.4309	0.3959	0.4007	574	115	15	38	13

(a) The validation R^2 statistic was negative, indicating the prediction errors were larger than if the mean of measured data were used as the predictor.

Table 5.5. IHLW PCT-Boron 8-Term Reduced LM Model and Performance Summary.

ln(PCT-Boron) Reduced LM Model Term	Coefficient Estimate	Coefficient Standard Deviation
Al_2O_3	-16.0111	1.7061
B_2O_3	6.0139	0.8922
Li_2O	20.5142	2.3325
MnO	3.7888	1.4656
Na_2O	12.2908	0.9975
SiO_2	-3.9574	0.3704
ThO_2	6.1476	1.9076
ZrO_2	-9.6868	1.3711

Statistic from Modeling Data	Value
R^2	0.722
R^2_A	0.700
R^2_P	0.667
RMSE	0.3791
LOF p-value	0.4878
N	97

Statistics from Data Splitting						
Statistic	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.734	0.700	0.720	0.726	0.726	0.721
R^2_A	0.709	0.671	0.693	0.700	0.700	0.695
R^2_P	0.667	0.626	0.652	0.656	0.661	0.652
RMSE	0.3821	0.3967	0.3859	0.3808	0.3669	0.3825
R^2_V	0.609	0.795	0.712	0.677	0.671	0.693

	R^2 for Validation					RMSE for Validation					Number of Points				
Validation Set	V1	V2a	V2b	V3a	V3b	V1	V2a	V2b	V3a	V3b	V1	V2a	V2b	V3a	V3b
VSL Validation	0.165	0.552	0.563	0.610	0.600	0.8800	0.3856	0.4028	0.3836	0.4117	75	18	15	15	13
Hanford CVS	0.037	(a)	NA	NA	NA	1.4712	1.2108	NA	NA	NA	146	23	0	0	0
DWPF PCT Model	0.366	0.391	NA	(a)	NA	1.1345	0.4318	NA	0.2560	NA	177	45	0	3	0
WVDP Sets	0.738	0.451	NA	0.280	NA	0.5598	0.3549	NA	0.3488	NA	110	29	0	20	0
RPP-WTP LAW	(a)	NA	NA	NA	NA	0.4923	NA	NA	NA	NA	66	0	0	0	0
All	0.342	0.355	0.563	0.470	0.600	1.0661	0.6490	0.4028	0.3568	0.4117	574	115	15	38	13

(a) The validation R^2 statistic was negative, indicating the prediction errors were larger than if the mean of measured data were used as the predictor.

Table 5.6. Summary of Various IHLW PCT-Boron LM and Reduced PQM Models.

Statistics for Modeling Data	Full 19-term LM	Reduced 8-term LM	Reduced 9-term PQM	Reduced 10-term PQM	Reduced 11-term PQM	Reduced 12-term PQM	Reduced 13-term PQM	Reduced 14-term PQM	Reduced 15-term PQM	Reduced 16-term PQM
R^2	0.751	0.722	0.743	0.753	0.763	0.784	0.807	0.814	0.822	0.824
R^2_A	0.694	0.700	0.719	0.728	0.735	0.756	0.779	0.785	0.792	0.792
R^2_P	0.567	0.667	0.684	0.688	0.685	0.722	0.739	0.744	0.747	0.743
RMSE	0.3834	0.3791	0.3669	0.3613	0.3564	0.3425	0.3254	0.3209	0.3160	0.3163
Model Terms (Quadratic terms written in element form to save space)	Al_2O_3, B_2O_3, CdO, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, Sb_2O_3, SeO_2, SiO_2, SrO, ThO_2, Tl_2O, UO_3, ZnO, ZrO_2, Spike	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn, Na*Na	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn, Na*Na. Li*Li	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Na*Th, Al*Na, B*Mn, B*Li	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Na*Th, Al*Na, B*Mn, Li*Li, Na*Na	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Na*Th, Al*Na, B*Mn, Li*Li, Na*Na, Si*Zr	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Na*Th, Al*Na, B*Mn, Li*Li, Na*Na, Si*Zr, B*Na	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Na*Th, Al*Na, B*Mn, Li*Li, Na*Na, Si*Zr, B*Na, Li*Zr
Statistic Averages Over Five Splits of the Modeling Data										
R^2	0.758	0.721	0.742	0.753	0.764	0.784	0.806	0.816	0.827	0.829
R^2_A	0.688	0.695	0.714	0.722	0.731	0.750	0.772	0.781	0.790	0.789
R^2_P	0.522	0.652	0.669	0.672	0.668	0.704	0.717	0.725	0.733	0.727
RMSE	0.3865	0.3825	0.3703	0.3646	0.3589	0.3462	0.3306	0.3237	0.3169	0.3174
R^2_V	0.567	0.693	0.717	0.707	0.684	0.733	0.769	0.696	0.676	0.676

Table 5.7. IHLW PCT-Lithium 19-Term Full LM Model and Performance Summary.

ln(PCT-Lithium) Full LM Model Term	Coefficient Estimate	Coefficient Standard Deviation
Al_2O_3	-14.3939	1.8748
B_2O_3	4.0295	0.9922
CdO	-4.5337	6.4914
Cr_2O_3	11.2836	27.1364
Fe_2O_3	-1.1063	1.2414
Li_2O	19.1382	2.5112
MnO	2.2379	1.7304
Na_2O	9.0235	1.1511
NiO	-1.5333	10.3583
Sb_2O_3	-38.3310	38.5317
SeO_2	11.2773	49.4561
SiO_2	-2.4897	0.4351
SrO	-0.5293	1.5160
ThO_2	3.4967	2.5290
Tl_2O	30.7031	41.4841
UO_3	-3.2673	2.7620
ZnO	-2.9129	3.6118
ZrO_2	-7.4205	1.4483
Spike	5.9190	7.6297

Statistic from Modeling Data	Value
R^2	0.666
R^2_A	0.589
R^2_P	0.422
RMSE	0.3058
LOF p-value	0.0007
N	97

Statistics from Data Splitting						
Statistic	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.684	0.624	0.649	0.679	0.724	0.672
R^2_A	0.594	0.515	0.547	0.586	0.644	0.577
R^2_P	0.389	0.191	0.273	0.406	0.491	0.350
RMSE	0.3099	0.3268	0.3193	0.3063	0.2855	0.3096
R^2_V	0.351	0.797	0.688	0.268	0.127	0.446

	R^2 for Validation					RMSE for Validation					Number of Points				
Validation Set	V1	V2a	V2b	V3a	V3b	V1	V2a	V2b	V3a	V3b	V1	V2a	V2b	V3a	V3b
VSL Validation	0.326	0.539	0.575	0.645	0.640	0.8017	0.2981	0.2992	0.2752	0.2923	70	18	15	15	13
Hanford CVS	0.149	0.148	NA	NA	NA	1.1435	0.9021	NA	NA	NA	146	23	0	0	0
DWPF PCT Model	0.418	0.221	NA	(a)	NA	0.9405	0.3921	NA	0.1735	NA	173	45	0	3	0
WVDP Sets	0.544	0.069	NA	(a)	NA	0.7129	0.3898	NA	0.3997	NA	110	29	0	20	0
RPP-WTP LAW	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	0	0	0	0	0
All	0.401	0.415	0.575	0.145	0.640	0.9442	0.5245	0.2992	0.3411	0.2923	499	115	15	38	13

(a) The validation R^2 statistic was negative, indicating the prediction errors were larger than if the mean of measured data were used as the predictor.

Table 5.8. IHLW PCT-Lithium 8-Term Reduced LM Model and Performance Summary.

ln(PCT-Lithium) Reduced LM Model Term	Coefficient Estimate	Coefficient Standard Deviation
Al_2O_3	-11.5792	1.3358
B_2O_3	3.0320	0.6986
Li_2O	15.7575	1.8263
MnO	1.4622	1.1476
Na_2O	7.4435	0.7810
SiO_2	-2.3693	0.2900
ThO_2	2.5351	1.4937
ZrO_2	-6.0292	1.0736

Statistic from Modeling Data	Value
R^2	0.641
R^2_A	0.612
R^2_P	0.571
RMSE	0.2968
LOF p-value	0.0010
N	97

Statistics from Data Splitting						
Statistic	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.653	0.601	0.626	0.612	0.703	0.639
R^2_A	0.620	0.563	0.590	0.575	0.674	0.604
R^2_P	0.575	0.502	0.536	0.518	0.632	0.552
RMSE	0.2998	0.3103	0.3038	0.3103	0.2732	0.2995
R^2_V	0.474	0.775	0.673	0.734	0.232	0.578

	R^2 for Validation					RMSE for Validation					Number of Points				
Validation Set	**V1**	**V2a**	**V2b**	**V3a**	**V3b**	**V1**	**V2a**	**V2b**	**V3a**	**V3b**	**V1**	**V2a**	**V2b**	**V3a**	**V3b**
VSL Validation	0.296	0.554	0.586	0.644	0.637	0.8190	0.2934	0.2951	0.2755	0.2936	70	18	15	15	13
Hanford CVS	(a)	(a)	NA	NA	NA	1.2656	1.0014	NA	NA	NA	146	23	0	0	0
DWPF PCT Model	0.324	0.345	NA	(a)	NA	1.0141	0.3597	NA	0.1051	NA	173	45	0	3	0
WVDP Sets	0.519	0.320	NA	(a)	NA	0.7321	0.3332	NA	0.3389	NA	110	29	0	20	0
RPP-WTP LAW	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	0	0	0	0	0
All	0.303	0.377	0.586	0.329	0.637	1.0185	0.5410	0.2951	0.3021	0.2936	499	115	15	38	13

(a) The validation R^2 statistic was negative, indicating the prediction errors were larger than if the mean of measured data were used as the predictor.

Table 5.9. Summary of Various IHLW PCT-Lithium LM and Reduced PQM Models.

Statistics for Modeling Data	Full 19-term LM	Reduced 8-term LM	Reduced 9-term PQM	Reduced 10-term PQM	Reduced 11-term PQM	Reduced 12-term PQM	Reduced 13-term PQM	Reduced 14-term PQM	Reduced 15-term PQM	Reduced 16-term PQM
R^2	0.666	0.641	0.688	0.711	0.728	0.740	0.788	0.802	0.814	0.818
R^2_A	0.589	0.612	0.659	0.681	0.696	0.706	0.758	0.771	0.782	0.785
R^2_P	0.422	0.571	0.622	0.641	0.651	0.663	0.724	0.733	0.740	0.740
RMSE	0.3058	0.2968	0.2783	0.2693	0.2628	0.2585	0.2344	0.2282	0.2226	0.2211
Model Terms (Quadratic terms written in element form to save space)	Al_2O_3, B_2O_3, CdO, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, Sb_2O_3, SeO_2, SiO_2, SrO, ThO_2, Tl_2O, UO_3, ZnO, ZrO_2, Spike	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, B*Li	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, B*Li, Mn*Mn	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, B*Li, Mn*Mn, Al*Na	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, B*Li, Mn*Mn, Al*Na, Na*Na	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Al*Na, Na*Na, Na*Si, Na*Th, Li*Li	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Al*Na, Na*Na, Na*Si, Na*Th, Li*Li, Mn*Mn	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Al*Na, Na*Na, Na*Si, Na*Th, Li*Li, Mn*Mn, Li*Mn	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Al*Na, Na*Na, Na*Si, Na*Th, Li*Li, Mn*Mn, Li*Mn, Na*Zr
Statistic Averages Over Five Splits of the Modeling Data										
R^2	0.672	0.639	0.691	0.714	0.732	0.744	0.794	0.807	0.819	0.826
R^2_A	0.577	0.604	0.656	0.678	0.694	0.704	0.757	0.769	0.781	0.785
R^2_P	0.350	0.552	0.610	0.626	0.637	0.650	0.713	0.720	0.724	0.724
RMSE	0.3096	0.2995	0.2792	0.2703	0.2636	0.2595	0.2348	0.2290	0.2229	0.2207
R^2_V	0.446	0.578	0.596	0.630	0.639	0.636	0.700	0.724	0.717	0.692

Table 5.10. IHLW PCT-Sodium 19-Term Full LM Model and Performance Summary.

ln(PCT-Sodium) Full LM Model Term	Coefficient Estimate	Coefficient Standard Deviation
Al_2O_3	-16.9891	1.5624
B_2O_3	2.1490	0.8268
CdO	-6.3774	5.4094
Cr_2O_3	7.3584	22.6136
Fe_2O_3	-1.6188	1.0345
Li_2O	24.2897	2.0926
MnO	3.5492	1.4420
Na_2O	16.2065	0.9592
NiO	2.6846	8.6319
Sb_2O_3	-3.4238	32.1096
SeO_2	47.0475	41.2132
SiO_2	-4.3716	0.3626
SrO	1.2144	1.2633
ThO_2	3.6820	2.1075
Tl_2O	23.2167	34.5698
UO_3	-3.5564	2.3017
ZnO	0.0494	3.0098
ZrO_2	-11.2921	1.2069
Spike	8.4368	6.3581

Statistic from Modeling Data	Value
R^2	0.865
R^2_A	0.833
R^2_P	0.775
RMSE	0.2548
LOF p-value	0.0010
N	97

Statistics from Data Splitting						
Statistic	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.872	0.878	0.880	0.863	0.855	0.870
R^2_A	0.836	0.843	0.845	0.823	0.812	0.832
R^2_P	0.765	0.753	0.792	0.730	0.726	0.753
RMSE	0.2586	0.2455	0.2426	0.2604	0.2672	0.2549
R^2_V	0.740	0.776	0.689	0.853	0.864	0.784

	R^2 for Validation					RMSE for Validation					Number of Points				
Validation Set	V1	V2a	V2b	V3a	V3b	V1	V2a	V2b	V3a	V3b	V1	V2a	V2b	V3a	V3b
VSL Validation	0.356	0.704	0.712	0.768	0.766	0.7389	0.2854	0.3004	0.2676	0.2847	75	18	15	15	13
Hanford CVS	0.020	(a)	NA	NA	NA	1.4231	1.1630	NA	NA	NA	146	23	0	0	0
DWPF PCT Model	0.340	0.350	NA	(a)	NA	1.0884	0.3497	NA	0.2761	NA	177	45	0	3	0
WVDP Sets	0.445	0.184	NA	0.052	NA	0.7360	0.3460	NA	0.2867	NA	110	29	0	20	0
RPP-WTP LAW	(a)	NA	NA	NA	NA	0.5687	NA	NA	NA	NA	66	0	0	0	0
All	0.289	0.298	0.712	0.561	0.766	1.0453	0.6011	0.3004	0.2785	0.2847	574	115	15	38	13

(a) The validation R^2 statistic was negative, indicating the prediction errors were larger than if the mean of measured data were used as the predictor.

Table 5.11. IHLW PCT-Sodium 8-Term Reduced LM Model and Performance Summary.

ln(PCT-Sodium) Reduced LM Model Term	Coefficient Estimate	Coefficient Standard Deviation
Al_2O_3	-13.7309	1.1574
B_2O_3	1.7213	0.6053
Li_2O	19.9566	1.5824
MnO	3.6828	0.9943
Na_2O	13.2619	0.6767
SiO_2	-3.8031	0.2513
ThO_2	3.1327	1.2942
ZrO_2	-8.9994	0.9302

Statistic from Modeling Data	Value
R^2	0.843
R^2_A	0.830
R^2_P	0.813
RMSE	0.2572
LOF p-value	0.0009
N	97

Statistics from Data Splitting						
Statistic	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.838	0.858	0.868	0.835	0.828	0.845
R^2_A	0.822	0.844	0.855	0.820	0.811	0.830
R^2_P	0.799	0.822	0.840	0.796	0.786	0.809
RMSE	0.2690	0.2449	0.2346	0.2627	0.2680	0.2558
R^2_V	0.869	0.758	0.708	0.868	0.896	0.820

	R^2 for Validation					RMSE for Validation					Number of Points				
Validation Set	V1	V2a	V2b	V3a	V3b	V1	V2a	V2b	V3a	V3b	V1	V2a	V2b	V3a	V3b
VSL Validation	0.333	0.704	0.695	0.734	0.728	0.7517	0.2855	0.3091	0.2864	0.3073	75	18	15	15	13
Hanford CVS	0.032	(a)	NA	NA	NA	1.4150	1.1333	NA	NA	NA	146	23	0	0	0
DWPF PCT Model	0.300	0.422	NA	(a)	NA	1.1211	0.3642	NA	0.2377	NA	177	45	0	3	0
WVDP Sets	0.552	0.409	NA	0.228	NA	0.6613	0.2945	NA	0.2586	NA	110	29	0	20	0
RPP-WTP LAW	(a)	NA	NA	NA	NA	0.5646	NA	NA	NA	NA	66	0	0	0	0
All	0.290	0.332	0.695	0.592	0.728	1.0446	0.5860	0.3091	0.2684	0.3073	574	115	15	38	13

(a) The validation R^2 statistic was negative, indicating the prediction errors were larger than if the mean of measured data were used as the predictor.

Table 5.12. Summary of Various IHLW PCT-Sodium LM and Reduced PQM Models.

Statistics for Modeling Data	Full 19-term LMM	Reduced 8-term LMM	Reduced 9-term PQM	Reduced 10-term PQM	Reduced 11-term PQM	Reduced 12-term PQM	Reduced 13-term PQM	Reduced 14-term PQM	Reduced 15-term PQM	Reduced 16-term PQM
R^2	0.865	0.843	0.860	0.871	0.878	0.883	0.890	0.896	0.900	0.904
R^2_A	0.833	0.830	0.847	0.857	0.864	0.868	0.874	0.880	0.883	0.886
R^2_P	0.775	0.813	0.828	0.836	0.839	0.843	0.851	0.856	0.854	0.858
RMSE	0.2548	0.2572	0.2442	0.2359	0.2303	0.2271	0.2219	0.2167	0.2135	0.2112
Model Terms (Quadratic terms written in element form to save space)	Al_2O_3, B_2O_3, CdO, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, Sb_2O_3, SeO_2, SiO_2, SrO, ThO_2, Tl_2O, UO_3, ZnO, ZrO_2, Spike	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn, Na*Na	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn, Na*Na, Li*Li	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn, Na*Na, Li*Li, Al*Zr	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn, Na*Na, Li*Li, Al*Zr, Na*Th	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn, Na*Na, Li*Li, Na*Zr, Mn*Na, B*Th	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn, Na*Na, Li*Li, Na*Zr, B*Th, Al*Zr, B*Na	Al_2O_3, B_2O_3, Li_2O, MnO, Na_2O, SiO_2, ThO_2, ZrO_2, Mn*Mn, Na*Na, Li*Li, Na*Zr, B*Th, Al*Zr, B*Na, Na*Si
Statistic Averages Over Five Splits of the Modeling Data										
R^2	0.870	0.845	0.863	0.875	0.882	0.887	0.894	0.899	0.906	0.908
R^2_A	0.832	0.830	0.848	0.859	0.866	0.869	0.876	0.880	0.886	0.887
R^2_P	0.753	0.809	0.825	0.832	0.834	0.838	0.848	0.849	0.853	0.853
RMSE	0.2549	0.2558	0.2420	0.2331	0.2276	0.2249	0.2192	0.2156	0.2099	0.2091
R^2_V	0.784	0.820	0.827	0.829	0.828	0.832	0.834	0.849	0.821	0.838

Table 5.13. HLW03-06 Composition in Formats Needed for Use in IHLW PCT Models.

Component	HLW03-06 Composition (wt%) From Table 5.1	HLW03-06 Composition (mass fractions) For Use In PCT Full LM Models	HLW03-06 Composition (mass fractions) For Use In PCT Reduced LM Models
Al_2O_3	8.532	0.08532	0.09538
B_2O_3	5.018	0.05018	0.05610
CdO	1.636	0.01636	NA [(a)]
Cr_2O_3	0.502	0.00502	NA
Fe_2O_3	2.007	0.02007	NA
Li_2O	6.022	0.06022	0.06733
MnO	7.027	0.07027	0.07855
Na_2O	4.015	0.04015	0.04489
NiO	1.004	0.01004	NA
Sb_2O_3	0.020	0.00020	NA
SeO_2	0.020	0.00020	NA
SiO_2	53.200	0.53200	0.59475
SrO	5.205	0.05205	NA
ThO_2	1.448	0.01448	0.01619
Tl_2O	0.019	0.00019	NA
UO_3	0.000	0.00000	NA
ZnO	0.000	0.00000	NA
ZrO_2	4.187	0.04187	0.04681
Spike	0.136	0.00136	NA

(a) NA indicates terms not included in reduced PCT models.

Table 5.14. Predicted PCT Releases and Corresponding 95% UCIs and 95% SUCIs for HLW03-06 Composition Used in IHLW PCT Models.

Model	Predicted ln(PCT) in ln(g/l)	Predicted PCT in g/l	95% UCI on Mean ln(PCT) in ln(g/l)	95% UCI on Median PCT in g/l	95% SUCI on Mean ln(PCT) in ln(g/l)	95% SUCI on Median PCT in g/l
PCT-Boron Full LM Model	-1.5035	0.2223	-1.0755	0.3411	-0.1192	0.8876
PCT-Boron Reduced LM Model	-1.6668	0.1889	-1.4351	0.2381	-1.1467	0.3177
PCT-Lithium Full LM Model	-1.0126	0.3633	-0.6711	0.5111	0.0916	1.0960
PCT-Lithium Reduced LM Model	-1.0747	0.3414	-0.8933	0.4093	-0.6675	0.5130
PCT-Sodium Full LM Model	-1.7088	0.1811	-1.4242	0.2407	-0.7886	0.4545
PCT-Sodium Reduced LM Model	-1.6173	0.1984	-1.4601	0.2322	-1.2645	0.2824

Table 6.1. Temperature and Volume %-Crystallinity Data for IHLW Phase 1 Combined Matrix Glasses.

Glass ID	Retained for Model Development	Temperature in (°C)													Crystal
		650	700	750	800	850[(b)]	875	900[(b)]	950[(b)]	1000[(b)]	1050	1100	1150	1200	
HLW02-01	Yes	NA[(a)]	NA	3	NA	1.88	NA	NA	0.27, 0.5	NA	NA	NA	NA	NA	Spinel
HLW02-02	Yes	NA	NA	NA	NA	1.1	NA	1.1	0.5	NA	NA	NA	NA	NA	Spinel
HLW02-03	Yes	NA	NA	1.8	NA	0.7	NA	NA	0.2	NA	NA	NA	NA	NA	Spinel
HLW02-04	Yes	NA	NA	23.4	14.2	0.1, 0.7	NA	NA	NA	NA	NA	NA	NA	NA	Spinel
HLW02-05	No	NA	NA	0.1	NA	0.1	NA	0.1	0.1	NA	NA	NA	NA	NA	Noble metal
HLW02-06	Yes	NA	NA	NA	NA	5.1	NA	3.2	2.8, 2.4	NA	0.8	NA	NA	NA	Spinel
HLW02-07	Yes	NA	NA	1	NA	0.8	NA	0.5	0.4	NA	NA	NA	NA	NA	Spinel
HLW02-08	Yes	NA	NA	1.2	NA	0.6	NA	NA	0.1	NA	NA	NA	NA	NA	Spinel
HLW02-09	Yes	NA	NA	NA	NA	2.9	NA	4.4, 3.5	1.2	0.2	NA	NA	NA	NA	Spinel
HLW02-10	No	NA	0.4	0.6	NA	0.1	NA	0.1	0.1	NA	NA	NA	NA	NA	Spinel
HLW02-11	Yes	NA	1.8	1.2	NA	1	NA	NA	0.1	NA	NA	NA	NA	NA	Spinel
HLW02-12	Yes	NA	NA	NA	NA	4.4	NA	3.3	NA	NA	1	NA	NA	NA	Spinel
HLW02-13	Yes	NA	NA	NA	NA	5.6	4.3	0.2	NA	1.0	0.3	NA	NA	NA	Spinel
HLW02-14	No	NA	NA	NA	NA	1.7	NA	NA	1.4, 1.1	0.2	NA	NA	NA	NA	ZrSiO4+ Spinel
HLW02-15	Yes	NA	NA	NA	NA	3.7	NA	3.1	2.7	NA	0.9	NA	NA	NA	Spinel
HLW02-16	Yes	NA	NA	NA	NA	4	NA	3.6	3.1, 1.3	0.7	NA	NA	NA	NA	Spinel+ZrO_2
HLW02-17	Yes	NA	NA	NA	NA	NA	NA	2.07	0.9, 1.2	0.2	0.4	NA	NA	NA	Spinel
HLW02-18	Yes	NA	NA	2.2	NA	1.8	NA	NA	1	NA	NA	NA	NA	NA	Spinel
HLW02-19	Yes	NA	NA	NA	NA	1.6, 2.4	NA	1.2	0.8, 0.6	NA	NA	NA	NA	NA	Spinel
HLW02-20	Yes	NA	NA	NA	NA	6.4	NA	1.65	0.8, 2.1	NA	NA	NA	NA	NA	Spinel
HLW02-21	No	NA	NA	0.2	0.2	NA	NA	0.2	NA	NA	NA	NA	NA	NA	Spinel
HLW02-22	Yes	NA	NA	NA	NA	1.6	NA	0.7	1.5	NA	0.2	NA	NA	NA	Spinel
HLW02-23	Yes	NA	NA	NA	NA	2.4	NA	1.7	1.1, 0.8	NA	NA	NA	NA	NA	Spinel
HLW02-24	Yes	NA	NA	NA	NA	2.3	NA	1.24	0.61	NA	NA	NA	NA	NA	Spinel
HLW02-25	Yes	NA	NA	NA	NA	2	NA	0.5	1.0	NA	NA	NA	NA	NA	Spinel
HLW02-26	Yes	NA	NA	NA	NA	3.9	NA	2.47	0.9, 1.6	0.8	NA	NA	NA	NA	Spinel
HLW02-27	Yes	NA	NA	NA	NA	2.5	NA	1.28	1.5	0.5	0.2	NA	NA	NA	Spinel+$ZrSiO_4$
HLW02-28	Yes	NA	NA	NA	NA	1.9	NA	1.1	0.9	0.1	NA	NA	NA	NA	Spinel
HLW02-29	Yes	NA	NA	NA	NA	3.5	NA	1.86	0.7,0.6,0.8	NA	0.2	NA	NA	NA	Spinel
HLW02-30	Yes	NA	NA	2.3	NA	1.1	NA	NA	0.8	NA	NA	NA	NA	NA	Spinel
HLW02-31	Yes	NA	1.2	1.3	NA	0.99	NA	NA	0.2	NA	NA	NA	NA	NA	Spinel
HLW02-32	Yes	NA	1.1	NA	1.4	0.27	NA	0.4	0.4	NA	NA	NA	NA	NA	Spinel
HLW02-33	Yes	NA	NA	NA	NA	5.8	NA	2.74	0.14,1,5,1.7	NA	NA	NA	NA	NA	Spinel
HLW02-34	Yes	NA	NA	NA	NA	6.2	NA	2.46	0.11,0.6,1.5	NA	NA	NA	NA	NA	Spinel
HLW02-35	Yes	NA	NA	NA	NA	7.2	NA	NA	1.7,2.3	0.8	NA	NA	NA	NA	Spinel

Table 6.1. Temperature and Volume %-Crystallinity Data for IHLW Phase 1 Combined Matrix Glasses (continued).

Glass ID	Retained for Model Development	Temperature in (°C)													Crystal
		650	700	750	800	850[b]	875	900[b]	950[b]	1000[b]	1050	1100	1150	1200	
HLW02-36	Yes	NA[a]	NA	1.9	NA	1.4	NA	0.3, 0.6	0.8	NA	NA	NA	NA	NA	Spinel
HLW02-37	Yes	NA	NA	NA	NA	2.9	NA	2.1	0.8	NA	0.6	NA	NA	NA	Spinel
HLW02-38	Yes	NA	NA	NA	NA	2.7	NA	1.25	1.61, 1.5	NA	0.2	NA	NA	NA	Spinel
HLW02-39	Yes	NA	NA	NA	NA	2.5	NA	1.79	1.95, 1.6	NA	0.2	NA	NA	NA	Spinel
HLW02-40	Yes	NA	NA	4	NA	1.95	NA	NA	1.6	0.4	NA	NA	NA	NA	Spinel
HLW02-41	Yes	NA	NA	NA	NA	2.4	NA	1.04	0.6, 0.6	NA	0.1	NA	NA	NA	Spinel
HLW02-42	Yes	NA	2.1	1.1	NA	0.66	NA	0.3	0.5	NA	NA	NA	NA	NA	Spinel
HLW02-43	Yes	NA	NA	NA	NA	2.6	NA	0.58	0.31, 0.9	NA	NA	NA	NA	NA	Spinel
HLW02-44	Yes	NA	NA	1.3	1.1	0.8	NA	0.57	NA	NA	NA	NA	NA	NA	Spinel
HLW02-45	Yes	NA	NA	NA	NA	2.4	NA	0.95	0.8	NA	NA	NA	NA	NA	Spinel
HLW02-46	Yes	NA	NA	NA	NA	2.9	NA	1.6	1.07, 0.9	NA	0.2	NA	NA	NA	Spinel
HLW02-47	No	4.5	4.9	NA	2.4	0.8	NA	NA	NA	NA	NA	NA	NA	NA	Spinel
HLW02-48	Yes	NA	NA	2.7	NA	1.5	NA	NA	1.4	0.7	NA	NA	NA	NA	Spinel
HLW02-49	Yes	NA	NA	NA	NA	3.68	NA	1.73	2.1,0.9,2.4	NA	0.8	NA	NA	NA	Spinel
HLW02-50	Yes	NA	NA	NA	NA	5.3	NA	1.96	1.52, 0.8	NA	0.9	NA	NA	NA	Spinel
HLW02-51	Yes	NA	NA	NA	NA	2	1.2	0.8	0.8	NA	NA	NA	NA	NA	Spinel
HLW02-52	Yes	NA	NA	2.5	NA	1.3	NA	2.1	1.2	NA	0.4	NA	NA	NA	Spinel
HLW02-53	Yes	NA	NA	NA	NA	2.1	NA	1.4, 1.4	1.0, 0.8	0.4, 0.9	NA	NA	NA	NA	Spinel
HLW02-54	Yes	NA	NA	NA	NA	2.6	NA	1.1	0.1	NA	NA	NA	NA	NA	Spinel
HLW02-55	Yes	NA	1.9	1.1	NA	1.4	NA	NA	0.2	NA	NA	NA	NA	NA	Spinel
HLW02-56	Yes	NA	1.4	0.9	NA	1	NA	0.4	0.5	NA	NA	NA	NA	NA	Spinel
HLW02-57	Yes	NA	1.3	0.9	NA	0.3	NA	NA	NA	NA	NA	NA	NA	NA	Spinel
HLW03-01	No	NA	NA	13	NA	10	NA	NA	1.4	NA	2.2	1.1	0.7	NA	Spinel
HLW03-02	Yes	NA	NA	NA	NA	7.3	NA	NA	4.6, 2.9	NA	2	3.3	3.3	4	Spinel +ZrO2
HLW03-03	Yes	NA	NA	NA	NA	NA	NA	NA	2.6, 2.8	NA	2.5	NA	2	0.05	Spinel
HLW03-04	Yes	NA	NA	NA	8.3	2.4, 2.8	NA	NA	0.6	NA	0.4	NA	NA	NA	Spinel
HLW03-05	Yes	NA	NA	NA	NA	2.1	NA	1.2	0.5	NA	NA	NA	NA	NA	Spinel
HLW03-06	Yes	NA	NA	NA	NA	NA	NA	2.0, 1.9	1.0, 0.9	0.9	NA	NA	NA	NA	Spinel
HLW03-07	Yes	NA	NA	9.9	NA	6.2	NA	NA	6	NA	4.2	NA	2.9	1	Spinel
HLW03-08	No	NA	NA	NA	NA	NA	NA	NA	12.2	NA	6.6	7.3	9.8	4.2	ZrO2
HLW03-09	No	0.2	NA	0.1	NA	0.2	NA	NA	0.1	NA	NA	NA	NA	NA	Noble Metal
HLW03-10	No	NA	NA	10.3	NA	12.5	NA	NA	8.7	NA	3.7	2.9	3.5	1.4	Spinel+ZrO_2 (ThO_2)
HLW03-11	No	0.4	NA	0.4	NA	0.3	NA	NA	0.2	NA	NA	NA	NA	NA	ThO_2+ Noble metal
HLW03-12	Yes	NA	NA	1.2	NA	0.7	NA	0.8	0.6	NA	NA	NA	NA	NA	Spinel
HLW03-13	Yes	NA	NA	NA	NA	7.9	NA	NA	5.3	NA	5	NA	3.5	0.6	Spinel + ThO_2 (UO_2)

Table 6.1. Temperature and Volume %-Crystallinity Data for IHLW Phase 1 Combined Matrix Glasses (continued).

Glass ID	Retained for Model Development	Temperature in (°C)													Crystal
		650	700	750	800	850[b]	875	900[b]	950[b]	1000[b]	1050	1100	1150	1200	
HLW03-14	Yes	NA[a]	NA	NA	NA	4.6	NA	NA	3.5, 2.9	1.5	2.2	0.5	NA	NA	Spinel + ZrO_2
HLW03-15	Yes	NA	NA	NA	NA	NA	NA	NA	2.7	NA	0.9	0.3	NA	NA	Spinel + ThO_2
HLW03-16	Yes	NA	NA	4.6	NA	2.8, 2.8	NA	NA	1.9	NA	0.9	NA	NA	NA	Spinel
HLW03-17	Yes	NA	NA	NA	NA	5.7	NA	NA	2.4, 1.7	NA	0.5	NA	NA	NA	Spinel
HLW03-18	Yes	NA	NA	NA	NA	2.4	NA	NA	0.5, 0.7	NA	0.5	NA	NA	NA	Spinel
HLW03-19	Yes	NA	NA	NA	NA	1.5	NA	NA	0.8	NA	0.6	NA	NA	NA	Spinel
HLW03-20	Yes	NA	NA	NA	NA	1	NA	1	0.3	NA	NA	NA	NA	NA	Spinel
HLW03-21	Yes	NA	NA	NA	2	1	NA	0.3	0.2	NA	NA	NA	NA	NA	Spinel
HLW03-22	Yes	NA	NA	4.4	NA	2.3	NA	0.6	0.5	NA	NA	NA	NA	NA	Spinel
HLW03-23	Yes	NA	NA	1.5	1.3	0.9, 0.6	NA	NA	0.4	NA	NA	NA	NA	NA	Spinel
HLW03-24	Yes	NA	NA	2.3	1.6	0,6, 0.4	NA	NA	NA	NA	NA	NA	NA	NA	Spinel
HLW03-25	Yes	NA	NA	1.6	0.2	0.2	NA	NA	0.1	NA	NA	NA	NA	NA	Spinel
HLW03-26	Yes	NA	NA	1.2	1	0.8	NA	0.4	0.3	NA	NA	NA	NA	NA	Spinel + ThO_2
HLW03-27	Yes	NA	NA	NA	NA	1.7	NA	NA	1.6	NA	0.6	NA	NA	NA	Spinel + ThO_2
HLW03-28	Yes	NA	NA	1.4	1.3	1.0, 0.5	NA	NA	0.2	NA	NA	NA	NA	NA	Spinel
HLW03-29	Yes	NA	NA	1.4	1.7	0.7	NA	NA	0.4	NA	NA	NA	NA	NA	Spinel
HLW03-30	Yes	NA	NA	1	0.9	0.6	NA	NA	0.2	NA	NA	NA	NA	NA	Spinel
HLW03-31	No	NA	NA	2.6	NA	2.4	NA	NA	1.6	1.8	0.7	NA	0.9	NA	Spinel + ZrO_2
HLW03-32	No	NA	NA	5	NA	4.6	NA	3.6	1.6	NA	2	1.5	NA	NA	Spinel + ZrO_2
HLW03-33	No	NA	NA	5.5	NA	2.7	NA	NA	3.9	NA	1.8	NA	1.1	NA	$ZrSiO_4$+ThO_2+Spinel
HLW03-34	No	NA	NA	NA	3	1.7	NA	NA	1	NA	0.3	NA	NA	NA	ThO_2 + Spinel
HLW03-35	No	NA	NA	NA	NA	NA	NA	NA	6.2	NA	3	2.4	0.4	NA	$ZrSiO_4$+ThO_2+ZrO_2
HLW03-36	No	NA	NA	NA	NA	10	NA	NA	6.1	NA	3.4	NA	3.5	0.1	$ZrSiO_4$ (ThO_2) + Spinel
HLW03-37	Yes	NA	NA	NA	NA	1.9	NA	0.9	0.3	NA	NA	NA	NA	NA	Spinel
HLW03-38	Yes	NA	NA	6.5	NA	3.8	NA	NA	2.5	NA	1.4	2	NA	NA	Spinel + ZrO_2
HLW03-39	Yes	NA	NA	2.8	NA	1.8	NA	NA	0.4	NA	NA	NA	NA	NA	Spinel
HLW03-40	Yes	NA	NA	5.6	NA	2.5	NA	NA	1.3	NA	0.4	NA	NA	NA	Spinel + ThO_2
HLW03-41	Yes	NA	NA	NA	1.5	0.8	NA	NA	0.4	NA	NA	NA	NA	NA	Spinel
HLW03-42	Yes	NA	NA	NA	NA	3	NA	NA	1.2, 1.1	NA	0.3	NA	NA	NA	Spinel
HLW03-43	Yes	NA	NA	NA	NA	1.8	NA	1.6	0.6	0.9	NA	NA	NA	NA	Spinel
HLW03-44	No	0.3	NA	NA	NA	0.1	NA	NA	0.1	NA	NA	NA	NA	NA	Noble Metal
HLW03-45	Yes	NA	NA	NA	1.3	1.3	NA	0.3	NA	NA	NA	NA	NA	NA	Spinel + ThO_2

[a] NA indicates that no volume %-crystallinity data were collected for specified temperatures.
[b] More than one set of data were collected for selected glasses at these temperatures. All data were used in regression.

Table 6.2. Intercepts, Slopes, Predicted $T_{1\%}$ (Spinel) Values, Standard Deviations of $T_{1\%}$ Values, and Number of Temperature vs. Vol%-Crystallinity Points for IHLW Phase 1 Combined Matrix Glasses.

Glass ID	Retained for $T_{1\%}$ Model Development	Intercept[a]	Slope[a]	Estimated $T_{1\%}$ (Spinel) (°C)	SD($T_{1\%}$) (°C)	Number of Points	$T_{1\%}$ Data Splitting Validation Set
HLW02-01	Yes	980.50[b]	-74.69[b]	905.8[b]	6.46[b]	4	NA [g]
HLW02-02	Yes	1012.50	-125.00	887.5	21.65	3	1
HLW02-03	Yes	957.46	-119.40	838.1	17.47	3	2
HLW02-04	Yes	853.06	-4.23	848.8	4.02	4	NA [g]
HLW02-05	No	NA [c]	NA [c]	NA [c]	NA [c]	4	NA [d]
HLW02-06	Yes	1073.28	-46.60	1026.7	14.78	5	5
HLW02-07	Yes	1066.48	-302.20	764.3	19.81	4	1
HLW02-08	Yes	964.84	-181.32	783.5	5.52	3	NA [g]
HLW02-09	Yes	984.27	-26.34	957.9	24.71	5	1
HLW02-10	No	926.89	-372.64	554.2	112.16	5	NA [f]
HLW02-11	Yes	968.40	-152.10	816.3	17.56	4	1
HLW02-12	Yes	1106.76	-59.80	1047.0	11.36	3	4
HLW02-13	Yes	993.53	-25.67	967.9	33.96	5	3
HLW02-14	No	1029.17	-83.33	945.8	20.08	4	NA [e]
HLW02-15	Yes	1119.38	-69.95	1049.4	15.02	4	3
HLW02-16	Yes	1017.04	-34.27	982.8	21.99	5	1
HLW02-17	Yes	1035.03	-68.17	966.9	13.82	5	NA [g]
HLW02-18	Yes	1117.86	-160.71	957.1	25.75	3	3
HLW02-19	Yes	983.79	-63.48	920.3	12.07	5	1
HLW02-20	Yes	958.02	-16.63	941.4	18.63	4	5
HLW02-21	No	NA [c]	NA [c]	NA [c]	NA [c]	3	NA [d]
HLW02-22	Yes	1030.78	-93.28	937.5	35.73	4	2
HLW02-23	Yes	1012.50	-66.67	945.8	6.59	4	3
HLW02-24	Yes	980.12	-57.92	922.2	6.77	3	5
HLW02-25	Yes	950.00	-42.86	907.1	31.94	3	5
HLW02-26	Yes	1011.84	-42.32	969.5	11.26	5	2
HLW02-27	Yes	1048.20	-82.10	966.1	14.34	5	4
HLW02-28	Yes	1010.37	-85.37	925.0	8.28	4	4
HLW02-29	Yes	1003.13	-48.14	955.0	14.56	6	4
HLW02-30	Yes	1016.67	-119.05	897.6	31.41	3	5
HLW02-31	Yes	999.98	-203.23	796.7	27.96	4	4
HLW02-32	Yes	937.78	-137.06	800.7	40.94	5	3
HLW02-33	Yes	967.39	-19.94	947.4	9.06	5	1
HLW02-34	Yes	958.60	-17.75	940.8	7.18	5	1
HLW02-35	Yes	1001.98	-21.49	980.5	9.99	4	2
HLW02-36	Yes	969.40	-99.40	870.0	20.98	5	3
HLW02-37	Yes	1051.47	-71.23	980.2	25.51	4	3
HLW02-38	Yes	1049.09	-75.13	974.0	18.70	5	1
HLW02-39	Yes	1071.30	-81.65	989.6	16.41	5	4
HLW02-40	Yes	1028.87	-71.13	957.7	23.79	4	2
HLW02-41	Yes	1012.25	-76.22	936.0	16.61	5	3
HLW02-42	Yes	951.15	-129.99	821.2	23.68	5	NA [g]
HLW02-43	Yes	955.36	-39.06	916.3	15.97	4	4
HLW02-44	Yes	1013.24	-199.73	813.5	2.95	4	NA [g]
HLW02-45	Yes	970.86	-51.23	919.6	19.63	3	2
HLW02-46	Yes	1032.92	-69.66	963.3	13.11	5	NA [g]
HLW02-47	No	892.14	-45.12	847.0	29.90	4	NA [h]
HLW02-48	Yes	1086.52	-126.36	960.2	28.14	4	5
HLW02-49	Yes	1036.12	-48.81	987.3	26.13	6	5
HLW02-50	Yes	1006.15	-31.56	974.6	28.25	5	5
HLW02-51	Yes	968.75	-62.50	906.3	15.83	4	1
HLW02-52	Yes	1077.78	-118.52	959.3	34.32	5	NA [g]
HLW02-53	Yes	1044.28	-94.99	949.3	8.52	7	NA [g]
HLW02-54	Yes	950.00	-39.47	910.5	4.84	3	NA [g]
HLW02-55	Yes	964.71	-132.35	832.4	36.51	4	NA [g]
HLW02-56	Yes	1018.10	-223.93	794.2	28.67	5	NA [g]
HLW02-57	Yes	892.76	-151.32	741.4	5.05	3	NA [g]

Table 6.2. Intercepts, Slopes, Predicted $T_{1\%}$ (Spinel) Values, Standard Deviations of $T_{1\%}$ Values, and Number of Temperature vs. Vol%-Crystallinity Points for IHLW Phase 1 Combined Matrix Glasses (continued).

Glass ID	Retained for $T_{1\%}$ Model Development	Intercept[a]	Slope[a]	Estimated $T_{1\%}$(Spinel) (°C)	SD($T_{1\%}$) (°C)	Number of Points	$T_{1\%}$ Data Splitting Validation Set
HLW03-01	No	1100.22	-26.45	1073.8	35.06	6	NA [h]
HLW03-02	Yes	1198.60	-41.61	1157.0	89.51	7	3
HLW03-03	Yes	1230.17	-85.51	1144.7	44.47	5	4
HLW03-04	Yes	970.80	-24.41	946.4	38.69	5	2
HLW03-05	Yes	978.76	-62.18	916.6	3.17	3	3
HLW03-06	Yes	1028.83	-66.29	962.5	12.08	5	NA [g]
HLW03-07	Yes	1268.10	-54.92	1213.2	33.53	6	2
HLW03-08	No	1270.28	-22.48	1247.8	94.80	5	NA [e]
HLW03-09	No	950.00	-1000.00	-50.0	1204.16	4	NA [d]
HLW03-10	No	1225.22	-35.50	1189.7	42.20	7	NA [h]
HLW03-11	No	1213.64	-1272.73	-59.1	214.17	4	NA [d]
HLW03-12	Yes	1106.02	-295.18	810.8	27.47	4	2
HLW03-13	Yes	1265.24	-50.50	1214.7	42.87	5	1
HLW03-14	Yes	1125.22	-56.01	1069.2	21.82	6	1
HLW03-15	Yes	1112.50	-60.90	1051.6	5.90	3	2
HLW03-16	Yes	1102.60	-81.77	1020.8	19.59	5	1
HLW03-17	Yes	1040.06	-34.98	1005.1	19.44	4	2
HLW03-18	Yes	1026.45	-74.58	951.9	27.01	4	5
HLW03-19	Yes	1144.78	-201.49	943.3	25.03	3	4
HLW03-20	Yes	982.14	-107.14	875.0	25.00	3	2
HLW03-21	Yes	939.54	-73.76	865.8	12.70	4	4
HLW03-22	Yes	951.27	-45.52	905.7	13.35	4	2
HLW03-23	Yes	981.22	-150.23	831.0	13.73	5	3
HLW03-24	Yes	877.82	-53.33	824.5	4.40	4	4
HLW03-25	Yes	882.88	-86.43	796.4	45.18	4	5
HLW03-26	Yes	1000.00	-202.70	797.3	8.41	5	NA [g]
HLW03-27	Yes	1143.24	-148.65	994.6	40.74	3	3
HLW03-28	Yes	956.18	-132.02	824.2	15.52	5	5
HLW03-29	Yes	965.14	-121.56	843.6	26.98	4	1
HLW03-30	Yes	996.45	-235.48	761.0	10.06	4	2
HLW03-31	No	1242.38	-170.43	1072.0	35.95	6	NA [h]
HLW03-32	No	1162.43	-75.11	1087.3	43.85	6	NA [h]
HLW03-33	No	1188.52	-79.51	1109.0	63.45	5	NA [e]
HLW03-34	No	1050.06	-91.71	958.4	23.07	4	NA [e]
HLW03-35	No	1167.91	-35.14	1132.8	10.29	4	NA [e]
HLW03-36	No	1211.33	-37.08	1174.2	32.79	5	NA [e]
HLW03-37	Yes	963.27	-61.22	902.0	5.84	3	4
HLW03-38	Yes	1152.82	-65.68	1087.1	43.44	5	5
HLW03-39	Yes	987.61	-82.57	905.0	9.45	3	3
HLW03-40	Yes	1033.20	-54.37	978.8	28.91	4	4
HLW03-41	Yes	982.80	-129.03	853.8	21.67	3	5
HLW03-42	Yes	1046.92	-69.23	977.7	13.79	4	NA [g]
HLW03-43	Yes	1042.12	-95.61	946.5	23.51	4	NA [g]
HLW03-44	No	1025.00	-1250.00	-225.0	363.15	3	NA [d]
HLW03-45	Yes	922.50	-75.00	847.5	20.46	3	NA [g]

[a] The intercept and slope are from fitting the model in Equation (6.1) to the temperature versus spinel percent crystallinity data for each glass as given in Table 6.1.

[b] Estimated $T_{1\%}$ values in this table have been rounded to one decimal place; intercepts, slopes, and standard deviations have been rounded to two decimal places.

[c] NA entries result when volume %-crystallinity values are the same over all available temperatures for a particular glass melt. In such cases, regression cannot be used to obtain slope, intercept, and estimated $T_{1\%}$ values. Furthermore, the standard deviation of the $T_{1\%}$ values cannot be calculated.

[d] Glasses that had undetermined $T_{1\%}$ values.

[e] Glasses that had non-spinel primary phases.

[f] Glass was removed from model development dataset because it had an unusually low $T_{1\%}$ value.

[g] Glasses not included in data splitting validation sets because they were replicates. These glasses were included in the modeling splits rather than the validation splits.

[h] Glasses dropped as outliers from initial regression involving linear mixture model with 19 components.

Table 6.3. $T_{1\%}$ (Spinel) Data and Standard Deviations for Replicates Among IHLW Phase 1 Combined Matrix Glasses.

Glass IDs of Replicate Pairs	Retained For $T_{1\%}$ (Spinel) Model Development	Estimated $T_{1\%}$ (Spinel) Values and SDs (ºC)
HLW02-52	Yes	959.3[(a)]
HLW02-01	Yes	905.8
		SD = 37.79[(a)]
HLW02-53	Yes	949.3
HLW02-17	Yes	966.9
		SD = 12.43
HLW02-54	Yes	910.5
HLW02-04	Yes	848.8
		SD = 43.62
HLW02-55	Yes	832.4
HLW02-42	Yes	821.2
		SD = 7.91
HLW02-56	Yes	794.2
HLW02-44	Yes	813.5
		SD = 13.68
HLW02-57	Yes	741.4
HLW02-08	Yes	783.5
		SD = 29.75
HLW03-42	Yes	977.7
HLW02-46	Yes	963.3
		SD = 10.20
HLW03-43	Yes	946.5
HLW03-06	Yes	962.5
		SD = 11.33
HLW03-44	No	NA [(b)]
HLW03-11	No	NA [(b)]
HLW03-45	Yes	847.5
HLW03-26	Yes	797.3
		SD = 35.50
Pooled Over 9 Replicate Pairs Used In (Spinel) $T_{1\%}$ Model Development		**SD = 26.06**

(a) Estimated $T_{1\%}$ values in this table have been rounded to one decimal place; standard deviations have been rounded to two decimal places.

(b) These glasses had undetermined $T_{1\%}$ values. The volume %-crystallinity values were less than 1% at all temperatures observed. As noted, these glasses were not retained for $T_{1\%}$ model development

Table 6.4. Compositions of IHLW $T_{1\%}$ (Spinel) Validation Glasses, 19 Normalized[(a)] Components Wt%.

Glass ID	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike	Retained For Validation Analysis
MS-7a	8.048	7.042	0.000	0.302	11.569	4.567	0.503	15.392	0.956	0.000	0.000	45.584	0.000	0.000	0.000	0.000	0.000	6.036	0.000	Yes
MS-7d	8.048	7.042	0.000	0.302	11.569	4.567	0.503	15.392	0.956	0.000	0.000	45.584	0.000	0.000	0.000	0.000	0.000	6.036	0.000	Yes
MS-7e	8.048	7.042	0.000	0.302	11.569	4.567	0.503	15.392	0.956	0.000	0.000	45.584	0.000	0.000	0.000	0.000	0.000	6.036	0.000	Yes
MS7-H-Al	11.065	6.810	0.000	0.292	11.196	4.416	0.483	14.888	0.925	0.000	0.000	44.090	0.000	0.000	0.000	0.000	0.000	5.834	0.000	Yes
MS7-L-Al	5.032	7.276	0.000	0.312	11.885	4.720	0.523	15.910	0.986	0.000	0.000	47.117	0.000	0.000	0.000	0.000	0.000	6.239	0.000	Yes
MS7-H-Cr	7.948	7.042	0.000	0.503	11.559	4.557	0.503	15.372	0.956	0.000	0.000	45.533	0.000	0.000	0.000	0.000	0.000	6.026	0.000	Yes
MS7-L-Cr	8.069	7.053	0.000	0.101	11.591	4.578	0.503	15.424	0.956	0.000	0.000	45.679	0.000	0.000	0.000	0.000	0.000	6.047	0.000	Yes
MS7-L-Fe	8.371	7.325	0.000	0.312	8.049	4.749	0.523	16.008	0.996	0.000	0.000	47.389	0.000	0.000	0.000	0.000	0.000	6.278	0.000	Yes
MS7-H-Li	7.926	6.930	0.000	0.302	11.386	6.035	0.493	15.158	0.945	0.000	0.000	44.880	0.000	0.000	0.000	0.000	0.000	5.944	0.000	Yes
MS7-L-Li	8.179	7.153	0.000	0.302	11.761	3.018	0.513	15.644	0.976	0.000	0.000	46.318	0.000	0.000	0.000	0.000	0.000	6.137	0.000	Yes
MS7-H-Mg	8.051	7.041	0.000	0.299	11.566	4.567	0.505	15.390	0.959	0.000	0.000	45.583	0.000	0.000	0.000	0.000	0.000	6.041	0.000	Yes
MS7-L-Mg	8.050	7.040	0.000	0.300	11.570	4.570	0.500	15.390	0.960	0.000	0.000	45.580	0.000	0.000	0.000	0.000	0.000	6.040	0.000	Yes
MS7-H-Na	7.785	6.820	0.000	0.292	11.195	4.426	0.483	18.105	0.925	0.000	0.000	44.126	0.000	0.000	0.000	0.000	0.000	5.844	0.000	Yes
MS7-L-Na	8.362	7.315	0.000	0.312	12.025	4.749	0.523	12.075	0.996	0.000	0.000	47.374	0.000	0.000	0.000	0.000	0.000	6.269	0.000	Yes
MS7-H-Ni	7.977	6.981	0.000	0.302	11.468	4.527	0.503	15.260	1.811	0.000	0.000	45.187	0.000	0.000	0.000	0.000	0.000	5.985	0.000	Yes
MS7-L-Ni	8.099	7.093	0.000	0.302	11.650	4.598	0.503	15.493	0.302	0.000	0.000	45.885	0.000	0.000	0.000	0.000	0.000	6.076	0.000	Yes
SP-Al-1	4.143	7.561	0.756	0.238	13.506	3.242	0.394	16.996	0.559	0.093	0.093	49.726	0.031	0.000	0.000	0.000	0.041	1.999	0.621	Yes
SP-Cr-1-o	8.294	7.260	0.724	0.000	12.958	3.113	0.372	16.308	0.538	0.093	0.093	47.673	0.031	0.000	0.000	0.000	0.041	1.913	0.589	Yes
SP-Cr-1-r	8.294	7.260	0.724	0.000	12.958	3.113	0.372	16.308	0.538	0.093	0.093	47.673	0.031	0.000	0.000	0.000	0.041	1.913	0.589	Yes
SP-Li-3-o	8.273	7.239	0.724	0.228	12.927	3.102	0.372	16.267	0.538	0.093	0.093	47.570	0.031	0.000	0.000	0.000	0.041	1.913	0.589	Yes
SP-Li-3-r	8.273	7.239	0.724	0.228	12.927	3.102	0.372	16.267	0.538	0.093	0.093	47.570	0.031	0.000	0.000	0.000	0.041	1.913	0.589	Yes
SP-Mg-1	8.275	7.237	0.716	0.228	12.927	3.105	0.374	16.270	0.540	0.093	0.093	47.565	0.031	0.000	0.000	0.000	0.042	1.910	0.592	Yes
SP-Mn-1	8.305	7.271	0.724	0.228	12.980	3.113	0.000	16.331	0.538	0.093	0.093	47.751	0.031	0.000	0.000	0.000	0.041	1.913	0.590	Yes
SP-Mn-3	7.963	6.961	0.692	0.217	12.435	2.985	4.131	15.658	0.516	0.093	0.093	45.765	0.031	0.000	0.000	0.000	0.041	1.838	0.578	Yes
SP-Na-1	9.057	7.926	0.788	0.249	14.161	3.403	0.405	8.300	0.591	0.104	0.104	52.090	0.031	0.000	0.000	0.000	0.041	2.096	0.654	Yes
SP-Na-3	7.836	6.866	0.681	0.217	12.255	2.942	0.351	20.648	0.506	0.083	0.093	45.075	0.031	0.000	0.000	0.000	0.041	1.807	0.568	Yes
SPA-18	6.578	8.968	0.000	0.329	15.349	4.155	1.096	17.421	0.548	0.033	0.066	38.965	1.557	0.000	0.000	0.000	1.085	3.289	0.559	No
SPA-38	8.273	7.239	0.724	0.228	12.927	3.102	0.372	16.267	0.538	0.083	0.093	47.580	0.031	0.000	0.000	0.000	0.041	1.913	0.589	Yes
WTP-TL-16	11.160	15.218	1.015	0.507	13.189	6.087	5.073	4.058	0.000	0.071	0.122	40.641	0.000	0.000	0.000	0.000	2.536	0.000	0.325	Yes
WTP-TL-17	11.160	15.218	0.000	0.507	6.655	0.000	0.000	15.218	1.015	0.071	0.122	38.551	8.623	0.000	0.000	0.000	2.536	0.000	0.325	Yes
WTP-TL-19	2.029	15.218	1.015	0.507	3.044	0.000	5.073	15.218	1.015	0.071	0.122	50.279	0.000	0.000	0.000	0.000	0.000	6.087	0.325	Yes
WTP-TL-20	2.029	4.058	1.015	0.507	13.189	6.087	0.000	4.058	1.015	0.071	0.122	50.279	8.623	0.000	0.000	0.000	2.536	6.087	0.325	Yes
WTP-TL-21	2.029	4.058	1.015	0.507	13.190	0.020	5.073	15.219	0.000	0.071	0.122	53.764	2.070	0.000	0.000	0.000	2.537	0.000	0.325	Yes
WTP-TL-23	8.877	6.848	0.761	0.386	8.045	4.565	3.804	6.848	0.761	0.071	0.122	49.964	6.473	0.000	0.000	0.000	0.629	1.522	0.325	Yes
WTP-TL-24	4.312	6.848	0.254	0.122	10.652	1.522	3.804	11.342	0.761	0.071	0.122	49.964	6.473	0.000	0.000	0.000	1.907	1.522	0.325	Yes
WTP-TL-27	8.877	12.428	0.254	0.122	10.652	4.565	3.804	6.848	0.254	0.071	0.122	43.056	2.151	0.000	0.000	0.000	1.907	4.565	0.325	Yes
WTP-TL-28	4.312	6.848	0.254	0.122	10.652	4.565	3.804	6.848	0.254	0.071	0.122	48.879	6.473	0.000	0.000	0.000	1.907	4.565	0.325	Yes
WTP-TL-29	4.312	12.428	0.761	0.386	10.652	1.522	3.804	6.848	0.254	0.071	0.122	49.964	5.275	0.000	0.000	0.000	0.629	2.648	0.325	Yes
WTP-TL-30	8.877	12.428	0.254	0.386	5.580	4.565	1.603	6.848	0.761	0.071	0.122	49.559	2.151	0.000	0.000	0.000	1.907	4.565	0.325	Yes

[(a)] Normalized to sum to 100% over the 19 components listed in this table.

Table 6.5. Temperature and Volume %-Crystallinity Data for IHLW $T_{1\%}$ (Spinel) Validation Glasses.

Glass ID	Vol%	Temp
MS-7a	1.19	864
MS-7a	1.13	893
MS-7a	0.93	934
MS-7a	0.7	971
MS-7a	0.5	1014
MS-7a	0.11	1062
MS-7d	0.74	959
MS-7d	0.52	1000
MS-7d	0.33	1045
MS-7d	0.51	1011
MS-7d	0.62	985
MS-7d	0.81	919
MS-7e	1.83	734
MS-7e	1.83	734
MS-7e	1.91	750
MS-7e	1.8	750
MS-7e	1.75	801
MS-7e	1.62	801
MS-7e	1.56	801
MS-7e	1.45	801
MS-7e	1.42	801
MS-7e	1.74	801
MS-7e	1.39	853
MS-7e	1.11	853
MS-7e	1.17	853
MS-7e	1.5	853
MS-7e	1.49	853
MS-7e	1.22	928
MS-7e	0.85	950
MS-7e	0.94	950
MS-7e	0.68	977
MS-7e	0.46	1005
MS-7e	0.12	1039
MS-7e	0.21	1052
MS7-H-Al	3.24	730
MS7-H-Al	2.68	839
MS7-H-Al	2.4	946
MS7-H-Al	1.62	987
MS7-H-Al	1.43	997
MS7-H-Al	1.14	1040
MS7-H-Al	0.59	1092
MS7-H-Al	0.36	1118
MS7-H-Cr	2.83	730
MS7-H-Cr	2.01	875
MS7-H-Cr	1.74	905

Glass ID	Vol%	Temp
MS7-H-Cr	1.49	949
MS7-H-Cr	1.07	1000
MS7-H-Cr	0.55	1047
MS7-H-Cr	0.19	1096
MS7-H-Li	2.95	705
MS7-H-Li	1.72	839
MS7-H-Li	1.28	905
MS7-H-Li	0.85	925
MS7-H-Li	0.97	942
MS7-H-Li	0.56	987
MS7-H-Li	0.11	1047
MS7-H-Mg	2.89	808
MS7-H-Mg	2.23	924
MS7-H-Mg	1.92	946
MS7-H-Mg	1.56	1000
MS7-H-Mg	0.87	1060
MS7-H-Mg	0.2	1133
MS7-H-Na	2.37	750
MS7-H-Na	1.36	860
MS7-H-Na	0.92	905
MS7-H-Na	0.32	969
MS7-H-Ni	4.02	808
MS7-H-Ni	4.01	812
MS7-H-Ni	3.86	840
MS7-H-Ni	3.86	870
MS7-H-Ni	3.49	915
MS7-H-Ni	3.61	930
MS7-H-Ni	2.75	1000
MS7-H-Ni	2.52	1041
MS7-H-Ni	1.48	1047
MS7-H-Ni	1.69	1060
MS7-H-Ni	0.55	1133
MS7-H-Ni	2.03	1000
MS7-H-Ni	2.77	915
MS7-H-Ni	3.42	808
MS7-L-Al	1.72	798
MS7-L-Al	1.0	875
MS7-L-Al	0.98	919
MS7-L-Al	0.39	964
MS7-L-Al	0.17	1000
MS7-L-Cr	2.71	730
MS7-L-Cr	1.79	860
MS7-L-Cr	1.3	905
MS7-L-Cr	1.1	925
MS7-L-Cr	0.59	969

Glass ID	Vol%	Temp
MS7-L-Cr	0.22	1006
MS7-L-Fe	1.76	808
MS7-L-Fe	1.53	840
MS7-L-Fe	0.76	919
MS7-L-Fe	0.39	946
MS7-L-Fe	0.39	960
MS7-L-Fe	0.16	1000
MS7-L-Li	2.63	750
MS7-L-Li	1.94	875
MS7-L-Li	1.65	919
MS7-L-Li	1.77	949
MS7-L-Li	1.34	964
MS7-L-Li	1.09	1000
MS7-L-Li	0.24	1096
MS7-L-Mg	2.14	808
MS7-L-Mg	1.96	854
MS7-L-Mg	1.53	924
MS7-L-Mg	1.03	997
MS7-L-Mg	0.21	1046
MS7-L-Na	3.7	728
MS7-L-Na	3.37	860
MS7-L-Na	2.94	905
MS7-L-Na	2.75	919
MS7-L-Na	1.93	969
MS7-L-Na	1.35	1006
MS7-L-Na	0.83	1092
MS7-L-Na	0.79	1118
MS7-L-Na	0.44	1155
MS7-L-Na	2.11	949
MS7-L-Na	1.68	1019
MS7-L-Ni	1.32	750
MS7-L-Ni	0.82	860
MS7-L-Ni	0.43	919
MS7-L-Ni	0.16	949
MS7-L-Ni	0.19	964
MS7-L-Ni	0.12	1006
SPA-18	0.99	875
SPA-18	0.69	900
SPA-18	0.59	926
SPA-18	0.24	951
SPA-38	1.05	851
SPA-38	0.65	901
SPA-38	0.32	951
SPA-38	0.21	975
SPA-38	0.15	1003

Glass ID	Vol%	Temp
SP-Al-1	0.1	952
SP-Al-1	0.19	898
SP-Al-1	0.33	854
SP-Al-1	0.6	808
SP-Al-1	0.82	717
SP-Cr-1-o	0.18	897
SP-Cr-1-o	0.38	848
SP-Cr-1-o	0.59	797
SP-Cr-1-o	0.92	744
SP-Cr-1-o	0.83	701
SP-Cr-1-r	0.29	897
SP-Cr-1-r	0.61	848
SP-Cr-1-r	0.95	797
SP-Cr-1-r	1.5	744
SP-Cr-1-r	1.34	701
SP-Li-3-o	0.72	938
SP-Li-3-o	0.77	892
SP-Li-3-o	1.08	793
SP-Li-3-o	1.71	740
SP-Li-3-r	0.27	951
SP-Li-3-r	0.47	897
SP-Li-3-r	1.39	737
SP-Li-3-r	1.35	701
SP-Mg-1	0.07	1028
SP-Mg-1	0.57	952
SP-Mg-1	0.96	898
SP-Mg-1	1.39	854
SP-Mg-1	1.81	808
SP-Mn-1	0.47	1028
SP-Mn-1	1.12	952
SP-Mn-1	0.78	943
SP-Mn-1	1.37	852
SP-Mn-1	1.66	808
SP-Mn-3	0.42	1028
SP-Mn-3	1.02	952
SP-Mn-3	1.29	900
SP-Mn-3	1.69	898
SP-Mn-3	2.17	854
SP-Mn-3	2.58	808
SP-Mn-3	2.84	736
SP-Na-1	1.19	1125
SP-Na-1	1.73	1028
SP-Na-1	2.84	952
SP-Na-1	3.74	898
SP-Na-1	4.57	808

Glass ID	Vol%	Temp
SP-Na-3	0.7	898
SP-Na-3	0.89	852
SP-Na-3	1.03	808
SP-Na-3	1.31	717
WTP-TL-16	2.35	1001
WTP-TL-16	1.55	1100
WTP-TL-16	0.93	1200
WTP-TL-16	0.46	1251
WTP-TL-16	0.36	1275
WTP-TL-17	0.56	894
WTP-TL-17	0.31	1002
WTP-TL-17	0.1	1100
WTP-TL-17	1.08	802
WTP-TL-17	0.05	1140
WTP-TL-19	0.87	894
WTP-TL-19	0.26	1002
WTP-TL-19	0.2	1025
WTP-TL-20	4.3	894
WTP-TL-20	2.2	1002
WTP-TL-20	0.72	1100
WTP-TL-20	0.26	1199
WTP-TL-21	0.62	901
WTP-TL-21	0.36	1002
WTP-TL-21	0.2	1100
WTP-TL-21	0.87	802
WTP-TL-23	1.4	901
WTP-TL-23	0.51	1000
WTP-TL-23	0.2	1100
WTP-TL-24	0.87	901
WTP-TL-24	0.2	1000
WTP-TL-24	0.1	1025
WTP-TL-27	3.14	899
WTP-TL-27	1.32	1001
WTP-TL-27	0.36	1101
WTP-TL-28	1.82	899
WTP-TL-28	0.67	1001
WTP-TL-28	0	1050
WTP-TL-29	1.51	899
WTP-TL-29	0.77	1001
WTP-TL-29	0.46	1101
WTP-TL-29	0.31	1200
WTP-TL-30	2.1	899
WTP-TL-30	1.02	1001
WTP-TL-30	0.41	1101
WTP-TL-30	0.15	1200

Table 6.6. Intercepts, Slopes, Predicted $T_{1\%}$ (Spinel) Values, Standard Deviations of $T_{1\%}$ (Spinel) Values, and Number of Temperature vs. Vol%-Crystallinity Points for IHLW $T_{1\%}$ Validation Glasses.

Glass ID	Retained for $T_{1\%}$ (Spinel) Model Validation	Intercept[(a)]	Slope[(a)]	Estimated $T_{1\%}$ (Spinel) (°C)	SD($T_{1\%}$) (°C)	Number of Points	Included in V2 Validation Subset	Included in V3 Validation Subset
MS-7a	Yes	1092.68[(b)]	-179.41[(b)]	913.3[(b)]	5.75[(b)]	6	Yes	Yes
MS-7d	Yes	1131.49	-246.44	885.0	10.90	6	Yes	Yes
MS-7e	Yes	1087.53	-177.74	909.8	6.50	22	Yes	Yes
MS7-H-Al	Yes	1176.97	-123.83	1053.1	14.87	8	No	No
MS7-L-Al	Yes	1019.89	-127.58	892.3	8.16	5	Yes	Yes
MS7-H-Cr	Yes	1133.11	-134.59	998.5	6.94	7	Yes	Yes
MS7-L-Cr	Yes	1038.80	-108.66	930.1	5.52	6	Yes	Yes
MS7-L-Fe	Yes	1004.07	-110.50	893.6	4.44	6	Yes	Yes
MS7-H-Li	Yes	1050.35	-118.77	931.6	5.12	7	Yes	No
MS7-L-Li	Yes	1149.48	-140.09	1009.4	12.78	7	Yes	Yes
MS7-H-Mg	Yes	1165.84	-116.24	1049.6	8.42	6	Yes	Yes
MS7-L-Mg	Yes	1093.89	-122.34	971.6	13.81	5	Yes	Yes
MS7-H-Na	Yes	1003.62	-106.73	896.9	0.66	4	No	No
MS7-L-Na	Yes	1191.86	-109.21	1082.7	13.18	11	Yes	No
MS7-H-Ni	Yes	1200.03	-90.40	1109.6	23.49	14	No	No
MS7-L-Ni	Yes	1003.59	-188.66	814.9	11.52	6	Yes	Yes
SP-Al-1	Yes	966.51	-295.85	670.7	19.98	5	Yes	Yes
SP-Cr-1-o	Yes	938.83	-243.84	695.0	21.79	5	No	No
SP-Cr-1-r	Yes	937.30	-149.15	788.2	12.41	5	No	No
SP-Li-3-o	Yes	1037.43	-183.82	853.6	21.22	4	Yes	Yes
SP-Li-3-r	Yes	1000.20	-205.41	794.8	11.89	4	Yes	Yes
SP-Mg-1	Yes	1028.38	-125.39	903.0	3.99	5	Yes	Yes
SP-Mn-1	Yes	1107.36	-176.63	930.7	13.76	5	Yes	Yes
SP-Mn-3	Yes	1065.35	-106.70	958.7	11.15	7	Yes	Yes
SP-Na-1	Yes	1203.97	-85.92	1118.1	18.24	5	No	No
SP-Na-3	Yes	1113.18	-299.67	813.5	3.27	4	No	No
SPA-18	No	978.18	-103.88	874.3	6.92	4	No	No
SPA-38	Yes	1012.07	-159.39	852.7	9.94	5	Yes	Yes
WTP-TL-16	Yes	1320.38	-137.15	1183.2	3.48	5	No	No
WTP-TL-17	Yes	1124.04	-324.85	799.2	32.58	5	No	No
WTP-TL-19	Yes	1057.02	-188.01	869.0	10.05	3	No	No
WTP-TL-20	Yes	1179.15	-69.73	1109.4	22.34	4	Yes	No
WTP-TL-21	Yes	1173.72	-434.09	739.6	16.33	4	No	No
WTP-TL-23	Yes	1108.46	-153.73	954.7	25.54	3	Yes	No
WTP-TL-24	Yes	1036.26	-156.22	880.0	7.89	3	Yes	No
WTP-TL-27	Yes	1113.58	-70.49	1043.1	15.86	3	Yes	Yes
WTP-TL-28	Yes	1052.71	-83.59	969.1	3.15	3	Yes	Yes
WTP-TL-29	Yes	1225.51	-229.85	995.7	28.46	4	Yes	No
WTP-TL-30	Yes	1182.65	-143.92	1038.7	21.30	4	Yes	No

(a) The intercept and slope are from fitting the model in Equation (6.1) to the temperature versus spinel percent crystallinity data for each glass as given in Table 6.5.

(b) Estimated $T_{1\%}$ values in this table have been rounded to one decimal place; intercepts, slopes, and standard deviations have been rounded to two decimal places.

Table 6.7. IHLW $T_{1\%}$ (Spinel) 19-Term Full LM Model and Performance Summary[(a)].

Spinel $T_{1\%}$ Full LM Model Term	Coefficient Estimate	Coefficient Standard Deviation
Al_2O_3	3158.2842	213.8396
B_2O_3	44.3634	113.5991
CdO	1153.5171	725.6121
Cr_2O_3	17884.1409	3039.4632
Fe_2O_3	3560.6972	148.8649
Li_2O	-2080.7112	285.7379
MnO	2158.5185	198.9088
Na_2O	-1218.7211	145.6210
NiO	11781.9930	1139.3105
Sb_2O_3	-4928.3481	4299.0866
SeO_2	12844.5691	5392.9761
SiO_2	578.7640	53.6079
SrO	-308.0047	158.8225
ThO_2	1439.1167	295.9473
Tl_2O	6704.0626	4596.5093
UO_3	1302.4434	301.2005
ZnO	4036.3993	453.4983
ZrO_2	1955.5781	185.5587
Spike	137.5979	810.5514

Statistic from Modeling Data	Value
R^2	0.912
R^2_A	0.888
R^2_P	0.853
RMSE	31.8791
LOF p-value	0.2377
N	85

Validation Dataset (# Glasses)	R^2_V	RMSE
V1 (38)	0.596	74.9016
V2 (27)	0.661	54.1070
V3 (20)	0.583	56.4402

Statistic from Data Splitting	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.905	0.918	0.914	0.922	0.921	0.916
R^2_A	0.872	0.889	0.885	0.895	0.894	0.887
R^2_P	0.813	0.844	0.833	0.854	0.850	0.839
RMSE	32.9981	30.8107	32.5239	31.1978	31.9727	31.9006
R^2_V	0.915	0.780	0.853	0.775	0.815	0.828

(a) Model and summary statistics were generated using estimated $T_{1\%}$ values as the response. Rounded versions of these $T_{1\%}$ values are given in Table 6.2. Conducting modeling with the rounded versions of the estimated $T_{1\%}$ values may result in slightly different summary statistic values.

Table 6.8. IHLW $T_{1\%}$ (Spinel) 13-Term Reduced LM Model and Performance Summary[(a)].

$T_{1\%}$ (Spinel) Reduced LM Model Term	Coefficient Estimate	Coefficient Standard Deviation
Al_2O_3	3139.3911	199.9823
B_2O_3	16.8471	107.8128
Cr_2O_3	17827.9333	2811.0551
Fe_2O_3	3616.2420	139.9543
Li_2O	-1982.3832	278.7899
MnO	2182.6998	191.3432
Na_2O	-1177.8694	137.3998
NiO	11230.9464	1080.7332
SiO_2	573.8247	50.2607
SrO	-164.6976	148.1791
ThO_2	1659.3672	248.1687
ZnO	3948.6108	438.1275
ZrO_2	2029.1022	179.3934

Statistic from Modeling Data	Value
R^2	0.901
R^2_A	0.884
R^2_P	0.860
RMSE	32.3888
LOF p-value	0.2214
N	85

Validation Dataset (# Glasses)	R^2_V	RMSE
V1 (38)	0.582	76.2025
V2 (27)	0.649	55.0890
V3 (20)	0.558	58.1024

Statistic from Data Splitting	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.894	0.908	0.898	0.903	0.910	0.903
R^2_A	0.873	0.889	0.877	0.883	0.891	0.883
R^2_P	0.838	0.866	0.839	0.851	0.864	0.851
RMSE	32.8796	30.7748	33.5740	32.8834	32.3304	32.4884
R^2_V	0.908	0.824	0.893	0.845	0.808	0.856

(a) Model and summary statistics were generated using estimated $T_{1\%}$ values as the response. Rounded versions of these $T_{1\%}$ values are given in Table 6.2. Conducting modeling with the rounded versions of the estimated $T_{1\%}$ values may result in slightly different summary statistic values.

Table 6.9. Summary of Various IHLW $T_{1\%}$ (Spinel) LM and Reduced PQM Models[(a)].

Statistics for Modeling Data	Full 19-term LM	Reduced 13-term LM	Reduced 14-term PQM	Reduced 15-term PQM	Reduced 16-term PQM	Reduced 17-term PQM	Reduced 18-term PQM	Reduced 19-term PQM	Reduced 20-term PQM	Reduced 21-term PQM
R^2	0.912	0.901	0.914	0.920	0.927	0.935	0.940	0.942	0.947	0.949
R^2_A	0.888	0.884	0.898	0.904	0.911	0.920	0.925	0.927	0.931	0.933
R^2_P	0.853	0.860	0.875	0.883	0.893	0.907	0.912	0.913	0.918	0.915
RMSE	31.8791	32.3888	30.4036	29.4826	28.4434	26.9212	26.1041	25.7757	25.0117	24.5962
Model Terms (Quadratic terms written in element form to save space)	Al_2O_3, B_2O_3, CdO, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, Sb_2O_3, SeO_2, SiO_2, SrO, ThO_2, Tl_2O, UO_3, ZnO, ZrO_2, Spike	Al_2O_3, B_2O_3, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, SiO_2, SrO, ThO_2, ZnO, ZrO_2	Al_2O_3, B_2O_3, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, SiO_2, SrO, ThO_2, ZnO, ZrO_2, B*Mn	Al_2O_3, B_2O_3, Cr2O3, Fe2O3, Li_2O, MnO, Na_2O, NiO, SiO_2, SrO, ThO_2, ZnO, ZrO_2, B*Mn, Al*Fe	Al_2O_3, B_2O_3, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, SiO_2, SrO, ThO_2, ZnO, ZrO_2, B*Mn, Zn*Zn, Li*Si	Al_2O_3, B_2O_3, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, SiO_2, SrO, ThO_2, ZnO, ZrO_2, B*Mn, Zn*Zn, Li*Si, Fe*Mn	Al_2O_3, B_2O_3, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, SiO_2, SrO, ThO_2, ZnO, ZrO_2, B*Mn, Zn*Zn, Li*Si, Fe*Mn, B*B	Al_2O_3, B_2O_3, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, SiO_2, SrO, ThO_2, ZnO, ZrO_2, B*Mn, Zn*Zn, Li*Si, Fe*Mn, B*Th, B*Zn	Al_2O_3, B_2O_3, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, SiO_2, SrO, ThO_2, ZnO, ZrO_2, B*Mn, Zn*Zn, Li*Si, Fe*Mn, B*Th, B*Zn, Zr*Zr	Al_2O_3, B_2O_3, Cr_2O_3, Fe_2O_3, Li_2O, MnO, Na_2O, NiO, SiO_2, SrO, ThO_2, ZnO, ZrO_2, B*Mn, Zn*Zn, Li*Si, Fe*Mn, B*Th, B*Zn, Zr*Zr, Li*Th
Statistic Averages Over Five Splits of the Modeling Data										
R^2	0.916	0.903	0.915	0.922	0.929	0.936	0.941	0.942	0.947	0.950
R^2_A	0.887	0.883	0.896	0.903	0.909	0.917	0.923	0.922	0.927	0.931
R^2_P	0.839	0.851	0.865	0.876	0.887	0.900	0.905	0.902	0.907	0.905
RMSE	31.9006	32.4884	30.6066	29.5903	28.5381	27.2603	26.3261	26.3976	25.5249	24.9418
R^2_V	0.828	0.856	0.875	0.871	0.885	0.901	0.894	0.915	0.907	0.895
Statistics for Secondary Validation Sets										
R^2 for V1	0.596	0.582	0.547	0.521	0.340	0.231	0.262	0.240	0.233	0.267
R^2 for V2	0.661	0.649	0.623	0.651	0.258	0.110	0.201	0.142	0.162	0.205
R^2 for V3	0.583	0.558	0.554	0.598	0.011	-0.182[(b)]	-0.060[(b)]	-0.116[(b)]	-0.065[(b)]	-0.019[(b)]
RMSE V1	74.8821	76.2048	79.2826	81.5185	95.7438	103.3263	101.2310	102.7622	103.2304	100.9211
RMSE V2	54.0944	55.0869	57.0200	54.8603	80.0457	87.6710	83.0795	86.0434	85.0588	82.8509
RMSE V3	56.4179	58.0998	58.3407	55.3891	86.8873	94.9748	89.9264	92.2874	90.1359	88.2020

(a) Summary statistics were generated using estimated $T_{1\%}$ values as the response. Rounded versions of these $T_{1\%}$ values are given in Table 6.2. Conducting modeling with the rounded versions of the estimated $T_{1\%}$ values may result in slightly different summary statistic values.

(b) R^2 statistics can take negative values for validation data, indicating that model predictions are worse than just using the mean of the validation response values (spinel $T_{1\%}$) as the predicted value for all validation glasses.

Table 6.10. HLW03-06 Composition in Formats Needed for Use in IHLW $T_{1\%}$ (Spinel) Models.

Component	HLW03-06 Composition (wt%) from Table 6.1	HLW03-06 Composition (mass fractions) for Use in $T_{1\%}$ Full LM Model	HLW03-06 Composition (mass fractions) for Use in $T_{1\%}$ Reduced LM Model
Al_2O_3	8.532	0.08532	0.08691
B_2O_3	5.018	0.05018	0.05112
CdO	1.636	0.01636	NA [(a)]
Cr_2O_3	0.502	0.00502	0.00511
Fe_2O_3	2.007	0.02007	0.02045
Li_2O	6.022	0.06022	0.06135
MnO	7.027	0.07027	0.07158
Na_2O	4.015	0.04015	0.04090
NiO	1.004	0.01004	0.01023
Sb_2O_3	0.020	0.00020	NA
SeO_2	0.020	0.00020	NA
SiO_2	53.200	0.53200	0.54193
SrO	5.205	0.05205	0.05303
ThO_2	1.448	0.01448	0.01475
Tl_2O	0.019	0.00019	NA
UO_3	0.000	0.00000	NA
ZnO	0.000	0.00000	0.00000
ZrO_2	4.187	0.04187	0.04265
Spike	0.136	0.00136	NA

[(a)] NA indicates terms not included in reduced $T_{1\%}$ model.

Table 6.11. Predicted $T_{1\%}$ Values and Corresponding 90% UCIs and 90% SUCIs for HLW03-06 Composition Used in IHLW $T_{1\%}$ (Spinel) Models.

Model	Predicted $T_{1\%}$ (Spinel) (°C)	90% UCI on Mean $T_{1\%}$ (Spinel) (°C)	90% SUCI on Mean $T_{1\%}$ (Spinel) (°C)
19-Term T1% Full LM Model	945.2	968.9	1037.0
13-Term T1% Reduced LM Model	953.4	975.9	1026.6

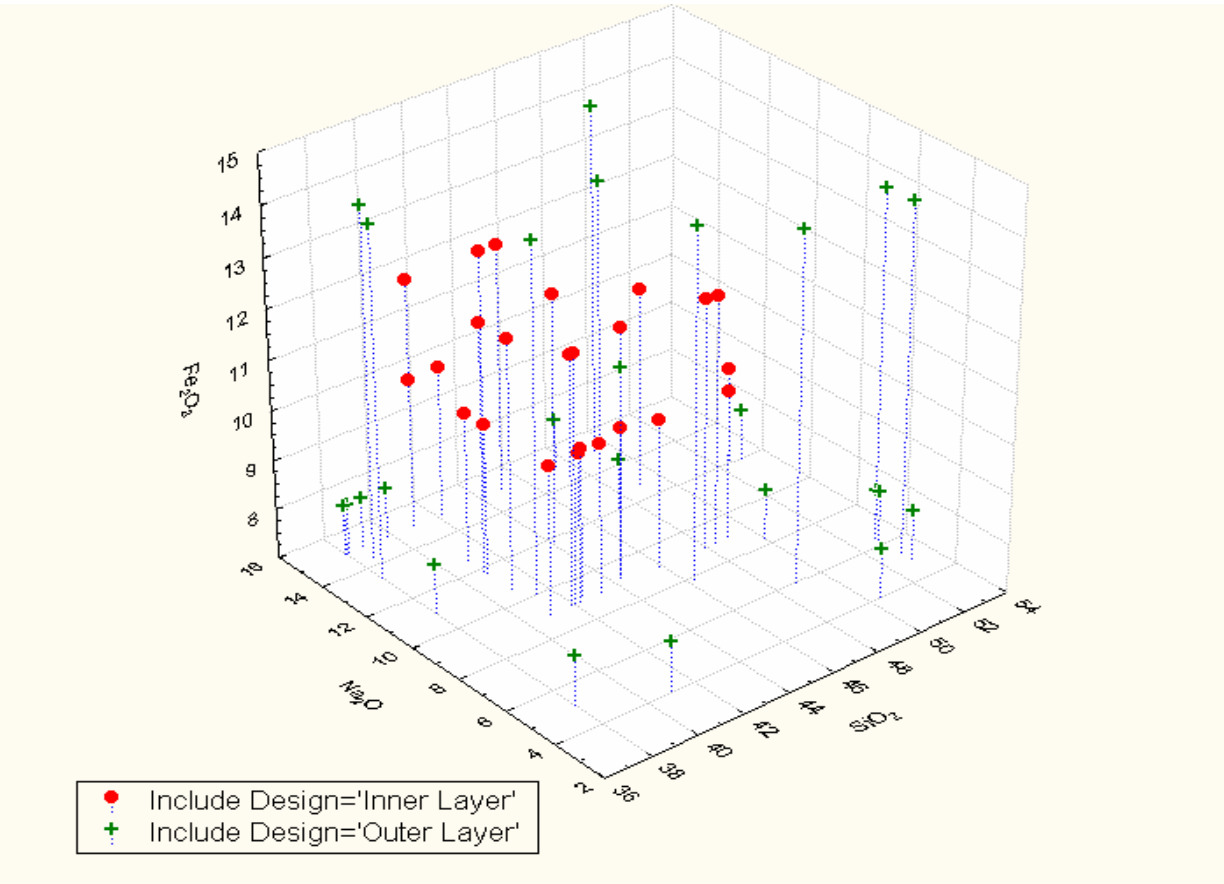

Figure 2.1. Scatter Plot Showing 3-Dimensional Distribution of (Na_2O-Li_2O-Fe_2O_3) for the Initial Test Matrix.

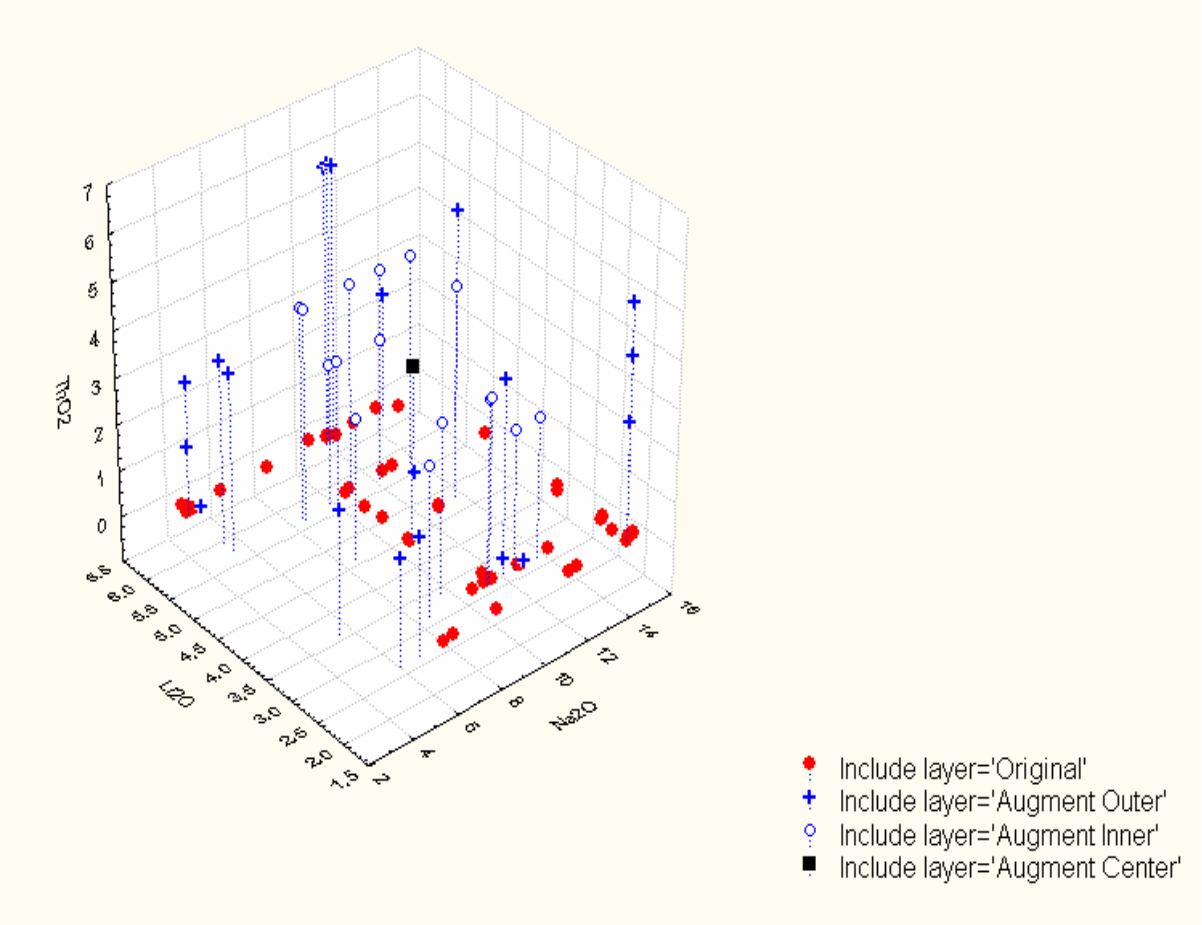

Figure 2.2. Scatter Plot Showing 3-Dimensional Distribution of (Na_2O-Li_2O-ThO_2) for the Augmentation Test Matrix.

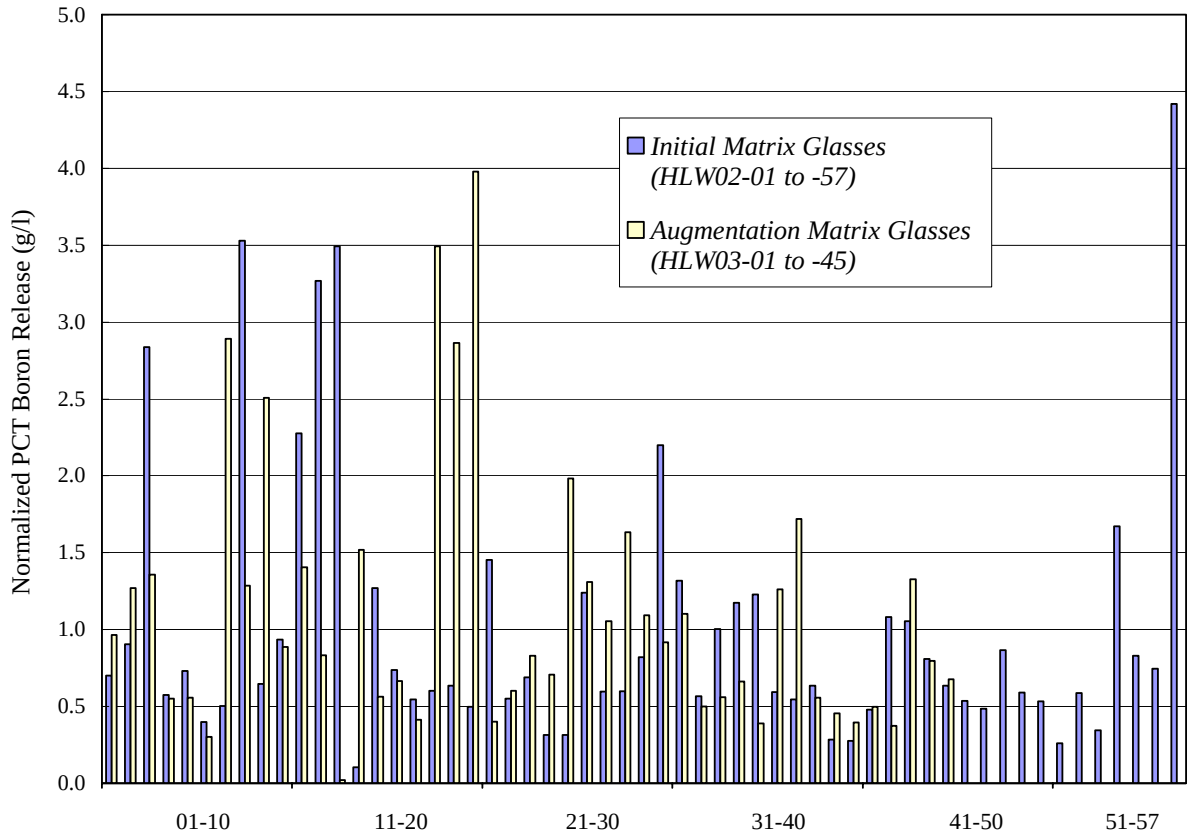

Figure 4.1. Normalized PCT Boron Releases for the IHLW Initial and Augmentation Matrix Glasses. (The index along the horizontal axis identifies the sample grouping (i.e., "01-10" identifies the samples HLW02-01 through -10 and HLW03-01 through -10, etc.).)

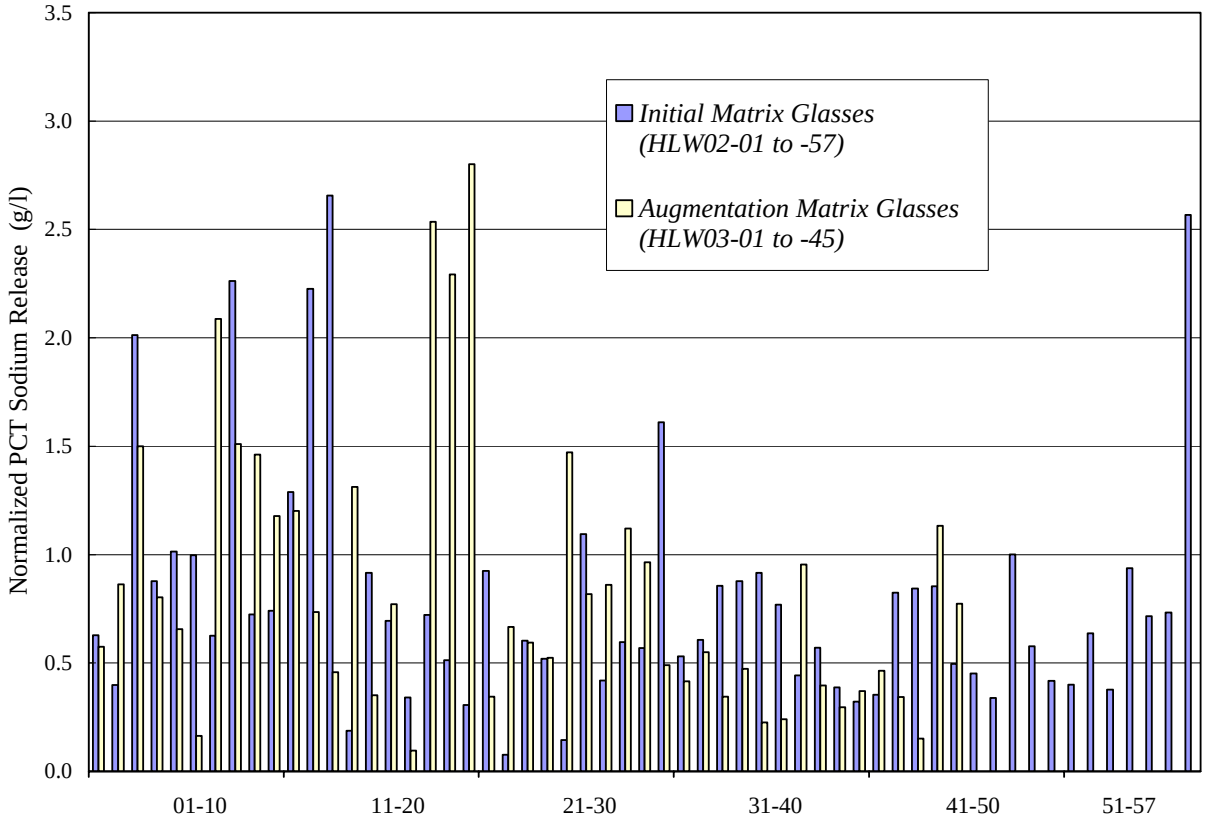

Figure 4.2. Normalized PCT Sodium Releases for the IHLW Initial and Augmentation Matrix Glasses. (The index along the horizontal axis identifies the sample grouping (i.e., "01-10" identifies the samples HLW02-01 through -10 and HLW03-01 through -10, etc.).)

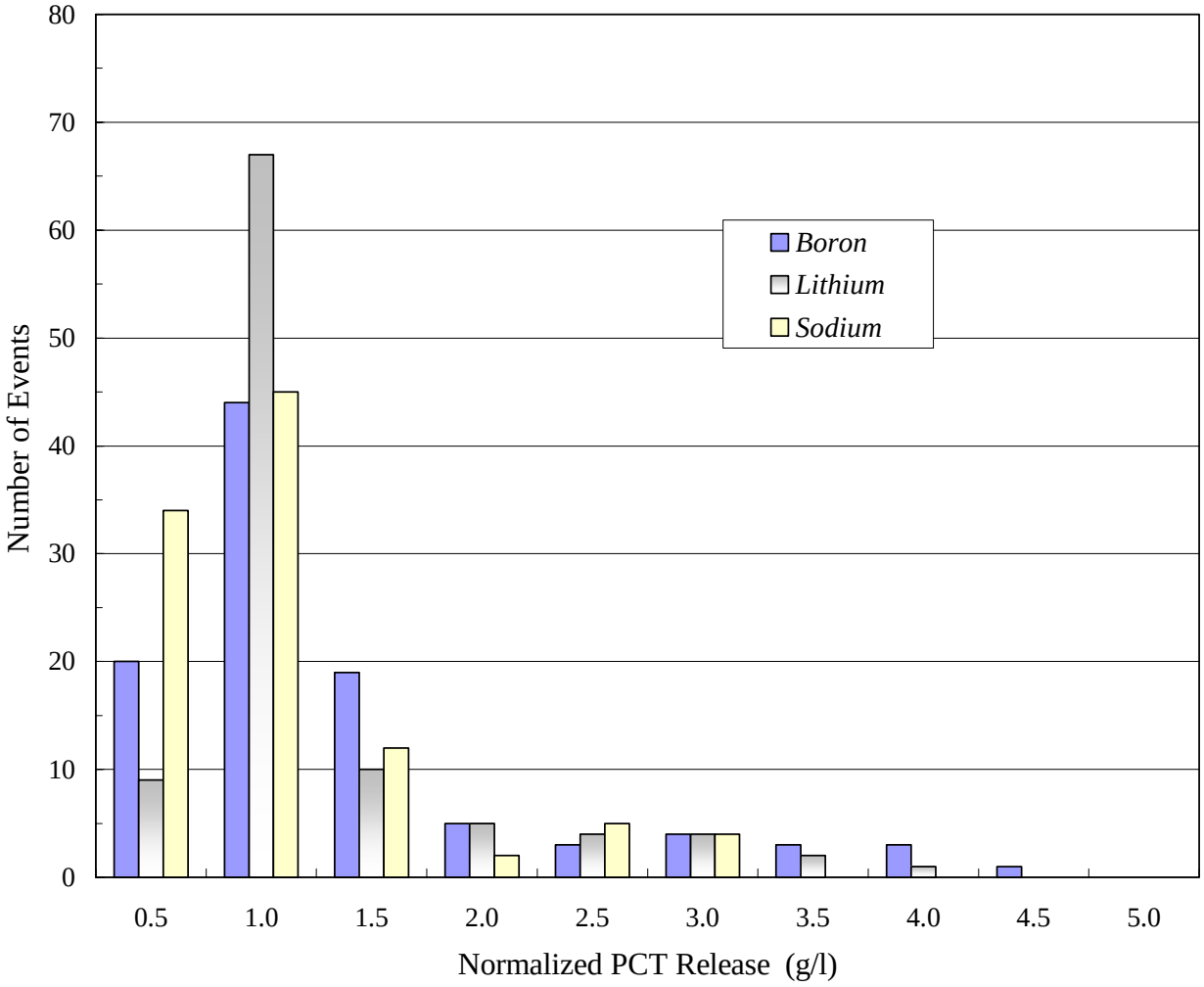

Figure 4.3 Distribution of Normalized PCT Releases of Boron, Lithium, and Sodium for the IHLW Combined Matrix Glasses.

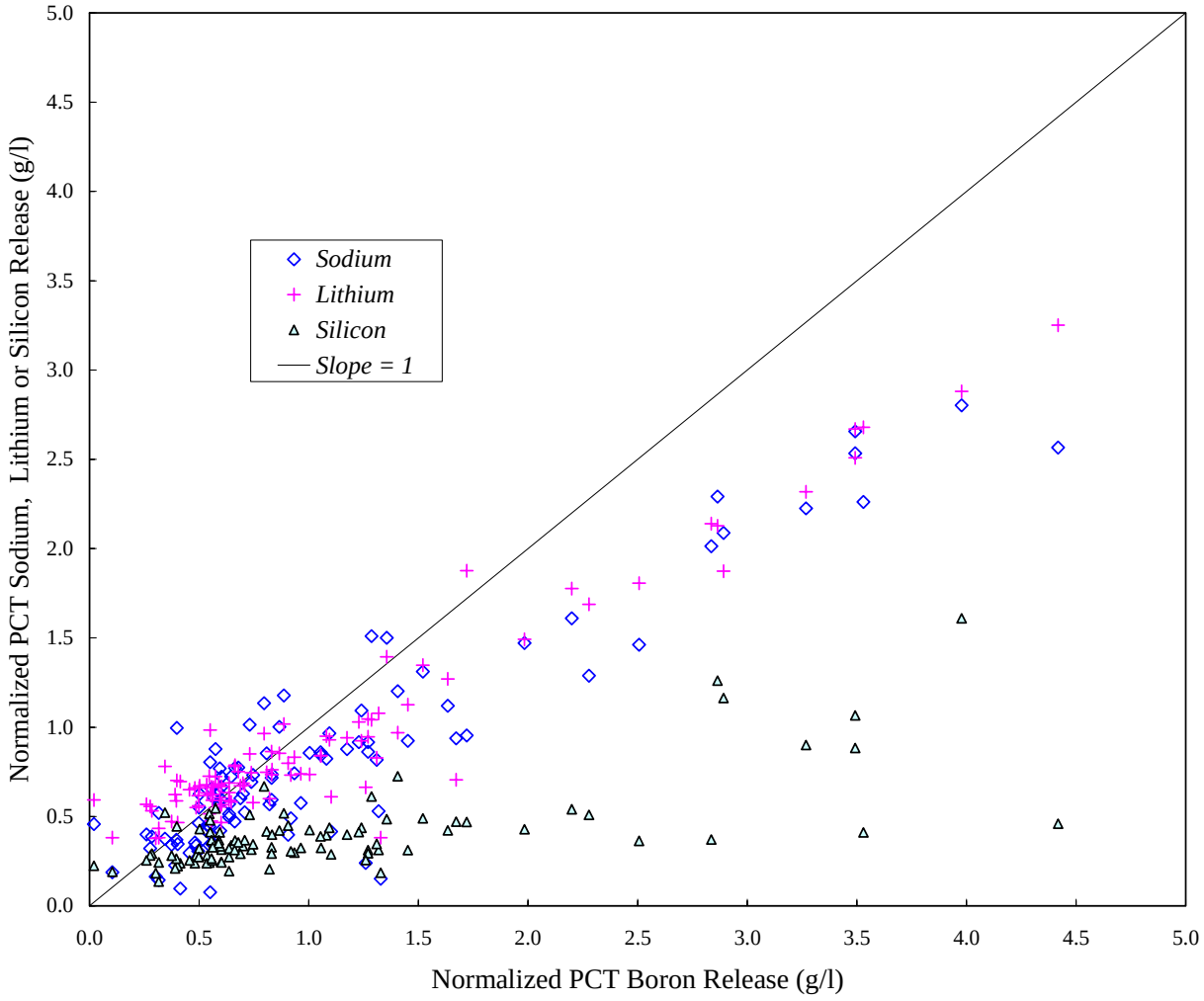

Figure 4.4. Comparison of Normalized PCT Releases of Sodium, Lithium, and Silicon with Normalized PCT Release of Boron.

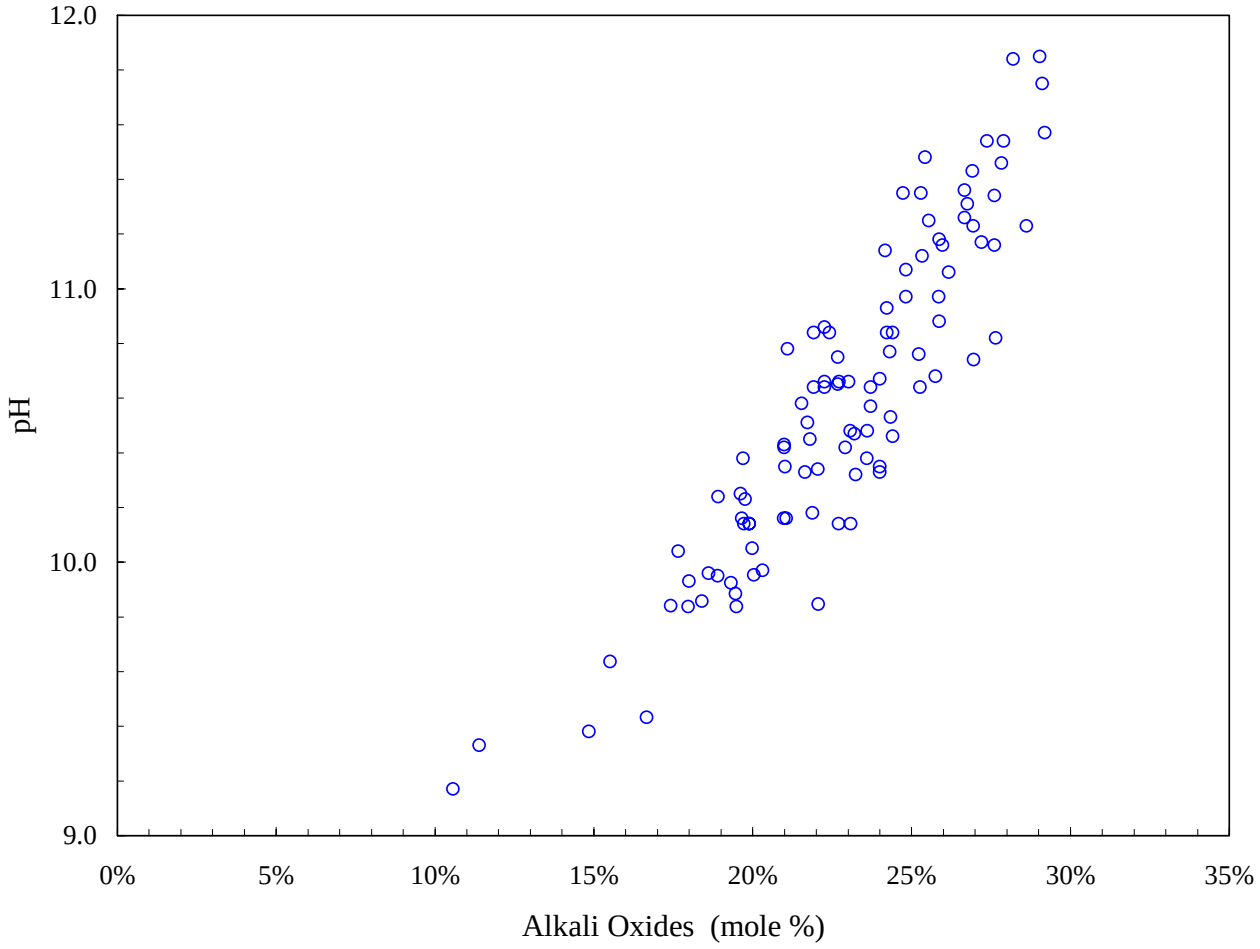

Figure 4.5. Measured pH of the PCT Leachates as a Function of Alkali Oxides.

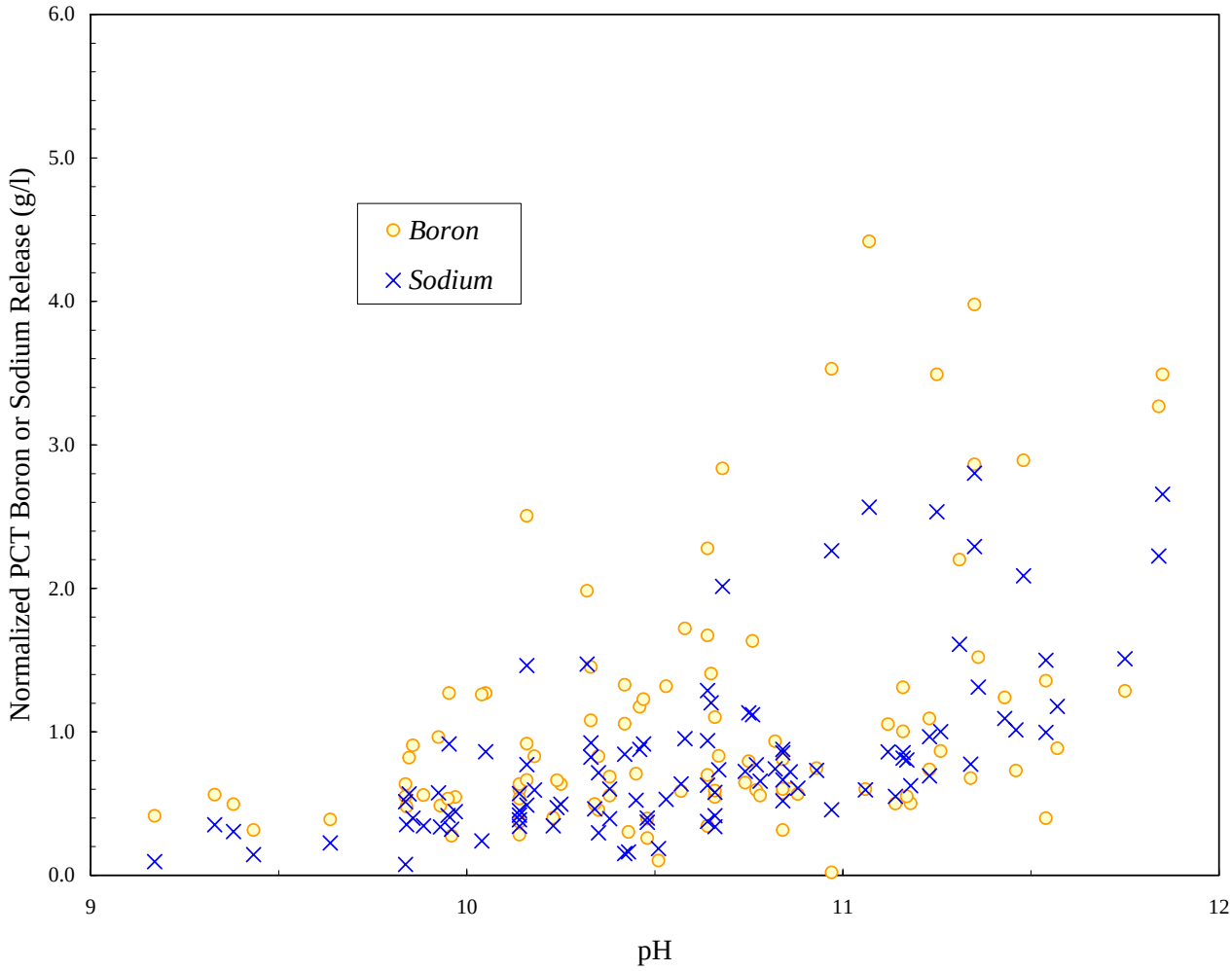

Figure 4.6. Normalized PCT Releases of Boron and Sodium as a Function of pH.

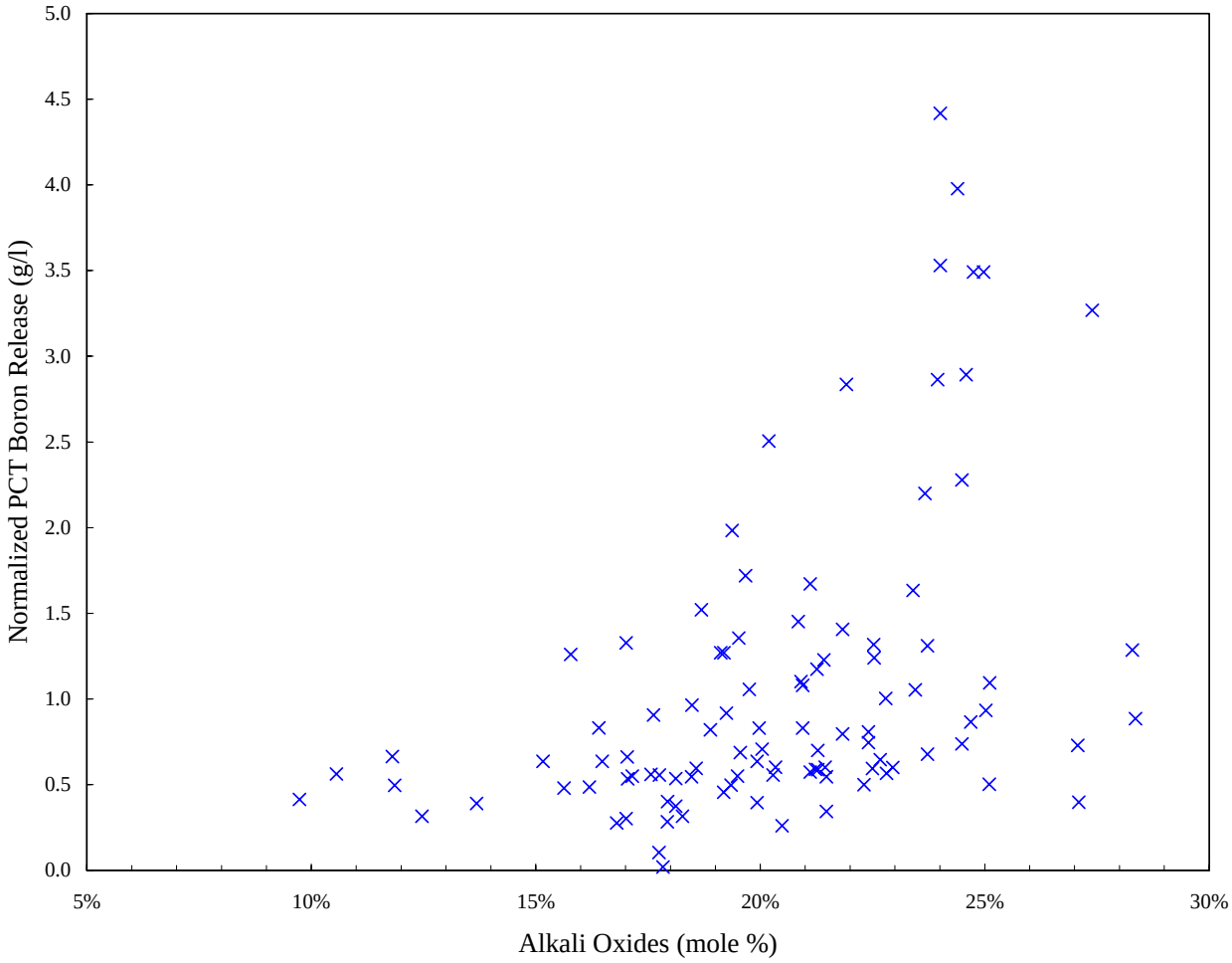

Figure 4.7. Correlation of Normalized PCT Boron Release with Alkali Content in the IHLW Matrix Glasses.

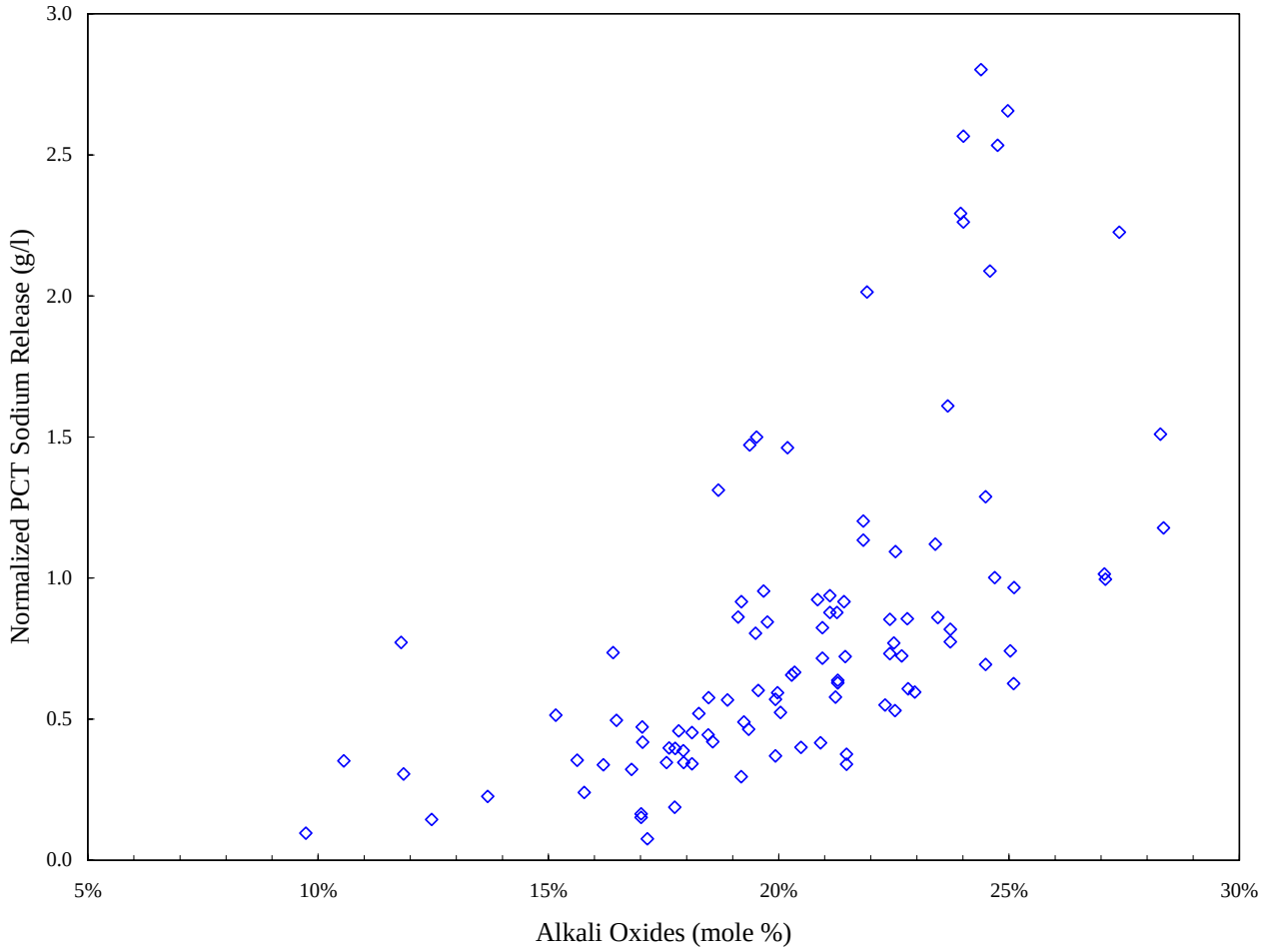

Figure 4.8. Correlation of Normalized PCT Sodium Release with Alkali Content in the IHLW Matrix Glasses.

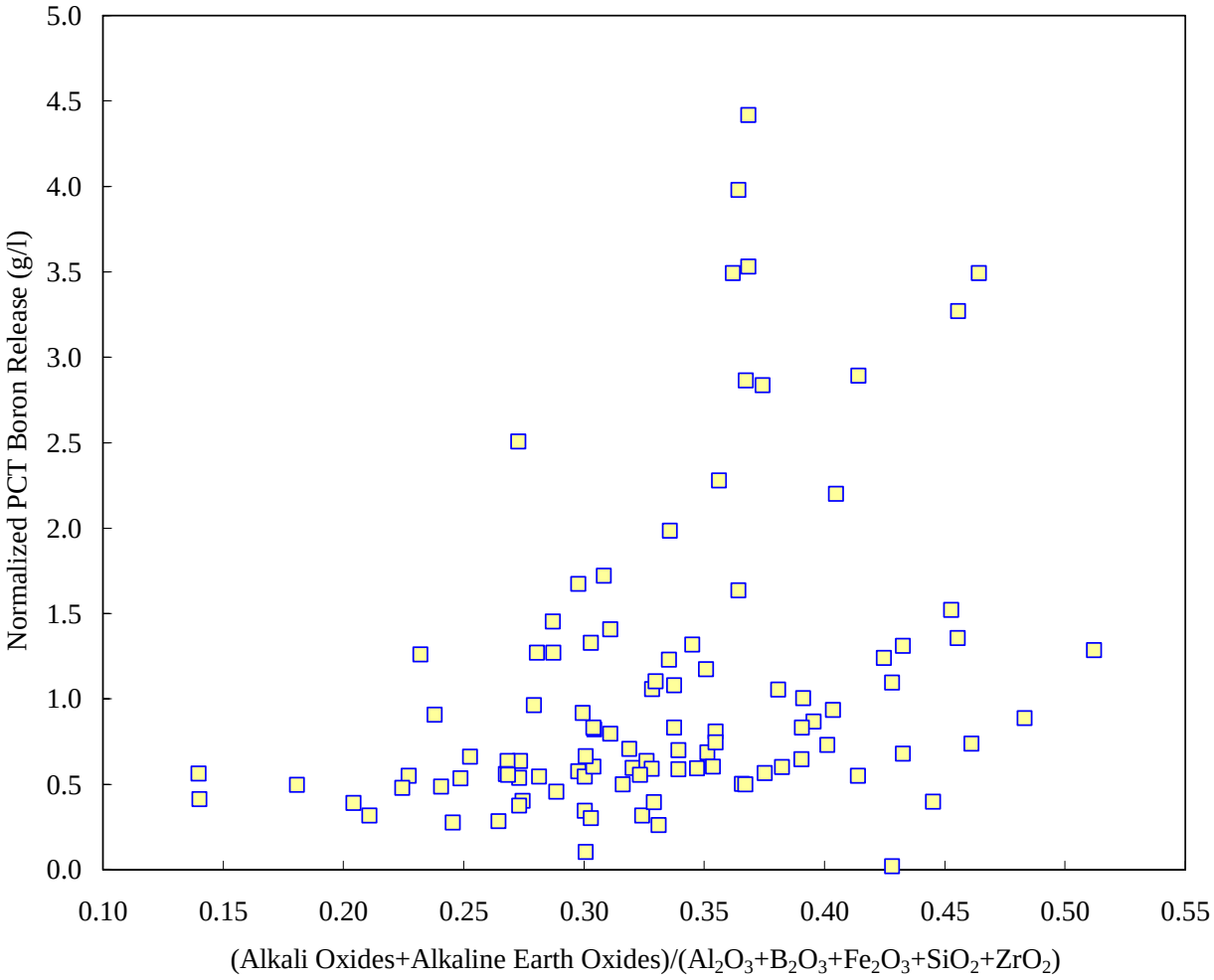

Figure 4.9. Correlation of Normalized PCT Boron Release with the Molar Ratio of (Alkali Oxides+Alkaline Oxides)/(Al_2O_3+B_2O_3+Fe_2O_3+SiO_2+ZrO_2) in the IHLW Matrix Glasses.

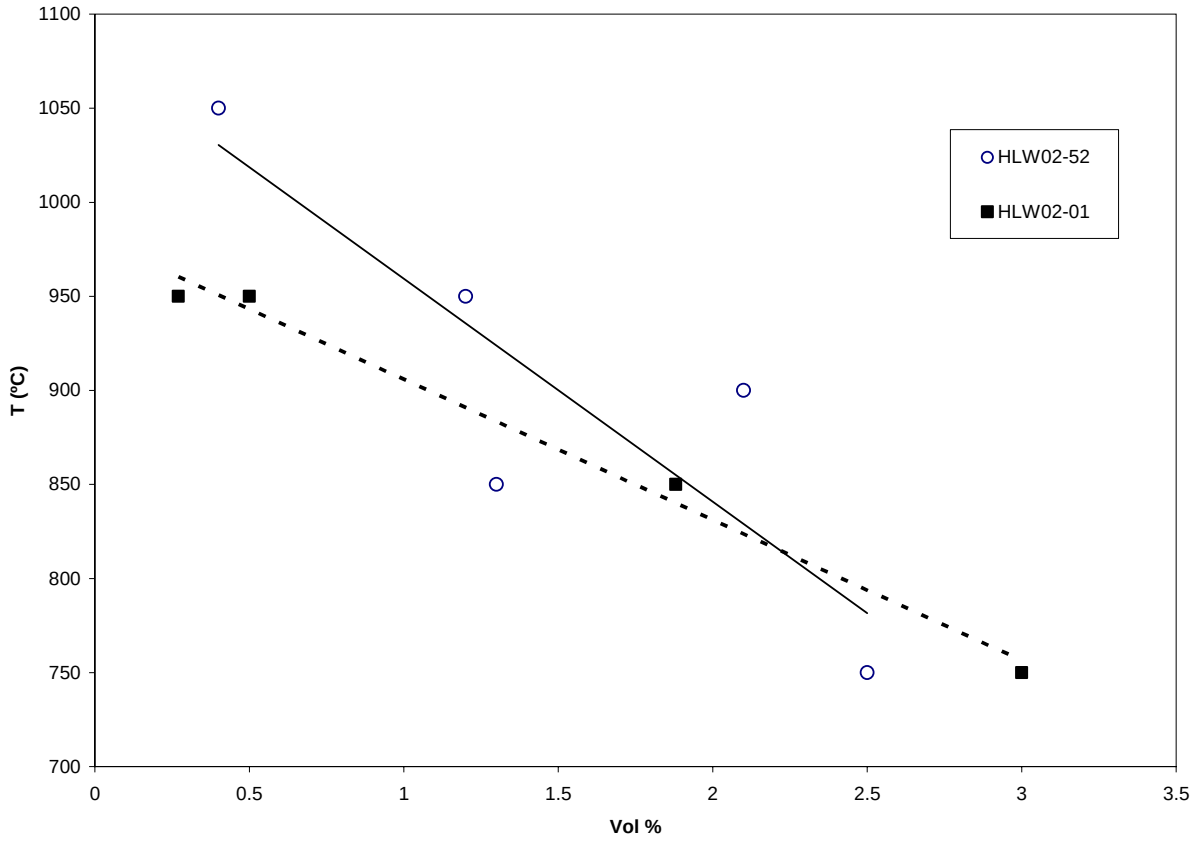

Figure 4.10. Volume % of Crystalline Phase in Heat-Treated HLW Matrix Glass (HLW02-01) and Replicate (HLW02-52).

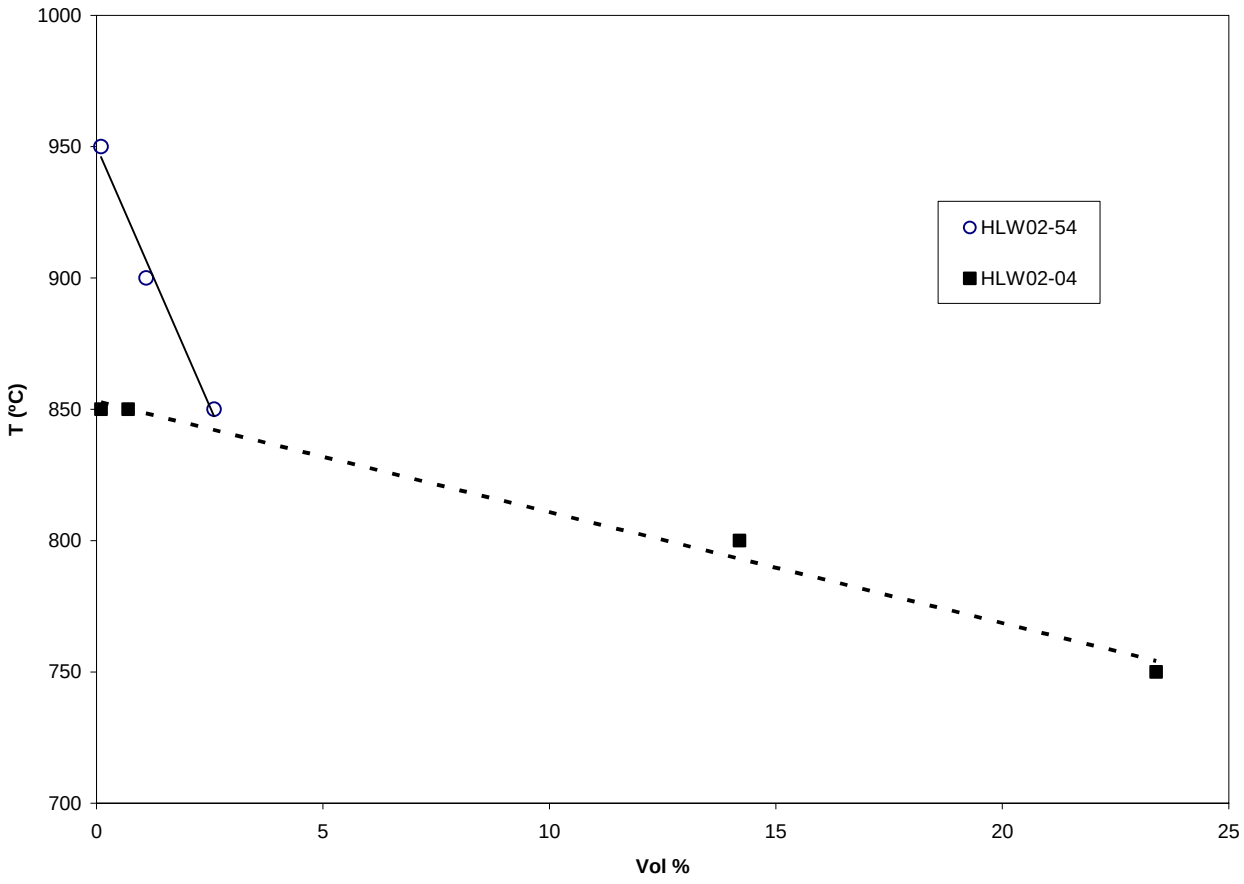

Figure 4.11. Volume % of Crystalline Phase in Heat-Treated HLW Matrix Glass (HLW02-04) and Replicate (HLW02-54).

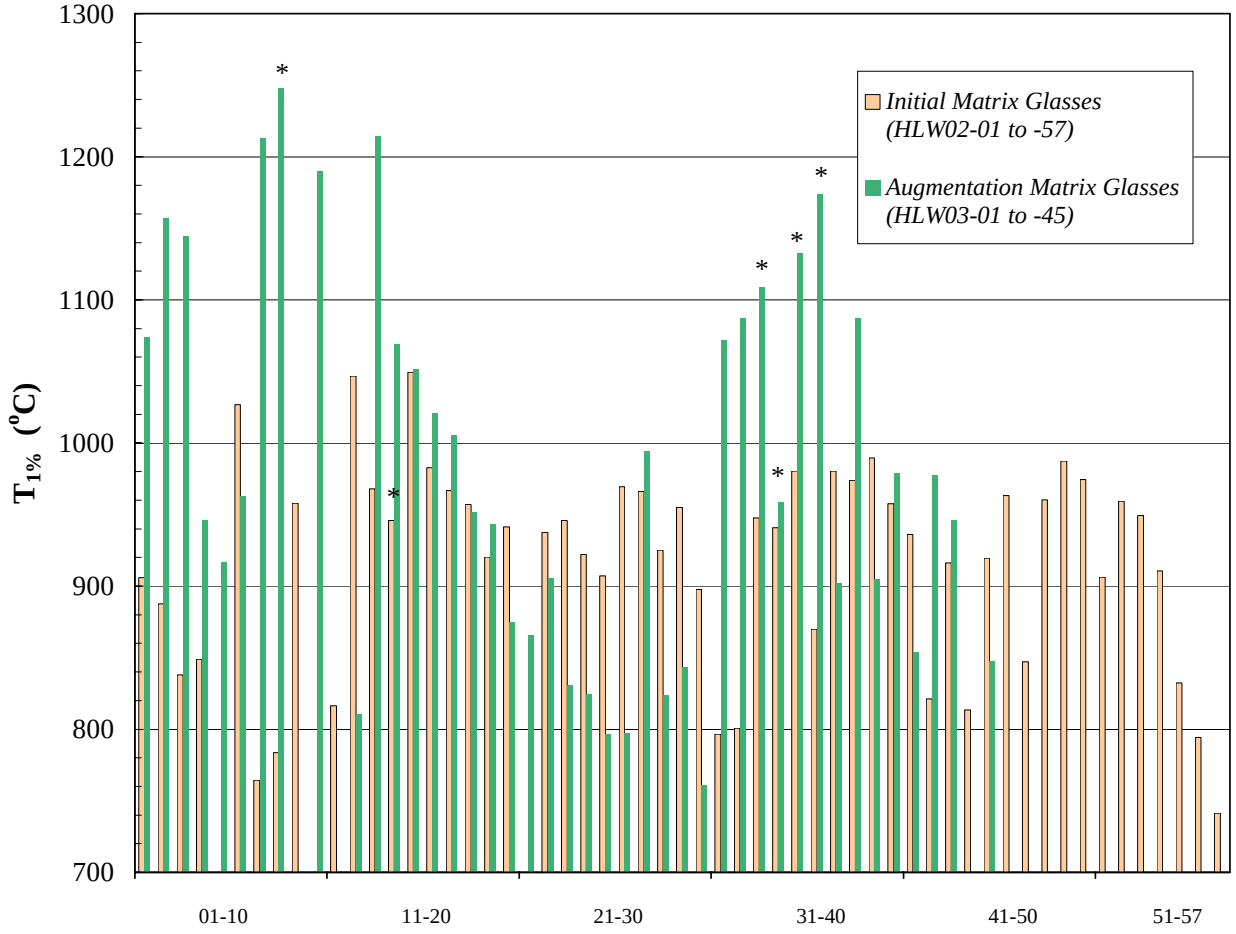

Figure 4.12. Estimated One-Percent Crystal Fraction Temperature ($T_{1\%}$) for the IHLW Combined Matrix (* indicates non-spinel dominant crystalline phase). (The index along the horizontal axis identifies the sample grouping (i.e., "01-10" identifies the samples HLW02-01 through -10 and HLW03-01 through -10, etc.).)

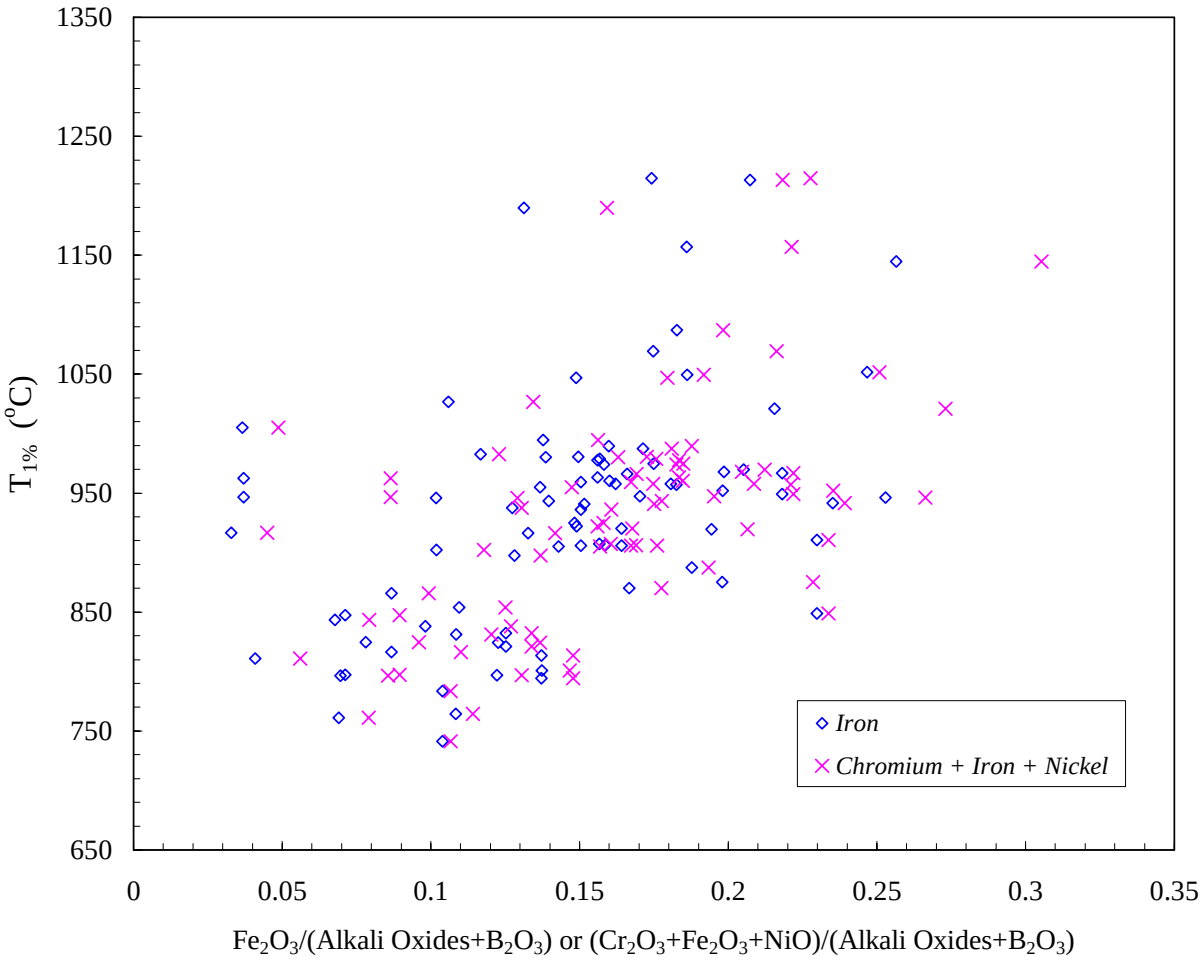

Figure 4.13. Correlation of Estimated $T_{1\%}$ to Molar Ratios of Fe_2O_3 and (Cr_2O_3+Fe_2O_3+NiO) to (Alkali Oxides + Boron Oxide).

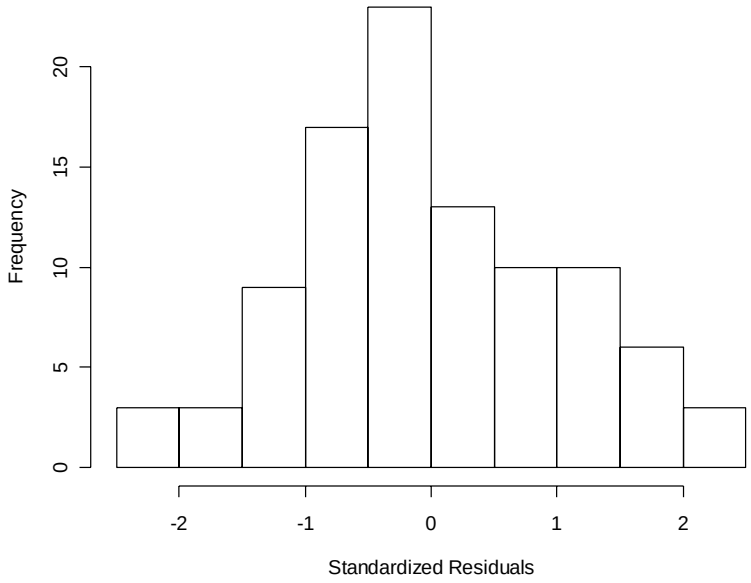

Figure 5.1. Histogram of Standardized Residuals for PCT-Boron 19-Term Full Linear Mixture (LM) Model.

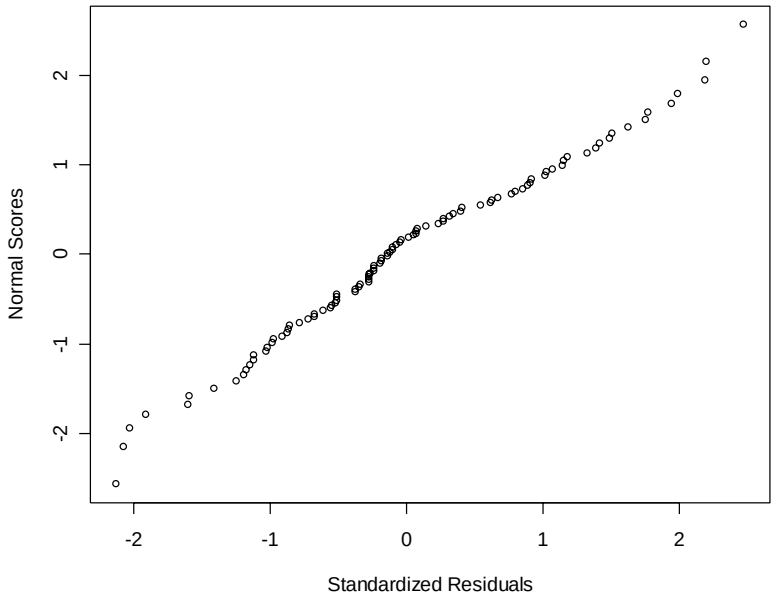

Figure 5.2. Normality Plot Associated with PCT-Boron 19-Term Full LM Model.

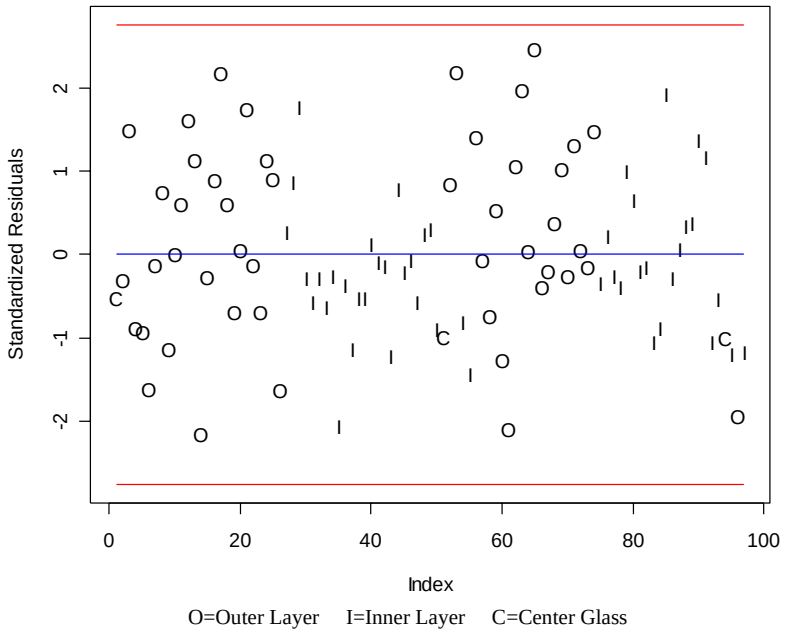

Figure 5.3. Plot of Standardized Residuals for PCT-Boron 19-Term Full LM Model.

Figure 5.4. Predicted Versus Measured Plot for PCT-Boron 19-Term Full LM Model.

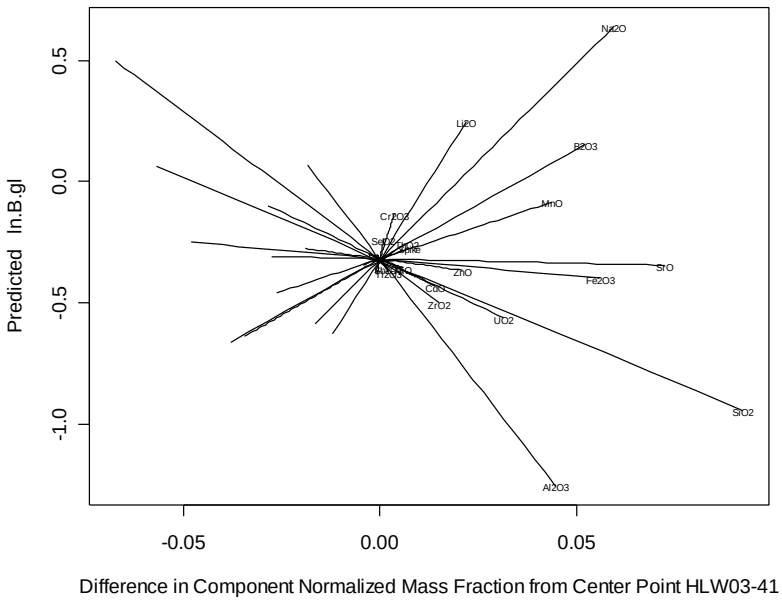

Figure 5.5. Trace Plot Associated with PCT-Boron 19-Term Full LM Model.

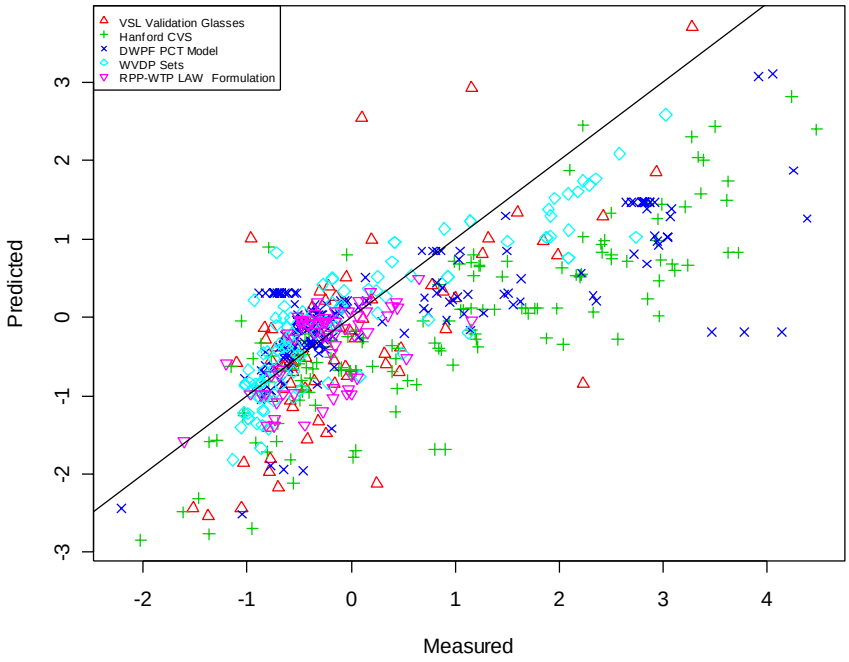

Figure 5.6 Predicted Versus Measured Plot for PCT-Boron 19-Term Full LM Model and Validation Set V1.

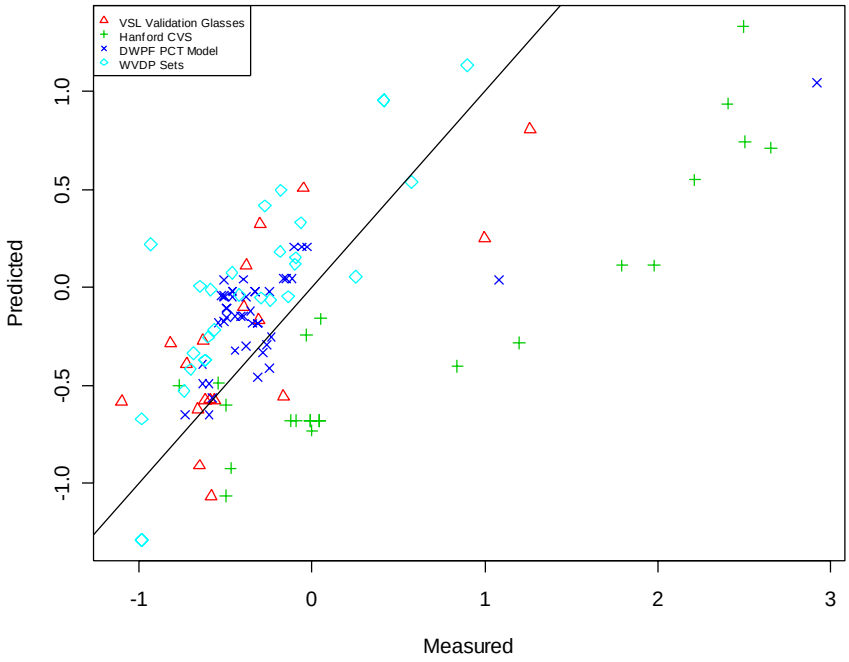

Figure 5.7. Predicted Versus Measured Plot for PCT-Boron 19-Term Full LM Model and Validation Set V2a.

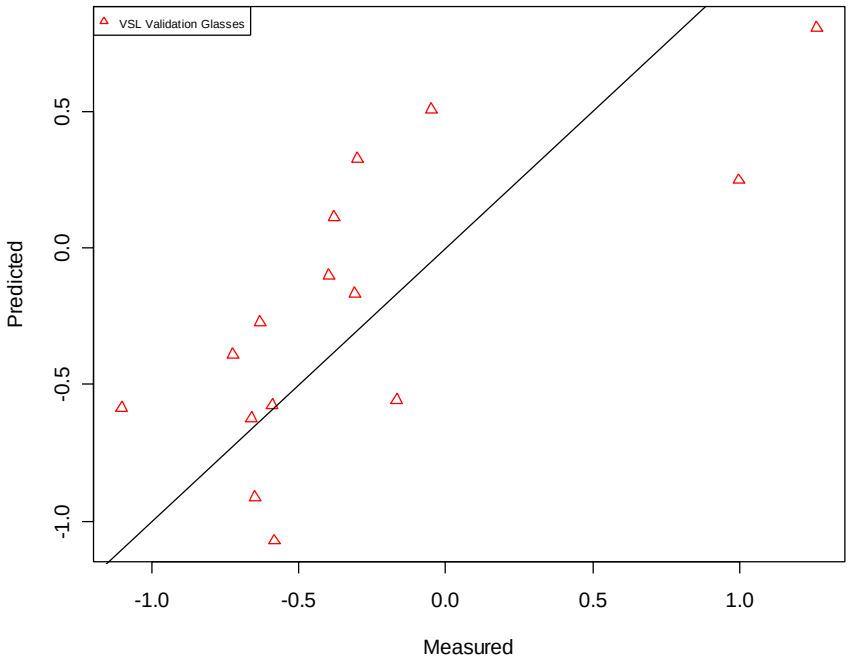

Figure 5.8. Predicted Versus Measured Plot for PCT-Boron 19-Term Full LM Model and Validation Set V2b.

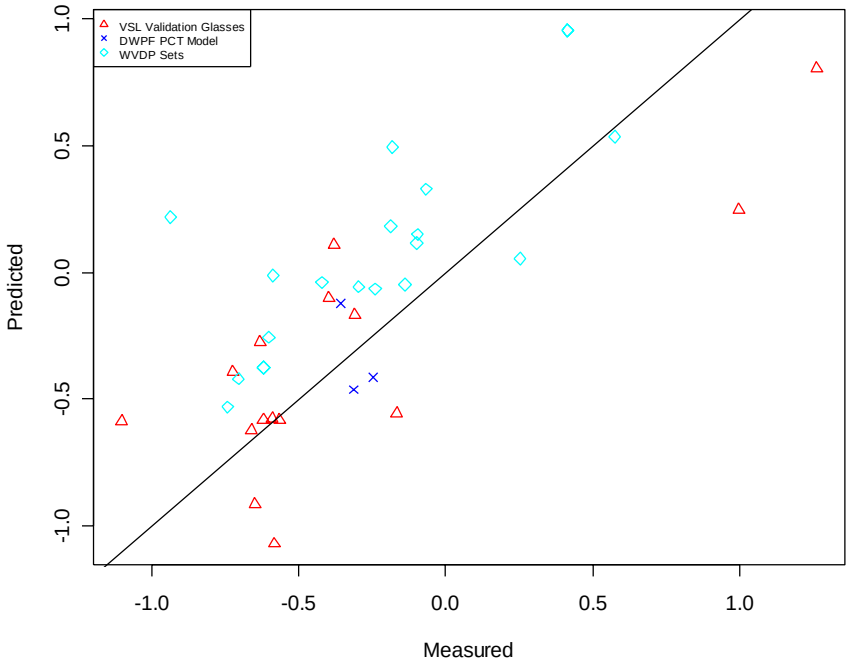

Figure 5.9. Predicted Versus Measured Plot for PCT-Boron 19-Term Full LM Model and Validation Set V3a.

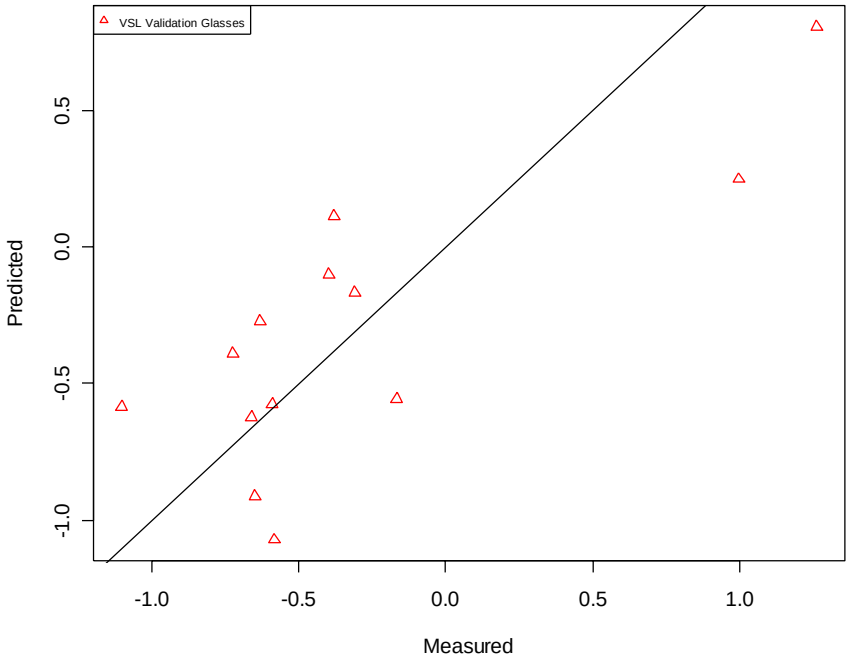

Figure 5.10. Predicted Versus Measured Plot for PCT-Boron 19-Term Full LM Model and Validation Set V3b.

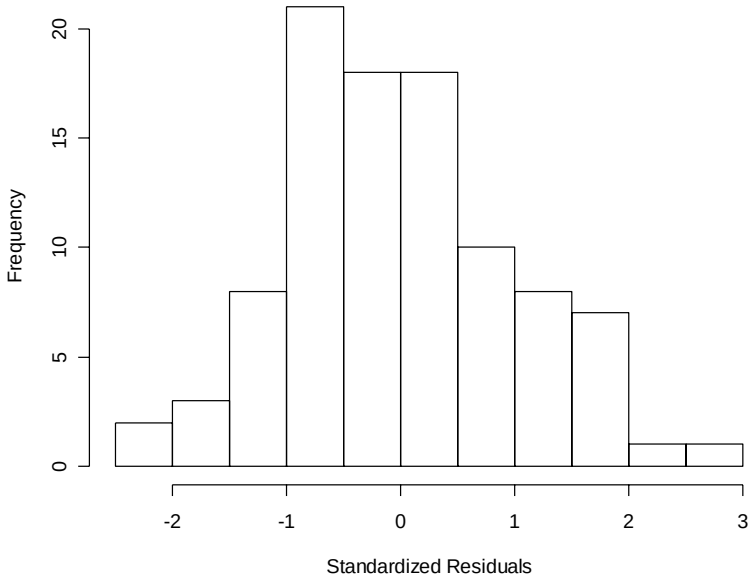

Figure 5.11. Histogram of Standardized Residuals for PCT-Boron 8-Term Reduced LM Model.

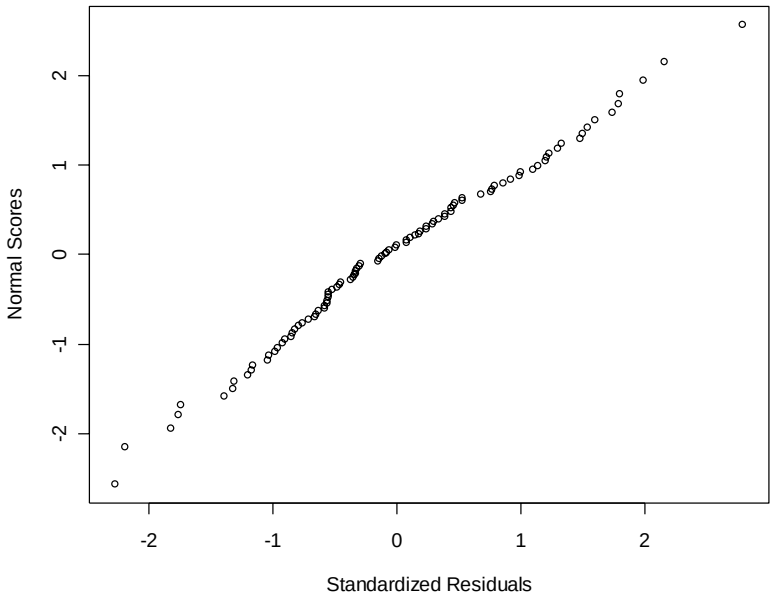

Figure 5.12. Normality Plot Associated with PCT-Boron 8-Term Reduced LM Model.

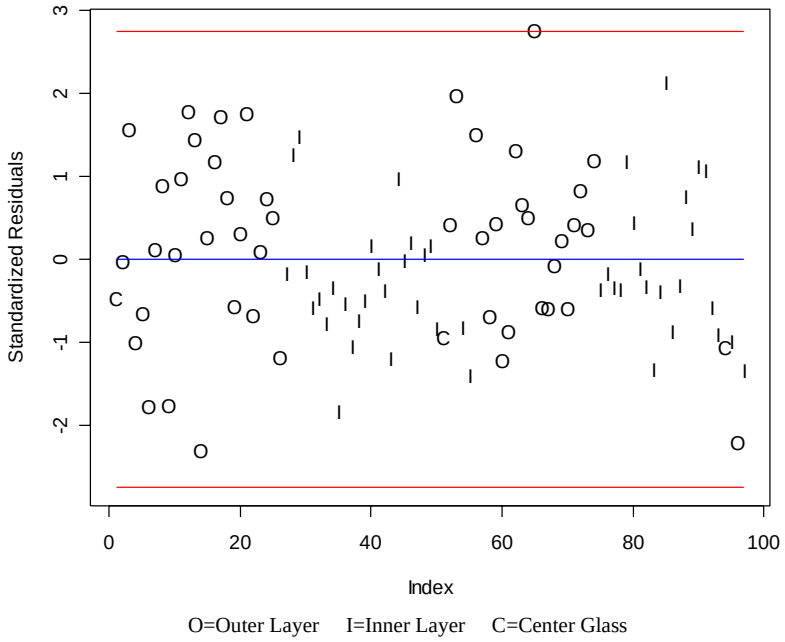

Figure 5.13. Plot of Standardized Residuals for PCT-Boron 8-Term Reduced LM Model.

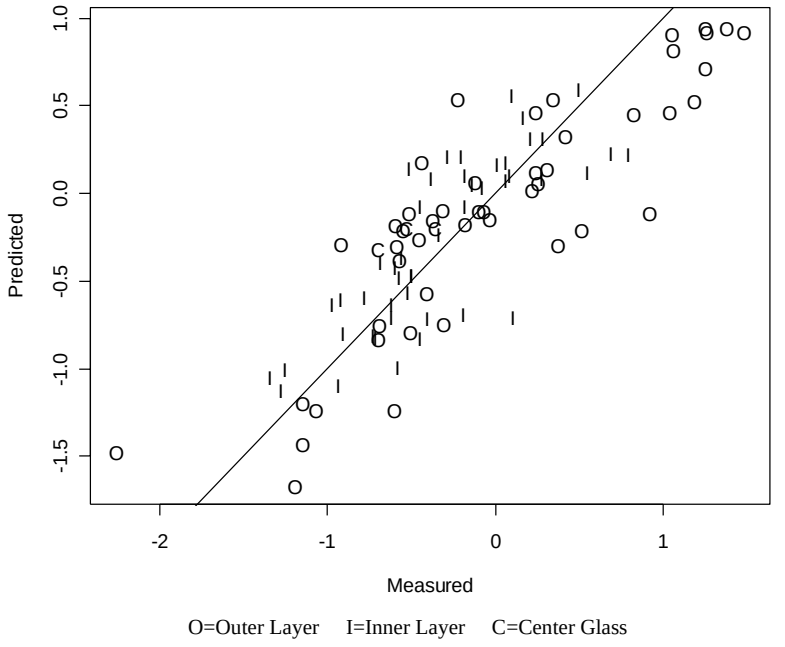

Figure 5.14. Predicted Versus Measured Plot for PCT-Boron 8-Term Reduced LM Model.

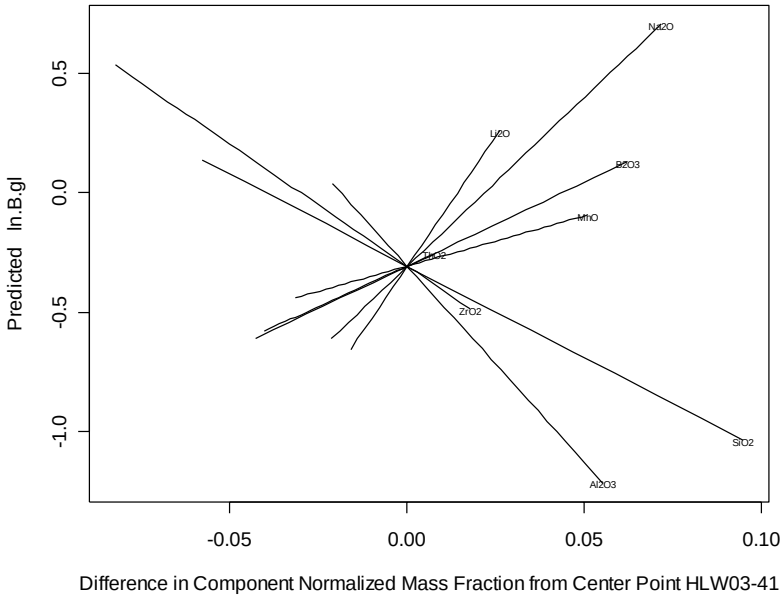

Figure 5.15. Trace Plot Associated with PCT-Boron 8-Term Reduced LM Model.

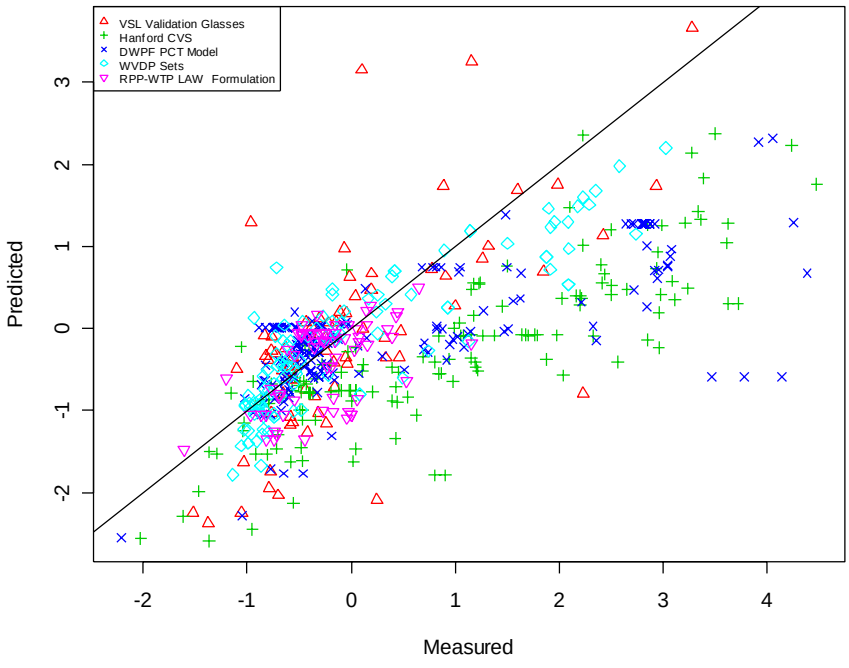

Figure 5.16. Predicted Versus Measured Plot for PCT-Boron 8-Term Reduced LM Model and Validation Set V1.

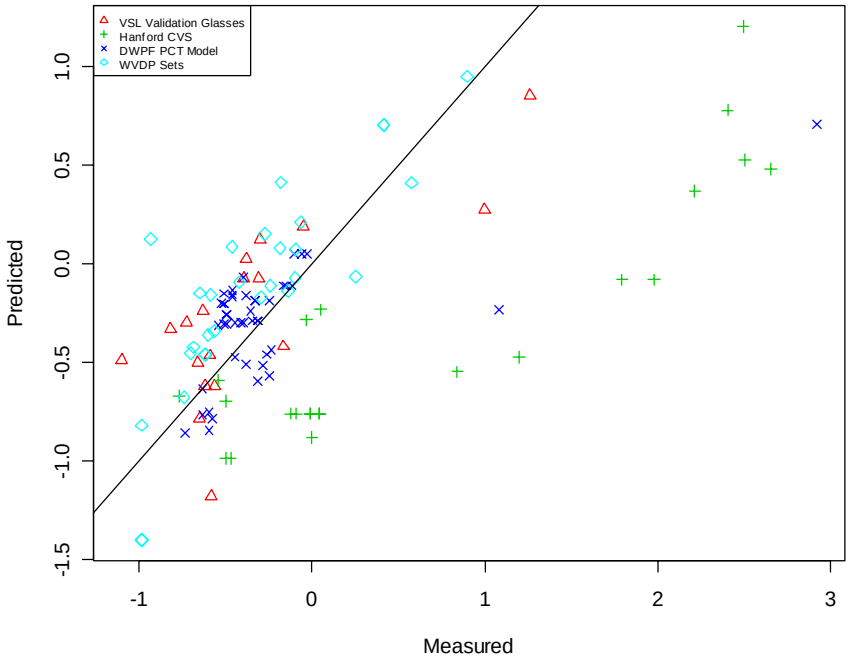

Figure 5.17. Predicted Versus Measured Plot for PCT-Boron 8-Term Reduced LM Model and Validation Set V2a.

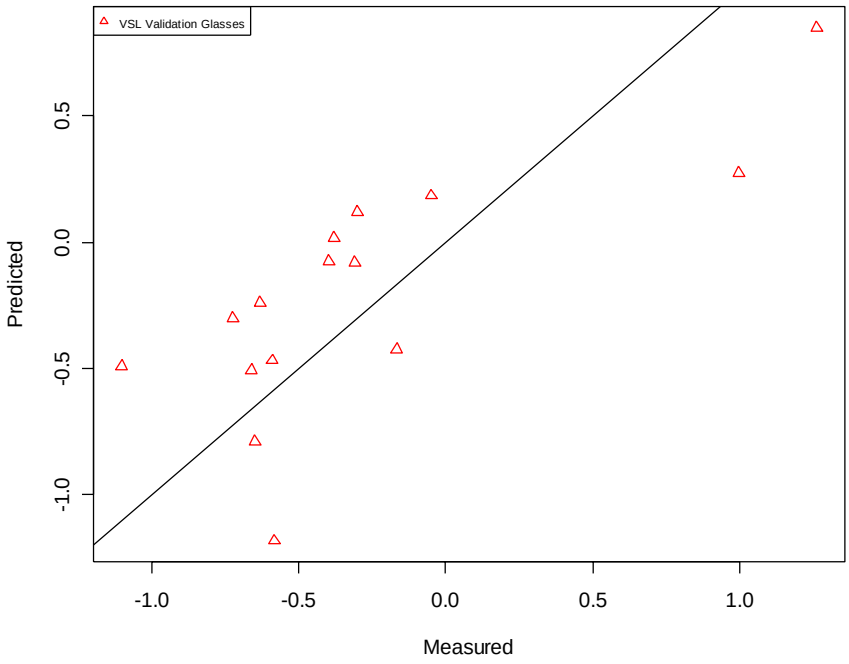

Figure 5.18. Predicted Versus Measured Plot for PCT-Boron 8-Term Reduced LM Model and Validation Set V2b.

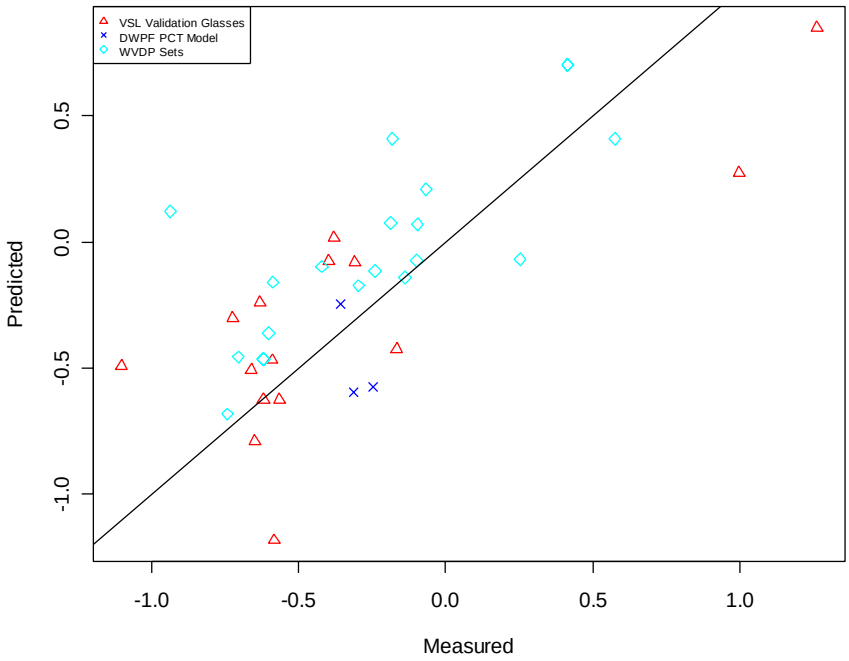

Figure 5.19. Predicted Versus Measured Plot for PCT-Boron 8-Term Reduced LM Model and Validation Set V3a.

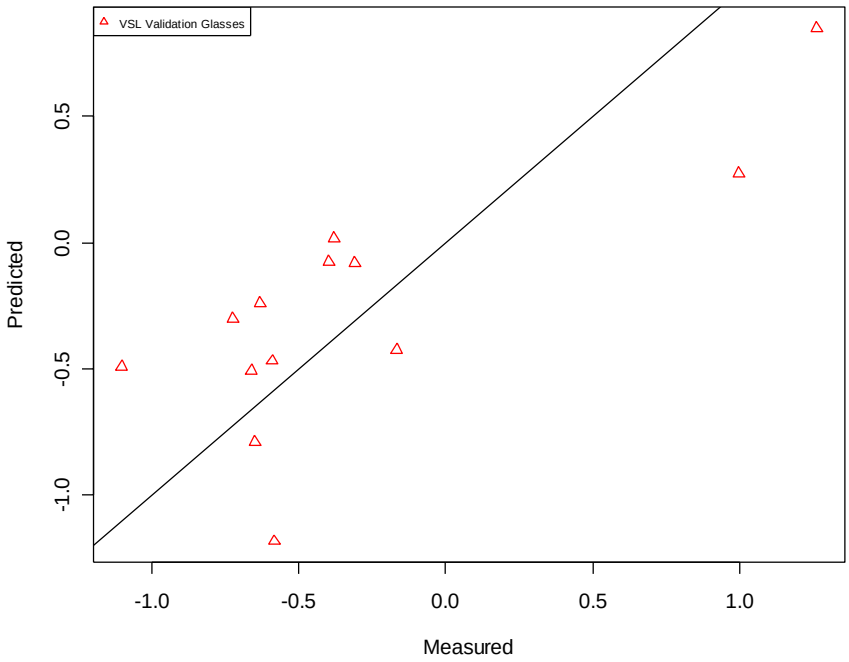

Figure 5.20. Predicted Versus Measured Plot for PCT-Boron 8-Term Reduced LM Model and Validation Set V3b.

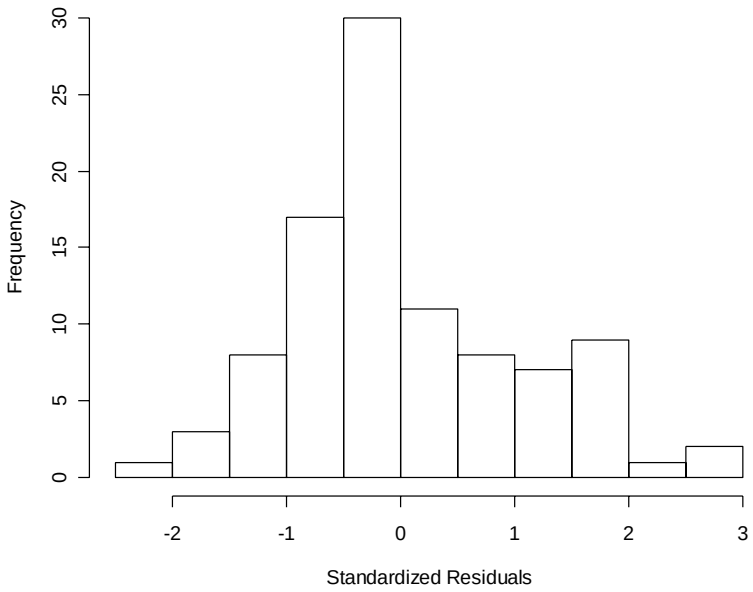

Figure 5.21. Histogram of Standardized Residuals for PCT-Lithium 19-Term Full LM Model.

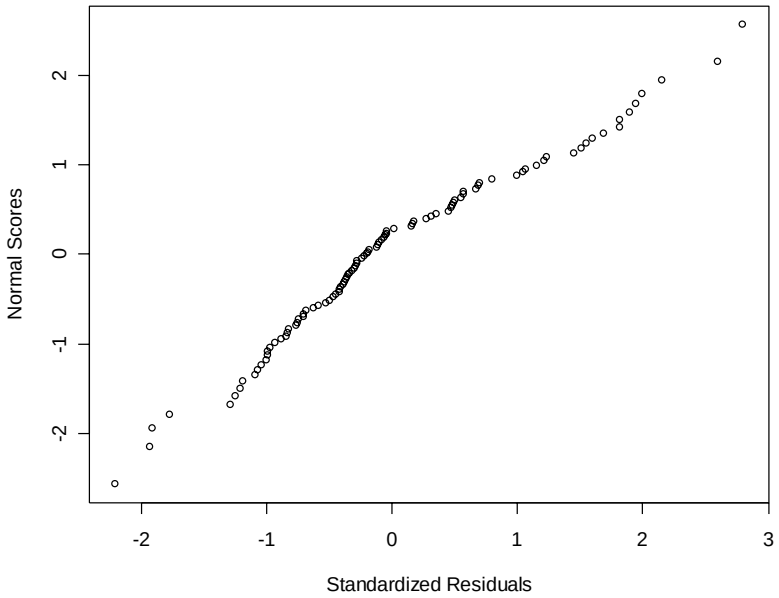

Figure 5.22. Normality Plot Associated with PCT-Lithium 19-Term Full LM Model.

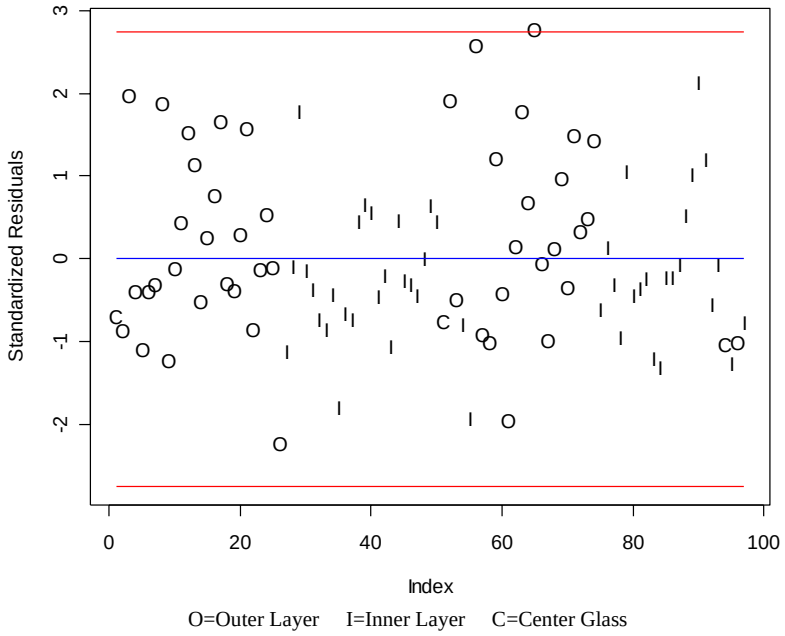

Figure 5.23. Plot of Standardized Residuals for PCT-Lithium 19-Term Full LM Model.

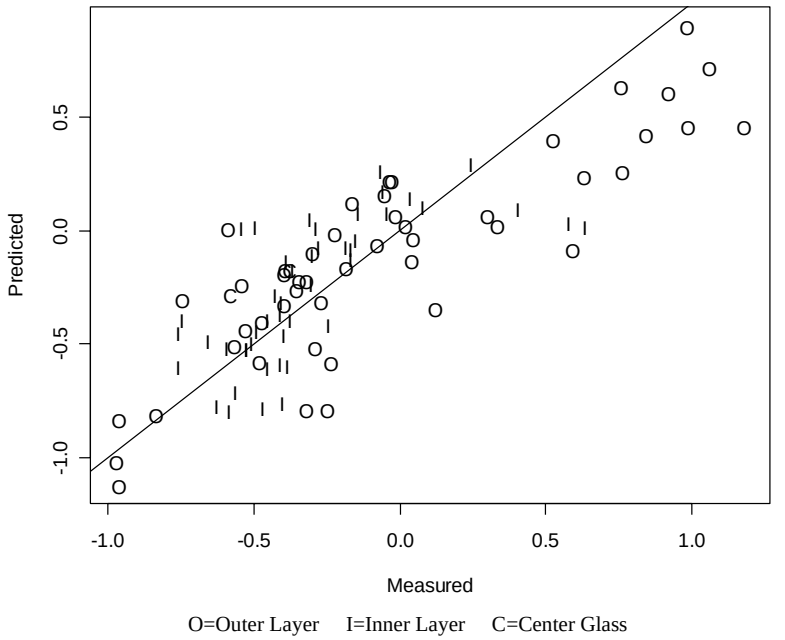

Figure 5.24. Predicted Versus Measured Plot for PCT-Lithium 19-Term Full LM Model.

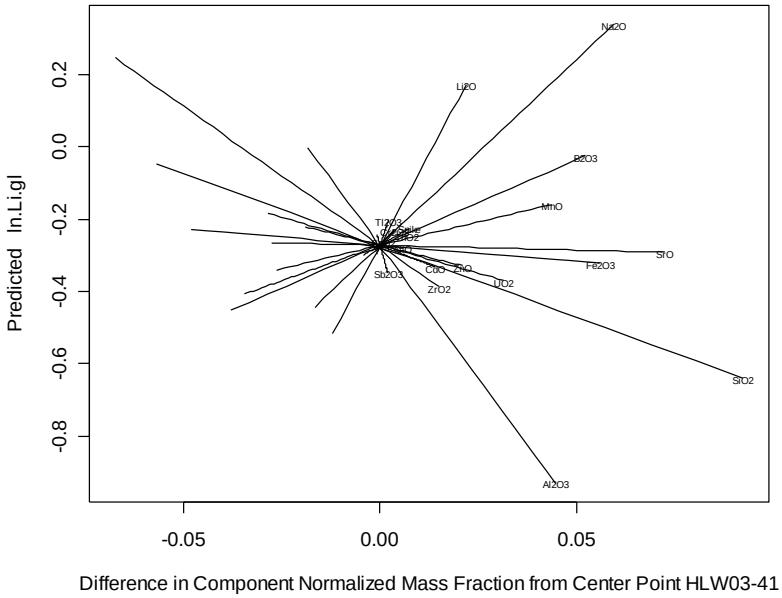

Figure 5.25. Trace Plot Associated with PCT-Lithium 19-Term Full LM Model.

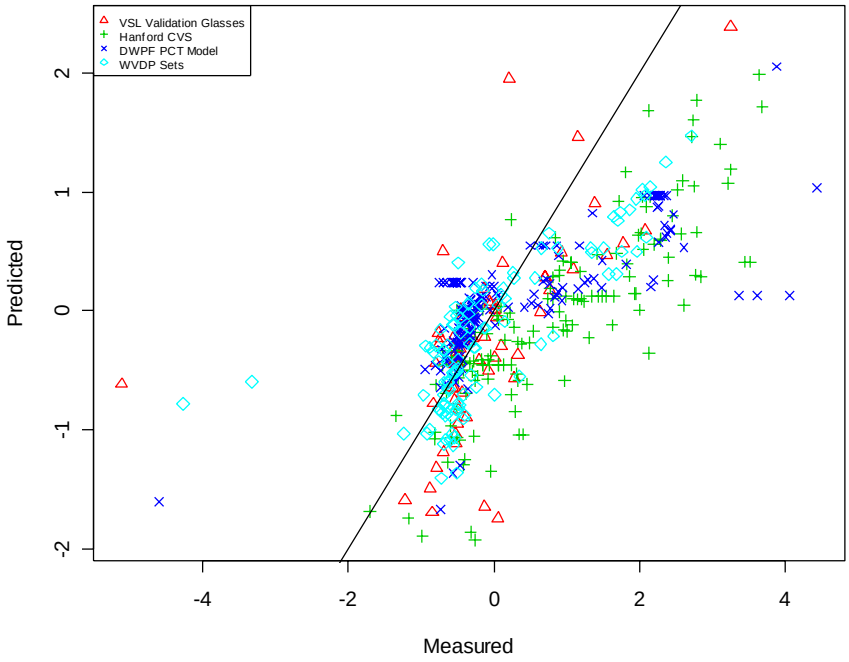

Figure 5.26. Predicted Versus Measured Plot for PCT-Lithium 19-Term Full LM Model and Validation Set V1.

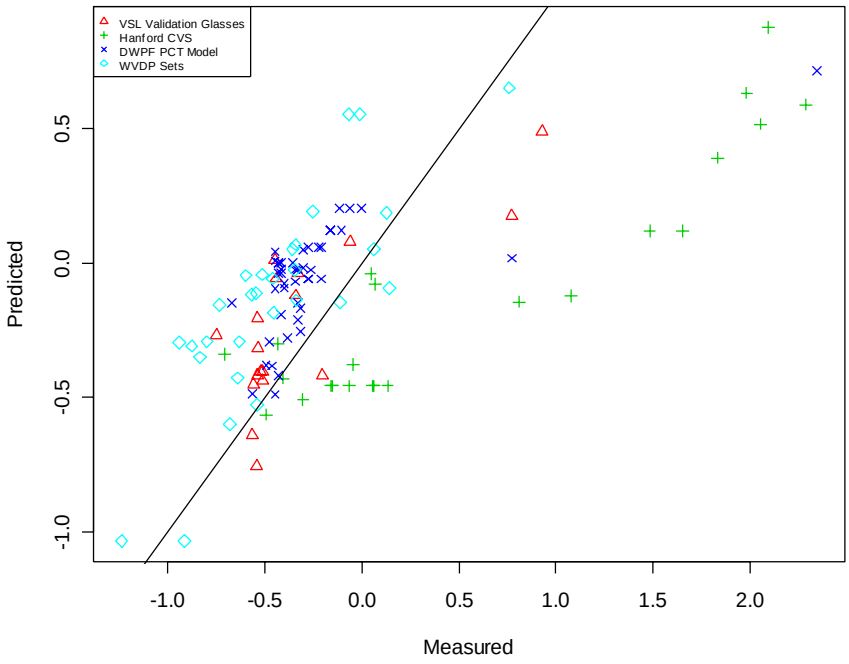

Figure 5.27. Predicted Versus Measured Plot for PCT-Lithium 19-Term Full LM Model and Validation Set V2a.

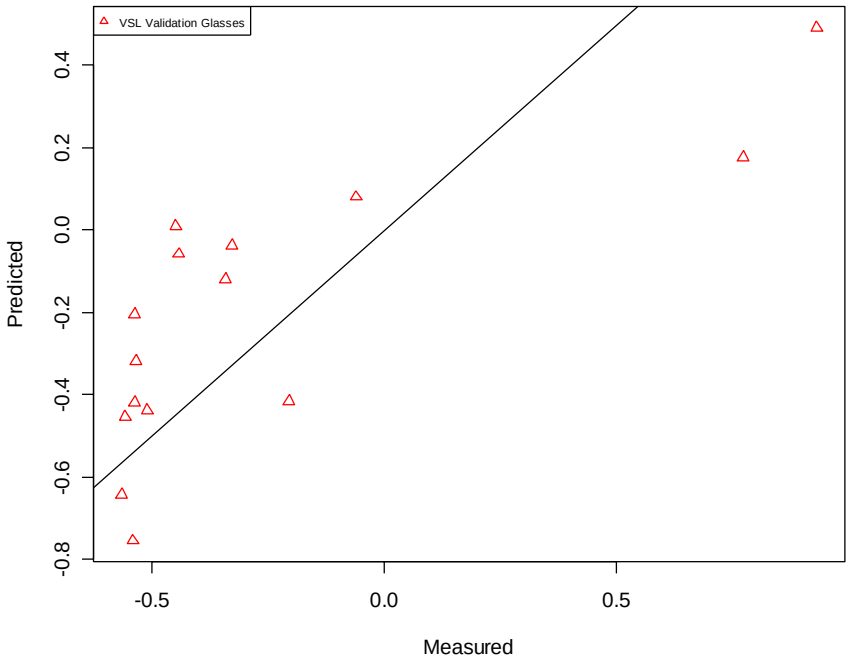

Figure 5.28. Predicted Versus Measured Plot for PCT-Lithium 19-Term Full LM Model and Validation Set V2b.

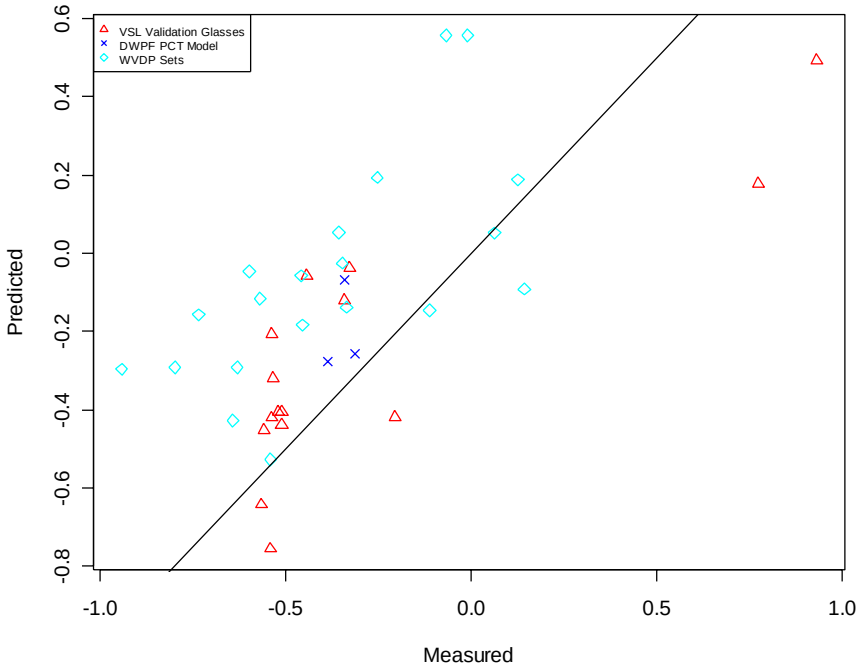

Figure 5.29. Predicted Versus Measured Plot for PCT-Lithium 19-Term Full LM Model and Validation Set V3a.

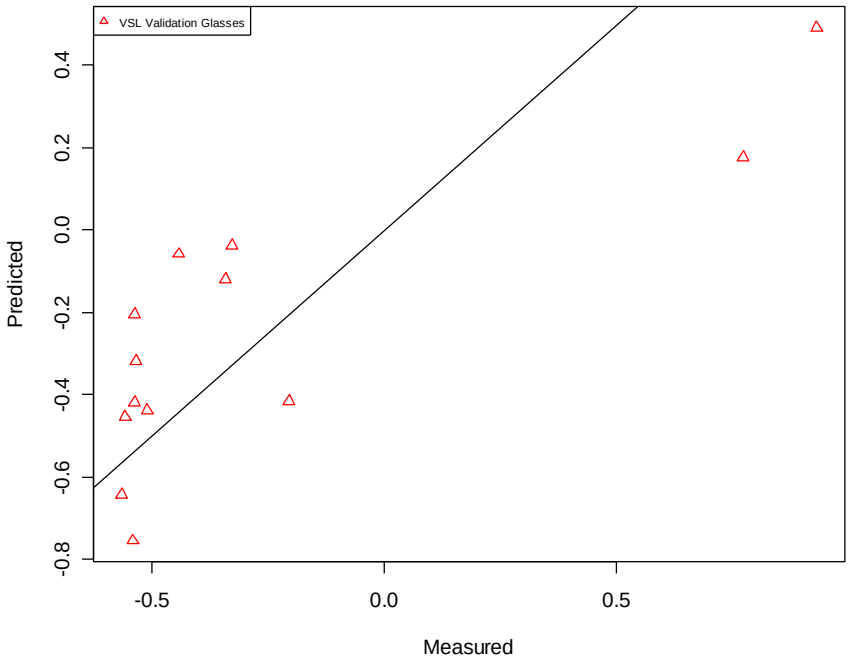

Figure 5.30. Predicted Versus Measured Plot for PCT-Lithium 19-Term Full LM Model and Validation Set V3b.

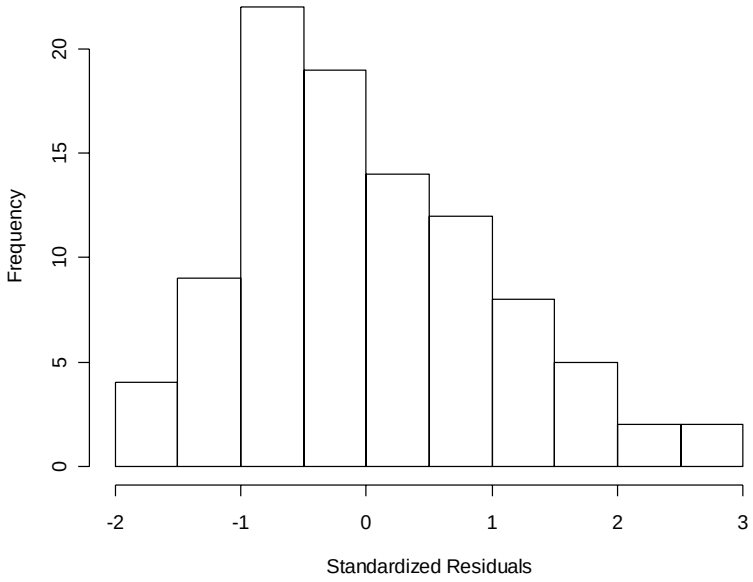

Figure 5.31. Histogram of Standardized Residuals for PCT-Lithium 8-Term Reduced LM Model.

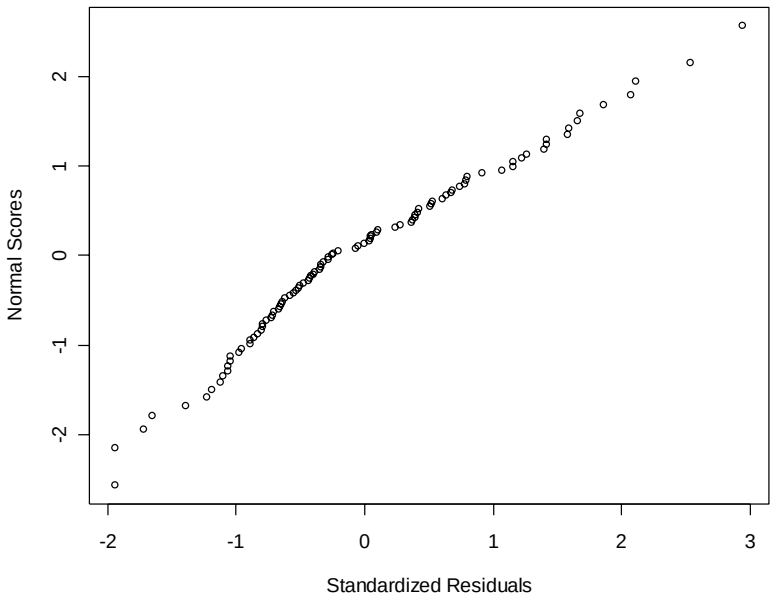

Figure 5.32. Normality Plot Associated with PCT-Lithium 8-Term Reduced LM Model.

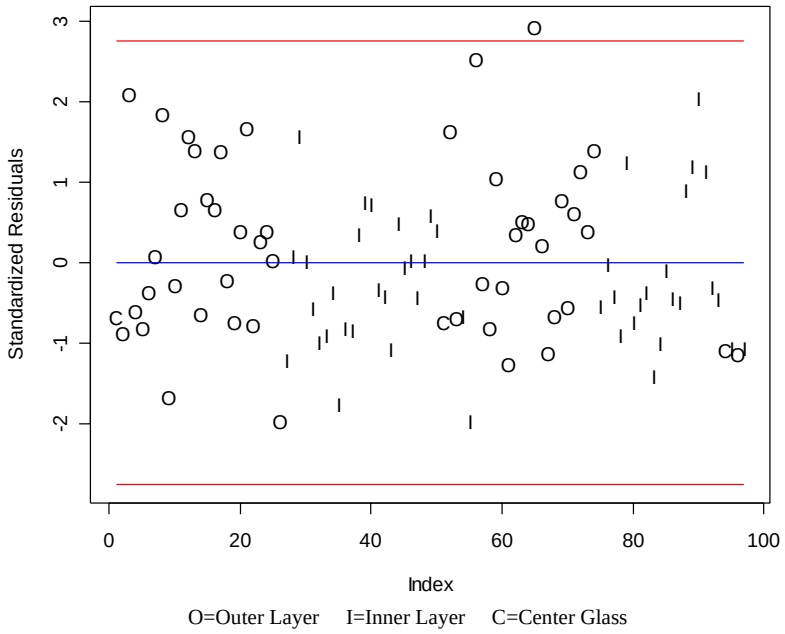

Figure 5.33. Plot of Standardized Residuals for PCT-Lithium 8-Term Reduced LM Model.

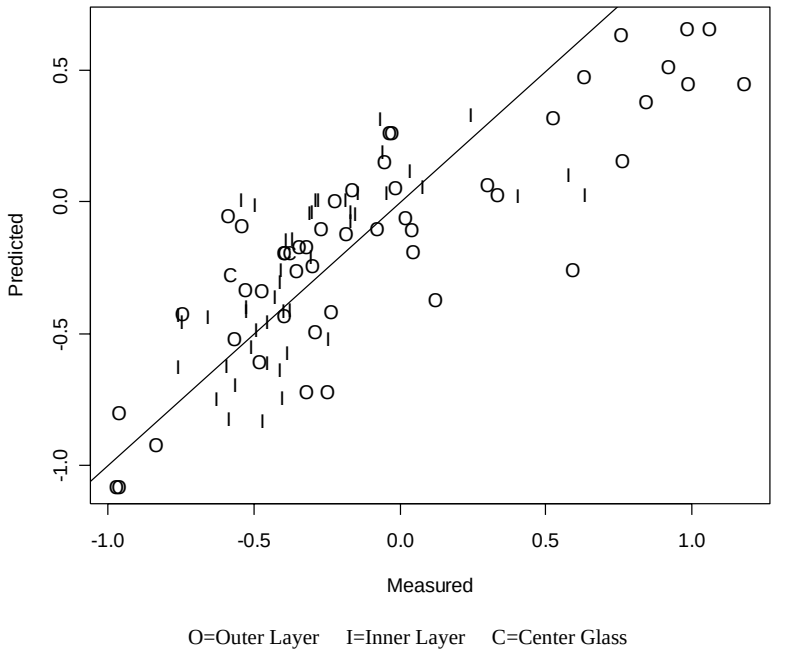

Figure 5.34. Predicted Versus Measured Plot for PCT-Lithium 8-Term Reduced LM Model.

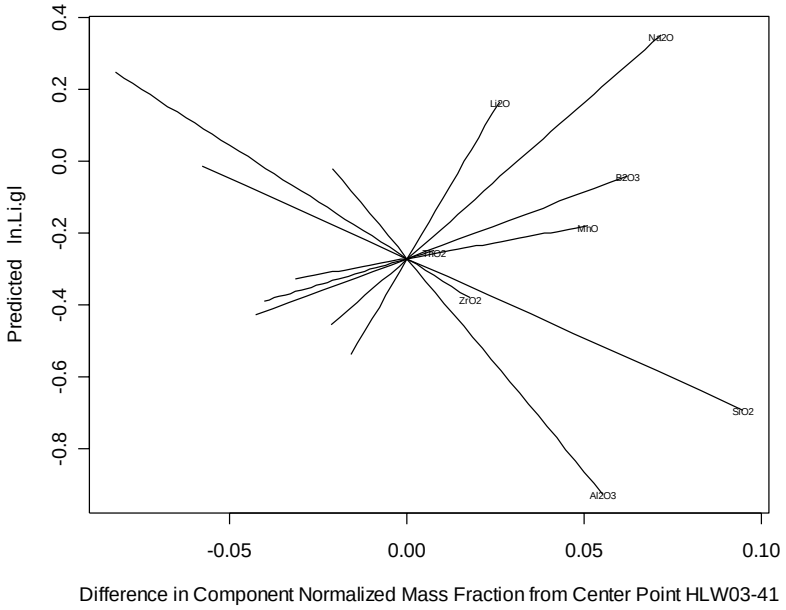

Figure 5.35. Trace Plot Associated with PCT-Lithium 8-Term Reduced LM Model.

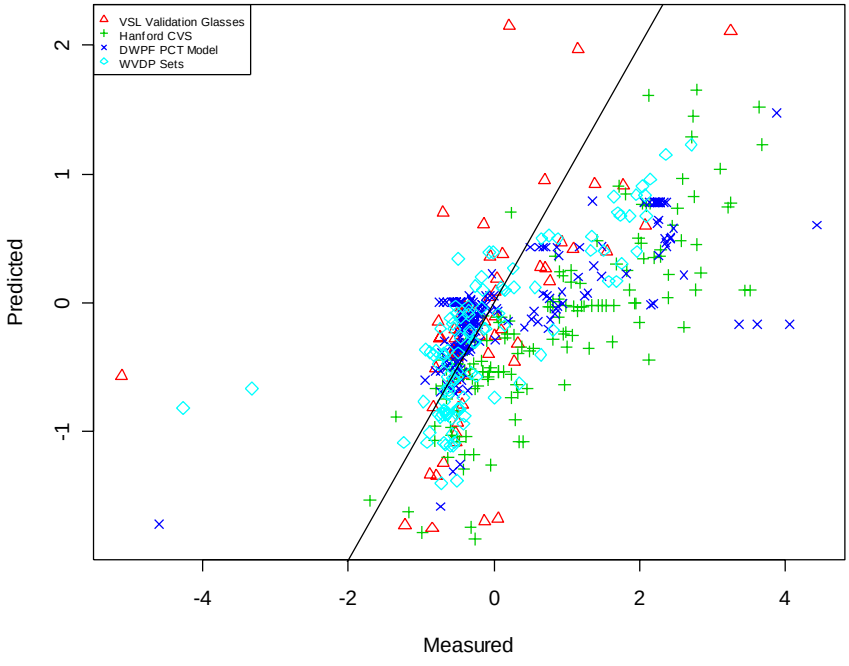

Figure 5.36. Predicted Versus Measured Plot for PCT-Lithium 8-Term Reduced LM Model and Validation Set V1.

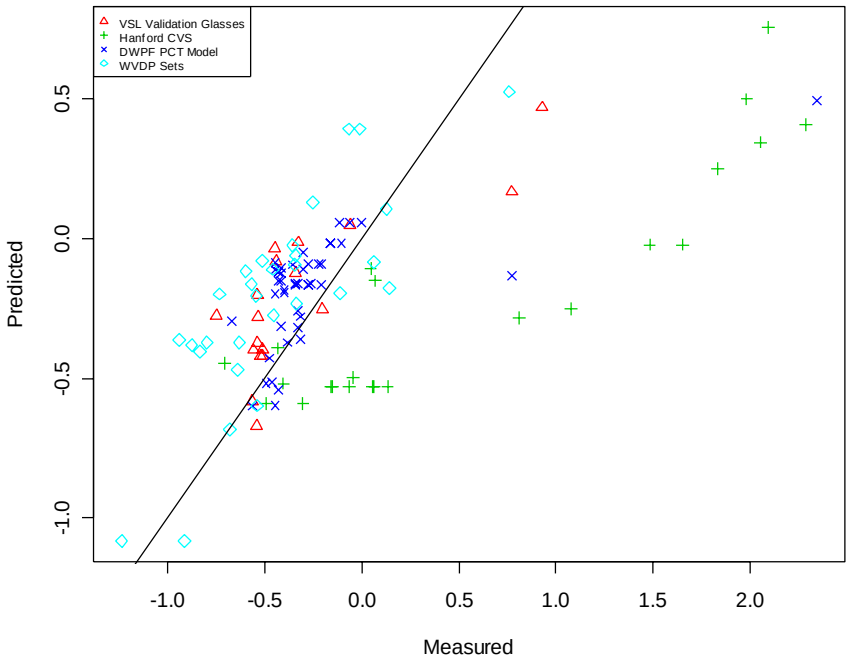

Figure 5.37. Predicted Versus Measured Plot for PCT-Lithium 8-Term Reduced LM Model and Validation Set V2a.

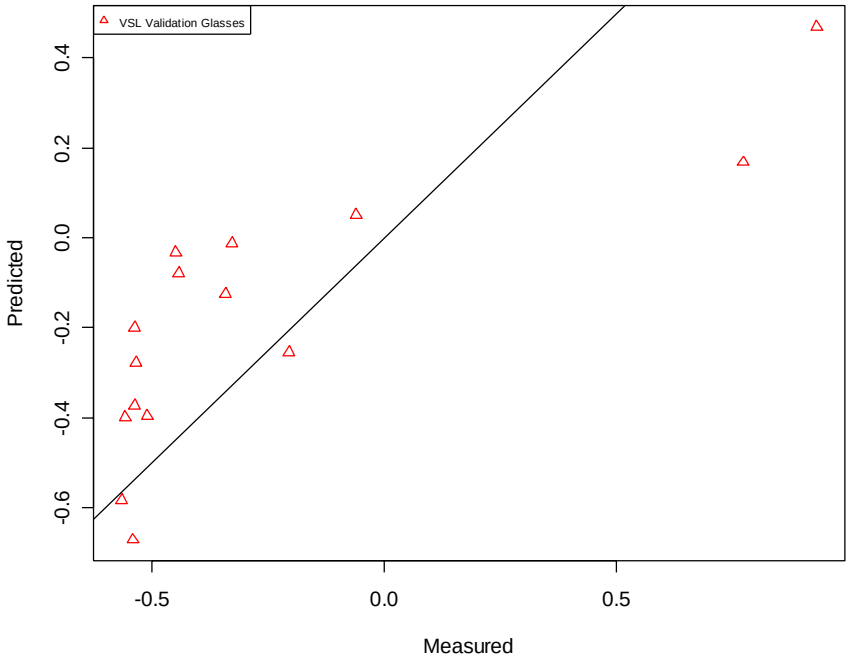

Figure 5.38. Predicted Versus Measured Plot for PCT-Lithium 8-Term Reduced LM Model and Validation Set V2b.

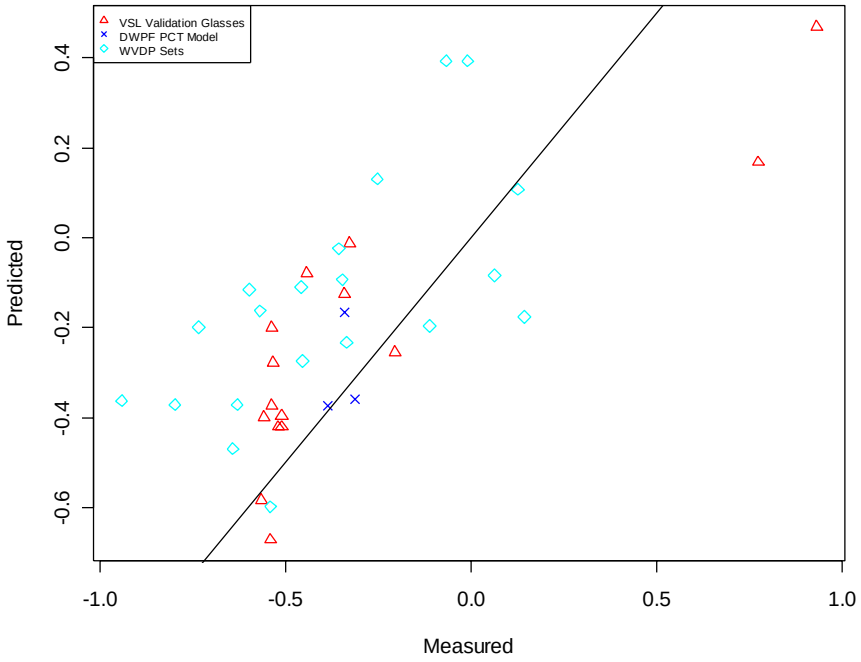

Figure 5.39. Predicted Versus Measured Plot for PCT-Lithium 8-Term Reduced LM Model and Validation Set V3a.

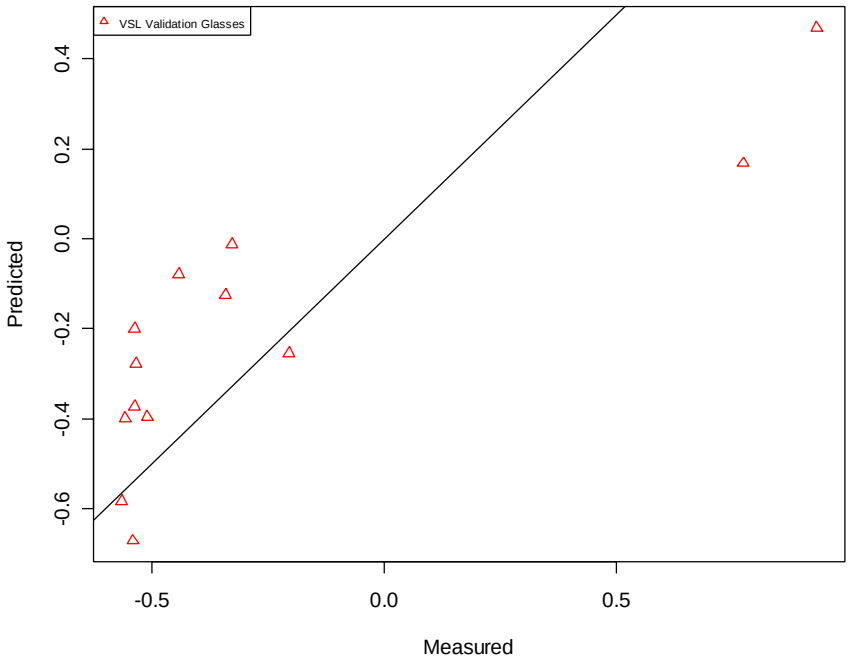

Figure 5.40. Predicted Versus Measured Plot for PCT-Lithium 8-Term Reduced LM Model and Validation Set V3b.

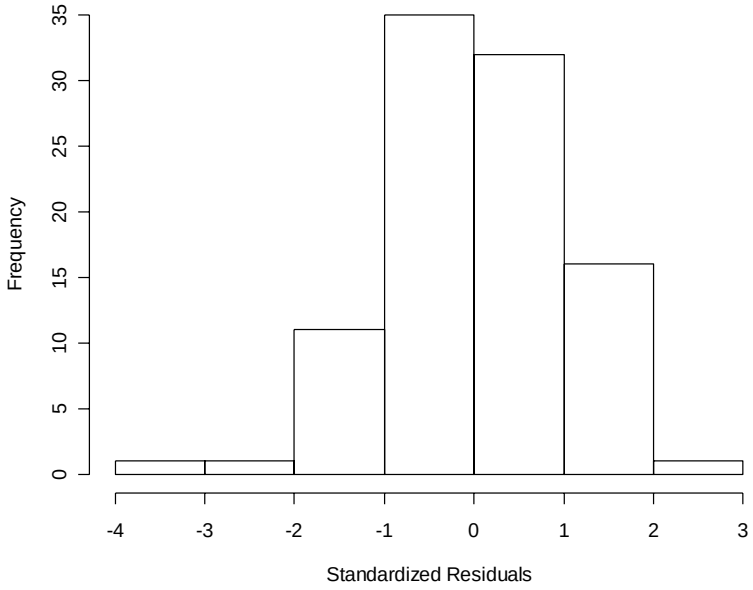

Figure 5.41. Histogram of Standardized Residuals for PCT-Sodium 19-Term Full LM Model.

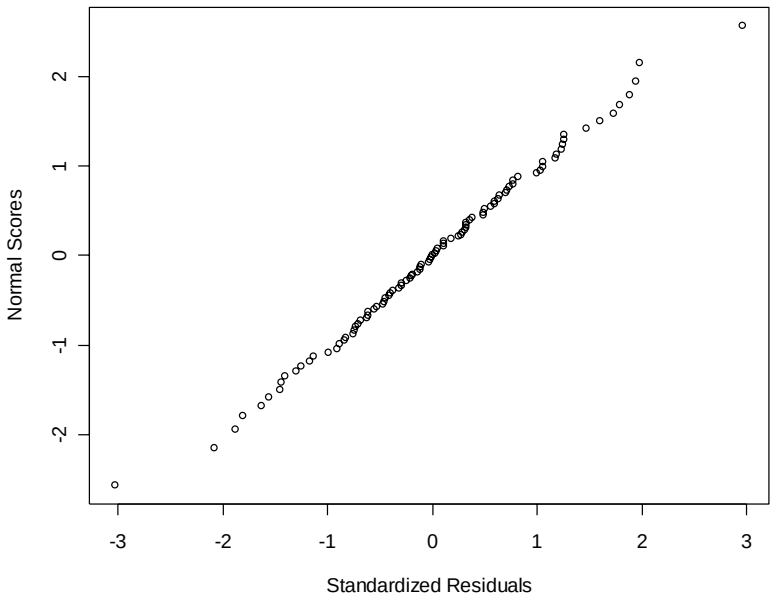

Figure 5.42. Normality Plot Associated with PCT-Sodium 19-Term Full LM Model.

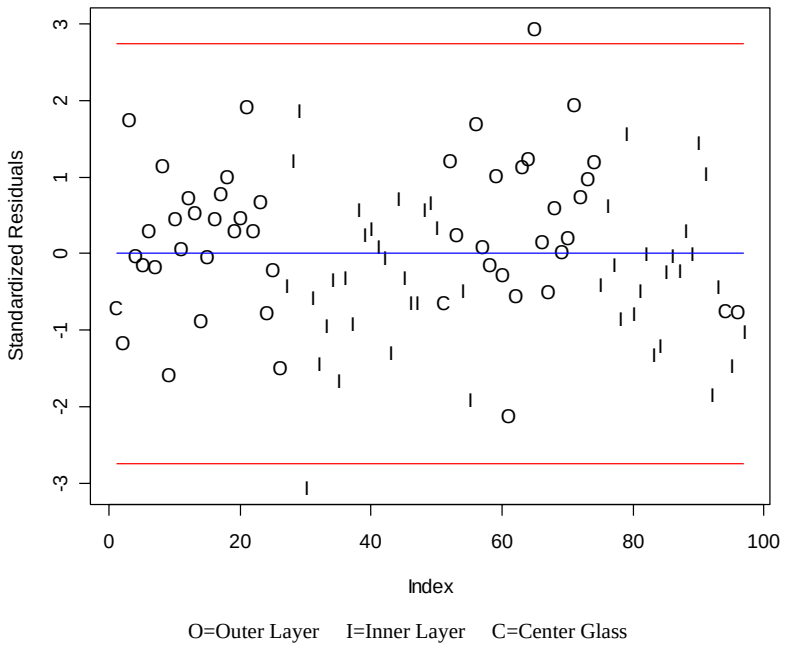

Figure 5.43. Plot of Standardized Residuals for PCT-Sodium 19-Term Full LM Model.

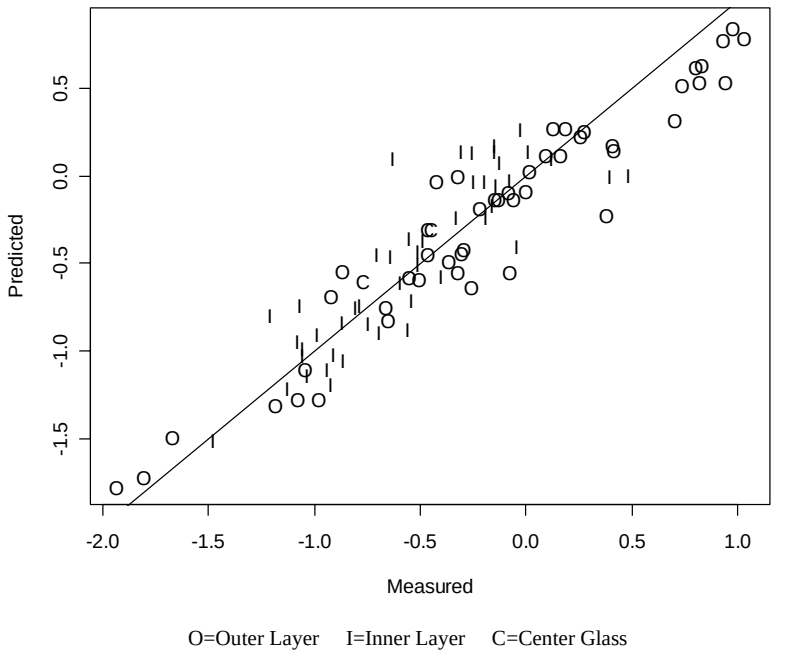

Figure 5.44. Predicted Versus Measured Plot for PCT-Sodium 19-Term Full LM Model.

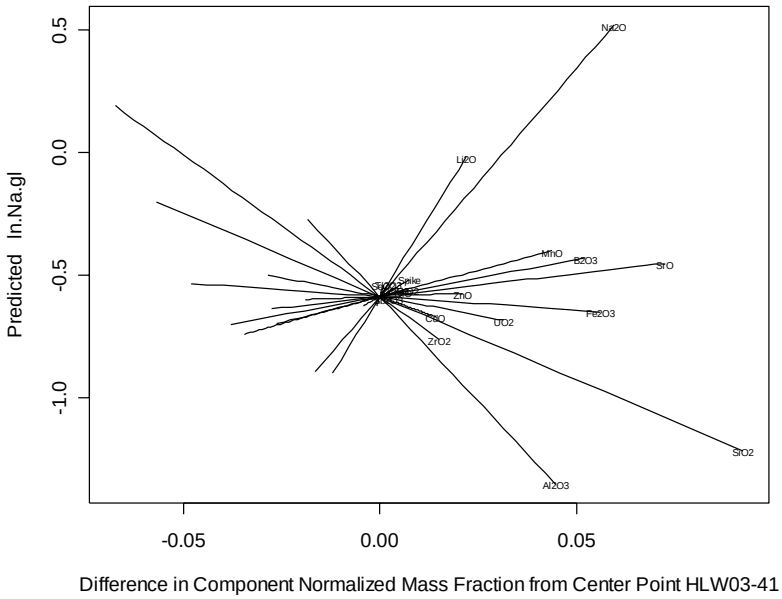

Figure 5.45. Trace Plot Associated with PCT-Sodium 19-Term Full LM Model.

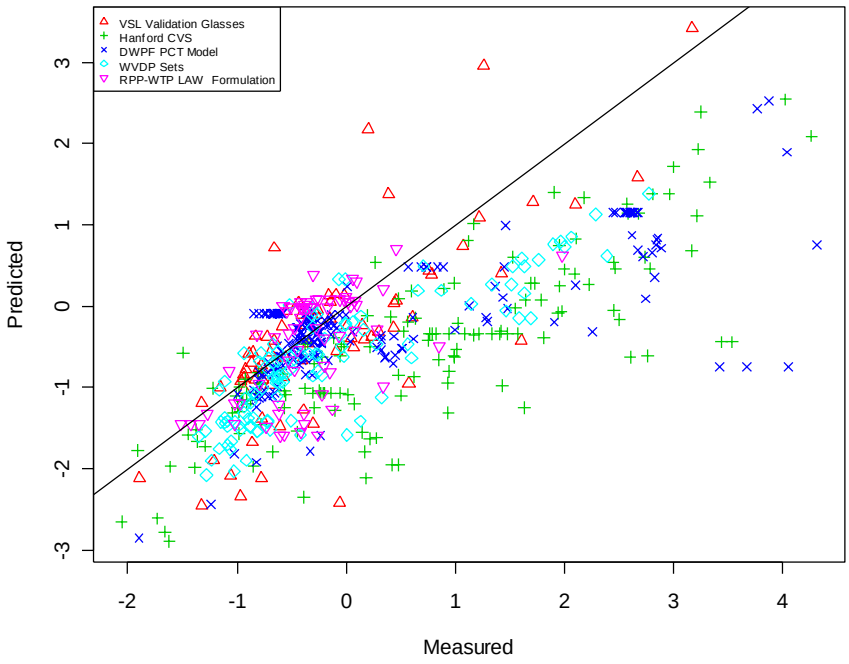

Figure 5.46. Predicted Versus Measured Plot for PCT-Sodium 19-Term Full LM Model and Validation Set V1.

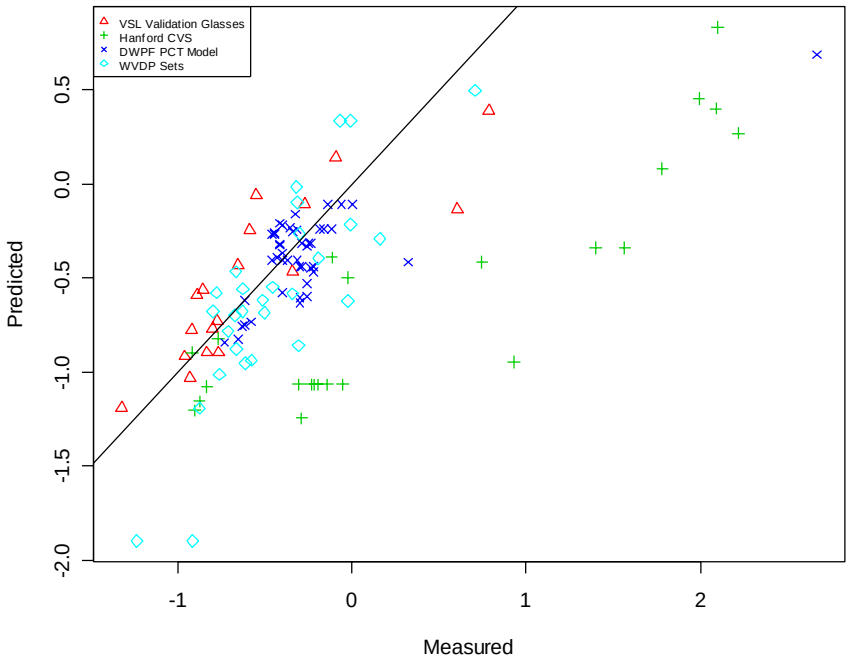

Figure 5.47. Predicted Versus Measured Plot for PCT-Sodium 19-Term Full LM Model and Validation Set V2a.

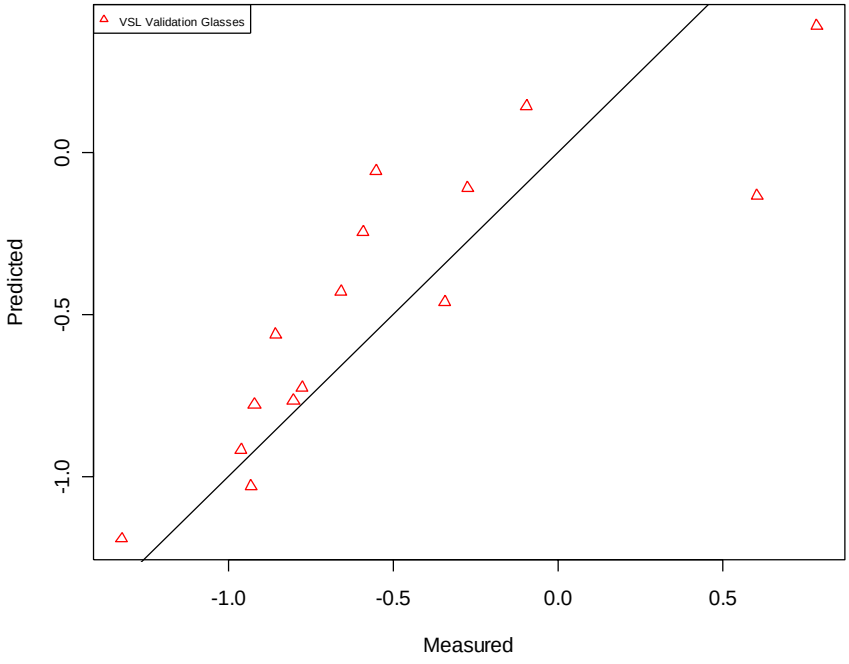

Figure 5.48. Predicted Versus Measured Plot for PCT-Sodium 19-Term Full LM Model and Validation Set V2b.

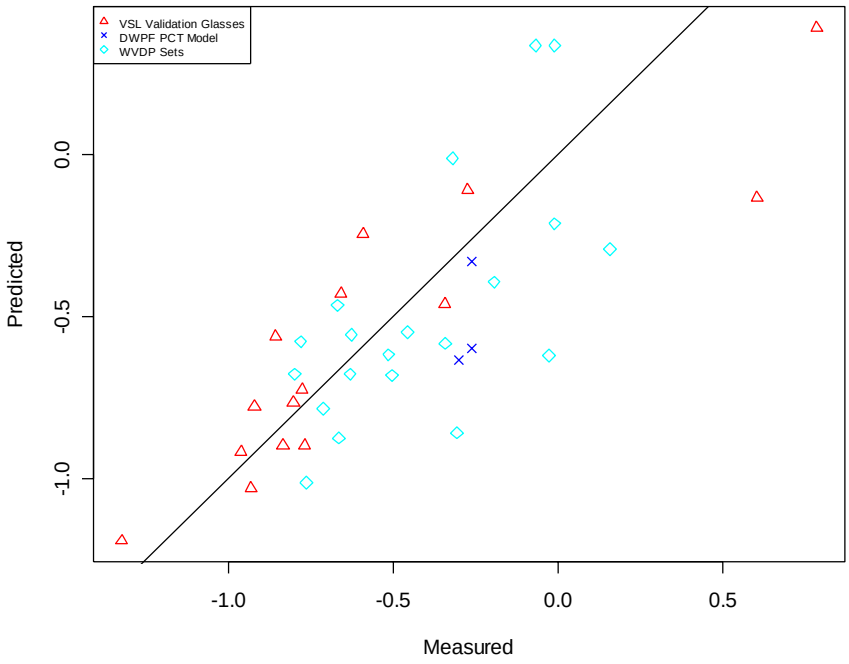

Figure 5.49. Predicted Versus Measured Plot for PCT-Sodium 19-Term Full LM Model and Validation Set V3a.

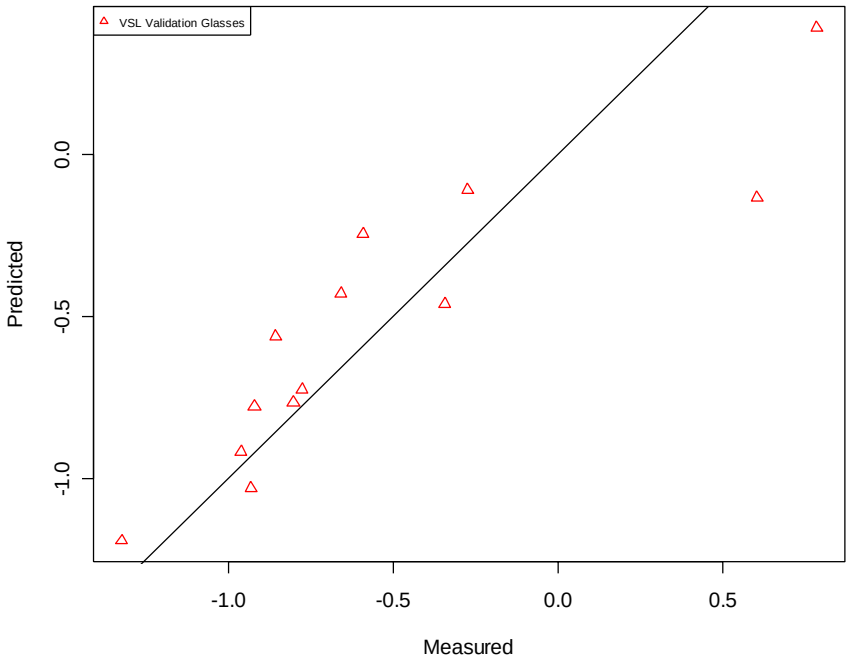

Figure 5.50. Predicted Versus Measured Plot for PCT-Sodium 19-Term Full LM Model and Validation Set V3b.

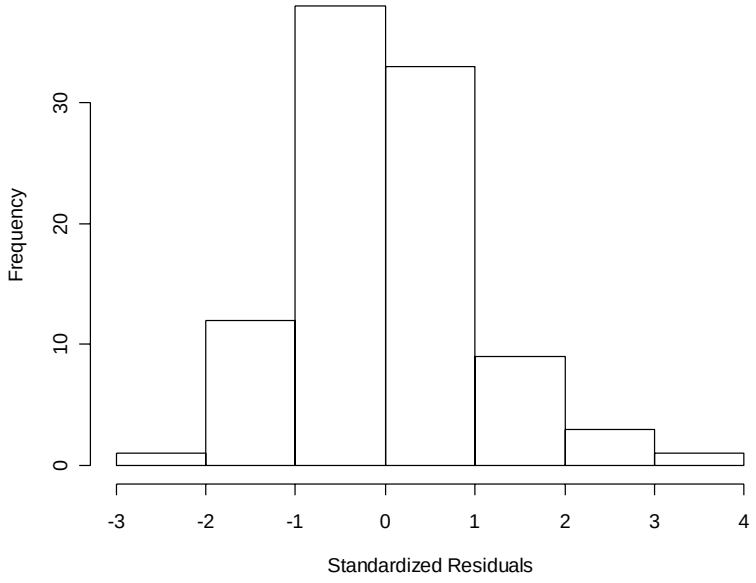

Figure 5.51. Histogram of Standardized Residuals for PCT-Sodium 8-Term Reduced LM Model.

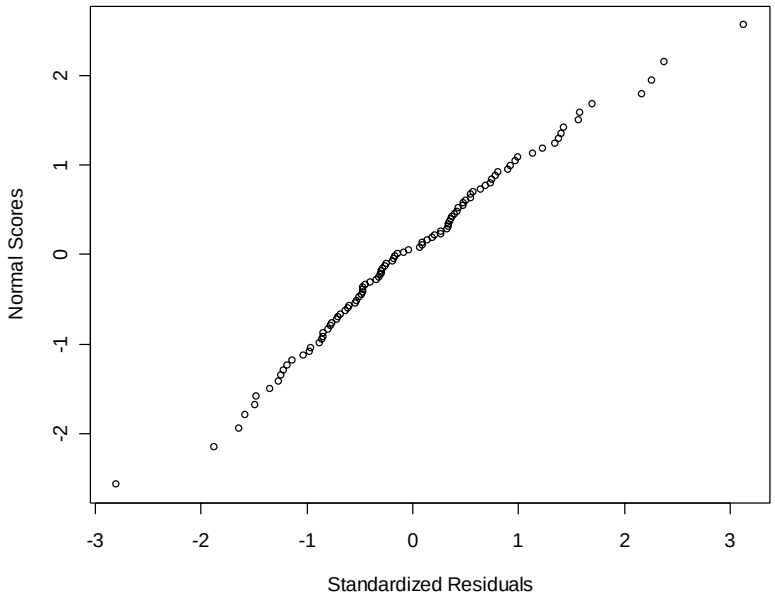

Figure 5.52. Normality Plot Associated with PCT-Sodium 8-Term Reduced LM Model.

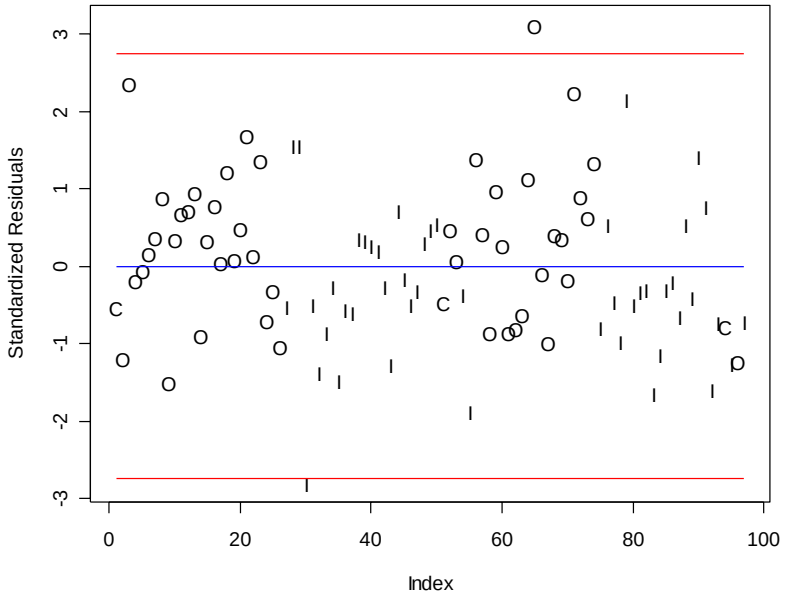

Figure 5.53. Plot of Standardized Residuals for PCT-Sodium 8-Term Reduced LM Model.

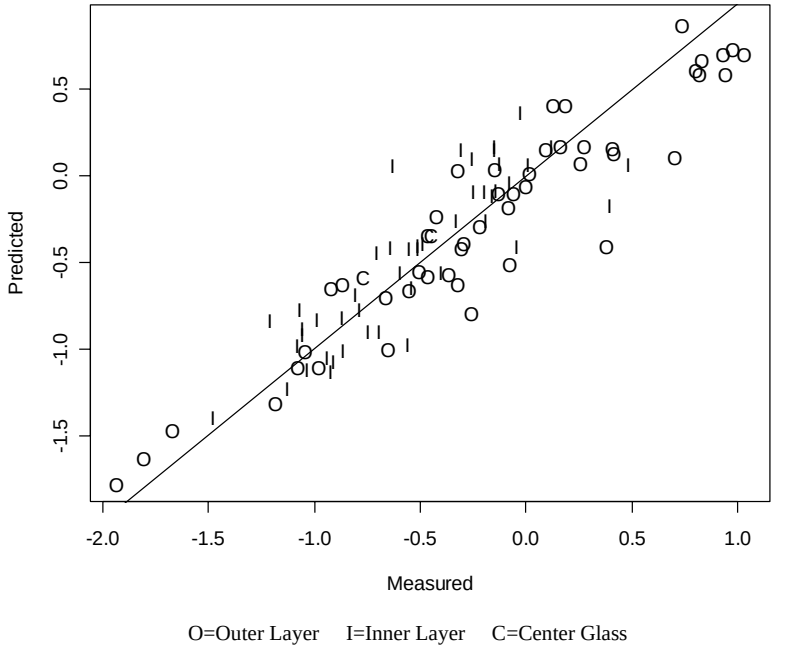

Figure 5.54. Predicted Versus Measured Plot for PCT-Sodium 8-Term Reduced LM Model.

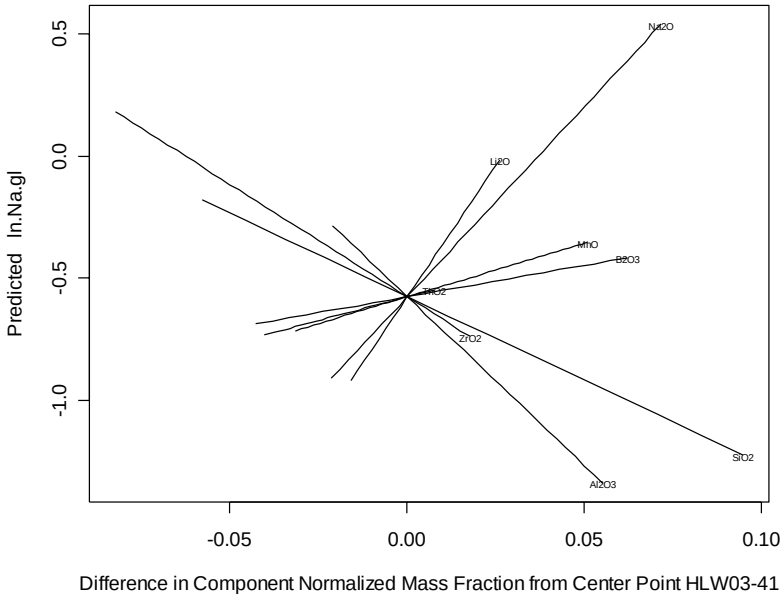

Figure 5.55. Trace Plot Associated with PCT-Sodium 8-Term Reduced LM Model.

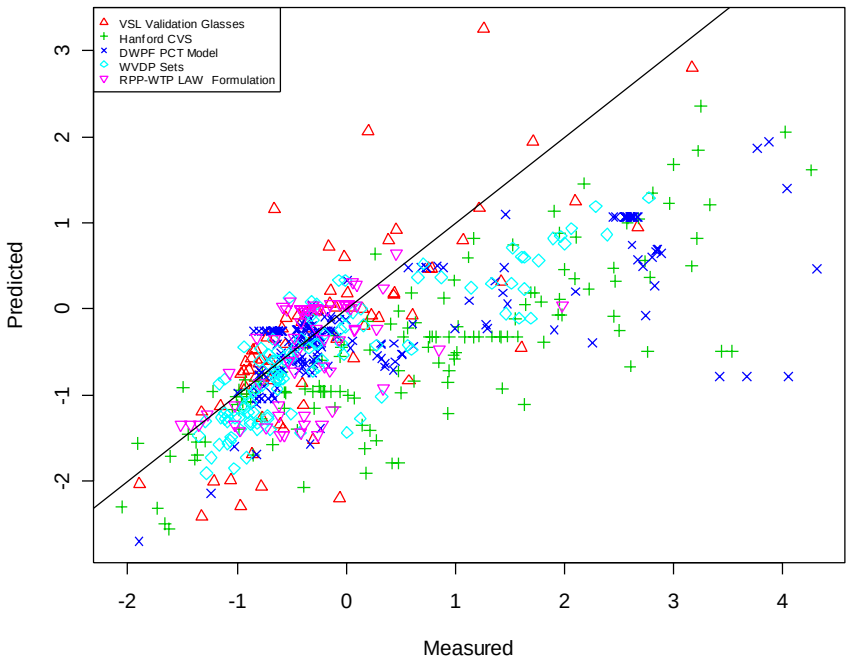

Figure 5.56. Predicted Versus Measured Plot for PCT-Sodium 8-Term Reduced LM Model and Validation Set V1.

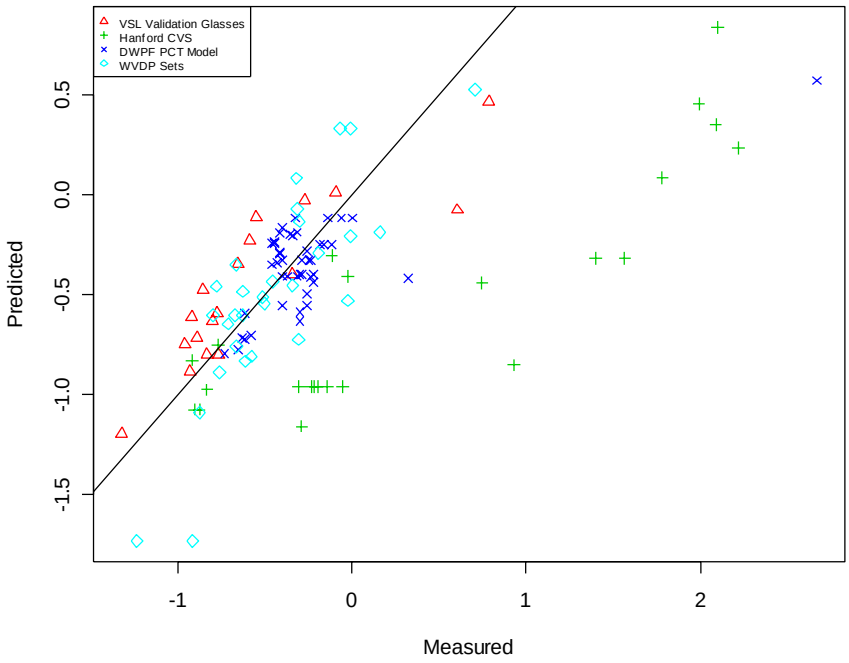

Figure 5.57. Predicted Versus Measured Plot for PCT-Sodium 8-Term Reduced LM Model and Validation Set V2a.

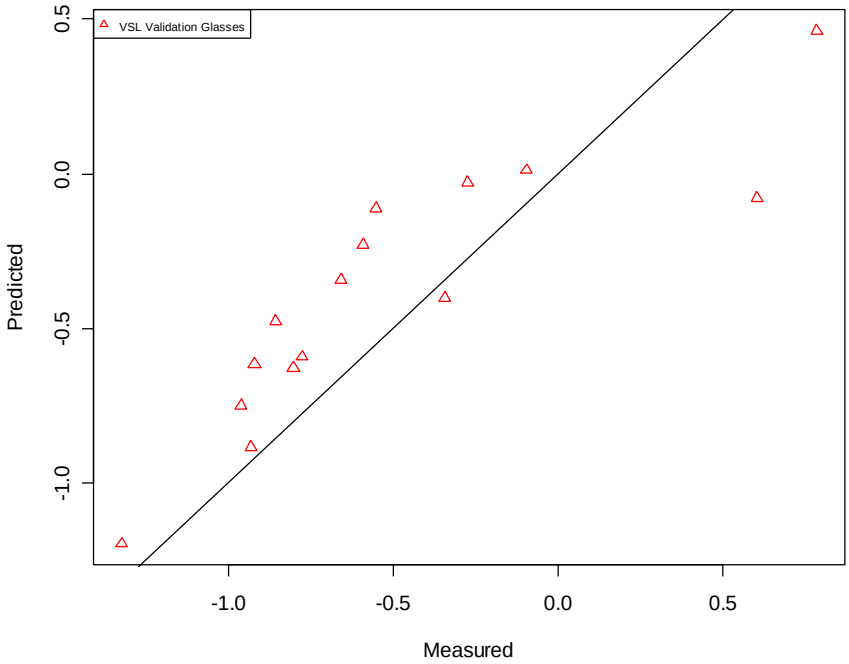

Figure 5.58. Predicted Versus Measured Plot for PCT-Sodium 8-Term Reduced LM Model and Validation Set V2b.

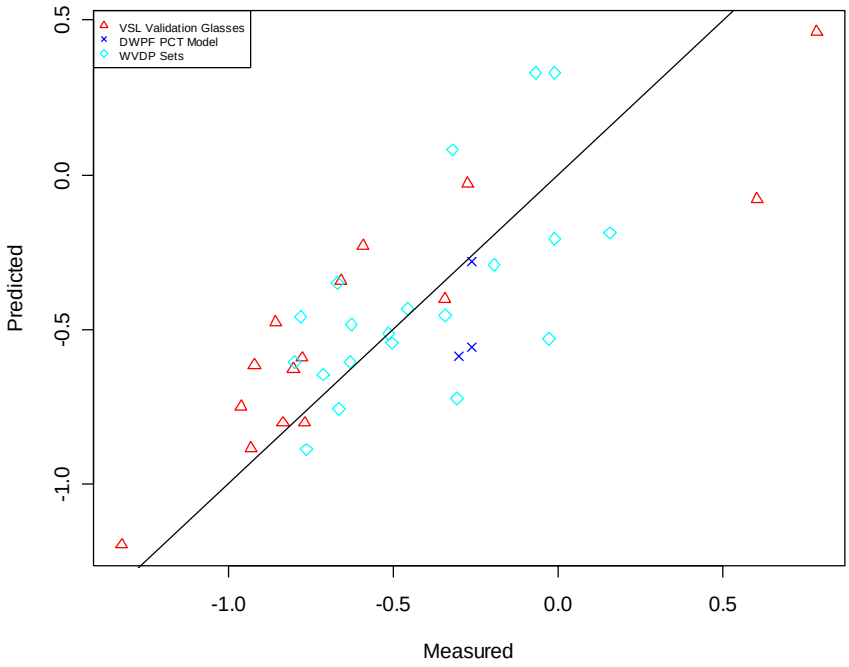

Figure 5.59. Predicted Versus Measured Plot for PCT-Sodium 8-Term Reduced LM Model and Validation Set V3a.

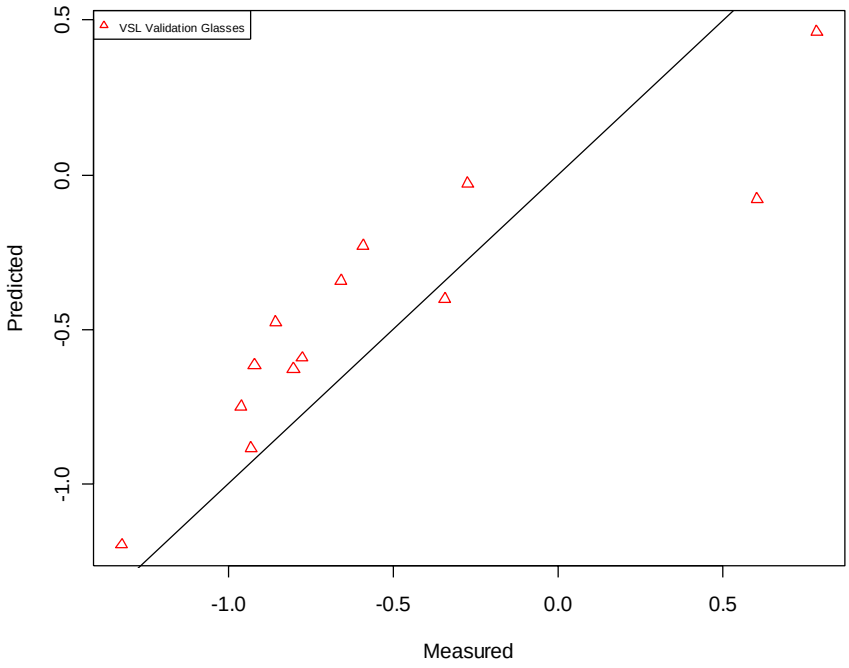

Figure 5.60. Predicted Versus Measured Plot for PCT-Sodium 8-Term Reduced LM Model and Validation Set V3b.

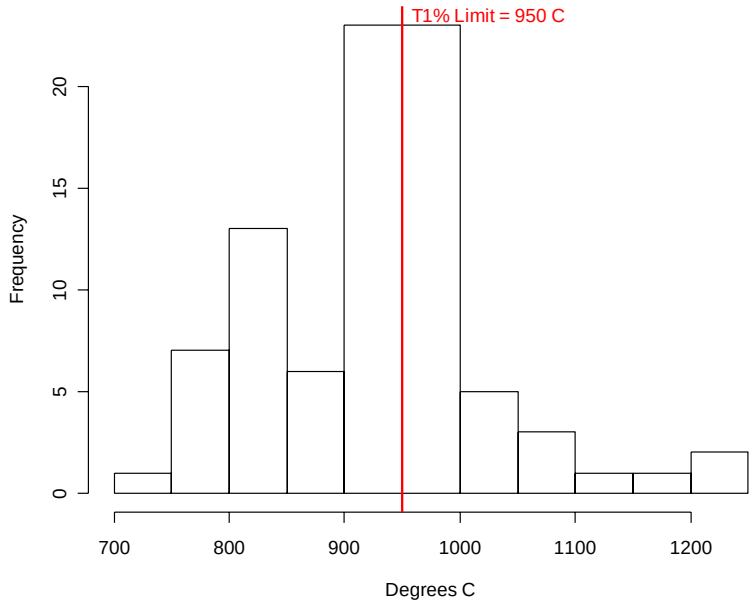

Figure 6.1. Histogram of Estimated $T_{1\%}$ Values for 85 Model Development Glasses.

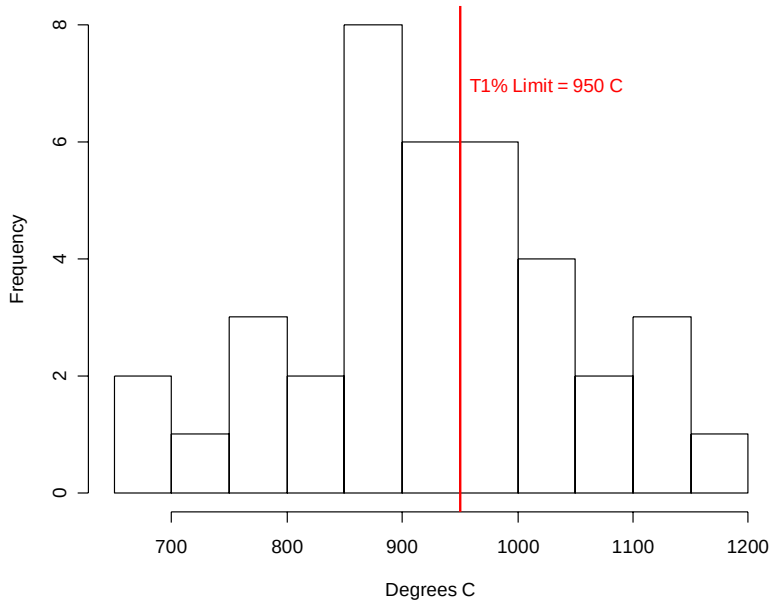

Figure 6.2. Histogram of Estimated $T_{1\%}$ Values for 38 Validation Glasses.

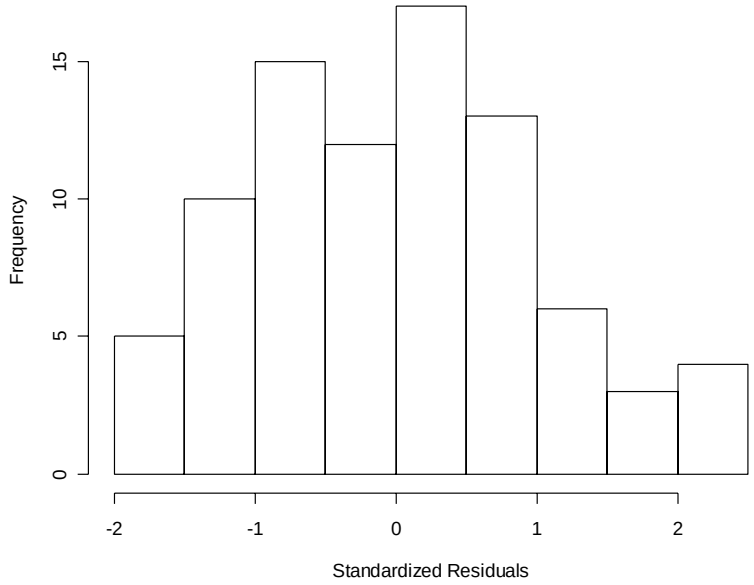

Figure 6.3. Histogram of Standardized Residuals for $T_{1\%}$ (Spinel) 19-Term Full LM Model.

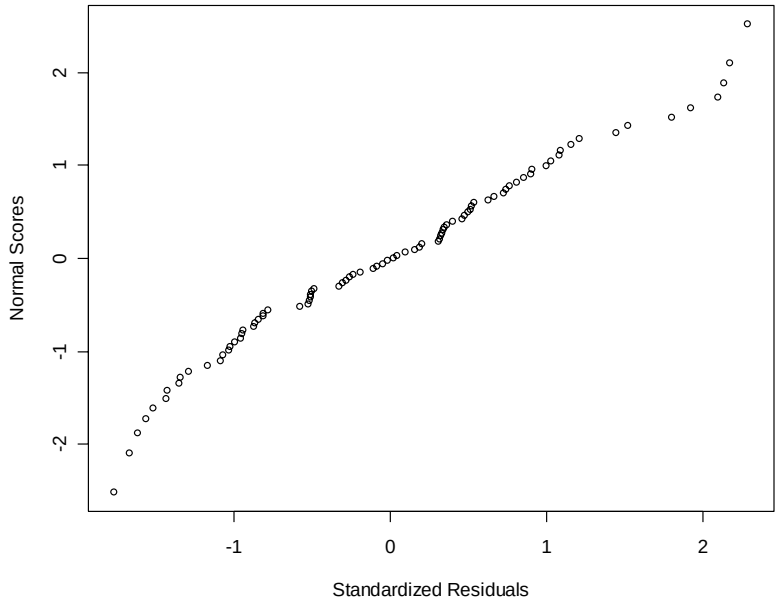

Figure 6.4. Normality Plot Associated with $T_{1\%}$ (Spinel) 19-Term Full LM Model.

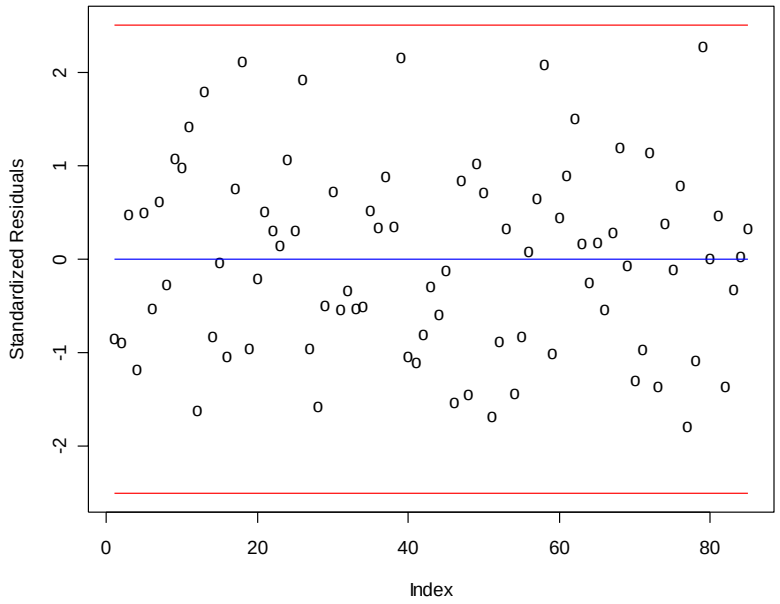

Figure 6.5. Plot of Standardized Residuals for $T_{1\%}$ (Spinel) 19-Term Full LM Model.

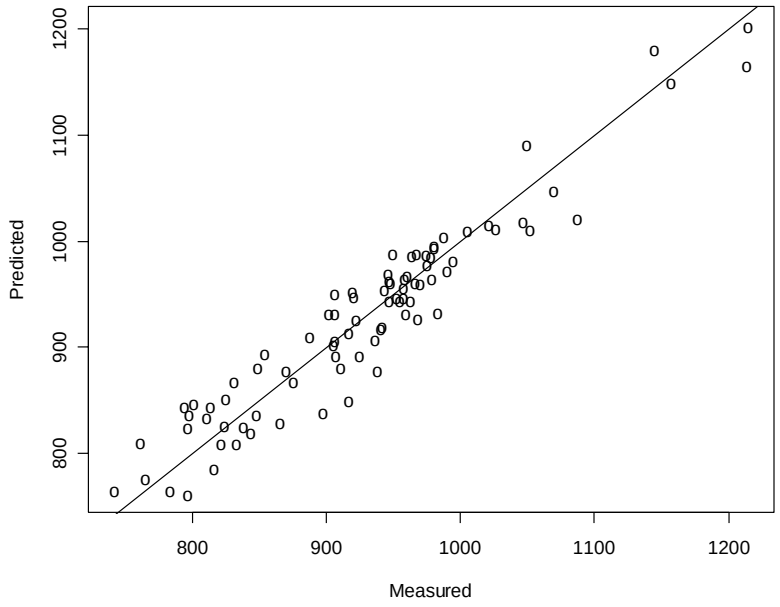

Figure 6.6. Predicted Versus Measured Plot for $T_{1\%}$ (Spinel) 19-Term Full LM Model.

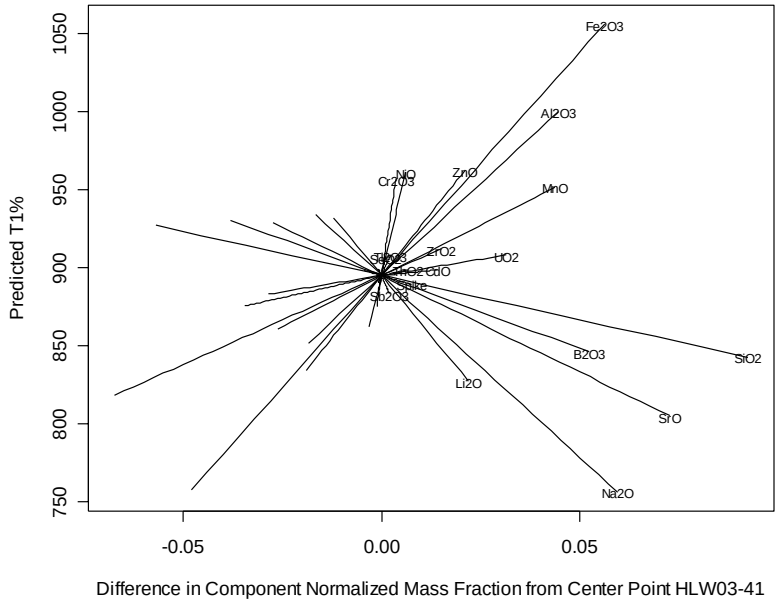

Figure 6.7. Trace Plot Associated with $T_{1\%}$ (Spinel) 19-Term Full LM Model.

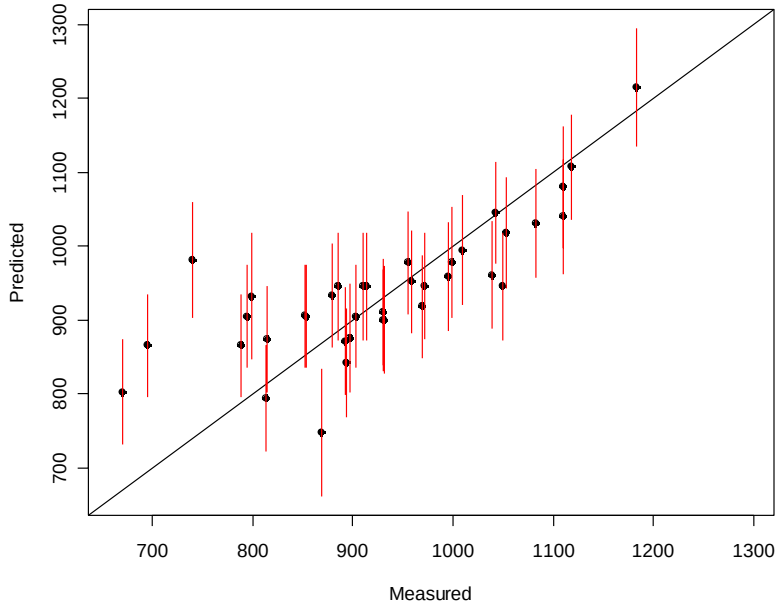

Figure 6.8. Predicted Versus Measured Plot for $T_{1\%}$ (Spinel) 19-Term Full LM Model and Validation Set V1.

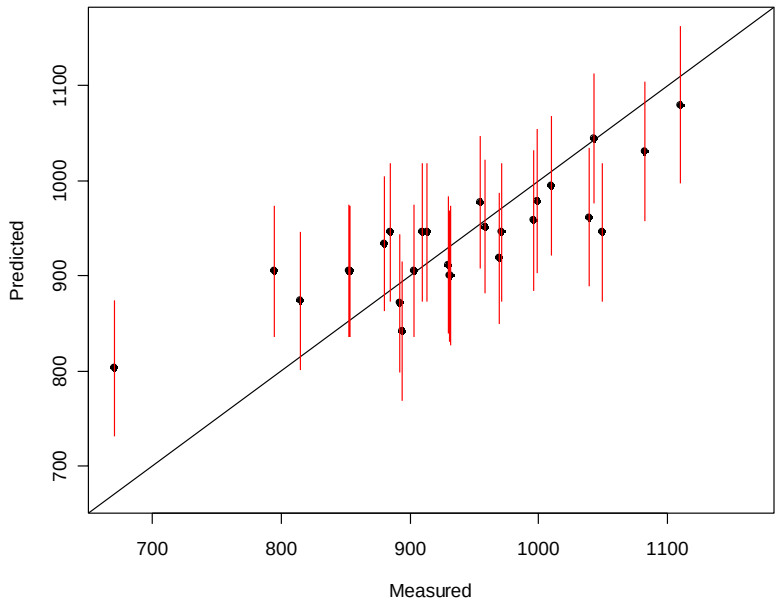

Figure 6.9. Predicted Versus Measured Plot for $T_{1\%}$ (Spinel) 19-Term Full LM Model and Validation Set V2.

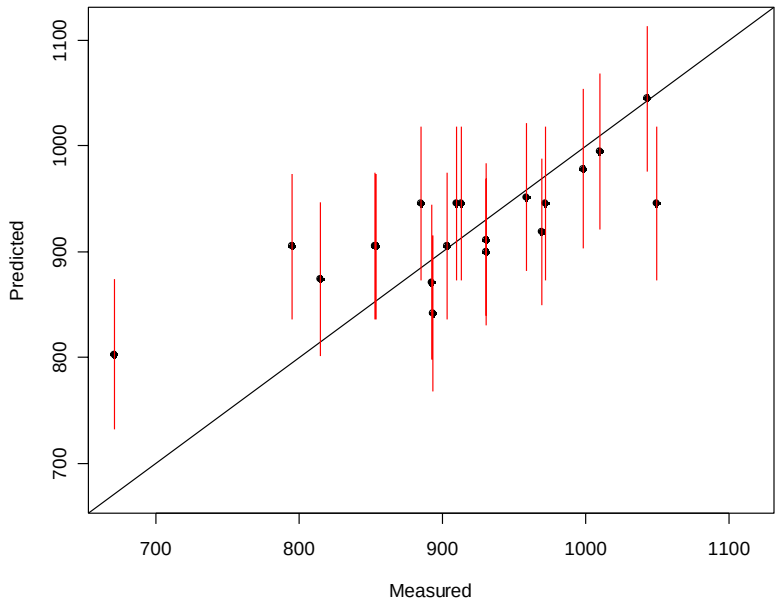

Figure 6.10. Predicted Versus Measured Plot for $T_{1\%}$ (Spinel) 19-Term Full LM Model and Validation Set V3.

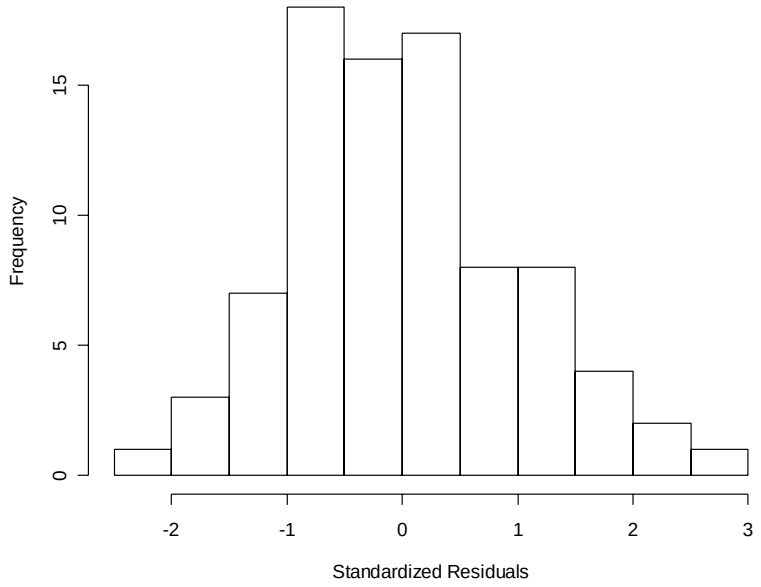

Figure 6.11. Histogram of Standardized Residuals for $T_{1\%}$ (Spinel) 13-Term Reduced LM Model.

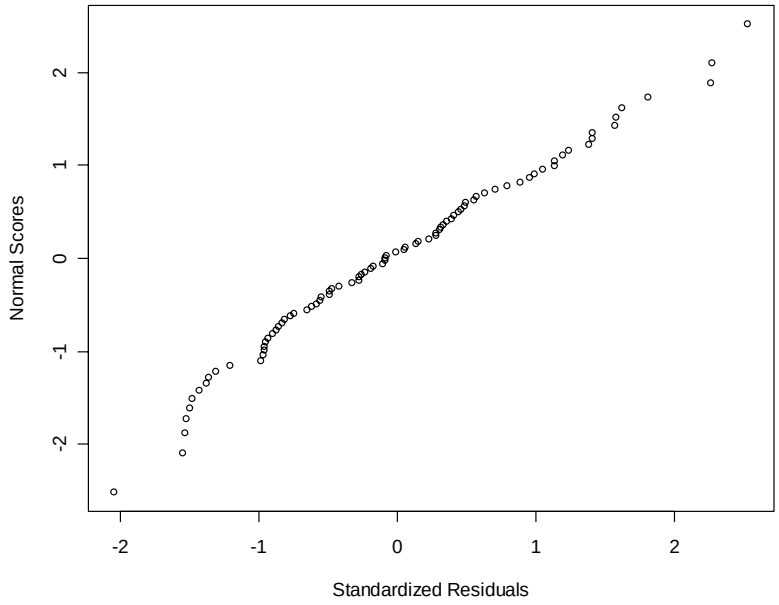

Figure 6.12. Normality Plot Associated with $T_{1\%}$ (Spinel) 13-Term Reduced LM Model.

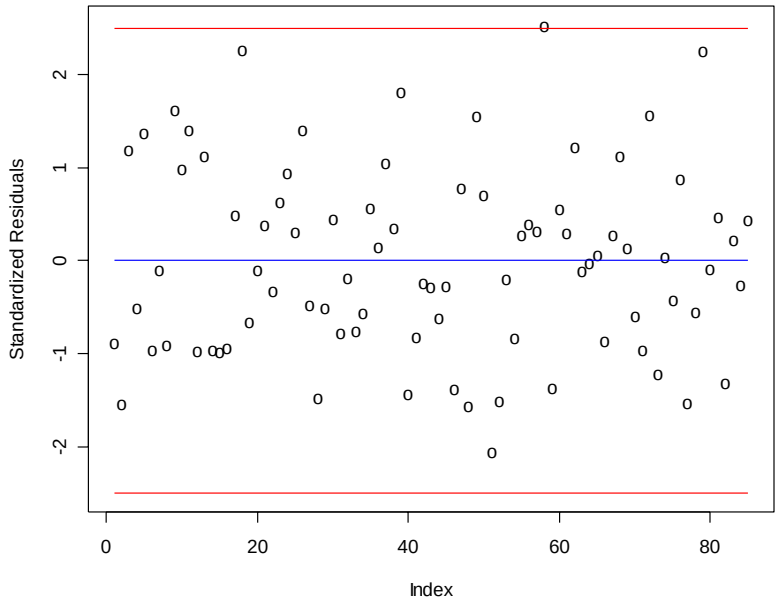

Figure 6.13. Plot of Standardized Residuals for $T_{1\%}$ (Spinel) 13-Term Reduced LM Model.

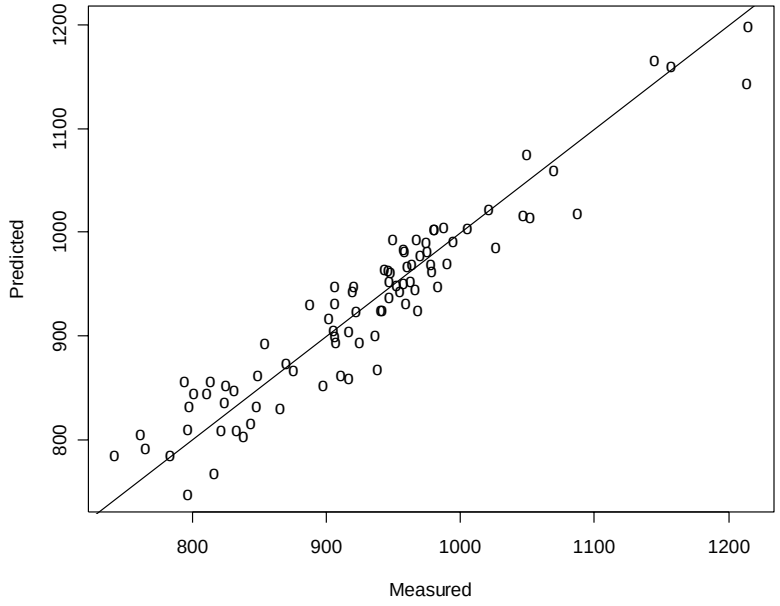

Figure 6.14. Predicted Versus Measured Plot for $T_{1\%}$ (Spinel) 13-Term Reduced LM Model.

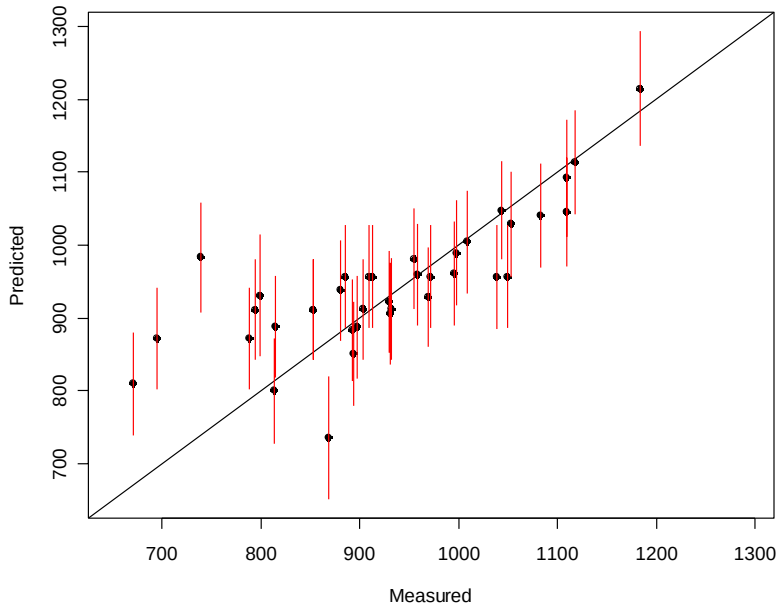

Figure 6.15. Predicted Versus Measured Plot for $T_{1\%}$ (Spinel) 13-Term Reduced LM Model and Validation Set V1.

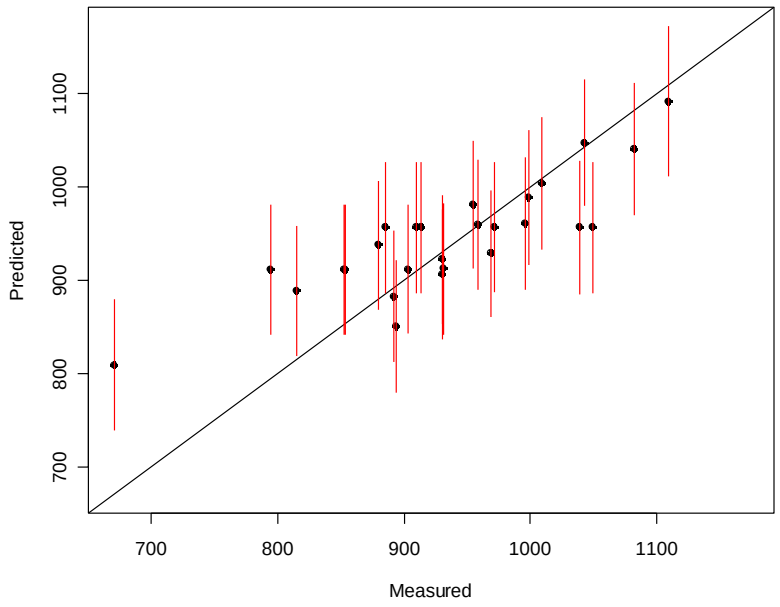

Figure 6.16. Predicted Versus Measured Plot for $T_{1\%}$ (Spinel) 13-Term Reduced LM Model and Validation Set V2.

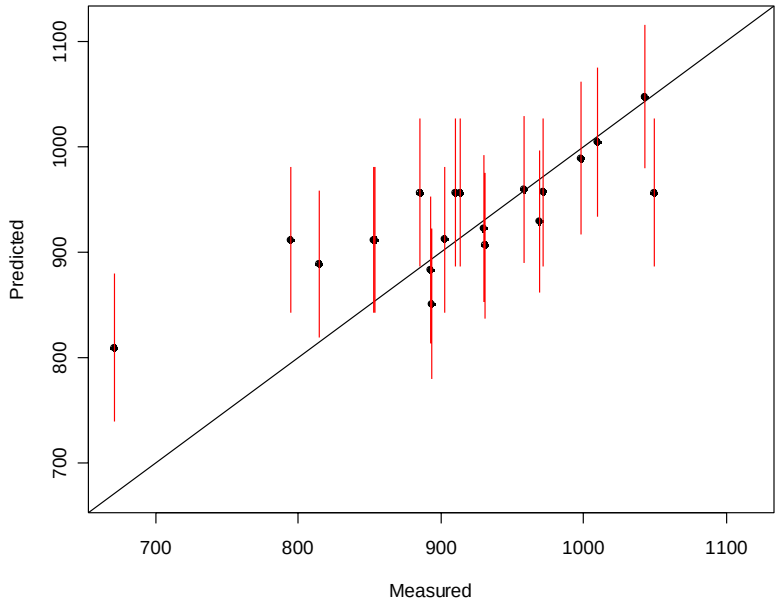

Figure 6.17. Predicted Versus Measured Plot for $T_{1\%}$ (Spinel) 13-Term Reduced LM Model and Validation Set V3.

APPENDIX A

Compositions and PCT Release Data for Validation Glasses Used for Phase 1 IHLW PCT Models

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Compositions and PCT Release Data for Validation Glasses Used for Phase 1 IHLW PCT Models

This appendix contains the compositions and corresponding PCT release data for the 574 validation glasses used for model validation of the Phase 1 IHLW PCT property-composition models that are recommended in this report.

The compositions and PCT releases for the 574 validation glasses are described and presented in the report (and appendix):

> Vienna, J. D., D.-S. Kim, and P. Hrma, *Database and Interim Glass Property Models for Hanford HLW and LAW Glasses*, PNNL-14060, Pacific Northwest National Laboratory, September 2002.

The above-mentioned report actually presents data describing 576 glasses. However, two of the glasses were listed twice in the summary tables, WVDG-40 and WVDG-46. Therefore, 574 glasses were actually used for IHLW PCT model validation.

Table A.1 gives the compositions of the 574 validation glasses in normalized wt% format, normalized over the 19 components of the IHLW design matrix. The compositions for these glasses presented in the report by Vienna referenced above originally involved 66 components. However, for the model development calculations relative to full linear mixture (LM) models, the compositions were normalized over the 19 components included in the IHLW design matrix, and converted to mass fractions that sum to 1 for each of the validation glasses. For consistency with the compositions given in Table 5.1 for the IHLW design matrix glasses (those glasses used for IHLW model development), the compositions of the validation glasses are given as wt% values. These compositions are based on components in the revised (new) oxide forms for Phase 1 IHLW modeling.

Table A.2 contains PCT release data for the 574 validation glasses for the elemental releases of PCT-Boron, PCT-Lithium, and PCT-Sodium. PCT releases are given in unnormalized units of ppm and in normalized units of g/L.

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt%.

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
HLW98-02	0.117	0.116	0.007	0.003	0.128	0.021	0.009	0.142	0.005	0.002	0.002	0.351	0.029	0.000	0.004	0.000	0.021	0.032	0.011
HLW98-04	0.125	0.138	0.003	0.001	0.100	0.000	0.004	0.125	0.003	0.000	0.001	0.419	0.013	0.000	0.000	0.000	0.021	0.040	0.007
HLW98-12	0.077	0.155	0.005	0.001	0.131	0.072	0.003	0.030	0.005	0.003	0.002	0.423	0.018	0.000	0.006	0.005	0.021	0.040	0.003
HLW98-20	0.094	0.126	0.000	0.002	0.103	0.016	0.004	0.151	0.002	0.000	0.000	0.458	0.012	0.000	0.000	0.000	0.021	0.003	0.009
HLW98-21	0.070	0.072	0.005	0.001	0.117	0.062	0.003	0.068	0.004	0.003	0.002	0.523	0.013	0.000	0.000	0.000	0.021	0.036	0.002
HLW98-22	0.055	0.124	0.000	0.001	0.151	0.031	0.002	0.089	0.001	0.000	0.000	0.414	0.104	0.000	0.000	0.000	0.021	0.002	0.005
HLW98-23	0.050	0.123	0.000	0.001	0.136	0.031	0.002	0.080	0.001	0.000	0.000	0.455	0.094	0.000	0.000	0.000	0.021	0.002	0.005
HLW98-27B	0.080	0.041	0.004	0.001	0.133	0.046	0.023	0.147	0.006	0.002	0.002	0.440	0.025	0.000	0.000	0.000	0.020	0.029	0.003
HLW98-32A	0.138	0.091	0.008	0.001	0.112	0.071	0.014	0.036	0.007	0.003	0.001	0.459	0.023	0.000	0.000	0.000	0.020	0.015	0.002
HLW98-34	0.109	0.071	0.000	0.002	0.119	0.041	0.045	0.095	0.002	0.000	0.000	0.415	0.075	0.000	0.000	0.000	0.020	0.001	0.005
HLW98-50	0.025	0.111	0.001	0.001	0.046	0.040	0.009	0.137	0.003	0.000	0.000	0.459	0.000	0.047	0.000	0.044	0.020	0.055	0.002
HLW98-51R	0.024	0.091	0.001	0.001	0.047	0.051	0.026	0.087	0.002	0.000	0.000	0.483	0.034	0.041	0.000	0.039	0.020	0.049	0.003
HLW98-53A	0.082	0.073	0.008	0.001	0.118	0.061	0.015	0.100	0.007	0.003	0.001	0.468	0.024	0.000	0.000	0.000	0.020	0.016	0.002
HLW98-56	0.077	0.071	0.014	0.001	0.119	0.071	0.003	0.097	0.008	0.000	0.000	0.504	0.000	0.000	0.000	0.018	0.000	0.017	0.001
HLW98-58	0.077	0.041	0.014	0.001	0.123	0.051	0.010	0.140	0.008	0.000	0.000	0.486	0.014	0.000	0.000	0.019	0.001	0.017	0.001
HLW98-60	0.077	0.041	0.014	0.001	0.121	0.051	0.006	0.134	0.008	0.000	0.000	0.483	0.007	0.000	0.000	0.019	0.021	0.017	0.001
HLW98-61	0.078	0.041	0.014	0.001	0.125	0.051	0.010	0.142	0.008	0.000	0.000	0.480	0.015	0.000	0.000	0.017	0.000	0.015	0.002
HLW98-62	0.100	0.123	0.001	0.001	0.040	0.051	0.018	0.099	0.003	0.000	0.000	0.438	0.021	0.000	0.000	0.000	0.021	0.083	0.001
HLW99-15	0.000	0.226	0.034	0.000	0.023	0.011	0.002	0.226	0.034	0.002	0.002	0.350	0.002	0.000	0.002	0.000	0.023	0.000	0.064
HLW99-27	0.000	0.188	0.035	0.000	0.147	0.082	0.002	0.059	0.035	0.002	0.002	0.352	0.002	0.000	0.002	0.000	0.023	0.000	0.067
HLW99-52	0.027	0.217	0.033	0.000	0.022	0.000	0.002	0.174	0.033	0.002	0.002	0.402	0.002	0.000	0.002	0.000	0.022	0.000	0.062
HLWD1-01	0.084	0.094	0.017	0.003	0.132	0.001	0.027	0.088	0.010	0.000	0.000	0.403	0.002	0.000	0.000	0.052	0.000	0.065	0.022
HLWD1-02	0.084	0.094	0.017	0.003	0.132	0.001	0.027	0.145	0.010	0.000	0.000	0.346	0.002	0.000	0.000	0.053	0.000	0.065	0.022
HLWD1-03	0.084	0.151	0.017	0.003	0.132	0.001	0.027	0.088	0.010	0.000	0.000	0.346	0.002	0.000	0.000	0.053	0.000	0.065	0.022
HLWD1-04	0.090	0.099	0.018	0.003	0.140	0.001	0.029	0.093	0.010	0.000	0.000	0.367	0.002	0.000	0.000	0.056	0.000	0.069	0.023
HLWD1-05	0.084	0.094	0.017	0.003	0.132	0.035	0.027	0.088	0.010	0.000	0.000	0.369	0.002	0.000	0.000	0.053	0.000	0.065	0.022
HLWD1-07	0.037	0.076	0.024	0.005	0.211	0.032	0.039	0.079	0.001	0.000	0.000	0.356	0.034	0.000	0.000	0.075	0.000	0.000	0.032
HLWD1-08	0.036	0.108	0.023	0.004	0.206	0.032	0.038	0.046	0.013	0.000	0.000	0.355	0.034	0.000	0.000	0.073	0.000	0.000	0.031
HLWD1-09	0.036	0.054	0.023	0.004	0.206	0.032	0.038	0.100	0.013	0.000	0.000	0.355	0.034	0.000	0.000	0.073	0.000	0.000	0.031
HLWD1-10	0.037	0.112	0.024	0.005	0.213	0.000	0.039	0.048	0.014	0.000	0.000	0.365	0.037	0.000	0.000	0.075	0.000	0.000	0.032
HLWD1-11	0.124	0.064	0.000	0.001	0.278	0.032	0.005	0.155	0.003	0.000	0.000	0.301	0.027	0.000	0.000	0.003	0.000	0.002	0.005
HLWD1-13	0.044	0.077	0.000	0.007	0.264	0.036	0.063	0.121	0.025	0.000	0.000	0.341	0.021	0.000	0.000	0.000	0.000	0.000	0.000
HLWD1-14R	0.039	0.167	0.000	0.000	0.078	0.032	0.000	0.147	0.002	0.000	0.000	0.284	0.019	0.004	0.000	0.100	0.000	0.127	0.000
HLWD1-17R	0.039	0.167	0.000	0.000	0.245	0.032	0.000	0.098	0.002	0.000	0.000	0.294	0.019	0.004	0.000	0.100	0.000	0.000	0.000
HLWD1-18	0.170	0.160	0.000	0.007	0.050	0.033	0.058	0.100	0.023	0.000	0.000	0.250	0.019	0.000	0.000	0.000	0.000	0.130	0.000
HLWD1-19RW	0.045	0.078	0.000	0.008	0.246	0.037	0.000	0.224	0.002	0.009	0.006	0.280	0.031	0.000	0.004	0.000	0.005	0.000	0.025
HLWD1-20R	0.045	0.079	0.000	0.000	0.057	0.037	0.000	0.227	0.002	0.010	0.006	0.329	0.027	0.000	0.004	0.000	0.005	0.147	0.025
HLWD1-21R	0.102	0.157	0.000	0.001	0.227	0.042	0.004	0.116	0.002	0.000	0.000	0.315	0.021	0.000	0.000	0.002	0.000	0.002	0.009
HLWD1-23	0.064	0.164	0.007	0.003	0.151	0.043	0.004	0.144	0.005	0.001	0.002	0.338	0.029	0.001	0.005	0.030	0.001	0.001	0.010
HLWD1-25	0.077	0.124	0.008	0.004	0.183	0.022	0.005	0.174	0.006	0.002	0.002	0.347	0.035	0.000	0.000	0.000	0.000	0.000	0.012

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
HLWD1-27	0.068	0.123	0.007	0.003	0.160	0.022	0.004	0.152	0.005	0.001	0.001	0.371	0.031	0.001	0.005	0.031	0.001	0.001	0.011
HLWD2-01	0.093	0.074	0.013	0.005	0.175	0.032	0.022	0.079	0.010	0.000	0.000	0.353	0.032	0.000	0.000	0.042	0.000	0.051	0.017
HLWD2-02	0.019	0.066	0.021	0.008	0.266	0.033	0.034	0.078	0.017	0.000	0.000	0.330	0.034	0.000	0.000	0.066	0.000	0.000	0.028
HLWD2-03	0.181	0.074	0.000	0.000	0.053	0.035	0.000	0.213	0.002	0.000	0.000	0.309	0.020	0.004	0.000	0.108	0.000	0.000	0.000
HLWD2-04	0.090	0.070	0.042	0.000	0.251	0.033	0.000	0.201	0.002	0.000	0.000	0.251	0.019	0.000	0.000	0.000	0.000	0.000	0.041
HLWD2-05R	0.044	0.076	0.000	0.007	0.098	0.036	0.063	0.218	0.025	0.000	0.000	0.272	0.021	0.000	0.000	0.000	0.000	0.141	0.000
HLWD2-06	0.099	0.130	0.004	0.006	0.185	0.032	0.002	0.123	0.013	0.001	0.001	0.366	0.015	0.001	0.002	0.015	0.000	0.001	0.005
HLWD3-01	0.093	0.079	0.012	0.002	0.108	0.001	0.019	0.218	0.007	0.000	0.000	0.337	0.028	0.000	0.000	0.036	0.000	0.045	0.015
HLWD3-02	0.051	0.078	0.014	0.003	0.128	0.000	0.024	0.172	0.008	0.000	0.000	0.436	0.021	0.002	0.000	0.045	0.000	0.000	0.019
HLWD3-03	0.188	0.088	0.046	0.000	0.121	0.036	0.000	0.110	0.002	0.000	0.000	0.342	0.021	0.000	0.000	0.000	0.000	0.000	0.045
HLWD3-04	0.192	0.192	0.000	0.000	0.102	0.037	0.000	0.113	0.002	0.009	0.007	0.283	0.027	0.000	0.004	0.000	0.005	0.000	0.025
HLWD3-06	0.044	0.185	0.046	0.000	0.055	0.036	0.000	0.109	0.002	0.000	0.000	0.338	0.021	0.000	0.000	0.000	0.000	0.120	0.045
HLWD3-07	0.161	0.114	0.000	0.000	0.190	0.031	0.000	0.190	0.002	0.000	0.000	0.294	0.018	0.000	0.000	0.000	0.000	0.000	0.000
HLWD3-08	0.180	0.093	0.005	0.008	0.111	0.000	0.006	0.232	0.004	0.001	0.001	0.301	0.024	0.001	0.003	0.021	0.001	0.002	0.008
HLW98-75	0.056	0.068	0.001	0.000	0.131	0.051	0.002	0.137	0.007	0.000	0.000	0.486	0.000	0.000	0.000	0.000	0.020	0.041	0.001
HLW98-77	0.053	0.121	0.001	0.000	0.124	0.036	0.002	0.118	0.006	0.000	0.000	0.481	0.000	0.000	0.000	0.000	0.020	0.039	0.001
HLW98-80	0.056	0.126	0.001	0.000	0.126	0.033	0.004	0.121	0.005	0.000	0.000	0.488	0.000	0.000	0.000	0.000	0.020	0.018	0.001
HLW98-83	0.015	0.122	0.000	0.000	0.131	0.028	0.025	0.120	0.004	0.001	0.002	0.522	0.000	0.000	0.000	0.000	0.021	0.001	0.007
HLW98-84	0.053	0.114	0.000	0.000	0.130	0.028	0.031	0.122	0.004	0.001	0.002	0.486	0.000	0.000	0.000	0.000	0.021	0.001	0.007
HLW98-86	0.054	0.096	0.000	0.001	0.128	0.031	0.041	0.121	0.002	0.002	0.004	0.481	0.009	0.000	0.000	0.000	0.021	0.003	0.006
HLW98-87	0.079	0.104	0.007	0.001	0.121	0.036	0.003	0.114	0.005	0.000	0.000	0.458	0.002	0.000	0.000	0.010	0.021	0.037	0.002
HLW98-88	0.077	0.109	0.007	0.001	0.117	0.039	0.003	0.120	0.005	0.000	0.000	0.452	0.002	0.000	0.000	0.010	0.021	0.036	0.002
HLW98-89	0.034	0.092	0.000	0.001	0.090	0.029	0.012	0.109	0.004	0.000	0.000	0.451	0.000	0.041	0.000	0.026	0.020	0.089	0.002
HLW98-94	0.096	0.117	0.007	0.000	0.107	0.039	0.002	0.121	0.006	0.000	0.000	0.448	0.000	0.000	0.000	0.000	0.021	0.033	0.002
HLW98-95	0.075	0.109	0.007	0.001	0.115	0.038	0.003	0.122	0.005	0.000	0.000	0.457	0.002	0.000	0.000	0.009	0.021	0.035	0.002
HLW98-96	0.034	0.102	0.000	0.001	0.090	0.031	0.012	0.109	0.004	0.000	0.000	0.438	0.000	0.041	0.000	0.026	0.020	0.089	0.002
HLW98-96A	0.036	0.109	0.000	0.001	0.097	0.034	0.013	0.116	0.005	0.000	0.000	0.470	0.000	0.000	0.000	0.000	0.022	0.096	0.002
HLW98-96B	0.036	0.109	0.000	0.001	0.097	0.034	0.013	0.116	0.005	0.000	0.000	0.470	0.000	0.000	0.000	0.000	0.022	0.096	0.002
HLW98-97	0.100	0.113	0.007	0.000	0.112	0.040	0.001	0.124	0.006	0.000	0.000	0.439	0.000	0.000	0.000	0.000	0.021	0.034	0.002
HLW98-T05	0.055	0.120	0.001	0.000	0.128	0.031	0.017	0.122	0.004	0.001	0.001	0.487	0.000	0.000	0.000	0.000	0.020	0.010	0.004
HLW98-V01	0.062	0.114	0.001	0.000	0.146	0.034	0.002	0.114	0.007	0.000	0.000	0.454	0.000	0.000	0.000	0.000	0.019	0.045	0.001
HLW98-V07	0.067	0.121	0.001	0.000	0.149	0.031	0.004	0.117	0.005	0.000	0.000	0.463	0.000	0.000	0.000	0.000	0.019	0.021	0.001
HLW98-V13	0.053	0.108	0.000	0.001	0.154	0.027	0.037	0.117	0.005	0.001	0.003	0.466	0.000	0.000	0.000	0.000	0.020	0.002	0.008
HLW98-V19	0.060	0.091	0.000	0.001	0.152	0.029	0.039	0.116	0.002	0.003	0.004	0.461	0.011	0.000	0.000	0.000	0.020	0.003	0.006
HLW98-V24	0.048	0.103	0.000	0.001	0.104	0.033	0.027	0.129	0.001	0.002	0.003	0.512	0.008	0.000	0.000	0.000	0.023	0.002	0.004
CVS1-1	0.070	0.126	0.006	0.001	0.062	0.041	0.001	0.110	0.005	0.000	0.000	0.528	0.001	0.000	0.000	0.000	0.000	0.047	0.002
CVS1-2	0.168	0.056	0.002	0.000	0.022	0.078	0.000	0.056	0.001	0.000	0.000	0.616	0.000	0.000	0.000	0.000	0.000	0.000	0.001
CVS1-3	0.153	0.219	0.001	0.000	0.022	0.077	0.000	0.055	0.001	0.000	0.000	0.460	0.000	0.000	0.000	0.000	0.000	0.011	0.000
CVS1-4	0.000	0.224	0.002	0.000	0.022	0.011	0.000	0.101	0.001	0.000	0.000	0.638	0.000	0.000	0.000	0.000	0.000	0.000	0.001
CVS1-5	0.081	0.050	0.001	0.000	0.151	0.070	0.000	0.070	0.001	0.000	0.000	0.574	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
CVS1-6	0.000	0.214	0.014	0.002	0.021	0.075	0.002	0.054	0.011	0.000	0.000	0.471	0.002	0.000	0.000	0.000	0.000	0.128	0.005
CVS1-7	0.000	0.056	0.002	0.000	0.038	0.011	0.000	0.108	0.001	0.000	0.000	0.638	0.000	0.000	0.000	0.000	0.000	0.146	0.001
CVS1-8	0.000	0.055	0.001	0.000	0.164	0.011	0.000	0.092	0.001	0.000	0.000	0.587	0.000	0.000	0.000	0.000	0.000	0.088	0.000
CVS1-9	0.000	0.230	0.016	0.003	0.164	0.012	0.003	0.063	0.012	0.000	0.000	0.492	0.002	0.000	0.000	0.000	0.000	0.000	0.005
CVS1-10	0.128	0.091	0.014	0.002	0.021	0.011	0.002	0.102	0.011	0.000	0.000	0.610	0.002	0.000	0.000	0.000	0.000	0.000	0.005
CVS1-11	0.165	0.183	0.013	0.002	0.024	0.012	0.002	0.089	0.010	0.000	0.000	0.496	0.002	0.000	0.000	0.000	0.000	0.000	0.004
CVS1-12	0.000	0.197	0.002	0.000	0.168	0.078	0.000	0.082	0.001	0.000	0.000	0.470	0.000	0.000	0.000	0.000	0.000	0.000	0.001
CVS1-13	0.004	0.201	0.001	0.000	0.020	0.010	0.000	0.187	0.001	0.000	0.000	0.574	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS1-14	0.024	0.201	0.001	0.000	0.020	0.010	0.000	0.187	0.001	0.000	0.000	0.423	0.000	0.000	0.000	0.000	0.000	0.131	0.000
CVS1-15	0.000	0.059	0.016	0.003	0.023	0.082	0.003	0.142	0.012	0.000	0.000	0.654	0.002	0.000	0.000	0.000	0.000	0.000	0.005
CVS1-16	0.158	0.055	0.001	0.000	0.094	0.011	0.000	0.205	0.001	0.000	0.000	0.474	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS1-17	0.000	0.060	0.016	0.003	0.168	0.012	0.003	0.174	0.012	0.000	0.000	0.545	0.002	0.000	0.000	0.000	0.000	0.000	0.005
CVS1-18	0.000	0.059	0.014	0.002	0.024	0.083	0.002	0.141	0.011	0.000	0.000	0.501	0.002	0.000	0.000	0.000	0.000	0.155	0.005
CVS1-19	0.070	0.126	0.006	0.001	0.062	0.041	0.001	0.110	0.005	0.000	0.000	0.528	0.001	0.000	0.000	0.000	0.000	0.047	0.002
CVS1-20	0.070	0.126	0.006	0.001	0.062	0.041	0.001	0.110	0.005	0.000	0.000	0.528	0.001	0.000	0.000	0.000	0.000	0.047	0.002
CVS1-21	0.000	0.224	0.002	0.000	0.022	0.011	0.000	0.101	0.001	0.000	0.000	0.638	0.000	0.000	0.000	0.000	0.000	0.000	0.001
CVS1-22	0.000	0.055	0.001	0.000	0.164	0.011	0.000	0.092	0.001	0.000	0.000	0.587	0.000	0.000	0.000	0.000	0.000	0.088	0.000
CVS1-23	0.049	0.102	0.006	0.001	0.126	0.040	0.001	0.112	0.004	0.000	0.000	0.550	0.001	0.000	0.000	0.000	0.000	0.007	0.002
CVS2-1	0.089	0.097	0.012	0.002	0.045	0.067	0.002	0.078	0.009	0.000	0.000	0.582	0.002	0.000	0.000	0.000	0.000	0.011	0.004
CVS2-2	0.120	0.077	0.004	0.001	0.049	0.066	0.001	0.097	0.003	0.000	0.000	0.549	0.000	0.000	0.000	0.000	0.000	0.033	0.001
CVS2-3	0.114	0.146	0.004	0.001	0.050	0.048	0.001	0.077	0.003	0.000	0.000	0.514	0.000	0.000	0.000	0.000	0.000	0.041	0.001
CVS2-4	0.068	0.120	0.004	0.001	0.044	0.059	0.001	0.077	0.003	0.000	0.000	0.613	0.000	0.000	0.000	0.000	0.000	0.011	0.001
CVS2-5	0.088	0.174	0.012	0.002	0.044	0.022	0.002	0.111	0.009	0.000	0.000	0.521	0.002	0.000	0.000	0.000	0.000	0.011	0.004
CVS2-6	0.018	0.079	0.010	0.002	0.136	0.043	0.002	0.079	0.007	0.000	0.000	0.608	0.001	0.000	0.000	0.000	0.000	0.011	0.003
CVS2-7	0.101	0.179	0.009	0.002	0.042	0.062	0.002	0.074	0.007	0.000	0.000	0.508	0.001	0.000	0.000	0.000	0.000	0.011	0.003
CVS2-8	0.065	0.075	0.004	0.001	0.122	0.064	0.001	0.106	0.003	0.000	0.000	0.548	0.000	0.000	0.000	0.000	0.000	0.011	0.001
CVS2-9	0.014	0.096	0.003	0.001	0.072	0.061	0.001	0.094	0.003	0.000	0.000	0.552	0.000	0.000	0.000	0.000	0.000	0.102	0.001
CVS2-10	0.106	0.173	0.004	0.001	0.068	0.020	0.001	0.133	0.003	0.000	0.000	0.478	0.001	0.000	0.000	0.000	0.000	0.010	0.001
CVS2-11	0.011	0.086	0.010	0.002	0.046	0.068	0.002	0.095	0.008	0.000	0.000	0.561	0.001	0.000	0.000	0.000	0.000	0.107	0.003
CVS2-12	0.100	0.188	0.004	0.001	0.044	0.052	0.001	0.077	0.003	0.000	0.000	0.518	0.000	0.000	0.000	0.000	0.000	0.011	0.001
CVS2-13	0.099	0.077	0.004	0.001	0.044	0.025	0.001	0.187	0.003	0.000	0.000	0.546	0.000	0.000	0.000	0.000	0.000	0.011	0.001
CVS2-14	0.027	0.146	0.007	0.001	0.044	0.054	0.001	0.089	0.005	0.000	0.000	0.511	0.001	0.000	0.000	0.000	0.000	0.111	0.002
CVS2-15	0.085	0.079	0.012	0.002	0.045	0.024	0.002	0.192	0.009	0.000	0.000	0.533	0.002	0.000	0.000	0.000	0.000	0.011	0.004
CVS2-16	0.024	0.111	0.008	0.001	0.076	0.040	0.001	0.119	0.006	0.000	0.000	0.567	0.001	0.000	0.000	0.000	0.000	0.041	0.003
CVS2-17	0.070	0.126	0.006	0.001	0.062	0.041	0.001	0.110	0.005	0.000	0.000	0.528	0.001	0.000	0.000	0.000	0.000	0.047	0.002
CVS2-18	0.024	0.111	0.008	0.001	0.076	0.040	0.001	0.119	0.006	0.000	0.000	0.567	0.001	0.000	0.000	0.000	0.000	0.041	0.003
CVS2-19	0.025	0.111	0.007	0.001	0.077	0.039	0.001	0.119	0.006	0.000	0.000	0.563	0.000	0.000	0.000	0.000	0.005	0.041	0.003
CVS2-20	0.010	0.050	0.001	0.000	0.060	0.067	0.000	0.104	0.001	0.000	0.000	0.574	0.000	0.000	0.000	0.000	0.000	0.131	0.000
CVS2-21	0.075	0.144	0.001	0.000	0.022	0.077	0.000	0.055	0.001	0.000	0.000	0.624	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-22	0.043	0.059	0.016	0.003	0.023	0.082	0.003	0.086	0.012	0.000	0.000	0.667	0.002	0.000	0.000	0.000	0.000	0.000	0.005

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
CVS2-23	0.063	0.057	0.001	0.000	0.022	0.011	0.000	0.219	0.001	0.000	0.000	0.624	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-24	0.102	0.213	0.013	0.002	0.021	0.075	0.002	0.078	0.010	0.000	0.000	0.476	0.002	0.000	0.000	0.000	0.000	0.000	0.004
CVS2-25	0.004	0.057	0.009	0.001	0.170	0.079	0.001	0.095	0.007	0.000	0.000	0.573	0.001	0.000	0.000	0.000	0.000	0.000	0.003
CVS2-26	0.028	0.219	0.001	0.000	0.022	0.077	0.000	0.056	0.001	0.000	0.000	0.485	0.000	0.000	0.000	0.000	0.000	0.109	0.000
CVS2-27	0.086	0.055	0.001	0.000	0.022	0.017	0.000	0.219	0.001	0.000	0.000	0.598	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-28	0.059	0.054	0.014	0.002	0.021	0.013	0.002	0.214	0.011	0.000	0.000	0.601	0.002	0.000	0.000	0.000	0.000	0.000	0.005
CVS2-29	0.000	0.234	0.016	0.003	0.023	0.012	0.003	0.079	0.012	0.000	0.000	0.514	0.002	0.000	0.000	0.000	0.000	0.098	0.005
CVS2-30	0.046	0.201	0.001	0.000	0.133	0.010	0.000	0.084	0.001	0.000	0.000	0.522	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-31	0.058	0.202	0.001	0.000	0.022	0.036	0.000	0.055	0.001	0.000	0.000	0.624	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-32	0.003	0.050	0.001	0.000	0.020	0.043	0.000	0.201	0.001	0.000	0.000	0.548	0.000	0.000	0.000	0.000	0.000	0.131	0.000
CVS2-33	0.104	0.064	0.016	0.003	0.023	0.043	0.003	0.234	0.012	0.000	0.000	0.492	0.002	0.000	0.000	0.000	0.000	0.000	0.005
CVS2-34	0.140	0.175	0.001	0.000	0.020	0.037	0.000	0.201	0.001	0.000	0.000	0.423	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-35	0.147	0.055	0.001	0.000	0.069	0.047	0.000	0.219	0.001	0.000	0.000	0.460	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-36	0.010	0.055	0.001	0.000	0.164	0.077	0.000	0.098	0.001	0.000	0.000	0.593	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-37	0.141	0.084	0.001	0.000	0.020	0.070	0.000	0.107	0.001	0.000	0.000	0.574	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-38	0.030	0.121	0.001	0.000	0.156	0.011	0.000	0.114	0.001	0.000	0.000	0.563	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-39	0.028	0.055	0.001	0.000	0.081	0.077	0.000	0.149	0.001	0.000	0.000	0.530	0.000	0.000	0.000	0.000	0.000	0.077	0.000
CVS2-40	0.110	0.070	0.004	0.001	0.022	0.046	0.001	0.165	0.003	0.000	0.000	0.554	0.001	0.000	0.000	0.000	0.000	0.022	0.001
CVS2-41	0.110	0.076	0.004	0.001	0.033	0.077	0.001	0.086	0.003	0.000	0.000	0.585	0.001	0.000	0.000	0.000	0.000	0.022	0.001
CVS2-42	0.033	0.055	0.004	0.001	0.110	0.077	0.001	0.069	0.003	0.000	0.000	0.623	0.001	0.000	0.000	0.000	0.000	0.022	0.001
CVS2-43	0.054	0.159	0.004	0.001	0.032	0.070	0.001	0.054	0.003	0.000	0.000	0.545	0.001	0.000	0.000	0.000	0.000	0.075	0.001
CVS2-44	0.068	0.118	0.004	0.001	0.022	0.077	0.001	0.055	0.003	0.000	0.000	0.626	0.001	0.000	0.000	0.000	0.000	0.022	0.001
CVS2-45	0.067	0.125	0.011	0.002	0.035	0.067	0.002	0.057	0.008	0.000	0.000	0.599	0.001	0.000	0.000	0.000	0.000	0.023	0.004
CVS2-46	0.081	0.137	0.010	0.002	0.022	0.076	0.002	0.063	0.007	0.000	0.000	0.574	0.001	0.000	0.000	0.000	0.000	0.022	0.003
CVS2-47	0.045	0.057	0.011	0.002	0.023	0.049	0.002	0.144	0.008	0.000	0.000	0.599	0.001	0.000	0.000	0.000	0.000	0.057	0.004
CVS2-48	0.096	0.161	0.008	0.001	0.022	0.044	0.001	0.108	0.006	0.000	0.000	0.526	0.001	0.000	0.000	0.000	0.000	0.022	0.003
CVS2-49	0.083	0.144	0.004	0.001	0.055	0.044	0.001	0.102	0.003	0.000	0.000	0.539	0.001	0.000	0.000	0.000	0.000	0.021	0.001
CVS2-50	0.070	0.126	0.006	0.001	0.062	0.041	0.001	0.110	0.005	0.000	0.000	0.528	0.001	0.000	0.000	0.000	0.000	0.047	0.002
CVS2-51	0.025	0.111	0.007	0.001	0.077	0.039	0.001	0.119	0.006	0.000	0.000	0.563	0.000	0.000	0.000	0.000	0.005	0.041	0.003
CVS2-52	0.024	0.085	0.008	0.001	0.075	0.082	0.001	0.047	0.006	0.000	0.000	0.625	0.001	0.000	0.000	0.000	0.000	0.040	0.003
CVS2-53	0.087	0.095	0.012	0.002	0.044	0.065	0.002	0.076	0.009	0.000	0.000	0.570	0.002	0.000	0.000	0.020	0.000	0.011	0.004
CVS2-54	0.025	0.110	0.007	0.001	0.077	0.039	0.001	0.119	0.006	0.000	0.000	0.559	0.000	0.000	0.000	0.006	0.005	0.041	0.003
CVS2-55	0.025	0.110	0.000	0.009	0.077	0.039	0.024	0.118	0.000	0.000	0.000	0.558	0.000	0.000	0.000	0.000	0.000	0.041	0.000
CVS2-56	0.024	0.108	0.000	0.007	0.076	0.038	0.039	0.117	0.000	0.000	0.000	0.550	0.000	0.000	0.000	0.000	0.000	0.040	0.000
CVS2-57	0.025	0.113	0.000	0.006	0.079	0.040	0.000	0.122	0.000	0.000	0.000	0.573	0.000	0.000	0.000	0.000	0.000	0.042	0.000
CVS2-58	0.168	0.224	0.002	0.000	0.022	0.078	0.000	0.056	0.001	0.000	0.000	0.437	0.000	0.000	0.000	0.000	0.000	0.011	0.001
CVS2-59	0.120	0.180	0.001	0.000	0.021	0.076	0.000	0.133	0.001	0.000	0.000	0.458	0.000	0.000	0.000	0.000	0.000	0.008	0.000
CVS2-60	0.094	0.089	0.001	0.000	0.020	0.075	0.000	0.175	0.001	0.000	0.000	0.535	0.000	0.000	0.000	0.000	0.000	0.008	0.000
CVS2-61	0.164	0.067	0.002	0.000	0.020	0.074	0.000	0.121	0.001	0.000	0.000	0.532	0.000	0.000	0.000	0.000	0.000	0.018	0.001
CVS2-62	0.053	0.187	0.001	0.000	0.021	0.017	0.000	0.119	0.001	0.000	0.000	0.591	0.000	0.000	0.000	0.000	0.000	0.008	0.000

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
CVS2-63	0.201	0.192	0.002	0.000	0.022	0.006	0.000	0.213	0.001	0.000	0.000	0.362	0.000	0.000	0.000	0.000	0.000	0.000	0.001
CVS2-64	0.030	0.053	0.013	0.001	0.085	0.067	0.000	0.097	0.010	0.000	0.000	0.594	0.000	0.000	0.000	0.000	0.002	0.045	0.003
CVS2-65	0.020	0.115	0.000	0.005	0.001	0.071	0.000	0.087	0.000	0.000	0.000	0.543	0.000	0.000	0.000	0.000	0.000	0.157	0.000
CVS2-66	0.122	0.095	0.000	0.011	0.040	0.054	0.012	0.125	0.005	0.000	0.000	0.533	0.000	0.000	0.000	0.000	0.000	0.003	0.001
CVS2-67	0.206	0.160	0.000	0.001	0.000	0.059	0.000	0.110	0.000	0.000	0.000	0.464	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-68	0.166	0.137	0.000	0.030	0.005	0.070	0.002	0.080	0.000	0.000	0.000	0.509	0.000	0.000	0.000	0.000	0.001	0.000	0.000
CVS2-69	0.087	0.083	0.001	0.025	0.035	0.076	0.013	0.071	0.000	0.000	0.004	0.601	0.000	0.000	0.000	0.000	0.000	0.001	0.004
CVS2-70	0.184	0.143	0.001	0.012	0.008	0.070	0.003	0.082	0.001	0.000	0.004	0.490	0.000	0.000	0.000	0.000	0.000	0.001	0.003
CVS2-71	0.030	0.053	0.009	0.002	0.085	0.067	0.002	0.097	0.007	0.000	0.000	0.598	0.001	0.000	0.000	0.000	0.000	0.045	0.003
CVS2-72	0.123	0.096	0.006	0.001	0.041	0.055	0.001	0.127	0.005	0.000	0.000	0.541	0.001	0.000	0.000	0.000	0.000	0.003	0.002
CVS2-73	0.169	0.139	0.006	0.001	0.005	0.072	0.001	0.082	0.004	0.000	0.000	0.519	0.001	0.000	0.000	0.000	0.000	0.000	0.002
CVS2-74	0.088	0.084	0.013	0.002	0.036	0.077	0.002	0.071	0.010	0.000	0.000	0.609	0.002	0.000	0.000	0.000	0.000	0.001	0.004
CVS2-75	0.186	0.145	0.004	0.001	0.008	0.071	0.001	0.083	0.003	0.000	0.000	0.496	0.001	0.000	0.000	0.000	0.000	0.001	0.001
CVS2-76	0.021	0.064	0.003	0.000	0.111	0.067	0.000	0.191	0.002	0.000	0.000	0.533	0.000	0.000	0.000	0.000	0.000	0.005	0.001
CVS2-77	0.021	0.064	0.013	0.002	0.005	0.075	0.002	0.193	0.010	0.000	0.000	0.489	0.002	0.000	0.000	0.000	0.000	0.118	0.004
CVS2-78	0.021	0.170	0.003	0.000	0.074	0.027	0.000	0.053	0.002	0.000	0.000	0.595	0.000	0.000	0.000	0.000	0.000	0.053	0.001
CVS2-79	0.021	0.172	0.013	0.002	0.113	0.013	0.002	0.054	0.010	0.000	0.000	0.589	0.002	0.000	0.000	0.000	0.000	0.005	0.004
CVS2-80	0.021	0.170	0.003	0.000	0.111	0.019	0.000	0.053	0.002	0.000	0.000	0.539	0.000	0.000	0.000	0.000	0.000	0.080	0.001
CVS2-81	0.022	0.067	0.012	0.002	0.116	0.078	0.002	0.192	0.009	0.000	0.000	0.488	0.002	0.000	0.000	0.000	0.000	0.006	0.004
CVS2-82	0.021	0.101	0.003	0.000	0.005	0.074	0.000	0.191	0.002	0.000	0.000	0.595	0.000	0.000	0.000	0.000	0.000	0.005	0.001
CVS2-83	0.022	0.106	0.013	0.002	0.006	0.078	0.002	0.201	0.010	0.000	0.000	0.547	0.002	0.000	0.000	0.000	0.000	0.006	0.005
CVS2-84	0.020	0.061	0.003	0.000	0.107	0.072	0.000	0.184	0.002	0.000	0.000	0.466	0.000	0.000	0.000	0.000	0.000	0.082	0.001
CVS2-85	0.180	0.063	0.006	0.001	0.005	0.074	0.001	0.190	0.005	0.000	0.000	0.465	0.001	0.000	0.000	0.000	0.000	0.005	0.002
CVS2-86	0.184	0.065	0.007	0.001	0.005	0.015	0.001	0.194	0.005	0.000	0.000	0.515	0.001	0.000	0.000	0.000	0.000	0.005	0.002
CVS2-87	0.102	0.083	0.003	0.000	0.026	0.019	0.000	0.186	0.002	0.000	0.000	0.515	0.000	0.000	0.000	0.000	0.000	0.063	0.001
CVS2-88	0.111	0.064	0.003	0.000	0.027	0.074	0.000	0.149	0.002	0.000	0.000	0.488	0.000	0.000	0.000	0.000	0.000	0.080	0.001
CVS2-89	0.021	0.124	0.003	0.000	0.111	0.011	0.000	0.191	0.002	0.000	0.000	0.467	0.000	0.000	0.000	0.000	0.000	0.067	0.001
CVS2-90	0.020	0.164	0.003	0.000	0.103	0.072	0.000	0.055	0.002	0.000	0.000	0.573	0.000	0.000	0.000	0.000	0.000	0.005	0.001
CVS2-91	0.022	0.179	0.013	0.002	0.006	0.011	0.002	0.117	0.010	0.000	0.000	0.625	0.002	0.000	0.000	0.000	0.000	0.006	0.005
CVS2-92	0.022	0.179	0.013	0.002	0.006	0.078	0.002	0.112	0.010	0.000	0.000	0.491	0.002	0.000	0.000	0.000	0.000	0.078	0.005
CVS2-93	0.022	0.144	0.013	0.002	0.106	0.076	0.002	0.138	0.010	0.000	0.000	0.475	0.002	0.000	0.000	0.000	0.000	0.005	0.004
CVS2-94	0.075	0.170	0.003	0.000	0.029	0.056	0.000	0.191	0.002	0.000	0.000	0.467	0.000	0.000	0.000	0.000	0.000	0.005	0.001
CVS2-95	0.038	0.116	0.000	0.000	0.093	0.045	0.014	0.174	0.006	0.000	0.000	0.510	0.000	0.000	0.000	0.000	0.000	0.004	0.000
CVS2-96	0.070	0.126	0.006	0.001	0.062	0.041	0.001	0.110	0.005	0.000	0.000	0.528	0.001	0.000	0.000	0.000	0.000	0.047	0.002
CVS2-97	0.025	0.111	0.007	0.001	0.077	0.039	0.001	0.119	0.006	0.000	0.000	0.563	0.000	0.000	0.000	0.000	0.005	0.041	0.003
CVS2-98	0.140	0.175	0.001	0.000	0.020	0.037	0.000	0.201	0.001	0.000	0.000	0.423	0.000	0.000	0.000	0.000	0.000	0.000	0.000
CVS2-99	0.056	0.103	0.003	0.002	0.108	0.038	0.004	0.104	0.003	0.000	0.000	0.553	0.000	0.000	0.000	0.000	0.001	0.021	0.004
CVS2-100	0.030	0.078	0.008	0.001	0.130	0.063	0.002	0.066	0.007	0.000	0.000	0.564	0.001	0.000	0.000	0.000	0.000	0.047	0.003
CVS2-101	0.038	0.116	0.000	0.000	0.093	0.045	0.014	0.174	0.006	0.000	0.000	0.510	0.000	0.000	0.000	0.000	0.000	0.004	0.000
CVS2-102	0.024	0.111	0.008	0.001	0.076	0.040	0.001	0.119	0.006	0.000	0.000	0.567	0.001	0.000	0.000	0.000	0.000	0.041	0.003

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
CVS2-103	0.032	0.144	0.011	0.002	0.098	0.051	0.002	0.154	0.008	0.000	0.000	0.441	0.001	0.000	0.000	0.000	0.000	0.053	0.004
CVS2-104	0.029	0.133	0.010	0.002	0.091	0.048	0.002	0.143	0.008	0.000	0.000	0.482	0.001	0.000	0.000	0.000	0.000	0.049	0.003
CVS2-105	0.027	0.123	0.009	0.002	0.084	0.044	0.002	0.131	0.007	0.000	0.000	0.522	0.001	0.000	0.000	0.000	0.000	0.045	0.003
CVS2-106	0.023	0.103	0.008	0.001	0.070	0.037	0.001	0.110	0.006	0.000	0.000	0.601	0.001	0.000	0.000	0.000	0.000	0.038	0.003
CVS2-107	0.026	0.053	0.009	0.001	0.081	0.042	0.001	0.127	0.007	0.000	0.000	0.604	0.001	0.000	0.000	0.000	0.000	0.043	0.003
CVS2-108	0.023	0.158	0.008	0.001	0.072	0.038	0.001	0.113	0.006	0.000	0.000	0.537	0.001	0.000	0.000	0.000	0.000	0.039	0.003
CVS2-109	0.022	0.210	0.007	0.001	0.068	0.035	0.001	0.106	0.006	0.000	0.000	0.504	0.001	0.000	0.000	0.000	0.000	0.036	0.002
CVS2-110	0.026	0.120	0.009	0.002	0.082	0.043	0.001	0.053	0.007	0.000	0.000	0.609	0.001	0.000	0.000	0.000	0.000	0.044	0.003
CVS2-111	0.023	0.107	0.008	0.001	0.073	0.038	0.001	0.158	0.006	0.000	0.000	0.541	0.001	0.000	0.000	0.000	0.000	0.039	0.003
CVS2-112	0.022	0.100	0.008	0.001	0.068	0.036	0.001	0.211	0.006	0.000	0.000	0.508	0.001	0.000	0.000	0.000	0.000	0.037	0.003
CVS2-113	0.025	0.115	0.009	0.001	0.078	0.011	0.001	0.123	0.007	0.000	0.000	0.584	0.001	0.000	0.000	0.000	0.000	0.042	0.003
CVS2-114	0.024	0.109	0.008	0.001	0.074	0.063	0.001	0.116	0.006	0.000	0.000	0.553	0.001	0.000	0.000	0.000	0.000	0.040	0.003
CVS2-115	0.024	0.108	0.008	0.001	0.073	0.074	0.001	0.115	0.006	0.000	0.000	0.547	0.001	0.000	0.000	0.000	0.000	0.039	0.003
CVS2-116	0.024	0.111	0.008	0.001	0.076	0.040	0.001	0.119	0.006	0.000	0.000	0.567	0.001	0.000	0.000	0.000	0.000	0.041	0.003
CVS2-117	0.024	0.111	0.008	0.001	0.076	0.040	0.001	0.119	0.006	0.000	0.000	0.567	0.001	0.000	0.000	0.000	0.000	0.041	0.003
CVS2-118	0.024	0.111	0.008	0.001	0.076	0.040	0.001	0.119	0.006	0.000	0.000	0.567	0.001	0.000	0.000	0.000	0.000	0.041	0.003
CVS2-119	0.000	0.114	0.009	0.001	0.078	0.041	0.001	0.122	0.007	0.000	0.000	0.581	0.001	0.000	0.000	0.000	0.000	0.042	0.003
CVS2-120	0.053	0.108	0.008	0.001	0.074	0.039	0.001	0.116	0.006	0.000	0.000	0.550	0.001	0.000	0.000	0.000	0.000	0.040	0.003
CVS2-121	0.105	0.102	0.008	0.001	0.070	0.036	0.001	0.109	0.006	0.000	0.000	0.520	0.001	0.000	0.000	0.000	0.000	0.037	0.003
CVS2-122	0.158	0.096	0.007	0.001	0.066	0.034	0.001	0.103	0.006	0.000	0.000	0.489	0.001	0.000	0.000	0.000	0.000	0.035	0.002
CVS2-123	0.025	0.111	0.007	0.001	0.077	0.039	0.001	0.119	0.006	0.000	0.000	0.563	0.000	0.000	0.000	0.000	0.005	0.041	0.003
HG-1-1-7	0.057	0.073	0.000	0.004	0.136	0.046	0.023	0.096	0.009	0.000	0.000	0.546	0.000	0.000	0.000	0.000	0.003	0.002	0.006
HG-1-2-7	0.053	0.071	0.000	0.003	0.124	0.048	0.024	0.090	0.008	0.000	0.000	0.568	0.000	0.000	0.000	0.000	0.004	0.001	0.005
HG-1-3-7	0.052	0.072	0.000	0.003	0.123	0.048	0.023	0.092	0.008	0.000	0.000	0.571	0.000	0.000	0.000	0.000	0.004	0.000	0.005
HG-2-1-7	0.053	0.070	0.000	0.003	0.126	0.047	0.024	0.091	0.008	0.000	0.000	0.569	0.000	0.000	0.000	0.000	0.004	0.000	0.005
HG-2-2-7	0.056	0.062	0.000	0.003	0.132	0.045	0.025	0.106	0.008	0.000	0.000	0.550	0.000	0.000	0.000	0.000	0.004	0.002	0.005
HG-2-3-7	0.055	0.062	0.000	0.003	0.130	0.046	0.025	0.107	0.008	0.000	0.000	0.556	0.000	0.000	0.000	0.000	0.004	0.001	0.004
HG-3-1-7	0.058	0.063	0.000	0.003	0.135	0.045	0.025	0.104	0.008	0.000	0.000	0.548	0.000	0.000	0.000	0.000	0.005	0.002	0.005
HG-3-2-7	0.059	0.064	0.000	0.003	0.140	0.044	0.026	0.101	0.008	0.000	0.000	0.544	0.000	0.000	0.000	0.000	0.004	0.002	0.005
HG-3-3-7	0.059	0.066	0.000	0.002	0.139	0.044	0.026	0.099	0.008	0.000	0.000	0.545	0.000	0.000	0.000	0.000	0.004	0.002	0.005
AH-165 Al-7	0.137	0.075	0.000	0.000	0.049	0.043	0.027	0.108	0.007	0.000	0.000	0.547	0.000	0.000	0.000	0.000	0.000	0.008	0.000
AH-165 AV-7	0.053	0.067	0.000	0.000	0.118	0.051	0.026	0.102	0.010	0.000	0.000	0.564	0.000	0.000	0.000	0.000	0.000	0.008	0.000
AH-165 FE-7	0.015	0.075	0.000	0.000	0.175	0.042	0.011	0.110	0.030	0.000	0.000	0.534	0.000	0.000	0.000	0.000	0.000	0.009	0.000
AH-131 Al-7	0.139	0.111	0.000	0.000	0.048	0.042	0.026	0.145	0.006	0.000	0.000	0.478	0.000	0.000	0.000	0.000	0.000	0.004	0.000
AH-131 AV-7	0.045	0.078	0.000	0.000	0.122	0.044	0.027	0.101	0.011	0.000	0.000	0.564	0.000	0.000	0.000	0.000	0.000	0.009	0.000
AH-131 FE-7	0.023	0.075	0.000	0.000	0.178	0.042	0.009	0.112	0.026	0.000	0.000	0.526	0.000	0.000	0.000	0.000	0.000	0.009	0.000
AH-168 Al-7	0.068	0.139	0.000	0.000	0.025	0.054	0.011	0.120	0.003	0.000	0.000	0.572	0.000	0.000	0.000	0.000	0.000	0.009	0.000
AH-168 AV-7	0.057	0.109	0.000	0.000	0.115	0.043	0.027	0.103	0.010	0.000	0.000	0.528	0.000	0.000	0.000	0.000	0.000	0.007	0.000
AH-168 FE-7	0.025	0.117	0.000	0.000	0.167	0.042	0.010	0.110	0.029	0.000	0.000	0.494	0.000	0.000	0.000	0.000	0.000	0.007	0.000
AH-200 Al-7	0.144	0.110	0.000	0.000	0.048	0.029	0.027	0.114	0.007	0.000	0.000	0.521	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
AH-200 AV-7	0.055	0.111	0.000	0.000	0.128	0.029	0.027	0.105	0.011	0.000	0.000	0.533	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AH-200 FE-7	0.022	0.109	0.000	0.000	0.177	0.028	0.010	0.114	0.028	0.000	0.000	0.511	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AH-202 Al-7	0.150	0.080	0.000	0.000	0.047	0.045	0.027	0.079	0.007	0.000	0.000	0.565	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AH-202-AV-7	0.053	0.080	0.000	0.000	0.128	0.046	0.028	0.071	0.011	0.000	0.000	0.583	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AH-202 FE-7	0.015	0.076	0.000	0.000	0.178	0.046	0.010	0.082	0.029	0.000	0.000	0.564	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AH-1-7	0.074	0.110	0.000	0.000	0.128	0.048	0.025	0.127	0.010	0.000	0.000	0.470	0.000	0.000	0.000	0.000	0.000	0.007	0.000
AH-2-7	0.070	0.141	0.000	0.000	0.121	0.040	0.028	0.109	0.010	0.000	0.000	0.473	0.000	0.000	0.000	0.000	0.000	0.007	0.000
AH-4-7	0.050	0.076	0.000	0.000	0.118	0.044	0.023	0.106	0.010	0.000	0.000	0.573	0.001	0.000	0.000	0.000	0.000	0.000	0.000
AH-5-7	0.059	0.074	0.000	0.000	0.122	0.040	0.028	0.099	0.010	0.000	0.000	0.567	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AH-6-7	0.060	0.100	0.000	0.000	0.126	0.049	0.029	0.112	0.010	0.000	0.000	0.506	0.001	0.000	0.000	0.000	0.000	0.007	0.000
AH-7-7	0.067	0.122	0.000	0.000	0.120	0.033	0.028	0.098	0.010	0.000	0.000	0.521	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AH-8-7	0.063	0.108	0.000	0.000	0.124	0.034	0.029	0.105	0.010	0.000	0.000	0.526	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AH-9-7	0.065	0.093	0.000	0.000	0.124	0.037	0.028	0.098	0.010	0.000	0.000	0.543	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AH-10-7	0.055	0.081	0.000	0.000	0.121	0.048	0.029	0.073	0.010	0.000	0.000	0.582	0.001	0.000	0.000	0.000	0.000	0.000	0.000
AH-11-7	0.061	0.129	0.000	0.000	0.119	0.039	0.028	0.069	0.010	0.000	0.000	0.543	0.001	0.000	0.000	0.000	0.000	0.000	0.000
AH-12-7	0.065	0.093	0.000	0.000	0.124	0.037	0.028	0.098	0.010	0.000	0.000	0.544	0.000	0.000	0.000	0.000	0.000	0.000	0.000
AH-13-7	0.070	0.070	0.000	0.000	0.148	0.036	0.035	0.096	0.012	0.000	0.000	0.532	0.001	0.000	0.000	0.000	0.000	0.000	0.000
AH-14-7	0.076	0.089	0.000	0.000	0.150	0.042	0.036	0.105	0.012	0.000	0.000	0.483	0.001	0.000	0.000	0.000	0.000	0.006	0.000
AH-15-7	0.075	0.100	0.000	0.000	0.148	0.030	0.035	0.102	0.012	0.000	0.000	0.496	0.001	0.000	0.000	0.000	0.000	0.000	0.000
AH-16-7	0.069	0.078	0.000	0.001	0.145	0.044	0.035	0.071	0.012	0.000	0.000	0.544	0.001	0.000	0.000	0.000	0.000	0.000	0.000
AH-17-7	0.061	0.087	0.000	0.001	0.122	0.050	0.029	0.071	0.010	0.000	0.000	0.562	0.000	0.000	0.000	0.000	0.000	0.007	0.000
SFRIT1	0.049	0.091	0.000	0.001	0.152	0.035	0.021	0.124	0.012	0.000	0.000	0.513	0.000	0.000	0.000	0.000	0.000	0.001	0.001
SFRIT2	0.049	0.091	0.000	0.001	0.152	0.035	0.021	0.124	0.012	0.000	0.000	0.513	0.000	0.000	0.000	0.000	0.000	0.001	0.001
SFRIT3	0.049	0.091	0.000	0.001	0.152	0.035	0.021	0.124	0.012	0.000	0.000	0.513	0.000	0.000	0.000	0.000	0.000	0.001	0.001
202P w/o Mn-7	0.048	0.097	0.000	0.001	0.120	0.038	0.000	0.103	0.008	0.000	0.000	0.575	0.000	0.000	0.000	0.000	0.000	0.000	0.010
202G w/o Mn-7	0.050	0.065	0.000	0.001	0.131	0.041	0.000	0.089	0.007	0.000	0.000	0.609	0.000	0.000	0.000	0.000	0.000	0.000	0.006
200R-7	0.051	0.105	0.000	0.000	0.136	0.033	0.024	0.147	0.006	0.000	0.000	0.499	0.000	0.000	0.000	0.000	0.000	0.000	0.000
NBS SRM 623-7	0.064	0.109	0.000	0.000	0.000	0.000	0.000	0.065	0.000	0.000	0.000	0.740	0.000	0.000	0.000	0.000	0.000	0.000	0.022
165 CGW STD-7	0.043	0.069	0.000	0.000	0.133	0.051	0.026	0.107	0.010	0.000	0.000	0.554	0.000	0.000	0.000	0.000	0.000	0.005	0.000
ARM-1-7 (4/88)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
ARM-1-7 (5/89)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
ARM-1-7 (7/90)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
ARM-1-7 (12/90)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
ARM-1-7 (5/91)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
ARM-1-7 (10/91)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
ARM-1-7 (10/92)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
ARM-1-7 (4/93)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
ARM-1-7 (6/93)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
ARM-1-7 (8/93)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
ARM-1-7	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
T-ARM-1	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
SS-ARM-1(2)	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
SS-ARM-1	0.068	0.137	0.000	0.000	0.000	0.062	0.000	0.117	0.000	0.000	0.000	0.564	0.005	0.000	0.000	0.000	0.018	0.022	0.008
EA-1-7(2)	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
EA-1-7	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
EA-2-7	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
EA-7	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
T-EA	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
SS-EA-19	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
SS-EA-15	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
SS-EA-1-7	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
SS-EA-2-7	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
SRS-SEA-A-7	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
SRS-SEA-B-7	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
CUASEA-A-7	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
CUASEA-B-7	0.039	0.118	0.000	0.000	0.094	0.044	0.014	0.175	0.006	0.000	0.000	0.507	0.000	0.000	0.000	0.000	0.000	0.005	0.000
131-TDS-EA-7	0.059	0.131	0.000	0.000	0.147	0.050	0.033	0.150	0.015	0.000	0.000	0.410	0.000	0.000	0.000	0.000	0.000	0.004	0.000
131-TDS-3A-SOPER-7	0.057	0.111	0.000	0.001	0.117	0.043	0.035	0.141	0.016	0.000	0.000	0.475	0.000	0.000	0.000	0.000	0.000	0.004	0.000
BLEND 1-7	0.045	0.087	0.000	0.002	0.118	0.048	0.018	0.099	0.010	0.000	0.000	0.564	0.000	0.000	0.000	0.000	0.000	0.001	0.007
BLEND 1-7 (2)	0.045	0.087	0.000	0.002	0.118	0.048	0.018	0.099	0.010	0.000	0.000	0.564	0.000	0.000	0.000	0.000	0.000	0.001	0.007
BLEND 1.6-7	0.045	0.087	0.000	0.002	0.118	0.048	0.018	0.099	0.010	0.000	0.000	0.564	0.000	0.000	0.000	0.000	0.000	0.001	0.007
BATCH 1-7	0.053	0.084	0.000	0.001	0.139	0.048	0.019	0.098	0.008	0.000	0.000	0.544	0.000	0.000	0.000	0.000	0.000	0.001	0.006
BATCH 1-7 (2)	0.053	0.084	0.000	0.001	0.139	0.048	0.019	0.098	0.008	0.000	0.000	0.544	0.000	0.000	0.000	0.000	0.000	0.001	0.006
BATCH 1-1.6	0.053	0.084	0.000	0.001	0.139	0.048	0.019	0.098	0.008	0.000	0.000	0.544	0.000	0.000	0.000	0.000	0.000	0.001	0.006
BATCH 2-7	0.050	0.085	0.000	0.002	0.120	0.049	0.015	0.099	0.010	0.000	0.000	0.562	0.000	0.000	0.000	0.000	0.000	0.002	0.006
BATCH 2-7 (2)	0.050	0.085	0.000	0.002	0.120	0.049	0.015	0.099	0.010	0.000	0.000	0.562	0.000	0.000	0.000	0.000	0.000	0.002	0.006
BATCH 2-1.6	0.050	0.085	0.000	0.002	0.120	0.049	0.015	0.099	0.010	0.000	0.000	0.562	0.000	0.000	0.000	0.000	0.000	0.002	0.006
BATCH 3-7	0.037	0.083	0.000	0.002	0.127	0.049	0.016	0.098	0.011	0.000	0.000	0.569	0.000	0.000	0.000	0.000	0.000	0.001	0.006
BATCH 3-7 (2)	0.037	0.083	0.000	0.002	0.127	0.049	0.016	0.098	0.011	0.000	0.000	0.569	0.000	0.000	0.000	0.000	0.000	0.001	0.006
BATCH 3-7 (3)	0.037	0.083	0.000	0.002	0.127	0.049	0.016	0.098	0.011	0.000	0.000	0.569	0.000	0.000	0.000	0.000	0.000	0.001	0.006
BATCH 4-7	0.038	0.089	0.000	0.002	0.128	0.047	0.028	0.100	0.012	0.000	0.000	0.547	0.000	0.000	0.000	0.000	0.000	0.002	0.008
BATCH 4-7 (2)	0.038	0.089	0.000	0.002	0.128	0.047	0.028	0.100	0.012	0.000	0.000	0.547	0.000	0.000	0.000	0.000	0.000	0.002	0.008
BATCH 4-7 (3)	0.038	0.089	0.000	0.002	0.128	0.047	0.028	0.100	0.012	0.000	0.000	0.547	0.000	0.000	0.000	0.000	0.000	0.002	0.008
HM-1-7	0.076	0.075	0.000	0.001	0.083	0.049	0.019	0.091	0.004	0.000	0.000	0.594	0.000	0.000	0.000	0.000	0.000	0.003	0.004
HM-1-7 (2)	0.076	0.075	0.000	0.001	0.083	0.049	0.019	0.091	0.004	0.000	0.000	0.594	0.000	0.000	0.000	0.000	0.000	0.003	0.004
HM-1.6-7	0.076	0.075	0.000	0.001	0.083	0.049	0.019	0.091	0.004	0.000	0.000	0.594	0.000	0.000	0.000	0.000	0.000	0.003	0.004
PUREX 1-7	0.032	0.112	0.000	0.002	0.143	0.035	0.018	0.136	0.013	0.000	0.000	0.502	0.000	0.000	0.000	0.000	0.000	0.000	0.007
PUREX 1-7 (2)	0.032	0.112	0.000	0.002	0.143	0.035	0.018	0.136	0.013	0.000	0.000	0.502	0.000	0.000	0.000	0.000	0.000	0.000	0.007
PUREX 1.6-7	0.032	0.112	0.000	0.002	0.143	0.035	0.018	0.136	0.013	0.000	0.000	0.502	0.000	0.000	0.000	0.000	0.000	0.000	0.007
PUREX SRSS 1.6	0.032	0.112	0.000	0.002	0.143	0.035	0.018	0.136	0.013	0.000	0.000	0.502	0.000	0.000	0.000	0.000	0.000	0.000	0.007

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
PUREX SRST-4.0	0.032	0.112	0.000	0.002	0.143	0.035	0.018	0.136	0.013	0.000	0.000	0.502	0.000	0.000	0.000	0.000	0.000	0.000	0.007
PUREX CUA	0.032	0.112	0.000	0.002	0.143	0.035	0.018	0.136	0.013	0.000	0.000	0.502	0.000	0.000	0.000	0.000	0.000	0.000	0.007
BLEND 1-3457	0.057	0.074	0.000	0.002	0.137	0.045	0.023	0.108	0.009	0.000	0.000	0.541	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 1-3479	0.057	0.075	0.000	0.002	0.136	0.045	0.023	0.107	0.009	0.000	0.000	0.542	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 1-3498	0.057	0.075	0.000	0.002	0.138	0.045	0.024	0.116	0.010	0.000	0.000	0.530	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 1-3510	0.058	0.075	0.000	0.002	0.140	0.045	0.024	0.116	0.010	0.000	0.000	0.528	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 1-3526	0.055	0.077	0.000	0.002	0.135	0.045	0.024	0.117	0.010	0.000	0.000	0.532	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 2-3611	0.055	0.072	0.000	0.003	0.130	0.045	0.023	0.109	0.010	0.000	0.000	0.550	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 2-3622	0.053	0.074	0.000	0.002	0.126	0.046	0.023	0.110	0.010	0.000	0.000	0.553	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 2-3635	0.054	0.073	0.000	0.002	0.123	0.046	0.023	0.111	0.010	0.000	0.000	0.555	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 2-3654	0.052	0.073	0.000	0.002	0.124	0.046	0.023	0.113	0.010	0.000	0.000	0.553	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 2-3666	0.053	0.074	0.000	0.003	0.125	0.046	0.023	0.111	0.010	0.000	0.000	0.552	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 2-3676	0.052	0.074	0.000	0.002	0.123	0.047	0.023	0.111	0.010	0.000	0.000	0.556	0.000	0.000	0.000	0.000	0.000	0.000	0.003
BLEND 3-3768	0.053	0.075	0.000	0.003	0.125	0.047	0.024	0.112	0.010	0.000	0.000	0.546	0.000	0.000	0.000	0.000	0.000	0.001	0.003
BLEND 3-3789	0.057	0.076	0.000	0.003	0.133	0.046	0.026	0.112	0.011	0.000	0.000	0.531	0.000	0.000	0.000	0.000	0.000	0.000	0.004
BLEND 3-3793	0.059	0.076	0.000	0.003	0.139	0.045	0.027	0.113	0.011	0.000	0.000	0.522	0.000	0.000	0.000	0.000	0.000	0.000	0.004
BLEND 3-3802B	0.059	0.076	0.000	0.003	0.141	0.045	0.027	0.109	0.010	0.000	0.000	0.525	0.000	0.000	0.000	0.000	0.000	0.000	0.004
HM 1-3824	0.060	0.073	0.000	0.002	0.117	0.048	0.026	0.104	0.008	0.000	0.000	0.558	0.000	0.000	0.000	0.000	0.000	0.000	0.003
HM 1-3829	0.064	0.071	0.000	0.002	0.117	0.048	0.027	0.100	0.008	0.000	0.000	0.559	0.000	0.000	0.000	0.000	0.000	0.000	0.003
HM 1-3851	0.065	0.070	0.000	0.002	0.114	0.048	0.027	0.106	0.008	0.000	0.000	0.557	0.000	0.000	0.000	0.000	0.000	0.000	0.003
HM 1-3855	0.069	0.069	0.000	0.002	0.106	0.048	0.028	0.106	0.007	0.000	0.000	0.562	0.000	0.000	0.000	0.000	0.000	0.000	0.002
HM-2-1 (3979C)	0.078	0.069	0.000	0.005	0.103	0.046	0.028	0.106	0.007	0.000	0.000	0.551	0.002	0.000	0.000	0.000	0.001	0.001	0.003
HM-2-2 (4099A)	0.080	0.069	0.000	0.005	0.103	0.045	0.029	0.108	0.007	0.000	0.000	0.546	0.002	0.000	0.000	0.000	0.001	0.001	0.003
HM-2-3 (4120B)	0.078	0.070	0.000	0.004	0.098	0.048	0.028	0.110	0.006	0.000	0.000	0.550	0.002	0.000	0.000	0.000	0.001	0.001	0.003
HM-3-1 (4176)	0.081	0.068	0.000	0.004	0.099	0.044	0.027	0.113	0.006	0.000	0.000	0.553	0.002	0.000	0.000	0.000	0.001	0.001	0.003
HM-3-2 (4225)	0.090	0.070	0.000	0.004	0.105	0.045	0.029	0.111	0.006	0.000	0.000	0.534	0.002	0.000	0.000	0.000	0.001	0.001	0.003
HM-3-3 (4357)	0.095	0.070	0.000	0.004	0.109	0.044	0.031	0.106	0.006	0.000	0.000	0.527	0.002	0.000	0.000	0.000	0.001	0.001	0.003
HM-4-1 (5260)	0.055	0.104	0.000	0.005	0.088	0.046	0.016	0.099	0.006	0.000	0.000	0.564	0.001	0.000	0.000	0.000	0.001	0.012	0.003
HM-4-2 (5641)	0.066	0.096	0.000	0.007	0.083	0.045	0.017	0.097	0.010	0.000	0.000	0.565	0.001	0.000	0.000	0.000	0.001	0.007	0.003
HM-4-3 (5748)	0.059	0.092	0.000	0.004	0.076	0.047	0.017	0.098	0.005	0.000	0.000	0.591	0.001	0.000	0.000	0.000	0.001	0.005	0.003
PX 1-1 (4643)	0.057	0.079	0.000	0.005	0.114	0.046	0.034	0.105	0.017	0.000	0.000	0.533	0.000	0.000	0.000	0.000	0.002	0.001	0.007
PX 1-2 (4726)	0.052	0.078	0.000	0.006	0.118	0.046	0.034	0.106	0.018	0.000	0.000	0.533	0.000	0.000	0.000	0.000	0.002	0.001	0.007
PX 1-3 (4776)	0.046	0.077	0.000	0.006	0.106	0.048	0.030	0.102	0.017	0.000	0.000	0.559	0.000	0.000	0.000	0.000	0.002	0.001	0.007
PX 2-1 (4455)	0.089	0.072	0.000	0.004	0.099	0.045	0.029	0.109	0.007	0.000	0.000	0.540	0.002	0.000	0.000	0.000	0.001	0.001	0.003
PX 2-2 (4509)	0.074	0.076	0.000	0.005	0.116	0.046	0.032	0.101	0.012	0.000	0.000	0.530	0.001	0.000	0.000	0.000	0.001	0.001	0.005
PX 2-3 (4566)	0.064	0.079	0.000	0.005	0.117	0.046	0.035	0.105	0.016	0.000	0.000	0.523	0.001	0.000	0.000	0.000	0.002	0.001	0.006
PX 3-1 (5780)	0.043	0.083	0.000	0.004	0.092	0.049	0.018	0.089	0.007	0.000	0.000	0.604	0.001	0.000	0.000	0.000	0.001	0.007	0.003
PX 3-2 (5818)	0.039	0.081	0.000	0.004	0.100	0.049	0.018	0.086	0.008	0.000	0.000	0.604	0.001	0.000	0.000	0.000	0.001	0.007	0.003
PX 3-3 (5880)	0.033	0.076	0.000	0.003	0.104	0.050	0.017	0.093	0.009	0.000	0.000	0.601	0.000	0.000	0.000	0.000	0.001	0.009	0.003
PX 4-1 (6390)	0.031	0.087	0.000	0.004	0.113	0.053	0.018	0.095	0.010	0.000	0.000	0.574	0.000	0.000	0.000	0.000	0.001	0.009	0.005

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
PX 4-2 (6434)	0.028	0.087	0.000	0.004	0.114	0.052	0.018	0.094	0.011	0.000	0.000	0.576	0.000	0.000	0.000	0.000	0.001	0.009	0.005
PX 4-3 (6458)	0.028	0.087	0.000	0.004	0.115	0.052	0.018	0.090	0.011	0.000	0.000	0.579	0.000	0.000	0.000	0.000	0.001	0.008	0.006
PX 5-1 (6787)	0.036	0.087	0.000	0.004	0.102	0.053	0.017	0.090	0.012	0.000	0.000	0.586	0.000	0.000	0.000	0.000	0.001	0.007	0.006
PX 5-2 (6795)	0.038	0.085	0.000	0.004	0.119	0.048	0.019	0.124	0.014	0.000	0.000	0.531	0.000	0.000	0.000	0.000	0.001	0.010	0.007
PX 5-3 (6812)	0.036	0.085	0.000	0.004	0.128	0.046	0.021	0.141	0.014	0.000	0.000	0.508	0.000	0.000	0.000	0.000	0.001	0.008	0.007
PX 5-4 (6820)	0.034	0.085	0.000	0.004	0.121	0.048	0.020	0.142	0.014	0.000	0.000	0.516	0.000	0.000	0.000	0.000	0.001	0.008	0.007
PX 5-5 (6839)	0.032	0.083	0.000	0.004	0.116	0.047	0.020	0.146	0.013	0.000	0.000	0.520	0.000	0.000	0.000	0.000	0.001	0.010	0.007
PX 5-6 (6862)	0.030	0.085	0.000	0.005	0.101	0.049	0.017	0.137	0.012	0.000	0.000	0.548	0.000	0.000	0.000	0.000	0.001	0.009	0.006
PX 5-7 (6871)	0.028	0.089	0.000	0.004	0.097	0.050	0.017	0.139	0.011	0.000	0.000	0.551	0.000	0.000	0.000	0.000	0.001	0.008	0.006
PX 5-8 (6884)	0.030	0.101	0.000	0.005	0.101	0.047	0.017	0.145	0.013	0.000	0.000	0.527	0.000	0.000	0.000	0.000	0.001	0.008	0.006
PX 5-9 (6960)	0.028	0.115	0.000	0.004	0.097	0.046	0.016	0.144	0.012	0.000	0.000	0.522	0.000	0.000	0.000	0.000	0.001	0.008	0.006
PX 5-10 (6972)	0.028	0.116	0.000	0.005	0.092	0.046	0.016	0.143	0.012	0.000	0.000	0.528	0.000	0.000	0.000	0.000	0.001	0.008	0.006
PX 6-1 (7340)	0.022	0.091	0.000	0.004	0.105	0.052	0.018	0.115	0.012	0.000	0.000	0.564	0.000	0.000	0.000	0.000	0.001	0.011	0.005
BATCH 1 STUDY-6-7	0.029	0.129	0.000	0.001	0.050	0.053	0.009	0.103	0.003	0.000	0.000	0.612	0.000	0.000	0.000	0.000	0.000	0.002	0.011
BATCH 1 STUDY-10B-7	0.029	0.107	0.000	0.001	0.049	0.057	0.008	0.089	0.003	0.000	0.000	0.651	0.000	0.000	0.000	0.000	0.001	0.002	0.005
BATCH 1 STUDY-15-7	0.027	0.085	0.000	0.000	0.047	0.059	0.008	0.076	0.003	0.000	0.000	0.688	0.000	0.000	0.000	0.000	0.001	0.002	0.003
H-GLAS-0112	0.043	0.087	0.000	0.005	0.103	0.049	0.027	0.099	0.015	0.000	0.000	0.556	0.000	0.000	0.000	0.000	0.003	0.006	0.007
H-GLAS-0130	0.040	0.099	0.000	0.004	0.100	0.049	0.022	0.093	0.014	0.000	0.000	0.562	0.000	0.000	0.000	0.000	0.003	0.006	0.006
H-GLAS-0162	0.033	0.120	0.000	0.004	0.089	0.049	0.013	0.082	0.010	0.000	0.000	0.562	0.000	0.000	0.000	0.000	0.005	0.027	0.004
H-GLAS-0244	0.045	0.098	0.000	0.004	0.115	0.047	0.019	0.096	0.009	0.000	0.000	0.545	0.000	0.000	0.000	0.000	0.003	0.014	0.005
H-GLAS-0254	0.033	0.125	0.000	0.004	0.085	0.050	0.012	0.079	0.009	0.000	0.000	0.568	0.000	0.000	0.000	0.000	0.003	0.029	0.004
H-GLAS-0278	0.033	0.122	0.000	0.004	0.091	0.048	0.010	0.078	0.009	0.000	0.000	0.568	0.000	0.000	0.000	0.000	0.003	0.030	0.004
H-GLAS-0293	0.030	0.126	0.000	0.004	0.097	0.049	0.010	0.083	0.009	0.000	0.000	0.569	0.000	0.000	0.000	0.000	0.003	0.016	0.004
H-GLAS-0308	0.032	0.129	0.000	0.005	0.086	0.051	0.010	0.081	0.010	0.000	0.000	0.554	0.000	0.000	0.000	0.000	0.004	0.033	0.004
H-GLAS-0334	0.031	0.132	0.000	0.005	0.099	0.050	0.009	0.082	0.010	0.000	0.000	0.557	0.000	0.000	0.000	0.000	0.003	0.018	0.003
H-GLAS-0352	0.030	0.134	0.000	0.004	0.095	0.050	0.008	0.081	0.010	0.000	0.000	0.546	0.000	0.000	0.000	0.000	0.003	0.036	0.003
H-GLAS-0387	0.029	0.138	0.000	0.004	0.082	0.051	0.007	0.078	0.008	0.000	0.000	0.559	0.000	0.000	0.000	0.000	0.003	0.038	0.003
H-GLAS-0421	0.031	0.140	0.000	0.005	0.091	0.052	0.007	0.081	0.009	0.000	0.000	0.560	0.000	0.000	0.000	0.000	0.003	0.019	0.003
H-GLAS-0466	0.029	0.140	0.000	0.004	0.094	0.051	0.007	0.080	0.008	0.000	0.000	0.543	0.000	0.000	0.000	0.000	0.003	0.039	0.004
FRIT-202-CLEAR	0.004	0.080	0.000	0.000	0.000	0.068	0.000	0.059	0.000	0.000	0.000	0.789	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FRIT-202-INT	0.004	0.080	0.000	0.000	0.000	0.068	0.000	0.059	0.000	0.000	0.000	0.789	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FRIT-202-WHITE	0.004	0.080	0.000	0.000	0.000	0.068	0.000	0.059	0.000	0.000	0.000	0.789	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FRIT-165-7	0.000	0.095	0.000	0.000	0.000	0.071	0.000	0.124	0.000	0.000	0.000	0.701	0.000	0.000	0.000	0.000	0.000	0.010	0.000
FRIT-131-7	0.004	0.157	0.000	0.000	0.001	0.056	0.002	0.206	0.001	0.000	0.000	0.569	0.000	0.000	0.000	0.000	0.000	0.005	0.000
MG 9-7	0.002	0.062	0.000	0.000	0.000	0.000	0.000	0.286	0.000	0.000	0.000	0.650	0.000	0.000	0.000	0.000	0.000	0.000	0.000
MG 18-7	0.010	0.178	0.000	0.000	0.000	0.000	0.000	0.285	0.000	0.000	0.000	0.527	0.000	0.000	0.000	0.000	0.000	0.000	0.000
MG 25-7	0.133	0.141	0.000	0.000	0.098	0.000	0.000	0.159	0.000	0.000	0.000	0.468	0.000	0.000	0.000	0.000	0.000	0.000	0.000
MG 28-7	0.146	0.092	0.000	0.000	0.135	0.000	0.000	0.168	0.000	0.000	0.000	0.458	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PNL 1	0.083	0.178	0.000	0.002	0.166	0.025	0.009	0.062	0.003	0.000	0.000	0.425	0.003	0.019	0.000	0.007	0.003	0.014	0.003
PNL 2	0.048	0.186	0.000	0.002	0.096	0.026	0.009	0.115	0.003	0.000	0.000	0.465	0.003	0.020	0.000	0.007	0.003	0.015	0.003

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
PNL 3	0.086	0.186	0.000	0.002	0.096	0.057	0.009	0.115	0.003	0.000	0.000	0.395	0.003	0.020	0.000	0.007	0.003	0.015	0.003
PNL 4	0.048	0.103	0.000	0.002	0.173	0.026	0.009	0.064	0.003	0.000	0.000	0.521	0.003	0.020	0.000	0.007	0.003	0.015	0.003
PNL 5	0.046	0.178	0.000	0.002	0.092	0.055	0.009	0.062	0.003	0.000	0.000	0.505	0.003	0.019	0.000	0.007	0.003	0.014	0.003
PNL 6	0.083	0.099	0.000	0.002	0.092	0.046	0.009	0.111	0.003	0.000	0.000	0.507	0.003	0.019	0.000	0.007	0.003	0.014	0.003
PNL 7	0.086	0.103	0.000	0.002	0.096	0.026	0.009	0.064	0.003	0.000	0.000	0.520	0.003	0.060	0.000	0.007	0.003	0.015	0.003
PNL 8	0.046	0.178	0.000	0.002	0.166	0.025	0.009	0.111	0.003	0.000	0.000	0.375	0.003	0.057	0.000	0.007	0.003	0.014	0.003
PNL 9	0.086	0.103	0.000	0.002	0.173	0.027	0.009	0.115	0.003	0.000	0.000	0.390	0.003	0.060	0.000	0.007	0.003	0.015	0.003
PNL 10	0.046	0.099	0.000	0.002	0.092	0.055	0.009	0.111	0.003	0.000	0.000	0.497	0.003	0.057	0.000	0.007	0.003	0.014	0.003
Alkali1	0.072	0.115	0.000	0.002	0.137	0.039	0.009	0.081	0.003	0.000	0.000	0.468	0.003	0.044	0.000	0.007	0.003	0.016	0.003
Alkali2	0.064	0.160	0.000	0.002	0.136	0.045	0.009	0.083	0.003	0.000	0.000	0.424	0.003	0.044	0.000	0.007	0.003	0.016	0.003
Alkali3	0.065	0.146	0.000	0.002	0.142	0.037	0.009	0.090	0.003	0.000	0.000	0.438	0.003	0.036	0.000	0.007	0.003	0.017	0.003
Alkali4	0.069	0.121	0.000	0.002	0.126	0.038	0.009	0.085	0.003	0.000	0.000	0.475	0.003	0.040	0.000	0.007	0.003	0.017	0.003
Alkali5	0.068	0.158	0.000	0.002	0.120	0.040	0.009	0.087	0.003	0.000	0.000	0.442	0.003	0.042	0.000	0.007	0.003	0.014	0.003
Alkali6	0.071	0.130	0.000	0.002	0.148	0.042	0.009	0.085	0.003	0.000	0.000	0.442	0.003	0.038	0.000	0.007	0.003	0.015	0.003
Alkali7	0.064	0.153	0.000	0.002	0.127	0.044	0.009	0.090	0.003	0.000	0.000	0.430	0.003	0.046	0.000	0.007	0.003	0.018	0.003
Alkali8	0.062	0.138	0.000	0.002	0.127	0.036	0.009	0.099	0.003	0.000	0.000	0.449	0.003	0.043	0.000	0.007	0.003	0.016	0.003
Alkali9	0.073	0.137	0.000	0.002	0.117	0.037	0.009	0.079	0.003	0.000	0.000	0.463	0.003	0.046	0.000	0.007	0.003	0.018	0.003
Ref6Qtr2	0.066	0.142	0.000	0.002	0.132	0.041	0.009	0.088	0.003	0.000	0.000	0.450	0.003	0.039	0.000	0.007	0.003	0.014	0.003
WVDG-1	0.095	0.131	0.000	0.002	0.127	0.019	0.011	0.099	0.003	0.000	0.000	0.468	0.000	0.031	0.000	0.006	0.000	0.006	0.001
WVDG-2	0.093	0.132	0.000	0.002	0.127	0.019	0.012	0.098	0.003	0.000	0.000	0.472	0.000	0.030	0.000	0.006	0.000	0.006	0.001
WVDG-3	0.079	0.102	0.000	0.003	0.119	0.026	0.016	0.108	0.004	0.000	0.000	0.499	0.000	0.030	0.000	0.006	0.000	0.007	0.001
WVDG-4	0.091	0.128	0.000	0.002	0.120	0.019	0.012	0.125	0.003	0.000	0.000	0.456	0.000	0.032	0.000	0.006	0.000	0.006	0.001
WVDG-5	0.075	0.134	0.000	0.002	0.129	0.019	0.012	0.098	0.003	0.000	0.000	0.480	0.000	0.034	0.000	0.007	0.000	0.006	0.001
WVDG-6	0.093	0.132	0.000	0.002	0.126	0.019	0.012	0.099	0.003	0.000	0.000	0.472	0.000	0.030	0.000	0.006	0.000	0.006	0.001
WVDG-7	0.096	0.131	0.000	0.002	0.125	0.018	0.011	0.094	0.003	0.000	0.000	0.465	0.000	0.041	0.000	0.005	0.000	0.007	0.001
WVDG-8	0.098	0.082	0.000	0.002	0.134	0.020	0.012	0.102	0.003	0.000	0.000	0.501	0.000	0.030	0.000	0.007	0.001	0.006	0.001
WVDG-11R	0.115	0.120	0.000	0.002	0.131	0.029	0.012	0.105	0.003	0.000	0.000	0.446	0.000	0.024	0.000	0.007	0.000	0.005	0.001
WVDG-12R	0.116	0.119	0.000	0.002	0.130	0.028	0.012	0.105	0.003	0.000	0.000	0.442	0.000	0.028	0.000	0.008	0.001	0.006	0.001
WVDG-13R	0.117	0.119	0.000	0.002	0.131	0.029	0.012	0.103	0.003	0.000	0.000	0.443	0.000	0.027	0.000	0.008	0.000	0.006	0.001
WVDG-14R	0.116	0.120	0.000	0.002	0.131	0.029	0.012	0.104	0.003	0.000	0.000	0.439	0.000	0.028	0.000	0.007	0.000	0.008	0.001
WVDG-15	0.106	0.139	0.000	0.003	0.098	0.030	0.023	0.113	0.006	0.000	0.000	0.441	0.000	0.018	0.000	0.011	0.000	0.008	0.004
WVDG-16	0.103	0.138	0.000	0.001	0.158	0.021	0.020	0.095	0.002	0.000	0.000	0.437	0.000	0.018	0.000	0.002	0.000	0.002	0.004
WVDG-17	0.105	0.109	0.000	0.003	0.099	0.026	0.023	0.118	0.006	0.000	0.000	0.443	0.000	0.052	0.000	0.001	0.001	0.008	0.004
WVDG-18	0.100	0.112	0.000	0.001	0.153	0.026	0.005	0.118	0.002	0.000	0.000	0.458	0.000	0.021	0.000	0.001	0.000	0.002	0.001
WVDG-19	0.133	0.110	0.000	0.001	0.154	0.023	0.004	0.107	0.002	0.000	0.000	0.392	0.000	0.057	0.000	0.011	0.000	0.002	0.004
WVDG-20	0.140	0.121	0.000	0.003	0.100	0.023	0.005	0.099	0.007	0.000	0.000	0.457	0.000	0.021	0.000	0.011	0.000	0.009	0.004
WVDG-21	0.135	0.108	0.000	0.001	0.158	0.025	0.022	0.113	0.002	0.000	0.000	0.404	0.000	0.017	0.000	0.010	0.001	0.002	0.002
WVDG-22	0.137	0.127	0.000	0.003	0.154	0.020	0.022	0.091	0.006	0.000	0.000	0.410	0.000	0.019	0.000	0.001	0.000	0.008	0.001
WVDG-23	0.102	0.135	0.000	0.001	0.154	0.019	0.005	0.089	0.002	0.000	0.000	0.425	0.000	0.054	0.000	0.011	0.000	0.003	0.001
WVDG-24	0.132	0.142	0.000	0.001	0.093	0.022	0.021	0.102	0.002	0.000	0.000	0.451	0.000	0.020	0.000	0.011	0.000	0.002	0.001

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
WVDG-25	0.101	0.118	0.000	0.001	0.094	0.022	0.021	0.099	0.002	0.000	0.000	0.489	0.000	0.047	0.000	0.001	0.000	0.003	0.001
WVDG-26	0.134	0.146	0.000	0.001	0.095	0.022	0.005	0.099	0.002	0.000	0.000	0.447	0.000	0.041	0.000	0.001	0.000	0.003	0.004
WVDG-27	0.137	0.142	0.000	0.003	0.098	0.026	0.005	0.115	0.007	0.000	0.000	0.415	0.000	0.039	0.000	0.001	0.001	0.009	0.002
WVDG-28	0.105	0.116	0.000	0.003	0.132	0.022	0.005	0.096	0.006	0.000	0.000	0.472	0.000	0.019	0.000	0.011	0.001	0.008	0.002
WVDG-29	0.102	0.126	0.000	0.001	0.096	0.028	0.004	0.118	0.002	0.000	0.000	0.492	0.000	0.021	0.000	0.001	0.000	0.003	0.004
WVDG-30	0.110	0.130	0.000	0.002	0.126	0.023	0.011	0.105	0.004	0.000	0.000	0.439	0.000	0.036	0.000	0.007	0.000	0.005	0.003
WVDG-33	0.091	0.100	0.000	0.001	0.127	0.032	0.012	0.116	0.003	0.000	0.000	0.470	0.000	0.037	0.000	0.006	0.000	0.004	0.001
WVDG-34	0.059	0.123	0.000	0.004	0.111	0.035	0.018	0.126	0.009	0.000	0.000	0.455	0.001	0.022	0.000	0.022	0.001	0.012	0.002
WVDG-35	0.109	0.078	0.000	0.001	0.163	0.034	0.017	0.123	0.002	0.000	0.000	0.413	0.000	0.030	0.000	0.028	0.000	0.002	0.001
WVDG-36	0.063	0.119	0.000	0.004	0.162	0.024	0.001	0.085	0.009	0.000	0.000	0.453	0.001	0.064	0.000	0.002	0.001	0.011	0.001
WVDG-37	0.111	0.087	0.000	0.004	0.109	0.037	0.001	0.133	0.009	0.000	0.000	0.469	0.001	0.023	0.000	0.002	0.001	0.012	0.001
WVDG-38	0.115	0.085	0.000	0.004	0.108	0.031	0.015	0.112	0.009	0.000	0.000	0.459	0.001	0.046	0.000	0.001	0.001	0.012	0.001
WVDG-39	0.113	0.126	0.000	0.001	0.105	0.034	0.001	0.124	0.002	0.000	0.000	0.428	0.000	0.058	0.000	0.001	0.000	0.003	0.001
WVDG-40	0.066	0.081	0.000	0.001	0.166	0.029	0.001	0.105	0.002	0.000	0.000	0.479	0.000	0.045	0.000	0.021	0.000	0.002	0.001
WVDG-41	0.065	0.080	0.000	0.001	0.105	0.035	0.001	0.127	0.002	0.000	0.000	0.498	0.000	0.058	0.000	0.023	0.000	0.003	0.001
WVDG-42	0.066	0.080	0.000	0.004	0.113	0.035	0.019	0.125	0.009	0.000	0.000	0.473	0.001	0.059	0.000	0.002	0.001	0.012	0.002
WVDG-43	0.108	0.134	0.000	0.001	0.103	0.024	0.017	0.088	0.002	0.000	0.000	0.453	0.000	0.045	0.000	0.022	0.000	0.002	0.001
WVDG-44	0.088	0.122	0.000	0.001	0.168	0.032	0.001	0.115	0.002	0.000	0.000	0.404	0.000	0.039	0.000	0.024	0.000	0.002	0.001
WVDG-45	0.114	0.079	0.000	0.001	0.172	0.036	0.018	0.130	0.002	0.000	0.000	0.423	0.000	0.020	0.000	0.001	0.000	0.003	0.000
WVDG-46	0.076	0.133	0.000	0.001	0.113	0.031	0.017	0.112	0.002	0.000	0.000	0.488	0.000	0.023	0.000	0.001	0.000	0.002	0.001
WVDG-47	0.062	0.123	0.000	0.001	0.163	0.025	0.017	0.089	0.002	0.000	0.000	0.492	0.000	0.021	0.000	0.001	0.000	0.002	0.000
WVDG-48	0.111	0.125	0.000	0.005	0.109	0.027	0.001	0.097	0.010	0.000	0.000	0.449	0.001	0.024	0.000	0.024	0.001	0.013	0.002
FY92-5	0.080	0.117	0.000	0.002	0.160	0.057	0.009	0.098	0.003	0.000	0.000	0.413	0.003	0.030	0.000	0.007	0.003	0.015	0.003
FY92-6	0.054	0.117	0.000	0.002	0.109	0.026	0.009	0.115	0.003	0.000	0.000	0.504	0.003	0.030	0.000	0.007	0.003	0.015	0.003
FY92-7	0.054	0.117	0.000	0.002	0.160	0.026	0.009	0.064	0.003	0.000	0.000	0.504	0.003	0.030	0.000	0.007	0.003	0.015	0.003
FY92-9	0.052	0.112	0.000	0.002	0.154	0.055	0.009	0.062	0.003	0.000	0.000	0.475	0.003	0.048	0.000	0.007	0.003	0.014	0.003
FY92-10	0.080	0.172	0.000	0.002	0.109	0.026	0.009	0.064	0.003	0.000	0.000	0.455	0.003	0.050	0.000	0.007	0.003	0.015	0.003
FY92Ref5	0.071	0.141	0.000	0.002	0.132	0.030	0.009	0.108	0.003	0.000	0.000	0.451	0.003	0.039	0.000	0.007	0.000	0.004	0.002
Ratio2	0.074	0.122	0.000	0.002	0.178	0.041	0.009	0.097	0.003	0.000	0.000	0.432	0.003	0.014	0.000	0.007	0.003	0.013	0.003
Ratio4	0.063	0.124	0.000	0.002	0.111	0.045	0.009	0.080	0.003	0.000	0.000	0.480	0.003	0.048	0.000	0.007	0.003	0.021	0.003
Ratio5	0.057	0.160	0.000	0.002	0.142	0.045	0.009	0.099	0.003	0.000	0.000	0.426	0.003	0.031	0.000	0.007	0.003	0.011	0.003
LoTh2	0.068	0.128	0.000	0.002	0.142	0.043	0.009	0.097	0.003	0.000	0.000	0.464	0.003	0.015	0.000	0.007	0.003	0.015	0.003
LoTh4	0.067	0.151	0.000	0.002	0.115	0.036	0.009	0.097	0.003	0.000	0.000	0.472	0.003	0.020	0.000	0.007	0.003	0.013	0.003
LoTh5	0.060	0.156	0.000	0.002	0.150	0.035	0.009	0.076	0.003	0.000	0.000	0.455	0.003	0.026	0.000	0.007	0.003	0.013	0.003
HiFe2	0.059	0.121	0.000	0.002	0.171	0.044	0.009	0.097	0.003	0.000	0.000	0.433	0.003	0.034	0.000	0.007	0.003	0.013	0.003
HiFe3	0.061	0.124	0.000	0.002	0.163	0.047	0.009	0.102	0.003	0.000	0.000	0.429	0.003	0.032	0.000	0.007	0.003	0.012	0.003
HiFe4	0.059	0.160	0.000	0.002	0.148	0.045	0.009	0.090	0.003	0.000	0.000	0.423	0.003	0.035	0.000	0.007	0.003	0.010	0.003
PNL190	0.055	0.117	0.000	0.002	0.109	0.057	0.009	0.115	0.003	0.000	0.000	0.453	0.003	0.050	0.000	0.007	0.003	0.015	0.003
FY93-1	0.083	0.178	0.000	0.002	0.166	0.025	0.009	0.062	0.003	0.000	0.000	0.425	0.003	0.019	0.000	0.007	0.003	0.014	0.003
FY93-2	0.048	0.186	0.000	0.002	0.096	0.026	0.009	0.115	0.003	0.000	0.000	0.465	0.003	0.020	0.000	0.007	0.003	0.015	0.003

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
FY93-3	0.086	0.186	0.000	0.002	0.096	0.057	0.009	0.115	0.003	0.000	0.000	0.395	0.003	0.020	0.000	0.007	0.003	0.015	0.003
FY93-4	0.048	0.103	0.000	0.002	0.173	0.026	0.009	0.064	0.003	0.000	0.000	0.521	0.003	0.020	0.000	0.007	0.003	0.015	0.003
FY93-5	0.046	0.178	0.000	0.002	0.092	0.055	0.009	0.062	0.003	0.000	0.000	0.505	0.003	0.019	0.000	0.007	0.003	0.014	0.003
FY93-6	0.083	0.099	0.000	0.002	0.092	0.046	0.009	0.111	0.003	0.000	0.000	0.507	0.003	0.019	0.000	0.007	0.003	0.014	0.003
FY93-7	0.086	0.103	0.000	0.002	0.096	0.026	0.009	0.064	0.003	0.000	0.000	0.520	0.003	0.060	0.000	0.007	0.003	0.015	0.003
FY93-8	0.046	0.178	0.000	0.002	0.166	0.025	0.009	0.111	0.003	0.000	0.000	0.375	0.003	0.057	0.000	0.007	0.003	0.014	0.003
FY93-9	0.086	0.103	0.000	0.002	0.173	0.027	0.009	0.115	0.003	0.000	0.000	0.390	0.003	0.060	0.000	0.007	0.003	0.015	0.003
FY93-10	0.046	0.099	0.000	0.002	0.092	0.055	0.009	0.111	0.003	0.000	0.000	0.497	0.003	0.057	0.000	0.007	0.003	0.014	0.003
FY94-1	0.082	0.100	0.000	0.002	0.073	0.031	0.009	0.093	0.003	0.000	0.000	0.530	0.003	0.053	0.000	0.007	0.003	0.008	0.003
FY94-2	0.082	0.079	0.000	0.002	0.193	0.044	0.009	0.058	0.003	0.000	0.000	0.477	0.003	0.030	0.000	0.007	0.003	0.008	0.003
FY94-3	0.062	0.204	0.000	0.002	0.120	0.031	0.009	0.120	0.003	0.000	0.000	0.404	0.003	0.022	0.000	0.007	0.003	0.008	0.003
FY94-4	0.047	0.188	0.000	0.002	0.187	0.051	0.009	0.100	0.003	0.000	0.000	0.380	0.003	0.010	0.000	0.007	0.003	0.008	0.003
FY94-5	0.061	0.079	0.000	0.002	0.074	0.050	0.009	0.120	0.003	0.000	0.000	0.533	0.003	0.035	0.000	0.007	0.003	0.019	0.003
FY94-6	0.084	0.077	0.000	0.002	0.190	0.051	0.009	0.065	0.003	0.000	0.000	0.427	0.003	0.056	0.000	0.007	0.003	0.021	0.003
FY94-7	0.068	0.190	0.000	0.002	0.072	0.026	0.009	0.072	0.003	0.000	0.000	0.472	0.003	0.051	0.000	0.007	0.003	0.020	0.003
FY94-8	0.048	0.195	0.000	0.002	0.189	0.041	0.009	0.093	0.003	0.000	0.000	0.374	0.003	0.012	0.000	0.007	0.003	0.021	0.003
FY94-9	0.051	0.151	0.000	0.002	0.156	0.038	0.009	0.068	0.003	0.000	0.000	0.460	0.003	0.027	0.000	0.007	0.003	0.020	0.003
FY94-10	0.066	0.201	0.000	0.002	0.071	0.052	0.009	0.084	0.003	0.000	0.000	0.452	0.003	0.039	0.000	0.007	0.003	0.008	0.003
Sigma1	0.048	0.210	0.000	0.002	0.131	0.057	0.009	0.123	0.003	0.000	0.000	0.384	0.003	0.010	0.000	0.007	0.003	0.008	0.003
Sigma2	0.048	0.210	0.000	0.002	0.083	0.057	0.009	0.123	0.003	0.000	0.000	0.384	0.003	0.058	0.000	0.007	0.003	0.008	0.003
Sigma3	0.051	0.085	0.000	0.002	0.195	0.055	0.009	0.122	0.003	0.000	0.000	0.411	0.003	0.043	0.000	0.007	0.003	0.009	0.003
Sigma4	0.055	0.206	0.000	0.002	0.123	0.056	0.009	0.115	0.003	0.000	0.000	0.396	0.003	0.011	0.000	0.007	0.003	0.009	0.003
Sigma5	0.051	0.201	0.000	0.002	0.135	0.055	0.009	0.117	0.003	0.000	0.000	0.392	0.003	0.010	0.000	0.007	0.003	0.009	0.003
Sigma6	0.052	0.195	0.000	0.002	0.116	0.054	0.009	0.113	0.003	0.000	0.000	0.407	0.003	0.025	0.000	0.007	0.003	0.009	0.003
Sigma7	0.057	0.190	0.000	0.002	0.126	0.055	0.009	0.120	0.003	0.000	0.000	0.402	0.003	0.012	0.000	0.007	0.003	0.009	0.003
Sigma8	0.053	0.178	0.000	0.002	0.145	0.054	0.009	0.108	0.003	0.000	0.000	0.412	0.003	0.011	0.000	0.007	0.003	0.009	0.003
Sigma9	0.058	0.172	0.000	0.002	0.104	0.053	0.009	0.110	0.003	0.000	0.000	0.417	0.003	0.048	0.000	0.007	0.003	0.009	0.003
Sigma10	0.056	0.176	0.000	0.002	0.094	0.052	0.009	0.106	0.003	0.000	0.000	0.423	0.003	0.056	0.000	0.007	0.003	0.009	0.003
LAWA41	0.069	0.083	0.000	0.000	0.077	0.000	0.000	0.222	0.000	0.000	0.000	0.482	0.000	0.000	0.000	0.000	0.033	0.033	0.000
LAWA42	0.070	0.102	0.000	0.000	0.095	0.000	0.000	0.225	0.000	0.000	0.000	0.427	0.000	0.000	0.000	0.000	0.041	0.041	0.000
LAWA43	0.133	0.082	0.000	0.000	0.076	0.000	0.000	0.222	0.000	0.000	0.000	0.421	0.000	0.000	0.000	0.000	0.033	0.033	0.000
LAWA44	0.067	0.096	0.000	0.000	0.075	0.000	0.000	0.216	0.000	0.000	0.000	0.481	0.000	0.000	0.000	0.000	0.032	0.032	0.000
LAWA45	0.065	0.125	0.000	0.000	0.073	0.000	0.000	0.210	0.000	0.000	0.000	0.468	0.000	0.000	0.000	0.000	0.026	0.031	0.000
LAWA46	0.067	0.097	0.000	0.000	0.076	0.000	0.000	0.217	0.000	0.000	0.000	0.484	0.000	0.000	0.000	0.000	0.027	0.032	0.000
LAWA47	0.067	0.097	0.000	0.000	0.076	0.000	0.000	0.217	0.000	0.000	0.000	0.484	0.000	0.000	0.000	0.000	0.027	0.032	0.000
LAWA48	0.067	0.097	0.000	0.000	0.076	0.000	0.000	0.217	0.000	0.000	0.000	0.484	0.000	0.000	0.000	0.000	0.027	0.032	0.000
LAWA49	0.065	0.094	0.000	0.000	0.105	0.000	0.000	0.210	0.000	0.000	0.000	0.468	0.000	0.000	0.000	0.000	0.026	0.031	0.000
LAWA50	0.065	0.094	0.000	0.000	0.126	0.000	0.000	0.210	0.000	0.000	0.000	0.447	0.000	0.000	0.000	0.000	0.026	0.031	0.000
LAWA51	0.065	0.126	0.000	0.000	0.073	0.000	0.000	0.189	0.000	0.000	0.000	0.489	0.000	0.000	0.000	0.000	0.026	0.031	0.000
LAWA52	0.070	0.070	0.000	0.000	0.085	0.000	0.000	0.227	0.000	0.000	0.000	0.479	0.000	0.000	0.000	0.000	0.034	0.034	0.000

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
LAWA60	0.094	0.124	0.000	0.000	0.000	0.000	0.000	0.222	0.000	0.000	0.000	0.493	0.000	0.000	0.000	0.000	0.033	0.033	0.000
LAWA64	0.064	0.064	0.000	0.000	0.078	0.000	0.000	0.208	0.000	0.000	0.000	0.440	0.082	0.000	0.000	0.000	0.031	0.031	0.000
LAWA76	0.070	0.125	0.000	0.000	0.085	0.057	0.000	0.115	0.000	0.000	0.000	0.479	0.000	0.000	0.000	0.000	0.034	0.034	0.000
LAWA81	0.067	0.096	0.000	0.000	0.075	0.000	0.000	0.216	0.000	0.000	0.000	0.481	0.000	0.000	0.000	0.000	0.032	0.032	0.000
LAWA82	0.067	0.096	0.000	0.000	0.075	0.000	0.000	0.216	0.000	0.000	0.000	0.481	0.000	0.000	0.000	0.000	0.032	0.032	0.000
LAWA83	0.068	0.098	0.000	0.000	0.055	0.000	0.000	0.221	0.000	0.000	0.000	0.492	0.000	0.000	0.000	0.000	0.033	0.033	0.000
LAWA84	0.070	0.100	0.000	0.000	0.034	0.000	0.000	0.226	0.000	0.000	0.000	0.503	0.000	0.000	0.000	0.000	0.033	0.034	0.000
LAWA85	0.067	0.096	0.000	0.000	0.054	0.000	0.000	0.216	0.000	0.000	0.000	0.481	0.022	0.000	0.000	0.000	0.032	0.032	0.000
LAWA86	0.068	0.098	0.000	0.000	0.033	0.000	0.000	0.221	0.000	0.000	0.000	0.492	0.022	0.000	0.000	0.000	0.033	0.033	0.000
LAWA87	0.049	0.098	0.000	0.000	0.077	0.000	0.000	0.220	0.000	0.000	0.000	0.490	0.000	0.000	0.000	0.000	0.033	0.033	0.000
LAWA88	0.067	0.106	0.000	0.000	0.061	0.000	0.000	0.219	0.000	0.000	0.000	0.482	0.000	0.000	0.000	0.000	0.032	0.033	0.000
LAWA89	0.067	0.106	0.000	0.000	0.061	0.000	0.000	0.219	0.000	0.000	0.000	0.482	0.000	0.000	0.000	0.000	0.032	0.033	0.000
LAWA90	0.067	0.106	0.000	0.000	0.061	0.000	0.000	0.219	0.000	0.000	0.000	0.482	0.000	0.000	0.000	0.000	0.032	0.033	0.000
LAWA93	0.070	0.126	0.000	0.000	0.085	0.057	0.000	0.114	0.000	0.000	0.000	0.479	0.000	0.000	0.000	0.000	0.034	0.034	0.000
LAWA96	0.072	0.091	0.000	0.000	0.035	0.000	0.000	0.231	0.000	0.000	0.000	0.503	0.000	0.000	0.000	0.000	0.034	0.035	0.000
LAWA98S	0.066	0.118	0.000	0.000	0.082	0.034	0.000	0.162	0.000	0.000	0.000	0.471	0.000	0.000	0.000	0.000	0.034	0.033	0.000
LAWA99S	0.067	0.119	0.000	0.000	0.050	0.022	0.000	0.164	0.000	0.000	0.000	0.477	0.000	0.000	0.000	0.000	0.034	0.034	0.033
LAWA100S	0.067	0.119	0.000	0.000	0.083	0.022	0.000	0.164	0.000	0.000	0.000	0.477	0.000	0.000	0.000	0.000	0.034	0.034	0.000
LAWA101S	0.068	0.120	0.000	0.000	0.084	0.012	0.000	0.166	0.000	0.000	0.000	0.482	0.000	0.000	0.000	0.000	0.034	0.034	0.000
LAWA102S	0.066	0.110	0.000	0.000	0.059	0.027	0.000	0.159	0.000	0.000	0.000	0.511	0.000	0.000	0.000	0.000	0.034	0.033	0.000
LAWA104	0.071	0.093	0.000	0.000	0.073	0.000	0.000	0.237	0.000	0.000	0.000	0.464	0.000	0.000	0.000	0.000	0.031	0.031	0.000
LAWA105	0.076	0.089	0.000	0.000	0.070	0.000	0.000	0.259	0.000	0.000	0.000	0.446	0.000	0.000	0.000	0.000	0.030	0.030	0.000
LAWB30	0.097	0.113	0.000	0.001	0.093	0.046	0.000	0.089	0.000	0.000	0.000	0.480	0.000	0.000	0.000	0.000	0.046	0.035	0.000
LAWB31	0.069	0.135	0.000	0.001	0.080	0.033	0.000	0.088	0.000	0.000	0.000	0.524	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWB32	0.069	0.169	0.000	0.001	0.047	0.033	0.000	0.088	0.000	0.000	0.000	0.524	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWB33	0.070	0.138	0.000	0.001	0.059	0.034	0.000	0.090	0.000	0.000	0.000	0.537	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWB34	0.070	0.138	0.000	0.001	0.059	0.034	0.000	0.090	0.000	0.000	0.000	0.537	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWB35	0.070	0.138	0.000	0.001	0.059	0.034	0.000	0.090	0.000	0.000	0.000	0.537	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWB37	0.070	0.138	0.000	0.001	0.059	0.034	0.000	0.090	0.000	0.000	0.000	0.537	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWB38	0.070	0.137	0.000	0.001	0.058	0.043	0.000	0.089	0.000	0.000	0.000	0.531	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWB39	0.068	0.133	0.000	0.001	0.057	0.033	0.000	0.087	0.000	0.000	0.000	0.517	0.000	0.000	0.000	0.000	0.034	0.034	0.037
LAWB40	0.068	0.133	0.000	0.001	0.057	0.070	0.000	0.087	0.000	0.000	0.000	0.517	0.000	0.000	0.000	0.000	0.034	0.034	0.000
LAWB41	0.069	0.136	0.000	0.001	0.058	0.051	0.000	0.089	0.000	0.000	0.000	0.527	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWB45	0.069	0.139	0.000	0.001	0.059	0.052	0.000	0.073	0.000	0.000	0.000	0.537	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWB51S	0.068	0.141	0.000	0.001	0.060	0.053	0.000	0.056	0.000	0.000	0.000	0.549	0.000	0.000	0.000	0.000	0.036	0.036	0.000
LAWB52S	0.068	0.112	0.000	0.001	0.076	0.066	0.000	0.056	0.000	0.000	0.000	0.549	0.000	0.000	0.000	0.000	0.036	0.036	0.000
LAWB53S	0.070	0.114	0.000	0.001	0.061	0.067	0.000	0.057	0.000	0.000	0.000	0.558	0.000	0.000	0.000	0.000	0.036	0.036	0.000
LAWC12 for AN107	0.129	0.098	0.000	0.000	0.061	0.000	0.001	0.215	0.000	0.000	0.000	0.423	0.000	0.000	0.000	0.000	0.046	0.026	0.000
LAWC13	0.070	0.071	0.000	0.000	0.040	0.000	0.000	0.229	0.000	0.000	0.000	0.485	0.000	0.000	0.000	0.000	0.035	0.035	0.034
LAWC14	0.068	0.068	0.000	0.000	0.039	0.000	0.000	0.222	0.000	0.000	0.000	0.470	0.000	0.000	0.000	0.000	0.034	0.034	0.063

Table A.1. Compositions of IHLW Phase 1 Validation Glasses, 19 Normalized Components Wt% (cont.).

Glass	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
LAWC15	0.067	0.096	0.000	0.000	0.075	0.000	0.000	0.215	0.000	0.000	0.000	0.481	0.000	0.000	0.000	0.000	0.032	0.032	0.000
LAWC16S	0.068	0.112	0.000	0.000	0.083	0.044	0.000	0.131	0.000	0.000	0.000	0.494	0.000	0.000	0.000	0.000	0.034	0.034	0.000
LAWC17S	0.069	0.113	0.000	0.000	0.050	0.033	0.000	0.132	0.000	0.000	0.000	0.500	0.000	0.000	0.000	0.000	0.034	0.034	0.034
LAWC18S	0.069	0.113	0.000	0.000	0.084	0.033	0.000	0.132	0.000	0.000	0.000	0.500	0.000	0.000	0.000	0.000	0.034	0.034	0.000
LAWC19S	0.070	0.115	0.000	0.000	0.085	0.023	0.000	0.134	0.000	0.000	0.000	0.505	0.000	0.000	0.000	0.000	0.034	0.034	0.000
LAWC20S	0.069	0.113	0.000	0.000	0.084	0.000	0.000	0.132	0.000	0.000	0.000	0.500	0.000	0.000	0.000	0.000	0.034	0.034	0.034
LAWC21S	0.068	0.112	0.000	0.000	0.072	0.030	0.000	0.132	0.000	0.000	0.000	0.519	0.000	0.000	0.000	0.000	0.033	0.034	0.000
LAWC22	0.067	0.110	0.000	0.000	0.059	0.027	0.000	0.158	0.000	0.000	0.000	0.511	0.000	0.000	0.000	0.000	0.034	0.033	0.000
LAWC23	0.070	0.115	0.000	0.000	0.074	0.000	0.000	0.136	0.000	0.000	0.000	0.535	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWC24	0.070	0.115	0.000	0.000	0.074	0.000	0.000	0.136	0.000	0.000	0.000	0.535	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWC25	0.070	0.115	0.000	0.000	0.074	0.000	0.000	0.136	0.000	0.000	0.000	0.535	0.000	0.000	0.000	0.000	0.035	0.035	0.000
LAWABP1	0.109	0.101	0.000	0.000	0.027	0.000	0.000	0.219	0.000	0.000	0.000	0.458	0.000	0.000	0.000	0.000	0.028	0.057	0.000
PNLREF (LD6-5412)	0.129	0.054	0.000	0.000	0.000	0.000	0.000	0.215	0.000	0.000	0.000	0.601	0.001	0.000	0.000	0.000	0.000	0.000	0.000
TFA-BASE (HLP-01)	0.074	0.106	0.000	0.001	0.058	0.000	0.000	0.211	0.000	0.000	0.000	0.518	0.000	0.000	0.000	0.000	0.016	0.016	0.000

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses.

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
HLW98-02	24.030	6.040	66.840	0.704	0.646	0.668	No	No	No	No
HLW98-04	18.340	NA	40.220	0.454	NA	0.460	No	No	No	No
HLW98-12	26.690	18.520	6.853	0.572	0.570	0.316	No	No	No	No
HLW98-20	21.870	3.120	53.160	0.586	0.448	0.498	No	No	No	No
HLW98-21	12.130	16.260	13.110	0.558	0.582	0.266	Yes	Yes	Yes	Yes
HLW98-22	16.150	6.467	27.750	0.434	0.464	0.434	No	No	No	No
HLW98-23	16.400	6.590	23.850	0.440	0.472	0.410	Yes	No	No	No
HLW98-27B	9.833	13.230	82.430	0.788	0.630	0.770	No	No	No	No
HLW98-32A	13.850	13.510	3.987	0.496	0.416	0.150	No	No	No	No
HLW98-34	10.100	8.047	27.190	0.464	0.434	0.392	No	No	No	No
HLW98-50	120.700	47.100	221.200	3.534	2.534	2.194	Yes	Yes	Yes	Yes
HLW98-51R	75.850	50.260	116.800	2.714	2.164	1.830	Yes	Yes	Yes	Yes
HLW98-53A	19.070	22.700	52.280	0.846	0.814	0.710	Yes	Yes	Yes	Yes
HLW98-56	30.300	28.810	64.670	1.394	0.886	0.914	No	No	No	No
HLW98-58	11.760	25.660	137.300	0.946	1.104	1.346	No	No	No	No
HLW98-60	12.010	23.440	115.800	0.966	1.008	1.178	No	No	No	No
HLW98-61	5.767	15.400	71.690	0.464	0.662	0.694	No	No	No	No
HLW98-62	21.190	14.270	33.070	0.568	0.614	0.462	No	No	No	No
HLW99-15	1648.000	120.100	3511.000	26.516	25.838	23.650	No	No	No	No
HLW99-27	55.010	40.020	45.350	1.106	1.230	1.222	No	No	No	No
HLW99-52	1169.000	0.807	1713.000	18.810	NA	14.424	No	No	No	No
HLWD1-01	6.630	0.180	15.590	0.252	0.428	0.266	No	No	No	No
HLWD1-02	20.500	0.250	65.050	0.786	0.594	0.674	No	No	No	No
HLWD1-03	14.950	0.190	20.310	0.356	0.452	0.348	No	No	No	No
HLWD1-04	9.060	0.370	22.170	0.348	0.880	0.380	No	No	No	No
HLWD1-05	17.130	8.940	31.690	0.656	0.608	0.544	No	No	No	No
HLWD1-07	22.180	14.300	53.870	1.038	1.044	1.012	No	No	No	No
HLWD1-08	19.710	9.140	17.960	0.646	0.668	0.572	No	No	No	No
HLWD1-09	14.980	13.010	66.690	0.982	0.950	0.984	No	No	No	No
HLWD1-10	21.040	0.120	21.800	0.730	NA	0.738	No	No	No	No
HLWD1-11	30.210	18.620	137.500	1.594	1.324	1.260	No	No	No	No
HLWD1-13	8.060	7.330	40.940	0.382	0.494	0.518	No	No	No	No
HLWD1-14R	123.700	27.490	162.300	2.474	1.892	1.540	No	No	No	No
HLWD1-17R	121.800	29.260	111.100	2.436	2.014	1.580	No	No	No	No
HLWD1-18	60.760	15.490	66.810	1.276	1.056	0.940	No	No	No	No
HLWD1-19RW	65.040	45.580	490.000	3.186	3.162	3.514	No	No	No	No
HLWD1-20R	25.130	16.370	207.300	1.218	1.124	1.472	No	No	No	No
HLWD1-21R	57.640	19.530	72.240	1.212	1.022	0.860	No	No	No	No
HLWD1-23	239.900	75.110	341.900	4.964	3.994	3.374	No	No	No	No
HLWD1-25	135.800	28.950	352.900	3.738	2.970	2.904	No	No	No	No
HLWD1-27	75.120	18.970	216.100	2.174	2.030	2.122	No	No	No	No
HLWD2-01	9.630	6.880	22.580	0.460	0.500	0.422	No	No	No	No
HLWD2-02	17.660	12.240	45.160	0.938	0.868	0.854	No	No	No	No
HLWD2-03	9.300	9.900	147.600	0.452	0.682	1.050	No	No	No	No
HLWD2-04	150.400	86.140	776.900	7.306	5.926	5.524	No	No	No	No
HLWD2-05R	235.300	118.000	1159.000	11.290	8.018	8.142	No	No	No	No
HLWD2-06	17.340	6.650	40.810	0.466	0.478	0.484	No	No	No	No
HLWD3-01	35.670	0.390	226.000	1.612	1.388	1.552	No	No	No	No
HLWD3-02	19.980	0.070	102.800	0.894	NA	0.868	No	No	No	No
HLWD3-03	5.170	4.320	21.190	0.218	0.294	0.298	No	No	No	No
HLWD3-04	27.860	8.630	39.500	0.556	0.594	0.562	No	No	No	No
HLWD3-06	55.980	14.850	75.030	1.120	1.022	1.068	No	No	No	No
HLWD3-07	48.670	13.480	163.200	1.378	0.928	1.160	No	No	No	No

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses (cont.).

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
HLWD3-08	256.500	0.620	814.900	9.300	NA	4.980	No	No	No	No
HLW98-75	15.260	16.820	76.330	0.734	0.720	0.760	Yes	Yes	Yes	Yes
HLW98-77	19.680	9.580	36.640	0.532	0.584	0.424	Yes	Yes	Yes	Yes
HLW98-80	26.130	10.750	46.190	0.672	0.710	0.518	Yes	Yes	Yes	Yes
HLW98-83	237.100	60.850	362.300	6.370	4.726	4.136	No	No	No	No
HLW98-84	25.640	8.180	51.210	0.740	0.638	0.576	Yes	Yes	No	No
HLW98-86	23.520	9.240	56.670	0.806	0.660	0.646	No	No	No	No
HLW98-87	16.370	9.280	32.370	0.522	0.568	0.394	Yes	Yes	Yes	Yes
HLW98-88	17.020	9.990	38.920	0.516	0.572	0.448	Yes	Yes	Yes	Yes
HLW98-89	9.400	7.960	30.540	0.332	0.600	0.382	Yes	Yes	Yes	Yes
HLW98-94	30.400	0.110	156.000	0.850	0.006	1.774	No	No	No	No
HLW98-95	18.290	10.210	40.770	0.554	0.584	0.460	Yes	Yes	Yes	Yes
HLW98-96	15.220	8.450	31.860	0.484	0.586	0.398	Yes	Yes	Yes	Yes
HLW98-96A	18.330	8.780	38.070	0.568	0.594	0.464	Yes	No	Yes	No
HLW98-96B	17.250	8.800	35.350	0.538	0.600	0.434	Yes	No	Yes	No
HLW98-97	22.100	10.590	45.220	0.644	0.588	0.500	No	No	No	No
HLW98-T05	25.150	8.970	49.440	0.684	0.642	0.554	Yes	Yes	Yes	Yes
HLW98-V01	19.690	8.980	32.470	0.564	0.582	0.390	No	No	No	No
HLW98-V07	21.180	8.590	35.840	0.572	0.600	0.420	No	No	No	No
HLW98-V13	28.470	8.880	56.130	0.866	0.736	0.662	No	No	No	No
HLW98-V19	21.550	9.880	61.180	0.780	0.748	0.730	No	No	No	No
HLW98-V24	29.900	14.180	85.270	0.952	0.940	0.910	Yes	Yes	No	No
CVS1-1	NA	NA	NA	1.042	1.058	0.806	Yes	No	No	No
CVS1-2	NA	NA	NA	0.132	0.308	0.128	No	No	No	No
CVS1-3	NA	NA	NA	1.728	1.582	1.160	No	No	No	No
CVS1-4	NA	NA	NA	41.278	33.870	34.068	No	No	No	No
CVS1-5	NA	NA	NA	0.710	0.924	0.382	No	No	No	No
CVS1-6	NA	NA	NA	12.226	9.784	6.092	No	No	No	No
CVS1-7	NA	NA	NA	0.574	0.662	0.678	No	No	No	No
CVS1-8	NA	NA	NA	2.476	1.488	1.610	No	No	No	No
CVS1-9	NA	NA	NA	21.986	17.204	15.794	No	No	No	No
CVS1-10	NA	NA	NA	0.254	0.772	0.190	No	No	No	No
CVS1-11	NA	NA	NA	0.198	0.374	0.198	No	No	No	No
CVS1-12	NA	NA	NA	9.324	8.342	8.790	No	No	No	No
CVS1-13	NA	NA	NA	28.144	25.806	24.826	No	No	No	No
CVS1-14	NA	NA	NA	19.694	16.022	11.580	No	No	No	No
CVS1-15	NA	NA	NA	37.556	22.396	27.990	No	No	No	No
CVS1-16	NA	NA	NA	1.046	0.532	1.080	No	No	No	No
CVS1-17	NA	NA	NA	4.470	4.150	4.608	No	No	No	No
CVS1-18	NA	NA	NA	22.476	16.130	16.080	No	No	No	No
CVS1-19	NA	NA	NA	1.046	1.066	0.866	Yes	No	No	No
CVS1-20	NA	NA	NA	0.910	0.936	0.792	Yes	No	No	No
CVS1-21	NA	NA	NA	37.700	31.182	31.072	No	No	No	No
CVS1-22	NA	NA	NA	2.238	1.408	1.520	No	No	No	No
CVS1-23	NA	NA	NA	1.050	1.070	0.974	Yes	No	No	No
CVS2-1	NA	NA	NA	0.624	0.738	0.416	Yes	No	No	No
CVS2-2	NA	NA	NA	0.256	0.552	0.376	No	No	No	No
CVS2-3	NA	NA	NA	0.274	0.444	0.250	No	No	No	No
CVS2-4	NA	NA	NA	0.316	0.600	0.364	No	No	No	No
CVS2-5	NA	NA	NA	0.568	0.764	0.568	No	No	No	No
CVS2-6	NA	NA	NA	2.370	2.606	2.568	No	No	No	No
CVS2-7	NA	NA	NA	1.480	1.624	0.686	No	No	No	No
CVS2-8	NA	NA	NA	0.968	1.046	0.890	Yes	No	No	No

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses (cont.).

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
CVS2-9	NA	NA	NA	1.120	1.240	0.748	No	No	No	No
CVS2-10	NA	NA	NA	2.664	2.644	1.656	No	No	No	No
CVS2-11	NA	NA	NA	3.174	3.128	2.740	No	No	No	No
CVS2-12	NA	NA	NA	0.388	0.524	0.368	No	No	No	No
CVS2-13	NA	NA	NA	0.720	0.724	0.956	No	No	No	No
CVS2-14	NA	NA	NA	3.312	2.936	2.536	Yes	No	No	No
CVS2-15	NA	NA	NA	0.662	0.902	1.216	No	No	No	No
CVS2-16	NA	NA	NA	5.874	4.698	4.364	No	No	No	No
CVS2-17	NA	NA	NA	0.990	1.142	0.948	Yes	No	No	No
CVS2-18	NA	NA	NA	5.156	4.188	3.772	No	No	No	No
CVS2-19	NA	NA	NA	3.980	3.308	2.962	No	No	No	No
CVS2-20	NA	NA	NA	0.694	0.772	0.558	No	No	No	No
CVS2-21	NA	NA	NA	7.708	5.068	4.178	No	No	No	No
CVS2-22	NA	NA	NA	19.292	10.906	12.194	No	No	No	No
CVS2-23	NA	NA	NA	0.346	1.208	1.618	No	No	No	No
CVS2-24	NA	NA	NA	9.044	6.452	4.120	No	No	No	No
CVS2-25	NA	NA	NA	9.324	5.530	7.052	No	No	No	No
CVS2-26	NA	NA	NA	3.256	2.872	2.698	No	No	No	No
CVS2-27	NA	NA	NA	6.540	3.670	4.684	No	No	No	No
CVS2-28	NA	NA	NA	10.288	7.364	7.076	No	No	No	No
CVS2-29	NA	NA	NA	2.572	2.710	2.546	No	No	No	No
CVS2-30	NA	NA	NA	13.024	8.388	5.104	No	No	No	No
CVS2-31	NA	NA	NA	0.822	0.920	0.636	No	No	No	No
CVS2-32	NA	NA	NA	19.292	11.054	11.792	No	No	No	No
CVS2-33	NA	NA	NA	3.446	2.876	3.216	No	No	No	No
CVS2-34	NA	NA	NA	8.680	6.936	5.400	No	No	No	No
CVS2-35	NA	NA	NA	0.640	1.160	1.820	No	No	No	No
CVS2-36	NA	NA	NA	0.960	1.260	1.308	No	No	No	No
CVS2-37	NA	NA	NA	0.492	0.600	0.354	No	No	No	No
CVS2-38	NA	NA	NA	2.238	1.452	1.614	No	No	No	No
CVS2-39	NA	NA	NA	25.402	13.056	15.336	No	No	No	No
CVS2-40	NA	NA	NA	0.674	0.656	0.798	No	No	No	No
CVS2-41	NA	NA	NA	0.354	0.520	0.376	No	No	No	No
CVS2-42	NA	NA	NA	3.388	2.440	2.674	No	No	No	No
CVS2-43	NA	NA	NA	1.534	1.394	0.902	No	No	No	No
CVS2-44	NA	NA	NA	0.510	0.588	0.388	No	No	No	No
CVS2-45	NA	NA	NA	1.000	0.956	0.748	Yes	No	No	No
CVS2-46	NA	NA	NA	0.634	0.692	0.376	No	No	No	No
CVS2-47	NA	NA	NA	2.318	2.248	2.110	Yes	No	No	No
CVS2-48	NA	NA	NA	0.614	0.636	0.568	No	No	No	No
CVS2-49	NA	NA	NA	0.606	0.668	0.434	Yes	No	No	No
CVS2-50	NA	NA	NA	0.884	0.852	0.736	Yes	No	No	No
CVS2-51	NA	NA	NA	3.528	2.992	2.566	No	No	No	No
CVS2-52	NA	NA	NA	1.114	1.108	0.520	No	No	No	No
CVS2-53	NA	NA	NA	0.608	0.610	0.404	Yes	No	No	No
CVS2-54	NA	NA	NA	5.522	3.430	3.224	No	No	No	No
CVS2-55	NA	NA	NA	2.684	2.254	1.760	No	No	No	No
CVS2-56	NA	NA	NA	2.838	2.436	1.892	No	No	No	No
CVS2-57	NA	NA	NA	2.328	2.162	1.684	No	No	No	No
CVS2-58	NA	NA	NA	1.556	1.272	1.240	No	No	No	No
CVS2-59	NA	NA	NA	3.182	2.574	2.444	No	No	No	No
CVS2-60	NA	NA	NA	3.248	2.316	3.046	No	No	No	No
CVS2-61	NA	NA	NA	0.444	0.560	0.460	No	No	No	No

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses (cont.).

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
CVS2-62	NA	NA	NA	2.004	1.724	1.856	No	No	No	No
CVS2-63	NA	NA	NA	0.664	0.444	0.780	No	No	No	No
CVS2-64	NA	NA	NA	0.758	0.752	0.684	No	No	No	No
CVS2-65	NA	NA	NA	0.670	0.710	0.400	No	No	No	No
CVS2-66	NA	NA	NA	0.420	0.494	0.446	No	No	No	No
CVS2-67	NA	NA	NA	1.024	0.960	0.428	No	No	No	No
CVS2-68	NA	NA	NA	0.616	0.680	0.254	No	No	No	No
CVS2-69	NA	NA	NA	0.452	0.604	0.224	No	No	No	No
CVS2-70	NA	NA	NA	0.624	0.762	0.256	No	No	No	No
CVS2-71	NA	NA	NA	0.822	0.854	0.700	No	No	No	No
CVS2-72	NA	NA	NA	0.420	0.452	0.456	No	No	No	No
CVS2-73	NA	NA	NA	0.488	0.602	0.148	No	No	No	No
CVS2-74	NA	NA	NA	0.452	0.558	0.294	No	No	No	No
CVS2-75	NA	NA	NA	0.556	0.668	0.200	No	No	No	No
CVS2-76	NA	NA	NA	29.742	15.142	25.082	No	No	No	No
CVS2-77	NA	NA	NA	19.024	12.442	13.104	No	No	No	No
CVS2-78	NA	NA	NA	1.868	1.396	1.186	No	No	No	No
CVS2-79	NA	NA	NA	1.488	1.368	1.320	No	No	No	No
CVS2-80	NA	NA	NA	1.528	1.344	1.200	No	No	No	No
CVS2-81	NA	NA	NA	33.226	16.128	25.648	No	No	No	No
CVS2-82	NA	NA	NA	88.000	39.938	70.754	No	No	No	No
CVS2-83	NA	NA	NA	69.312	38.456	55.780	No	No	No	No
CVS2-84	NA	NA	NA	24.920	13.364	16.472	No	No	No	No
CVS2-85	NA	NA	NA	0.912	0.844	1.498	No	No	No	No
CVS2-86	NA	NA	NA	0.230	0.182	0.508	No	No	No	No
CVS2-87	NA	NA	NA	0.356	0.262	0.572	No	No	No	No
CVS2-88	NA	NA	NA	0.616	0.752	0.946	No	No	No	No
CVS2-89	NA	NA	NA	3.432	2.472	2.696	No	No	No	No
CVS2-90	NA	NA	NA	11.154	7.528	6.962	No	No	No	No
CVS2-91	NA	NA	NA	17.284	13.548	13.476	No	No	No	No
CVS2-92	NA	NA	NA	37.180	24.884	23.584	No	No	No	No
CVS2-93	NA	NA	NA	26.454	15.514	20.020	No	No	No	No
CVS2-94	NA	NA	NA	8.140	6.132	6.700	No	No	No	No
CVS2-95	NA	NA	NA	19.952	8.542	14.518	No	No	No	No
CVS2-96	NA	NA	NA	0.986	0.858	0.820	Yes	No	No	No
CVS2-97	NA	NA	NA	2.868	2.104	2.268	No	No	No	No
CVS2-98	NA	NA	NA	9.040	6.994	5.592	No	No	No	No
CVS2-99	NA	NA	NA	0.464	0.492	0.398	Yes	No	No	No
CVS2-100	NA	NA	NA	0.652	0.686	0.452	No	No	No	No
CVS2-101	NA	NA	NA	17.288	7.662	13.172	No	No	No	No
CVS2-102	NA	NA	NA	5.344	3.842	3.354	No	No	No	No
CVS2-103	NA	NA	NA	12.146	8.132	8.164	Yes	No	No	No
CVS2-104	NA	NA	NA	11.096	7.266	7.336	Yes	No	No	No
CVS2-105	NA	NA	NA	9.180	6.264	5.948	Yes	No	No	No
CVS2-106	NA	NA	NA	3.302	2.696	2.330	No	No	No	No
CVS2-107	NA	NA	NA	1.576	1.324	1.240	No	No	No	No
CVS2-108	NA	NA	NA	4.288	3.292	2.774	No	No	No	No
CVS2-109	NA	NA	NA	11.414	8.988	7.168	No	No	No	No
CVS2-110	NA	NA	NA	0.628	0.804	0.236	No	No	No	No
CVS2-111	NA	NA	NA	12.270	7.788	8.086	Yes	No	No	No
CVS2-112	NA	NA	NA	28.800	15.588	19.206	No	No	No	No
CVS2-113	NA	NA	NA	1.224	1.260	1.020	No	No	No	No
CVS2-114	NA	NA	NA	14.232	9.856	9.198	Yes	No	No	No

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses (cont.).

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
CVS2-115	NA	NA	NA	18.812	11.674	11.530	No	No	No	No
CVS2-116	NA	NA	NA	6.024	4.406	4.060	Yes	No	No	No
CVS2-117	NA	NA	NA	3.180	2.674	2.198	No	No	No	No
CVS2-118	NA	NA	NA	7.260	5.218	4.788	Yes	No	No	No
CVS2-119	NA	NA	NA	7.606	5.376	5.148	No	No	No	No
CVS2-120	NA	NA	NA	0.582	0.648	0.462	Yes	No	No	No
CVS2-121	NA	NA	NA	0.398	0.622	0.274	No	No	No	No
CVS2-122	NA	NA	NA	0.386	0.726	0.178	No	No	No	No
CVS2-123	NA	NA	NA	2.946	2.250	2.150	No	No	No	No
HG-1-1-7	NA	NA	NA	0.680	0.660	0.670	Yes	No	No	No
HG-1-2-7	NA	NA	NA	0.730	0.670	0.690	No	No	No	No
HG-1-3-7	NA	NA	NA	0.680	0.620	0.650	No	No	No	No
HG-2-1-7	NA	NA	NA	0.690	0.640	0.670	No	No	No	No
HG-2-2-7	NA	NA	NA	0.770	0.730	0.800	Yes	No	No	No
HG-2-3-7	NA	NA	NA	0.790	0.720	0.790	Yes	No	No	No
HG-3-1-7	NA	NA	NA	0.750	0.720	0.770	Yes	No	No	No
HG-3-2-7	NA	NA	NA	0.780	0.730	0.770	Yes	No	Yes	No
HG-3-3-7	NA	NA	NA	0.730	0.680	0.740	Yes	No	Yes	No
AH-165 Al-7	NA	NA	NA	0.520	0.630	0.360	No	No	No	No
AH-165 AV-7	NA	NA	NA	0.640	0.660	0.530	No	No	No	No
AH-165 FE-7	NA	NA	NA	4.760	3.930	4.180	No	No	No	No
AH-131 Al-7	NA	NA	NA	0.720	0.700	0.690	No	No	No	No
AH-131 AV-7	NA	NA	NA	0.680	0.730	0.610	No	No	No	No
AH-131 FE-7	NA	NA	NA	3.580	3.200	3.090	No	No	No	No
AH-168 Al-7	NA	NA	NA	10.250	8.640	6.700	No	No	No	No
AH-168 AV-7	NA	NA	NA	0.800	0.750	0.590	No	No	No	No
AH-168 FE-7	NA	NA	NA	5.130	4.420	3.900	No	No	No	No
AH-200 Al-7	NA	NA	NA	0.460	0.570	0.440	No	No	No	No
AH-200 AV-7	NA	NA	NA	0.580	0.620	0.590	No	No	No	No
AH-200 FE-7	NA	NA	NA	5.100	4.380	4.380	No	No	No	No
AH-202 Al-7	NA	NA	NA	0.350	0.480	0.290	No	No	No	No
AH-202-AV-7	NA	NA	NA	0.520	0.590	0.510	No	No	No	No
AH-202 FE-7	NA	NA	NA	3.160	2.550	2.710	No	No	No	No
AH-1-7	NA	NA	NA	0.580	0.710	0.730	No	No	No	No
AH-2-7	NA	NA	NA	0.950	0.950	0.870	No	No	No	No
AH-4-7	NA	NA	NA	0.530	0.610	0.630	No	No	No	No
AH-5-7	NA	NA	NA	0.420	0.520	0.490	No	No	No	No
AH-6-7	NA	NA	NA	0.690	0.730	0.700	No	No	No	No
AH-7-7	NA	NA	NA	0.440	0.490	0.450	No	No	No	No
AH-8-7	NA	NA	NA	0.500	0.550	0.490	No	No	No	No
AH-9-7	NA	NA	NA	0.440	0.510	0.460	No	No	No	No
AH-10-7	NA	NA	NA	0.430	0.520	0.430	No	No	No	No
AH-11-7	NA	NA	NA	0.470	0.570	0.450	No	No	No	No
AH-12-7	NA	NA	NA	0.850	0.610	0.730	No	No	No	No
AH-13-7	NA	NA	NA	0.430	0.520	0.470	No	No	No	No
AH-14-7	NA	NA	NA	0.520	0.580	0.610	No	No	No	No
AH-15-7	NA	NA	NA	0.430	0.480	0.450	No	No	No	No
AH-16-7	NA	NA	NA	0.420	0.480	0.440	No	No	No	No
AH-17-7	NA	NA	NA	0.360	0.450	0.370	No	No	No	No
SFRIT1	NA	NA	NA	0.750	0.690	0.710	No	No	No	No
SFRIT2	NA	NA	NA	0.730	0.700	0.700	No	No	No	No
SFRIT3	NA	NA	NA	0.760	0.820	0.870	No	No	No	No
202P w/o Mn-7	NA	NA	NA	0.640	0.510	0.740	Yes	No	No	No

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses (cont.).

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
202G w/o Mn-7	NA	NA	NA	0.390	0.390	0.520	No	No	No	No
200R-7	NA	NA	NA	1.150	0.970	1.010	No	No	No	No
NBS SRM 623-7	NA	NA	NA	0.110	0.010	0.150	No	No	No	No
165 CGW STD-7	NA	NA	NA	0.840	0.730	0.820	No	No	No	No
ARM-1-7 (4/88)	NA	NA	NA	0.580	0.750	0.690	No	No	No	No
ARM-1-7 (5/89)	NA	NA	NA	0.590	0.560	0.470	No	No	No	No
ARM-1-7 (7/90)	NA	NA	NA	0.480	0.570	0.510	No	No	No	No
ARM-1-7 (12/90)	NA	NA	NA	0.500	0.590	0.520	No	No	No	No
ARM-1-7 (5/91)	NA	NA	NA	0.540	0.630	0.540	No	No	No	No
ARM-1-7 (10/91)	NA	NA	NA	0.510	0.600	0.540	No	No	No	No
ARM-1-7 (10/92)	NA	NA	NA	0.440	0.500	0.450	No	No	No	No
ARM-1-7 (4/93)	NA	NA	NA	0.480	0.580	0.500	No	No	No	No
ARM-1-7 (6/93)	NA	NA	NA	0.470	0.520	0.480	No	No	No	No
ARM-1-7 (8/93)	NA	NA	NA	0.410	0.470	0.430	No	No	No	No
ARM-1-7	NA	NA	NA	0.510	0.600	0.510	No	No	No	No
T-ARM-1	NA	NA	NA	0.490	0.600	0.530	No	No	No	No
SS-ARM-1(2)	NA	NA	NA	0.530	0.630	0.550	No	No	No	No
SS-ARM-1	NA	NA	NA	0.540	0.640	0.560	No	No	No	No
EA-1-7(2)	NA	NA	NA	14.000	7.850	11.520	No	No	No	No
EA-1-7	NA	NA	NA	16.790	10.690	14.490	No	No	No	No
EA-2-7	NA	NA	NA	15.210	9.430	12.780	No	No	No	No
EA-7	NA	NA	NA	17.720	9.890	13.890	No	No	No	No
T-EA	NA	NA	NA	14.750	8.520	11.820	No	No	No	No
SS-EA-19	NA	NA	NA	16.410	9.120	13.090	No	No	No	No
SS-EA-15	NA	NA	NA	16.790	9.740	13.600	No	No	No	No
SS-EA-1-7	NA	NA	NA	18.500	10.280	14.330	No	No	No	No
SS-EA-2-7	NA	NA	NA	17.760	9.770	13.720	No	No	No	No
SRS-SEA-A-7	NA	NA	NA	16.450	9.340	12.850	No	No	No	No
SRS-SEA-B-7	NA	NA	NA	16.990	9.120	13.510	No	No	No	No
CUASEA-A-7	NA	NA	NA	16.850	9.670	12.950	No	No	No	No
CUASEA-B-7	NA	NA	NA	16.460	9.210	13.420	No	No	No	No
131-TDS-EA-7	NA	NA	NA	4.430	3.850	4.280	No	No	No	No
131-TDS-3A-SOPER-7	NA	NA	NA	2.810	2.450	2.300	No	No	No	No
BLEND 1-7	NA	NA	NA	0.720	0.810	0.780	Yes	No	No	No
BLEND 1-7 (2)	NA	NA	NA	0.780	0.800	0.790	Yes	No	No	No
BLEND 1.6-7	NA	NA	NA	0.720	0.760	0.750	Yes	No	No	No
BATCH 1-7	NA	NA	NA	0.730	0.810	0.800	Yes	No	No	No
BATCH 1-7 (2)	NA	NA	NA	0.730	0.760	0.750	Yes	No	No	No
BATCH 1-1.6	NA	NA	NA	0.710	0.760	0.740	Yes	No	No	No
BATCH 2-7	NA	NA	NA	0.660	0.770	0.730	Yes	No	No	No
BATCH 2-7 (2)	NA	NA	NA	0.670	0.720	0.690	Yes	No	No	No
BATCH 2-1.6	NA	NA	NA	0.640	0.710	0.670	Yes	No	No	No
BATCH 3-7	NA	NA	NA	0.860	0.900	0.890	Yes	No	No	No
BATCH 3-7 (2)	NA	NA	NA	0.890	0.850	0.850	Yes	No	No	No
BATCH 3-7 (3)	NA	NA	NA	0.850	0.850	0.830	Yes	No	No	No
BATCH 4-7	NA	NA	NA	0.970	1.000	1.000	Yes	No	No	No
BATCH 4-7 (2)	NA	NA	NA	0.900	0.890	0.870	Yes	No	No	No
BATCH 4-7 (3)	NA	NA	NA	0.940	0.940	0.940	Yes	No	No	No
HM-1-7	NA	NA	NA	0.460	0.620	0.490	No	No	No	No
HM-1-7 (2)	NA	NA	NA	0.460	0.570	0.460	No	No	No	No
HM-1.6-7	NA	NA	NA	0.430	0.560	0.440	No	No	No	No
PUREX 1-7	NA	NA	NA	2.190	1.860	2.090	No	No	No	No
PUREX 1-7 (2)	NA	NA	NA	1.970	1.650	1.760	No	No	No	No

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses (cont.).

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
PUREX 1.6-7	NA	NA	NA	4.460	3.250	4.260	No	No	No	No
PUREX SRSS 1.6	NA	NA	NA	2.380	2.040	2.080	No	No	No	No
PUREX SRST-4.0	NA	NA	NA	2.260	1.960	1.990	No	No	No	No
PUREX CUA	NA	NA	NA	2.850	2.370	2.420	No	No	No	No
BLEND 1-3457	NA	NA	NA	0.600	0.670	0.650	Yes	No	No	No
BLEND 1-3479	NA	NA	NA	0.580	0.640	0.630	Yes	No	No	No
BLEND 1-3498	NA	NA	NA	0.630	0.700	0.670	Yes	No	No	No
BLEND 1-3510	NA	NA	NA	0.680	0.740	0.730	Yes	No	No	No
BLEND 1-3526	NA	NA	NA	0.670	0.740	0.720	Yes	No	No	No
BLEND 2-3611	NA	NA	NA	0.610	0.670	0.670	Yes	No	No	No
BLEND 2-3622	NA	NA	NA	0.610	0.660	0.660	Yes	No	No	No
BLEND 2-3635	NA	NA	NA	0.610	0.650	0.660	Yes	No	No	No
BLEND 2-3654	NA	NA	NA	0.600	0.650	0.640	Yes	No	No	No
BLEND 2-3666	NA	NA	NA	0.600	0.650	0.640	Yes	No	No	No
BLEND 2-3676	NA	NA	NA	0.590	0.640	0.630	Yes	No	No	No
BLEND 3-3768	NA	NA	NA	0.600	0.640	0.660	Yes	No	No	No
BLEND 3-3789	NA	NA	NA	0.630	0.660	0.700	Yes	No	No	No
BLEND 3-3793	NA	NA	NA	0.630	0.660	0.710	Yes	No	No	No
BLEND 3-3802B	NA	NA	NA	0.700	0.710	0.770	Yes	No	Yes	No
HM 1-3824	NA	NA	NA	0.590	0.630	0.620	No	No	No	No
HM 1-3829	NA	NA	NA	0.570	0.630	0.610	No	No	No	No
HM 1-3851	NA	NA	NA	0.520	0.600	0.550	No	No	No	No
HM 1-3855	NA	NA	NA	0.530	0.600	0.550	No	No	No	No
HM-2-1 (3979C)	NA	NA	NA	0.530	0.610	0.540	Yes	No	No	No
HM-2-2 (4099A)	NA	NA	NA	0.550	0.630	0.560	Yes	No	No	No
HM-2-3 (4120B)	NA	NA	NA	0.530	0.620	0.540	Yes	No	No	No
HM-3-1 (4176)	NA	NA	NA	0.560	0.650	0.530	Yes	No	No	No
HM-3-2 (4225)	NA	NA	NA	0.550	0.640	0.520	Yes	No	No	No
HM-3-3 (4357)	NA	NA	NA	0.510	0.590	0.530	No	No	No	No
HM-4-1 (5260)	NA	NA	NA	0.750	0.760	0.640	No	No	No	No
HM-4-2 (5641)	NA	NA	NA	0.530	0.570	0.520	No	No	No	No
HM-4-3 (5748)	NA	NA	NA	0.700	0.710	0.650	No	No	No	No
PX 1-1 (4643)	NA	NA	NA	0.720	0.780	0.730	No	No	No	No
PX 1-2 (4726)	NA	NA	NA	0.710	0.760	0.720	No	No	No	No
PX 1-3 (4776)	NA	NA	NA	0.790	0.830	0.770	No	No	No	No
PX 2-1 (4455)	NA	NA	NA	0.480	0.570	0.480	Yes	No	No	No
PX 2-2 (4509)	NA	NA	NA	0.580	0.650	0.610	No	No	No	No
PX 2-3 (4566)	NA	NA	NA	0.730	0.780	0.730	No	No	No	No
PX 3-1 (5780)	NA	NA	NA	0.840	0.820	0.670	No	No	No	No
PX 3-2 (5818)	NA	NA	NA	1.080	1.010	0.850	No	No	No	No
PX 3-3 (5880)	NA	NA	NA	1.350	1.210	1.040	No	No	No	No
PX 4-1 (6390)	NA	NA	NA	2.270	1.970	1.840	No	No	No	No
PX 4-2 (6434)	NA	NA	NA	4.540	3.630	3.600	No	No	No	No
PX 4-3 (6458)	NA	NA	NA	4.370	3.490	3.650	No	No	No	No
PX 5-1 (6787)	NA	NA	NA	1.070	1.050	1.060	No	No	No	No
PX 5-2 (6795)	NA	NA	NA	9.160	6.190	8.170	No	No	No	No
PX 5-3 (6812)	NA	NA	NA	19.200	10.610	16.470	No	No	No	No
PX 5-4 (6820)	NA	NA	NA	21.000	11.290	17.880	No	No	No	No
PX 5-5 (6839)	NA	NA	NA	21.030	11.400	16.970	No	No	No	No
PX 5-6 (6862)	NA	NA	NA	18.970	10.810	15.120	No	No	No	No
PX 5-7 (6871)	NA	NA	NA	18.580	10.420	14.430	Yes	No	No	No
PX 5-8 (6884)	NA	NA	NA	21.580	11.800	17.150	No	No	No	No
PX 5-9 (6960)	NA	NA	NA	17.140	9.580	13.700	No	No	No	No

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses (cont.).

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
PX 5-10 (6972)	NA	NA	NA	21.900	9.490	17.370	No	No	No	No
PX 6-1 (7340)	NA	NA	NA	15.120	9.610	16.830	No	No	No	No
BATCH 1 STUDY-6-7	NA	NA	NA	17.190	13.620	15.450	No	No	No	No
BATCH 1 STUDY-10B-7	NA	NA	NA	10.530	8.990	9.530	No	No	No	No
BATCH 1 STUDY-15-7	NA	NA	NA	1.660	1.520	1.420	No	No	No	No
H-GLAS-0112	NA	NA	NA	0.880	0.830	0.750	No	No	No	No
H-GLAS-0130	NA	NA	NA	1.160	1.030	0.920	No	No	No	No
H-GLAS-0162	NA	NA	NA	2.010	1.670	1.380	No	No	No	No
H-GLAS-0244	NA	NA	NA	2.950	2.170	1.380	Yes	No	No	No
H-GLAS-0254	NA	NA	NA	2.100	1.820	1.430	No	No	No	No
H-GLAS-0278	NA	NA	NA	2.500	2.120	1.540	No	No	No	No
H-GLAS-0293	NA	NA	NA	3.080	2.580	1.850	No	No	No	No
H-GLAS-0308	NA	NA	NA	2.020	1.730	1.320	No	No	No	No
H-GLAS-0334	NA	NA	NA	2.410	2.150	1.550	No	No	No	No
H-GLAS-0352	NA	NA	NA	2.660	2.360	1.670	No	No	No	No
H-GLAS-0387	NA	NA	NA	2.580	2.310	1.570	No	No	No	No
H-GLAS-0421	NA	NA	NA	2.280	2.080	1.370	No	No	No	No
H-GLAS-0466	NA	NA	NA	2.790	2.410	1.660	No	No	No	No
FRIT-202-CLEAR	NA	NA	NA	31.960	28.890	30.380	No	No	No	No
FRIT-202-INT	NA	NA	NA	43.900	37.270	39.080	No	No	No	No
FRIT-202-WHITE	NA	NA	NA	63.070	58.260	57.440	No	No	No	No
FRIT-165-7	NA	NA	NA	80.320	84.310	74.160	No	No	No	No
FRIT-131-7	NA	NA	NA	50.300	48.600	43.130	No	No	No	No
MG 9-7	NA	NA	NA	70.240	NA	56.420	No	No	No	No
MG 18-7	NA	NA	NA	57.820	NA	47.770	No	No	No	No
MG 25-7	NA	NA	NA	0.830	NA	0.790	No	No	No	No
MG 28-7	NA	NA	NA	0.630	NA	0.720	No	No	No	No
PNL 1	NA	NA	NA	1.088	1.008	0.656	No	No	No	No
PNL 2	NA	NA	NA	8.088	5.404	4.852	No	No	No	No
PNL 3	NA	NA	NA	6.532	4.530	3.794	No	No	No	No
PNL 4	NA	NA	NA	0.478	0.500	0.380	No	No	No	No
PNL 5	NA	NA	NA	2.534	1.762	1.316	No	No	No	No
PNL 6	NA	NA	NA	0.538	0.532	0.450	Yes	No	Yes	No
PNL 7	NA	NA	NA	0.372	0.400	0.290	Yes	No	No	No
PNL 8	NA	NA	NA	3.150	2.394	1.924	No	No	No	No
PNL 9	NA	NA	NA	0.862	0.770	0.754	No	No	No	No
PNL 10	NA	NA	NA	1.514	0.990	0.934	Yes	No	Yes	No
Alkali1	NA	NA	NA	0.502	0.434	0.560	Yes	No	No	No
Alkali2	NA	NA	NA	1.294	0.860	0.948	No	No	No	No
Alkali3	NA	NA	NA	0.908	0.632	0.710	Yes	No	Yes	No
Alkali4	NA	NA	NA	0.548	0.390	0.514	Yes	No	Yes	No
Alkali5	NA	NA	NA	1.272	0.842	0.954	No	No	No	No
Alkali6	NA	NA	NA	0.656	0.480	0.604	Yes	No	Yes	No
Alkali7	NA	NA	NA	1.778	1.134	1.172	Yes	No	Yes	No
Alkali8	NA	NA	NA	0.936	0.700	0.824	Yes	No	Yes	No
Alkali9	NA	NA	NA	0.568	0.416	0.542	Yes	No	No	No
Ref6Qtr2	NA	NA	NA	0.830	0.706	0.634	Yes	No	Yes	No
WVDG-1	NA	NA	NA	0.360	0.500	0.318	No	No	No	No
WVDG-2	NA	NA	NA	0.414	0.622	0.362	No	No	No	No
WVDG-3	NA	NA	NA	0.476	0.582	0.466	Yes	No	Yes	No
WVDG-4	NA	NA	NA	0.522	0.606	0.532	No	No	No	No
WVDG-5	NA	NA	NA	0.428	0.570	0.396	No	No	No	No
WVDG-6	NA	NA	NA	0.398	0.606	0.338	No	No	No	No

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses (cont.).

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
WVDG-7	NA	NA	NA	0.360	0.534	0.338	No	No	No	No
WVDG-8	NA	NA	NA	0.346	0.546	0.348	No	No	No	No
WVDG-11R	NA	NA	NA	0.410	0.492	0.408	No	No	No	No
WVDG-12R	NA	NA	NA	0.434	0.526	0.428	No	No	No	No
WVDG-13R	NA	NA	NA	0.474	0.558	0.486	No	No	No	No
WVDG-14R	NA	NA	NA	0.576	0.666	0.604	No	No	No	No
WVDG-15	NA	NA	NA	0.592	0.600	0.528	No	No	No	No
WVDG-16	NA	NA	NA	0.378	0.470	0.330	No	No	No	No
WVDG-17	NA	NA	NA	0.584	0.584	0.546	No	No	No	No
WVDG-18	NA	NA	NA	0.450	0.538	0.438	No	No	No	No
WVDG-19	NA	NA	NA	0.428	0.564	0.414	No	No	No	No
WVDG-20	NA	NA	NA	0.320	0.484	0.278	No	No	No	No
WVDG-21	NA	NA	NA	0.450	0.504	0.444	No	No	No	No
WVDG-22	NA	NA	NA	0.420	0.600	0.358	No	No	No	No
WVDG-23	NA	NA	NA	0.506	0.614	0.374	No	No	No	No
WVDG-24	NA	NA	NA	0.426	0.572	0.346	No	No	No	No
WVDG-25	NA	NA	NA	0.376	0.506	0.328	No	No	No	No
WVDG-26	NA	NA	NA	0.370	0.514	0.312	No	No	No	No
WVDG-27	NA	NA	NA	0.618	0.654	0.486	No	No	No	No
WVDG-28	NA	NA	NA	0.402	0.578	0.338	No	No	No	No
WVDG-29	NA	NA	NA	0.434	0.036	0.428	No	No	No	No
WVDG-30	NA	NA	NA	0.418	0.014	0.392	No	No	No	No
WVDG-33	NA	NA	NA	0.494	0.526	0.490	Yes	No	Yes	No
WVDG-34	NA	NA	NA	0.834	0.776	0.726	Yes	No	Yes	No
WVDG-35	NA	NA	NA	0.800	0.788	0.798	No	No	No	No
WVDG-36	NA	NA	NA	0.488	0.502	0.328	No	No	No	No
WVDG-37	NA	NA	NA	0.462	0.534	0.534	No	No	No	No
WVDG-38	NA	NA	NA	0.394	0.480	0.394	No	No	No	No
WVDG-39	NA	NA	NA	0.542	0.498	0.494	No	No	No	No
WVDG-40	NA	NA	NA	0.610	0.610	0.578	No	No	No	No
WVDG-41	NA	NA	NA	0.628	0.598	0.738	Yes	No	No	No
WVDG-42	NA	NA	NA	0.760	0.710	0.728	Yes	No	No	No
WVDG-43	NA	NA	NA	0.416	0.514	0.276	No	No	No	No
WVDG-44	NA	NA	NA	0.714	0.716	0.662	No	No	No	No
WVDG-45	NA	NA	NA	0.520	0.530	0.600	No	No	No	No
WVDG-46	NA	NA	NA	0.744	0.634	0.598	Yes	No	Yes	No
WVDG-47	NA	NA	NA	0.448	0.466	0.312	No	No	No	No
WVDG-48	NA	NA	NA	0.358	0.412	0.258	No	No	No	No
FY92-5	NA	NA	NA	1.388	1.168	1.058	No	No	No	No
FY92-6	NA	NA	NA	0.556	0.714	0.534	Yes	No	Yes	No
FY92-7	NA	NA	NA	0.422	0.528	0.416	No	No	No	No
FY92-9	NA	NA	NA	0.524	0.590	0.392	No	No	No	No
FY92-10	NA	NA	NA	1.644	1.422	1.138	No	No	No	No
FY92Ref5	NA	NA	NA	0.392	0.550	0.512	Yes	No	Yes	No
Ratio2	NA	NA	NA	3.092	2.258	1.818	No	No	No	No
Ratio4	NA	NA	NA	0.522	0.580	0.510	Yes	No	No	No
Ratio5	NA	NA	NA	0.488	0.610	0.594	No	No	No	No
LoTh2	NA	NA	NA	0.786	0.566	0.458	Yes	No	Yes	No
LoTh4	NA	NA	NA	1.288	1.154	0.974	Yes	No	Yes	No
LoTh5	NA	NA	NA	0.484	0.866	0.770	No	No	No	No
HiFe2	NA	NA	NA	1.176	1.110	0.996	No	No	No	No
HiFe3	NA	NA	NA	0.836	0.846	0.764	No	No	No	No
HiFe4	NA	NA	NA	1.482	1.304	1.144	No	No	No	No

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses (cont.).

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
PNL190	NA	NA	NA	2.454	2.138	2.028	Yes	No	No	No
FY93-1	NA	NA	NA	1.088	0.656	1.008	No	No	No	No
FY93-2	NA	NA	NA	8.088	4.852	5.404	No	No	No	No
FY93-3	NA	NA	NA	6.532	3.794	4.530	No	No	No	No
FY93-4	NA	NA	NA	0.478	0.380	0.500	No	No	No	No
FY93-5	NA	NA	NA	2.534	1.316	1.762	No	No	No	No
FY93-6	NA	NA	NA	0.538	0.450	0.532	Yes	No	Yes	No
FY93-7	NA	NA	NA	0.372	0.290	0.400	Yes	No	No	No
FY93-8	NA	NA	NA	3.150	1.924	2.394	No	No	No	No
FY93-9	NA	NA	NA	0.862	0.754	0.770	No	No	No	No
FY93-10	NA	NA	NA	1.514	0.934	0.990	Yes	No	Yes	No
FY94-1	NA	NA	NA	0.372	0.506	0.416	Yes	No	No	No
FY94-2	NA	NA	NA	0.430	0.594	0.444	No	No	No	No
FY94-3	NA	NA	NA	8.114	7.118	5.106	No	No	No	No
FY94-4	NA	NA	NA	6.672	5.210	4.592	No	No	No	No
FY94-5	NA	NA	NA	0.906	1.064	0.990	Yes	No	Yes	No
FY94-6	NA	NA	NA	0.576	0.728	0.532	No	No	No	No
FY94-7	NA	NA	NA	2.094	1.898	1.386	No	No	No	No
FY94-8	NA	NA	NA	4.484	3.840	3.130	No	No	No	No
FY94-9	NA	NA	NA	0.870	0.894	0.736	Yes	No	Yes	No
FY94-10	NA	NA	NA	6.770	5.770	4.302	No	No	No	No
Sigma1	NA	NA	NA	13.218	10.624	9.840	No	No	No	No
Sigma2	NA	NA	NA	20.556	15.070	15.930	No	No	No	No
Sigma3	NA	NA	NA	15.484	8.142	10.858	No	No	No	No
Sigma4	NA	NA	NA	9.310	7.678	7.102	No	No	No	No
Sigma5	NA	NA	NA	10.536	8.524	7.860	No	No	No	No
Sigma6	NA	NA	NA	9.842	7.938	7.366	No	No	No	No
Sigma7	NA	NA	NA	8.858	7.090	6.652	No	No	No	No
Sigma8	NA	NA	NA	6.814	5.460	5.118	No	No	No	No
Sigma9	NA	NA	NA	7.084	5.666	4.970	No	No	No	No
Sigma10	NA	NA	NA	8.056	6.490	5.826	No	No	No	No
LAWA41	NA	NA	NA	0.940	NA	1.040	No	No	No	No
LAWA42	NA	NA	NA	1.560	NA	1.400	No	No	No	No
LAWA43	NA	NA	NA	0.760	NA	0.860	No	No	No	No
LAWA44	NA	NA	NA	0.740	NA	0.720	No	No	No	No
LAWA45	NA	NA	NA	1.540	NA	1.020	No	No	No	No
LAWA46	NA	NA	NA	0.860	NA	0.700	No	No	No	No
LAWA47	NA	NA	NA	0.760	NA	0.660	No	No	No	No
LAWA48	NA	NA	NA	0.780	NA	0.660	No	No	No	No
LAWA49	NA	NA	NA	0.620	NA	0.580	No	No	No	No
LAWA50	NA	NA	NA	0.620	NA	0.600	No	No	No	No
LAWA51	NA	NA	NA	0.700	NA	0.520	No	No	No	No
LAWA52	NA	NA	NA	0.860	NA	1.100	No	No	No	No
LAWA60	NA	NA	NA	0.580	NA	0.620	No	No	No	No
LAWA64	NA	NA	NA	0.760	NA	1.000	No	No	No	No
LAWA76	NA	NA	NA	1.420	NA	1.320	No	No	No	No
LAWA81	NA	NA	NA	0.780	NA	0.840	No	No	No	No
LAWA82	NA	NA	NA	0.680	NA	0.660	No	No	No	No
LAWA83	NA	NA	NA	0.620	NA	0.680	No	No	No	No
LAWA84	NA	NA	NA	0.600	NA	0.660	No	No	No	No
LAWA85	NA	NA	NA	0.680	NA	0.700	No	No	No	No
LAWA86	NA	NA	NA	0.780	NA	0.780	No	No	No	No
LAWA87	NA	NA	NA	1.200	NA	1.100	No	No	No	No

Table A.2. PCT Release Data and Validation Subset Indicators for IHLW Phase 1 Validation Glasses (cont.).

Glass	PCT-B (ppm)	PCT-Li (ppm)	PCT-Na (ppm)	PCT-B (g/L)	PCT-Li (g/L)	PCT-Na (g/L)	Included In V2a	Included In V2b	Included In V3a	Included In V3b
LAWA88	NA	NA	NA	0.860	NA	0.860	No	No	No	No
LAWA89	NA	NA	NA	1.160	NA	0.940	No	No	No	No
LAWA90	NA	NA	NA	0.980	NA	0.980	No	No	No	No
LAWA93	NA	NA	NA	1.060	NA	1.080	No	No	No	No
LAWA96	NA	NA	NA	0.620	NA	0.760	No	No	No	No
LAWA98S	NA	NA	NA	0.720	NA	0.560	No	No	No	No
LAWA99S	NA	NA	NA	1.480	NA	1.080	No	No	No	No
LAWA100S	NA	NA	NA	1.080	NA	0.760	No	No	No	No
LAWA101S	NA	NA	NA	0.860	NA	0.640	No	No	No	No
LAWA102S	NA	NA	NA	0.540	NA	0.440	No	No	No	No
LAWA104	NA	NA	NA	1.160	NA	1.060	No	No	No	No
LAWA105	NA	NA	NA	1.920	NA	1.580	No	No	No	No
LAWB30	NA	NA	NA	0.480	NA	0.480	No	No	No	No
LAWB31	NA	NA	NA	0.420	NA	0.220	No	No	No	No
LAWB32	NA	NA	NA	0.500	NA	0.280	No	No	No	No
LAWB33	NA	NA	NA	0.380	NA	0.240	No	No	No	No
LAWB34	NA	NA	NA	0.440	NA	0.260	No	No	No	No
LAWB35	NA	NA	NA	1.000	NA	0.680	No	No	No	No
LAWB37	NA	NA	NA	0.520	NA	0.360	No	No	No	No
LAWB38	NA	NA	NA	0.500	NA	0.360	No	No	No	No
LAWB39	NA	NA	NA	1.000	NA	0.800	No	No	No	No
LAWB40	NA	NA	NA	3.180	NA	2.340	No	No	No	No
LAWB41	NA	NA	NA	1.700	NA	1.400	No	No	No	No
LAWB45	NA	NA	NA	1.060	NA	0.880	No	No	No	No
LAWB51S	NA	NA	NA	0.960	NA	0.660	No	No	No	No
LAWB52S	NA	NA	NA	0.980	NA	0.680	No	No	No	No
LAWB53S	NA	NA	NA	0.840	NA	0.540	No	No	No	No
LAWC12 for AN107	NA	NA	NA	0.840	NA	0.818	No	No	No	No
LAWC13	NA	NA	NA	0.708	NA	0.740	No	No	No	No
LAWC14	NA	NA	NA	1.080	NA	7.218	No	No	No	No
LAWC15	NA	NA	NA	0.658	NA	0.670	No	No	No	No
LAWC16S	NA	NA	NA	1.168	NA	0.816	No	No	No	No
LAWC17S	NA	NA	NA	0.798	NA	0.588	No	No	No	No
LAWC18S	NA	NA	NA	0.826	NA	0.590	No	No	No	No
LAWC19S	NA	NA	NA	0.464	NA	0.450	No	No	No	No
LAWC20S	NA	NA	NA	0.488	NA	0.378	No	No	No	No
LAWC21S	NA	NA	NA	0.300	NA	0.344	No	No	No	No
LAWC22	NA	NA	NA	1.036	NA	0.938	No	No	No	No
LAWC23	NA	NA	NA	0.478	NA	0.546	No	No	No	No
LAWC24	NA	NA	NA	0.442	NA	0.564	No	No	No	No
LAWC25	NA	NA	NA	0.640	NA	0.770	No	No	No	No
LAWABP1	NA	NA	NA	0.580	NA	0.620	No	No	No	No
PNLREF (LD6-5412)	NA	NA	NA	0.200	NA	0.540	No	No	No	No
TFA-BASE (HLP-01)	NA	NA	NA	0.780	NA	0.660	No	No	No	No

APPENDIX B

Data from X-Ray Fluorescence (XRF) Analyses of IHLW Combined Matrix Test Glasses

Oxide	Analyzed XRF (wt%) of Initial Matrix Glasses					
	HLW02-01	**HLW02-02**	**HLW02-03**	**HLW02-04**	**HLW02-05**	**HLW02-06**
Ag_2O	0.13	0.25	0.23	0.03	0.02	0.03
Al_2O_3	5.99	4.13	4.36	4.17	3.99	7.97
As_2O_3	0.11	0.19	0.20	0.01	0.02	0.02
B_2O_3*	9.93	14.00	14.00	5.00	5.00	5.00
BaO	0.23	0.39	0.36	0.05	0.05	0.04
Bi_2O_3	0.01	0.01	0.01	0.01	0.01	0.01
CaO	0.52	0.50	0.54	0.52	0.55	0.54
CdO	0.99	1.86	1.84	2.06	0.06	2.01
CeO_2	0.05	0.05	0.03	0.05	0.03	0.04
Cl	0.13	0.15	0.11	0.14	0.15	0.11
Co_3O_4*	0.02	0.02	0.02	0.02	0.02	0.02
Cr_2O_3	0.12	0.21	0.22	0.02	0.22	0.02
Cs_2O	0.01	0.02	0.01	0.02	0.02	0.02
CuO	0.08	0.12	0.12	0.01	0.02	0.01
F	NA	NA	NA	NA	NA	NA
Er_2O_3	0.01	0.02	-	0.01	-	0.01
Eu_2O_3	-	-	-	-	-	-
Fe_2O_3	11.41	14.18	8.23	14.72	9.29	8.66
Gd_2O_3	-	-	-	-	-	-
GeO_2			0.00	-	-	
HfO_2	0.05	-	0.13	-	0.12	0.13
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.07	0.06	0.08	0.04	0.10	0.05
La_2O_3	0.29	0.29	0.30	0.33	0.28	0.30
Li_2O*	4.00	6.00	2.00	2.00	6.00	4.74
MgO	0.08	0.12	-	-	0.15	-
MnO	2.63	0.01	-	0.59	0.01	5.69
MoO_3	-	-	-		0.01	
Na_2O	11.18	4.44	15.01	15.30	13.57	14.55
Nd_2O_3	-	-	-	-	-	-
NiO	0.57		1.05	0.11	0.16	1.13
OsO_4	-	-	-	-	-	-
P_2O_5	0.43	0.43	0.42	0.42	0.43	0.43
PbO	0.21	0.36	0.37	0.04	0.04	0.04
PdO	0.11	0.10	0.05	0.11	0.10	0.09
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.05	0.05	0.04	0.05	0.05	0.05
RuO_4*	0.08	0.08	0.05	0.09	0.07	0.07
Sb_2O_3	0.14	0.24	0.03	0.27	0.01	0.03
SeO_2	0.12	0.02	0.22	0.28	0.05	0.29
SiO_2	41.90	49.56	36.27	51.06	50.47	38.89
Sm_2O_3	-	-	-	0.02	-	-
SnO_2	-	-	-	-	-	-
SO_3	0.08	0.10	0.08	0.09	0.09	0.09
SrO	2.83	0.01	4.93	0.01		0.00
Tb_4O_7	-	0.01	-	0.02	0.01	0.01
TeO_2	-	-	-	-	-	-
ThO_2	-	-	-	-	-	-
TiO_2	0.06	0.04	0.08	0.06	0.06	0.05
Tl_2O_3	0.08	0.02	0.13	0.18	0.01	0.06
V_2O_5	0.05	0.11	0.11	0.01	-	0.01
Y_2O_3	-	-	-	-	0.01	0.01
ZnO	1.92	1.84	1.88	1.94	2.05	2.04
ZrO_2	3.32	0.01	6.46	-	6.65	6.74
TOTAL	99.98	100.00	99.96	99.85	99.98	100.00

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co and Ru are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Initial Matrix Glasses					
	HLW02-07	**HLW02-08**	**HLW02-09**	**HLW02-10**	**HLW02-11**	**HLW02-12**
Ag_2O	0.26	0.02	0.02	0.02	0.02	0.23
Al_2O_3	8.11	3.77	7.93	8.02	4.29	4.18
As_2O_3	0.20	0.02	0.01	0.02	-	0.22
B_2O_3*	5.00	14.00	11.59	14.00	14.00	5.00
BaO	0.44	0.05	-	-	0.04	0.40
Bi_2O_3	-	-	0.01	0.01	-	0.01
CaO	0.53	0.55	0.52	0.53	0.53	0.53
CdO	0.06	0.07	0.07	1.96	0.06	1.86
CeO_2	0.04	0.05	0.06	0.05	0.04	0.05
Cl	0.15	0.13	0.12	0.14	0.12	0.07
Co_3O_4*	0.02	0.02	0.02	0.02	0.02	0.02
Cr_2O_3	0.23	0.20	0.02	0.02	0.02	0.22
Cs_2O	0.02	0.01	-	0.01	0.01	0.01
CuO	0.12	0.02	0.02	0.02	0.01	0.12
F	NA	NA	NA	NA	NA	NA
Er_2O_3	-	0.01	0.01	0.01	-	0.02
Eu_2O_3	-	-	-	-	-	-
Fe_2O_3	8.57	10.26	14.13	8.52	8.31	11.79
Gd_2O_3	-	-	-	-	-	-
GeO_2	-	-	-	-	-	0.00
HfO_2	0.03	0.13	-	0.12	0.12	0.13
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.11	0.08	0.10	0.05	0.11	0.06
La_2O_3	0.31	0.28	0.32	0.33	0.31	0.32
Li_2O*	6.00	3.31	2.27	6.00	6.00	6.00
MgO	0.09	0.11	0.10	-	-	-
MnO	-	5.56	0.01	0.01	0.01	5.43
MoO_3	-	0.01	-	-	-	-
Na_2O	12.40	14.76	15.95	10.59	11.49	12.89
Nd_2O_3	-	-	-	-	-	-
NiO	0.11	0.16	1.03	0.11	1.09	1.05
OsO_4	-	-	-	-	-	0.01
P_2O_5	0.43	0.42	0.42	0.44	0.43	0.42
PbO	0.38	0.04	0.04	0.05	0.04	0.38
PdO	0.10	0.10	0.10	0.11	0.09	0.09
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.05	0.05	0.03	0.05	0.04	0.05
RuO_4*	0.09	0.06	0.05	0.08	0.06	0.04
Sb_2O_3	0.25	0.25	0.25	0.03	0.24	0.02
SeO_2	0.03	0.02	0.03	0.26	0.23	0.15
SiO_2	51.72	36.86	36.93	36.68	44.02	39.81
Sm_2O_3	0.01	0.01	0.02	0.01	0.01	0.01
SnO_2	-	-	-	-	-	-
SO_3	0.09	0.08	0.08	0.08	0.08	0.08
SrO	-	0.01	5.69	3.25	0.01	0.00
Tb_4O_7	-	0.01	0.01	0.01	0.01	0.02
TeO_2	-	0.01	0.01	0.01	0.01	-
ThO_2	-	0.01	-	-	-	-
TiO_2	0.06	0.05	0.05	0.07	0.07	0.07
Tl_2O_3	0.19	-	-	-	0.15	-
V_2O_5	0.11	-	0.01	0.01	0.01	0.11
Y_2O_3	0.00	0.01	-	0.01	0.01	0.01
ZnO	1.97	2.01	1.86	1.94	1.90	1.93
ZrO_2	1.66	6.41	0.02	6.33	5.99	6.19
TOTAL	99.93	99.99	99.92	99.94	99.98	99.95

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co and Ru are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Initial Matrix Glasses					
	HLW02-13	**HLW02-14**	**HLW02-15**	**HLW02-16**	**HLW02-17**	**HLW02-18**
Ag_2O	0.26	0.02	0.26	0.24	0.03	0.23
Al_2O_3	4.02	4.25	7.70	7.26	8.22	4.40
As_2O_3	0.19	-	0.20	0.22	0.03	0.22
B_2O_3*	5.00	5.00	14.00	5.00	5.00	5.00
BaO	0.43	-	0.41	0.41	0.06	0.39
Bi_2O_3	-	0.01	-	0.01	0.01	0.01
CaO	0.52	0.53	0.53	0.52	0.52	0.52
CdO	0.07	1.96	0.06	1.93	2.04	0.06
CeO_2	0.05	0.03	0.06	0.05	0.05	0.03
Cl	0.10	0.13	0.13	0.09	0.18	0.18
Co_3O_4*	0.02	0.01	0.02	0.02	0.02	0.01
Cr_2O_3	0.23	0.02	0.38	0.43	0.02	0.22
Cs_2O	0.01	0.01	0.02	0.01	0.03	0.01
CuO	0.12	0.02	0.13	0.12	0.01	0.12
F	NA	NA	NA	NA	NA	NA
Er_2O_3	0.01	0.01	0.01	-	0.01	-
Eu_2O_3	0.01	-	-	-	-	-
Fe_2O_3	14.71	8.44	14.73	9.07	13.74	11.24
Gd_2O_3	-	-	-	-	0.01	-
GeO_2	-	-	-	-	-	-
HfO_2	0.02	0.12	-	0.13	-	0.11
HgO	-	-	-	-	-	-
IrO_2	-	-	0.01	-	-	-
K_2O	0.10	0.07	0.09		0.05	0.12
La_2O_3	0.32	0.31	0.31	0.33	0.27	0.28
Li_2O*	6.00	6.00	2.00	6.00	6.00	2.01
MgO	-	0.08	-	-	0.13	0.10
MnO	5.51	2.75	5.20	5.57	-	-
MoO_3	-	-	-	-	-	-
Na_2O	10.39	4.19	13.29	10.08	8.53	15.34
Nd_2O_3	-	-	-	-	-	-
NiO	0.11	0.11	0.15	0.17	0.10	1.06
OsO_4	-	-	-	-	-	-
P_2O_5	0.42	0.43	0.43	0.40	0.44	0.44
PbO	0.39	0.03	0.40	0.41	0.04	0.36
PdO	0.11	0.09	0.29	0.09	0.11	0.08
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.05	0.04	0.05	0.03	0.05	0.05
RuO_4*	0.08	0.07	0.08	0.04	0.09	0.08
Sb_2O_3	-	0.25	0.01	0.26	0.03	0.23
SeO_2	0.16	0.03	0.12	0.19	0.03	0.03
SiO_2	40.90	50.33	36.38	36.28	52.06	48.43
Sm_2O_3	0.03	-	0.02	0.01	0.02	0.01
SnO_2	-	-	-	-	-	-
SO_3	0.09	0.09	0.08	0.08	0.10	0.08
SrO	6.00	5.88	0.01	5.90	0.01	
Tb_4O_7	0.02	-	0.02	0.01	0.01	0.01
TeO_2	-	-	-	-	-	-
ThO_2	-	-	-	-	-	-
TiO_2	0.05	0.07	0.04	0.06	0.04	0.07
Tl_2O_3	0.06	0.17	0.17	-	0.02	0.02
V_2O_5	0.11	-	0.11	0.11	0.01	0.11
Y_2O_3	-	0.01	-	0.01	0.00	-
ZnO	1.94	1.94	2.02	1.98	1.85	1.88
ZrO_2	1.29	6.43	0.02	6.39	0.01	6.44
TOTAL	99.90	99.91	99.90	99.93	99.99	100.00

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co and Ru are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Initial Matrix Glasses					
	HLW02-19	**HLW02-20R1**	**HLW02-21R1**	**HLW02-22**	**HLW02-23R1**	**HLW02-24**
Ag_2O	0.02	0.02	0.04	0.03	0.02	0.18
Al_2O_3	3.62	4.26	7.81	8.28	8.07	8.15
As_2O_3	0.01	0.02	0.02	0.02	-	0.17
B_2O_3*	14.00	14.00	14.00	14.00	14.00	5.00
BaO	-	-	0.06	0.07	-	0.35
Bi_2O_3	0.01	0.01	0.01	0.01	0.01	0.01
CaO	0.51	0.51	0.53	0.53	0.53	0.54
CdO	1.93	0.07	0.07	0.07	1.95	0.05
CeO_2	0.04	0.04	0.05	0.04	0.05	0.05
Cl	0.11	0.18	0.16	0.14	0.11	0.15
Co_3O_4*	0.02	0.02	0.02	0.02	0.01	0.02
Cr_2O_3	0.22	0.03	0.20	0.02	0.03	0.16
Cs_2O	0.01	0.01	0.02	0.02	0.01	0.02
CuO	0.01	0.01	0.02	0.01	0.02	0.09
F	NA	NA	NA	NA	NA	NA
Er_2O_3	0.01	0.01	-	0.01	0.01	-
Eu_2O_3	-	-	-	-	-	0.01
Fe_2O_3	11.88	14.17	9.18	9.87	8.47	8.26
Gd_2O_3	-	-	-	-		-
GeO_2	-	-	-	-	0.00	-
HfO_2	0.12	-	0.03	-	0.03	0.02
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.03	0.12	0.09	0.12	0.06	0.11
La_2O_3	0.33	0.30	0.28	0.28	0.31	0.31
Li_2O*	2.00	2.00	2.00	6.00	6.00	2.00
MgO	0.11	0.12	0.10	0.12	0.12	-
MnO	5.54	-	-	-	5.52	5.41
MoO_3	0.01	-	-	-	-	
Na_2O	8.87	6.68	15.45	4.42	5.23	12.92
Nd_2O_3	-	-	-	-	-	-
NiO	0.17	0.09	0.16	0.11	1.11	0.10
OsO_4	-	-	-	-	-	-
P_2O_5	0.41	0.43	0.43	0.44	0.42	0.42
PbO	0.04	0.04	0.05	0.03	0.04	0.29
PdO	0.11	0.10	0.13	0.12	0.11	0.10
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.05	0.06	0.06	0.06	0.04	0.05
RuO_4*	0.08	0.09	0.10	0.09	0.06	0.08
Sb_2O_3	0.24	0.02	0.03	0.30	-	0.02
SeO_2	0.10	0.02	0.04	0.10	0.01	0.23
SiO_2	34.95	50.79	44.91	52.46	37.83	45.24
Sm_2O_3	0.01	0.02	0.01	-	-	-
SnO_2	-	-	-	-	-	-
SO_3	0.07	0.10	0.08	0.09	0.08	0.09
SrO	5.85	3.62	0.02	0.10	5.90	5.76
Tb_4O_7	0.02	0.02	0.01	0.01	0.01	
TeO_2	-	-	-	-	-	-
ThO_2	-	-	-	-	-	-
TiO_2	0.06	0.06	0.04	0.05	0.07	0.06
Tl_2O_3	0.01	0.02	0.02	0.02	0.10	0.01
V_2O_5	0.01	0.01	0.02	0.01	-	0.09
Y_2O_3	0.01	-	-	0.00	0.00	-
ZnO	1.97	1.85	2.04	1.94	1.96	1.91
ZrO_2	6.37	0.01	1.69	0.01	1.60	1.57
TOTAL	99.95	99.94	99.98	100.00	99.89	99.97

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co and Ru are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Initial Matrix Glasses					
	HLW02-25R1	**HLW02-26**	**HLW02-27**	**HLW02-28**	**HLW02-29R1**	**HLW02-30**
Ag_2O	0.03	0.27	0.03	0.04	0.17	0.04
Al_2O_3	8.10	3.92	3.81	6.99	6.65	5.28
As_2O_3	0.01	0.22	-	0.03	0.15	0.03
B_2O_3*	14.00	5.00	14.00	8.00	13.00	9.72
BaO	-	0.40	-	-	0.28	-
Bi_2O_3	0.01	-	0.01	0.01	-	0.01
CaO	0.54	0.53	0.48	0.54	0.57	0.52
CdO	2.06	1.96	0.05	1.33	0.68	1.24
CeO_2	0.05	0.03	0.04	0.04	0.05	0.05
Cl	0.15	0.10	0.12	0.14	0.13	0.13
Co_3O_4*	0.02	0.02	0.02	0.02	0.02	0.02
Cr_2O_3	0.03	0.23	0.02	0.05	0.36	0.04
Cs_2O	0.02	-	0.01	0.01	0.02	
CuO	0.02	0.12	0.01	0.05	0.09	0.03
F	NA	NA	NA	NA	NA	NA
Er_2O_3	-	0.01	0.01	0.01	0.01	0.01
Eu_2O_3	-	-	-	-	-	-
Fe_2O_3	10.02	13.39	11.76	11.12	11.30	10.14
Gd_2O_3	-	-	-	-	-	-
GeO_2	-	-	-	-	-	-
HfO_2	-	0.14	0.12	0.09	0.09	0.09
HgO	-	-	-	-	-	-
IrO_2	-	-	0.01	-	-	-
K_2O	0.04	0.05	0.09	0.07	0.07	0.08
La_2O_3	0.32	0.31	0.28	0.34	0.33	0.30
Li_2O*	2.00	2.00	5.99	2.50	3.75	5.00
MgO	0.10	-	-	0.06	-	0.07
MnO	0.40	5.58	3.37	1.58	1.72	3.71
MoO_3	-	-	-	-	-	-
Na_2O	6.79	13.80	4.62	14.80	9.07	11.69
Nd_2O_3	-	-	-	-	-	-
NiO	0.10	0.11	0.10	0.34	0.40	0.32
OsO_4	-	-	-	-	-	-
P_2O_5	0.43	0.42	0.40	0.43	0.47	0.43
PbO	0.04	0.39	0.03	0.08	0.26	0.08
PdO	0.12	0.07	0.11	0.11	0.12	0.11
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	0.01	-
Rh_2O_3	0.06	0.05	0.05	0.05	0.04	0.04
RuO_4*	0.09	0.06	0.07	0.07	0.08	0.07
Sb_2O_3	0.26	0.02	0.02	0.06	0.06	0.17
SeO_2	0.02	0.03	0.12	0.08	0.16	0.05
SiO_2	45.83	35.40	41.06	39.54	38.48	39.71
Sm_2O_3	-	-	-	-	-	0.01
SnO_2	-	-	-	-	-	-
SO_3	0.10	0.09	0.09	0.09	0.08	0.09
SrO	5.88	6.01	5.10	4.20	4.18	3.88
Tb_4O_7	-	-	-	-	-	0.01
TeO_2	-	-	-	-	-	0.01
ThO_2	-	-	-	-	-	-
TiO_2	0.06	0.07	0.07	0.07	0.06	0.06
Tl_2O_3	0.28	0.05	0.15	0.08	0.04	0.01
V_2O_5	-	-	-	0.02	0.07	0.02
Y_2O_3	-	-	-	0.01	0.01	-
ZnO	1.91	2.00	1.74	1.97	2.05	1.86
ZrO_2	0.01	6.92	5.93	4.90	4.89	4.79
TOTAL	99.90	99.91	99.86	99.88	99.93	99.91

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co and Ru are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Initial Matrix Glasses					
	HLW02-31	**HLW02-32R1**	**HLW02-33**	**HLW02-34R1**	**HLW02-35**	**HLW02-36**
Ag_2O	0.05	0.06	0.05	0.16	0.16	0.16
Al_2O_3	5.23	6.72	5.59	5.08	6.28	5.36
As_2O_3	0.04	0.04	0.03	0.14	0.13	0.14
B_2O_3*	13.00	8.00	13.00	13.00	13.00	8.67
BaO	-	-	-	0.28	0.30	0.30
Bi_2O_3	0.01	0.01	-	0.01	0.01	0.01
CaO	0.51	0.53	0.48	0.53	0.52	0.52
CdO	0.63	1.35	0.60	1.32	0.67	1.32
CeO_2	0.05	0.05	0.05	0.06	0.05	0.05
Cl	0.14	0.13	0.14	0.10	0.13	0.13
Co_3O_4*	0.02	0.02	0.02	0.02	0.02	0.02
Cr_2O_3	0.04	0.24	0.04	0.16	0.15	0.15
Cs_2O	0.01	0.02	0.02	0.01	0.02	0.02
CuO	0.03	0.03	0.03	0.08	0.09	0.08
F	NA	NA	NA	NA	NA	NA
Er_2O_3	-	0.01	0.01	-	0.01	0.01
Eu_2O_3	-	-	-	-	-	-
Fe_2O_3	10.27	11.31	11.54	12.79	12.57	12.34
Gd_2O_3	-	-	-	-	-	-
GeO_2	-	-	-	-	-	-
HfO_2	0.09	0.02	0.04	0.02	0.03	0.03
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.09	0.04	0.08	0.06	0.10	0.07
La_2O_3	0.32	0.34	0.30	0.31	0.33	0.30
Li_2O*	2.50	5.00	2.50	3.96	5.00	2.50
MgO	-	-	-	-	0.07	-
MnO	1.65	1.72	3.53	1.67	3.85	1.63
MoO_3	-	-	-	-	-	-
Na_2O	15.72	11.01	14.57	10.84	8.99	15.45
Nd_2O_3	-	-	-	-	-	-
NiO	0.31	0.39	0.79	0.90	0.86	0.32
OsO_4	-	-	-	-	-	-
P_2O_5	0.44	0.41	0.40	0.41	0.43	0.42
PbO	0.08	0.08	0.07	0.25	0.26	0.25
PdO	0.12	0.12	0.15	0.11	0.10	0.11
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.05	0.05	0.03	0.04	0.05	0.04
RuO_4*	0.08	0.09	0.05	0.07	0.07	0.07
Sb_2O_3	0.06	0.18	0.35	0.06	0.19	0.06
SeO_2	0.19	0.24	0.17	0.05	0.05	0.19
SiO_2	39.52	43.58	37.49	39.65	39.65	43.87
Sm_2O_3	-	-	-	-	-	-
SnO_2	-	-	-	-	-	-
SO_3	0.09	0.09	0.08	0.07	0.08	0.08
SrO	1.71	4.24	3.76	4.16	1.73	1.72
Tb_4O_7			0.01		0.01	-
TeO_2	0.01	0.01	0.01	-	-	-
ThO_2	-	-	-	-	-	-
TiO_2	0.07	0.06	0.05	0.05	0.06	0.05
Tl_2O_3	0.13	0.03	0.02	0.01	0.09	0.03
V_2O_5	0.02	0.02	0.02	0.07	0.07	0.07
Y_2O_3	0.00	0.00	-	0.00	-	-
ZnO	1.90	2.00	1.77	1.97	1.94	1.89
ZrO_2	4.74	1.68	2.10	1.44	1.89	1.60
TOTAL	99.90	99.91	99.91	99.93	100.00	99.99

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co and Ru are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Initial Matrix Glasses					
	HLW02-37	**HLW02-38**	**HLW02-39**	**HLW02-40**	**HLW02-41**	**HLW02-42**
Ag_2O	0.05	0.17	0.05	0.17	0.05	0.05
Al_2O_3	6.18	6.47	7.17	7.07	6.53	5.01
As_2O_3	0.04	0.14	0.04	0.11	0.02	0.04
B_2O_3*	13.00	13.00	8.99	9.83	13.00	13.00
BaO	-	0.31	-	0.29	0.10	-
Bi_2O_3	0.01	0.01	0.01	-	-	0.01
CaO	0.51	0.55	0.52	0.52	0.52	0.52
CdO	0.67	1.39	1.34	1.28	0.65	0.65
CeO_2	0.04	0.06	0.04	0.05	0.04	0.04
Cl	0.15	0.17	0.17	0.14	0.17	0.11
Co_3O_4*	0.02	0.02	0.02	0.02	0.02	0.02
Cr_2O_3	0.05	0.16	0.05	0.15	0.05	0.26
Cs_2O	0.02	0.02	0.02	0.02	0.02	0.01
CuO	0.02	0.08	0.03	0.08	0.24	0.03
F	NA	NA	NA	NA	NA	NA
Er_2O_3	-	0.01	0.01	0.01	-	0.01
Eu_2O_3	-	-	-	-	-	-
Fe_2O_3	10.54	13.16	10.47	10.44	10.15	11.02
Gd_2O_3	-	-	-	-	-	-
GeO_2	-	-	-	-	-	-
HfO_2	0.09	0.03	0.03	0.02	0.02	0.05
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.08	0.06	0.07	0.08	0.11	0.08
La_2O_3	0.34	0.33	0.31	0.30	0.30	0.32
Li_2O*	2.50	2.50	2.50	2.63	2.50	5.00
MgO	0.07	-	0.09	0.08	0.10	0.11
MnO	3.87	1.74	1.67	1.65	1.59	1.69
MoO_3	-	-	-	-	-	-
Na_2O	11.37	8.91	11.50	10.18	9.91	9.45
Nd_2O_3	-	-	-	-	-	-
NiO	0.88	0.84	0.87	0.32	0.32	0.39
OsO_4	-	-	-	-	-	-
P_2O_5	0.43	0.44	0.42	0.44	0.45	0.42
PbO	0.07	0.29	0.07	0.24	0.07	0.08
PdO	0.08	0.09	0.13	0.11	0.12	0.11
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.06	0.07	0.06	0.05	0.06	0.05
RuO_4*	0.09	0.08	0.09	0.09	0.09	0.08
Sb_2O_3	0.18	0.19	0.06	0.18	0.06	0.06
SeO_2	0.05	0.19		0.04	0.04	0.06
SiO_2	39.40	40.15	47.63	47.86	47.14	42.28
Sm_2O_3	-	-	-	-	-	-
SnO_2	-	-	-	-	-	-
SO_3	0.08	0.09	0.09	0.09	0.09	0.07
SrO	1.75	4.30	1.75	1.71	1.68	4.07
Tb_4O_7	0.01	-	-	-	-	-
TeO_2	-	-	-	-	-	-
ThO_2	-	-	-	-	-	-
TiO_2	0.07	0.06	0.05	0.05	0.07	0.06
Tl_2O_3	0.04	0.05	0.05	0.13	0.20	0.12
V_2O_5	0.02	0.08	0.02	0.07	0.02	0.02
Y_2O_3	0.00	-	0.00	-	-	-
ZnO	1.96	2.03	1.93	1.91	1.86	1.94
ZrO_2	5.11	1.79	1.60	1.59	1.62	2.65
TOTAL	99.89	99.99	99.90	99.98	99.98	99.90

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co and Ru are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Initial Matrix Glasses					
	HLW02-43	**HLW02-44**	**HLW02-45**	**HLW02-46**	**HLW02-47**	**HLW02-48**
Ag_2O	0.05	0.16	0.05	0.05	0.16	0.16
Al_2O_3	6.35	4.95	5.63	5.65	5.41	5.70
As_2O_3	0.05	0.14	0.04	0.03	0.14	0.12
B_2O_3*	13.00	9.07	8.00	9.15	9.81	8.00
BaO	-	0.24	-	0.09	0.25	0.25
Bi_2O_3	0.01	0.01	0.01	0.01	-	-
CaO	0.52	0.52	0.52	0.53	0.51	0.52
CdO	1.34	1.30	1.28	0.63	0.63	0.65
CeO_2	0.06	0.06	0.04	0.04	0.04	0.04
Cl	0.14	0.13	0.15	0.15	0.13	0.12
Co_3O_4*	0.02	0.02	0.02	0.02	0.02	0.02
Cr_2O_3	0.04	0.26	0.05	0.05	0.14	0.15
Cs_2O	0.01	0.01	0.02	0.02	0.01	0.01
CuO	0.04	0.08	0.03	0.03	0.08	0.08
F	NA	NA	NA	NA	NA	NA
Er_2O_3	-	0.01	0.01	-	0.01	-
Eu_2O_3	-	-	-	-	-	-
Fe_2O_3	10.33	11.02	10.88	9.82	10.30	12.75
Gd_2O_3	-	-	-	-	-	-
GeO_2	-	-	-	-	-	-
HfO_2	0.03	0.05	0.02	0.05	0.04	0.10
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.07	0.04	0.09	0.11	0.09	0.09
La_2O_3	0.33	0.33	0.30	0.32	0.29	0.32
Li_2O*	2.50	2.50	2.50	3.70	2.50	3.34
MgO	-	0.06	0.10	0.08	0.11	-
MnO	3.84	3.93	3.71	3.73	3.82	1.69
MoO_3	-	-	-	-	-	-
Na_2O	12.95	15.09	10.03	9.71	9.90	14.78
Nd_2O_3	-	-	-	-	-	-
NiO	0.33	0.38	0.31	0.81	0.31	0.90
OsO_4	-	-	-	-	-	-
P_2O_5	0.42	0.40	0.42	0.43	0.43	0.42
PbO	0.07	0.27	0.07	0.08	0.26	0.25
PdO	0.11	0.08	0.19	0.08	0.10	0.14
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.04	0.06	0.05	0.05	0.05	0.04
RuO_4*	0.07	0.08	0.09	0.09	0.09	0.06
Sb_2O_3	0.18	0.17	0.05	0.06	0.06	0.17
SeO_2	0.05	0.06	0.11	0.11	0.04	0.20
SiO_2	39.26	41.58	47.58	47.57	47.53	39.42
Sm_2O_3	-	-	-	-	-	-
SnO_2	-	-	-	-	-	-
SO_3	0.08	0.08	0.09	0.08	0.08	0.08
SrO	3.99	1.80	3.86	1.70	1.71	2.05
Tb_4O_7	0.02	0.02	0.01	0.01	0.01	
TeO_2	-	-	-	-	-	-
ThO_2	-	-	-	-	-	-
TiO_2	0.06	0.06	0.07	0.07	0.06	0.06
Tl_2O_3	0.02	-	0.04	0.14	0.12	0.08
V_2O_5	0.02	0.07	0.03	0.02	0.07	0.08
Y_2O_3	0.00	0.00	-	-	-	-
ZnO	1.89	2.01	1.84	1.90	1.90	1.98
ZrO_2	1.55	2.90	1.61	2.75	2.74	5.16
TOTAL	99.84	100.00	99.89	99.95	99.96	99.98

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co and Ru are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Initial Matrix Glasses					
	HLW02-49	**HLW02-50**	**HLW02-51R1**	**HLW02-52**	**HLW02-53**	**HLW02-54**
Ag_2O	0.05	0.04	0.05	0.13	0.03	0.02
Al_2O_3	6.77	5.93	6.85	6.06	7.80	4.40
As_2O_3	0.04	0.02	0.03	0.10	0.02	
B_2O_3*	8.74	13.00	8.00	9.93	5.00	5.00
BaO	-	-	-	0.23	0.05	0.04
Bi_2O_3	0.01	-	0.01	0.01	0.01	-
CaO	0.52	0.52	0.53	0.53	0.52	0.51
CdO	0.65	0.60	0.67	1.00	2.08	2.06
CeO_2	0.04	0.03	0.04	0.04	0.05	0.05
Cl	0.13	0.14	0.12	0.13	0.17	0.16
Co_3O_4*	0.02	0.02	0.02	0.01	0.02	0.02
Cr_2O_3	0.25	0.04	0.22	0.12	0.20	0.02
Cs_2O	0.01	0.01	0.02	0.02	0.01	0.01
CuO	0.04	0.03	0.03	0.07	0.02	0.01
F	NA	NA	NA	NA	NA	NA
Er_2O_3	0.01	-	0.02	-	0.01	0.01
Eu_2O_3	-	-	-	-	-	-
Fe_2O_3	12.99	11.85	11.44	11.40	15.16	14.45
Gd_2O_3	-	-	-	-	-	-
GeO_2	-	-	-	-	-	-
HfO_2	0.06	0.08	0.09	0.06	-	-
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.08	0.09	0.06	0.08	-	0.04
La_2O_3	0.31	0.31	0.31	0.32	0.28	0.28
Li_2O*	5.00	2.50	4.58	4.00	6.00	2.00
MgO	0.08	0.11	-	-	-	-
MnO	3.79	1.57	1.93	2.63	0.03	0.56
MoO_3	-	-	-	-	-	-
Na_2O	9.87	11.04	9.64	11.09	8.19	15.59
Nd_2O_3	-	-	-	-	-	-
NiO	0.38	0.29	0.05	0.56	0.16	0.11
OsO_4	-	-	-	-	-	-
P_2O_5	0.42	0.46	0.42	0.42	0.43	0.41
PbO	0.08	0.06	0.08	0.20	0.04	0.03
PdO	0.11	0.10	0.12	0.11	0.12	0.09
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.06	0.05	0.05	0.05	0.05	0.06
RuO_4*	0.08	0.08	0.07	0.07	0.09	0.09
Sb_2O_3	0.06	0.16	0.18	0.14	0.03	0.27
SeO_2	0.05	0.05	0.17	0.14	0.04	0.27
SiO_2	42.05	42.26	42.90	42.07	51.10	51.13
Sm_2O_3	0.02	-	-	-	0.02	0.01
SnO_2	-	-	-	-	-	-
SO_3	0.09	0.09	0.07	0.08	0.09	0.10
SrO	1.74	1.63	4.10	2.82	0.02	-
Tb_4O_7	0.02	-	-	-	0.02	-
TeO_2	0.01	-	0.01	0.01	0.01	-
ThO_2	-	-	-	-	-	-
TiO_2	0.05	0.07	0.05	0.06	0.04	0.05
Tl_2O_3	0.10	0.16	0.09	0.06	0.02	0.20
V_2O_5	0.02	0.02	0.03	0.06	0.02	-
Y_2O_3	0.01	-	0.01	0.00	-	-
ZnO	1.94	1.82	1.96	1.93	1.98	1.90
ZrO_2	3.18	4.69	4.79	3.16	0.02	0.01
TOTAL	99.91	99.90	99.77	99.90	99.92	99.95

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co and Ru are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Initial Matrix Glasses		
	HLW02-55	**HLW02-56**	**HLW02-57**
Ag_2O	0.05	0.16	0.02
Al_2O_3	5.62	5.25	4.08
As_2O_3	0.04	0.15	0.02
B_2O_3*	13.00	9.07	14.00
BaO	-	0.28	0.05
Bi_2O_3	0.01	0.01	0.01
CaO	0.55	0.54	0.51
CdO	0.67	1.33	0.06
CeO_2	0.04	0.03	0.05
Cl	0.12	0.12	0.11
Co_3O_4*	0.02	0.02	0.02
Cr_2O_3	0.05	0.15	0.03
Cs_2O	0.02	0.01	-
CuO	0.03	0.08	0.01
F	NA	NA	NA
Er_2O_3	0.01	-	0.01
Eu_2O_3	-	-	-
Fe_2O_3	10.72	10.70	9.47
Gd_2O_3	-	-	-
GeO_2	-	-	-
HfO_2	0.05	0.05	0.12
HgO	-	-	-
IrO_2	-	-	-
K_2O	0.12	0.06	0.09
La_2O_3	0.33	0.30	0.27
Li_2O*	2.50	2.50	3.31
MgO	0.09	0.06	0.11
MnO	1.69	3.93	5.38
MoO_3	-	-	-
Na_2O	9.20	14.86	15.61
Nd_2O_3	-	-	-
NiO	0.33	0.33	0.10
OsO_4	-	-	-
P_2O_5	0.45	0.42	0.42
PbO	0.08	0.26	0.04
PdO	0.25	0.09	0.10
Pr_6O_{11}	-	-	-
PtO_2	-	-	-
Re_2O_7	-	-	-
Rh_2O_3	0.04	0.05	0.05
RuO_4*	0.08	0.07	0.06
Sb_2O_3	0.05	0.21	0.24
SeO_2	0.06	0.06	0.02
SiO_2	44.21	42.11	37.36
Sm_2O_3	-	-	0.02
SnO_2	-	-	-
SO_3	0.09	0.08	0.07
SrO	4.21	1.79	0.01
Tb_4O_7	-	0.01	0.02
TeO_2	-	0.01	0.01
ThO_2	-	-	-
TiO_2	0.08	0.05	0.05
Tl_2O_3	0.13	0.02	-
V_2O_5	0.03	0.08	-
Y_2O_3	-	-	0.01
ZnO	1.98	1.98	1.91
ZrO_2	2.90	2.74	6.15
TOTAL	99.87	100.00	99.97

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co and Ru are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Augmentation Matrix Glasses					
	HLW03-01	**HLW03-02**	**HLW03-03**	**HLW03-04**	**HLW03-05**	**HLW03-06**
Ag_2O	0.23	0.03	0.02	0.24	0.25	0.02
Al_2O_3	7.25	1.94	1.89	1.92	7.23	7.49
As_2O_3	0.22	0.01	0.02	0.20	0.20	-
Au	-	-	-	-	-	-
B_2O_3	13.73	13.66	4.88	4.90	4.81	4.91
BaO	0.35	0.04	-	-	0.38	-
Bi_2O_3	0.01	0.01	0.01	-	-	0.01
CaO	0.52	0.50	0.51	0.53	0.52	0.52
CdO	0.06	1.92	2.01	0.05	2.05	2.14
CeO_2	0.05	0.05	0.03	0.07	0.06	0.04
Cl	0.07	0.07	0.06	0.07	0.11	0.14
Co_3O_4*	0.03	0.02	0.02	0.02	0.02	0.01
Cr_2O_3	0.38	0.70	0.61	0.76	0.87	0.90
Cs_2O	0.01	0.01	-	0.01	0.01	0.01
CuO	0.13	0.02	0.01	0.12	0.13	0.03
Er_2O_3	0.01	-	-	-	-	-
Eu_2O_3	0.01	-	-	-	-	-
F	NA	NA	NA	NA	NA	NA
Fe_2O_3	15.85	14.47	14.08	14.90	3.06	3.27
GeO_2	-	-	-	-	-	0.00
HfO_2	0.06	0.24	0.16	0.07	-	0.10
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	0.01	-
K_2O	0.07	0.06	0.04	0.07	-	0.05
La_2O_3	0.32	0.29	0.34	0.33	0.35	0.32
Li_2O	5.88	2.47	2.68	5.85	1.92	5.89
MgO	0.06	0.09	-	-	-	0.12
MnO	6.90	7.32	7.31	3.49	7.89	7.82
MoO_3	-	0.01	-	-	-	-
Na_2O	3.87	11.61	10.26	4.11	14.11	3.89
NiO	0.23	1.06	0.95	0.17	0.21	1.24
P_2O_5	0.42	0.42	0.39	0.39	0.41	0.43
PbO	0.39	0.04	0.03	0.40	0.38	0.04
PdO	0.07	0.09	0.08	0.07	0.11	0.10
Pr_6O_{11}	-	-	-	0.02	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	0.01
Rh_2O_3	0.05	0.05	0.03	0.09	0.05	0.06
RuO_4*	0.08	0.06	0.06	0.03	0.07	0.08
Sb_2O_3	0.03	0.35	0.02	0.02	0.36	0.02
SeO_2	0.06	0.02	0.14	0.21	0.20	0.02
SiO_2	32.90	32.05	31.90	38.10	44.89	46.94
Sm_2O_3	0.02	0.01	-	-	-	-
SO_3	0.06	0.06	0.09	0.08	0.05	0.09
SrO	0.03	0.02	11.49	12.19	0.02	6.49
Tb_4O_7	0.02	0.01	0.02	-	-	-
TeO_2	0.01	-	-	-	-	-
ThO_2	2.70	-	-	-	4.51	1.50
TiO_2	0.05	0.04	0.05	0.06	0.05	0.06
Tl_2O_3	0.16	0.12	0.07	0.11	0.33	-
U_3O_8*	0.02	-	-	6.04	0.01	-
V_2O_5	0.11	-	0.01	0.11	0.12	0.01
Y_2O_3	0.01	0.01	-	-	-	0.01
ZnO	3.14	0.01	1.83	0.01	4.04	0.02
ZrO_2	3.29	9.98	7.32	3.19	0.03	5.00
TOTAL	99.90	99.95	99.42	99.00	99.82	99.77

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co, Ru and U are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Augmentation Matrix Glasses					
	HLW03-07	**HLW03-08**	**HLW03-09**	**HLW03-10R1**	**HLW03-11**	**HLW03-12**
Ag_2O	0.01	0.20	0.03	0.22	0.01	-
Al_2O_3	4.67	8.05	7.07	8.13	2.25	1.90
As_2O_3	0.01	0.21	-	0.22	-	-
Au	-	-	-	-	0.01	-
B_2O_3	4.98	4.83	13.69	4.93	4.98	4.97
BaO	0.03	0.33	0.05	0.35	0.03	-
Bi_2O_3	0.01	0.01	-	0.01	0.01	-
CaO	0.51	0.53	0.54	0.52	0.54	0.50
CdO	0.05	1.72	0.07	0.06	0.06	0.05
CeO_2	0.06	0.02	0.05	0.04	0.06	0.05
Cl	0.13	0.10	0.12	0.11	0.13	0.10
Co_3O_4*	0.02	0.01	0.02	0.02	0.02	0.02
Cr_2O_3	0.79	0.57	0.39	0.03	0.33	0.90
Cs_2O	0.01	-	0.02	-	-	0.01
CuO	0.01	0.12	0.02	0.12	0.02	0.01
Er_2O_3	0.01	-	-	0.02	-	-
Eu_2O_3	0.02	0.01	-	0.01	-	-
F	NA	NA	NA	NA	NA	NA
Fe_2O_3	15.40	2.18	5.25	10.20	11.87	3.26
GeO_2	-	-	-	-	-	-
HfO_2	-	0.20	-	0.17	-	0.09
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.09	0.11	0.09	0.10	0.10	0.08
La_2O_3	0.33	0.32	0.32	0.31	0.30	0.32
Li_2O	4.77	5.15	1.98	5.91	1.99	5.03
MgO	-	0.08	-	0.08	0.07	0.08
MnO	7.78	7.36	0.05	7.41	0.05	7.68
MoO_3	-	-	-	-	-	-
Na_2O	11.82	14.47	14.29	12.98	14.12	3.78
NiO	0.19	0.12	0.24	0.99	0.22	0.22
P_2O_5	0.41	0.44	0.44	0.44	0.42	0.38
PbO	0.05	0.37	0.03	0.38	0.04	0.04
PdO	0.08	0.05	0.13	0.08	0.09	0.08
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	0.01
Rh_2O_3	0.08	0.03	0.06	0.04	0.09	0.15
RuO_4*	0.04	0.05	0.10	0.05	0.07	0.04
Sb_2O_3	0.02	0.30	0.41	0.02	0.02	0.35
SeO_2	0.16	0.02	0.21	0.02	0.28	0.02
SiO_2	37.75	34.45	50.87	34.45	49.21	38.35
Sm_2O_3	0.02	-	-	-	-	-
SO_3	0.09	0.08	0.08	0.08	0.07	0.05
SrO	0.02	0.02	0.04	0.03	0.06	12.35
Tb_4O_7	0.01	-	-	0.02	0.01	-
TeO_2	-	-	0.01	-	-	-
ThO_2	-	4.44	2.66	2.51	5.49	3.98
TiO_2	0.05	0.06	0.05	0.05	0.06	0.05
Tl_2O_3	-	-	0.34	-	0.01	-
U_3O_8*	6.32	0.01	0.03	1.14	6.89	6.36
V_2O_5	-	0.10	-	-	-	-
Y_2O_3	-	0.01	-	-	-	-
ZnO	3.17	3.61	0.01	0.01	0.03	3.94
ZrO_2	-	9.24	0.08	7.62	-	4.30
TOTAL	99.99	99.97	99.81	99.98	99.99	99.51

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co, Ru and U are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Augmentation Matrix Glasses					
	HLW03-13	**HLW03-14**	**HLW03-15**	**HLW03-16**	**HLW03-17**	**HLW03-18**
Ag_2O	-	0.02	0.03	0.24	0.24	0.03
Al_2O_3	7.11	2.44	2.08	2.05	7.58	2.07
As_2O_3	-	-	-	0.22	0.23	-
Au	-	-	-	-	-	-
B_2O_3	4.98	4.97	13.66	4.90	13.80	4.97
BaO	-	-	0.04	-	0.38	0.04
Bi_2O_3	0.01	0.01	-	0.01	0.01	-
CaO	0.51	0.52	0.51	0.50	0.53	0.51
CdO	0.04	0.06	1.87	0.05	0.05	0.06
CeO_2	0.05	0.05	0.05	0.03	0.04	0.05
Cl	0.12	0.07	0.13	0.10	0.10	0.09
Co_3O_4*	0.02	0.02	0.02	0.02	0.01	0.02
Cr_2O_3	0.88	0.05	0.30	0.34	0.33	0.97
Cs_2O	0.01	0.01	0.02	0.01	0.01	0.02
CuO	0.02	0.02	0.02	0.13	0.12	0.01
Er_2O_3	0.01	0.01	0.01	0.01	-	-
Eu_2O_3	-	-	-	-	-	-
F	NA	NA	NA	NA	NA	NA
Fe_2O_3	9.83	9.40	15.07	9.20	3.12	16.12
GeO_2	-	-	-	-	-	-
HfO_2	0.02	-	-	-	0.03	-
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.06	0.12	0.06	0.10	0.10	0.09
La_2O_3	0.32	0.35	0.29	0.31	0.29	0.32
Li_2O	5.23	2.50	1.95	2.86	1.97	5.92
MgO	-	0.09	0.08	0.08	0.09	0.06
MnO	7.51	7.52	1.57	7.52	7.86	0.05
MoO_3	-	-	-	-	-	-
Na_2O	4.00	9.75	5.66	3.67	4.47	10.21
NiO	1.10	1.03	0.19	1.16	0.43	1.22
P_2O_5	0.41	0.40	0.42	0.40	0.43	0.43
PbO	0.03	0.03	0.03	0.41	0.40	0.02
PdO	0.06	0.07	0.12	0.08	0.07	0.10
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.11	0.05	0.05	0.11	0.08	0.05
RuO_4*	0.07	0.05	0.09	0.05	0.05	0.08
Sb_2O_3	0.02		0.33	0.35	0.02	0.03
SeO_2	0.12	0.02	0.01	0.10	0.00	0.02
SiO_2	32.71	32.44	49.29	38.53	43.08	50.16
Sm_2O_3	0.03	0.02	-	-	-	-
SO_3	0.06	0.08	0.08	0.07	0.07	0.07
SrO	12.06	11.86	0.02	12.25	0.18	0.02
Tb_4O_7	0.01	0.01	-	-	-	0.01
TeO_2	-	-	-	-	-	-
ThO_2	3.78	3.92	1.93	2.82	2.43	5.75
TiO_2	0.05	0.06	0.04	0.06	0.06	0.05
Tl_2O_3	-	0.10	0.41	-	0.02	0.21
U_3O_8*	6.14	-	-	6.26	5.33	0.01
V_2O_5	-	-	0.02	0.11	0.11	0.01
Y_2O_3	-	-	-	-	-	0.01
ZnO	1.07	3.81	3.27	2.75	3.99	0.03
ZrO_2	0.86	7.40	0.04	1.25	1.90	0.04
TOTAL	99.41	99.46	99.76	99.07	99.99	99.90

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co, Ru and U are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Augmentation Matrix Glasses					
	HLW03-19	**HLW03-20**	**HLW03-21**	**HLW03-22**	**HLW03-23**	**HLW03-24**
Ag_2O	0.03	0.23	0.04	0.15	0.04	0.05
Al_2O_3	2.17	2.07	5.33	4.34	4.57	2.96
As_2O_3	0.01	0.22	0.04	0.14	0.03	0.04
Au	-	-	0.01	-	-	-
B_2O_3	4.91	4.81	6.95	6.90	11.93	6.95
BaO	0.02	0.34	-	-	-	-
Bi_2O_3	0.01	0.01	0.01	0.01	-	0.01
CaO	0.51	0.53	0.53	0.53	0.51	0.52
CdO	1.92	1.85	0.36	0.38	0.12	0.37
CeO_2	0.05	0.05	0.03	0.05	0.05	0.04
Cl	0.12	0.08	0.13	0.12	0.13	0.13
Co_3O_4*	0.02	0.02	0.01	0.02	0.01	0.02
Cr_2O_3	0.86	0.41	0.10	0.44	0.56	0.42
Cs_2O	0.01	0.01	0.01	0.01	0.01	0.01
CuO	0.01	0.13	0.03	0.09	0.03	0.02
Er_2O_3	-	-	0.01	-	0.01	-
Eu_2O_3	-	-	-	-	-	0.01
F	NA	NA	NA	NA	NA	NA
Fe_2O_3	11.27	15.47	5.40	11.63	9.28	6.31
GeO_2	-	-	-	-	-	-
HfO_2	-	-	0.15	0.15	0.13	0.13
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.08	0.08	0.14	0.09	0.07	0.07
La_2O_3	0.29	0.32	0.32	0.31	0.32	0.32
Li_2O	5.89	5.77	2.48	2.45	2.48	4.96
MgO	0.08	0.05	0.06	-	-	0.09
MnO	0.26	0.04	5.05	1.68	1.70	5.08
MoO_3	-	-	-	-	-	-
Na_2O	10.32	9.53	10.19	10.91	12.21	7.92
NiO	1.22	1.21	0.35	0.45	0.44	0.67
P_2O_5	0.43	0.41	0.43	0.40	0.43	0.43
PbO	0.03	0.37	0.07	0.27	0.08	0.08
PdO	0.10	0.09	0.11	0.08	0.08	0.09
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.05	0.06	0.07	0.08	0.06	0.06
RuO_4*	0.08	0.06	0.09	0.05	0.05	0.07
Sb_2O_3	0.02	0.32	0.05	0.06	0.07	0.05
SeO_2	0.02	0.23	0.06	0.20	0.17	0.04
SiO_2	49.53	46.94	46.87	36.32	37.96	45.26
Sm_2O_3	0.01	-	-	-	-	-
SO_3	0.06	0.05	0.07	0.07	0.06	0.07
SrO	0.03	0.20	1.91	5.67	1.85	1.87
Tb_4O_7	-	-	-	-	-	0.01
TeO_2	-	-	-	-	0.01	-
ThO_2	5.48	7.03	2.62	3.01	2.72	2.96
TiO_2	0.06	0.05	0.07	0.06	0.06	0.06
Tl_2O_3	-	0.22	0.03	0.01	0.03	0.02
U_3O_8*	0.01	0.48	1.73	4.28	4.06	2.11
V_2O_5	0.02	0.11	0.01	0.07	0.01	0.01
Y_2O_3	0.01	0.01	0.01	-	0.01	0.02
ZnO	3.95	0.01	1.01	1.02	1.03	3.03
ZrO_2	0.01	0.02	6.90	7.07	6.44	6.50
TOTAL	99.98	99.89	99.82	99.53	99.81	99.83

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co, Ru and U are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Augmentation Matrix Glasses					
	HLW03-25	**HLW03-26**	**HLW03-27**	**HLW03-28**	**HLW03-29**	**HLW03-30**
Ag_2O	0.16	0.14	0.16	0.07	0.04	0.04
Al_2O_3	2.85	5.18	4.53	2.46	3.39	3.04
As_2O_3	0.15	0.15	0.15	0.06	0.03	0.03
Au	-	-	0.01	-	-	-
B_2O_3	11.84	6.91	6.91	11.93	6.95	11.90
BaO	-	-	0.27	-	-	-
Bi_2O_3	0.01	-	-	0.02	0.01	0.01
CaO	0.53	0.53	0.52	0.66	0.52	0.52
CdO	0.12	0.12	0.13	0.19	0.36	0.12
CeO_2	0.05	0.05	0.02	0.07	0.03	0.02
Cl	0.11	0.11	0.09	0.12	0.10	0.12
Co_3O_4*	0.02	0.01	0.02	0.03	0.02	0.02
Cr_2O_3	0.37	0.15	0.52	0.58	0.24	0.43
Cs_2O	-	-	0.02		-	0.01
CuO	0.09	0.08	0.09	0.07	0.03	0.03
Er_2O_3	-	-	0.01	-	-	-
Eu_2O_3	-	-	-	-	-	-
F	NA	NA	NA	NA	NA	NA
Fe_2O_3	6.25	5.40	11.29	16.07	5.40	6.36
GeO_2	-	-	0.00	-	-	-
HfO_2	0.13	0.14	0.14	0.19	0.19	0.17
HgO	-	-	-	-	-	-
IrO_2		-	-	-	-	-
K_2O	0.11	0.10	0.10	0.08	0.11	0.08
La_2O_3	0.33	0.31	0.32	0.43	0.32	0.33
Li_2O	2.46	4.92	4.05	4.96	4.96	4.95
MgO	-		-	-	0.08	-
MnO	1.74	1.70	1.76	2.38	3.97	5.01
MoO_3	-	-	-	-	-	-
Na_2O	10.85	9.79	11.03	3.61	11.39	6.78
NiO	0.66	0.57	0.66	0.95	0.35	0.44
P_2O_5	0.43	0.42	0.42	0.40	0.43	0.41
PbO	0.27	0.26	0.28	0.12	0.08	0.07
PdO	0.10	0.06	0.08	0.14	0.07	0.11
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.07	0.07	0.05	0.09	0.07	0.07
RuO_4*	0.06	0.03	0.06	0.11	0.04	0.08
Sb_2O_3	0.05	0.17	0.17	0.29	0.05	0.17
SeO_2	0.16	0.23	0.19	0.05	0.05	0.11
SiO_2	38.23	38.49	37.20	32.34	38.86	40.29
Sm_2O_3	-	-	-	-	-	-
SO_3	0.06	0.06	0.06	0.40	0.07	0.05
SrO	5.72	5.50	1.92	2.80	1.86	1.87
Tb_4O_7	-	-	-	-	-	0.01
TeO_2	-	-	0.01	0.01	-	-
ThO_2	2.97	4.26	4.17	4.52	3.84	4.10
TiO_2	0.06	0.07	0.05	0.08	0.06	0.07
Tl_2O_3	0.06	0.03	0.02	0.03	0.01	0.09
U_3O_8*	2.16	4.05	2.14	3.13	4.16	1.93
V_2O_5	0.08	0.07	0.07	0.02	0.01	-
Y_2O_3	0.01	0.01	0.01	0.02	0.01	0.02
ZnO	3.04	2.95	3.08	1.18	2.98	1.02
ZrO_2	7.15	6.50	7.14	9.08	8.80	8.88
TOTAL	99.48	99.58	99.91	99.70	99.90	99.74

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co, Ru and U are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Augmentation Matrix Glasses					
	HLW03-31	**HLW03-32**	**HLW03-33**	**HLW03-34**	**HLW03-35**	**HLW03-36**
Ag_2O	0.04	0.14	0.04	0.16	0.05	0.14
Al_2O_3	5.21	4.59	4.48	2.78	4.46	4.59
As_2O_3	0.03	0.13	0.03	0.14	0.04	0.14
Au	-	-	-	0.01	-	-
B_2O_3	6.94	6.91	11.93	6.91	10.41	6.90
BaO	-	0.21	-	-	-	0.24
Bi_2O_3	0.01	0.01	0.01	-	0.01	0.01
CaO	0.52	0.51	0.52	0.52	0.53	0.52
CdO	0.11	0.12	0.12	0.12	0.12	0.34
CeO_2	0.03	0.04	0.04	0.04	0.03	0.04
Cl	0.14	0.09	0.13	0.10	0.12	0.16
Co_3O_4*	0.01	0.02	0.02	0.02	0.02	0.02
Cr_2O_3	0.22	0.41	0.64	0.58	0.36	0.57
Cs_2O	-	-	0.02	0.01	0.01	-
CuO	0.02	0.09	0.03	0.08	0.03	0.09
Er_2O_3	0.01	-	-	-	-	0.01
Eu_2O_3	0.01	-	-	-	-	-
F	NA	NA	NA	NA	NA	NA
Fe_2O_3	5.31	6.36	11.84	11.55	6.26	11.15
GeO_2	0.00	-	-	-	0.00	-
HfO_2	0.22	0.22	0.11	0.14	0.15	0.12
HgO	-	-	-	-	-	-
IrO_2	-	-	-	-	-	-
K_2O	0.14	0.10	0.07	0.08	0.09	0.08
La_2O_3	0.33	0.33	0.33	0.29	0.33	0.32
Li_2O	4.96	4.93	3.91	2.47	2.48	2.70
MgO		0.10	0.08	0.08	0.07	0.08
MnO	4.91	3.33	1.71	1.68	5.14	1.69
MoO_3	-	-	0.02	-	-	-
Na_2O	8.49	9.12	6.89	9.34	6.53	8.09
NiO	0.55	0.66	0.63	0.66	0.66	0.64
P_2O_5	0.45	0.43	0.42	0.42	0.42	0.42
PbO	0.07	0.26	0.07	0.26	0.07	0.26
PdO	0.08	0.06	0.08	0.08	0.10	0.08
Pr_6O_{11}	-	-	-	-	-	-
PtO_2	-	-	-	-	-	-
Re_2O_7	-	-	-	-	-	-
Rh_2O_3	0.05	0.05	0.06	0.06	0.07	0.05
RuO_4*	0.07	0.04	0.07	0.08	0.08	0.07
Sb_2O_3	0.16	0.17	0.17	0.05	0.06	0.17
SeO_2	0.16	0.05	0.05	0.12	0.03	0.05
SiO_2	43.33	37.23	37.73	45.02	45.27	44.66
Sm_2O_3	-	-	-	-	0.02	-
SO_3	0.07	0.05	0.06	0.05	0.06	0.06
SrO	1.81	1.83	1.84	1.80	1.91	1.80
Tb_4O_7	-			-	0.01	-
TeO_2	-	0.01	0.01	-	-	0.01
ThO_2	2.24	4.13	2.90	3.91	3.21	3.77
TiO_2	0.07	0.05	0.06	0.05	0.05	0.06
Tl_2O_3	0.14	0.04	0.04	0.11	0.15	0.06
U_3O_8*	2.00	4.06	3.29	2.02	2.15	2.51
V_2O_5	0.01	0.06	0.01	0.07	0.01	0.07
Y_2O_3	0.01	-	0.01	0.01	-	0.01
ZnO	0.99	2.96	3.01	1.00	1.10	0.99
ZrO_2	9.86	10.02	6.38	6.77	7.06	6.16
TOTAL	99.78	99.92	99.85	99.87	99.73	99.90

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co, Ru and U are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Augmentation Matrix Glasses					
	HLW03-37	**HLW03-38**	**HLW03-39**	**HLW03-40**	**HLW03-41**	**HLW03-42**
Ag_2O	0.16	0.14	0.15	0.04	0.10	0.06
Al_2O_3	2.71	4.70	2.85	4.54	3.58	4.95
As_2O_3	0.16	0.14	0.13	0.04	0.08	0.03
Au	-	-	-	-	-	-
B_2O_3	11.84	6.90	6.88	6.94	8.75	9.15
BaO	0.25	0.23	0.24	-	-	-
Bi_2O_3	0.01	0.01	0.01	0.01	0.01	-
CaO	0.50	0.53	0.53	0.53	0.52	0.53
CdO	0.12	0.34	0.36	0.36	0.27	0.69
CeO_2	0.03	0.05	0.03	0.05	0.04	0.05
Cl	0.10	0.15	0.12	0.12	0.12	0.15
Co_3O_4*	0.01	0.02	0.02	0.02	0.02	0.02
Cr_2O_3	0.22	0.55	0.54	0.46	0.48	0.25
Cs_2O	0.01	-	-	-	-	0.02
CuO	0.08	0.09	0.08	0.03	0.06	0.03
Er_2O_3	-	-	-	-	-	-
Eu_2O_3	-	-	-	-	-	-
F	NA	NA	NA	NA	NA	NA
Fe_2O_3	8.16	11.45	9.98	11.06	8.51	11.18
GeO_2	-		-	-	-	-
HfO_2	0.18	0.16	0.15	0.12	0.15	0.06
HgO	-		-	-	-	-
IrO_2	-		-	-	-	-
K_2O	0.07	0.07	0.07	0.06	0.07	0.07
La_2O_3	0.31	0.32	0.32	0.31	0.34	0.33
Li_2O	4.87	2.46	4.86	4.89	3.72	3.70
MgO	0.04	0.07	0.08	-	0.06	-
MnO	1.67	1.71	1.68	1.70	3.10	3.96
MoO_3	-		-	-	-	-
Na_2O	6.42	9.75	6.41	6.64	8.67	9.12
NiO	0.59	0.43	0.43	0.67	0.56	0.96
P_2O_5	0.43	0.42	0.42	0.45	0.43	0.42
PbO	0.27	0.27	0.26	0.07	0.17	0.07
PdO	0.07	0.09	0.07	0.08	0.09	0.14
Pr_6O_{11}		-	-	-	-	-
PtO_2		-	-	-	-	-
Re_2O_7		-	-	-	-	-
Rh_2O_3	0.07	0.06	0.06	0.08	0.07	0.05
RuO_4*	0.06	0.08	0.06	0.07	0.06	0.08
Sb_2O_3	0.05	0.05	0.16	0.17	0.12	0.06
SeO_2	0.16	0.14	0.13	0.14	0.10	0.15
SiO_2	37.72	40.11	44.34	40.16	40.09	46.24
Sm_2O_3	-	-	-	-	-	0.01
SO_3	0.06	0.06	0.05	0.07	0.05	0.09
SrO	1.92	1.88	1.80	4.07	3.44	1.84
Tb_4O_7	-	-	-	-	-	0.01
TeO_2	-	-	0.01	-	-	0.01
ThO_2	4.25	3.77	5.55	4.20	3.21	-
TiO_2	0.04	0.06	0.07	0.06	0.06	0.05
Tl_2O_3	0.11	0.06	0.13	0.02	0.06	0.18
U_3O_8*	4.11	4.07	2.41	4.12	3.02	-
V_2O_5	0.08	0.06	0.06	0.01	0.04	0.02
Y_2O_3	-	0.01	0.02	0.01	0.01	-
ZnO	3.06	0.99	1.00	1.01	1.99	2.02
ZrO_2	8.90	7.48	7.35	6.36	7.48	2.96
TOTAL	99.87	99.90	99.86	99.74	99.70	99.71

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co, Ru and U are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Oxide	Analyzed XRF (wt%) of Augmentation Matrix Glasses		
	HLW03-43	**HLW03-44**	**HLW03-45**
Ag_2O	0.02	0.02	0.15
Al_2O_3	7.45	2.40	4.52
As_2O_3	0.02	-	0.15
Au	-	0.01	0.01
B_2O_3	4.91	4.98	6.91
BaO	-	0.05	-
Bi_2O_3	0.01	0.01	0.01
CaO	0.52	0.54	0.53
CdO	2.08	0.07	0.14
CeO_2	0.03	0.05	0.03
Cl	0.13	0.13	0.11
Co_3O_4*	0.02	0.02	0.02
Cr_2O_3	0.86	0.32	0.55
Cs_2O	0.01	0.01	-
CuO	0.03	0.02	0.09
Er_2O_3	-	0.01	-
Eu_2O_3	0.02	-	-
F	NA	NA	NA
Fe_2O_3	3.09	11.53	6.25
GeO_2	-	-	-
HfO_2	0.10	-	0.15
HgO	-	-	-
IrO_2	-	-	-
K_2O	0.06	0.11	0.10
La_2O_3	0.33	0.29	0.31
Li_2O	5.89	1.99	4.92
MgO	0.09	0.14	0.04
MnO	7.67	0.07	1.77
MoO_3	-	-	-
Na_2O	4.12	14.75	10.09
NiO	1.20	0.20	0.66
P_2O_5	0.43	0.42	0.42
PbO	0.04	0.04	0.27
PdO	0.09	0.10	0.08
Pr_6O_{11}	-	-	-
PtO_2	-	-	-
Re_2O_7	-	-	-
Rh_2O_3	0.05	0.09	0.07
RuO_4*	0.08	0.07	0.04
Sb_2O_3	0.02	0.03	0.18
SeO_2	0.02	0.28	0.19
SiO_2	47.25	49.04	37.28
Sm_2O_3	-	-	-
SO_3	0.08	0.07	0.07
SrO	6.35	0.04	5.50
Tb_4O_7	-	0.01	-
TeO_2	-	0.01	-
ThO_2	1.49	5.16	3.80
TiO_2	0.06	0.05	0.05
Tl_2O_3	-	0.02	0.02
U_3O_8*	0.05	6.80	3.94
V_2O_5	0.01	0.01	0.07
Y_2O_3	0.00	-	-
ZnO	0.05	0.04	3.04
ZrO_2	5.00	0.04	7.05
TOTAL	99.73	100.01	99.57

Note: – signifies empty data field, NA = Not Analyzed, * Target values are used for B_2O_3 and Li_2O while analyses for Co, Ru and U are reported in chemical forms determined by the XRF software, which are different than those found in matrix design.

Appendix C

Statistical Methods Used to Develop, Evaluate, and Validate Property-Composition Models

Appendix C

Statistical Methods Used to Develop, Evaluate, and Validate Property-Composition Models

This appendix presents various statistical methods used for developing, evaluating, and validating waste glass property-composition models. Section C.1 discusses mixture experiments, introduces two general forms of mixture experiment models, and two variants of one of the model forms appropriate for assessing the presence of "block effects". Section C.2 discusses the least squares regression methods used to fit models to data and corresponding assumptions. Section C.3 discusses the statistical methods and summary statistics used for model evaluation based on the data used to fit a model. Section C.4 discusses statistical methods for model augmentation (i.e., adding terms to a model) and model reduction (i.e., removing unneeded terms from a model). Section C.5 discusses the statistical methods and summary statistics used for model validation based on data not used to fit a model. Section C.6 discusses several statistical intervals used to assess uncertainties in model predictions.

C.1 Mixture Experiments, Model Forms, and Assessing Block Effects

A *mixture experiment* involves mixing two or more components in various proportions, and then measuring one or more responses variables for the resulting end-product mixtures. If the proportions of q mixture components are denoted x_i, $i = 1, 2, \ldots, q$, then these proportions are subject to the basic "mixture constraints"

$$0 \le x_i \le 1 \quad and \quad \sum_{i=1}^{q} x_i = 1. \tag{C.1}$$

Often in practice, the component proportions will be subject to additional single-component constraints

$$0 \le L_i \le x_i \le U_i \le 1 \tag{C.2}$$

and/or multiple-component constraints that can be written in the general form

$$\sum_{i=1}^{q} A_{ki} x_i + A_{k0} \ge 0, \quad k = 1, 2, \ldots, K. \tag{C.3}$$

In Equation (C.2) L_i and U_i denote, respectively, the lower and upper constraints on the i^{th} component ($i = 1, 2, \ldots, q$). In Equation (C.3), the A_{ki} ($i = 1, 2, \ldots, q$) and A_{k0} denote the coefficients of the k^{th} multiple-component constraint. Cornell (2002) provides a comprehensive discussion of statistical methods for the design, modeling, and data analysis of mixture experiments.

Section C.1.1 introduces the linear mixture (LM) model and partial quadratic mixture (PQM) model forms for mixture experiment data. Section C.1.2 discusses two variations of the LM model that can be used to assess modeling data collected in two or more blocks (e.g., at different times or under different conditions) for "block effects".

C.1.1 Linear and Partial Quadratic Mixture Model Forms

The LM model form is given by

$$f(y) = \sum_{i=1}^{q} b_i x_i + \varepsilon \tag{C.4}$$

while the PQM model form is given by

$$f(y) = \sum_{i=1}^{q} b_i x_i + \text{Selected}\left\{ \sum_{i=1}^{q} b_{ii} x_i^2 + \sum_{i<j}^{q-1} \sum^{q} b_{ij} x_i x_j \right\} + \varepsilon \ . \tag{C.5}$$

In Equations (C.4) and (C.5), y is a property or response variable that can be measured for each end-product mixture; $f(y)$ is some mathematical transformation of y (which could be the identity transformation); the x_i (i = 1, 2, …, q) are proportions of q components subject to the constraints in Equation (C.1) and possibly constraints of the forms in Equations (C.2) and/or (C.3); the b_i (i = 1, 2, …, q), the b_{ii} (selected), and the b_{ij} (selected) are coefficients to be estimated from data; and ε is a random error for each data point. Many statistical methods exist for the case where the ε are independent (i.e., not correlated) and normally distributed with mean 0 and standard deviation σ. In Equation (C.5), "Selected" means that only some of the terms in curly brackets are included in the model. The subset is selected using standard stepwise regression or related methods (Draper and Smith 1998; Montgomery et al. 2001). LM models and PQM models are discussed in more detail and illustrated, respectively, by Cornell (2002) and Piepel et al. (2002).

Cornell (2002) discusses many other empirical mixture model forms that can be more appropriate than models of the forms in Equations (C.4) and (C.5) in certain specialized conditions. However, models of the form in Equations (C.4) and (C.5) are widely used in many application areas (including waste glass property modeling) and have been shown to perform very well.

C.1.2 Variants of the Linear Mixture Model for Assessing Block Effects

Two variants of the LM model, useful in assessing the presence or absence of "block effects" in a modeling dataset comprised of two subsets of data collected at different times and/or locations (i.e., "blocks"), are presented in this section. These LM model variants can easily be extended for use with modeling datasets comprised of three or more subsets of data.

The following model form is applicable if: (1) the LM model accounts for the majority of the compositional dependence of $f(y)$ and (2) there is a constant difference in $f(y)$ values for one subset of data compared to the other:

$$f(y) = b_0 B + \sum_{i=1}^{q} b_i x_i + \varepsilon , \tag{C.6}$$

where $B = 0$ for one of the two subsets of modeling data, and $B = 1$ for the other subset. If there is a reason to believe one subset is unbiased and the other biased, then $B = 0$ should be used for the subset believed to be unbiased. In Equation (C.6), b_0 is a coefficient estimated from the modeling data that gives the estimated magnitude of the constant difference in $f(y)$ values between the two subsets. If the b_0 coefficient is statistically different from zero, then that is an indication there is a significant constant difference between the $f(y)$ values for one subset of the modeling data compared to the other.

The following model form is applicable if: (1) the LM model accounts for the majority of the compositional dependence of $f(y)$ and (2) the difference in $f(y)$ values for one subset of data compared to the other depends on the composition of the mixture:

$$f(y) = \sum_{i=1}^{q} b_i^0 x_i + \sum_{i=1}^{q} b_i^1 x_i B + \varepsilon , \tag{C.7}$$

where the choice of $B = 0$ or $B = 1$ is the same as previously discussed. In Equation (C.7), the b_i^0 coefficient represents the linear blending effect of the i^{th} component for the subset of modeling data represented by $B = 0$. The b_i^1 coefficient represents the change or bias in the linear blending effect of the i^{th} component for the subset of modeling data represented by $B = 1$. If any of the b_i^1 coefficients ($i = 1, 2, \ldots, q$) are statistically different from zero, that is an indication that there are compositionally-dependent differences in the $f(y)$ values for one subset of the modeling data compared to the other.

The model forms in Equations (C.6) and (C.7) are intended for use in assessing whether data collected at different times, locations, or conditions are subject to effects (biases) related to the change in time, location, or conditions of data collection. If significant bias is indicated by such models, it should ideally be confirmed by other means (e.g., results on a standard collected at different times, locations, and conditions). It is beyond the scope of this discussion to address what to do when biased data are detected and confirmed. The appropriate steps will depend on the specific situation, the intended use of the data, and any requirements or limitations regarding the use of biased (or bias-corrected) data.

C.2 Least Squares Regression Methods and Assumptions for Fitting Models

Empirical or semi-empirical property-composition models are typically fitted to data sets using unweighted least squares (ULS) or weighted least squares (WLS) regression (Draper and

Smith 1998 or Montgomery et al. 2001). The underlying assumptions of ULS and WLS regression are:

(i) The predictor variable values (e.g., mass fractions of glass components) are known or measured without uncertainty, or at least that the uncertainty is small relative to the uncertainty in response variable (glass property) values

(ii) The testing and/or measurement errors in a response variable (glass property) over a model development data set are independently distributed. For ULS regression, the additional assumption is made that the errors are identically distributed (i.e., with zero mean and the same variance). For WLS regression, the errors are also assumed to have zero mean, but the variance can be different for different data points.

(iii) The errors from (ii) are normally (Gaussian) distributed.

Regarding assumption (i), the true composition of glasses in a model development data set are generally not known, and so any representation of glass composition selected (e.g., target compositions, analyzed compositions, or adjusted and normalized versions of analyzed compositions) will be subject to uncertainty. Weier and Piepel (2002) discuss a procedure for performing adjustments and weighted normalization of analyzed glass compositions that corrects for biases and reduces uncertainties in analyzed glass compositions. As long as representations of glass composition do not have significant biases (or those biases are appropriately corrected), it is generally expected that uncertainties will be small compared to uncertainties in glass property values. Further, uncertainties in glass compositions are expected to be small compared to errors in using empirical or semi-empirical model forms to approximate the true (but unknown) property-composition relationships. Hence, assumption (i) is sufficiently satisfied for most waste glass property-composition modeling situations.

The portion of assumption (ii) having to do with the independence of errors in testing and measuring properties may not be completely satisfied when model development data sets are comprised of subsets of data generated at different times or locations (e.g., different laboratories). There is the potential for errors in testing and measuring properties to vary for different subsets of data, and be more alike within the same subset of data. However, this issue has generally not been a problem in many past property-composition modeling efforts. If needed, *generalized least squares* methods that account for correlations among data points could be applied.

The "identically distributed" portion of assumption (ii) for ULS regression is not valid for some properties, because the variance of errors in testing and measurement of properties depends on the value of the property. For example, the variances of viscosity and durability results for waste glasses tend to increase as the values of these properties increase. In cases where the identically distributed (equal variance) assumption is violated, it can often be remedied by applying an appropriate mathematical transformation to the property values (e.g., a logarithmic transformation). The Box-Cox family of transformations contains transformations (including the logarithmic transformation) appropriate for many models (see Draper and Smith 1998). Such transformations also often yield better fitting empirical or semi-empirical property-composition

models. In some cases, a property transformation used in a particular model form may be preferred for some reason (e.g., provides a better fit), but does not satisfy the constant variance assumption of (ii). Or, it may be that the difference in variances across response values in the modeling data set cannot be rectified by a response transformation. In such cases, other regression methods such as WLS regression or generalized linear models (Myers et al. 2002) could be applied.

The assumption of normally distributed measurement and testing errors in the measured response variable values allows the use of normal theory regression tests and uncertainty equations associated with the fitted regression model. For example, normal theory confidence intervals and prediction intervals can be used (see Section C.6).

As discussed in preceding text, ULS regression requires that all response values for the modeling data have constant variance (i.e., uncertainty). WLS regression accounts for response values having different variations by using a weight for each data point (w_i). Often, w_i is chosen to be proportional to the reciprocal of the variance (squared standard deviation) of the response for the i^{th} data point (y_i).

$$w_i = \frac{\lambda}{Var(y_i)} = \frac{\lambda}{[SD(y_i)]^2}$$

where λ is a proportionality constant (which could be 1). Thus, in such a WLS regression the weighted response values $\sqrt{w_i}\, y_i$ then have equal variance. However, other methods for selecting weights can be applicable for various situations.

In summary, assumptions of ULS regression may not be completely satisfied for typical property-composition data sets and models. Violations of the constant variance assumption for property values over a modeling data set can sometimes be addressed by appropriate property transformations so that ULS regression may be used. Other violations may be small enough that ULS regression methods can still be used without significant consequence. However, if there are large enough differences in variances of property values across a modeling data set that cannot be addressed by a property transformation, then WLS regression methods should be used.

C.3 Statistical Methods for Model Evaluation

There are many statistical methods (both numerical and graphical) for assessing models. *Evaluation methods* assess a model with the data used to develop the model. Such data are referred to as *model development data*. The goals of model evaluation are to assess: (1) how well a model fits the data used to develop it, (2) how well the least squares or other regression method assumptions are satisfied (see Section C.2), and (3) whether there are any outlying or influential data points that significantly affect the fitted model. Problems detected by model evaluation such as violation of assumptions, detection of outlying data points, or detection of model inadequacy require implementing various remedies in the model development process until the problem(s) are corrected. When the model being evaluated acceptably fits the data used to develop the

model, *model validation* methods should be applied using data not used to develop the model. Such data are referred to as *model validation data*. If model validation data are not available, *crossvalidation methods* can be applied using the model development data. Crossvalidation methods leave out one or more data points at a time, so that some of the data are used for model development and some for model validation. Such methods are also referred to as data-splitting validation methods, where part of the data is used for model development and evaluation, while the other part is used for validation. Draper and Smith (1998) and Montgomery et al. (2001) discuss statistical methods for evaluating and validating models.

Model evaluation techniques include predicted versus measured (PvM) property plots, standardized residual plots, outlier diagnostics, three R^2 statistics, root mean squared error (*RMSE*), and statistical lack-of-fit (LOF) tests. Each of these is explained briefly below. The following notation is used in the subsequent descriptions and definitions:

n = the number of data points used to fit a model,

p = the number of parameters in a model form estimated via regression on the data,

y_i = the measured property value (mathematically transformed, if appropriate for the model form used) for the i^{th} data point,

$\hat{y}_i$ = the predicted property value (mathematically transformed, if appropriate for the model form used) for the i^{th} data point made using the model fitted to all n data points,

r_i = the residual for the i^{th} data point = $y_i - \hat{y}_i$,

$\hat{y}_{(i)}$ = the predicted property value (mathematically transformed, if appropriate for the model form used) for the i^{th} data point made using a model fitted to all n data points except the i^{th},

w_i = the weight applied to the i^{th} data point in cases where WLS regression is used. Typically, w_i is proportional to the reciprocal of the variance of the response variable for the i^{th} data point,

$\bar{y}$ = the unweighted average (mean) of the n measured property values (mathematically transformed, if appropriate for the model form used),

$\bar{y}_w$ = the weighted average (mean) of the n measured property values (mathematically transformed, if appropriate for the model form used)

$$\bar{y}_w = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i} \tag{C.8}$$

The model evaluation methods are now briefly described.

- *Predicted versus measured (PvM) property plots* show how well model predicted values $\hat{y}_i$ compare to the measured values y_i for the glasses in the model development data set. Predicted property values $\hat{y}_i$ are plotted on the *y*-axis and measured property values y_i are plotted on the *x*-axis. A line with slope one is included in the plot for reference purposes, and represents the ideal of predicted values equaling measured values. Plotted points falling above this line correspond to glasses for which the model over-predicts the property, while plotted points falling below this line represent glasses for which the model under-predicts the property. A preponderance of plotted points in a portion of the plot falling above or below the line indicates that the model tends to yield biased predictions for that range of property values. Plotted points far from the line are outlying or potentially influential data points.

  For WLS regression, an *ordinary (unweighted) PvM plot* of $\hat{y}_i$ versus y_i could be viewed as is done for ULS regression. Or, a *weighted PvM plot* of $\sqrt{w_i}\,\hat{y}_i$ versus $\sqrt{w_i}\,y_i$ could be viewed. The unweighted PvM plot has the advantage of retaining the units of the response (or its transformation), but the disadvantage that points with smaller weights (i.e., higher uncertainties) may appear farther from the line with slope one. However, rather than considering this a disadvantage, it may be better thought of as showing the penalty paid in obtaining predictions having more uncertainty for modeling data points with smaller weights (i.e., higher uncertainty). The weighted PvM plot would show the model predictive performance for the modeling data points after accounting for (i.e., removing the scatter due to) the differing weights (i.e., uncertainties).

- *RMSE* is given by

$$RMSE_U = \sqrt{\frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{n - p}} \tag{C.9a}$$

  for ULS regression, and by

$$RMSE_W = \sqrt{\frac{\sum_{i=1}^{n} w_i (\hat{y}_i - y_i)^2}{n - p}} \tag{C.9b}$$

  for WLS regression. If the fitted model is adequate and does not have a statistically significant lack-of-fit, this statistic provides an estimate of the experimental and

measurement uncertainty standard deviation associated with melting glasses and measuring the associated property. The statistic *RMSE* is included as standard output in most regression software, and has units the same as the property values y_i (including any mathematical transformation of the property in the model form) for ULS regression and the units of $\sqrt{w_i}\, y_i$ for WLS regression.

- *Standardized residual plots* display standardized residuals (s_i, differences in predicted and measured property values divided by their standard deviations) versus various quantities, such as: glass component mass fractions (x_i), predicted property values ($\hat{y}_i$), or an index associated with each data point. The formula for a standardized residual is given by

$$s_i = \frac{r_i}{RMSE_U \left[1 - \boldsymbol{a}_i^T \left(\boldsymbol{A}^T \boldsymbol{A} \right)^{-1} \boldsymbol{a}_i \right]^{0.5}} \tag{C.10a}$$

for ULS regression, and by

$$s_i = \frac{\sqrt{w_i}\, r_i}{RMSE_W \left[1 - w_i \boldsymbol{a}_i^T \left(\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A} \right)^{-1} \boldsymbol{a}_i \right]^{0.5}} \tag{C.10b}$$

for WLS regression. In Equations (C.10a) and (C.10b): s_i, w_i, and r_i are as previously described; $RMSE_U$ and $RMSE_W$ are respectively given by Equations (C.9a) and (C.9b); $\boldsymbol{a}_i$ is the composition (column) vector for the i^{th} modeling data point expanded in the form of the model; $\boldsymbol{A}$ is an $n \times p$ matrix of the compositions in the modeling data set expanded in the form of the model; and $\boldsymbol{W}$ is an $n \times n$ matrix with the weights w_i along the main diagonal, and zeros elsewhere.

Patterns in the s_i versus $\hat{y}_i$ plot can indicate a violation of the least squares regression assumptions and suggest a property transformation to remedy the situation. Patterns in the s_i versus x_i plots can indicate inadequacies of the model or least squares assumptions. Standardized residuals are typically used in residual plots because the majority should fall within the range of ± 2.0 or 2.5. Comparing standardized residuals to such a range provides an easy criterion for judging whether a data point is possibly outlying or influential.

- *Normality plots* display normal scores versus the ordered (from smallest to largest) standardized residuals (from Equations (C.10a) or (C.10b) for ULS and WLS regression, respectively) for the *n* data points used to fit the model being assessed. Normal scores are the expected values of a sample of size *n* from standard normal distribution (with mean 0 and standard deviation 1). The plotted points are compared to the ideal of a straight line corresponding to a normal distribution. A straight middle portion of the plot with curved "tails" on each end of the plot indicate the presence of outlying data points, which cause a heavier-tailed distribution than the normal distribution.

- *Outlier diagnostics and plots* indicate data points that are outlying or influential with respect to property value or composition. There are too many of these diagnostics and plots to discuss here, but several produced by the R software (Ihaka and Gentleman 1996) and the SAS software (2001) were considered in this work. Draper and Smith (1998) and Montgomery et al. (2001) discuss outlier diagnostics and plots for ULS regression, but software such as R and SAS produce the appropriate weighted versions of diagnostics and plots for WLS as well as ULS regression.

- *R^2 statistics* quantify the proportion of variation in the property values y_i (for ULS regression) or weighted property values $\sqrt{w_i}\,y_i$ (for WLS regression) accounted for by the fitted model. Three R^2 statistics are used, as discussed later in this section.

- A *statistical lack-of-fit (LOF) test* checks whether the differences (for ULS regression) or weighted differences (for WLS regression) between measured and predicted property values from a fitted model are larger than expected based on the experimental and measurement uncertainty in the data. If the predicted versus measured differences are larger than data uncertainty at a high enough statistical confidence (e.g., greater than 90%), the model is said to have a statistically significant LOF. Replicate data points containing all applicable sources of experimental and measurement uncertainty[1] are required to perform statistical LOF tests. This process is conducted using a LOF F-test given by

$$F = \frac{(\text{SSE} - \text{SSPE})/(n - p - f)}{\text{SSPE}/f} = \frac{\left[\left(\sum_{i=1}^{n}(\hat{y}_i - y_i)^2 - \sum_{k=1}^{K}\sum_{j=1}^{m_k}(y_{kj} - \bar{y}_k)^2\right)\Big/(n-p-f)\right]}{\sum_{k=1}^{K}\sum_{j=1}^{m_k}(y_{kj} - \bar{y}_k)^2\Big/f} \qquad \text{(C.11a)}$$

  for ULS regression, and by

[1] To be appropriate replicate data points, two or more glass samples of the same composition must be batched and melted at different times, and have their properties measured at different times. It is insufficient, for example, to batch and melt a glass once, and measure its properties several times (because the batching and melting sources of uncertainty are not included in the data). Similarly, replicate samples should not be measured at the same time (or close in time) because all sources of measurement uncertainty will not be included in the data.

$$F = \frac{(\text{SSE} - \text{SSPE})/(n - p - f)}{\text{SSPE}/f}$$

$$= \frac{\left[\left(\sum_{i=1}^{n} w_i(\hat{y}_i - y_i)^2 - \sum_{k=1}^{K}\sum_{j=1}^{m_k} w_j(y_{kj} - \bar{y}_k)^2\right) \Big/ (n - p - f)\right]}{\sum_{k=1}^{K}\sum_{j=1}^{m_k} w_j(y_{kj} - \bar{y}_k)^2 \Big/ f} \qquad \text{(C.11b)}$$

for WLS regression. In Equations (C.11a) and C.11b): SSE = sum of squares error; SSPE = sum of squared pure error (i.e., from replicates); n and p are as described previously such that $n–p$ is the degrees of freedom for SSE; and the degrees of freedom for pure error is given by $f = \sum_{k=1}^{K}(m_k - 1)$, where m_k is the number of replicate data points in the k^{th} replicate set, k = 1, 2, …, K. In practice, if the F-test is statistically significant at a significance level of 0.05 or smaller (i.e., 95% confidence or higher), then it would be concluded that the fitted model has a statistically significant LOF for the modeling dataset. See Draper and Smith (1998) or Montgomery et al. (2001) for additional discussion of the statistical test for model LOF.

Even when a fitted model has a statistically significant LOF, the LOF may not be "practically significant". An example of such a situation is when a fitted model yields biased predictions for higher and/or lower values of a property or in a particular subregion of compositions, but the model will not be applied to such areas in practice. Another example is when the model fits the data very well (e.g., $R^2 > 0.95$) without bias over the model's region of validity, but the LOF is statistically significant because the experimental and measurement uncertainty is very small (e.g., because glasses can be batched, melted, and properties measured with excellent repeatability). Finally, a statistically significant LOF may not be practically significant if the uncertainty in model predictions is considerably smaller than uncertainty that can be tolerated and still meet requirements.

The model evaluation techniques discussed in the preceding bullets are included in, or can be obtained from, the output of the R software (Ihaka and Gentleman 1996) and SAS software (2001). See Draper and Smith (1998) or Montgomery et al. (2001) for further discussion of the concepts.

Three different R^2 statistics are useful in evaluating models fitted to glass property-composition data. The *(ordinary) R^2 statistic* is given by

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \qquad \text{(C.12a)}$$

for ULS regression, and by

$$R^2 = 1 - \frac{\sum_{i=1}^{n} w_i (\hat{y}_i - y_i)^2}{\sum_{i=1}^{n} w_i (y_i - \bar{y}_w)^2} \tag{C.12b}$$

for WLS regression, where $\bar{y}_w$ in Equation (C.12b) is the weighted mean whose formula is given in Equation (C.8). R^2 is interpreted as the fraction of variability in the unweighted (for ULS regression) or weighted (for WLS regression) property data (transformed if appropriate) accounted for by the fitted model. The *adjusted R^2 statistic* is given by

$$R_A^2 = 1 - \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2 \Big/ (n-p)}{\sum_{i=1}^{n} (y_i - \bar{y})^2 \Big/ (n-1)} \tag{C.13a}$$

for ULS regression, and by

$$R_A^2 = 1 - \frac{\sum_{i=1}^{n} w_i (\hat{y}_i - y_i)^2 \Big/ (n-p)}{\sum_{i=1}^{n} w_i (y_i - \bar{y}_w)^2 \Big/ (n-1)} \tag{C.13b}$$

for WLS regression. R_A^2 is interpreted as the adjusted fraction of variability in the unweighted or weighted property data (transformed if appropriate) accounted for by the fitted model. The adjustment is for the number of parameters (p) and number of data points (n) used in fitting the model. The *predicted R^2 statistic* is given by

$$R_P^2 = 1 - \frac{\sum_{i=1}^{n} (\hat{y}_{(i)} - y_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}, \tag{C.14a}$$

for ULS regression, and by

$$R_P^2 = 1 - \frac{\sum_{i=1}^{n} w_i (\hat{y}_{(i)} - y_i)^2}{\sum_{i=1}^{n} w_i (y_i - \bar{y}_w)^2}, \tag{C.14b}$$

for WLS regression. R_P^2 is interpreted as the leave-one-out crossvalidation fraction of variability in the unweighted or weighted property data (transformed if appropriate) accounted for by the fitted model. This statistic is calculated by a method equivalent to leaving each data point out of the model fit, and then evaluating how well the model predicts the property for that data point. R_P^2 estimates the fraction of variability that would be explained in predicting new observations drawn from the same composition space.

Generally R^2 statistics take values between 0 and 1. However, R_A^2 and R_P^2 can take negative values for a poor fitting model, a model that contains many more terms than needed to fit the data, or a model fitted to data with one or more very influential data points. Among the three R^2 statistics, typically $R^2 > R_A^2 > R_P^2$. More than a minor difference between R^2 and R_A^2 indicates that the model may contain more terms than needed to achieve the same goodness of fit. A substantial difference between R^2 and R_P^2 is indicative of one or more data points being very influential in determining the fit of the model. Some reduction from R^2 to R_P^2 is expected because R^2 corresponds to using all data to fit the model, whereas R_P^2 corresponds to leaving each data point out of the fit when evaluating the performance of the model for that point. In general, a model will tend to predict better for data used to fit it than for data not used to fit it. R_P^2 is a crossvalidation evaluation method.

C.4 Statistical Methods for Model Reduction and Augmentation

Section C.4.1 discusses methods for identifying and removing unnecessary terms from mixture experiment models. Section C.4.2 discusses methods for augmenting linear mixture models with quadratic terms.

C.4.1 Statistical Methods for Reducing Mixture Experiment Models

In evaluating a fitted regression model, it may often be determined that there are unnecessary terms in the model. Such terms may not improve, and can even degrade, the predictive performance of the model in applications to data not used to develop the model.

The most basic statistical method to identify unnecessary terms in a model is a *t-test* to perform a hypothesis test of whether the coefficient of a model term is statistically different from zero. The t-test computes a t-statistic equal to a model coefficient divided by the standard deviation of the coefficient. The t-statistic is then compared to the Student-t probability distribution to determine the probability of getting a t-statistic at least that large. The resulting probability is referred to as a *p-value*, and represents the probability of incorrectly deciding a coefficient is significantly different than zero. Most regression software outputs estimated model coefficients, coefficient standard deviations, t-statistics, and p-values. Typically, practitioners require a p-value to be smaller than 0.05 or 0.01 as strong evidence that the coefficient is significantly different than zero, and thus that the corresponding model term is needed. If there are not too many potentially unnecessary terms in a model, a practitioner can assess the t-statistics and p-values for the coefficients in a "full" model, and remove the model term whose coefficient is least statistically significant. Then, the model would be refitted without that term, and the t-statistics and p-values again considered, deleting the model term with the least statistically significant coefficient. This process continues until all terms in the model have p-values lower than 0.05, say. *Backward elimination* (Draper and Smith 1998, Montgomery et al. 2001) is a widely used statistical method for removing unneeded terms from a model. This method basically automates the process just described, where the practitioner sets a stopping criterion.

Unfortunately, there are some model forms for which the model reduction methods just described are inappropriate. In general, these are model forms where a model coefficient being small (e.g., near zero) does not imply the corresponding model term is unneeded. That, is some model forms may have terms with significant effects even though the coefficients of those terms are small. One class of models in this category relevant to this work is the class of *mixture experiment models* (Cornell 2002), of which LM and PQM models are given in Section C.1.1. The LM model (or the linear blending portion of a PQM model) is of the form $\sum_{i=1}^{q} b_i x_i$, where the b_i are coefficients and the x_i are proportions of the mixture components (e.g., mass fractions of waste glass components) that must sum to one (i.e., $\sum_{i=1}^{q} x_i = 1$). When each x_i can vary from zero to one, the coefficient b_i represents the estimated response variable value for pure component i [i.e., when $x_i = 1$ and $x_j = 0$ ($j \neq i$)]. When the ranges of the mixture component proportions x_i are constrained, each b_i represents extrapolated response values for pure component i. Because hypotheses concerning LM model coefficients (or the coefficients of linear terms in PQM models) equaling zero are not related to the importance or non-importance of a given component, it is inappropriate to use t-tests or the standard backward elimination method to reduce the linear portion of a mixture experiment model. However, mixture models can contain nonlinear terms in the components (such as in the PQM model form discussed in Section C.1.1), and it is appropriate to use t-tests or the standard stepwise, forward, or backward elimination *variable selection methods* (see Draper and Smith 1998 or Montgomery et al. 2001) on such terms.

Component response trace plots (Cornell 2002) provide for graphically assessing the effects of mixture components on a response variable of interest. These plots are generally produced using a fitted mixture model. The model is used to predict, for each component, the response for a series of compositions lying along an *effect direction* for that component. The most commonly used effect direction corresponds to subtracting or adding a component to a reference (or baseline) mixture. Along such a direction, the component of interest is varied within the allowable composition region of interest. The changes in the component of interest are offset by changes in the remaining components, such that they remain in the same relative proportions as in the reference mixture. The predicted response values along the effect direction for a given component form a *component response trace*. The response traces for the components varied in a mixture experiment plotted together form the *component response trace plot*. The predicted response values are plotted on the y-axis and changes in each component from its reference mixture value are plotted on the x-axis. Components with steeper response traces have stronger effects on the response. A response trace that is nearly horizontal indicates the corresponding component has little or no effect on the response. Components whose response traces are very close may have similar effects on the response. Thus, component response trace plots can be used to guide the reduction of components appearing in a mixture experiment model (e.g., see Piepel and Redgate 1997).

A special backward elimination method for mixture experiments can be used to reduce linear mixture models and linear portions of mixture models. The reduction method is performed in stages. In the first stage, each mixture component in turn is dropped from the model, the

remaining mixture component proportions are renormalized to sum to one, and then a linear mixture model without the dropped component is fitted to the data. The dropped mixture component that causes the smallest increase in the error sums of squares (the quantity being minimized in ULS regression) is then the first component to be permanently dropped from the model. Similar stages continue, with one component dropped at the end of each stage, until dropping a component causes the full-reduced model F-test (Draper and Smith 1998, Montgomery et al. 2001) to declare a statistically significant increase in the error sum of squares. This then signals the stopping point for the backward elimination algorithm. After each component is dropped, the remaining components are renormalized according to the mixture experiment definition that a response variable depends only on the relative proportions of the mixture components that affect the response variable (Cornell 2002). Hence, only the normalized proportions of components affecting the response are used in developing mixture experiment models.

C.4.2 Statistical Methods for Adding Terms to Models

It is often of interest to add additional terms onto a starting model in the hopes of improving the predictive performance of the starting model. For example, a linear mixture model may be considered as a starting model. However, if it has a significant LOF, adding nonlinear composition terms may be considered in hopes of improving the predictive performance of the model. *Stepwise regression* is the most commonly used method to add terms to an existing starting model. In stepwise regression, certain terms can be forced into the model, and a candidate list of possible terms to add is identified. The procedure identifies the term from the candidate list that, if added to the model, would yield the greatest reduction in the error sum of squares (i.e., the sum of squared differences in measured and model-predicted values across the modeling data set). If the reduction is statistically significant, that term is added to the model. Stepwise regression proceeds in stages, with one additional term being added at each stage unless the user-selected stopping criterion is reached. After adding a term, stepwise regression checks all other terms in the model to assess if they are still statistically significant. If not, a term can be removed during a stage.

The stepwise regression algorithm requires that a significance level be specified for terms to enter the model, and that a significance level be specified for terms to remain in the model. In each iteration of a stepwise regression application, t-tests are conducted for each term already in the model and for terms being considered for inclusion in the model. To describe the results of these t-tests, a p-value is calculated for each of the terms. Loosely speaking, the p-values represent the probability that the respective model terms do <u>not</u> make a significant contribution to the predictive ability of the model. Terms whose corresponding p-values are small (often <0.05 is considered sufficiently small) are considered important in the model. The significance levels specified for the stepwise regression algorithm indicate how small p-values must be for the corresponding terms to be included in the model. The statistical literature generally indicates that the stepwise algorithm is somewhat liberal in allowing terms into models. Yet, models containing unnecessary terms are undesirable because they tend to have inflated prediction variance. Thus, it is typically advisable to use tight significance levels such as 0.05 or 0.01 when applying the stepwise regression algorithm.

One particular variation of stepwise regression that can be used to select terms for model building is what the SAS statistical software package (SAS 2001) refers to as the Maximum R-squared Improvement (MAXR) selection method. For the MAXR criterion (as with other criteria for stepwise regression), terms can enter and leave (being replaced by another term) the model. Sequential changes to the model are based on maximal increases to the model's R^2 value, and MAXR tries to find the "best" model having a specified numbers of terms. However, MAXR is not the same as the "best subsets" algorithm because it does not consider all possible models with a given number of terms. Therefore, MAXR is not guaranteed to find the model with the highest R^2 value among all models having a given number of terms. This method tends to have a better chance of finding more nearly optimal models than does the stepwise selection method using other criteria (Freund and Littell, 1995). The MAXR method does not require significance levels to control term selection, but does require the user to identify any terms to force into the model and to specify the number of terms to include in models being considered.

The standard stepwise regression procedure (regardless of the criterion used for model term selection) is not appropriate for linear mixture models or linear portions of other mixture experiment models for similar reasons as described previously with regard to the standard backward elimination method. However, it is appropriate for adding nonlinear mixture terms or non-mixture terms to mixture models.

C.5 Statistical Methods for Model Validation

Model validation methods assess how well a fitted model predicts property values for glasses not used in fitting the model. The glasses used for validation ideally should be in the same composition region as the data used to fit the property-composition models, because (in general) fitted empirical and semi-empirical models should not be used to extrapolate much beyond the region covered by the modeling data. Also, ideally the validation data should be evenly distributed over the model composition region of model validity to properly assess predictive ability over the region. However, this is difficult to achieve in practice because validation data is typically not designed, but often consists of whatever extra data are available.

Validation generally consists of using a fitted model to predict property values for a set of validation data, and then comparing the predicted property values to the measured values from the validation database. Assessment of these comparisons is aided by plotting the predicted versus the measured property values for each data point. Such *predicted versus measured plots* are the same as described in Section C.3, except model validation data are used instead of model development data. Also, similarly as described in Section C.3, *unweighted PvM plots* or *weighted PvM plots* may be produced and viewed to validate models fitted by WLS regression.

Statistical comparisons of predicted and measured response values are also useful to see if differences are larger than their expected uncertainties. One such comparison is the *validation* R^2 statistic, which in general is given by

$$R_V^2 = 1 - \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}. \qquad \text{(C.15a)}$$

However, in cases where WLS regression is used to fit the model and corresponding weights are available, a weighted version of the *validation* R^2 statistics is given by

$$R_V^2 = 1 - \frac{\sum_{i=1}^{n} w_i (\hat{y}_i - y_i)^2}{\sum_{i=1}^{n} w_i (y_i - \bar{y}_w)^2}. \qquad \text{(C.15b)}$$

R_V^2 is interpreted as the fraction of variability in the unweighted or weighted property values (transformed if appropriate) in the validation data accounted for by the fitted model. Note that R_V^2 is defined exactly the same as the ordinary R^2 defined in Equations (C.12a) and (C.12b), except that model validation data are used to assess model predictive performance instead of the model development data. Hence, the y_i, $\hat{y}_i$, $\bar{y}$, w_i, and $\bar{y}_w$ values in Equations (C.15a) and (C.15b) correspond to the model validation data.

Generally $R_V^2 \le R_P^2 \le R_A^2 \le R^2 \le 1$. However, R_V^2 can take negative values (when a model predicts a validation set very poorly) and can take values larger than R_P^2, R_A^2, or R^2 (when a model predicts a particular validation dataset better than estimated by these statistics based on the modeling data).

Another useful statistical technique, which can be combined with the plot of predicted versus measured property values for the validation data set, is to include error bars consisting of 95% two-sided prediction intervals (95% PIs) on the predicted values. Then, if the error bar for a given validation data point overlaps a line with slope one superimposed on the PvM plot, the model is validated for that data point. Draper and Smith (1998) and Montgomery et al. (2001) provide additional discussion of 95% PIs for regression models. The formulas for a 95% two-sided PI in the ULS and WLS cases are given in Section C.6 following.

C.6 Statistical Methods for Describing Uncertainties in Model Predictions

Several types of statistical intervals are available to describe the uncertainty associated with model predictions. Each type of statistical interval has a particular interpretation. The following two types of statistical intervals are used to describe the uncertainty associated with model predictions at a single specific composition.

A *100(1–α)% upper confidence interval (UCI)* for the true mean response value for a given glass composition $\boldsymbol{x} = (x_1, x_2, \ldots, x_q)$ is given by

$$\begin{aligned} \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p}\sqrt{\boldsymbol{a}^T \boldsymbol{C}_U\ \boldsymbol{a}} &= \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p}\sqrt{\boldsymbol{a}^T [(\boldsymbol{A}^T \boldsymbol{A})^{-1} MSE_U]\,\boldsymbol{a}} \\ &= \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p} RMSE_U \sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{a}} \end{aligned}, \qquad \text{(C.16a)}$$

for ULS regression, and by

$$\begin{aligned} \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p}\sqrt{\boldsymbol{a}^T \boldsymbol{C}_W\ \boldsymbol{a}} &= \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p}\sqrt{\boldsymbol{a}^T [(\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A})^{-1} MSE_W]\,\boldsymbol{a}} \\ &= \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p} RMSE_W \sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A})^{-1} \boldsymbol{a}} \end{aligned}, \qquad \text{(C.16b)}$$

for WLS regression. In Equations (C.16a) and (C.16b)

$\hat{y}(\boldsymbol{x})$ = the model predicted value at composition $\boldsymbol{x}$,

$100(1-\alpha)$ = the desired confidence (e.g., 90%) for the confidence interval, where α denotes the significance level (e.g., $\alpha = 0.10$ for 90% confidence),

$t_{1-\alpha,n-p}$ = the $100(1-\alpha)$-percentile of the Student's t-distribution with n-p degrees of freedom,

n = the number of data points used to fit the model,

p = the number of parameters estimated in the model,

$\boldsymbol{C_U}$ = the estimated variance-covariance matrix for a model fitted by ULS regression = $(\boldsymbol{A}^T \boldsymbol{A})^{-1} MSE_U$,

$\boldsymbol{C_W}$ = the estimated variance-covariance matrix for a model fitted by WLS regression = $(\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A})^{-1} MSE_W$,

$\boldsymbol{a^T}$ = the vector transpose of the glass composition vector $\boldsymbol{x}$ expanded in the form of the model,

$\boldsymbol{A^T}$ = the matrix transpose of the composition matrix (used to estimate the model coefficients via regression) expanded in the form of the model,

$\boldsymbol{W}$ = an $n \times n$ diagonal weight matrix with entries w_i, $i = 1, 2, \ldots, n$ (i.e., the weights associated with the model development set of n data points),

MSE = mean squared error, which is obtained from the ULS (MSE_U) or WLS (MSE_W) regression fit of the model,

$RMSE$ = the root mean squared error = $\sqrt{MSE}$, with $RMSE_U$ and $RMSE_W$ resulting from ULS and WLS regression fits of a model, respectively.

A $100(1-\alpha)$% UCI is appropriate when an uncertainty statement is desired about the true mean response for a given composition $\boldsymbol{x}$.

A *100(1–α)% two-sided prediction interval (PI)* for an individual response value for a given composition $\boldsymbol{x}$ is given by

$$\hat{y}(\boldsymbol{x}) \mp t_{1-\alpha/2,n-p}\sqrt{MSE_U + \boldsymbol{a}^T \boldsymbol{C}_U\ \boldsymbol{a}} = \hat{y}(\boldsymbol{x}) \mp t_{1-\alpha/2,n-p} RMSE_U \sqrt{1 + \boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{a}}\ , \quad \text{(C.17a)}$$

for ULS regression, and by

$$\hat{y}(\boldsymbol{x}) \mp t_{1-\alpha/2,n-p}\sqrt{\frac{MSE_W}{w_i} + \boldsymbol{a}^T \boldsymbol{C}_W\ \boldsymbol{a}} = \hat{y}(\boldsymbol{x}) \mp t_{1-\alpha/2,n-p} RMSE_W \sqrt{\frac{1}{w_i} + \boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A})^{-1} \boldsymbol{a}}\ , \quad \text{(C.17b)}$$

for WLS regression, where the notation is defined as in the preceding UCI definition. Note that the w_i under the square root applies when PIs are calculated for modeling data, validation data, or application data (i.e., data used in applying the models and PIs) with weights. In situations where validation or application data do not have weights, w_i should be set to 1. A 100(1−α)% PI is appropriately used when comparing a model predicted response value for a given composition to an individual measurement of the response for that composition. This type of application arises in validating the predictive performance of a model for one or more glass compositions not used to fit the model. Specifically, Equations (C.17a) and (C.17b) can be used to produce 95% PIs displayed as error bars in PvM plots, as described at the end of Section C.5.

At times it is desirable to describe the uncertainty associated with predictions obtained for a specified group of compositions. For example, a statement may be desired that indicates with high confidence that the predicted response value for every composition $\boldsymbol{x}$ in a specified group of compositions (or composition region) is below a particular regulatory limit. Such a confidence statement requires a statistical interval called a simultaneous upper confidence interval. The formula for a *100(1–α)% upper simultaneous confidence interval (SUCI)* is given by

$$\hat{y}(\boldsymbol{x}) + \sqrt{pF_{1-2\alpha;p,n-p}}\sqrt{\boldsymbol{a}^T \boldsymbol{C}_U\ \boldsymbol{a}} = \hat{y}(\boldsymbol{x}) + RMSE_U \sqrt{pF_{1-2\alpha;p,n-p}}\sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{a}} \quad \text{(C.18a)}$$

for ULS regression, and by

$$\hat{y}(\boldsymbol{x}) + \sqrt{pF_{1-2\alpha;p,n-p}}\sqrt{\boldsymbol{a}^T \boldsymbol{C}_W\ \boldsymbol{a}} = \hat{y}(\boldsymbol{x}) + RMSE_W \sqrt{pF_{1-2\alpha;p,n-p}}\sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A})^{-1} \boldsymbol{a}} \quad \text{(C.18b)}$$

for WLS regression. In Equations (C.18a) and (C.18b):

$\hat{y}(\boldsymbol{x})$ = the predicted response for each composition $\boldsymbol{x}$ in the specified composition set or region,

$F_{1-2\alpha,p,n-p}$ = the 100(1–2α)-percentile of the F-distribution with p and $n–p$ degrees of freedom.

The remaining notation in Equations (C.18a) and (C.18b) is the same as defined previously.

Equations (C.16), (C.17), and (C.18) yield statistical intervals in transformed units when a transformed property is modeled. For example, a natural logarithm transformation of a response y [i.e., ln(y)] is often used for property-composition models. Hence, the statistical intervals calculated using the preceding equations would be in ln(y) units. The statistical intervals can be transformed back to the original units of y by exponentiating the endpoint(s) of the statistical interval. However, the process of back-transforming (exponentiating) a statistical interval can change its interpretation. For example, if a 90% UCI in ln(y) units has the value "v", the back-transformed 90% UCI in the original units of y is given by e^v. The 90% UCI in units of ln(y) is a statement about the true mean response in ln(y) units for a given glass composition $\boldsymbol{x}$. However, the resulting back-transformed interval is a 90% UCI on the true median response value for the given composition $\boldsymbol{x}$, under the assumption that experimental errors in the data used to develop the model are lognormally distributed. This assumption corresponds to the assumption of the natural-log-transformed response data being normally distributed. This change in interpretation occurs because the mean and median of a normal distribution are the same, but the mean of a lognormal distribution is larger than the median of a lognormal distribution.

Hence, back-transforming a 90% UCI on a mean response for a given composition $\boldsymbol{x}$ (in ln-units) yields a 90% UCI on the median response for a given composition $\boldsymbol{x}$ in original units, which in turn underestimates a 90% UCI on the mean response for a given composition $\boldsymbol{x}$ in original units. Back-transforming *100(1–α)% SUCIs* given by Equation (C.18) in log-transformed units has a similar change in interpretation. Whereas the original *100(1–α)% SUCIs* are statements about the true mean values of responses in log-transformed response units for multiple compositions $\boldsymbol{x}$, the back-transformed *100(1–α)% SUCIs* are statements about the true median values of responses in original response units for multiple compositions $\boldsymbol{x}$. However, a *100(1–α)% PI* given by Equation (C.17) in log-transformed units does not have a change in interpretation when back-transforming, because the original statement (in log-transformed units) and the back-transformed statement (in original units) are both about a true individual response value.

Alternatives exist to using normal-theory-based Equations (C.16) through (C.18) and back-transforming them when a transformed response variable is modeled. One alternative is to modify the statistical interval equations so that the statistical statement is about the true mean response value in the original units for a given composition $\boldsymbol{x}$ [Equation C.16)] or set of compositions $\boldsymbol{x}$ [Equation (C.18)]. Although this type of alternative is discussed in the literature for non-regression problems (e.g., Gilbert 1987), no references were found for the regression context. Another alternative, the *generalized linear model* regression approach (Myers et al. 2002), avoids directly transforming the response variable and instead uses the transformation indirectly. These alternative approaches were not pursued in this work. However, the interested reader may refer to the references given.

Note that Equations (C.16) through (C.18) require knowledge of the variance-covariance matrix $\boldsymbol{C_U} = MSE_U(\boldsymbol{A}^T\boldsymbol{A})^{-1}$ for ULS regression and $\boldsymbol{C_W} = MSE_W(\boldsymbol{A}^T\boldsymbol{W}\boldsymbol{A})^{-1}$ for WLS regression. The MSE_U and MSE_W are mean squared errors equal to the squares of $RMSE_U$ and $RMSE_W$ given

by Equations (C.9a) and (C.9b). This information is included in the regression software output that comes with the estimates of the p model coefficients. A variance-covariance matrix is a $p \times p$ matrix with coefficient variances along the diagonal, and covariances between coefficient pairs in the off-diagonal entries.

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APPENDIX D

Variance-Covariance Matrices Associated With Coefficients of Phase 1 IHLW PCT and $T_{1\%}$ Models

APPENDIX D

Variance-Covariance Matrices Associated With Coefficients of Phase 1 IHLW PCT and $T_{1\%}$ Models

This appendix contains the variance-covariance matrices for the PCT and $T_{1\%}$ property-composition models for IHLW glasses that are recommended in this report.

Tables D.1 and D.2, respectively, contain the variance-covariance matrices for the two recommended ln(PCT-Boron) models: (1) the 19-term full linear mixture (LM) model given in Table 5.4, and (2) the 8-term reduced LM model given in Table 5.5. Tables D.3 and D.4, respectively, contain the variance-covariance matrices for the two recommended ln(PCT-Lithium) models: (1) the 19-term full LM model given in Table 5.7, and (2) the 8-term reduced LM model given in Table 5.8. Tables D.5 and D.6, respectively, contain the variance-covariance matrices for the two recommended ln(PCT-Sodium) models: (1) the 19-term full LM model given in Table 5.10, and (2) the 8-term reduced LM model given in Table 5.11.

Tables D.7 and D.8, respectively, contain the variance-covariance matrices for the two recommended $T_{1\%}$ spinel crystallinity models: (1) the 19-term full LM model given in Table 6.7, and (2) the 13-term reduced LM model given in Table 6.8.

Table D.1. Variance-Covariance Matrix Associated with the Estimated Model Coefficients (in Table 5.4) for the IHLW PCT-Boron 19-Term Full LM Model.

Term [(a)]	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
Al_2O_3	5.5244	-0.9478	-1.6181	10.9882	1.0643	-2.3858	-1.1572	-1.0586	2.3725	14.4595	-1.4187	-0.3538	-0.0659	1.4100	15.9993	1.1433	-0.0329	0.9627	-5.2234
B_2O_3	-0.9478	1.5471	1.8851	3.9748	-0.6216	0.7323	0.3371	0.3099	-1.1165	-12.3536	-2.5636	-0.1228	0.0848	0.3415	-7.4452	0.1793	-1.1029	-0.8049	2.0111
CdO	-1.6181	1.8851	66.2262	-67.3619	-1.6592	0.6654	0.0859	1.1455	-4.0807	-91.0989	-73.0249	-0.7416	-0.8154	0.7393	31.4307	11.1071	-2.6863	-0.5907	8.8578
Cr_2O_3	10.9882	3.9748	-67.3619	1157.3414	3.9445	-18.0070	-20.9536	-7.3246	-21.0921	68.8684	385.6416	0.2001	-0.9597	-3.9920	-283.5005	-24.4608	-1.9079	6.6270	-73.2404
Fe_2O_3	1.0643	-0.6216	-1.6592	3.9445	2.4222	-1.2936	-0.0891	-0.6527	-2.3828	15.3361	-0.7518	-0.2935	-0.0286	1.7470	-15.9408	-0.6541	0.1849	0.8563	-3.1041
Li_2O	-2.3858	0.7323	0.6654	-18.0070	-1.2936	9.9108	0.3374	2.2854	-5.6153	4.0732	-17.1556	-0.6284	0.7331	-0.8292	11.9410	0.4738	-2.1392	-2.3794	-0.4865
MnO	-1.1572	0.3371	0.0859	-20.9536	-0.0891	0.3374	4.7061	0.1488	-2.2427	-7.3269	-5.8852	0.1056	-0.7315	0.6940	-15.7529	-0.4773	-1.9689	-1.2500	0.6487
Na_2O	-1.0586	0.3099	1.1455	-7.3246	-0.6527	2.2854	0.1488	2.0824	-3.4548	-5.6081	-23.2255	-0.3245	0.7642	-0.0080	10.6438	0.4960	-1.1557	-1.0545	0.0003
NiO	2.3725	-1.1165	-4.0807	-21.0921	-2.3828	-5.6153	-2.2427	-3.4548	168.6306	27.4996	35.8826	0.3698	-5.8272	-9.8643	16.4980	9.3891	8.6819	-1.5382	-0.7852
Sb_2O_3	14.4595	-12.3536	-91.0989	68.8684	15.3361	4.0732	-7.3269	-5.6081	27.4996	2333.4178	273.5021	-4.1363	3.4168	-4.2316	-313.4611	-10.6886	-20.2193	4.1003	-79.8272
SeO_2	-1.4187	-2.5636	-73.0249	385.6416	-0.7518	-17.1556	-5.8852	-23.2255	35.8826	273.5021	3844.1096	2.2589	-10.1199	10.6025	-945.5139	-73.5548	25.9363	8.2273	-142.0299
SiO_2	-0.3538	-0.1228	-0.7416	0.2001	-0.2935	-0.6284	0.1056	-0.3245	0.3698	-4.1363	2.2589	0.2976	-0.1522	-0.4932	-3.9589	-0.3747	-0.1168	0.1394	0.7409
SrO	-0.0659	0.0848	-0.8154	-0.9597	-0.0286	0.7331	-0.7315	0.7642	-5.8272	3.4168	-10.1199	-0.1522	3.6121	1.8237	-13.3975	-1.9698	-2.1051	-0.4355	-0.3425
ThO_2	1.4100	0.3415	0.7393	-3.9920	1.7470	-0.8292	0.6940	-0.0080	-9.8643	-4.2316	10.6025	-0.4932	1.8237	10.0519	-47.7675	-5.3621	-2.0023	-0.6369	-3.0462
Tl_2O	15.9993	-7.4452	31.4307	-283.5005	-15.9408	11.9410	-15.7529	10.6438	16.4980	-313.4611	-945.5139	-3.9589	-13.3975	-47.7675	2704.6934	77.2297	30.1474	0.4459	5.7554
UO_3	1.1433	0.1793	11.1071	-24.4608	-0.6541	0.4738	-0.4773	0.4960	9.3891	-10.6886	-73.5548	-0.3747	-1.9698	-5.3621	77.2297	11.9899	1.1821	-0.4849	2.1154
ZnO	-0.0329	-1.1029	-2.6863	-1.9079	0.1849	-2.1392	-1.9689	-1.1557	8.6819	-20.2193	25.9363	-0.1168	-2.1051	-2.0023	30.1474	1.1821	20.5020	0.7084	-3.6245
ZrO_2	0.9627	-0.8049	-0.5907	6.6270	0.8563	-2.3794	-1.2500	-1.0545	-1.5382	4.1003	8.2273	0.1394	-0.4355	-0.6369	0.4459	-0.4849	0.7084	3.2965	-1.7371
Spike	-5.2234	2.0111	8.8578	-73.2404	-3.1041	-0.4865	0.6487	0.0003	-0.7852	-79.8272	-142.0299	0.7409	-0.3425	-3.0462	5.7554	2.1154	-3.6245	-1.7371	91.4898

(a) The variance-covariance matrix for the 19-term model is for renormalized mass fractions of the listed components.

Table D.2. Variance-Covariance Matrix Associated with the Estimated Model Coefficients (in Table 5.5) for the IHLW PCT-Boron 8-Term Reduced LM Model.

Term [(a)]	Al_2O_3	B_2O_3	Li_2O	MnO	Na_2O	SiO_2	ThO_2	ZrO_2
Al_2O_3	2.9107	-0.4115	-1.2015	-0.2953	-0.5616	-0.0653	1.0062	0.3466
B_2O_3	-0.4115	0.7961	0.2909	0.1557	0.0865	-0.1463	0.3776	-0.3723
Li_2O	-1.2015	0.2909	5.4405	-0.2057	0.9592	-0.5017	-0.2438	-1.0954
MnO	-0.2953	0.1557	-0.2057	2.1481	0.0215	-0.0587	0.2270	-0.7287
Na_2O	-0.5616	0.0865	0.9592	0.0215	0.9950	-0.2315	0.0945	-0.4691
SiO_2	-0.0653	-0.1463	-0.5017	-0.0587	-0.2315	0.1372	-0.2555	0.1555
ThO_2	1.0062	0.3776	-0.2438	0.2270	0.0945	-0.2555	3.6391	-0.8087
ZrO_2	0.3466	-0.3723	-1.0954	-0.7287	-0.4691	0.1555	-0.8087	1.8799

(a) The variance-covariance matrix for the 8-term model is for renormalized mass fractions of the listed components.

Table D.3. Variance-Covariance Matrix Associated with the Estimated Model Coefficients (in Table 5.7) for the IHLW PCT-Lithium 19-Term Full LM Model.

Term [(a)]	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
Al_2O_3	3.5151	-0.6031	-1.0296	6.9915	0.6772	-1.5180	-0.7363	-0.6736	1.5095	9.2002	-0.9027	-0.2251	-0.0419	0.8972	10.1799	0.7274	-0.0209	0.6125	-3.3235
B_2O_3	-0.6031	0.9844	1.1994	2.5291	-0.3955	0.4659	0.2145	0.1972	-0.7104	-7.8603	-1.6312	-0.0782	0.0539	0.2173	-4.7372	0.1141	-0.7018	-0.5122	1.2796
CdO	-1.0296	1.1994	42.1381	-42.8607	-1.0557	0.4234	0.0546	0.7288	-2.5965	-57.9639	-46.4639	-0.4719	-0.5188	0.4704	19.9986	7.0672	-1.7093	-0.3758	5.6360
Cr_2O_3	6.9915	2.5291	-42.8607	736.3866	2.5098	-11.4574	-13.3322	-4.6604	-13.4203	43.8192	245.3739	0.1273	-0.6106	-2.5400	-180.3841	-15.5638	-1.2140	4.2166	-46.6010
Fe_2O_3	0.6772	-0.3955	-1.0557	2.5098	1.5412	-0.8231	-0.0567	-0.4153	-1.5161	9.7580	-0.4784	-0.1868	-0.0182	1.1116	-10.1427	-0.4162	0.1176	0.5449	-1.9751
Li_2O	-1.5180	0.4659	0.4234	-11.4574	-0.8231	6.3060	0.2147	1.4541	-3.5729	2.5917	-10.9157	-0.3999	0.4664	-0.5276	7.5978	0.3015	-1.3611	-1.5139	-0.3095
MnO	-0.7363	0.2145	0.0546	-13.3322	-0.0567	0.2147	2.9944	0.0947	-1.4270	-4.6619	-3.7446	0.0672	-0.4654	0.4416	-10.0232	-0.3037	-1.2527	-0.7953	0.4128
Na_2O	-0.6736	0.1972	0.7288	-4.6604	-0.4153	1.4541	0.0947	1.3250	-2.1982	-3.5683	-14.7778	-0.2065	0.4862	-0.0051	6.7724	0.3156	-0.7353	-0.6709	0.0002
NiO	1.5095	-0.7104	-2.5965	-13.4203	-1.5161	-3.5729	-1.4270	-2.1982	107.2954	17.4973	22.8312	0.2353	-3.7077	-6.2764	10.4972	5.9740	5.5241	-0.9787	-0.4996
Sb_2O_3	9.2002	-7.8603	-57.9639	43.8192	9.7580	2.5917	-4.6619	-3.5683	17.4973	1484.6939	174.0224	-2.6318	2.1740	-2.6925	-199.4472	-6.8009	-12.8650	2.6089	-50.7920
SeO_2	-0.9027	-1.6312	-46.4639	245.3739	-0.4784	-10.9157	-3.7446	-14.7778	22.8312	174.0224	2445.9083	1.4373	-6.4390	6.7461	-601.6063	-46.8010	16.5026	5.2348	-90.3700
SiO_2	-0.2251	-0.0782	-0.4719	0.1273	-0.1868	-0.3999	0.0672	-0.2065	0.2353	-2.6318	1.4373	0.1893	-0.0968	-0.3138	-2.5190	-0.2384	-0.0743	0.0887	0.4714
SrO	-0.0419	0.0539	-0.5188	-0.6106	-0.0182	0.4664	-0.4654	0.4862	-3.7077	2.1740	-6.4390	-0.0968	2.2983	1.1604	-8.5245	-1.2534	-1.3394	-0.2771	-0.2179
ThO_2	0.8972	0.2173	0.4704	-2.5400	1.1116	-0.5276	0.4416	-0.0051	-6.2764	-2.6925	6.7461	-0.3138	1.1604	6.3957	-30.3932	-3.4118	-1.2740	-0.4052	-1.9382
Tl_2O	10.1799	-4.7372	19.9986	-180.3841	-10.1427	7.5978	-10.0232	6.7724	10.4972	-199.4472	-601.6063	-2.5190	-8.5245	-30.3932	1720.9270	49.1393	19.1820	0.2837	3.6620
UO_3	0.7274	0.1141	7.0672	-15.5638	-0.4162	0.3015	-0.3037	0.3156	5.9740	-6.8009	-46.8010	-0.2384	-1.2534	-3.4118	49.1393	7.6288	0.7522	-0.3085	1.3460
ZnO	-0.0209	-0.7018	-1.7093	-1.2140	0.1176	-1.3611	-1.2527	-0.7353	5.5241	-12.8650	16.5026	-0.0743	-1.3394	-1.2740	19.1820	0.7522	13.0449	0.4507	-2.3062
ZrO_2	0.6125	-0.5122	-0.3758	4.2166	0.5449	-1.5139	-0.7953	-0.6709	-0.9787	2.6089	5.2348	0.0887	-0.2771	-0.4052	0.2837	-0.3085	0.4507	2.0975	-1.1053
Spike	-3.3235	1.2796	5.6360	-46.6010	-1.9751	-0.3095	0.4128	0.0002	-0.4996	-50.7920	-90.3700	0.4714	-0.2179	-1.9382	3.6620	1.3460	-2.3062	-1.1053	58.2126

(a) The variance-covariance matrix for the 19-term model is for renormalized mass fractions of the listed components.

Table D.4. Variance-Covariance Matrix Associated with the Estimated Model Coefficients (in Table 5.8) for the IHLW PCT-Lithium 8-Term Reduced LM Model.

Term [(a)]	Al_2O_3	B_2O_3	Li_2O	MnO	Na_2O	SiO_2	ThO_2	ZrO_2
Al_2O_3	1.7844	-0.2523	-0.7366	-0.1810	-0.3443	-0.0400	0.6169	0.2125
B_2O_3	-0.2523	0.4880	0.1784	0.0955	0.0530	-0.0897	0.2315	-0.2283
Li_2O	-0.7366	0.1784	3.3354	-0.1261	0.5880	-0.3076	-0.1494	-0.6716
MnO	-0.1810	0.0955	-0.1261	1.3169	0.0132	-0.0360	0.1392	-0.4468
Na_2O	-0.3443	0.0530	0.5880	0.0132	0.6100	-0.1419	0.0579	-0.2876
SiO_2	-0.0400	-0.0897	-0.3076	-0.0360	-0.1419	0.0841	-0.1566	0.0953
ThO_2	0.6169	0.2315	-0.1494	0.1392	0.0579	-0.1566	2.2310	-0.4958
ZrO_2	0.2125	-0.2283	-0.6716	-0.4468	-0.2876	0.0953	-0.4958	1.1525

(a) The variance-covariance matrix for the 8-term model is for renormalized mass fractions of the listed components.

Table D.5. Variance-Covariance Matrix Associated with the Estimated Model Coefficients (in Table 5.10) for the IHLW PCT-Sodium 19-Term Full LM Model.

Term [(a)]	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
Al_2O_3	2.4410	-0.4188	-0.7150	4.8551	0.4703	-1.0542	-0.5113	-0.4678	1.0483	6.3890	-0.6269	-0.1563	-0.0291	0.6230	7.0693	0.5052	-0.0145	0.4254	-2.3080
B_2O_3	-0.4188	0.6836	0.8329	1.7563	-0.2747	0.3236	0.1490	0.1369	-0.4933	-5.4585	-1.1327	-0.0543	0.0374	0.1509	-3.2897	0.0792	-0.4873	-0.3557	0.8886
CdO	-0.7150	0.8329	29.2621	-29.7640	-0.7331	0.2940	0.0379	0.5061	-1.8031	-40.2522	-32.2661	-0.3277	-0.3603	0.3267	13.8877	4.9077	-1.1870	-0.2610	3.9138
Cr_2O_3	4.8551	1.7563	-29.7640	511.3727	1.7429	-7.9564	-9.2584	-3.2364	-9.3196	30.4296	170.3962	0.0884	-0.4240	-1.7639	-125.2650	-10.8080	-0.8430	2.9281	-32.3614
Fe_2O_3	0.4703	-0.2747	-0.7331	1.7429	1.0703	-0.5716	-0.0394	-0.2884	-1.0529	6.7763	-0.3322	-0.1297	-0.0127	0.7719	-7.0435	-0.2890	0.0817	0.3784	-1.3716
Li_2O	-1.0542	0.3236	0.2940	-7.9564	-0.5716	4.3791	0.1491	1.0098	-2.4811	1.7998	-7.5802	-0.2777	0.3239	-0.3664	5.2762	0.2094	-0.9452	-1.0513	-0.2150
MnO	-0.5113	0.1490	0.0379	-9.2584	-0.0394	0.1491	2.0794	0.0657	-0.9909	-3.2374	-2.6004	0.0467	-0.3232	0.3066	-6.9604	-0.2109	-0.8700	-0.5523	0.2866
Na_2O	-0.4678	0.1369	0.5061	-3.2364	-0.2884	1.0098	0.0657	0.9201	-1.5265	-2.4780	-10.2622	-0.1434	0.3377	-0.0035	4.7030	0.2192	-0.5106	-0.4659	0.0001
NiO	1.0483	-0.4933	-1.8031	-9.3196	-1.0529	-2.4811	-0.9909	-1.5265	74.5097	12.1508	15.8548	0.1634	-2.5748	-4.3586	7.2896	4.1486	3.8361	-0.6797	-0.3469
Sb_2O_3	6.3890	-5.4585	-40.2522	30.4296	6.7763	1.7998	-3.2374	-2.4780	12.1508	1031.0236	120.8472	-1.8276	1.5097	-1.8697	-138.5032	-4.7228	-8.9339	1.8117	-35.2717
SeO_2	-0.6269	-1.1327	-32.2661	170.3962	-0.3322	-7.5802	-2.6004	-10.2622	15.8548	120.8472	1698.5247	0.9981	-4.4715	4.6847	-417.7765	-32.5003	11.4600	3.6352	-62.7561
SiO_2	-0.1563	-0.0543	-0.3277	0.0884	-0.1297	-0.2777	0.0467	-0.1434	0.1634	-1.8276	0.9981	0.1315	-0.0673	-0.2179	-1.7493	-0.1655	-0.0516	0.0616	0.3273
SrO	-0.0291	0.0374	-0.3603	-0.4240	-0.0127	0.3239	-0.3232	0.3377	-2.5748	1.5097	-4.4715	-0.0673	1.5960	0.8058	-5.9197	-0.8704	-0.9301	-0.1924	-0.1513
ThO_2	0.6230	0.1509	0.3267	-1.7639	0.7719	-0.3664	0.3066	-0.0035	-4.3586	-1.8697	4.6847	-0.2179	0.8058	4.4414	-21.1061	-2.3693	-0.8847	-0.2814	-1.3460
Tl_2O	7.0693	-3.2897	13.8877	-125.2650	-7.0435	5.2762	-6.9604	4.7030	7.2896	-138.5032	-417.7765	-1.7493	-5.9197	-21.1061	1195.0722	34.1241	13.3207	0.1970	2.5430
UO_3	0.5052	0.0792	4.9077	-10.8080	-0.2890	0.2094	-0.2109	0.2192	4.1486	-4.7228	-32.5003	-0.1655	-0.8704	-2.3693	34.1241	5.2977	0.5223	-0.2142	0.9347
ZnO	-0.0145	-0.4873	-1.1870	-0.8430	0.0817	-0.9452	-0.8700	-0.5106	3.8361	-8.9339	11.4600	-0.0516	-0.9301	-0.8847	13.3207	0.5223	9.0588	0.3130	-1.6015
ZrO_2	0.4254	-0.3557	-0.2610	2.9281	0.3784	-1.0513	-0.5523	-0.4659	-0.6797	1.8117	3.6352	0.0616	-0.1924	-0.2814	0.1970	-0.2142	0.3130	1.4565	-0.7675
Spike	-2.3080	0.8886	3.9138	-32.3614	-1.3716	-0.2150	0.2866	0.0001	-0.3469	-35.2717	-62.7561	0.3273	-0.1513	-1.3460	2.5430	0.9347	-1.6015	-0.7675	40.4249

(a) The variance-covariance matrix for the 19-term model is for renormalized mass fractions of the listed components.

Table D.6. Variance-Covariance Matrix Associated with the Estimated Model Coefficients (in Table 5.11) for the IHLW PCT-Sodium 8-Term Reduced LM Model.

Term [(a)]	Al_2O_3	B_2O_3	Li_2O	MnO	Na_2O	SiO_2	ThO_2	ZrO_2
Al_2O_3	1.3396	-0.1894	-0.5530	-0.1359	-0.2585	-0.0300	0.4631	0.1595
B_2O_3	-0.1894	0.3664	0.1339	0.0717	0.0398	-0.0673	0.1738	-0.1714
Li_2O	-0.5530	0.1339	2.5039	-0.0947	0.4414	-0.2309	-0.1122	-0.5042
MnO	-0.1359	0.0717	-0.0947	0.9886	0.0099	-0.0270	0.1045	-0.3354
Na_2O	-0.2585	0.0398	0.4414	0.0099	0.4579	-0.1065	0.0435	-0.2159
SiO_2	-0.0300	-0.0673	-0.2309	-0.0270	-0.1065	0.0631	-0.1176	0.0716
ThO_2	0.4631	0.1738	-0.1122	0.1045	0.0435	-0.1176	1.6748	-0.3722
ZrO_2	0.1595	-0.1714	-0.5042	-0.3354	-0.2159	0.0716	-0.3722	0.8652

(a) The variance-covariance matrix for the 8-term model is for renormalized mass fractions of the listed components.

Table D.7. Variance-Covariance Matrix Associated with the Estimated Model Coefficients (in Table 6.7) for the IHLW $T_{1\%}$ (Spinel) 19-Term Full LM Model.

Term [(a)]	Al_2O_3	B_2O_3	CdO	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	Sb_2O_3
Al_2O_3	45727.382	-6968.791	-14362.099	72384.332	11649.046	-16092.612	-6642.384	-10699.179	2733.994	45727.382
B_2O_3	-6968.791	12904.748	14867.090	43625.589	-5297.785	5511.193	1067.520	4649.728	-15419.564	-6968.791
CdO	-14362.099	14867.090	526512.991	-431345.533	-10280.438	20979.494	-12534.728	12542.300	-77801.400	-14362.099
Cr_2O_3	72384.332	43625.589	-431345.533	9238336.611	24063.138	-210101.633	-212167.320	-78989.431	-247136.648	72384.332
Fe_2O_3	11649.046	-5297.785	-10280.438	24063.138	22160.760	-12560.279	4152.172	-10750.406	710.114	11649.046
Li_2O	-16092.612	5511.193	20979.494	-210101.633	-12560.279	81646.130	4175.107	20334.554	-53796.951	-16092.612
MnO	-6642.384	1067.520	-12534.728	-212167.320	4152.172	4175.107	39564.713	1385.908	-19323.259	-6642.384
Na_2O	-10699.179	4649.728	12542.300	-78989.431	-10750.406	20334.554	1385.908	21205.463	-32124.779	-10699.179
NiO	2733.994	-15419.564	-77801.400	-247136.648	710.114	-53796.951	-19323.259	-32124.779	1298028.444	2733.994
Sb_2O_3	174253.064	-101734.904	-504657.822	1191037.612	62753.402	-6054.573	-37251.672	-75350.720	347213.206	174253.064
SeO_2	-92145.746	66283.721	-142573.106	2457817.643	-81555.916	-195345.047	-47105.280	-114945.031	27310.429	-92145.746
SiO_2	-4893.388	-1247.160	-8137.590	-6530.453	-2909.532	-5400.037	-185.421	-1250.173	3044.527	-4893.388
SrO	-4859.604	2212.523	2888.371	-31082.262	-4639.992	5385.351	-6928.103	6831.775	-42996.378	-4859.604
ThO_2	17344.066	5051.171	8252.219	-76277.228	15702.097	-7740.251	13743.846	-892.860	-86262.074	17344.066
Tl_2O	195765.754	-57234.890	-120652.094	-1777365.649	-144276.052	96416.408	-109346.930	14771.430	112725.665	195765.754
UO_3	-1068.452	867.780	85032.202	-223900.899	-6956.236	8781.898	-8492.362	9904.248	59629.980	-1068.452
ZnO	14510.661	-13438.160	-13156.404	318443.504	13678.445	-16371.489	-23664.649	-26026.279	75725.225	14510.661
ZrO_2	14325.677	-9123.090	-7869.884	103360.032	10261.180	-19191.046	-9537.202	-15668.493	1383.054	14325.677
Spike	-10832.051	4278.418	7171.867	-366541.172	4536.173	1815.611	18606.466	-12428.275	29715.039	-10832.051

Term [(a)]	SeO_2	SiO_2	SrO	ThO_2	Tl_2O	UO_3	ZnO	ZrO_2	Spike
Al_2O_3	174253.064	-92145.746	-4893.388	-4859.604	17344.066	195765.754	-1068.452	14510.661	14325.677
B_2O_3	-101734.904	66283.721	-1247.160	2212.523	5051.171	-57234.890	867.780	-13438.160	-9123.090
CdO	-504657.822	-142573.106	-8137.590	2888.371	8252.219	-120652.094	85032.202	-13156.404	-7869.884
Cr_2O_3	1191037.612	2457817.643	-6530.453	-31082.262	-76277.228	-1777365.649	-223900.899	318443.504	103360.032
Fe_2O_3	62753.402	-81555.916	-2909.532	-4639.992	15702.097	-144276.052	-6956.236	13678.445	10261.180
Li_2O	-6054.573	-195345.047	-5400.037	5385.351	-7740.251	96416.408	8781.898	-16371.489	-19191.046
MnO	-37251.672	-47105.280	-185.421	-6928.103	13743.846	-109346.930	-8492.362	-23664.649	-9537.202
Na_2O	-75350.720	-114945.031	-1250.173	6831.775	-892.860	14771.430	9904.248	-26026.279	-15668.493
NiO	347213.206	27310.429	3044.527	-42996.378	-86262.074	112725.665	59629.980	75725.225	1383.054
Sb_2O_3	18482145.841	-415990.837	-37191.088	6970.067	-71021.334	-704546.655	-76330.072	31343.316	89932.588
SeO_2	-415990.837	29084190.943	19713.085	-65195.329	88055.785	-4877959.306	-423975.083	126524.401	-37142.458
SiO_2	-37191.088	19713.085	2873.812	-5.215	-5685.697	-14528.787	-907.599	-4717.421	239.673
SrO	6970.067	-65195.329	-5.215	25224.593	5705.834	-85521.252	-10052.593	-12675.980	-5750.747
ThO_2	-71021.334	88055.785	-5685.697	5705.834	87584.776	-331015.428	-39989.737	-15701.744	-5769.651
Tl_2O	-704546.655	-4877959.306	-14528.787	-85521.252	-331015.428	21127898.004	460060.865	116938.237	6644.427
UO_3	-76330.072	-423975.083	-907.599	-10052.593	-39989.737	460060.865	90721.745	-15257.660	-7735.341
ZnO	31343.316	126524.401	-4717.421	-12675.980	-15701.744	116938.237	-15257.660	205660.723	26939.111
ZrO_2	89932.588	-37142.458	239.673	-5750.747	-5769.651	6644.427	-7735.341	26939.111	34432.032
Spike	-336111.616	-960681.966	-1125.155	-24.216	12512.242	-208667.641	-21228.607	-31065.673	-2064.286

(a) The variance-covariance matrix for the 19-term model is for renormalized mass fractions of the listed components.

Table D.8. Variance-Covariance Matrix Associated with the Estimated Model Coefficients (in Table 6.8) for the IHLW $T_{1\%}$ (Spinel) 13-Term Reduced LM Model.

Term [(a)]	Al_2O_3	B_2O_3	Cr_2O_3	Fe_2O_3	Li_2O	MnO	Na_2O	NiO	SiO_2	SrO	ThO_2	ZnO	ZrO_2
Al_2O_3	39992.909	-5075.531	60716.306	11410.817	-16248.996	-5665.023	-9710.608	2328.464	-4243.028	-4348.698	17906.571	11794.418	12285.345
B_2O_3	-5075.531	11623.598	51548.156	-4780.188	5640.621	1054.819	4289.680	-12650.786	-1300.153	2194.716	3805.827	-12681.181	-8268.532
Cr_2O_3	60716.306	51548.156	7902030.634	2333.775	-175685.606	-218713.378	-56477.457	-115282.377	-10913.197	-49519.707	-141680.067	253610.606	79910.553
Fe_2O_3	11410.817	-4780.188	2333.775	19587.201	-11957.796	2556.677	-10165.583	2969.610	-2864.739	-5760.462	11671.596	14289.791	9182.871
Li_2O	-16248.996	5640.621	-175685.606	-11957.796	77723.820	5230.997	18571.431	-51070.347	-4831.802	4972.204	-5147.366	-15456.735	-18696.699
MnO	-5665.023	1054.819	-218713.378	2556.677	5230.997	36612.234	2276.790	-18073.880	-512.806	-7697.565	9417.878	-23530.066	-9474.590
Na_2O	-9710.608	4289.680	-56477.457	-10165.583	18571.431	2276.790	18878.713	-33920.311	-1286.116	7086.883	2401.917	-24040.203	-14543.966
NiO	2328.464	-12650.786	-115282.377	2969.610	-51070.347	-18073.880	-33920.311	1167984.233	1617.943	-29646.191	-44903.868	91373.502	8571.847
SiO_2	-4243.028	-1300.153	-10913.197	-2864.739	-4831.802	-512.806	-1286.116	1617.943	2526.134	62.590	-5347.860	-4518.647	485.446
SrO	-4348.698	2194.716	-49519.707	-5760.462	4972.204	-7697.565	7086.883	-29646.191	62.590	21957.044	-500.430	-13174.706	-6688.603
ThO_2	17906.571	3805.827	-141680.067	11671.596	-5147.366	9417.878	2401.917	-44903.868	-5347.860	-500.430	61587.691	-20849.327	-9167.297
ZnO	11794.418	-12681.181	253610.606	14289.791	-15456.735	-23530.066	-24040.203	91373.502	-4518.647	-13174.706	-20849.327	191955.677	24836.208
ZrO_2	12285.345	-8268.532	79910.553	9182.871	-18696.699	-9474.590	-14543.966	8571.847	485.446	-6688.603	-9167.297	24836.208	32181.983

(a) The variance-covariance matrix for the 13-term model is for renormalized mass fractions of the listed components.

Appendix E

Example Illustrating the Use of Equations (6.1) to (6.3) for Calculating Estimated $T_{1\%}$ Values and Corresponding Standard Deviations

Appendix E

Example Illustrating the Use of Equations (6.1) to (6.3) for Calculating Estimated $T_{1\%}$ Values and Corresponding Standard Deviations

Estimated $T_{1\%}$ values were used as the response in developing the $T_{1\%}$-composition models. These estimated $T_{1\%}$ values were obtained using temperature versus volume %-crystallinity data (see Tables 6.1 and 6.5) and simple linear regression as indicated in Equation (6.1). Corresponding standard deviations for the estimated $T_{1\%}$ values were calculated using Equations (6.2) and (6.3). This process was used for both modeling and validation datasets. This appendix illustrates the use of Equations (6.1) to (6.3) for calculating the estimated $T_{1\%}$ value and corresponding standard deviation for one of the glasses of the IHLW Combined Matrix.

The specific glass selected to illustrate the estimation process is HLW02-52. The temperature versus volume %-crystallinity data for HLW02-52, as given in Table 6.1, are provided below.

Temperature (°C)	750	850	900	950	1050
Volume %-Crystallinity	2.5	1.3	2.1	1.2	0.4

Simple linear regression using the above data with temperature as the response results in the regression line

$$\hat{T} = 1077.78 - 118.52v, \tag{E.1}$$

where v is the volume %-crystallinity and $\hat{T}$ is the corresponding temperature estimate. As explained in Section 6.1.1, this regression equation form can be considered an inverse regression because temperature would typically be the more suitable predictor variable. For a volume %-crystallinity value of 1, the above regression line in Equation (E.1) produces an estimated $T_{1\%}$ value of

$$\hat{T} = 1077.78 - 118.52(1) = 1077.78 - 118.52 = 959.3\,^{o}\text{C}$$

Note that the intercept (1077.78), slope (–118.52), and estimated $T_{1\%}$ value (959.3) for HLW02-52 are given in Table 6.2.

A graphical depiction of the temperature versus volume %-crystallinity data for HLW02-52, together with the calculated regression line in Equation (E.1) is shown in Figure E.1. The black diagonal line in Figure E.1 is the regression line used to obtain the estimated $T_{1\%}$ value for HLW02-52. The dashed line in Figure E.1 represents using the regression line to calculate the estimated $T_{1\%}$ value for HLW02-52. As depicted in Figure E.1, the dashed red line corresponds to a volume %-crystallinity value of 1.0, and results in an estimated temperature of 959.3ºC.

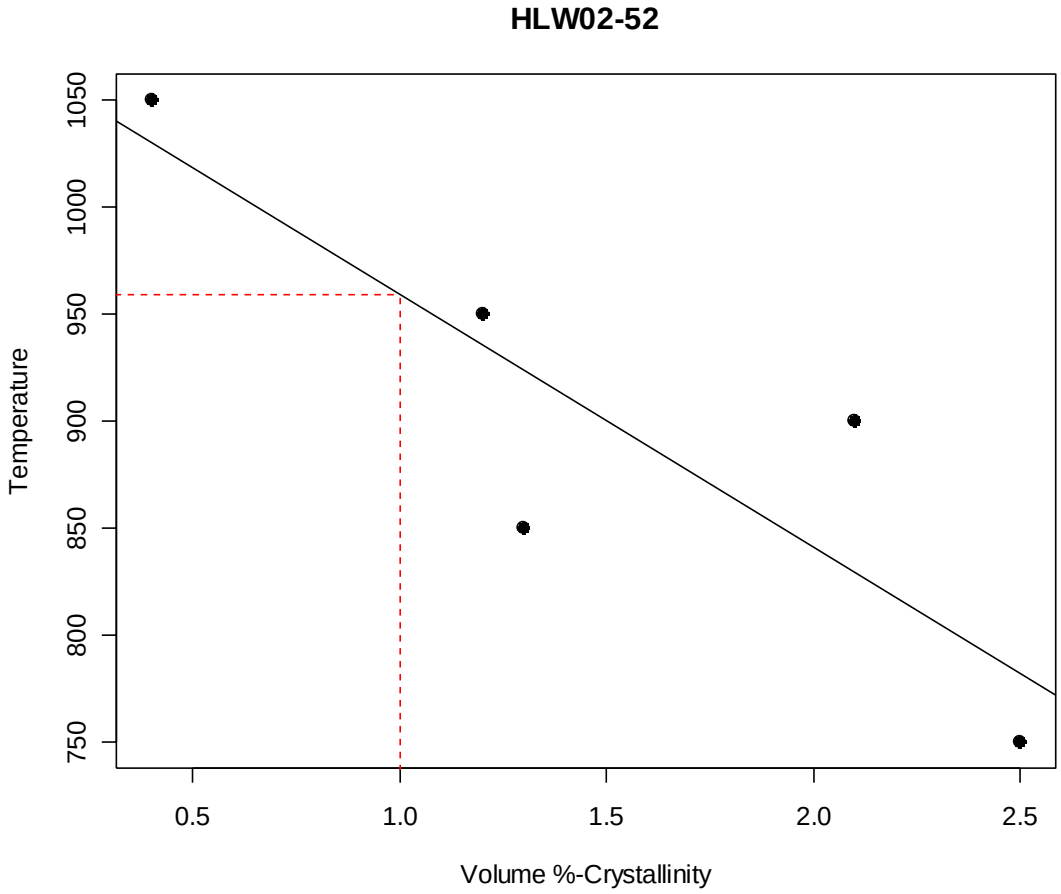


Figure E.1. Temperature versus Volume %-Crystallinity Data, Regression Line, and Estimated $T_{1\%}$ Value for HLW02-52.

The standard deviation associated with the estimated $T_{1\%}$ value for HLW02-52 is calculated using Equations (6.2) and (6.3). Equation (6.3) is used first to calculate the mean squared error (*MSE*)[(a)], which is then substituted into Equation (6.2) to calculate the standard deviation associated with the estimated $T_{1\%}$ value for HLW02-52. As indicated in Equation (6.3), estimated $T_{1\%}$ values are needed for each of the five temperature versus volume %-crystallinity data points available for HLW02-52. These estimated $T_{1\%}$ values are obtained by applying the regression Equation (E.1) to each of the five volume %-crystallinity values for HLW02-52. The estimated temperature calculations are shown below.

Volume %-Crystallinity	Estimated Temperature [(a)]
2.5	1077.7778 – 118.5185(2.5) = 781.482
1.3	1077.7778 – 118.5185(1.3) = 923.704
2.1	1077.7778 – 118.5185(2.1) = 828.889
1.2	1077.7778 – 118.5185(1.2) = 935.556
0.4	1077.7778 – 118.5185(0.4) = 1030.370

(a) Intercepts, slopes, and estimated $T_{1\%}$ values are given in greater decimal accuracy here than were used in Table 6.2 in order to ensure two decimal accuracy in the calculated standard deviation below.

Thus, using Equation (6.3) yields

$$MSE = \frac{\sum_{i=1}^{n}(T_i - \hat{T}_i)^2}{n-2}$$

$$= \frac{(750-781.482)^2 + (850-923.704)^2 + (900-828.889)^2 + (950-935.556)^2 + (1050-1030.370)^2}{5-2}$$

$$= \frac{991.116 + 5432.280 + 5056.774 + 208.629 + 385.337}{3}$$

$$= \frac{12074.136}{3} = 4024.712$$

Prior to using Equation (6.2) to calculate the standard deviation associated with the estimated $T_{1\%}$ value for HLW02-52, the mean volume %-crystallinity value is needed. This is calculated as

$$\bar{v} = \frac{\sum_{i=1}^{n} v_i}{n} = \frac{2.5+1.3+2.1+1.2+0.4}{5} = 1.5$$

Substituting *MSE* and $\bar{v}$ into Equation (6.2), and using $v_0 = 1$, the standard deviation associated with the estimated $T_{1\%}$ value for HLW02-52 is calculated as follows

(a) Although Equation (6.3) can be used to calculate the *MSE*, it (or its square root, known as *RMSE*) is typically included in the output of many regression software routines.

$$SD(T_{1\%}) = \sqrt{MSE * \left(\frac{1}{n} + \frac{(v_0 - \bar{v})^2}{\sum_{i=1}^{n} (v_i - \bar{v})^2} \right)}$$

$$= \sqrt{4024.712 * \left(\frac{1}{5} + \frac{(1-1.5)^2}{(2.5-1.5)^2 + (1.3-1.5)^2 + (2.1-1.5)^2 + (1.2-1.5)^2 + (0.4-1.5)^2} \right)}$$

$$= \sqrt{4024.712 * \left(0.2 + \frac{0.25}{2.7} \right)}$$

$$= 34.32$$

This calculated standard deviation is as given in Table 6.2.

The process described above was used, where possible, to calculate estimated $T_{1\%}$ values and their corresponding standard deviations for both modeling and validation glasses. There were two glasses from the modeling dataset (IHLW Combined Matrix glasses) for which the inverse regression process could not be used to calculate the estimated $T_{1\%}$ value and corresponding standard deviation. These two glasses were HLW02-05 and HLW02-21. For HLW02-05, the temperature versus volume %-crystallinity data had volume %-crystallinity values all equal to 0.1. Similarly, HLW02-21 had volume %-crystallinity values all equal to 0.2.

conferences

R&T Subcontractor Document Review Record

1) To Be Completed by Cognizant R&T Personnel		
Document Number VSL-05R5780-1	Revision 0	Document Title Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%)

Test Spec:	24590-HLW-TSP-RT-01-006, Rev 1, HLW Property Composition Modeling 24590-WTP-TSP-RT-02-001, Rev 0, Statistics for HLW & LAW Glass Property-Composition Modeling 24590-WTP-TEF-RT-03-078 (Changed from T-L to T-1%)	Scoping Statement(s):	VSL-13, HLW Glass Property Composition Modeling VSL-14, HLW Processing Properties Models B-72, Demonstrate Compliance with Glass Durability Requirements for IHLW (PCT and TCLP composition model for IHLW)

R&T Contact:	Keith Abel	MS5-L	371-3086	2/11/05
	Name (Print)	MSIN	Telephone Number	Date

Review Distribution

Organization	Contact	MSIN	Required?
Process Operations	D McLaughlin	MS4-B2	Yes ☒ No ☐
Quality Assurance	M Mitchell	MS14-4B	Yes ☐ No ☒
Environmental and Nuclear Safety	E Sauceda	MS4-C1	Yes ☒ No ☐
Commissioning and Training	K Vacca	MS12-B	Yes ☐ No ☒
Engineering	M Ongpin	MS4-A2	Yes ☒ No ☐
R&T Functional Manager	C Musick	MS5-L	Yes ☒ No ☐
			Yes ☐ No ☐
			Yes ☐ No ☐
			Yes ☐ No ☐
			Yes ☐ No ☐

Comments Due By: 2/28/05

Required Reviewers are required to respond to the R&T Contact.

2) To be Completed by Reviewer			
Reviewer E·SAUCEDA/PDC	E4NS	3/2/05	
Name (Print)	Organization	Date	

☒ Accepted, No Comments	☐ Accepted, Comments Not Significant	☐ Significant Comments, Form 24590-MGT-F00006 Attached	☐ Significant Comments, Comments Marked on Document

R&T Subcontractor Document Review Record

Document Number	Revision	Document Title
VSL-05R5780-1	0	Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%)

3) To be Completed by Reviewer*

My significant comments have been addressed.

Acceptance: _____ _____ _____

Print/Type Name *Signature* *Date*

** An e-mail to the R&T contact stating that significant comments are addressed can substitute for this acceptance.*

Abel, Keith H.

From: Beaumier, Cynthia
Sent: Wednesday, March 02, 2005 7:09 AM
To: Abel, Keith H.
Subject: FW: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1, Rev. 0

Importance: High

There are no operations comments on the document listed below.

Thanks.

-----Original Message-----
From: Jenkins, Terri **On Behalf Of** Vacca, Karen
Sent: Thursday, February 24, 2005 9:17 AM
To: Beaumier, Cynthia
Subject: FW: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1, Rev. 0
Importance: High

-----Original Message-----
From: **Abel, Keith H.**
Sent: Thursday, February 24, 2005 9:00 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Mclaughlin, Doris; Yorgesen, Jack
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Vienna, John; 'Joseph H Westsik Jr (E-mail)'; Westsik, Joseph; Kaiser, Bruce
Subject: RE: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1, Rev. 0
Importance: High

All,

Just a note of reminder. Comments are requested early next week on the Duratek (VSL-Battelle) report draft.

Thanks,

Keith

-----Original Message-----
From: Abel, Keith H.
Sent: Friday, February 11, 2005 9:08 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Mclaughlin, Doris; Yorgesen, Jack
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Musick, Chris A; Vienna, John; 'Joseph H Westsik Jr (E-mail)'; Gimpel, Rod; Westsik, Joseph; Kaiser, Bruce; Reynolds, Jacob
Subject: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1 , Rev. 0

We are requesting your assistance in review and finalization of the VSL and Battelle joint report **Development of *Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%)*, VSL-05R5780-1 , Rev. A.** The Document Review Record Form, the Comment Resolution Form for comments and an electronic version of the report are at the location shown below. I have also placed a copy of the Test Specifications, Test Plans and the one Test Exceptions related to the work at the link below. This report describes initial laboratory work at VSL determining HLW glass PCT and 1% Crystalinity. Also included is statistical work at Battelle to develop models describing the relationship between IHLW glass composition and (1) PCT release and (2) 1% Crystalinity temperature or T-1%.

\\wtps0166\R&T\HLW_PCT_Liquidus_Report0205

We appreciate your assistance in finalizing this document.

Comments are due no later than February 28, 2005

If you have any questions regarding this review request, please contact me (371-3086) or Chris Musick (371-3881)

Please provide comments to me by e-mail using the DRR and/or the CRF, also located at the hypertext link above.

Thank you for your assistance in the review and finalization of this document.

Keith Abel

Abel, Keith H.

From: Yorgesen, Jack
Sent: Monday, March 21, 2005 1:30 PM
To: Abel, Keith H.
Subject: RE: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1, Rev. 0

Keith,

Engineering gives its concurrence on document "Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%)", VSL-05R5780-1, Rev. 0.

Bret Yorgesen
Bechtel National
Process Engineering
371-3774

-----Original Message-----
From: Abel, Keith H.
Sent: Monday, March 21, 2005 10:01 AM
To: Yorgesen, Jack
Subject: RE: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1, Rev. 0

Jack,

Although there were no comments from Engineering staff as you stated below, I did receive comments from Rod Gimpel and Jake Reynolds in Process Operations. I have resolved their comments as of last Friday; they both signed off on their Comment Resolution Forms.

Therefore, would you please provide Engineering concurrence that the document should proceed to completion of Rev 0.

Thank you,

Keith Abel

-----Original Message-----
From: Yorgesen, Jack
Sent: Wednesday, March 02, 2005 1:50 PM
To: Abel, Keith H.
Subject: RE: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1, Rev. 0

No comments from Engineering on this document.

-----Original Message-----
From: Abel, Keith H.
Sent: Thursday, February 24, 2005 9:00 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Mclaughlin, Doris; Yorgesen, Jack
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Vienna, John; 'Joseph H Westsik Jr (E-mail)'; Westsik, Joseph; Kaiser, Bruce
Subject: RE: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1, Rev. 0
Importance: High

All,

Just a note of reminder. Comments are requested early next week on the Duratek (VSL-Battelle) report draft.

Thanks,

Keith

-----Original Message-----

From: Abel, Keith H.
Sent: Friday, February 11, 2005 9:08 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Mclaughlin, Doris; Yorgesen, Jack
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Musick, Chris A; Vienna, John; 'Joseph H Westsik Jr (E-mail)'; Gimpel, Rod; Westsik, Joseph; Kaiser, Bruce; Reynolds, Jacob
Subject: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1 , Rev. 0

We are requesting your assistance in review and finalization of the VSL and Battelle joint report **Development of *Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%)*, VSL- 05R5780-1 , Rev. A .** The Document Review Record Form, the Comment Resolution Form for comments and an electronic version of the report are at the location shown below. I have also placed a copy of the Test Specifications, Test Plans and the one Test Exceptions related to the work at the link below. This report describes initial laboratory work at VSL determining HLW glass PCT and 1% Crystalinity. Also included is statistical work at Battelle to develop models describing the relationship between IHLW glass composition and (1) PCT release and (2) 1% Crystalinity temperature or T-1%.

\\wtps0166\R&T\HLW_PCT_Liquidus_Report0205

We appreciate your assistance in finalizing this document.

Comments are due no later than February 28, 2005

If you have any questions regarding this review request, please contact me (371-3086) or Chris Musick (371-3881)

Please provide comments to me by e-mail using the DRR and/or the CRF, also located at the hypertext link above.

Thank you for your assistance in the review and finalization of this document.

Keith Abel

Abel, Keith H.

From: Yorgesen, Jack
Sent: Wednesday, March 02, 2005 1:50 PM
To: Abel, Keith H.
Subject: RE: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1, Rev. 0

No comments from Engineering on this document.

-----Original Message-----
From: Abel, Keith H.
Sent: Thursday, February 24, 2005 9:00 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Mclaughlin, Doris; Yorgesen, Jack
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Vienna, John; 'Joseph H Westsik Jr (E-mail)'; Westsik, Joseph; Kaiser, Bruce
Subject: RE: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1, Rev. 0
Importance: High

All,

Just a note of reminder. Comments are requested early next week on the Duratek (VSL-Battelle) report draft.

Thanks,

Keith

-----Original Message-----
From: Abel, Keith H.
Sent: Friday, February 11, 2005 9:08 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Mclaughlin, Doris; Yorgesen, Jack
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Musick, Chris A; Vienna, John; 'Joseph H Westsik Jr (E-mail)'; Gimpel, Rod; Westsik, Joseph; Kaiser, Bruce; Reynolds, Jacob
Subject: Document Review: Development of Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%), VSL-05R5780-1 , Rev. 0

We are requesting your assistance in review and finalization of the VSL and Battelle joint report **Development of *Phase 1 IHLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%)*, VSL- 05R5780-1 , Rev. A .** The Document Review Record Form, the Comment Resolution Form for comments and an electronic version of the report are at the location shown below. I have also placed a copy of the Test Specifications, Test Plans and the one Test Exceptions related to the work at the link below. This report describes initial laboratory work at VSL determining HLW glass PCT and 1% Crystalinity. Also included is statistical work at Battelle to develop models describing the relationship between IHLW glass composition and (1) PCT release and (2) 1% Crystalinity temperature or T-1%.

\\wtps0166\R&T\HLW_PCT_Liquidus_Report0205

We appreciate your assistance in finalizing this document.

Comments are due no later than February 28, 2005

If you have any questions regarding this review request, please contact me (371-3086) or Chris Musick (371-3881)

Please provide comments to me by e-mail using the DRR and/or the CRF, also located at the hypertext link above.

Thank you for your assistance in the review and finalization of this document.

Abel, Keith H.

From: Vienna, John
Sent: Friday, March 18, 2005 7:07 AM
To: Abel, Keith H.
Subject: RE: Comment Responses for HLW PCT 1% Crystallinity Report

Responses are acceptable. There was a question about normalization of PCT responses for validation glasses. All validation glasses except DWPF glasses are normalized to target composition. For DWPF glasses (Jantzen et al. 1995) only analyzed compositions were available. -John

-----Original Message-----
From: Abel, Keith H.
Sent: Thursday, March 17, 2005 3:29 PM
To: Vienna, John; John Vienna (E-mail)
Subject: Comment Responses for HLW PCT 1% Crystallinity Report

John,

Attached are the responses to your comments on the VSL/Battelle report. Please let me know if this set of responses resolve your comments on the report.

Thanks,

Keith

<< File: comres_vienna.doc >>

Abel, Keith H.

From: Westsik, Joseph H Jr [joseph.westsik@pnl.gov]
Sent: Friday, March 18, 2005 10:54 AM
To: Abel, Keith H.
Subject: RE: FW: Comment Responses HLW PCT 1% Crystallinity Report

Keith,
My comments have been resolved on the report "Development of Phase 1 HLW Models for PCT Response and One-Percent Crystal Fraction Temperature (T1%)", VSL-05R5780-1.

Joe

-----Original Message-----
From: Abel, Keith H. [mailto:khabel@bechtel.com]
Sent: Friday, March 18, 2005 10:29 AM
To: Westsik, Joseph H Jr
Subject: FW: FW: Comment Responses HLW PCT 1% Crystallinity Report

Joe,

Here is the note Ian sent in today regarding your unresolved comment. Let me know if your comments are now resolved.

Thanks,

Keith

-----Original Message-----
From: ianp@vsl.cua.edu [mailto:ianp@vsl.cua.edu]
Sent: Friday, March 18, 2005 6:30 AM
To: Abel, Keith H.
Cc: Westsik, Joseph; iJOSEPH@duratekinc.com; wingk@vsl.cua.edu
Subject: Re: FW: Comment Responses HLW PCT 1% Crystallinity Report

Keith:

No problem. I have added our response into the comment file (in blue). We will change the date as Joe requested.

Regards,

Ian.

On 17 Mar 2005 at 16:24, Abel, Keith H. wrote:

From: "Abel, Keith H." <khabel@bechtel.com>
To: "Ian Pegg (E-mail)" <ianp@vsl.cua.edu>, "Innocent Joseph (E-mail)" <ijoseph@duratekinc.com>
Copies to: "Westsik, Joseph" <jhwestsi@bechtel.com>
Subject: FW: Comment Responses HLW PCT 1% Crystallinity Report
Date sent: Thu, 17 Mar 2005 16:24:25 -0800

> Ian & Innocent,
>
> I have the comment responses out for resolution. Joe Westsik is not
> satisfied with the response on his comment #31. See the attachment

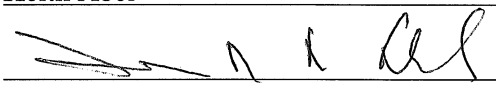
> and
let
> me know if you can accommodate his request and explanation.
>
> Thanks,
>
> Keith
>
> > -----Original Message-----
> > From: Westsik, Joseph
> > Sent: Thursday, March 17, 2005 4:19 PM
> > To: Abel, Keith H.
> > Subject: RE: Comment Responses HLW PCT 1% Crystallinity Report
> >
> > Keith,
> > All comments have been resolved except for #31. I have added some
> > text
in
> > red to explain.
> >
> > Joe
> >
> > <<comres_westsik jhw.doc>>
> >
> > -----Original Message-----
> > From: Abel, Keith H.
> > Sent: Thursday, March 17, 2005 3:27 PM
> > To: Westsik, Joseph; Joseph H Westsik Jr (E-mail)
> > Subject: Comment Responses HLW PCT 1% Crystallinity Report
> >
> > Joe,
> >
> > Attached are the comment responses from Duratek/VSL/Battelle for
> > your review. Please let me know if your comments are resolved with
> > this set
of
> > responses.
> >
> > Keith
> >
> > << File: comres_westsik.doc >>
>
>

R&T Technology Issues Summary

Test Report Title: Development of Phase 1 HLW Models for PCT Response and one-Percent Crystal Fraction Temperature (T1%)

Test Report Number: VSL-05R5780-1, Rev 0

Prepared By: Keith Abel **Date:** 04/13/05

Signature: 

Does the Testing or Report reveal any new discoveries, technology issues, or suggest potential follow-on work?	**Yes**	**No**
	☒	☐

If yes, describe the suggested activity.

This report documents the development of initial, or Phase 1, models for application to IHLW PCT response and One Percent Crystallinity Fraction Temperature. There is a planned Phase 2 effort for final IHLW model development and validation. The Phase 2 effort is currently scheduled for completion in 2007.

If appropriate, is a Request for Technology Development attached.	**Yes**	**No**
	☐	☒

Additional comments (include researcher recommendations):