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Mixture Models Versus Free Energy of Hydration Models for Waste Glass Durability

Greg Piepel
Trish Redgate
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March 1996

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Richland, Washington 99352

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Mixture Models Versus Free Energy of Hydration Models for Waste Glass Durability

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Abstract

Two approaches for modeling high-level waste glass durability as a function of glass composition are compared. The *mixture approach* utilizes first-order mixture (FOM) or second-order mixture (SOM) polynomials in composition, whereas the *free energy of hydration (FEH) approach* assumes durability is linearly related to the FEH of glass. Both approaches fit their models to data using least squares regression.

The mixture and FEH approaches are used to model glass durability as a function of glass composition for several simulated waste glass data sets. The resulting FEH and FOM model coefficients and goodness-of-fit statistics are compared, both within and across data sets. The goodness-of-fit statistics show that the FOM model fits/predicts durability in each data set better (sometimes much better) than the FEH model. Considerable differences also exist between some FEH and FOM model component coefficients for each of the data sets. These differences are due to the mixture approach having a greater flexibility to account for the effect of a glass component depending on the level and range of the component and on the levels of other glass components. The mixture approach can also account for higher-order (e.g., curvilinear or interactive) effects of components, whereas the FEH approach cannot. SOM models were developed for three of the data sets, and are shown to improve on the corresponding FOM models. Thus, the mixture approach has much more flexibility than the FEH approach for approximating the relationship between glass composition and durability for various glass composition regions.

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Summary

Two approaches for modeling high-level waste glass durability as a function of glass composition are compared. The *mixture approach* fits first- or second-order polynomials in composition to durability data using least squares regression. The *free energy of hydration (FEH) approach* assumes durability is linearly related to the FEH of glass, with the line fitted to data by least squares regression. The FEH of a glass is calculated as a composition-weighted linear combination of free energies of hydration of the glass components. The FEH approach is shown to be a restricted version of the first-order mixture (FOM) approach.

The mixture and FEH approaches are compared in terms of their ability to model Product Consistency Test (PCT) normalized boron releases as a function of glass composition for several simulated waste glass data sets. Least squares regression was used to fit FEH and FOM models to each data set. Goodness-of-fit statistics show that the FOM model fits/predicts PCT boron release in each data set better (sometimes much better) than the FEH model. The model R^2 (proportion of variation in PCT boron releases accounted for by a model) statistics are summarized in Table S.1 to illustrate this point.

Considerable differences also exist between some FEH and FOM model component coefficients for each of the data sets. Comparing FOM coefficients across the data sets shows that the effect of a glass component on PCT normalized boron release can depend on the level and range of the component and on the levels of other glass components. The FEH approach has a limited ability to represent such behavior for different glass composition regions, due to its reliance on assumed constant effects of each component. The mixture approach, on the other hand, determines the effects of glass components on durability from a given data set. It can also account for higher-order (e.g., curvilinear or interactive) effects of components. Second-order mixture (SOM) models were developed for three of the data sets, and are shown to improve on the corresponding FOM models (see R^2 statistics in Table S.1).

It is concluded that the mixture approach is more flexible than the FEH approach for approximating the relationship between glass composition and durability for various glass composition regions.

Table S.1. R^2 Statistics for FEH, FOM, and SOM Models Fitted to Several Data Sets

	Data Set											
Model	#1	#2	#3	#4	#5	#6	#7	#8	#9	#10	#11a	#11b
FEH	.472	.129	.113	.537	.741	.400	.730	.326	.506	.620	.763	.764
FOM	.954	.794	.694	.911	.899	.810	.880	.917	.980	.842	.961	.961
SOM	n.a.	n.a.	n.a.	n.a.	n.a.	.892	.931	n.a.	n.a.	.923	n.a.	n.a.

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1. Introduction

Nuclear waste glasses must satisfy several property constraints in order to be processable in a melter and acceptable for eventual disposal in a geologic repository. While these properties can be experimentally measured for any glass composition of interest, it is desirable to develop models that predict glass properties as functions of glass composition. If a model that adequately approximates the true relationship between a glass property and glass composition can be developed, property values can then be predicted for any composition within the model's domain (the composition region where the model is applicable). Predictive glass property models are very useful in formulating glass compositions with desired properties, and can be used in operating and controlling a nuclear waste vitrification plant.

A very important waste glass property is chemical durability (resistance to dissolution in water). The normalized elemental release of boron (B) from a 7-day Product Consistency Test (PCT)[1] is used as a measure glass durability in this report. Using several data sets, the performance of two approaches for modeling and predicting the PCT B release of simulated high-level nuclear waste glasses as a function of glass composition are compared. The *mixture* and *free energy of hydration* (FEH) modeling approaches are described in Section 2. There are many options for mixture models[2], but attention is restricted in this report to Scheffé first-order mixture (FOM) and second-order mixture (SOM) models, as described in Section 2. Section 3 compares the mathematical forms of the FEH and FOM models, and describes how to compare their coefficients. The data sets used to compare the fits and coefficients of FEH and mixture (FOM and SOM) models are discussed in Section 4. Section 5 describes the goodness-of-fit statistics used to assess how well the FEH and mixture models fit/predict the various data sets. Section 6 presents the results of fitting FEH and FOM models to each of the data sets, and SOM models to three of the data sets. The results are discussed in Section 7. Conclusions are given in Section 8. References are listed in Section 9.

2. Mixture and Free Energy of Hydration Models

The mathematical forms of first-order and second-order mixture models considered in this report are presented in Section 2.1. The mathematical form of the FEH model is discussed in Section 2.2.

2.1 Mixture Models

Many model forms have been proposed in the statistics literature for modeling mixture properties as functions of composition. Cornell[2] discusses many of these mixture model forms, the most widely used being the first- and second-order canonical polynomial models of Scheffé. As used in this report for modeling PCT elemental releases, the Scheffé first-order mixture (FOM) model is

$$\ln(NR) = \sum_{i=1}^{q} b_i x_i \qquad (1)$$

and the Scheffé second-order mixture (SOM) model is

$$\ln(NR) = \sum_{i=1}^{q} b_i x_i + \sum_{i=1}^{q-1} \sum_{j>i}^{q} b_{ij} x_i x_j \qquad (2)$$

In (1) and (2), ln(NR) is the natural logarithm of a normalized elemental release from the PCT (g/m^2), q is the number of mixture (glass) components, x_i is the mole fraction of the i-th glass component such that $x_1 + x_2 + \ldots + x_q = 1$, b_i is the coefficient of the first-order blending term involving x_i, and b_{ij} is the coefficient of the second-order blending term involving x_i and x_j. The coefficients b_i for a first-order model or b_i and b_{ij} for a second-order model are determined by fitting a model to an appropriate set of glass composition and PCT release data using least squares regression. Third- and higher-order Scheffé mixture models exist, as do other non-polynomial mixture models[2], but such models are not considered in this report.

Either mass or mole fractions of glass components may be used in models (1) and (2); both were used by Hrma, Piepel, et al.[3] In this report, mole fractions are used to allow a direct comparison of mixture models with free energy of hydration models (which use mole fractions). Also, note that the full SOM model (2) does not normally contain squared terms. That is, normally $j > i$ in the $x_i x_j$ terms of (2), so that x_i^2 terms (when $i = j$) are excluded. The squared terms are excluded when all $x_i x_j$ ($j > i$) terms are present, because otherwise the model would be overparameterized and unique coefficient estimates could not be obtained. However, reduced forms of (2) containing selected squared (x_i^2) and/or crossproduct ($x_i x_j$) terms can be used[3,4].

2.2 Free Energy of Hydration Model

The free energy of hydration (FEH) model[5] applied in this report has the form.

$$\ln(NR) = a + b \{ \sum_{i \neq SiO_2}^{k} (\Delta G_i) x_i + (\Delta G_{SiO_2}) [x_{SiO_2} - \sum_{i \in S}^{k} x_i] \} \quad (3)$$

where ln(NR) and x_i are as defined for (1) and (2), ΔG_i is the FEH value for the i-th glass component (kcal/mol), k is the number of glass components for which ΔG_i values are available, and "a" and "b" are coefficients determined by fitting the model (3) to a set of glass composition and PCT release data using least squares regression. The last summation sign in (3) is over each glass component i assumed to be associated with SiO_2 in glass dissolution reactions, which is denoted $i \in S$. Further information about the FEH model can be found in the THERMO report by Jantzen et al.[5]. The component FEH values ΔG_i used in this work were current as of early 1995, and are documented in Table 1.

2.3 Numbers of Components and Logarithm of Durability

Note that the number of glass components included in a FEH model is denoted by k in (3), whereas the number of glass components in FOM and SOM models is denoted by q in (1) and (2). The FEH approach accounts for the effects of many glass components, as indicated in Table I. In practice, however, many minor components have little or no practical effect on PCT normalized releases. The mixture models (1) and (2) can accommodate this by combining minor components in a catch-all component Others. The number of terms in mixture models can also be reduced by combining components with nearly identical effects, or by removing components with negligible effects (and renormalizing the composition to a total mole fraction of unity). Hence, while it is possible (assuming an adequate data set) to fit a mixture model using all k components used by the FEH approach, this is usually not done. In practice, very good mixture models can be obtained with $q < k$ (sometimes $q << k$).

The natural logarithm of normalized elemental release is used in Eqs. (1), (2), and (3) for two reasons. First, a logarithmic transformation of the dependent variable in a regression model (normalized PCT release in this report) stabilizes the variances of measured values when the variances increase with the magnitudes of measured values. Stabilized variances are a requirement for unweighted least squares regression. Second, a natural logarithmic transformation (log base e) is preferred over a common logarithmic transformation (log base 10) because of the relationship

$$SD[\ln(NR)] \approx RSD[NR], \quad (4)$$

where SD denotes "standard deviation" and RSD denotes "relative standard deviation". Thus, a standard deviation in ln(NR) units can be interpreted as a relative standard deviation in NR units. This fact will be used in Sections 5 and 7.

Table 1. Component Free Energy of Hydration Values (ΔG_i) Used In This Work

Oxide (i)	ΔG_i (kcal/mol)	Oxide (i)	ΔG_i (kcal/mol)	Oxide (i)	ΔG_i (kcal/mol)
Ag_2O	0.0	K_2O	-xx.xx	Rh_2O_3	0.0
Al_2O_3	xx.xx	La_2O_3	-xx.xx	RuO_2	xx.x
As_2O_3	-xx.xx	Li_2O	-xx.xx	Sb_2O_3	-xx.xx
B_2O_3	-xx.xx	MgO	-x.xx	SeO_2	-x.x
BaO	-xx.xx	MnO	-xx.xx	SiO_2	x.xx
Bi_2O_3	0.0	MoO_3	xx.xx	Sm_2O_3	0.0
CaO	-x.xx	Na_2O	-xx.xx	SO_3	0.0
CdO	x.xx	Nd_2O_3	-xx.xx	SrO	-xx.xx
Ce_2O_3	-xx.xx	NiO	x.xx	TeO_2	xx.xx
CoO	-x.xx	P_2O_5	-xx.xx	ThO_2	xx.xx
Cr_2O_3	xx.xx	PbO	xx.xx	TiO_2	xx.xx
Cs_2O	-xx.xx	PdO	0.0	U_3O_8	-xx.xx
CuO	-x.xx	PdO_2	0.0	WO_3	0.0
F	0.0	Pr_6O_{11}	0.0	Y_2O_3	-xx.xx
FeO	-xx.xx	Rb_2O	-xx.xx	ZnO	x.xx
Fe_2O_3	xx.xx	RhO_2	0.0	ZrO_2	xx.xx

Note 1: Jantzen et al.[5] and various information therein has not yet been cleared for public release or reference. Hence, the component FEH values and designators of which components occur in silicate species could not be included in this report. If and when release of this information is authorized, a completed version of this table will be made available to those requesting it from the first author.

Note 2: $\Delta G_i = 0.0$ where values were not given or were given as zero by Jantzen et al.[5].

3. Comparing Mixture and Free Energy of Hydration Model Forms

Section 3.1 shows how a FEH model can be rewritten in the form of a FOM model so that their coefficients can be compared. Section 3.2 discusses two approaches for deriving quantities from FOM models that can be compared to the component free energies of hydration used in FEH models. Section 3.3 discusses a hybrid FEH/FOM modeling approach. Section 3.4 discusses the results in the other subsections.

3.1 Writing the FEH Model in the Form of a FOM Model

The FOM model in Eq. (1) and the FEH model in Eq. (3) are both seen to be first-order functions of composition. To facilitate comparing FEH and FOM models and their coefficients later in the report, this section shows how the FEH model may be rewritten in the form of the FOM model.

By moving the constant b inside the summation, the FEH model (3) may be written as

$$\ln(NR) = a + \sum_{i \neq SiO_2}^{k} b(\Delta G_i) x_i + b(\Delta G_{SiO_2}) [x_{SiO_2} - \sum_{i \in S}^{k} x_i] . \quad (5a)$$

Collecting the $\Delta G_i x_i$ terms yields

$$\ln(NR) = a + \sum_{i=1}^{k} b(\Delta G_i) x_i - b(\Delta G_{SiO_2}) \sum_{i \in S}^{k} x_i . \quad (5b)$$

Assuming the complete composition of each glass is known such that $\Sigma x_i = 1$, and multiplying the constant a by $1 = \Sigma x_i$, yields

$$\begin{aligned} \ln(NR) &= \sum_{i=1}^{k} a x_i + \sum_{i=1}^{k} b(\Delta G_i) x_i - b(\Delta G_{SiO_2}) \sum_{i \in S}^{k} x_i \\ &= \sum_{i=1}^{k} [a + b(\Delta G_i)] x_i - b(\Delta G_{SiO_2}) \sum_{i \in S}^{k} x_i . \end{aligned} \quad (5c)$$

Finally, collecting terms according to whether each component i falls in the silica association group ($i \in S$) or in the non-silica association group ($i \notin S$) yields

$$\begin{aligned} \ln(NR) &= \sum_{i \in S}^{k} [a + b(\Delta G_i)] x_i + \sum_{i \in S}^{k} [a + b(\Delta G_i - \Delta G_{SiO_2})] x_i \\ &= \sum_{i \notin S}^{k} c_i x_i + \sum_{i \in S}^{k} d_i x_i \end{aligned} \quad (5d)$$

where $c_i = a + b(\Delta G_i)$ and $d_i = a + b(\Delta G_i - \Delta G_{SiO_2})$. Thus, the rewritten FEH model in

(5d) is seen to be of the same general form as the FOM model in (1), except that the terms fall into two groups (depending on whether or not each component is assumed to be associated with SiO_2 in glass dissolution reactions).

For the FOM model (1) and the FEH model (3) fitted to the same data set via least squares regression, the b_i coefficient for each component from (1) can be compared with the corresponding coefficient c_i or d_i from the rewritten FEH model in (5d).

3.2 Deriving Coefficients from a FOM Model That Can Be Compared to Component Free Energy of Hydration Values

FEH and FOM models can also be compared by deriving coefficients $\Delta G_i'$ from a FOM model and comparing them to the ΔG_i component FEH values in Table 1. The $\Delta G_i'$ coefficients may be thought of as "data-determined" component FEH values. Two ways to derive such $\Delta G_i'$ coefficients are presented in this section.

One way to obtain $\Delta G_i'$ coefficients from a FOM model (1) fitted to a data set requires that the FEH model (3) also be fitted to the data set. Then, the b_i values from (1) and the a and b values from (3) are substituted into the coefficient relationships in (5d), which are then solved for $\Delta G_i'$. This yields

$$\Delta G_i' = \frac{b_i - a}{b} \quad for \quad i \notin S \tag{6a}$$

$$\Delta G_i' = \Delta G_{SiO_2}' + \frac{b_i - a}{b} \quad for \quad i \in S \tag{6b}$$

Because SiO_2 is not contained in the set S, Eq. (6a) is used to obtain $\Delta G_{SiO2}'$, which can then be used in determining the quantities in Eq. (6b). Note that in the case where a FOM model uses $q < k$ components, where $x_q = x_q + x_{q+1} + \ldots + x_k$, the $\Delta G_i'$ values for $i = q, q+1, \ldots, k$ are the same. The approach in (6a) and (6b) for deriving $\Delta G_i'$ values from the fitted FOM model (1) coefficients relies on the assumption that the a and b coefficients from the fitted FEH model (3) are appropriate.

Another way to obtain $\Delta G_i'$ coefficients from a FOM model (1) fitted to a data set is to assume that two or three of the ΔG_i values in Table 1 are applicable (or correct) for the data set (i.e., $\Delta G_i' = \Delta G_i$ for component i). Substituting the two or three ΔG_i values assumed to be correct into Eqs. (6a) and (6b) allows solving for the values of a and b. Then, the remaining $\Delta G_i'$ coefficients can be derived from the FOM model coefficients using Eqs. (6a) and (6b). Whether two or three ΔG_i values must be assumed applicable (or correct) to uniquely solve for each $\Delta G_i'$ depends on whether the corresponding glass components are in the group S or not. Several cases are considered below.

Case 1: Two components j and k are sufficient if $j \notin S$ and $k \notin S$. This includes the case where neither of j or k is SiO_2, as well as the cases where one of j or k is SiO_2. Simultaneously solving the corresponding Eqs. (6a) for j and k yields

$$b = \frac{b_j - b_k}{\Delta G_j - \Delta G_k} \tag{7a}$$

$$a = b_k - b\,\Delta G_k \tag{7b}$$

Then, $\Delta G'_j = \Delta G_j$, $\Delta G'_k = \Delta G_k$, and the remaining $\Delta G'_i$ for all $i \neq j,k$ are obtained by substituting the above values of a and b into Eqs. (6a) and (6b).

Case 2: Two components are also sufficient if $j \in S$ and $k = SiO_2$ (without loss of generality, since the names of j and k could be switched). Simultaneously solving the corresponding Eq. (6b) for j and Eq. (6a) for k yields

$$b = \frac{b_j - b_{SiO_2}}{\Delta G_j - 2\,\Delta G_{SiO_2}} \tag{8a}$$

$$a = b_{SiO_2} - b\,\Delta G_{SiO_2} \tag{8b}$$

Then, $\Delta G'_j = \Delta G_j$, $\Delta G'_{SiO2} = \Delta G_{SiO2}$, and the remaining $\Delta G'_i$ for all $i \neq j$ or SiO_2, are obtained by substituting the above values of a and b into Eqs. (6a) and (6b).

Case 3: Three components j, k, and h are sufficient if $j \notin S$ (where $j \neq SiO_2$), $k \in S$, and $h \in S$ (without loss of generality, since the names of j, k, and h could be switched). Simultaneously solving the corresponding Eq. (6a) for j and Eqs. (6b) for k and h yields

$$b = \frac{b_k - b_h}{\Delta G_k - \Delta G_h} \tag{9a}$$

$$a = b_j - b\,\Delta G_j \tag{9b}$$

$$\Delta G'_{SiO_2} = \Delta G_h - \frac{b_h - a}{b} \tag{9c}$$

Then, $\Delta G'_j = \Delta G_j$, $\Delta G'_k = \Delta G_k$, $\Delta G'_h = \Delta G_h$, and the remaining $\Delta G'_i$ for all $i \neq j,k,h$ are obtained by substituting the above values of a, b, and $\Delta G'_{SiO2}$ into Eqs. (6a) and (6b).

Any other combinations of two or three components either revert to one of the three cases above, or do not lead to a solution.

3.3 A Hybrid FEH/FOM Modeling Approach

A hybrid FEH/FOM modeling approach could be used. This would involve fitting (to a given data set of glass composition and PCT release data) a model of the form

$$\ln(NR) = \sum_{i \in S}^{k} g_i (\Delta G_i) x_i + \sum_{i \in S}^{k} g_i (\Delta G_i - \Delta G_{SiO_2}) x_i \qquad (10)$$

where ln(NR), x_i, ΔG_i, and k are as defined in Section 2, and g_i is the coefficient for the i-th glass component obtained as part of the least squares fit. Eq. (10) is a modification of Eq. (5d), where $c_i = g_i (\Delta G_i)$ and $d_i = g_i (\Delta G_i - \Delta G_{SiO2})$ would be the coefficients of the FOM model. In this model, a g_i coefficient may be thought of as a multiplicative factor that "adjusts" the assumed FEH value [(ΔG_i) or $(\Delta G_i - \Delta G_{SiO2})$] for component i for a particular data set (and the property-composition space it represents). A g_i value that is (is not) statistically different from 1.0 would indicate that the corresponding FEH value is not (is) reasonable for the particular data set.

3.4 Discussion

Only the results from Section 3.1 are used in the remainder of this report. It was beyond the scope of this work to apply the results presented in Sections 3.2 and 3.3 to the data sets discussed in Section 4. However, it was decided to include Sections 3.2 and 3.3 in this report so that the results would be documented for possible future use.

The main result from Section 3.1 used in the remainder of this report is that the FEH model [(3) rewritten as (5d)] has the same form as the FOM model (1). The main difference between the two models is that the FEH model assumes that FEH values for each component are applicable component coefficients, whereas the FOM model estimates component coefficients from experimental data. Differences between assumed and estimated component coefficients for a given data set may indicate that the assumed reactions leading to the particular FEH coefficient values are not appropriate for the glass composition space represented by the data set. Such indications may be useful in improving the theory or assumptions underlying the FEH model.

An additional advantage of the mixture approach is that it can account for second-order (or higher-order) effects (both curvature and interactions) of glass components by including squared terms and crossproduct terms in the model [as in (2)]. The FEH modeling approach presented in Section 2.2 (referred to as "preliminary" FEH by Jantzen et al.[5]) cannot account for second-order effects of components in this fashion. Jantzen et al.[5] discuss a modification of the "preliminary" FEH approach (referred to as "final" FEH) that essentially allows for adjusting the ΔG_i values in Table 1 based on pH effects on PCT releases. However, the work summarized in this report was well under way prior to the completion by Jantzen et al. of the "final" FEH approach. Hence, only the "preliminary" and not the "final" FEH modeling approach is compared to the mixture modeling approach in this report.

4. Data Sets

Several data sets (glass compositions in terms of mole fractions, and PCT normalized B releases) from the waste glass literature are used to compare the fitting and predictive abilities of mixture and FEH models. The data sets are briefly described in the following subsections. Listings of the mole fraction compositions and PCT normalized B releases for each data set are given in Appendix A.

The glass mole fraction compositions given in Appendix A for the various data sets required (in some cases) adjustments from the way they were reported in the documents from which they were taken. For most data sets, the compositions were reported in terms of mass fractions or mass percents, and had to be converted to mole fractions. In some data sets, the oxide forms of a small number of components were different than those assumed by the FEH approach (e.g., MnO_2 instead of MnO), and had to be converted to the FEH-assumed oxide forms.

Normalized B releases from the 7-day Product Consistency Test (PCT) are used in this report as indicators of glass durability. The PCT exposes crushed glass to deionized water at 90°C for seven days, and is responsive to both glass homogeneity and composition[1]: Normalized B releases in this report were obtained via the formula

$$NR = \frac{C}{f \cdot \frac{A}{V}} \tag{11}$$

where NR is the normalized B release (g/m^2), C is the concentration of B in the PCT solution (mg/L), f is the mass fraction of B in the glass (unitless), and A/V is the surface area to volume ratio for the PCT (assumed to be 2000 m^{-1} for this work). Boron release is commonly selected as a good indicator of PCT durability of borosilicate waste glasses for the following reasons: 1) all B dissolved from glass enters into solution and does not precipitate in the gel layer, 2) B is released only by dissolution of the glass network, not by a diffusion process, and 3) B concentration in solution is determined with very good analytical precision.

Appendix B contains scatterplot matrices of the glass mole fraction compositions for each data set. A scatterplot matrix is simply a matrix of scatterplots of all possible pairs of components. Because individual plots in a scatterplot matrix get quite small for large numbers of components, attention was limited to only those components used in the FOM model for each data set. Observations regarding scatterplot matrices for the various data sets are made in the following subsections.

Table 2 lists the ranges of the component mole fraction values and the range of normalized B release values for each of the data sets discussed below. These ranges provide a rough indication of the composition region and the range of normalized B releases covered by each data set.

Table 2. Ranges of Glass Components and PCT Normalized B Release

Component		CVS-I	CVS-II.1	CVS-II.2	CVS-II.3	CVS-II.4	CVS (all)
Al_2O_3	Low	.0000	.0062	.0000	.0112	.0000	.0000
	High	.0930	.0690	.0885	.1269	.1004	.1269
B_2O_3	Low	.0414	.0629	.0420	.0467	.0465	.0414
	High	.1953	.1648	.1974	.1661	.1882	.1974
BaO	Low	(b)	(b)	(b)	(b)	(b)	(b)
	High						
CaO	Low	.0000	.0000	.0000	.0000	.0086	.0000
	High	.1227	.0817	.0968	.1201	.0232	.1227
Cr_2O_3	Low	(b)	(b)	(b)	(b)	(b)	(b)
	High						
CuO	Low	(b)	(b)	(b)	(b)	(b)	(b)
	High						
Fe_2O_3	Low	.0072	.0154	.0072	.0002		.0002
	High	.0626	.0492	.0596	.0513		.0626
FeO	Low	(a)	(a)	(a)	(a)	(a)	(a)
	High						
K_2O	Low	(a)	(a)	(a)	(a)	(a)	(a)
	High						
Li_2O	Low	.0200	.0448	.0209	.0115	.0225	.0115
	High	.1526	.1294	.1639	.1518	.1466	.1639
MgO	Low	.0000	.0000	.0000	.0000	.0000	.0000
	High	.1343	.0779	.1288	.0668	.0320	.1343
MnO	Low	(b)	(b)	(b)	(b)	(b)	(b)
	High						
Na_2O	Low	.0484	.0696	.0451	.0518	.0527	.0451
	High	.2043	.1804	.2110	.2077	.2089	.2110
NiO	Low	(b)	(b)	(b)	(b)	(b)	(b)
	High						
P_2O_5	Low	(b)	(b)	(b)	(b)	(b)	(b)
	High						
SiO_2	Low	.4194	.4913	.3905	.3623	.4127	.3623
	High	.6417	.5849	.6208	.6266	.6225	.6417
ThO_2	Low	(a)	(a)	(a)	(a)	(a)	(a)
	High						
TiO_2	Low	(a)	(a)	(a)	(a)	(a)	(a)
	High						
U_3O_8	Low	(a)	(a)	(b)	(a)	(a)	(b)
	High						
ZrO_2	Low	.0000	.0050	.0000	.0000		.0000
	High	.0717	.0523	.0671	.0792		.0792
Others	Low	.0054	.0140	.0052	.0054	.0758	.0052
	High	.0624	.0485	.0615	.0561	.1181	.0624
PCT B	Low	0.066	0.128	0.173	0.115	0.193	0.066
(g/m^2)	High	20.639	2.937	12.701	44.000	14.400	44.000

(a) Component not included or determined for glasses in this data set.

(b) Component included in Others for this data set.

Table 2. Ranges of Glass Components and PCT Normalized B Release (cont.)

Component		Ramsey	WV87	WV88	WVDP	SRTC 137	SRTC 118	SRTC 111
Al_2O_3	Low	.0012	.0630	.0370	.0294	.0012	.0086	.0196
	High	.1568	.0924	.0737	.0612	.1016	.0885	.0885
B_2O_3	Low	.0409	.1017	.0707	.0723	.0491	.0553	.0553
	High	.1543	.1375	.1313	.2000	.1428	.1281	.1281
BaO	Low	(a)	.0152(c)	.0082(c)	(b)	(b)	(b)	(b)
	High		.0446(c)	.0418(c)				
CaO	Low	.0000	.0152(c)	.0082(c)	(b)	.0000	.0044	.0044
	High	.1040	.0446(c)	.0418(c)		.1027	.0180	.0180
Cr_2O_3	Low	(a)	(b)	(b)	(b)	.0000	.0000	.0000
	High					.0028	.0028	.0028
CuO	Low	(a)	(b)	(b)	(b)	.0000	.0000	.0000
	High					.0054	.0054	.0037
Fe_2O_3	Low	.0000	.0379	.0419	.0294	.0000	.0175	.0175
	High	.0975	.0685	.0738	.0857	.0600	.0600	.0600
FeO	Low	.0000	(a)	(a)	(a)	.0000	.0000	.0000
	High	.0340				.0789	.0790	.0127
K_2O	Low	(a)	.1584(c)	.1697(c)	.0232	.0000	.0000	.0000
	High		.2007(c)	.2493(c)	.0591	.0395	.0395	.0270
Li_2O	Low	(a)	.1584(c)	.1697(c)	.0572	.0000	.0576	.0587
	High		.2007(c)	.2493(c)	.1284	.1145	.1076	.1076
MgO	Low	(a)	.0152(c)	.0082(c)	(b)	.0000	.0084	.0084
	High		.0446(c)	.0418(c)		.0508	.0508	.0268
MnO	Low	(a)	.0040	.0009	(b)	.0000	.0000	.0119
	High		.0215	.0170		.0322	.0322	.0322
Na_2O	Low	.1344	.1584(c)	.1697(c)	.0646	.0660	.0691	.0691
	High	.273	.2007(c)	.2493(c)	.1342	.2576	.1702	.1702
NiO	Low	(a)	(b)	(b)	(b)	.0000	.0035	.0035
	High					.0256	.0256	.0147
P_2O_5	Low	(a)	.0063	.0003	(b)	(b)	(b)	(b)
	High		.0181	.0225				
SiO_2	Low	.4551	.4520	.4555	.4116	.4348	.4348	.4348
	High	.6049	.5382	.5432	.5928	.7754	.6000	.5957
ThO_2	Low	(a)	.0044	.0050	.0024	(a)	(a)	(a)
	High		.0152	.0167	.0164			
TiO_2	Low	(a)	(b)	(b)	(b)	.0000	.0000	.0000
	High					.0271	.0148	.0141
U_3O_8	Low	(a)	.0001	.0001	(b)	(a)	(a)	(a)
	High		.0009	.0022				
ZrO_2	Low	(a)	(b)	(b)	.0012	(b)	(b)	(b)
	High				.0122			
Others	Low	(a)	.0101	.0086	n.a.	.0000	.0000	.0000
	High		.0386	.0555		.0590	.0086	.0086
PCT B	Low	0.075	0.160	0.179	0.186	0.055	0.175	0.175
(g/m^2)	High	38.709	0.309	0.417	10.278	35.120	9.250	9.250

(a) Component not included or determined for glasses in this data set.

(b) Component included in Others for this data set.

(c) The ranges listed for BaO, CaO, and MgO are for BaO+CaO+MgO. The ranges listed for Na_2O, Li_2O, and K_2O are for Na_2O+Li_2O+K_2O.

4.1 CVS Data Set

The first five phases of the Composition Variation Study (CVS) performed at the Pacific Northwest Laboratory from 1989 to 1994 studied 147 simulated waste glass compositions[3]. The CVS primarily varied the 10 components SiO_2, B_2O_3, Al_2O_3, Fe_2O_3, ZrO_2, Na_2O, Li_2O, CaO, MgO, and Others (all remaining waste components treated as a single component), although the composition of the Others mix was varied in several glasses. The 147 CVS glasses were studied in five phases (named CVS-I, and CVS-II Phases 1, 2, 3, and 4). The majority of the 147 glasses were selected using statistical optimal design software so as to cover the boundary and interior of an explicitly-defined composition experimental region. CVS-I, part of CVS-II Phase 2, and CVS-II Phase 3 focused mainly on the boundary of the composition region. CVS-II Phase 1, part of CVS-II Phase 2, and CVS-II Phase 4 focused mainly on the interior of the composition region. CVS-II Phase 4 consisted of one-at-a-time variations of SiO_2, B_2O_3, Na_2O, Li_2O, CaO, MgO, and Al_2O_3 while keeping all remaining components in the same relative proportions as in a base composition near the center of the composition region. A detailed discussion of the experimental design of the CVS phases is contained in the report by Hrma, Piepel, et al.[3]

In this report, the five CVS phases are treated as five separate data sets and one combined data set. The mole fraction compositions and PCT normalized B, Li, and Na releases for the 147 CVS-I and CVS-II Phase 1-4 glasses are given in Tables A.1 to A.5 of Appendix A. The normalized releases are averages of duplicate PCT results. There are 14 replicate compositions (same compositions with different glass names) scattered throughout the five CVS phases, and it is important to realize that neither modeling approach (mixture or FEH) can account for experimental variability in ln(NR) values among replicates. Hence, R^2 values (defined in Section 5 and reported in Section 6) for the mixture and FEH models will be lower than they would be without replicates in the data set.

Although B, Li, and Na normalized releases are given in Tables A.1 to A.5, only B normalized releases are used in this report. The range of B normalized release values (g/m^2) are: 0.066 to 20.639 for CVS-I, 0.128 to 2.937 for CVS-II Phase 1, 0.173 to 12.701 for CVS-II Phase 2, 0.115 to 44.000 for CVS-II Phase 3, 0.193 to 14.400 for CVS-II Phase 4, and 0.066 to 44.000 for the combined CVS data set [denoted CVS(all)].

Figures B.1 to B.5 in Appendix B contain scatterplot matrices for the glass compositions in each of the five CVS phases, while Figure B.6 contains the scatterplot matrix for the compositions from all five CVS phases combined. Figures B.1 to B.3 show that CVS-I, CVS-II Phase 1, and CVS-II Phase 2 glasses cover their respective experimental regions quite well. Similarly, Figure B.6 shows that the combined data set covers the overall experimental region very well. This is expected, since statistical experimental design methods and software were employed to achieve good coverage of various experimental subregions and the overall experimental region. Some pairwise scatterplots in Figures B.1 to B.4 and B.6 do not have any points in the upper right hand corners, but this is due to using multicomponent constraints to exclude such compositions from study. Figures B.2 to B.4 and B.6 show only single points with the lowest SiO_2 level, but these compositions were specially selected outside the specified experimental region. Within the experimental region, the SiO_2 range is covered very well. Figure B.3 shows that CVS-II Phase 3

provides a good coverage of the experimental region relative to most pairs of components, but a somewhat uneven coverage for a few pairs. This is expected, since CVS-II Phase 3 compositions were selected to augment the data available through the completion of CVS-II Phase 2. Also, compositions with extreme glass property values were selected for CVS-II Phase 3. These goals for selecting points led to avoiding portions of composition space covered in previous CVS phases and focusing on undercovered portions, which caused a somewhat uneven coverage of composition space in CVS-II Phase 3. CVS-II Phase 4 varied selected components one-at-a-time while keeping all remaining components in the same relative proportions. This proportional adjustment leads to most points in Figure B.5 scatterplots lying along straight lines, and these lines are also visible in Figure B.6 for the combined data set. In summary, the data for each of the five CVS experimental phases (with the possible exception of CVS-II Phase 4), and the combined CVS data set, should provide good bases for fitting and comparing FOM and FEH models.

4.2 Ramsey Data Set

A paper by Öksoy, Pye, Bickford, and Ramsey[6] contains mole fraction compositions and unnormalized PCT releases for 30 glasses. The glasses are from a statistically-designed study of a seven-component glass composition region investigated by W.G. Ramsey [a Savannah River Technology Center (SRTC) staff member] as part of his Ph.D. research at Clemson University. Hence, the data set is referred to as the Ramsey data set in this report. Whereas most of the data sets used in this report are for glass systems with a large number of components, the Ramsey data set is different in that it is for a smaller system containing only seven components (Al_2O_3, B_2O_3, CaO, Fe_2O_3, FeO, Na_2O, and SiO_2).

The mole fraction compositions and PCT normalized Si, B, and Na releases for the 30 Ramsey glasses are listed in Table A.6 of Appendix A. The normalized releases were calculated by first averaging unnormalized releases from triplicate PCTs, and then normalizing the averages. Only the B normalized releases are used in this report. The range of B normalized release values for the Ramsey data set is 0.075 to 38.709 g/m^2.

The scatterplot matrix in Figure B.7 of Appendix B shows that the Ramsey data set does a good job of covering its experimental region and that there are no strong correlations among pairs of components, with one exception. Fe_2O_3 and FeO exhibit a fairly strong positive correlation. This could make it difficult for mixture models to properly separate the effects of these two variables on PCT durability.

4.3 West Valley 1987 and 1988 Data Sets

Pacific Northwest Laboratory (PNL) performed two composition variation studies for West Valley Nuclear Services in 1987 and 1988. Each of these studies investigated 16 glasses in different composition regions defined in terms of the 11 components Al_2O_3, B_2O_3, BaO+CaO+MgO, Fe_2O_3, K_2O+Li_2O+Na_2O, MnO_2, P_2O_5, SiO_2, ThO_2, UO_2, and Others (all remaining components). (Note that UO_2 was converted to U_3O_8 for the modeling work in this report to be consistent with Jantzen et al.[5]) In each of the 1987 and 1988 studies, 15 of the 16 glasses were selected by statistical methods to evenly cover the boundary of the experimental

region. A sixteenth composition from the center of each region was included in each of the experimental designs[7]. PNL tested these glasses with the PCT in 1991 and 1992, and the results were ultimately published in a 1994 report[8].

The mole fraction compositions and PCT averaged normalized B, Li, and Na releases for the WV87 and WV88 data sets are given in Tables A.7 and A.8 of Appendix A. Only B normalized releases are used in this report. The range of B normalized release values for the WV87 data set is 0.160 to 0.309 g/m^2, and for the WV88 data set is 0.179 to 0.417 g/m^2.

Scatterplot matrices for the WV87 and WV88 data sets are given in Figures B.8 and B.9 of Appendix B. Many of the pairwise plots in each figure reflect that the designs consist of 15 vertices (boundary points) and one center point of the respective experimental regions. Some pairwise plots show components having values intermediate in their ranges, but this is possible with vertices of polyhedral experimental regions. Strong correlations are seen in the plots corresponding to pairs of components that were grouped, i.e., BaO+CaO+MgO and K_2O+Li_2O+Na_2O. However, these strong correlations are of no consequence as long as the grouped components are treated as a single component in mixture modeling efforts. Overall, each data set covers its experimental region well, in keeping with the statistical experimental design methods used to select the compositions[7].

4.4 WVDP Data Set

West Valley Nuclear Services (WVNS) developed a data set consisting of 58 glass compositions and PCT elemental releases, and used this data set to develop PCT release models[9] for use in the West Valley Demonstration Plant (WVDP), a high-level nuclear waste glass facility. The 58 glasses were selected to evenly cover a glass composition region centered on the WVDP target glass composition with boundary taken to be three times the expected process variation. Although the WVDP target glass composition contains a large number of components, variations in many of them are not expected to significantly affect PCT releases. Thus, with the exception of three glasses, only nine components (SiO_2, Al_2O_3, ZrO_2, ThO_2, Na_2O, K_2O, Li_2O, B_2O_3, Fe_2O_3) were varied in the 58 WVDP glass compositions. This nature of the data set does not support treating the remaining components as a combined Others component as was done in the CVS (Section 4.1), because Others is necessarily also constant except for the three glasses. The variation in Others for the three glasses is small, hence the WVDP data set does not support the use of an Others component. For purposes of fitting mixture models, the compositions of the nine components (listed above) were normalized to a total mole fraction of 1.0.

The mole fraction compositions and PCT averaged normalized B, Li, and Na releases for the 58 WVDP glasses are given in Table A.9 of Appendix A. Only B normalized releases are used in this report. The range of B normalized release values for the WVDP data set is 0.186 to 10.278 g/m^2.

Composition #51 in Table A.9 was determined to be an outlier by WVNS and was not used in developing their PCT models. Regression diagnostics obtained in fitting the FOM model to all

58 data points confirmed that #51 was an outlier, and so it was not used for fitting mixture or FEH models in this report.

The scatterplot matrix for the WVDP data set (without observation #51) is given in Figure B.10 of Appendix B. The scatterplot matrix used the compositions normalized to a total mole fraction of 1.0 for the nine components shown in the plot. The scatterplot matrix shows that the WVDP data generally cover the underlying composition region quite well. The pairwise plots of Na_2O, K_2O, and Li_2O show positive correlations for subsets of the data, but there are sufficient additional data that this should not be a problem. The pairwise plots involving ZrO_2 show some patterns for small subsets of the data, but this likewise should not be a problem. However, the small mole fraction ranges of ZrO_2 and ThO_2 limit assessing component effects and making model predictions to the small ranges of these components.

4.5 SRTC/DWPF Homogenous Glasses Data Set

The Savannah River Technology Center (SRTC) tested the PCT durability of many glasses and developed PCT normalized release prediction models for the Defense Waste Processing Facility (DWPF) high-level nuclear waste glass plant[5]. SRTC separated their glasses into *homogeneous* and *inhomogeneous* sets. Glasses were classified as homogeneous if they contain no crystalline species and are not liquid-liquid phase separated. Glasses with crystallinity or phase separation were classified as inhomogeneous. PCT normalized releases are often (but not always) higher for inhomogeneous glasses than for homogeneous glasses, due to higher solubility in water of one of the phases. Because of this, Jantzen et al.[5] modeled PCT normalized releases of homogeneous and inhomogeneous glasses separately. Only the homogeneous data set is modeled here, because the inhomogeneous data set contains too few data points and has other limitations.

The SRTC homogeneous data set (as defined in early 1995) contains 137 glasses, with triplicate PCT tests performed on each (with a few exceptions). Of the 137 glasses, 43 are replicates (i.e., the same glasses tested by the PCT at different times). The averages of the triplicate PCT releases for each of the 137 glasses are used for modeling in this report. The triplicate PCT releases for each of the 137 glasses only contain short-term testing and analytical sources of variation, whereas the replicate glass releases contain longer-term sources of variation. Using averaged triplicate PCT releases for modeling avoids improperly diluting the experimental error variance estimate obtained (from the replicate glasses) in least squares regression. Note that R^2 values (see Section 5) for mixture and FEH models fitted to averages of triplicate PCT releases will be somewhat larger than if unaveraged triplicate results were used. This is because models cannot account for the experimental variation represented by triplicate PCT tests. However, even using averages of triplicate PCT results, R^2 values for this data will be lower than they would be if the 137 glasses did not include replicates. This should not be viewed negatively, because having replicates in a data set permits statistically testing fitted models for lack-of-fit. Statistical lack-of-fit tests are not considered in this report, but the interested reader should see Section 1.5 of Draper and Smith[10].

The mole fraction compositions and PCT averaged normalized B, Li, and Na releases for the 137 SRTC homogeneous glasses can be found in Table A.10 of Appendix A. Only the B

normalized releases are used in this report. The range of B normalized release values for the full SRTC homogeneous data set is 0.055 to 35.12 g/m^2. The range without the two sets of outlying compositions (as discussed in following paragraphs) is 0.175 to 9.25 g/m^2.

The scatterplot matrix for the 137-point SRTC homogeneous data set is given in Figure B.11 in Appendix B. The scatterplot matrix shows considerable clustering of the glass compositions, uncovered portions of glass composition space, and a few glasses with outlying values of several components (e.g., CaO, Li_2O, Na_2O, SiO_2, and Others). Of particular note is the CaO vs. Na_2O scatterplot, which shows a very strong positive correlation between these components due to a few compositions. The NBS623 glass, the 14 replicates of the ARM1 glass, and the series of four MG glasses (MG-9, MG-18, MG-25, and MG-28) were identified as being the outlying compositions. These compositions are very atypical of the other glasses in the data set, and of waste glasses expected to be produced by the DWPF. In fact, several components (not shown in Figure B.11) varied significantly over the data set only because of these few glasses. Such atypical, outlying compositions can have a major impact when models are fitted to the data.

Figure B.12 contains the scatterplot matrix without the 19 atypical NBS623, ARM1, and MG compositions (118 data points). Considerable clustering of compositions, uncovered or lightly-covered portions of composition space, and outlying component values are still evident in Figure B.12. Outlying compositions of particular note are the composition with a low SiO_2 value, the two compositions with larger MgO values, and the five compositions that have larger values of both NiO and FeO than the remaining glasses. The FeO vs. NiO scatterplot shows a very strong correlation between FeO and NiO, indicating that the data do not provide adequate support for separately determining the effects of FeO and NiO on durability.

In Section 6, FEH and FOM models are fitted to both the whole SRTC homogeneous data set (referred to as SRTC 137), and also the subset of data obtained by excluding the 19 atypical data points discussed above (referred to as SRTC 118). The scatterplot matrix in Figure B.11 indicates that extreme caution should be used regarding models developed from the whole data set. The scatterplot matrix in Figure B.12 after deleting the 19 atypical data points looks better, but still the data does not cover the composition space as well as might be desired. This could have undesirable effects on models developed using the SRTC 118 data. Hence, in Section 6 a FOM model is also fit to a data set obtained by deleting the two compositions with larger MgO values, and the five compositions with larger values of NiO and FeO (referred to as SRTC 111). A scatterplot matrix of the SRTC 111 composition data is given in Figure B.13.

5. Statistics Used to Compare Models

This section describes the goodness-of-fit statistics R^2, R^2(ADJ), R^2(PRESS), and s used to assess and compare the mixture and FEH models fitted to each of the data sets described in Section 4. Descriptions and formulas for these statistics are given below. The notation used in the formulas is defined following the formulas.

R^2 — The fraction of variability in the ln(NR) data accounted for by a fitted model.

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \tag{12}$$

R^2(ADJ) — The fraction of variability in the ln(NR) data accounted for by the fitted model, adjusted for the number of coefficients and number of data points used in fitting the model. R^2(ADJ) is also useful for comparing fitted models based on different numbers of coefficients.

$$R^2(ADJ) = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2/(n-p)}{\sum_{i=1}^{n} (y_i - \bar{y})^2/(n-1)} \tag{13}$$

R^2(PRESS) — The fraction of variability in the ln(NR) data accounted for by the fitted model, where each data point is "left out of the fit" in evaluating how well the model predicts the property for that data point. R^2(PRESS) estimates the fraction of variability that would be explained in predicting new observations drawn from the same composition space.

$$R^2(PRESS) = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_{(i)})^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \tag{14}$$

s — The square root of the mean squared error of the fitted model, which is a measure of the variability of model prediction errors.

$$s = \sqrt{\frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{n-p}} \tag{15}$$

In the preceding definitions,

n = the number of data points used to fit the model,

p = the number of fitted coefficients in the model,

y_i = the measured ln(NR) value for the i^{th} data point,

$\hat{y}_i$ = the predicted ln(NR) value for the i^{th} data point made using the model fitted to all n data points,

$\hat{y}_{(i)}$ = the predicted ln(NR) value for the i^{th} data point made using a model fitted to all n data points except the i^{th},

$\bar{y}$ = the average of the n measured ln(NR) values y_i.

The numerator of the ratio in (14) is referred to as the PRESS statistic, where PRESS is an acronym that stands for **PR**edicted **E**rror **S**ums of **S**quares. R^2(PRESS) is also referred to as cross-validation R^2 in the literature.

The R^2 statistic must be between 0 and 1 for models fitted to a data set by least squares. Generally, R^2(ADJ) and R^2(PRESS) also are between 0 and 1, but they can be negative for a poor-fitting model, a model that contains many more coefficients than needed to fit the data, or a model fitted to data with one or more very influential data points. The maximum possible values of the three R^2 statistics will be less than 1 for a data set that contains replicate compositions whose y_i = ln(NR) values are different due to experimental variation, since a model relating ln(NR) to composition cannot account for such experimental variation. Among the three R^2 statistics, $R^2 > R^2$(ADJ), and typically R^2(ADJ) > R^2(PRESS). More than a minor difference between R^2 and R^2(ADJ) indicates that the model may contain more coefficients than needed. A substantial difference between R^2 and R^2(PRESS) indicates that one or more data points are very influential in determining the fit of the model. Some reduction from R^2 to R^2(PRESS) is expected because R^2 corresponds to using all data to fit the model, whereas R^2(PRESS) 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. Technically, R^2(PRESS) evaluates model performance using data not used in fitting the model, so it can be considered a "model validation" rather than a "model evaluation" technique.

The s statistic has the same units as ln(NR) [ln(g/m^2) in this report], and estimates the experimental standard deviation when the corresponding model is appropriate (i.e., does not have a statistically significant lack-of-fit) for the data set. When a model is not appropriate (i.e., does have a statistically significant lack-of-fit), the s statistic will be larger than the experimental standard deviation. Experience with the PCT on high-level waste glasses indicates that the experimental relative standard deviation (RSD) for single PCT determinations (i.e., a single PCT and chemical analysis) conducted on the same glass at different times is approximately 0.06 - 0.14 (see Table F.5 in Appendix F of the report by Hrma, Piepel, et al.[3]). The work of Hrma, Piepel, et al.[3] (Table F.5) also shows that the RSD remains in the same 0.06 - 0.14 range for an average of two determinations conducted at the same time. Based on that work, it can be concluded that the RSD would be in the same 0.06 - 0.14 range for an average of three determinations conducted

at the same time. The RSDs do not decrease much because only short-term variation in PCT results is being averaged. Then, according to the relationship in (4), the experimental standard deviation [in ln(NR) units] is approximately equal to the experimental RSD (which is unitless). Hence, the experimental standard deviation in ln(NR) units is in the range 0.06 - 0.14 regardless of whether a single determination, an average of two same-time determinations, or an average of three same-time determinations is used to represent the PCT release of a glass. The s statistic for a fitted model can be compared to this 0.06 - 0.14 range to subjectively assess whether the fitted model may have a statistically significant lack-of-fit. Objective statistical tests for model lack-of-fit exist (see Section 1.5 of Draper and Smith[10]), but are not considered or applied in this report.

6. Mixture and Free Energy of Hydration Models Fitted to Data Sets

The results of fitting the FEH and FOM models to each of the data sets described in Section 4 are presented in this section. Results from fitting SOM models to three of the data sets are also presented. The results consist of the fitted model coefficients (obtained by unweighted least squares regression) and the goodness-of-fit statistics R^2, R^2(ADJ), R^2(PRESS), and s described in Section 5. The results are compared and discussed in Section 7.

Table 3 contains the results of fitting the FEH model (3) to each of the data sets described in Section 4. Included in Table 3 are the a and b coefficients and their standard deviations obtained by least squares regression, as well as the R^2, R^2(ADJ), R^2(PRESS), and s statistics.

Table 4 contains the results of fitting the FOM model (1) to each of the data sets described in Section 4. Included are the b_i coefficients and their standard deviations obtained by least squares regression, as well as the R^2, R^2(ADJ), R^2(PRESS), and s statistics. Also included in Table 4 for each data set are the c_i and d_i coefficients obtained via (5d) from the FEH fitted model for that data set along with the corresponding standard deviations of the coefficients. For each data set, the c_i and d_i coefficients calculated from the FEH model can be directly compared to the b_i coefficients from the FOM model. The standard deviations of the coefficients for a given component can be used to ascertain whether there is a significant difference between the coefficients for that component.

Ranges of coefficients and standard deviations for the Others component in the FEH model (converted to the form of a FOM model) are also included in Table 4. A single Others coefficient and standard deviation exists only if the "Others mix" is fixed for all glasses in a data set, as is the case for the CVS-I data set. However, the remaining data sets have different "Others mixes" for different glasses in the data sets. In such cases, an Others component coefficient was computed for each glass as a weighted average of the coefficients for each component making up Others, with the relative mole fractions of components in Others used as weights. Also, the coefficient for each component making up Others was computed per (5d) for each data set, with the results given in Table 5. A standard deviation was computed for each Others component coefficient for each glass. The ranges of Others coefficients and standard deviations obtained across all the glasses in each data set are summarized in Table 4.

Reduced SOM models (i.e., SOM models containing only some of the second-order terms) were fitted to the WVDP, CVS(all), and Ramsey data sets. The resulting fitted models and goodness-of-fit statistics are given in Table 6. Stepwise regression techniques[10] were used to add statistically significant second-order terms (squares or crossproducts of oxide component mole fractions) to FOM models.

The reduced SOM model given in Table 6 for the Ramsey data was obtained via stepwise regression using a very conservative stopping criterion. Stepwise regression with a less conservative stopping criterion, as well as all-subsets regression[10] (in which all possible combinations of second-order terms taken two, three, four, ... at-a-time are added to the first-order mixture model), suggested that adding up to six second-order terms may improve the model

fit. However, several models of each size (number of second-order terms added) have nearly identical R^2 values, and thus it was difficult to pick just one of them for inclusion in Table 6. To make this point clearer, the following chart shows the R^2 values for five options of adding five second-order terms to the first-order mixture model:

Total Number Model Terms	R^2	Second-Order Terms Added to First-Order Model
12	0.97634665	SiO_2*CaO, B_2O_3*Na_2O, B_2O_3*FeO, Na_2O*Fe_2O_3, Na_2O*Al_2O_3
12	0.97440217	SiO_2*Al_2O_3, Na_2O*Fe_2O_3, Na_2O*Al_2O_3, CaO*Fe_2O_3, CaO*Al_2O_3
12	0.97418499	SiO_2*Al_2O_3, Na_2O*FeO, Na_2O*Al_2O_3, CaO*Fe_2O_3, CaO*Al_2O_3
12	0.97415623	SiO_2*CaO, Na_2O*Fe_2O_3, Na_2O*Al_2O_3, CaO*Al_2O_3, B_2O_3*B_2O_3
12	0.97325151	SiO_2*CaO, B_2O_3*Na_2O, B_2O_3*Fe_2O_3, Na_2O*Fe_2O_3, Na_2O*Al_2O_3

Care must be taken regarding the interpretation of second-order terms in reduced SOM models. The second-order terms selected for the reduced SOM models are those that most improved the model fit for each data set, and are not necessarily interpretable or explainable from a glass science perspective. Squared and crossproduct terms are always correlated with each other and with the first-order terms. The magnitudes of these correlations are influenced by the magnitudes of correlations among the glass components for each data set. These correlations can cause stepwise regression to select second-order terms that may or may not directly represent the true underlying curvilinear or interactive behavior of components. The chart above for the Ramsey data set shows how several possible sets of second-order terms can yield similar goodness-of-fits. Our practical experience is that some but not all second-order terms selected by stepwise regression correspond to behavior expected from glass science principles. However, even if second-order terms indirectly rather than directly account for underlying nonlinear behavior, the resulting reduced SOM models are still useful for predicting ln(NR) values for glasses in the same composition region as the glasses used to develop the models.

Predicted versus measured plots are given in Appendix C for the free energy of hydration, FOM, and reduced second-order mixture models fitted to the various data sets. Such plots are useful in assessing how well the model fits the data set used to develop it. A discussion of what to look for in such plots is given at the start of Appendix C.

Table 3. Coefficients and Goodness-of-Fit Statistics for Free Energy of Hydration Models Fitted to ln(PCT Normalized B Release in g/m^2)

Coefficient	CVS-I	CVS-II.1	CVS-II.2	CVS-II.3	CVS-II.4	CVS (all)
a (intercept)	-2.3584	-2.2001	-1.1381	-2.7293	-2.7236	-2.3093
sd(a)	(0.7066)	(1.0687)	(0.5980)	(0.4639)	(0.4705)	(0.2734)
b (slope)	-0.5047	-0.3015	-0.2046	-0.4395	-0.5302	-0.4081
sd(b)	(0.1165)	(0.1898)	(0.0944)	(0.0638)	(0.0683)	(0.0415)
R^2	0.472	0.129	0.113	0.537	0.741	0.400
R^2(ADJ)	0.447	0.078	0.089	0.525	0.729	0.396
R^2(PRESS)	0.394	-0.316	-0.007	0.496	0.690	0.384
s	1.364	0.973	1.171	1.192	0.662	1.169

Coefficient	RAMSEY	WV87	WV88	WVDP	SRTC Homo 137 Obs.	SRTC Homo. 118 Obs.
a (intercept)	-3.5570	-2.1005	-2.2325	-3.8233	-4.8609	-5.1678
sd(a)	(0.3791)	(0.2298)	(0.2565)	(0.3898)	(0.2073)	(0.2398)
b (slope)	-0.4380	-0.1262	-0.1476	-0.4600	-0.6138	-0.6665
sd(b)	(0.0504)	(0.0485)	(0.0390)	(0.0485)	(0.0294)	(0.0344)
R^2	0.730	0.326	0.506	0.620	0.763	0.764
R^2(ADJ)	0.720	0.278	0.471	0.614	0.762	0.762
R^2(PRESS)	0.673	0.098	0.361	0.594	0.751	0.752
s	0.867	0.155	0.195	0.714	0.583	0.547

Table 4. Coefficients, Coefficient Standard Deviations (in parentheses), and Goodness-of-Fit Statistics for First-Order Mixture Models and Rewritten Free Energy of Hydration Models for ln(PCT Normalized B Release, g/m^2)

	CVS-I		CVS-II.1		CVS-II.2		CVS-II.3	
Component	Mixture	FEH	Mixture	FEH	Mixture	FEH	Mixture	FEH
Al_2O_3	-41.13	-21.38	-34.54	-13.56	-63.81	-8.85	-39.85	-19.29
	(3.49)	(5.04)	(15.28)	(8.20)	(10.91)	(4.13)	(3.40)	(2.84)
B_2O_3	9.42	2.91	11.59	0.94	19.17	1.00	17.48	1.85
	(1.75)	(0.64)	(6.87)	(0.96)	(3.58)	(0.46)	(2.53)	(0.30)
CaO	-3.46	4.61	-5.66	1.96	-14.41	1.69	-12.76	3.34
	(2.70)	(1.00)	(5.56)	(1.59)	(3.95)	(0.76)	(5.14)	(0.49)
Fe_2O_3	-14.84	-9.71	27.61	-6.59	-13.62	-4.12	-11.97	-9.13
	(5.23)	(2.36)	(21.96)	(3.81)	(10.75)	(1.95)	(6.80)	(1.37)
Li_2O	7.69	9.77	5.35	5.05	18.96	3.78	12.89	7.84
	(2.04)	(2.17)	(10.84)	(3.52)	(4.39)	(1.71)	(2.13)	(1.12)
MgO	8.92	0.96	-0.87	-0.22	5.14	0.21	11.68	0.16
	(2.08)	(0.31)	(6.31)	(0.30)	(3.02)	(0.19)	(4.80)	(0.18)
Na_2O	13.16	24.44	12.41	13.81	24.49	9.72	19.97	20.60
	(2.56)	(5.54)	(9.68)	(9.03)	(4.03)	(4.45)	(1.97)	(2.96)
SiO_2	-2.01	-4.40	-5.59	-3.42	-5.36	-1.97	-5.69	-4.51
	(0.88)	(1.15)	(4.25)	(1.83)	(1.41)	(0.97)	(1.00)	(0.71)
ZrO_2	-17.06	-11.19	0.92	-7.47	-40.24	-4.72	-28.41	-10.42
	(4.64)	(2.70)	(17.60)	(4.37)	(11.54)	(2.23)	(5.69)	(1.55)
Others	3.23[a]	0.96[b]	15.05[a]	-0.29 to -0.22[b]	-4.32[a]	-0.17 to 2.16[b]	-0.78[a]	-3.01 to 19.95[b]
	(4.71)	(0.31)	(13.95)	(0.27 to 0.30)	(7.54)	(0.19 to 0.97)	(6.23)	(0.18 to 2.87)
prevalent values				-0.22		0.21		0.16
				(0.30)		(0.19)		(0.18)
R^2	0.954	0.472	0.794	0.129	0.694	0.113	0.911	0.537
R^2(ADJ)	0.921	0.447	0.588	0.078	0.599	0.089	0.887	0.525
R^2(PRESS)	0.880	0.394	-0.281	-0.316	0.310	-0.007	0.848	0.496
s	0.515	1.364	0.651	0.973	0.777	1.171	0.582	1.192

(a) The Others coefficient in the first-order mixture model may be considered to be an average coefficient for all the components contained in Others.

(b) Others coefficients for FEH models were computed by forming a weighted average of the coefficients for the individual Others components, where the relative proportions of the Others components were used as weights. This can yield different weighted averages across the data points in the data set, so the ranges of coefficient values and standard deviations are reported. There is no range for CVS-I glasses, since the relative proportions of components in Others are the same for each of these glasses. For CVS-II.1, CVS II.2, and CVS II.3, the majority of glasses have the same relative proportions in Others as in CVS-I, and these "prevalent" coefficients and standard deviations are also shown.

Table 4. Coefficients, Coefficient Standard Deviations (in parentheses), and Goodness-of-Fit Statistics for First-Order Mixture Models and Rewritten Free Energy of Hydration Models for ln(PCT Normalized B Release, g/m^2) (continued)

	CVS-II.4		CVS(all)		RAMSEY	
Component	Mixture	FEH	Mixture	FEH	Mixture	FEH
Al_2O_3	-32.63	-22.70	-40.81	-17.69	-26.45	-20.06
	(4.94)	(3.03)	(2.31)	(1.82)	(2.78)	(2.25)
B_2O_3	11.42	2.81	12.82	1.95	8.80	1.01
	(3.98)	(0.30)	(1.23)	(0.20)	(2.94)	(0.24)
CaO	34.90	4.60	-7.79	3.33	-8.13	2.49
	(36.88)	(0.51)	(1.79)	(0.33)	(2.94)	(0.39)
Fe_2O_3	(b)	-10.44	-8.39	-8.25	-26.08	-9.93
		(1.45)	(3.98)	(0.87)	(7.80)	(1.09)
FeO	(a)	(a)	(a)	(a)	38.60	5.79
					(23.44)	(0.75)
Li_2O	22.35	10.02	10.63	7.50	(a)	(a)
	(4.57)	(1.20)	(1.28)	(0.75)		
MgO	27.65	0.77	7.01	0.38	(a)	(a)
	(21.08)	(0.14)	(1.46)	(0.10)		
Na_2O	22.45	25.42	17.53	19.36	17.31	19.70
	(3.66)	(3.18)	(1.18)	(1.95)	(2.78)	(2.34)
SiO_2	-2.98	-4.87	-4.05	-3.96	-3.57	-5.33
	(1.01)	(0.74)	(0.55)	(0.43)	(1.36)	(0.57)
ZrO_2	(b)	-12.00	-20.90	-9.45	(a)	(a)
		(1.65)	(3.54)	(0.99)		
Others	-41.04[c]	0.64 to 0.76[d]	0.98[c]	-2.57 to 18.75[d]	(e)	(e)
	(11.54)	(0.14 to 0.14)	(3.39)	(0.10 to 1.89)		
prevalent values		0.76		0.37		
		(0.14)		(0.10)		
R^2	0.899	0.741	0.810	0.400	0.880	0.730
R^2(ADJ)	0.852	0.729	0.798	0.396	0.848	0.720
R^2(PRESS)	0.709[f]	0.690	0.776	0.384	0.769	0.673
s	0.489	0.662	0.677	1.169	0.638	0.867

(a) Component not included or determined for glasses in this data set.

(b) Fe_2O_3 and ZrO_2 were included in the Others component for fitting the first-order mixture model, since CVS-II Phase 4 consisted of experiments varying SiO_2, B_2O_3, Na_2O, Li_2O, CaO, MgO, and Al_2O_3 one-at-a-time. Hence, the effects of Fe_2O_3 and ZrO_2 are highly correlated with the effect of Others, and cannot be separately estimated.

(c) The Others coefficient in the first-order mixture model may be considered to be an average coefficient for all the components contained in Others.

(d) Others coefficients for FEH models were computed by forming a weighted average of the coefficients for the individual Others components, where the relative proportions of the Others components were used as weights. This can yield different weighted averages across the data points in the data set, so the ranges of coefficient values and standard deviations are reported. For the CVS-II.4 and CVS(all) data sets, the majority of glasses have the same relative proportions in Others as in CVS-I and other CVS-II phases, and these "prevalent" coefficients and standard deviations are also shown.

(e) No other components in this data set.

(f) Computed in a modified way, since the data set does not support fitting a CaO model term when glass CVS2-116 is deleted from the data set. The PRESS contribution with CVS2-116 deleted was obtained by including CaO in Others. CaO was retained in the model for the remaining PRESS contributions.

Table 4. Coefficients, Coefficient Standard Deviations (in parentheses), and Goodness-of-Fit Statistics for First-Order Mixture Models and Rewritten Free Energy of Hydration Models for ln(PCT Normalized B Release, g/m^2) (continued)

	WV87		WV88		WVDP	
Component	Mixture(a)	FEH	Mixture(a)	FEH	Mixture	FEH
Al_2O_3	-9.77	-6.86	-14.69	-7.79	-14.07	-21.16
	(2.38)	(2.06)	(1.21)	(1.72)	(8.50)	(2.21)
B_2O_3	3.18	-0.78	1.79	-0.69	14.53	0.97
	(1.89)	(0.28)	(0.85)	(0.16)	(1.81)	(0.16)
BaO	-6.28	0.82	3.51	1.19	(b)	(b)
	(1.99)	(0.90)	(1.20)	(0.65)		
CaO	-6.28	-0.36	3.51	-0.19	(b)	(b)
	(1.99)	(0.45)	(1.20)	(0.29)		
Fe_2O_3	-0.29	-3.94	-0.39	-4.38	-10.63	-10.52
	(1.90)	(0.93)	(1.42)	(0.82)	(4.36)	(1.09)
K_2O	5.86	7.54	5.26	9.05	14.44	31.32
	(1.37)	(3.48)	(0.60)	(2.73)	(6.22)	(3.33)
Li_2O	5.86	0.93	5.26	1.32	9.08	7.24
	(1.37)	(0.94)	(0.60)	(0.69)	(2.80)	(0.79)
MgO	-6.28	-1.27	3.51	-1.26	(b)	(b)
	(1.99)	(0.10)	(1.20)	(0.05)		
MnO	1.10	0.98	8.98	1.38	(b)	(b)
	(3.09)	(0.96)	(2.47)	(0.70)		
Na_2O	5.86	4.60	5.26	5.60	7.29	20.60
	(1.37)	(2.35)	(0.60)	(1.82)	(3.50)	(2.20)
P_2O_5	-0.77	1.25	-9.96	1.69	(b)	(b)
	(4.95)	(1.06)	(2.17)	(0.78)		
SiO_2	-4.49	-2.61	-3.65	-2.83	-6.09	-5.69
	(0.60)	(0.42)	(0.38)	(0.41)	(0.98)	(0.58)
ThO_2	13.09	-4.53	8.13	-5.07	-5.36	-12.67
	(6.38)	(1.16)	(4.90)	(1.00)	(18.56)	(1.31)
U_3O_8	15.79	0.90	50.44	1.28	(b)	(b)
	(66.78)	(0.93)	(21.10)	(0.68)		
ZrO_2	(b)	(b)	(b)	(b)	-31.14	-11.87
					(30.22)	(1.23)
Others	3.52[c]	-2.64 to -2.48[d]	-3.05[c]	-2.81 to -2.78[d]	(c)	0.01 to 1.62[d]
	(2.07)	(0.37 to 0.44)	(0.92)	(0.40 to 0.41)		(0.10 to 0.22)
R^2	0.917	0.326	0.980	0.506	0.842	0.620
R^2(ADJ)	0.750	0.278	0.939	0.471	0.816	0.614
R^2(PRESS)	0.165	0.098	0.793	0.361	0.780	0.594
s	0.091	0.155	0.066	0.195	0.493	0.714

(a) BaO+CaO+MgO and K_2O+Li_2O+Na_2O were each treated as combined components, so that the same coefficients are listed for the separate components in each group.

(b) Included in the Others component for this data set--see Table 5.

(c) The Others coefficient in the first-order mixture model may be considered to be an average coefficient for all the components contained in Others.

(d) Others coefficients for FEH models were computed by forming a weighted average of the coefficients for the individual Others components, where the relative proportions of the Others components were used as weights. This can yield different weighted averages across the data points in the data set, so the ranges of coefficient values and standard deviations are reported.

(e) All Others components have constant mass fraction values except for minor variations in three glasses, and there is little variation in mole fractions. This is insufficient to estimate a separate coefficient for Others. The nine components varied in the WVDP data were renormalized to a total mole fraction of 1.0 and then the first-order mixture model was fitted.

Table 4. Coefficients, Coefficient Standard Deviations (in parentheses), and Goodness-of-Fit Statistics for First-Order Mixture Models and Rewritten Free Energy of Hydration Models for ln(PCT Normalized B Release, g/m^2) (continued)

	SRTC 137		SRTC 118		SRTC 111	
Component	Mixture	FEH	Mixture	FEH	Mixture	FEH[d]
Al_2O_3	-32.03	-27.99	-30.48	-30.28	-22.29	
	(2.04)	(1.31)	(2.77)	(1.53)	(3.26)	
B_2O_3	4.17	1.54	6.14	1.78	4.44	
	(1.83)	(0.12)	(2.52)	(0.13)	(2.54)	
CaO	-2.08	3.62	20.29	4.04	5.40	
	(3.42)	(0.21)	(11.21)	(0.25)	(11.16)	
Cr_2O_3	109.45	-12.20	76.65	-13.13	13.35	
	(65.13)	(0.55)	(71.02)	(0.65)	(70.85)	
CuO	133.56	1.69	72.90	1.95	44.86	
	(38.83)	(0.12)	(44.36)	(0.14)	(48.43)	
Fe_2O_3	-19.44	-13.80	-22.97	-14.87	-14.49	
	(3.06)	(0.63)	(4.61)	(0.74)	(4.64)	
FeO	29.35	8.23	24.73	9.05	61.42	
	(4.72)	(0.43)	(5.25)	(0.50)	(12.32)	
K_2O	-30.08	42.04	-21.89	45.76	-14.01	
	(7.37)	(2.05)	(8.19)	(2.39)	(8.03)	
Li_2O	5.39	9.90	5.41	10.85	3.20	
	(2.08)	(0.51)	(3.04)	(0.59)	(2.98)	
MgO	4.85	-0.82	7.91	-0.78	19.19	
	(5.06)	(0.05)	(6.19)	(0.05)	(8.93)	
MnO	18.75	10.14	14.12	11.12	-3.43	
	(7.10)	(0.52)	(7.43)	(0.61)	(9.37)	
Na_2O	21.07	27.73	19.56	30.22	16.98	
	(1.50)	(1.36)	(1.82)	(1.59)	(1.87)	
NiO	-48.18	-5.09	-40.15	-5.41	-0.09	
	(14.04)	(0.22)	(15.86)	(0.25)	(21.19)	
SiO_2	-3.62	-7.35	-4.20	-7.87	-4.47	
	(0.38)	(0.32)	(0.68)	(0.38)	(0.65)	
TiO_2	61.91	-14.85	56.79	-16.01	41.81	
	(12.68)	(0.68)	(12.78)	(0.80)	(12.74)	
Others	-54.24[a]	-15.60 to 18.94[b]	10.92[a]	-16.82 to 20.68[b]	30.01	
	(7.22)	(0.05 to 0.94)	(20.75)	(0.05 to 1.10)	(20.95)	
R^2	0.961[c]	0.763	0.961[c]	0.764	0.968	
R^2(ADJ)	0.956	0.762	0.955	0.762	0.963	
R^2(PRESS)	0.935	0.751	0.937	0.752	0.949	
s	0.251	0.583	0.237	0.547	0.215	

(a) The Others coefficient in the first-order mixture model may be considered to be an average coefficient for all the components contained in Others.

(b) Others coefficients for FEH models were computed by forming a weighted average of the coefficients for the individual Others components, where the relative proportions of the Others components were used as weights. This can yield different weighted averages across the data points in the data set, so the ranges of coefficient values and standard deviations are reported.

(c) Although the various R^2 values are nearly identical for the 137-, 118-, and 111-observation data sets, the models for 118 and 111 observations fit those data sets considerably better than the 137-observation model.

(d) The FEH model for SRTC 111 is essentially the same as for SRTC 118, and so is not reported here.

Table 5. Coefficients of Others Components for Free Energy of Hydration Models Written in the Form of First-Order Mixture Models for ln(PCT Normalized B Release in g/m^2)

Others Component[a]	CVS-I	CVS-II.1	CVS-II.2	CVS-II.3	CVS-II.4	CVS(all)
Ag_2O	(b)	(b)	(b)	-2.73	(b)	-2.31
As_2O_3	(b)	(b)	(b)	-17.52	(b)	-16.04
BaO	9.34	4.79	3.60	7.46	9.57	7.15
CdO	-1.49	-1.68	-0.78	-1.97	-1.81	-1.60
Ce_2O_3	20.34	11.36	8.06	17.04	21.12	16.05
CoO	(b)	(b)	(b)	0.07	(b)	0.29
Cr_2O_3	-8.39	-5.80	-3.58	-7.98	-9.06	-7.19
Cs_2O	38.21	22.03	15.31	32.60	39.89	30.49
CuO	3.03	1.02	1.05	1.96	2.94	2.05
F	-2.36	-2.20	-1.14	-2.73	-2.72	-2.31
FeO	(b)	(b)	(b)	(b)	(b)	(b)
K_2O	(b)	(b)	(b)	30.85	(b)	28.87
La_2O_3	21.76	12.21	8.64	18.27	22.61	17.19
MnO	9.98	5.17	3.86	8.01	10.23	7.66
MoO_3	-10.67	-7.16	-4.51	-9.96	-11.45	-9.03
Nd_2O_3	16.71	9.19	6.59	13.88	17.31	13.11
NiO	-2.55	-2.31	-1.21	-2.89	-2.92	-2.46
P_2O_5	11.04	5.80	4.29	8.94	11.35	8.53
PbO	(b)	(b)	(b)	-11.97	(b)	-10.89
PdO	-2.36	-2.20	-1.14	-2.73	-2.72	-2.31
PdO_2	(b)	(b)	(b)	(b)	(b)	(b)
Pr_6O_{11}	-2.36	-2.20	-1.14	-2.73	-2.72	-2.31
Rb_2O	41.16	23.80	16.50	35.17	43.00	32.88
RhO_2	(b)	(b)	(b)	(b)	(b)	(b)
Rh_2O_3	-2.36	-2.20	-1.14	-2.73	-2.72	-2.31
RuO_2	-31.28	-19.48	-12.86	-27.91	-33.10	-25.69
SO_3	-2.36	-2.20	-1.14	-2.73	-2.72	-2.31
Sb_2O_3	(b)	(b)	(b)	13.78	(b)	13.02
SeO_2	(b)	(b)	(b)	0.70	(b)	0.87
Sm_2O_3	-2.36	-2.20	-1.14	-2.73	-2.72	-2.31
SrO	7.59	3.75	2.90	5.94	7.73	5.74
TeO_2	(b)	(b)	(b)	-8.01	(b)	-7.21
ThO_2	(b)	(b)	(b)	(b)	(b)	(b)
TiO_2	(b)	(b)	(b)	-9.88	(b)	-8.95
U_3O_8	(b)	(b)	3.73	(b)	(b)	7.39
WO_3	(b)	(b)	(b)	(b)	(b)	(b)
Y_2O_3	4.16	1.69	1.50	2.94	4.12	2.96
ZnO	(b)	-2.48	-1.33	-3.13	-3.21	-2.68

(a) Component coefficients were computed according to the two parts of Equation (5d), depending on whether or not a component is in *S*, the group of components assumed to be associated with SiO_2 in glass dissolution reactions. Authorization has not been given to publish which components are in the group *S*. If and when such authorization is received, a revised version of this table may be requested from the first author.

(b) Component was not included or determined for glasses in this data set.

Table 5. Coefficients of Others Components for Free Energy of Hydration Models Written in the Form of First-Order Mixture Models for ln(PCT Normalized B Release in g/m^2) (continued)

Others Component[a]	Ramsey	WV87	WV88	WVDP	SRTC Homo. All 137 Obs.	SRTC Homo. 118 Obs.
Ag_2O	(b)	(b)	(b)	(b)	(b)	(b)
As_2O_3	(b)	(b)	(b)	(b)	(b)	(b)
BaO	(b)	(c)	(c)	6.84	9.37	10.28
CaO	(c)	(c)	(c)	2.53	(c)	(c)
CdO	(b)	(b)	(b)	(b)	(b)	(b)
Ce_2O_3	(b)	3.58	4.41	16.87	22.75	24.81
CoO	(b)	(b)	(b)	-0.89	(b)	(b)
Cr_2O_3	(b)	-3.61	-4.00	-9.32	(c)	(c)
Cs_2O	(b)	8.04	9.63	33.15	44.48	48.41
CuO	(b)	-0.75	-0.66	1.09	(c)	(c)
F	(b)	(b)	(b)	(b)	(b)	(b)
FeO	(c)	(b)	(b)	(b)	(c)	(c)
Fe_2O_3	(c)	(c)	(c)	(c)	(c)	(c)
K_2O	(b)	(c)	(c)	(c)	(c)	(c)
La_2O_3	(b)	3.93	4.82	18.16	24.47	26.68
MgO	(b)	(c)	(c)	-0.80	(c)	(c)
MnO	(b)	(c)	(c)	7.42	(c)	(c)
MoO_3	(b)	-4.18	-4.66	-11.39	-14.96	-16.14
Nd_2O_3	(b)	2.67	3.35	13.56	18.33	20.02
NiO	(b)	-2.15	-2.29	-3.99	(c)	(c)
P_2O_5	(b)	(c)	(c)	8.39	11.44	12.53
PbO	(b)	(b)	(b)	(b)	-17.77	-19.18
PdO	(b)	(b)	(b)	-3.82	(b)	(b)
PdO_2	(b)	(b)	(b)	(b)	(b)	(b)
Pr_6O_{11}	(b)	-2.10	-2.23	-3.82	(b)	(b)
Rb_2O	(b)	(b)	(b)	(b)	(b)	(b)
RhO_2	(b)	(b)	(b)	-3.82	(b)	(b)
Rh_2O_3	(b)	(b)	(b)	(b)	(b)	(b)
RuO_2	(b)	(b)	(b)	-30.18	(b)	(b)
SO_3	(b)	-2.10	-2.23	-3.82	(b)	(b)
Sb_2O_3	(b)	(b)	(b)	(b)	(b)	(b)
SeO_2	(b)	(b)	(b)	(b)	(b)	(b)
Sm_2O_3	(b)	-2.10	-2.23	-3.82	(b)	(b)
SrO	(b)	0.39	0.68	5.25	7.24	7.98
TeO_2	(b)	(b)	(b)	(b)	(b)	(b)
ThO_2	(b)	(c)	(c)	(c)	(b)	(b)
TiO_2	(b)	-4.15	-4.63	-11.31	(c)	(c)
U_3O_8	(b)	(c)	(c)	7.11	(b)	(b)
WO_3	(b)	(b)	(b)	(b)	(b)	(b)
Y_2O_3	(b)	-0.47	-0.33	2.12	(b)	(b)
ZnO	(b)	-2.22	-2.37	-4.25	-5.43	-5.78
ZrO_2	(b)	-4.31	-4.81	(c)	-15.60	-16.82

(a) Component coefficients were computed according to the two parts of Equation (5d), depending on whether or not a component is in *S*, the group of components assumed to be associated with SiO_2 in glass dissolution reactions. Authorization has not been given to publish which components are in the group *S*. If and when such authorization is received, a revised version of this table may be requested from the first author.

(b) Component was not included or determined for glasses in this data set.

(c) Component was not in Others component for this data set--see Table 4 for coefficient.

Table 6. Coefficients, Coefficient Standard Deviations (in parentheses), and Goodness-of-Fit Statistics for Reduced Second-Order Mixture Models for ln(PCT Normalized B Release, g/m^2)

WVDP		CVS(all)		RAMSEY	
Model Term	Coefficient (sd)	Model Term	Coefficient (sd)	Model Term	Coefficient (sd)
Al_2O_3	-21.89 (6.62)	Al_2O_3	-94.71 (7.85)	Al_2O_3	-56.16 (8.57)
B_2O_3	40.02 (6.83)	B_2O_3	11.78 (1.50)	B_2O_3	9.31 (2.35)
CaO	(b)	CaO	13.55 (4.67)	CaO	-7.63 (2.33)
Fe_2O_3	-73.47 (27.79)	Fe_2O_3	-18.85 (4.18)	Fe_2O_3	-25.59 (6.35)
FeO	(a)	FeO	(a)	FeO	10.28 (20.78)
K_2O	16.04 (5.22)	K_2O	(b)	K_2O	(a)
Li_2O	27.47 (9.45)	Li_2O	11.30 (1.03)	Li_2O	(a)
MgO	(b)	MgO	11.54 (1.63)	MgO	(a)
Na_2O	7.87 (3.07)	Na_2O	20.48 (1.13)	Na_2O	14.25 (2.33)
SiO_2	-5.18 (1.38)	SiO_2	-3.44 (0.51)	SiO_2	-1.24 (1.22)
ThO_2	-240.17 (72.48)	ThO_2	(a)	ThO_2	(a)
ZrO_2	-41.61 (26.97)	ZrO_2	-25.34 (2.81)	ZrO_2	(a)
Others	(c)	Others	3.43[d] (2.65)	Others	(e)
Fe_2O_3*Fe_2O_3	805.57 (221.73)	Al_2O_3*Al_2O_3	406.09 (54.04)	Al_2O_3*Al_2O_3	185.40 (59.64)
B_2O_3*K_2O	-228.91 (82.04)	Na_2O*CaO	-111.56 (27.93)	Al_2O_3*Fe_2O_3	186.30 (72.80)
ThO_2*ThO_2	11850.0 (3870.25)	B_2O_3*CaO	-82.09 (26.72)		
B_2O_3*Li_2O	-145.12 (70.02)	MgO*Al_2O_3	-109.80 (37.00)		
		Fe_2O_3*Al_2O_3	459.62 (137.24)		
		B_2O_3*Al_2O_3	85.79 (31.74)		
R^2	0.923		0.892		0.931
R^2(ADJ)	0.903		0.879		0.905
R^2(PRESS)	0.874		0.860		0.825
s	0.358		0.523		0.504

(a) Component was not included or determined for glasses in this data set.

(b) Included in Others component for this data set.

(c) Essentially only nine components were varied in the data set, and the mole fractions of these nine components were renormalized to a total mole fraction of 1.0 prior to fitting the model.

(d) The Others coefficient in the first-order mixture model may be considered to be an average coefficient for all the components contained in Others.

(e) No other components are in this data set.

7. Discussion

The following subsections discuss various aspects of the first-order mixture, second-order mixture, and free energy of hydration models fitted to the data sets described in Section 4.

7.1 Free Energy of Hydration Model Results

Table 3 shows that the fitted FEH models have R^2 values between 0.113 and 0.764 [i.e., the models account for between 11.3% and 76.4% of the variation in ln(NR) values in the various data sets]. The R^2(ADJ) value for the model fitted to each data set is close to the corresponding R^2 value since, with only two coefficients estimated from each data set, it is unlikely the data are overfitted (i.e., that there are unneeded coefficients). R^2(PRESS) values are reasonably close to the corresponding R^2(ADJ) and R^2 values, except for the CVS-II.1, CVS-II.2, WV87, and WV88 data sets. For the first three of these data sets, the FEH model fits the data very poorly, so poor validation performance (including negative R^2(PRESS) values for the CVS-II.1 and CVS-II.2 data sets) is not surprising. For the WV88 data set, the drop from R^2 and R^2(ADJ) to R^2(PRESS) is not as large, and the FEH model fits better than for the CVS-II.1, CVS-II.2, and WV87 data sets.

The s statistics in Table 3 are generally much larger than the 0.06 - 0.14 range suggested in Section 5 for subjectively assessing model lack-of-fit. The WV87 and WV88 data sets are exceptions, where the s values are only slightly larger than the 0.06 - 0.14 range. In general, the FEH models appear to have significant lack-of-fits for all of the data sets.

Predicted versus measured plots (see start of Appendix C for a discussion of such plots) for the FEH models are given in the odd numbered figures in Appendix C (i.e., Figures C.1, C.3, ... C.23). For the CVS-II.1, CVS-II.2, and WV-87 data sets, the FEH models yield roughly constant predictions that do not correlate with the variation in measured PCT normalized B releases. For the CVS-I, CVS-II.3, CVS(all), Ramsey, and WVDP data sets, the FEH models tend (in varying degrees) to overpredict lower PCT normalized B releases and underpredict higher releases. For the CVS-II.4 data set, the FEH model has a slight tendency to overpredict smaller and larger B releases and underpredict intermediate B releases. For the WV88 data set, the FEH model does not appear to be significantly biased, but has considerable uncertainty in predicted B releases. For the SRTC homogeneous data, both the 137-observation and 118-observation FEH models have biased prediction behavior below about 1 g/m^2.

7.2 First-Order Mixture Model Results

Table 4 shows that the fitted FOM models have R^2 values between 0.694 and 0.980 [i.e., the models account for between 69.4% and 98.0% of the variation in ln(NR) values in the various data sets]. Significant decreases in R^2(ADJ) compared to R^2 occur for the CVS-II.1, CVS-II.2, and WV87 data sets, indicating it may be possible to reduce the numbers of components (terms) in the models for these data sets. Significant decreases in R^2(PRESS) compared to the corresponding R^2(ADJ) and R^2 values occur for the CVS-II.1, CVS-II.2, CVS-II.4, WV87, and WV88 data sets, indicating the presence of influential data points. Because all of these data sets resulted from statistically designed experiments, having one or more compositions much different

from the others is not a potential explanation for influential points. One possible explanation is that data points can be influential for FOM models when the true behavior is really second-order. Another potential explanation exists for the CVS-I, CVS-II.4, WV87, and WV88 data sets, which contain only a few more points than model terms. In such cases, many data points can be influential due to the small size of the data set. The fact that influential data points exist for a given data set and model may or may not adversely affect the model's predictive ability.

The s statistics in Table 4 for the FOM models are generally larger than the 0.06 - 0.14 range suggested in Section 5 for subjectively assessing lack-of-fit of models. The WV87 and WV88 data sets are exceptions, where the s values are within the 0.06 - 0.14 range. This is likely due to the relatively small composition regions and narrow ranges of PCT normalized B releases for the WV87 and WV88 data sets. FOM models fitted to such data often perform extremely well. FOM models appear to have slight to moderate lack-of-fits for the other data sets, although not as large as the lack-of-fits for the FEH models. Such lack-of-fits are likely due to the presence of curvilinear and interactive effects of glass components on ln(PCT B normalized release).

Predicted versus measured plots (see start of Appendix C for a discussion of such plots) for the FOM models are given in the even numbered figures in Appendix C (i.e., Figures C.2, C.4, ... C.24). The FOM models do not show any significant prediction bias for any of the data sets, although there are indications of possible slight biases for certain data sets. The FOM models for the various CVS data sets show a slight tendency to underpredict very low PCT normalized B releases (< 0.2 g/m^2). The model for the Ramsey data shows a possible tendency to underpredict larger B releases (> 30-35 g/m^2). The uncertainty in model predictions (represented by the scatter of the points about the 45° line in the predicted versus measured plots) appears to be quite small for all data sets except CVS-II.2, CVS(all), and WVDP, for which moderate uncertainty is seen. Also worth noting is that the FOM model for the WVDP data significantly overpredicts the B release for data point #11 (Ratio5 glass). This point was not greatly influential, and so was retained for use in developing the models.

7.3 Second-Order Mixture Model Results

The reduced second-order mixture models fitted to the WVDP, CVS(all), and Ramsey data sets have R^2 values that are noticeably larger than the R^2 values corresponding to the FOM models (see Tables 4 and 6). The increase in R^2 was from 0.842 to 0.923 for the WVDP data, from 0.810 to 0.892 for the CVS(all) data, and from 0.880 to 0.931 for the Ramsey data. For all three data sets, the SOM model R^2(ADJ) and R^2(PRESS) values are typical amounts below the corresponding R^2 values, indicating that the reduced-second order models do not appear to overfit the data and that there are no highly influential data points. Hrma, Piepel, et al.[3] and subsequent unpublished PNL work have shown that indeed there are second-order component effects in the CVS durability data. Other work in the waste glass community has also demonstrated curvilinear and interactive effects of glass components on glass durability.

Although the second-order mixture models improve on the FOM models, the s statistics (0.358 for the WVDP data, 0.523 for the CVS(all) data, and 0.504 for the Ramsey data) indicate

that they still may have some lack of fit. However, this lack of fit may not be practically significant depending on how the models might be used.

Predicted versus measured plots are given in Figures C.25, C.26, and C.27 for the reduced second-order mixture models fitted to the WVDP, CVS(all), and Ramsey data sets. For the WVDP data, comparing Figure C.25 to the corresponding plot for the FOM model in Figure C.20 shows that the reduced second-order model has better precision. For the CVS(all) data, comparing Figure C.26 to the corresponding plot for the FOM model in Figure C.12 shows that the tendency for biased predictions at smaller and larger B release values was slightly reduced, and that precision is somewhat better. For the Ramsey data, comparing Figure C.27 to the corresponding plot for the FOM model in Figure C.14 shows that the second-order model has corrected the tendency toward underpredicting larger B releases.

7.4 Comparing Goodness-of-Fits of Mixture and Free Energy of Hydration Models

The FEH and FOM models are first compared by evaluating their goodness-of-fit statistics [R^2, R^2(ADJ), and s] and the predictive validation statistics [R^2(PRESS)] listed in Table 4. Comparing these statistics shows that the FOM model fits and predicts better (usually substantially better) than the FEH model for all data sets. This should not be surprising, given the Section 3 result that the FEH model is a restricted form of the FOM model. The FEH approach assumes that the effects of glass components on durability are adequately represented by component FEH values (all adjusted by the same slope "b" and intercept "a" estimated from each data set), whereas the FOM approach lets each data set indicate the effect of each component. For each data set where the FOM model performs much better than the FEH model, the implication is that the component FEH values do not adequately represent the effects of the components on durability over the composition region covered by the data set. Table 4 shows that the FOM component coefficients vary from data set to data set, which implies that the relative effects of components depend on the composition region covered by the data set. The FEH model approach considered in this report does not allow for the relative effects of components to depend on the composition region.

Predicted versus measured plots (Figures C.1 to C.24 in Appendix C) are also used to compare the performance of FEH and FOM models. The plots for the FEH and FOM models for a particular data set are given on the same page in Appendix C to facilitate their comparison. FOM model predictions for the various data sets are generally free from bias, whereas FEH model predictions are much more prone to bias. FOM model predictions are generally much more precise than FEH model predictions, evidenced by the tighter scatter of points about the 45° lines in Figures C.2, C.4, ..., C.22, and C.24 compared to Figures C.1, C.3, ..., C.21, and C.23.

The predicted versus measured plots for the reduced SOM models fitted to the WVDP, CVS(all), and Ramsey data sets given in Figures C.25, C.26, and C.27 improve slightly over the corresponding FOM plots, which in turn are better than the corresponding FEH plots.

The ideal basis to compare the performance of the FEH, FOM, and reduced SOM models would be to have some additional data for each data set that were not used to develop the models.

However, this is not possible, since all data in each data set were used to develop the models. Data from other data sets in this study that fall in the composition region for a given data set could be used to validate the fitted models, but doing so was beyond the scope of this effort. Additional cross-validation approaches (besides the leave-each-data-point-out PRESS approach) could also be used to validate the models, but again these were beyond the scope of this effort. However, Hrma, Piepel, et al.[3] (Section 12.8) used CVS-II Phase 3 data to validate FOM and reduced SOM models (for PCT normalized B release) fitted to CVS data through CVS-II Phase 2. The mixture models accurately predicted PCT normalized B releases within the uncertainty of the model predictions for nearly all the CVS-II Phase 3 validation data points. FOM and SOM models fitted to CVS data through CVS-II Phase 3 were validated using CVS-II Phase 4 data, and the results (although not published) were again very good. These very good validation performances indicate that FOM and SOM models can be very useful prediction tools.

7.5 Comparing FEH and FOM Model Coefficients

The FEH and FOM models fitted to the various data sets are written in the same mathematical form in Table 4, which allows directly comparing their coefficients. Coefficients of models written in the FOM model form do not directly estimate the effects of components on ln(NR), but can be used to estimate such effects. The effect of a given component is strongly determined by its FOM coefficient. However, it's effect is also determined by the component's value at the glass composition at which the effect is to be estimated, and the coefficients (and effects) of other components. Still, comparing FEH and FOM coefficients in Table 4 can indicate where the FEH theory and assumptions seem to hold, and where they do not. The standard deviations of the coefficients provided in Table 4 must be considered when comparing FEH and FOM coefficients. Differences between FEH and FOM model coefficients are only mentioned in the following discussion when they are significant after accounting for the uncertainties in the coefficients.

Al_2O_3 coefficients for FEH and FOM models agree fairly well for all data sets except the CVS data sets, where the Al_2O_3 coefficients are more negative in the FOM models than in the corresponding FEH models. The reason for this is not clear, but it could be due to the CVS data covering a wider range of compositions than the other data sets.

B_2O_3 coefficients are more positive for FOM models than FEH models for all of the data sets. This may indicate a need to reassess the FEH theory and assumptions for B_2O_3.

For all the CVS data sets except CVS-II Phase 1 (where CaO was varied a small amount in only one glass) and also the Ramsey data set, CaO coefficients are negative for FOM models but positive for FEH models. CaO was combined with BaO and MgO in the WV87 and WV88 data sets, so nothing specific can be said about CaO for those data sets. Neither can anything be said about the WVDP data set, where CaO was not studied. For the SRTC 137, 118, and 111 data sets, the CaO FOM model coefficient changes significantly as outlying data points are deleted. This is due to the effect of the outlying data points on correlations of CaO with other components, and also on the changes in the range of CaO values (see Table 2). However, with or

without the outlying data, the CaO coefficients in the FOM models have large enough uncertainties that they are not clearly different from the CaO coefficients in the FEH models.

Fe_2O_3 coefficients in the FEH and FOM models in Table 4 agree very well within their uncertainties except possibly for the Ramsey data set, where the coefficient in the FOM model is more negative than in the FEH model. The Fe_2O_3 coefficient in the FOM model for the CVS-II Phase 1 data set is positive, whereas for the rest of the CVS data sets and all other data sets it is negative. However, the standard deviation of the Fe_2O_3 FOM model coefficient is relatively large for the CVS-II Phase 1 data set, and thus the difference from FEH coefficient is not significant. The CVS-II Phase 1 study investigated a shrunken version of the CVS-I glass composition region, where additional constraints were imposed on glass composition (directly via component ranges, and indirectly via constraints on glass properties). The shrinkage of the composition region reduces the effects of some components, and the small data set size limits the accurate estimation of the reduced component effects.

Li_2O coefficients in the FEH and FOM models in Table 4 agree reasonably well within their uncertainties for all data sets except possibly CVS-II Phase 2 and Phase 4. The very poor fit of the FEH model to the CVS-II Phase 2 data ($R^2 = 0.113$) is likely the reason for the poor agreement of Li_2O coefficients for that data set. The reason for the difference in Li_2O coefficients for the CVS-II Phase 4 data set is not as clear, since the FEH model fits that data reasonably well ($R^2 = 0.741$). The four data points in CVS-II Phase 4 in which Li_2O was varied (see Section 4.1) show an almost perfect linear relationship between ln(NR) and Li_2O mole fraction value, and the FOM model Li_2O coefficient in Table 4 captures that relationship almost perfectly. Hence, the problem would appear to be with the Li_2O coefficient in the FEH model.

For the CVS data sets, the MgO coefficients for the FOM models are generally larger than for the FEH models, but the differences are not significant in all cases. The MgO coefficients in the FEH models for the WV87 and WV88 data sets have essentially identical small negative values, but in the FOM models the MgO coefficient is more negative for the WV87 data set, and positive for the WV88 data set. However, MgO+CaO+BaO were treated as one component in the WV87 and WV88 studies, which is a possible explanation for the differences. Also, the WV88 data set covers a larger composition region than the WV87 data set. MgO was not studied in the WVDP data set. For the SRTC 137 and SRTC 118 data sets, the MgO FOM model coefficients have relatively large standard deviations, and so the differences with respect to the FEH coefficients aren't significant. The MgO FOM model coefficient for the SRTC 111 data set is larger than the coefficients for the SRTC 137 and 118 data sets, due to the smaller upper limit for MgO. The standard deviation is still relatively large, but the difference from the FEH coefficient is borderline significant.

Na_2O coefficients in the FEH and FOM models in Table 4 agree very well within their uncertainties for all data sets except CVS-II Phase 2 (where the FOM model coefficient is larger), WVDP (where the FEH model coefficient is larger), and SRTC 118 and SRTC 111 (where the FEH model coefficients are larger). A possible explanation is that the upper limits of Na_2O for glasses in these data sets are lower than in the other data sets. For the CVS-II Phase 2 data, a likely explanation is the very poor fit of the FEH model ($R^2 = 0.113$).

SiO_2 coefficients in the FEH and FOM models in Table 4 agree very well within their uncertainties for all data sets except possibly the SRTC 137, 118, and 111 data sets. For these SRTC data sets, the SiO_2 coefficients for the FEH models are more negative than the coefficients for the FOM models. The reasons for this are not apparent.

ZrO_2 coefficients for FOM models were more negative than for FEH models for the CVS-I, CVS-II Phase 2, CVS-II Phase 3, CVS(all), and WVDP data sets, although the differences were only significant (when considering uncertainties) for the CVS-II Phase 2, CVS-II Phase 3, and CVS(all) data sets. ZrO_2 appears to have no effect on ln(NR) over the composition region covered by the CVS-II Phase 1 data set, which causes the FOM model to have a small ZrO_2 coefficient with a large standard deviation. ZrO_2 was not studied in the CVS-II Phase 4, Ramsey, WV87, WV88, and SRTC data sets.

K_2O was only studied in the WV87, WV88, WVDP, and SRTC data sets. In the WV87, WV88, and WVDP data sets, the K_2O coefficients were more positive for the FEH models than the FOM models, although the differences are not significant when accounting for the uncertainties in the coefficients. For the SRTC data, the K_2O coefficients for the FOM models are negative, while the coefficients for the FEH models are positive. K_2O, like other alkalis, is expected to increase PCT B release, so the negative K_2O coefficients for the FOM models is bothersome. However, the shortcomings of the SRTC data sets discussed in Section 4.5 are possible reasons. In particular, Figures B.11and B.12 show that the coverage of combinations of K_2O with other components is poor, and this can have significant effects on mixture model coefficients.

FeO was only studied in the Ramsey and SRTC data sets. The FeO coefficients were significantly more positive for the FOM models than the FEH models. This was especially true for the Ramsey and SRTC 111 data sets, which had smaller upper limits for FeO than the SRTC 137 and SRTC 118 data sets. These observations may indicate a need to reassess the FEH theory and assumptions for FeO.

ThO_2 was only studied in the WV87, WV88, and WVDP data sets. For the WV87 and WV88 data sets, the ThO_2 coefficients in the FOM models are positive, where the coefficients in the FEH models are negative. For the WVDP data set, the FOM and FEH model coefficients for ThO_2 are both negative, but not significantly different due to a large standard deviation of the FOM model coefficient. Other work not reported here indicates that ThO_2 appears to have no effect on ln(NR) over the composition region studied in the WVDP data set. These results suggest a possible need to reassess the FEH theory and assumptions for ThO_2.

MnO was only studied in the WV87, WV88, and SRTC data sets. Agreement between MnO coefficients in the FOM and FEH models is relatively good when accounting for uncertainty, except for the SRTC 111 data set. The MnO coefficient for the SRTC 111 data is noticeably different than for the SRTC 118 data, due to deleting two outlying data points with low MnO and high MgO values.

P_2O_5 and U_3O_8 were only studied in the WV87 and WV88 data sets, and the small composition regions and ranges of PCT NR releases in these data sets limit any conclusions. Hence, the results for these components are not discussed.

Cr_2O_3, CuO, NiO, and TiO_2 were only studied in the SRTC data. The FOM model coefficients of Cr_2O_3, CuO, and NiO change dramatically as the glasses with outlying values of these components are deleted going from SRTC 137 to SRTC 118 to SRTC 111. This is due to: (1) the narrowing of the ranges of these components, and (2) the "removal" of strong pairwise correlations among these and other components caused by the outlying points. The coefficients of Cr_2O_3 and CuO are large due their very small upper limits (see Table 2). Overall, the shortcomings of the SRTC data set limit the ability to make meaningful conclusions for Cr_2O_3, CuO, and NiO. The TiO_2 coefficients are positive and large for the FOM models (for the SRTC 137, 118, and 111 data sets) compared to the FEH models. The range of TiO_2 values in these glasses is small, and TiO_2 is somewhat correlated with certain other components (see Figures B.11 and B.12). This could cause the differences observed, but reassessing the FEH theory and assumptions for TiO_2 may be warranted.

The above comparisons show that FOM and FEH model coefficients agree in some cases and disagree in others, depending on the component and data set. For most components, the FOM and FEH model coefficients differed significantly for at least some of the data sets. This confirms that the "preliminary" FEH approach is not flexible enough to adapt to components having different effects for different data sets (and glass composition regions).

8. Conclusions

The free energy of hydration model considered in this report is a restricted form of the first-order mixture model, and thus does not have the flexibility to fit data sets as well as first- or second-order mixture models. The free energy of hydration approach is "restricted" by the assumption that the effects of glass components on durability are determined primarily by constant values of free energy of hydration for each component, which are applicable to all glass composition regions.

Work in the waste glass field has shown that glass components can have curvilinear and interactive effects on glass durability (resistance to dissolution in water). In other words, the effect of a glass component on durability can depend on the fraction of that component in the glass as well as on the fractions of other components in the glass. Neither the FEH nor FOM modeling approaches (as discussed in this report) can account for curvilinear or interactive effects of glass components (without fitting separate models for different composition regions or subregions). However, second-order and higher-order Scheffé mixture models (and other mixture model forms[2]) can directly account for curvilinear or interactive effects of glass components. The FEH approach discussed in this report is referred to as "preliminary FEH" by Jantzen et al.[5], and they also discuss "final FEH" which adjusts the preliminary FEH in some cases. These adjustments appear to provide some ability to account for curvilinear and interactive effects of glass components, but we have insufficient experience with the "final FEH" approach to comment further.

A properly-developed mixture model has a distinct advantage over a FEH model (of the type discussed in this report) when the goal is to predict PCT normalized releases for glass compositions within the same composition region used to fit the model. By properly-developed we mean that: (a) the data used to develop the mixture model should adequately cover the composition region of interest and should avoid unnecessary correlations among glass component mole (or mass) fractions, and (b) proper statistical approaches should be applied to fit the model, detect outliers or influential data points, detect model lack-of-fit, and validate performance of the model with data not used to fit it. If data to develop a mixture model are limited (in number, or due to poor coverage of the region of interest), or are available only for a composition region different than the one for which predictions are desired, then the FEH approach (or some other theoretical/structural approach) might (or might not) be preferable to a mixture approach. However, the FEH approach still requires fitting its model to data, and shortcomings in the data may also affect the performance of the FEH approach. The performance of the FEH approach also appears to depend on the composition region to which it is applied, and hence extrapolation may not be any more advisable than for the mixture approach.

In conclusion, the mixture approach is recommended over the FEH approach for predicting PCT releases of glass compositions within the same composition region as the data base available for modeling.

9. References

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Appendix A

Data Sets--Glass Compositions and PCT Normalized Releases

This appendix contains the glass compositions (mole fractions) and PCT normalized elemental releases for the data sets used in this report. Normalized releases for several elements are given in the tables, but only B normalized releases were used in this report.

In several of the references from which the data were taken, compositions were given in terms of weight percents (or weight fractions). In those cases, mole fraction compositions were computed and are given in the tables of this appendix. Also, in several of the references, PCT unnormalized releases or normalized releases that did not normalize for the surface area to volume ratio were given. In those cases, normalized releases in units of g/m^2 were computed and are given in the tables of this appendix.

Table A.1. CVS-I Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2)

Comp.	CVS1-1*	CVS1-2	CVS1-3	CVS1-4	CVS1-5	CVS1-6	CVS1-7	CVS1-8
SiO_2	0.512371	0.555060	0.419394	0.567939	0.612381	0.477042	0.622724	0.595322
B_2O_3	0.105186	0.043550	0.172363	0.171988	0.046361	0.187143	0.047144	0.047902
Na_2O	0.103769	0.048917	0.048401	0.086933	0.072905	0.052552	0.102097	0.090071
Li_2O	0.080686	0.142048	0.140550	0.020035	0.151218	0.152603	0.021967	0.022321
CaO	0.031444	0.108127	0.000000	0.021351	0.000000	0.000000	0.117051	0.000000
MgO	0.057752	0.000000	0.119089	0.118829	0.000000	0.000000	0.000000	0.132386
Fe_2O_3	0.022807	0.007594	0.007514	0.007498	0.060634	0.008158	0.013811	0.062648
Al_2O_3	0.039998	0.089206	0.082381	0.000000	0.050648	0.000000	0.000000	0.000000
ZrO_2	0.022325	0.000000	0.004869	0.000000	0.000000	0.063440	0.069254	0.043303
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000305	0.000071	0.000070	0.000070	0.000075	0.000760	0.000077	0.000078
CdO	0.002729	0.000634	0.000627	0.000626	0.000675	0.006813	0.000687	0.000698
Ce_2O_3	0.000204	0.000047	0.000047	0.000047	0.000050	0.000509	0.000051	0.000052
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000385	0.000089	0.000088	0.000088	0.000095	0.000960	0.000097	0.000098
Cs_2O	0.000249	0.000058	0.000057	0.000057	0.000062	0.000622	0.000063	0.000064
CuO	0.000883	0.000205	0.000203	0.000202	0.000218	0.002203	0.000222	0.000226
F	0.007376	0.001714	0.001696	0.001692	0.001824	0.018411	0.001855	0.001885
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000896	0.000208	0.000206	0.000206	0.000222	0.002237	0.000225	0.000229
MnO	0.000808	0.000188	0.000186	0.000185	0.000200	0.002016	0.000203	0.000206
MoO_3	0.000974	0.000226	0.000224	0.000223	0.000241	0.002430	0.000245	0.000249
Nd_2O_3	0.001713	0.000398	0.000394	0.000393	0.000424	0.004277	0.000431	0.000438
NiO	0.003599	0.000836	0.000827	0.000825	0.000890	0.008982	0.000905	0.000920
P_2O_5	0.000329	0.000076	0.000076	0.000075	0.000081	0.000821	0.000083	0.000084
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000192	0.000045	0.000044	0.000044	0.000047	0.000479	0.000048	0.000049
Pr_6O_{11}	0.000046	0.000011	0.000011	0.000010	0.000011	0.000114	0.000012	0.000012
Rb_2O	0.000126	0.000029	0.000029	0.000029	0.000031	0.000314	0.000032	0.000032
Rh_2O_3	0.000093	0.000022	0.000021	0.000021	0.000023	0.000231	0.000023	0.000024
RuO_2	0.000528	0.000123	0.000121	0.000121	0.000130	0.001317	0.000133	0.000135
SO_3	0.001607	0.000373	0.000369	0.000369	0.000398	0.004012	0.000404	0.000411
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000067	0.000016	0.000015	0.000015	0.000017	0.000168	0.000017	0.000017
SrO	0.000451	0.000105	0.000104	0.000103	0.000112	0.001125	0.000113	0.000115
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000104	0.000024	0.000024	0.000024	0.000026	0.000260	0.000026	0.000027
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	0.521	0.066	0.864	20.639	0.355	6.113	0.287	1.238
PCT Li	0.529	0.154	0.791	16.935	0.462	4.892	0.331	0.744
PCT Na	0.403	0.064	0.580	17.034	0.191	3.046	0.339	0.805

* The glass names are those used in the reference from which the data were taken.

Table A.1. CVS-I Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS1-9*	CVS1-10	CVS1-11	CVS1-12	CVS1-13	CVS1-14	CVS1-15	CVS1-16
SiO_2	0.472970	0.641699	0.473322	0.440542	0.594718	0.475321	0.536648	0.470582
B_2O_3	0.190688	0.082685	0.150660	0.159689	0.180097	0.195347	0.041435	0.046931
Na_2O	0.058733	0.103571	0.082047	0.074839	0.188334	0.204282	0.112723	0.197470
Li_2O	0.022644	0.022637	0.022660	0.147637	0.020980	0.022756	0.135149	0.021868
CaO	0.000000	0.000000	0.120743	0.112381	0.000000	0.000000	0.000000	0.000000
MgO	0.134302	0.000000	0.000000	0.000000	0.000000	0.000000	0.114512	0.129702
Fe_2O_3	0.059318	0.008472	0.008480	0.059198	0.007851	0.008516	0.007225	0.035108
Al_2O_3	0.000000	0.079609	0.092974	0.000000	0.002336	0.015872	0.000000	0.092414
ZrO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.071740	0.000000	0.000000
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000790	0.000790	0.000632	0.000074	0.000073	0.000079	0.000674	0.000076
CdO	0.007077	0.007074	0.005665	0.000659	0.000656	0.000711	0.006034	0.000683
Ce_2O_3	0.000529	0.000529	0.000423	0.000049	0.000049	0.000053	0.000451	0.000051
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000997	0.000997	0.000798	0.000093	0.000092	0.000100	0.000850	0.000096
Cs_2O	0.000646	0.000646	0.000517	0.000060	0.000060	0.000065	0.000551	0.000062
CuO	0.002288	0.002287	0.001832	0.000213	0.000212	0.000230	0.001951	0.000221
F	0.019123	0.019118	0.015310	0.001781	0.001772	0.001922	0.016305	0.001847
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.002324	0.002323	0.001860	0.000216	0.000215	0.000234	0.001981	0.000224
MnO	0.002094	0.002093	0.001676	0.000195	0.000194	0.000210	0.001785	0.000202
MoO_3	0.002524	0.002524	0.002021	0.000235	0.000234	0.000254	0.002152	0.000244
Nd_2O_3	0.004442	0.004441	0.003556	0.000414	0.000412	0.000446	0.003787	0.000429
NiO	0.009330	0.009327	0.007469	0.000869	0.000864	0.000938	0.007955	0.000901
P_2O_5	0.000853	0.000853	0.000683	0.000079	0.000079	0.000086	0.000728	0.000082
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000498	0.000497	0.000398	0.000046	0.000046	0.000050	0.000424	0.000048
Pr_6O_{11}	0.000119	0.000119	0.000095	0.000011	0.000011	0.000012	0.000101	0.000011
Rb_2O	0.000326	0.000326	0.000261	0.000030	0.000030	0.000033	0.000278	0.000031
Rh_2O_3	0.000240	0.000240	0.000192	0.000022	0.000022	0.000024	0.000205	0.000023
RuO_2	0.001368	0.001367	0.001095	0.000127	0.000127	0.000137	0.001166	0.000132
SO_3	0.004167	0.004165	0.003336	0.000388	0.000386	0.000419	0.003553	0.000402
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000175	0.000175	0.000140	0.000016	0.000016	0.000018	0.000149	0.000017
SrO	0.001169	0.001168	0.000936	0.000109	0.000108	0.000117	0.000997	0.000113
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000270	0.000270	0.000216	0.000025	0.000025	0.000027	0.000230	0.000026
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	10.993	0.127	0.099	4.662	14.072	9.847	18.778	0.523
PCT Li	8.602	0.386	0.187	4.171	12.903	8.011	11.198	0.266
PCT Na	7.897	0.095	0.099	4.395	12.413	5.790	13.995	0.540

* The glass names are those used in the reference from which the data were taken.

Table A.1. CVS-I Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS1-17*	CVS1-18	CVS1-19	CVS1-20	CVS1-21	CVS1-22	CVS1-23
SiO_2	0.520558	0.429600	0.512371	0.512371	0.567939	0.595322	0.563543
B_2O_3	0.049425	0.043993	0.105186	0.105186	0.171988	0.047902	0.090233
Na_2O	0.161552	0.117211	0.103769	0.103769	0.086933	0.090071	0.111531
Li_2O	0.023030	0.143492	0.080686	0.080686	0.020035	0.022321	0.082463
CaO	0.122713	0.021845	0.031444	0.031444	0.021351	0.000000	0.033863
MgO	0.000000	0.121581	0.057752	0.057752	0.118829	0.132386	0.013695
Fe_2O_3	0.060331	0.007671	0.022807	0.022807	0.007498	0.062648	0.048513
Al_2O_3	0.000000	0.000000	0.039998	0.039998	0.000000	0.000000	0.029387
ZrO_2	0.000000	0.064624	0.022325	0.022325	0.000000	0.043303	0.003360
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000803	0.000644	0.000305	0.000305	0.000070	0.000078	0.000301
CdO	0.007197	0.005766	0.002729	0.002729	0.000626	0.000698	0.002701
Ce_2O_3	0.000538	0.000431	0.000204	0.000204	0.000047	0.000052	0.000202
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.001014	0.000812	0.000385	0.000385	0.000088	0.000098	0.000381
Cs_2O	0.000657	0.000526	0.000249	0.000249	0.000057	0.000064	0.000246
CuO	0.002327	0.001864	0.000883	0.000883	0.000202	0.000226	0.000873
F	0.019450	0.015581	0.007376	0.007376	0.001692	0.001885	0.007299
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.002364	0.001893	0.000896	0.000896	0.000206	0.000229	0.000887
MnO	0.002129	0.001706	0.000808	0.000808	0.000185	0.000206	0.000799
MoO_3	0.002567	0.002057	0.000974	0.000974	0.000223	0.000249	0.000963
Nd_2O_3	0.004518	0.003619	0.001713	0.001713	0.000393	0.000438	0.001695
NiO	0.009489	0.007601	0.003599	0.003599	0.000825	0.000920	0.003561
P_2O_5	0.000868	0.000695	0.000329	0.000329	0.000075	0.000084	0.000326
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000506	0.000405	0.000192	0.000192	0.000044	0.000049	0.000190
Pr_6O_{11}	0.000121	0.000097	0.000046	0.000046	0.000010	0.000012	0.000045
Rb_2O	0.000331	0.000265	0.000126	0.000126	0.000029	0.000032	0.000124
Rh_2O_3	0.000244	0.000195	0.000093	0.000093	0.000021	0.000024	0.000092
RuO_2	0.001391	0.001114	0.000528	0.000528	0.000121	0.000135	0.000522
SO_3	0.004238	0.003395	0.001607	0.001607	0.000369	0.000411	0.001590
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000178	0.000142	0.000067	0.000067	0.000015	0.000017	0.000067
SrO	0.001189	0.000952	0.000451	0.000451	0.000103	0.000115	0.000446
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000274	0.000220	0.000104	0.000104	0.000024	0.000027	0.000103
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	2.235	11.238	0.523	0.455	18.850	1.119	0.525
PCT Li	2.075	8.065	0.533	0.468	15.591	0.704	0.535
PCT Na	2.304	8.040	0.433	0.396	15.536	0.760	0.487

* The glass names are those used in the reference from which the data were taken.

Table A.2. CVS-II Phase 1 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2)

Comp.	CVS2-1*	CVS2-2	CVS2-3	CVS2-4	CVS2-5	CVS2-6	CVS2-7	CVS2-8
SiO_2	0.537807	0.526245	0.497874	0.574264	0.528889	0.584895	0.514167	0.532857
B_2O_3	0.077626	0.063370	0.122109	0.096912	0.152730	0.065778	0.156707	0.062937
Na_2O	0.069834	0.089788	0.072735	0.069588	0.108974	0.073885	0.072479	0.099475
Li_2O	0.124156	0.126548	0.093753	0.110522	0.044759	0.083631	0.126925	0.125683
CaO	0.000000	0.078668	0.080387	0.076909	0.041498	0.081657	0.010757	0.000000
MgO	0.076707	0.000000	0.015979	0.000000	0.000000	0.007466	0.000000	0.077650
Fe_2O_3	0.015488	0.017760	0.018148	0.015433	0.016750	0.049158	0.016074	0.044683
Al_2O_3	0.048515	0.067993	0.065184	0.037406	0.052469	0.010202	0.059981	0.037447
ZrO_2	0.005018	0.015344	0.019234	0.005000	0.005427	0.005309	0.005208	0.005080
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000577	0.000184	0.000188	0.000180	0.000625	0.000490	0.000485	0.000183
CdO	0.005173	0.001648	0.001684	0.001611	0.005595	0.004386	0.004349	0.001637
Ce_2O_3	0.000387	0.000123	0.000126	0.000120	0.000418	0.000328	0.000325	0.000122
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000729	0.000232	0.000237	0.000227	0.000788	0.000618	0.000613	0.000231
Cs_2O	0.000472	0.000150	0.000154	0.000147	0.000511	0.000400	0.000397	0.000149
CuO	0.001673	0.000533	0.000544	0.000521	0.001809	0.001418	0.001406	0.000529
F	0.013981	0.004453	0.004550	0.004354	0.015120	0.011852	0.011753	0.004423
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.001699	0.000541	0.000553	0.000529	0.001837	0.001440	0.001428	0.000537
MnO	0.001531	0.000488	0.000498	0.000477	0.001655	0.001298	0.001287	0.000484
MoO_3	0.001845	0.000588	0.000601	0.000575	0.001996	0.001564	0.001551	0.000584
Nd_2O_3	0.003247	0.001034	0.001057	0.001011	0.003512	0.002753	0.002730	0.001027
NiO	0.006821	0.002173	0.002220	0.002124	0.007377	0.005782	0.005734	0.002158
P_2O_5	0.000624	0.000199	0.000203	0.000194	0.000675	0.000529	0.000524	0.000197
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000364	0.000116	0.000118	0.000113	0.000393	0.000308	0.000306	0.000115
Pr_6O_{11}	0.000087	0.000028	0.000028	0.000027	0.000094	0.000073	0.000073	0.000027
Rb_2O	0.000238	0.000076	0.000078	0.000074	0.000258	0.000202	0.000200	0.000075
Rh_2O_3	0.000175	0.000056	0.000057	0.000055	0.000190	0.000149	0.000147	0.000055
RuO_2	0.001000	0.000319	0.000325	0.000311	0.001081	0.000848	0.000841	0.000316
SO_3	0.003046	0.000970	0.000991	0.000949	0.003294	0.002582	0.002561	0.000964
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000128	0.000041	0.000042	0.000040	0.000138	0.000108	0.000107	0.000040
SrO	0.000855	0.000272	0.000278	0.000266	0.000924	0.000724	0.000718	0.000270
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000197	0.000063	0.000064	0.000061	0.000213	0.000167	0.000166	0.000062
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	0.312	0.128	0.137	0.158	0.284	1.185	0.740	0.484
PCT Li	0.369	0.276	0.222	0.300	0.382	1.303	0.812	0.523
PCT Na	0.208	0.188	0.125	0.182	0.284	1.284	0.343	0.445

* The glass names are those used in the reference from which the data were taken.

Table A.2. CVS-II Phase 1 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-9*	CVS2-10	CVS2-11	CVS2-12	CVS2-13	CVS2-14	CVS2-15	CVS2-16
SiO_2	0.582711	0.527333	0.517212	0.491330	0.516203	0.491918	0.517626	0.579488
B_2O_3	0.087399	0.164828	0.068192	0.153935	0.063168	0.121090	0.066128	0.098382
Na_2O	0.096090	0.142232	0.084960	0.071197	0.171503	0.083142	0.180389	0.118063
Li_2O	0.129421	0.045178	0.126931	0.098309	0.047304	0.104503	0.047100	0.081628
CaO	0.000000	0.000000	0.078906	0.078687	0.033607	0.057287	0.070482	0.009627
MgO	0.000000	0.000000	0.015684	0.015641	0.077935	0.031884	0.000000	0.013556
Fe_2O_3	0.028737	0.028278	0.015834	0.015790	0.015736	0.016094	0.016473	0.029285
Al_2O_3	0.008724	0.069048	0.006200	0.055706	0.055206	0.015313	0.048763	0.014736
ZrO_2	0.052309	0.005478	0.047968	0.005116	0.005098	0.052145	0.005337	0.020323
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000188	0.000227	0.000491	0.000184	0.000183	0.000343	0.000614	0.000450
CdO	0.001685	0.002033	0.004397	0.001648	0.001643	0.003071	0.005503	0.004027
Ce_2O_3	0.000126	0.000152	0.000328	0.000123	0.000123	0.000229	0.000411	0.000301
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000237	0.000287	0.000620	0.000232	0.000231	0.000433	0.000775	0.000567
Cs_2O	0.000154	0.000186	0.000401	0.000150	0.000150	0.000280	0.000502	0.000368
CuO	0.000545	0.000657	0.001422	0.000533	0.000531	0.000993	0.001779	0.001302
F	0.004554	0.005494	0.011881	0.004454	0.004439	0.008299	0.014870	0.010883
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000553	0.000668	0.001444	0.000541	0.000539	0.001008	0.001807	0.001322
MnO	0.000499	0.000602	0.001301	0.000488	0.000486	0.000909	0.001628	0.001191
MoO_3	0.000601	0.000725	0.001568	0.000588	0.000586	0.001095	0.001963	0.001437
Nd_2O_3	0.001058	0.001276	0.002760	0.001035	0.001031	0.001928	0.003454	0.002528
NiO	0.002222	0.002680	0.005796	0.002173	0.002166	0.004049	0.007255	0.005309
P_2O_5	0.000203	0.000245	0.000530	0.000199	0.000198	0.000370	0.000663	0.000486
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000118	0.000143	0.000309	0.000116	0.000115	0.000216	0.000387	0.000283
Pr_6O_{11}	0.000028	0.000034	0.000074	0.000028	0.000028	0.000051	0.000092	0.000067
Rb_2O	0.000078	0.000094	0.000202	0.000076	0.000076	0.000141	0.000253	0.000185
Rh_2O_3	0.000057	0.000069	0.000149	0.000056	0.000056	0.000104	0.000187	0.000137
RuO_2	0.000326	0.000393	0.000850	0.000319	0.000317	0.000594	0.001064	0.000778
SO_3	0.000992	0.001197	0.002589	0.000970	0.000967	0.001808	0.003240	0.002371
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000042	0.000050	0.000108	0.000041	0.000041	0.000076	0.000136	0.000099
SrO	0.000278	0.000336	0.000726	0.000272	0.000271	0.000507	0.000909	0.000665
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000064	0.000077	0.000168	0.000063	0.000063	0.000117	0.000210	0.000153
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	0.560	1.332	1.587	0.194	0.360	1.656	0.331	2.937
PCT Li	0.620	1.322	1.564	0.262	0.362	1.468	0.451	2.349
PCT Na	0.374	0.828	1.370	0.184	0.478	1.268	0.608	2.182

* The glass names are those used in the reference from which the data were taken.

Table A.2. CVS-II Phase 1 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-17*	CVS2-18	CVS2-19
SiO_2	0.512371	0.579488	0.578911
B_2O_3	0.105186	0.098382	0.098276
Na_2O	0.103769	0.118063	0.118920
Li_2O	0.080686	0.081628	0.081492
CaO	0.031444	0.009627	0.009546
MgO	0.057752	0.013556	0.013606
Fe_2O_3	0.022807	0.029285	0.029966
Al_2O_3	0.039998	0.014736	0.015047
ZrO_2	0.022325	0.020323	0.020769
Ag_2O	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000
BaO	0.000305	0.000450	0.000423
CdO	0.002729	0.004027	0.003316
Ce_2O_3	0.000204	0.000301	0.000032
CoO	0.000000	0.000000	0.000000
Cr_2O_3	0.000385	0.000567	0.000556
Cs_2O	0.000249	0.000368	0.000349
CuO	0.000883	0.001302	0.001301
F	0.007376	0.010883	0.006551
K_2O	0.000000	0.000000	0.000000
La_2O_3	0.000896	0.001322	0.003097
MnO	0.000808	0.001191	0.001191
MoO_3	0.000974	0.001437	0.001411
Nd_2O_3	0.001713	0.002528	0.001110
NiO	0.003599	0.005309	0.005262
P_2O_5	0.000329	0.000486	0.000457
PbO	0.000000	0.000000	0.000000
PdO	0.000192	0.000283	0.000000
Pr_6O_{11}	0.000046	0.000067	0.000121
Rb_2O	0.000126	0.000185	0.000000
Rh_2O_3	0.000093	0.000137	0.000000
RuO_2	0.000528	0.000778	0.000743
SO_3	0.001607	0.002371	0.003601
Sb_2O_3	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000
Sm_2O_3	0.000067	0.000099	0.000000
SrO	0.000451	0.000665	0.000000
TeO_2	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000
Y_2O_3	0.000104	0.000153	0.000000
ZnO	0.000000	0.000000	0.003945
PCT B	0.495	2.578	1.990
PCT Li	0.572	2.094	1.654
PCT Na	0.474	1.886	1.481

* The glass names are those used in the reference from which the data were taken.

Table A.3. CVS-II Phase 2 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2)

Comp.	CVS2-20*	CVS2-21	CVS2-22	CVS2-23	CVS2-24	CVS2-25	CVS2-26	CVS2-27
SiO_2	0.603222	0.545304	0.554513	0.592645	0.471671	0.534599	0.457421	0.550251
B_2O_3	0.045668	0.108492	0.041980	0.046841	0.182383	0.045601	0.178191	0.043465
Na_2O	0.105773	0.046371	0.069317	0.201588	0.075389	0.086154	0.051239	0.195287
Li_2O	0.142360	0.134655	0.136929	0.020906	0.148721	0.148738	0.145302	0.031392
CaO	0.000000	0.000000	0.000000	0.089118	0.000000	0.090575	0.088483	0.000000
MgO	0.000000	0.114094	0.116020	0.000000	0.000000	0.000000	0.000000	0.120123
Fe_2O_3	0.023891	0.007199	0.007321	0.007824	0.007951	0.059639	0.007768	0.007579
Al_2O_3	0.006236	0.038673	0.020925	0.035414	0.059836	0.002055	0.015634	0.046415
ZrO_2	0.067085	0.000000	0.000000	0.000000	0.000000	0.000000	0.050338	0.000000
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000074	0.000067	0.000682	0.000073	0.000696	0.000420	0.000072	0.000071
CdO	0.000665	0.000601	0.006113	0.000653	0.006235	0.003765	0.000649	0.000633
Ce_2O_3	0.000050	0.000045	0.000457	0.000049	0.000466	0.000281	0.000048	0.000047
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000094	0.000085	0.000861	0.000092	0.000879	0.000531	0.000091	0.000089
Cs_2O	0.000061	0.000055	0.000558	0.000060	0.000569	0.000344	0.000059	0.000058
CuO	0.000215	0.000194	0.001977	0.000211	0.002016	0.001217	0.000210	0.000205
F	0.001797	0.001625	0.016520	0.001766	0.016848	0.010175	0.001753	0.001710
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000218	0.000197	0.002008	0.000215	0.002047	0.001236	0.000213	0.000208
MnO	0.000197	0.000178	0.001809	0.000193	0.001845	0.001114	0.000192	0.000187
MoO_3	0.000237	0.000214	0.002181	0.000233	0.002224	0.001343	0.000231	0.000226
Nd_2O_3	0.000417	0.000377	0.003837	0.000410	0.003914	0.002363	0.000407	0.000397
NiO	0.000877	0.000793	0.008060	0.000861	0.008220	0.004964	0.000855	0.000834
P_2O_5	0.000080	0.000072	0.000737	0.000079	0.000752	0.000454	0.000078	0.000076
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000047	0.000042	0.000430	0.000046	0.000438	0.000265	0.000046	0.000044
Pr_6O_{11}	0.000011	0.000010	0.000102	0.000011	0.000104	0.000063	0.000011	0.000011
Rb_2O	0.000031	0.000028	0.000281	0.000030	0.000287	0.000173	0.000030	0.000029
Rh_2O_3	0.000023	0.000020	0.000207	0.000022	0.000211	0.000128	0.000022	0.000021
RuO_2	0.000129	0.000116	0.001182	0.000126	0.001205	0.000728	0.000125	0.000122
SO_3	0.000392	0.000354	0.003599	0.000385	0.003671	0.002217	0.000382	0.000373
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000016	0.000015	0.000151	0.000016	0.000154	0.000093	0.000016	0.000016
SrO	0.000110	0.000099	0.001010	0.000108	0.001030	0.000622	0.000107	0.000105
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000025	0.000023	0.000233	0.000025	0.000238	0.000143	0.000025	0.000024
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	0.347	3.854	9.646	0.173	4.522	4.662	1.628	3.270
PCT Li	0.386	2.534	5.453	0.604	3.226	2.765	1.436	1.835
PCT Na	0.279	2.089	6.097	0.809	2.060	3.526	1.349	2.342

* The glass names are those used in the reference from which the data were taken.

Table A.3. CVS-II Phase 2 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-28*	CVS2-29	CVS2-30	CVS2-31	CVS2-32	CVS2-33	CVS2-34	CVS2-35
SiO_2	0.611440	0.495802	0.593498	0.585354	0.575854	0.433951	0.450027	0.448238
B_2O_3	0.046957	0.194901	0.197388	0.163346	0.045638	0.048510	0.161186	0.046054
Na_2O	0.210979	0.073886	0.092234	0.049777	0.205049	0.200325	0.207746	0.206921
Li_2O	0.027569	0.022704	0.022994	0.068349	0.091016	0.075623	0.079502	0.091847
CaO	0.000000	0.096781	0.000000	0.088021	0.000000	0.000000	0.000000	0.091475
MgO	0.000000	0.000000	0.000000	0.000000	0.000000	0.123222	0.000000	0.000000
Fe_2O_3	0.008188	0.008497	0.056794	0.007728	0.007958	0.007775	0.008063	0.025378
Al_2O_3	0.035589	0.000000	0.030863	0.031831	0.001683	0.054310	0.087640	0.084273
ZrO_2	0.000000	0.045919	0.000000	0.000000	0.067041	0.000000	0.000000	0.000000
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000763	0.000792	0.000080	0.000072	0.000074	0.000725	0.000075	0.000075
CdO	0.006838	0.007095	0.000719	0.000645	0.000665	0.006493	0.000673	0.000671
Ce_2O_3	0.000511	0.000530	0.000054	0.000048	0.000050	0.000485	0.000050	0.000050
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000964	0.001000	0.000101	0.000091	0.000094	0.000915	0.000095	0.000095
Cs_2O	0.000624	0.000648	0.000066	0.000059	0.000061	0.000593	0.000061	0.000061
CuO	0.002211	0.002294	0.000232	0.000209	0.000215	0.002099	0.000218	0.000217
F	0.018479	0.019174	0.001942	0.001744	0.001796	0.017546	0.001820	0.001812
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.002246	0.002330	0.000236	0.000212	0.000218	0.002132	0.000221	0.000220
MnO	0.002023	0.002099	0.000213	0.000191	0.000197	0.001921	0.000199	0.000198
MoO_3	0.002439	0.002531	0.000256	0.000230	0.000237	0.002316	0.000240	0.000239
Nd_2O_3	0.004292	0.004454	0.000451	0.000405	0.000417	0.004076	0.000423	0.000421
NiO	0.009015	0.009355	0.000947	0.000851	0.000876	0.008560	0.000888	0.000884
P_2O_5	0.000824	0.000856	0.000087	0.000078	0.000080	0.000783	0.000081	0.000081
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000481	0.000499	0.000051	0.000045	0.000047	0.000456	0.000047	0.000047
Pr_6O_{11}	0.000115	0.000119	0.000012	0.000011	0.000011	0.000109	0.000011	0.000011
Rb_2O	0.000315	0.000327	0.000033	0.000030	0.000031	0.000299	0.000031	0.000031
Rh_2O_3	0.000232	0.000241	0.000024	0.000022	0.000023	0.000220	0.000023	0.000023
RuO_2	0.001322	0.001371	0.000139	0.000125	0.000128	0.001255	0.000130	0.000130
SO_3	0.004026	0.004178	0.000423	0.000380	0.000391	0.003823	0.000396	0.000395
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000169	0.000175	0.000018	0.000016	0.000016	0.000160	0.000017	0.000017
SrO	0.001129	0.001172	0.000119	0.000107	0.000110	0.001072	0.000111	0.000111
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000261	0.000270	0.000027	0.000025	0.000025	0.000247	0.000026	0.000026
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	5.144	1.286	6.512	0.411	9.646	1.723	4.340	0.320
PCT Li	3.682	1.355	4.194	0.460	5.527	1.438	3.468	0.580
PCT Na	3.538	1.273	2.552	0.318	5.896	1.608	2.700	0.910

* The glass names are those used in the reference from which the data were taken.

Table A.3. CVS-II Phase 2 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

	CVS2-36*	CVS2-37	CVS2-38	CVS2-39	CVS2-40	CVS2-41	CVS2-42	CVS2-43
SiO_2	0.561666	0.580749	0.555715	0.482977	0.515480	0.538664	0.576536	0.521806
B_2O_3	0.044710	0.073776	0.103340	0.043079	0.056406	0.060589	0.043840	0.131196
Na_2O	0.089493	0.104795	0.109273	0.131811	0.148726	0.076588	0.061554	0.049887
Li_2O	0.145833	0.143407	0.021710	0.140514	0.086581	0.142382	0.142994	0.135137
CaO	0.088806	0.000000	0.000000	0.000000	0.021916	0.054190	0.034831	0.022054
MgO	0.000000	0.000000	0.128764	0.119058	0.076236	0.030160	0.057551	0.046029
Fe_2O_3	0.058474	0.007667	0.058010	0.027870	0.007696	0.011418	0.038224	0.011617
Al_2O_3	0.005373	0.084056	0.017306	0.015178	0.060271	0.059611	0.017960	0.030325
ZrO_2	0.000000	0.000000	0.000000	0.034075	0.009975	0.009865	0.009908	0.035130
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000073	0.000071	0.000076	0.000070	0.000215	0.000213	0.000214	0.000217
CdO	0.000651	0.000640	0.000678	0.000627	0.001928	0.001907	0.001915	0.001940
Ce_2O_3	0.000049	0.000048	0.000051	0.000047	0.000144	0.000142	0.000143	0.000145
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000092	0.000090	0.000096	0.000088	0.000272	0.000269	0.000270	0.000273
Cs_2O	0.000059	0.000058	0.000062	0.000057	0.000176	0.000174	0.000175	0.000177
CuO	0.000211	0.000207	0.000219	0.000203	0.000623	0.000617	0.000619	0.000627
F	0.001759	0.001730	0.001833	0.001695	0.005210	0.005153	0.005176	0.005243
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000214	0.000210	0.000223	0.000206	0.000633	0.000626	0.000629	0.000637
MnO	0.000193	0.000189	0.000201	0.000186	0.000570	0.000564	0.000567	0.000574
MoO_3	0.000232	0.000228	0.000242	0.000224	0.000688	0.000680	0.000683	0.000692
Nd_2O_3	0.000409	0.000402	0.000426	0.000394	0.001210	0.001197	0.001202	0.001218
NiO	0.000858	0.000844	0.000894	0.000827	0.002542	0.002514	0.002525	0.002558
P_2O_5	0.000079	0.000077	0.000082	0.000076	0.000232	0.000230	0.000231	0.000234
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000046	0.000045	0.000048	0.000044	0.000136	0.000134	0.000135	0.000136
Pr_6O_{11}	0.000011	0.000011	0.000011	0.000011	0.000032	0.000032	0.000032	0.000033
Rb_2O	0.000030	0.000029	0.000031	0.000029	0.000089	0.000088	0.000088	0.000089
Rh_2O_3	0.000022	0.000022	0.000023	0.000021	0.000065	0.000065	0.000065	0.000066
RuO_2	0.000126	0.000124	0.000131	0.000121	0.000373	0.000369	0.000370	0.000375
SO_3	0.000383	0.000377	0.000399	0.000369	0.001135	0.001123	0.001128	0.001142
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000016	0.000016	0.000017	0.000015	0.000048	0.000047	0.000047	0.000048
SrO	0.000108	0.000106	0.000112	0.000104	0.000318	0.000315	0.000316	0.000320
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000025	0.000024	0.000026	0.000024	0.000073	0.000073	0.000073	0.000074
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	0.480	0.246	1.119	12.701	0.337	0.177	1.694	0.767
PCT Li	0.630	0.300	0.726	6.528	0.328	0.260	1.220	0.697
PCT Na	0.654	0.177	0.807	7.668	0.399	0.188	1.337	0.451

* The glass names are those used in the reference from which the data were taken.

Table A.3. CVS-II Phase 2 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-44*	CVS2-45	CVS2-46	CVS2-47	CVS2-48	CVS2-49	CVS2-50	CVS2-51
SiO_2	0.566725	0.538631	0.537222	0.551685	0.496072	0.537845	0.512371	0.578911
B_2O_3	0.092503	0.097027	0.110893	0.044969	0.131357	0.124169	0.105186	0.098276
Na_2O	0.048193	0.049270	0.057086	0.129007	0.099046	0.098360	0.103769	0.118920
Li_2O	0.139745	0.121611	0.143647	0.089893	0.082770	0.088044	0.080686	0.081492
CaO	0.053263	0.021781	0.021869	0.055825	0.056542	0.022718	0.031444	0.009546
MgO	0.029644	0.075766	0.030428	0.031070	0.031469	0.031610	0.057752	0.013606
Fe_2O_3	0.007482	0.011779	0.007680	0.007842	0.007942	0.020543	0.022807	0.029966
Al_2O_3	0.036501	0.035460	0.044864	0.024564	0.053116	0.049044	0.039998	0.015047
ZrO_2	0.009696	0.009913	0.009953	0.025407	0.010293	0.010340	0.022325	0.020769
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000209	0.000499	0.000468	0.000512	0.000404	0.000223	0.000305	0.000423
CdO	0.001874	0.004471	0.004194	0.004584	0.003621	0.001999	0.002729	0.003316
Ce_2O_3	0.000140	0.000334	0.000313	0.000342	0.000271	0.000149	0.000204	0.000032
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000264	0.000630	0.000591	0.000646	0.000510	0.000282	0.000385	0.000556
Cs_2O	0.000171	0.000408	0.000383	0.000418	0.000331	0.000182	0.000249	0.000349
CuO	0.000606	0.001446	0.001356	0.001482	0.001171	0.000646	0.000883	0.001301
F	0.005065	0.012083	0.011334	0.012387	0.009786	0.005401	0.007376	0.006551
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000616	0.001468	0.001377	0.001505	0.001189	0.000656	0.000896	0.003097
MnO	0.000555	0.001323	0.001241	0.001356	0.001071	0.000591	0.000808	0.001191
MoO_3	0.000669	0.001595	0.001496	0.001635	0.001292	0.000713	0.000974	0.001411
Nd_2O_3	0.001177	0.002807	0.002633	0.002877	0.002273	0.001255	0.001713	0.001110
NiO	0.002471	0.005895	0.005530	0.006043	0.004774	0.002635	0.003599	0.005262
P_2O_5	0.000226	0.000539	0.000506	0.000553	0.000437	0.000241	0.000329	0.000457
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000132	0.000314	0.000295	0.000322	0.000255	0.000141	0.000192	0.000000
Pr_6O_{11}	0.000031	0.000075	0.000070	0.000077	0.000061	0.000033	0.000046	0.000121
Rb_2O	0.000086	0.000206	0.000193	0.000211	0.000167	0.000092	0.000126	0.000000
Rh_2O_3	0.000064	0.000152	0.000142	0.000155	0.000123	0.000068	0.000093	0.000000
RuO_2	0.000362	0.000864	0.000811	0.000886	0.000700	0.000386	0.000528	0.000743
SO_3	0.001104	0.002633	0.002470	0.002699	0.002132	0.001177	0.001607	0.003601
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000046	0.000110	0.000103	0.000113	0.000089	0.000049	0.000067	0.000000
SrO	0.000310	0.000739	0.000693	0.000757	0.000598	0.000330	0.000451	0.000000
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000071	0.000170	0.000160	0.000175	0.000138	0.000076	0.000104	0.000000
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.003945
PCT B	0.255	0.500	0.317	1.159	0.307	0.303	0.442	1.764
PCT Li	0.294	0.478	0.346	1.124	0.318	0.334	0.426	1.496
PCT Na	0.194	0.374	0.188	1.055	0.284	0.217	0.368	1.283

* The glass names are those used in the reference from which the data were taken.

Table A.3. CVS-II Phase 2 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-52*	CVS2-53	CVS2-54	CVS2-55	CVS2-56	CVS2-57	CVS2-58
SiO_2	0.620786	0.538830	0.578728	0.574707	0.569131	0.585337	0.390482
B_2O_3	0.072955	0.077774	0.098245	0.097563	0.096616	0.099367	0.172825
Na_2O	0.045135	0.069967	0.118882	0.118056	0.116911	0.120240	0.048531
Li_2O	0.163937	0.124392	0.081466	0.080900	0.080116	0.082397	0.140927
CaO	0.000887	0.000000	0.009543	0.009477	0.009385	0.009652	0.021455
MgO	0.001388	0.076853	0.013602	0.013507	0.013376	0.013757	0.119408
Fe_2O_3	0.028028	0.015517	0.029956	0.029748	0.029460	0.030298	0.007534
Al_2O_3	0.014206	0.048607	0.015042	0.014937	0.014792	0.015214	0.088502
ZrO_2	0.019424	0.005028	0.020762	0.020618	0.020418	0.021000	0.004882
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000428	0.000579	0.000454	0.000000	0.000000	0.000000	0.000070
CdO	0.003836	0.005183	0.004068	0.000000	0.000000	0.000000	0.000629
Ce_2O_3	0.000287	0.000387	0.000304	0.000000	0.000000	0.000000	0.000047
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000541	0.000730	0.000573	0.003812	0.003020	0.002330	0.000089
Cs_2O	0.000350	0.000473	0.000371	0.000000	0.000000	0.000000	0.000057
CuO	0.001240	0.001676	0.001315	0.000000	0.000000	0.000000	0.000203
F	0.010366	0.014007	0.010993	0.010165	0.010066	0.010353	0.001700
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.001260	0.001702	0.001336	0.000000	0.000000	0.000000	0.000207
MnO	0.001135	0.001533	0.001204	0.020882	0.034320	0.000000	0.000186
MoO_3	0.001368	0.001849	0.001451	0.000000	0.000000	0.000000	0.000224
Nd_2O_3	0.002408	0.000000	0.000000	0.003214	0.000000	0.010055	0.000395
NiO	0.005057	0.006834	0.005363	0.000000	0.000000	0.000000	0.000829
P_2O_5	0.000463	0.000625	0.000491	0.000000	0.000000	0.000000	0.000076
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000270	0.000364	0.000286	0.000000	0.000000	0.000000	0.000044
Pr_6O_{11}	0.000064	0.000087	0.000068	0.000000	0.000000	0.000000	0.000011
Rb_2O	0.000177	0.000239	0.000187	0.000000	0.000000	0.000000	0.000029
Rh_2O_3	0.000130	0.000176	0.000138	0.000000	0.000000	0.000000	0.000021
RuO_2	0.000741	0.001002	0.000786	0.000000	0.000000	0.000000	0.000122
SO_3	0.002259	0.003052	0.002395	0.002412	0.002389	0.000000	0.000370
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000095	0.000128	0.000100	0.000000	0.000000	0.000000	0.000016
SrO	0.000634	0.000856	0.000672	0.000000	0.000000	0.000000	0.000104
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.001351	0.001061	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000146	0.000198	0.000155	0.000000	0.000000	0.000000	0.000024
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	0.557	0.304	2.761	1.342	1.419	1.164	0.778
PCT Li	0.554	0.305	1.715	1.127	1.218	1.081	0.636
PCT Na	0.260	0.202	1.612	0.880	0.946	0.842	0.620

* The glass names are those used in the reference from which the data were taken.

Table A.4. CVS-II Phase 3 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2)

Comp.	CVS2-59*	CVS2-60	CVS2-61	CVS2-62	CVS2-63	CVS2-64	CVS2-65	CVS2-66
SiO_2	0.446571	0.528447	0.546037	0.586772	0.362325	0.609524	0.560856	0.545773
B_2O_3	0.151175	0.075654	0.059254	0.160213	0.166126	0.047001	0.102172	0.083466
Na_2O	0.125328	0.167335	0.120282	0.114704	0.206488	0.095940	0.087498	0.123811
Li_2O	0.149043	0.149497	0.151771	0.032991	0.011496	0.138115	0.147088	0.110908
CaO	0.040964	0.006754	0.000000	0.056343	0.120111	0.002866	0.000787	0.010960
MgO	0.000760	0.000746	0.000000	0.000784	0.000000	0.001276	0.000626	0.009590
Fe_2O_3	0.007672	0.007530	0.007781	0.007914	0.008436	0.032687	0.000513	0.015396
Al_2O_3	0.069094	0.054545	0.099011	0.030989	0.118912	0.018158	0.012122	0.073335
ZrO_2	0.003729	0.003660	0.008823	0.003846	0.000000	0.022486	0.079220	0.001337
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000073	0.000075	0.000091	0.000070	0.000079	0.000000	0.000000	0.000209
CdO	0.000654	0.000673	0.000812	0.000628	0.000704	0.006476	0.000000	0.000000
Ce_2O_3	0.000049	0.000050	0.000061	0.000047	0.000053	0.000483	0.000000	0.000000
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000092	0.000095	0.000114	0.000088	0.000099	0.000477	0.001996	0.004486
Cs_2O	0.000060	0.000061	0.000074	0.000057	0.000064	0.000590	0.000000	0.000000
CuO	0.000211	0.000218	0.000263	0.000203	0.000228	0.000000	0.000000	0.000000
F	0.001766	0.001818	0.002195	0.001697	0.001904	0.001122	0.000000	0.002111
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000588	0.005844	0.000000
La_2O_3	0.000215	0.000221	0.000267	0.000206	0.000231	0.000549	0.000083	0.000829
MnO	0.000193	0.000199	0.000240	0.000186	0.000208	0.000000	0.000000	0.010581
MoO_3	0.000233	0.000240	0.000290	0.000224	0.000251	0.001066	0.000000	0.002768
Nd_2O_3	0.000410	0.000422	0.000510	0.000394	0.000442	0.002788	0.001160	0.000000
NiO	0.000862	0.000887	0.001071	0.000828	0.000929	0.008450	0.000000	0.004439
P_2O_5	0.000079	0.000081	0.000098	0.000076	0.000085	0.001681	0.000000	0.000000
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000802	0.000000	0.000000
PdO	0.000046	0.000047	0.000057	0.000044	0.000050	0.000279	0.000000	0.000000
Pr_6O_{11}	0.000011	0.000011	0.000014	0.000011	0.000012	0.000000	0.000000	0.000000
Rb_2O	0.000030	0.000031	0.000037	0.000029	0.000032	0.000000	0.000000	0.000000
Rh_2O_3	0.000022	0.000023	0.000028	0.000021	0.000024	0.000118	0.000035	0.000000
RuO_2	0.000126	0.000130	0.000157	0.000121	0.000136	0.000852	0.000000	0.000000
SO_3	0.000385	0.000396	0.000478	0.000370	0.000415	0.002236	0.000000	0.000000
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000016	0.000017	0.000020	0.000015	0.000017	0.000000	0.000000	0.000000
SrO	0.000108	0.000111	0.000134	0.000104	0.000116	0.000000	0.000000	0.000000
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.002240	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000025	0.000026	0.000031	0.000024	0.000027	0.000000	0.000000	0.000000
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.001152	0.000000	0.000000
PCT B	1.591	1.624	0.222	1.002	0.332	0.379	0.335	0.210
PCT Li	1.287	1.158	0.280	0.862	0.222	0.376	0.355	0.247
PCT Na	1.222	1.523	0.230	0.928	0.390	0.342	0.200	0.223

* The glass names are those used in the reference from which the data were taken.

Table A.4. CVS-II Phase 3 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-67*	CVS2-68	CVS2-69	CVS2-70	CVS2-71	CVS2-72	CVS2-73	CVS2-74
SiO_2	0.484279	0.518857	0.587706	0.509864	0.605472	0.546417	0.524842	0.586424
B_2O_3	0.144322	0.120392	0.069990	0.128550	0.046688	0.083565	0.121780	0.069837
Na_2O	0.110933	0.079541	0.066838	0.082685	0.095302	0.123957	0.080458	0.066693
Li_2O	0.123522	0.144074	0.148865	0.145946	0.137196	0.111039	0.145736	0.148541
CaO	0.002709	0.000772	0.008789	0.000900	0.002847	0.010973	0.000781	0.008770
MgO	0.000157	0.000307	0.004953	0.001253	0.001267	0.009602	0.000310	0.004943
Fe_2O_3	0.000159	0.001782	0.013049	0.003162	0.032470	0.015414	0.001802	0.013020
Al_2O_3	0.126855	0.099491	0.049930	0.112593	0.018037	0.073421	0.100639	0.049821
ZrO_2	0.000000	0.000050	0.000253	0.000256	0.022336	0.001339	0.000051	0.000253
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000340	0.000000	0.000000	0.000000	0.000000
BaO	0.000000	0.000000	0.000000	0.000000	0.000494	0.000313	0.000304	0.000666
CdO	0.000000	0.000000	0.000534	0.000538	0.004428	0.002800	0.002722	0.005964
Ce_2O_3	0.000000	0.000000	0.000000	0.000240	0.000331	0.000209	0.000203	0.000446
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000563	0.012071	0.009750	0.004852	0.000624	0.000395	0.000384	0.000840
Cs_2O	0.000000	0.000000	0.000000	0.000000	0.000404	0.000256	0.000248	0.000544
CuO	0.000000	0.000000	0.001437	0.001304	0.001432	0.000905	0.000880	0.001928
F	0.004280	0.018418	0.003609	0.000000	0.011966	0.007567	0.007356	0.016116
K_2O	0.000000	0.001065	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000000	0.000000	0.000000	0.000106	0.001454	0.000919	0.000894	0.001958
MnO	0.000000	0.001894	0.010728	0.002562	0.001310	0.000828	0.000805	0.001764
MoO_3	0.000000	0.000304	0.000000	0.000000	0.001579	0.000999	0.000971	0.002127
Nd_2O_3	0.000000	0.000000	0.000323	0.000103	0.002779	0.001758	0.001709	0.003744
NiO	0.000000	0.000000	0.000000	0.000693	0.005838	0.003692	0.003589	0.007863
P_2O_5	0.002203	0.000000	0.014309	0.000297	0.000534	0.000338	0.000328	0.000719
PbO	0.000000	0.000000	0.000410	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000000	0.000000	0.000700	0.000706	0.000311	0.000197	0.000191	0.000419
Pr_6O_{11}	0.000000	0.000000	0.000000	0.000000	0.000074	0.000047	0.000046	0.000100
Rb_2O	0.000000	0.000000	0.000000	0.000000	0.000204	0.000129	0.000125	0.000275
Rh_2O_3	0.000000	0.000000	0.000158	0.000166	0.000150	0.000095	0.000092	0.000202
RuO_2	0.000000	0.000000	0.000301	0.000337	0.000856	0.000541	0.000526	0.001153
SO_3	0.000018	0.000064	0.005361	0.000216	0.002607	0.001649	0.001603	0.003512
Sb_2O_3	0.000000	0.000000	0.000000	0.000106	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.002009	0.002007	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000000	0.000000	0.000000	0.000000	0.000109	0.000069	0.000067	0.000147
SrO	0.000000	0.000000	0.000000	0.000000	0.000731	0.000462	0.000450	0.000985
TeO_2	0.000000	0.000000	0.000000	0.000217	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000000	0.000000	0.000000	0.000000	0.000169	0.000107	0.000104	0.000227
ZnO	0.000000	0.000917	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	0.512	0.308	0.226	0.312	0.411	0.210	0.244	0.226
PCT Li	0.480	0.340	0.302	0.381	0.427	0.226	0.301	0.279
PCT Na	0.214	0.127	0.112	0.128	0.350	0.228	0.074	0.147

* The glass names are those used in the reference from which the data were taken.

Table A.4. CVS-II Phase 3 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-75*	CVS2-76	CVS2-77	CVS2-78	CVS2-79	CVS2-80	CVS2-81	CVS2-82
SiO_2	0.508511	0.517269	0.478355	0.598395	0.626631	0.568136	0.456525	0.533726
B_2O_3	0.128208	0.053380	0.054442	0.147557	0.157932	0.154619	0.053728	0.078144
Na_2O	0.082465	0.179876	0.183453	0.051795	0.055436	0.054273	0.174411	0.166309
Li_2O	0.145559	0.130997	0.147978	0.054575	0.027826	0.039626	0.146039	0.134149
CaO	0.000898	0.044177	0.005632	0.005724	0.006127	0.005998	0.005558	0.005106
MgO	0.001249	0.007684	0.007836	0.063719	0.008525	0.066768	0.061870	0.056833
Fe_2O_3	0.003153	0.040724	0.001978	0.028103	0.045183	0.044235	0.040990	0.001793
Al_2O_3	0.112294	0.012149	0.012391	0.012594	0.013479	0.013196	0.012228	0.011233
ZrO_2	0.000255	0.002513	0.056391	0.025896	0.002788	0.040949	0.002530	0.002324
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000224	0.000145	0.000664	0.000150	0.000722	0.000157	0.000594	0.000134
CdO	0.002008	0.001296	0.005946	0.001343	0.006468	0.001407	0.005320	0.001198
Ce_2O_3	0.000150	0.000097	0.000444	0.000100	0.000483	0.000105	0.000398	0.000089
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000283	0.000183	0.000838	0.000189	0.000911	0.000198	0.000750	0.000169
Cs_2O	0.000183	0.000118	0.000543	0.000123	0.000590	0.000128	0.000486	0.000109
CuO	0.000649	0.000419	0.001923	0.000434	0.002091	0.000455	0.001720	0.000387
F	0.005426	0.003501	0.016068	0.003629	0.017479	0.003803	0.014377	0.003237
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000659	0.000425	0.001953	0.000441	0.002124	0.000462	0.001747	0.000393
MnO	0.000594	0.000383	0.001759	0.000397	0.001914	0.000416	0.001574	0.000354
MoO_3	0.000716	0.000462	0.002121	0.000479	0.002307	0.000502	0.001898	0.000427
Nd_2O_3	0.001260	0.000813	0.003732	0.000843	0.004060	0.000883	0.003340	0.000752
NiO	0.002647	0.001708	0.007839	0.001771	0.008528	0.001855	0.007014	0.001579
P_2O_5	0.000242	0.000156	0.000717	0.000162	0.000780	0.000170	0.000642	0.000144
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000141	0.000091	0.000418	0.000094	0.000455	0.000099	0.000374	0.000084
Pr_6O_{11}	0.000034	0.000022	0.000100	0.000023	0.000108	0.000024	0.000089	0.000020
Rb_2O	0.000092	0.000060	0.000274	0.000062	0.000298	0.000065	0.000245	0.000055
Rh_2O_3	0.000068	0.000044	0.000202	0.000046	0.000219	0.000048	0.000180	0.000041
RuO_2	0.000388	0.000250	0.001149	0.000260	0.001250	0.000272	0.001028	0.000232
SO_3	0.001182	0.000763	0.003501	0.000791	0.003809	0.000829	0.003133	0.000705
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000050	0.000032	0.000147	0.000033	0.000160	0.000035	0.000131	0.000030
SrO	0.000332	0.000214	0.000982	0.000222	0.001068	0.000232	0.000879	0.000198
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000077	0.000049	0.000227	0.000051	0.000246	0.000054	0.000203	0.000046
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	0.278	14.871	9.512	0.934	0.744	0.764	16.613	44.000
PCT Li	0.334	7.571	6.221	0.698	0.684	0.672	8.064	19.969
PCT Na	0.100	12.541	6.552	0.593	0.660	0.600	12.824	35.377

* The glass names are those used in the reference from which the data were taken.

Table A.4. CVS-II Phase 3 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-83*	CVS2-84	CVS2-85	CVS2-86	CVS2-87	CVS2-88	CVS2-89	CVS2-90
SiO_2	0.488745	0.486090	0.453040	0.523892	0.548474	0.480202	0.500662	0.578967
B_2O_3	0.081867	0.055322	0.053318	0.056946	0.075997	0.054093	0.114998	0.142766
Na_2O	0.174049	0.186420	0.179668	0.191892	0.192066	0.142076	0.198554	0.054322
Li_2O	0.140192	0.150371	0.144925	0.030072	0.039838	0.147031	0.022880	0.145520
CaO	0.042747	0.005723	0.005516	0.047129	0.016156	0.044768	0.048765	0.005538
MgO	0.007435	0.007963	0.030699	0.008197	0.008204	0.007786	0.008481	0.007706
Fe_2O_3	0.001876	0.042206	0.001937	0.002069	0.010353	0.009826	0.044953	0.039210
Al_2O_3	0.011756	0.012591	0.103147	0.110165	0.064019	0.064634	0.013411	0.012185
ZrO_2	0.002432	0.041675	0.002510	0.002681	0.032901	0.038203	0.034900	0.002521
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000630	0.000150	0.000325	0.000347	0.000154	0.000147	0.000160	0.000145
CdO	0.005641	0.001343	0.002912	0.003110	0.001383	0.001313	0.001430	0.001299
Ce_2O_3	0.000421	0.000100	0.000218	0.000232	0.000103	0.000098	0.000107	0.000097
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000795	0.000189	0.000410	0.000438	0.000195	0.000185	0.000202	0.000183
Cs_2O	0.000515	0.000123	0.000266	0.000284	0.000126	0.000120	0.000131	0.000119
CuO	0.001824	0.000434	0.000941	0.001005	0.000447	0.000424	0.000462	0.000420
F	0.015244	0.003628	0.007868	0.008403	0.003738	0.003548	0.003865	0.003511
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.001852	0.000441	0.000956	0.001021	0.000454	0.000431	0.000470	0.000427
MnO	0.001669	0.000397	0.000861	0.000920	0.000409	0.000388	0.000423	0.000384
MoO_3	0.002012	0.000479	0.001039	0.001109	0.000493	0.000468	0.000510	0.000464
Nd_2O_3	0.003541	0.000843	0.001828	0.001952	0.000868	0.000824	0.000898	0.000816
NiO	0.007437	0.001770	0.003839	0.004100	0.001824	0.001731	0.001885	0.001713
P_2O_5	0.000680	0.000162	0.000351	0.000375	0.000167	0.000158	0.000172	0.000157
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000397	0.000094	0.000205	0.000219	0.000097	0.000092	0.000101	0.000091
Pr_6O_{11}	0.000095	0.000022	0.000049	0.000052	0.000023	0.000022	0.000024	0.000022
Rb_2O	0.000260	0.000062	0.000134	0.000143	0.000064	0.000060	0.000066	0.000060
Rh_2O_3	0.000191	0.000046	0.000099	0.000105	0.000047	0.000045	0.000048	0.000044
RuO_2	0.001090	0.000260	0.000563	0.000601	0.000267	0.000254	0.000276	0.000251
SO_3	0.003321	0.000791	0.001714	0.001831	0.000815	0.000773	0.000842	0.000765
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000139	0.000033	0.000072	0.000077	0.000034	0.000032	0.000035	0.000032
SrO	0.000932	0.000222	0.000481	0.000514	0.000228	0.000217	0.000236	0.000215
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000215	0.000051	0.000111	0.000119	0.000053	0.000050	0.000054	0.000050
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	34.656	12.460	0.456	0.115	0.178	0.308	1.716	5.577
PCT Li	19.228	6.682	0.422	0.091	0.131	0.376	1.236	3.764
PCT Na	27.890	8.236	0.749	0.254	0.286	0.473	1.348	3.481

* The glass names are those used in the reference from which the data were taken.

Table A.4. CVS-II Phase 3 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-91*	CVS2-92	CVS2-93	CVS2-94	CVS2-95	CVS2-96	CVS2-97	CVS2-98
SiO_2	0.589408	0.450082	0.468865	0.451923	0.504882	0.512371	0.578911	0.450027
B_2O_3	0.145341	0.141253	0.122961	0.141831	0.098986	0.105186	0.098276	0.161186
Na_2O	0.107135	0.099164	0.132123	0.179225	0.167079	0.103769	0.118920	0.207746
Li_2O	0.021164	0.143978	0.149987	0.108632	0.088762	0.080686	0.081492	0.079502
CaO	0.005638	0.005480	0.011189	0.044018	0.012488	0.031444	0.009546	0.000000
MgO	0.062762	0.060997	0.007943	0.007656	0.025531	0.057752	0.013606	0.000000
Fe_2O_3	0.001980	0.001924	0.039532	0.010473	0.036049	0.022807	0.029966	0.008063
Al_2O_3	0.012405	0.012056	0.012559	0.042549	0.022306	0.039998	0.015047	0.087640
ZrO_2	0.002566	0.034915	0.002598	0.002504	0.020599	0.022325	0.020769	0.000000
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000664	0.000646	0.000673	0.000144	0.000000	0.000305	0.000423	0.000075
CdO	0.005953	0.005785	0.006027	0.001291	0.000000	0.002729	0.003316	0.000673
Ce_2O_3	0.000445	0.000432	0.000450	0.000096	0.000000	0.000204	0.000032	0.000050
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000839	0.000815	0.000849	0.000182	0.000000	0.000385	0.000556	0.000095
Cs_2O	0.000543	0.000528	0.000550	0.000118	0.000000	0.000249	0.000349	0.000061
CuO	0.001925	0.001871	0.001949	0.000417	0.000000	0.000883	0.001301	0.000218
F	0.016086	0.015634	0.016286	0.003488	0.000000	0.007376	0.006551	0.001820
K_2O	0.000000	0.000000	0.000000	0.000000	0.000263	0.000000	0.000000	0.000000
La_2O_3	0.001955	0.001900	0.001979	0.000424	0.000780	0.000896	0.003097	0.000221
MnO	0.001761	0.001712	0.001783	0.000382	0.011706	0.000808	0.001191	0.000199
MoO_3	0.002123	0.002064	0.002150	0.000460	0.000000	0.000974	0.001411	0.000240
Nd_2O_3	0.003737	0.003631	0.003783	0.000810	0.000000	0.001713	0.001110	0.000423
NiO	0.007848	0.007627	0.007945	0.001702	0.005061	0.003599	0.005262	0.000888
P_2O_5	0.000718	0.000698	0.000727	0.000156	0.000000	0.000329	0.000457	0.000081
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000418	0.000407	0.000424	0.000091	0.000000	0.000192	0.000000	0.000047
Pr_6O_{11}	0.000100	0.000097	0.000101	0.000022	0.000000	0.000046	0.000121	0.000011
Rb_2O	0.000274	0.000266	0.000277	0.000059	0.000000	0.000126	0.000000	0.000031
Rh_2O_3	0.000202	0.000196	0.000204	0.000044	0.000000	0.000093	0.000000	0.000023
RuO_2	0.001151	0.001118	0.001165	0.000250	0.000000	0.000528	0.000743	0.000130
SO_3	0.003505	0.003406	0.003548	0.000760	0.000000	0.001607	0.003601	0.000396
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000147	0.000143	0.000149	0.000032	0.000000	0.000067	0.000000	0.000017
SrO	0.000983	0.000956	0.000995	0.000213	0.000000	0.000451	0.000000	0.000111
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.005508	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000227	0.000220	0.000230	0.000049	0.000000	0.000104	0.000000	0.000026
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.003945	0.000000
PCT B	8.642	18.590	13.227	4.070	9.976	0.493	1.434	4.520
PCT Li	6.774	12.442	7.757	3.066	4.271	0.429	1.052	3.497
PCT Na	6.738	11.792	10.010	3.350	7.259	0.410	1.134	2.796

* The glass names are those used in the reference from which the data were taken.

Table A.4. CVS-II Phase 3 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-99*	CVS2-100	CVS2-101
SiO_2	0.576620	0.591424	0.512060
B_2O_3	0.092683	0.070880	0.101150
Na_2O	0.105287	0.067351	0.171843
Li_2O	0.079332	0.133002	0.088901
CaO	0.011518	0.004162	0.013835
MgO	0.012721	0.001985	0.028025
Fe_2O_3	0.042490	0.051319	0.036932
Al_2O_3	0.034156	0.018704	0.022280
ZrO_2	0.010754	0.023974	0.002458
Ag_2O	0.000287	0.000087	0.000000
As_2O_3	0.000000	0.000000	0.000000
BaO	0.000218	0.000303	0.000000
CdO	0.001556	0.004153	0.000000
Ce_2O_3	0.000271	0.000000	0.000000
CoO	0.000401	0.000000	0.000000
Cr_2O_3	0.000877	0.000263	0.000000
Cs_2O	0.000000	0.000000	0.000000
CuO	0.000169	0.000254	0.000000
F	0.000000	0.000000	0.000000
K_2O	0.014986	0.011612	0.000268
La_2O_3	0.000287	0.000941	0.000542
MnO	0.003677	0.001609	0.012097
MoO_3	0.000045	0.000000	0.000000
Nd_2O_3	0.000910	0.002874	0.000000
NiO	0.002587	0.006159	0.004477
P_2O_5	0.002580	0.004134	0.000000
PbO	0.000597	0.000328	0.000000
PdO	0.000000	0.000000	0.000000
Pr_6O_{11}	0.000000	0.000000	0.000000
Rb_2O	0.000000	0.000000	0.000000
Rh_2O_3	0.000000	0.000000	0.000000
RuO_2	0.000000	0.000452	0.000000
SO_3	0.003326	0.002668	0.000000
Sb_2O_3	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000
Sm_2O_3	0.000000	0.000000	0.000000
SrO	0.000256	0.000322	0.000000
TeO_2	0.000000	0.000209	0.000000
TiO_2	0.001000	0.000670	0.005133
U_3O_8	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000
Y_2O_3	0.000000	0.000000	0.000000
ZnO	0.000411	0.000162	0.000000
PCT B	0.232	0.326	8.644
PCT Li	0.246	0.343	3.831
PCT Na	0.199	0.226	6.586

* The glass names are those used in the reference from which the data were taken.

Table A.5. CVS-II Phase 4 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2)

Comp.	CVS2-102*	CVS2-103	CVS2-104	CVS2-105	CVS2-106	CVS2-107	CVS2-108	CVS2-109
SiO_2	0.579488	0.453956	0.494661	0.534747	0.613270	0.612819	0.552342	0.521788
B_2O_3	0.098382	0.127752	0.118210	0.108843	0.090480	0.046526	0.140604	0.188172
Na_2O	0.118063	0.153307	0.141889	0.130626	0.108578	0.124849	0.112532	0.106305
Li_2O	0.081628	0.105996	0.098094	0.090321	0.075070	0.086327	0.077811	0.073499
CaO	0.009627	0.012503	0.011565	0.010652	0.008853	0.010177	0.009181	0.008667
MgO	0.013556	0.017595	0.016289	0.015000	0.012462	0.014337	0.012920	0.012205
Fe_2O_3	0.029285	0.038030	0.035196	0.032401	0.026932	0.030968	0.027914	0.026370
Al_2O_3	0.014736	0.019137	0.017710	0.016303	0.013555	0.015585	0.014048	0.013266
ZrO_2	0.020323	0.026390	0.024426	0.022483	0.018693	0.021492	0.019373	0.018297
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000450	0.000584	0.000540	0.000497	0.000413	0.000475	0.000428	0.000405
CdO	0.004027	0.005229	0.004840	0.004456	0.003704	0.004259	0.003838	0.003626
Ce_2O_3	0.000301	0.000391	0.000362	0.000333	0.000277	0.000318	0.000287	0.000271
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000567	0.000737	0.000682	0.000628	0.000522	0.000600	0.000541	0.000511
Cs_2O	0.000368	0.000477	0.000442	0.000407	0.000338	0.000389	0.000350	0.000331
CuO	0.001302	0.001691	0.001565	0.001441	0.001198	0.001377	0.001241	0.001172
F	0.010883	0.014132	0.013080	0.012040	0.010009	0.011509	0.010373	0.009799
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.001322	0.001717	0.001589	0.001463	0.001216	0.001399	0.001260	0.001191
MnO	0.001191	0.001547	0.001432	0.001318	0.001096	0.001260	0.001136	0.001073
MoO_3	0.001437	0.001865	0.001727	0.001589	0.001321	0.001519	0.001369	0.001293
Nd_2O_3	0.002528	0.003283	0.003038	0.002797	0.002325	0.002673	0.002409	0.002276
NiO	0.005309	0.006894	0.006381	0.005874	0.004883	0.005615	0.005060	0.004780
P_2O_5	0.000486	0.000631	0.000584	0.000537	0.000447	0.000514	0.000463	0.000437
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000283	0.000368	0.000340	0.000313	0.000260	0.000299	0.000270	0.000255
Pr_6O_{11}	0.000067	0.000088	0.000081	0.000075	0.000062	0.000071	0.000064	0.000061
Rb_2O	0.000185	0.000241	0.000223	0.000205	0.000170	0.000196	0.000177	0.000167
Rh_2O_3	0.000137	0.000177	0.000164	0.000151	0.000126	0.000144	0.000130	0.000123
RuO_2	0.000778	0.001011	0.000936	0.000861	0.000716	0.000823	0.000742	0.000701
SO_3	0.002371	0.003079	0.002850	0.002623	0.002181	0.002508	0.002260	0.002135
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000099	0.000129	0.000119	0.000110	0.000091	0.000105	0.000095	0.000089
SrO	0.000665	0.000864	0.000799	0.000736	0.000612	0.000703	0.000634	0.000599
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000153	0.000199	0.000184	0.000170	0.000141	0.000162	0.000146	0.000138
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	2.672	6.073	5.548	4.590	1.651	0.788	2.144	5.707
PCT Li	1.921	4.066	3.633	3.132	1.348	0.662	1.646	4.494
PCT Na	1.677	4.082	3.668	2.974	1.165	0.620	1.387	3.584

* The glass names are those used in the reference from which the data were taken.

Table A.5. CVS-II Phase 4 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-110*	CVS2-111	CVS2-112	CVS2-113	CVS2-114	CVS2-115	CVS2-116	CVS2-117
SiO_2	0.622469	0.553837	0.519827	0.616782	0.550790	0.538521	0.571568	0.587447
B_2O_3	0.105683	0.094027	0.088255	0.104716	0.093510	0.091424	0.097040	0.099732
Na_2O	0.052656	0.157087	0.208876	0.125657	0.112216	0.109716	0.116448	0.119682
Li_2O	0.087680	0.078025	0.073218	0.022525	0.127108	0.146550	0.080518	0.082755
CaO	0.010335	0.009201	0.008634	0.010250	0.009150	0.008947	0.023153	0.009759
MgO	0.014559	0.012964	0.012158	0.014429	0.012885	0.012603	0.013369	0.000000
Fe_2O_3	0.031456	0.027988	0.026270	0.031169	0.027835	0.027214	0.028885	0.029688
Al_2O_3	0.015831	0.014081	0.013218	0.015685	0.014006	0.013695	0.014537	0.014941
ZrO_2	0.021830	0.019422	0.018229	0.021631	0.019317	0.018887	0.020048	0.020604
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000483	0.000430	0.000403	0.000478	0.000427	0.000418	0.000443	0.000456
Bi_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
CdO	0.004326	0.003849	0.003612	0.004286	0.003828	0.003742	0.003972	0.004082
Ce_2O_3	0.000323	0.000288	0.000270	0.000320	0.000286	0.000280	0.000297	0.000305
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000610	0.000542	0.000509	0.000604	0.000539	0.000527	0.000560	0.000575
Cs_2O	0.000395	0.000351	0.000330	0.000391	0.000349	0.000342	0.000363	0.000373
CuO	0.001399	0.001245	0.001168	0.001386	0.001238	0.001210	0.001284	0.001320
F	0.011690	0.010401	0.009762	0.011583	0.010344	0.010113	0.010734	0.011032
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.001421	0.001264	0.001186	0.001408	0.001257	0.001229	0.001304	0.001341
MnO	0.001280	0.001139	0.001069	0.001268	0.001132	0.001107	0.001175	0.001208
MoO_3	0.001543	0.001373	0.001289	0.001529	0.001365	0.001335	0.001417	0.001456
Nd_2O_3	0.002715	0.002416	0.002268	0.002691	0.002403	0.002349	0.002493	0.002563
NiO	0.005703	0.005075	0.004763	0.005651	0.005046	0.004934	0.005237	0.005382
P_2O_5	0.000522	0.000464	0.000436	0.000517	0.000462	0.000451	0.000479	0.000492
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000304	0.000271	0.000254	0.000301	0.000269	0.000263	0.000279	0.000287
Pr_6O_{11}	0.000072	0.000064	0.000061	0.000072	0.000064	0.000063	0.000067	0.000068
Rb_2O	0.000199	0.000177	0.000166	0.000197	0.000176	0.000172	0.000183	0.000188
Rh_2O_3	0.000147	0.000131	0.000122	0.000145	0.000130	0.000127	0.000135	0.000138
RuO_2	0.000836	0.000744	0.000698	0.000828	0.000740	0.000723	0.000768	0.000789
SO_3	0.002547	0.002266	0.002127	0.002524	0.002254	0.002204	0.002339	0.002404
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000107	0.000095	0.000089	0.000106	0.000094	0.000092	0.000098	0.000101
SrO	0.000715	0.000636	0.000597	0.000708	0.000632	0.000618	0.000656	0.000674
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000165	0.000147	0.000138	0.000163	0.000146	0.000143	0.000151	0.000156
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PCT B	0.314	6.135	14.400	0.612	7.116	9.406	3.012	1.590
PCT Li	0.402	3.894	7.794	0.630	4.928	5.837	2.203	1.337
PCT Na	0.118	4.043	9.603	0.510	4.599	5.765	2.030	1.099

* The glass names are those used in the reference from which the data were taken.

Table A.5. CVS-II Phase 4 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	CVS2-118*	CVS2-119	CVS2-120	CVS2-121	CVS2-122	CVS2-123	CVS2-124
SiO_2	0.568631	0.588149	0.569204	0.549531	0.529092	0.578911	0.412660
B_2O_3	0.096540	0.099852	0.096636	0.093295	0.089825	0.098276	0.137413
Na_2O	0.115846	0.119827	0.115965	0.111955	0.107801	0.118920	0.164902
Li_2O	0.080095	0.082855	0.080185	0.077413	0.074533	0.081492	0.114012
CaO	0.009443	0.009775	0.009454	0.009133	0.008787	0.009546	0.013446
MgO	0.032046	0.013761	0.013318	0.012857	0.012379	0.013606	0.018934
Fe_2O_3	0.028737	0.029723	0.028766	0.027771	0.026739	0.029966	0.040904
Al_2O_3	0.014460	0.000000	0.032218	0.065664	0.100412	0.015047	0.020582
ZrO_2	0.019942	0.020627	0.019962	0.019273	0.018556	0.020769	0.028386
Ag_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
As_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
BaO	0.000441	0.000456	0.000442	0.000426	0.000410	0.000423	0.000628
CdO	0.003952	0.004087	0.003956	0.003819	0.003677	0.003316	0.005625
Ce_2O_3	0.000295	0.000305	0.000296	0.000285	0.000275	0.000032	0.000420
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000557	0.000576	0.000557	0.000538	0.000518	0.000556	0.000793
Cs_2O	0.000361	0.000373	0.000361	0.000349	0.000336	0.000349	0.000513
CuO	0.001278	0.001322	0.001279	0.001235	0.001189	0.001301	0.001819
F	0.010679	0.011046	0.010690	0.010320	0.009937	0.006551	0.015200
K_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.001298	0.001342	0.001299	0.001254	0.001207	0.003097	0.001847
MnO	0.001169	0.001209	0.001170	0.001130	0.001088	0.001191	0.001664
MoO_3	0.001410	0.001458	0.001411	0.001362	0.001312	0.001411	0.002006
Nd_2O_3	0.002481	0.002566	0.002483	0.002397	0.002308	0.001110	0.003531
NiO	0.005210	0.005389	0.005215	0.005035	0.004848	0.005262	0.007416
P_2O_5	0.000477	0.000493	0.000477	0.000460	0.000443	0.000457	0.000678
PbO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
PdO	0.000278	0.000287	0.000278	0.000268	0.000259	0.000000	0.000395
Pr_6O_{11}	0.000066	0.000068	0.000066	0.000064	0.000062	0.000121	0.000094
Rb_2O	0.000182	0.000188	0.000182	0.000176	0.000169	0.000000	0.000259
Rh_2O_3	0.000134	0.000139	0.000134	0.000129	0.000125	0.000000	0.000191
RuO_2	0.000764	0.000790	0.000765	0.000738	0.000711	0.000743	0.001087
SO_3	0.002327	0.002407	0.002329	0.002249	0.002165	0.003601	0.003312
Sb_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000097	0.000101	0.000098	0.000094	0.000091	0.000000	0.000139
SrO	0.000653	0.000675	0.000653	0.000631	0.000607	0.000000	0.000929
TeO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
TiO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
U_3O_8	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
WO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Y_2O_3	0.000151	0.000156	0.000151	0.000146	0.000140	0.000000	0.000214
ZnO	0.000000	0.000000	0.000000	0.000000	0.000000	0.003945	0.000000
PCT B	3.630	3.803	0.291	0.199	0.193	1.473	5.567
PCT Li	2.609	2.688	0.324	0.311	0.363	1.125	4.424
PCT Na	2.394	2.574	0.231	0.137	0.089	1.075	4.293

* The glass names are those used in the reference from which the data were taken.

Table A.6. Ramsey Glass Compositions (mole fractions) and PCT Normalized Si, B, and Na Releases (g/m^2)

# *	SiO_2	Al_2O_3	B_2O_3	Fe_2O_3	FeO	CaO	Na_2O	PCT Si	PCT B	PCT Na
1	0.6049	0.1046	0.1407	0	0	0	0.1499	0.093	0.555	0.239
2	0.5903	0.1038	0.0495	0	0	0.1035	0.1529	0.045	0.075	0.187
4	0.6009	0.1107	0.0430	0	0	0	0.2454	0.187	0.368	0.685
5	0.5887	0.0349	0.1365	0	0	0.0961	0.1438	0.179	0.361	0.364
6	0.5857	0.0296	0.1312	0.0871	0.0256	0	0.1407	0.162	0.817	0.512
7	0.5938	0.0062	0.1446	0	0	0	0.2555	15.029	29.834	25.044
8	0.5800	0.0252	0.0473	0.0828	0.0290	0.0934	0.1424	0.108	0.257	0.597
9	0.5953	0.0012	0.0491	0	0	0.1002	0.2543	16.036	38.709	27.827
10	0.5777	0.0165	0.0409	0.0794	0.0294	0	0.2561	0.710	1.702	1.508
11	0.4817	0.1084	0.1543	0	0	0.1040	0.1516	0.047	0.254	0.286
13	0.5000	0.1198	0.1390	0	0	0	0.2412	0.085	2.122	1.133
15	0.5036	0.1121	0.0453	0	0	0.0980	0.2410	0.126	0.174	0.762
16	0.5046	0.1084	0.0440	0.0874	0.0225	0	0.2331	0.218	0.493	0.620
17	0.4551	0.0810	0.1344	0.0715	0.0340	0.0896	0.1344	0.078	0.184	0.481
18	0.4912	0.0057	0.1429	0	0	0.1026	0.2576	7.624	31.162	22.973
19	0.4643	0.0260	0.1319	0.0901	0.0146	0	0.2730	0.367	5.016	2.621
20	0.4876	0.0067	0.0496	0.0975	0.0133	0.0992	0.2461	0.361	0.770	1.748
21	0.5684	0.0751	0.0861	0.0374	0.0080	0.0384	0.1865	0.126	0.275	0.378
22	0.4694	0.1295	0.0974	0.0489	0.0166	0.0532	0.1850	0.084	0.165	0.240
23	0.5047	0.1568	0.0774	0.0295	0.0162	0.0352	0.1802	0.086	0.152	0.205
24	0.5302	0.0500	0.1036	0.0527	0.0166	0.0560	0.1909	0.128	0.436	0.531
25	0.5212	0.0876	0.1357	0.0355	0.0111	0.0370	0.1720	0.103	0.417	0.353
26	0.5553	0.0755	0.0432	0.0493	0.0244	0.0563	0.1960	0.123	0.254	0.472
27	0.5112	0.0972	0.0795	0.0333	0.0122	0.0936	0.1731	0.058	0.137	0.277
28	0.5412	0.1016	0.0938	0.0496	0.0212	0	0.1926	0.134	0.307	0.312
29	0.5348	0.0817	0.0765	0.0784	0.0301	0.0345	0.1640	0.120	0.276	0.382
30	0.5542	0.0673	0.1130	0	0	0.0631	0.2025	0.138	0.847	0.817
31	0.5099	0.1002	0.0776	0.0346	0.0109	0.0368	0.2300	0.147	0.310	0.469
32	0.5264	0.1130	0.0943	0.0442	0.0282	0.0541	0.1400	0.050	0.123	0.202
33	0.5116	0.1234	0.0877	0.0372	0.0181	0.0430	0.1790	0.088	0.168	0.237

* The glass numbers are those used in the reference from which the data were taken. Note that three numbers are missing, so that there are only 30 glasses, not 33.

Table A.7. WV87 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2)

Comp.	WVDG-15*	WVDG-16	WVDG-17	WVDG-18	WVDG-19	WVDG-20	WVDG-21	WVDG-22
Al_2O_3	0.068181	0.067416	0.066961	0.066586	0.091558	0.087620	0.091514	0.092402
B_2O_3	0.130854	0.132033	0.101710	0.109363	0.110520	0.111342	0.107674	0.125261
BaO	0.001559	0.001521	0.001511	0.000514	0.001593	0.001476	0.000535	0.000541
CaO	0.017562	0.017808	0.018462	0.006903	0.017831	0.017441	0.006650	0.006720
Ce_2O_3	0.002609	0.000805	0.002860	0.000812	0.000843	0.002862	0.000845	0.002890
Cr_2O_3	0.001143	0.000336	0.001239	0.000377	0.000352	0.001249	0.000393	0.001289
Cs_2O	0.000308	0.000103	0.000334	0.000102	0.000108	0.000337	0.000106	0.000348
CuO	0.000182	0.000733	0.000182	0.000180	0.000672	0.000184	0.000656	0.000190
Fe_2O_3	0.039905	0.065822	0.040215	0.064826	0.067875	0.039993	0.068519	0.066219
K_2O	0.012608	0.010137	0.015911	0.013319	0.015964	0.017279	0.009740	0.014723
La_2O_3	0.000156	0.000045	0.000178	0.000044	0.000047	0.000157	0.000046	0.000162
Li_2O	0.066159	0.046593	0.056697	0.058541	0.052878	0.049830	0.057660	0.045907
MgO	0.000000	0.022065	0.023173	0.007827	0.024242	0.025715	0.009808	0.008976
MnO	0.020907	0.018698	0.020737	0.004453	0.004390	0.004366	0.021449	0.021327
MoO_3	0.000352	0.000101	0.000402	0.000100	0.000106	0.000355	0.000104	0.000367
Na_2O	0.118824	0.101615	0.123475	0.128857	0.121679	0.101631	0.125879	0.101056
Nd_2O_3	0.000517	0.000152	0.000559	0.000170	0.000159	0.000564	0.000177	0.000582
NiO	0.005138	0.001561	0.005622	0.001632	0.001635	0.005667	0.001697	0.005751
P_2O_5	0.006785	0.016587	0.006325	0.007829	0.007260	0.017175	0.017761	0.007593
Pr_6O_{11}	0.000050	0.000014	0.000057	0.000014	0.000015	0.000050	0.000015	0.000052
SO_3	0.003618	0.001093	0.003889	0.001164	0.001144	0.003920	0.001118	0.003954
SiO_2	0.479557	0.484669	0.476819	0.515456	0.457473	0.485304	0.466014	0.468904
Sm_2O_3	0.000062	0.000021	0.000083	0.000021	0.000022	0.000084	0.000021	0.000086
SrO	0.000210	0.000070	0.000279	0.000069	0.000074	0.000282	0.000072	0.000291
ThO_2	0.004553	0.004417	0.012860	0.005322	0.015149	0.005169	0.004492	0.004996
TiO_2	0.013051	0.004014	0.014317	0.004127	0.004204	0.014342	0.004294	0.014527
U_3O_8	0.000822	0.000117	0.000072	0.000080	0.000876	0.000856	0.000847	0.000102
Y_2O_3	0.000096	0.000032	0.000128	0.000032	0.000034	0.000129	0.000033	0.000134
ZnO	0.000178	0.000179	0.000534	0.000000	0.000000	0.000179	0.000550	0.000185
ZrO_2	0.004055	0.001242	0.004407	0.001280	0.001301	0.004443	0.001332	0.004465
PCT B	0.296	0.189	0.292	0.225	0.214	0.160	0.225	0.210
PCT Li	0.300	0.235	0.292	0.269	0.282	0.242	0.252	0.300
PCT Na	0.264	0.165	0.273	0.219	0.207	0.139	0.222	0.179

* The glass numbers are those used in the reference from which the data were taken.

Table A.7. WV87 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	WVDG-23*	WVDG-24	WVDG-25	WVDG-26	WVDG-27	WVDG-28	WVDG-29	WVDG-30
Al_2O_3	0.070257	0.086353	0.065548	0.086082	0.088273	0.069246	0.063024	0.072232
B_2O_3	0.136321	0.135709	0.112516	0.137478	0.133639	0.111683	0.113888	0.124804
BaO	0.000546	0.000513	0.000469	0.001400	0.000531	0.000523	0.001445	0.000954
CaO	0.006780	0.006117	0.006407	0.017092	0.006462	0.006243	0.016423	0.010955
Ce_2O_3	0.000928	0.000830	0.000919	0.000935	0.003094	0.002924	0.000885	0.001700
Cr_2O_3	0.000400	0.000376	0.000378	0.000424	0.001362	0.001296	0.000364	0.000770
Cs_2O	0.000108	0.000101	0.000102	0.000102	0.000367	0.000336	0.000098	0.000208
CuO	0.000000	0.000180	0.000181	0.000270	0.000744	0.000734	0.000174	0.000368
Fe_2O_3	0.067811	0.038800	0.039016	0.038836	0.040199	0.055311	0.037899	0.052577
K_2O	0.015016	0.019119	0.015411	0.020048	0.019236	0.010453	0.013526	0.014053
La_2O_3	0.000047	0.000044	0.000044	0.000066	0.000182	0.000179	0.000043	0.000090
Li_2O	0.045808	0.049029	0.048821	0.047877	0.056430	0.050039	0.059556	0.051399
MgO	0.010189	0.009930	0.009450	0.023960	0.011377	0.011220	0.023366	0.018328
MnO	0.004461	0.020058	0.019839	0.004525	0.004339	0.004363	0.003983	0.010095
MoO_3	0.000106	0.000099	0.000100	0.000149	0.000411	0.000405	0.000096	0.000203
Na_2O	0.100978	0.110234	0.105397	0.104911	0.120995	0.104266	0.119993	0.113637
Nd_2O_3	0.000181	0.000170	0.000171	0.000191	0.000615	0.000585	0.000165	0.000348
NiO	0.001832	0.001626	0.001828	0.001819	0.006138	0.005761	0.001761	0.003427
P_2O_5	0.017679	0.007099	0.015847	0.008164	0.018132	0.007862	0.015952	0.012469
Pr_6O_{11}	0.000015	0.000014	0.000014	0.000021	0.000058	0.000057	0.000014	0.000029
SO_3	0.001330	0.001160	0.001257	0.001251	0.004249	0.004009	0.001211	0.002375
SiO_2	0.497523	0.500751	0.538222	0.487522	0.451977	0.526601	0.514930	0.487625
Sm_2O_3	0.000022	0.000020	0.000021	0.000021	0.000085	0.000084	0.000020	0.000042
SrO	0.000073	0.000069	0.000069	0.000069	0.000285	0.000282	0.000067	0.000141
ThO_2	0.014256	0.005089	0.011867	0.010295	0.009691	0.004751	0.005062	0.009030
TiO_2	0.004759	0.004204	0.004587	0.004745	0.015550	0.014697	0.004420	0.008604
U_3O_8	0.000873	0.000820	0.000089	0.000088	0.000100	0.000864	0.000085	0.000533
Y_2O_3	0.000034	0.000032	0.000032	0.000032	0.000131	0.000129	0.000031	0.000065
ZnO	0.000187	0.000176	0.000000	0.000176	0.000545	0.000538	0.000170	0.000270
ZrO_2	0.001481	0.001276	0.001400	0.001451	0.004802	0.004558	0.001349	0.002671
PCT B	0.253	0.213	0.188	0.185	0.309	0.201	0.217	0.209
PCT Li	0.307	0.286	0.253	0.257	0.327	0.289	0.255**	0.270**
PCT Na	0.187	0.173	0.164	0.156	0.243	0.169	0.214	0.196

* The glass numbers are those used in the reference from which the data were taken.

** Approximated from Figure 4.4 of Ref. 8 due to errors for these values in Table 4.3 of Ref. 8.

Table A.8. WV88 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2)

Comp.	WVDG-33*	WVDG-34	WVDG-35	WVDG-36	WVDG-37	WVDG-38	WVDG-39	WVDG-40
Al_2O_3	0.057810	0.036690	0.072311	0.042298	0.069628	0.073673	0.070996	0.043326
B_2O_3	0.093011	0.112355	0.075571	0.117582	0.079496	0.079871	0.116084	0.078458
BaO	0.000281	0.000142	0.000480	0.000099	0.000093	0.000096	0.000423	0.000473
CaO	0.005115	0.002323	0.009185	0.002162	0.001776	0.002093	0.008477	0.009313
Ce_2O_3	0.001396	0.004015	0.000684	0.004139	0.003844	0.004113	0.001067	0.000885
Cr_2O_3	0.000613	0.001761	0.000290	0.001845	0.001685	0.001786	0.000474	0.000382
Cs_2O	0.000178	0.000488	0.000078	0.000484	0.000454	0.000495	0.000128	0.000103
CuO	0.000361	0.001001	0.000185	0.000953	0.000894	0.001014	0.000272	0.000182
Fe_2O_3	0.051415	0.044269	0.069024	0.069581	0.043521	0.044421	0.041857	0.069725
K_2O	0.026187	0.027808	0.028981	0.020438	0.029452	0.025388	0.027681	0.024411
La_2O_3	0.000088	0.000244	0.000045	0.000233	0.000218	0.000248	0.000066	0.000045
Li_2O	0.069833	0.074341	0.077322	0.054535	0.078560	0.067756	0.073761	0.065300
MgO	0.017436	0.008079	0.031767	0.007522	0.006354	0.007098	0.029309	0.032036
MnO	0.010558	0.016480	0.016505	0.001046	0.001064	0.016623	0.000911	0.001001
MoO_3	0.000199	0.000553	0.000102	0.000527	0.000494	0.000561	0.000150	0.000101
Na_2O	0.121598	0.129239	0.134630	0.094775	0.136696	0.117766	0.128301	0.113291
Nd_2O_3	0.000277	0.000796	0.000131	0.000833	0.000761	0.000807	0.000214	0.000172
NiO	0.002784	0.007943	0.001379	0.008219	0.007618	0.008151	0.002121	0.001748
P_2O_5	0.012478	0.009533	0.000311	0.003150	0.002506	0.003101	0.019333	0.003066
Pr_6O_{11}	0.000028	0.000078	0.000014	0.000074	0.000070	0.000079	0.000021	0.000014
SO_3	0.001881	0.005513	0.000919	0.005680	0.005331	0.005589	0.001440	0.001178
SiO_2	0.507219	0.481712	0.465367	0.518464	0.497252	0.499348	0.455540	0.535544
Sm_2O_3	0.000041	0.000104	0.000021	0.000109	0.000102	0.000105	0.000021	0.000021
SrO	0.000138	0.000349	0.000071	0.000366	0.000343	0.000354	0.000070	0.000070
ThO_2	0.009152	0.005262	0.007747	0.016678	0.005631	0.011474	0.013940	0.011511
TiO_2	0.007000	0.020195	0.003500	0.020775	0.019231	0.020658	0.005409	0.004449
U_3O_8	0.000443	0.001635	0.002180	0.000122	0.000123	0.000081	0.000089	0.001630
Y_2O_3	0.000064	0.000160	0.000033	0.000168	0.000158	0.000162	0.000032	0.000032
ZnO	0.000264	0.000711	0.000090	0.000745	0.000699	0.000721	0.000177	0.000178
ZrO_2	0.002153	0.006225	0.001075	0.006397	0.005946	0.006370	0.001637	0.001354
PCT B	0.247	0.417	0.400	0.244	0.231	0.197	0.271	0.305
PCT Li	0.263	0.388	0.394	0.251	0.267	0.240	0.249	0.305
PCT Na	0.245	0.363	0.399	0.164	0.267	0.197	0.247	0.289

* The glass numbers are those used in the reference from which the data were taken.

Table A.8. WV88 Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	WVDG-41*	WVDG-42	WVDG-43	WVDG-44	WVDG-45	WVDG-46	WVDG-47	WVDG-48
Al_2O_3	0.041905	0.039679	0.072406	0.060784	0.073694	0.047064	0.040476	0.068960
B_2O_3	0.075265	0.070678	0.131287	0.123049	0.077274	0.120428	0.116789	0.113100
BaO	0.000141	0.000475	0.000144	0.000146	0.000096	0.000447	0.000095	0.000486
CaO	0.002574	0.008839	0.002622	0.002524	0.002100	0.008312	0.002069	0.009041
Ce_2O_3	0.001006	0.003918	0.000876	0.000866	0.000877	0.000737	0.000759	0.004440
Cr_2O_3	0.000427	0.001727	0.000387	0.000392	0.000387	0.000316	0.000334	0.001962
Cs_2O	0.000128	0.000466	0.000104	0.000106	0.000104	0.000097	0.000103	0.000529
CuO	0.000272	0.000916	0.000185	0.000187	0.000185	0.000172	0.000182	0.001031
Fe_2O_3	0.042845	0.043502	0.043882	0.073748	0.071477	0.044602	0.067856	0.043143
K_2O	0.028733	0.026854	0.020921	0.027915	0.030001	0.024526	0.020559	0.021214
La_2O_3	0.000066	0.000224	0.000045	0.000046	0.000045	0.000042	0.000045	0.000252
Li_2O	0.076566	0.071722	0.055860	0.074537	0.080043	0.065613	0.054856	0.056643
MgO	0.009133	0.030204	0.008940	0.008871	0.007304	0.028404	0.007198	0.030895
MnO	0.000996	0.016351	0.016409	0.001114	0.017015	0.015455	0.016185	0.001029
MoO_3	0.000150	0.000506	0.000102	0.000104	0.000102	0.000095	0.000101	0.000570
Na_2O	0.133217	0.124671	0.096929	0.129682	0.139281	0.113924	0.095726	0.098408
Nd_2O_3	0.000193	0.000780	0.000175	0.000177	0.000175	0.000143	0.000151	0.000886
NiO	0.002029	0.007807	0.001772	0.001695	0.001773	0.001468	0.001456	0.008784
P_2O_5	0.019322	0.018899	0.012381	0.003254	0.020220	0.002849	0.020081	0.022483
Pr_6O_{11}	0.000021	0.000071	0.000014	0.000015	0.000014	0.000013	0.000014	0.000080
SO_3	0.001352	0.005372	0.001194	0.001210	0.001213	0.001028	0.000997	0.006147
SiO_2	0.540541	0.485292	0.513999	0.471114	0.465438	0.513421	0.543214	0.471566
Sm_2O_3	0.000021	0.000104	0.000021	0.000021	0.000021	0.000020	0.000021	0.000128
SrO	0.000070	0.000352	0.000071	0.000072	0.000071	0.000066	0.000070	0.000432
ThO_2	0.014405	0.013804	0.011529	0.010467	0.004989	0.005608	0.005357	0.005817
TiO_2	0.005059	0.019707	0.004417	0.004382	0.004421	0.003689	0.003813	0.022304
U_3O_8	0.001773	0.000108	0.001743	0.001977	0.000091	0.000093	0.000107	0.001749
Y_2O_3	0.000032	0.000161	0.000033	0.000033	0.000033	0.000030	0.000032	0.000198
ZnO	0.000177	0.000717	0.000181	0.000183	0.000181	0.000168	0.000178	0.000825
ZrO_2	0.001581	0.006093	0.001373	0.001330	0.001374	0.001168	0.001177	0.006898
PCT B	0.314	0.380	0.208	0.357	0.260	0.372	0.224	0.179
PCT Li	0.299	0.355	0.257	0.358	0.265	0.317	0.233	0.206
PCT Na	0.369	0.364	0.138	0.331	0.300	0.299	0.156	0.129

* The glass numbers are those used in the reference from which the data were taken.

Table A.9. WVDP Glass Compositions (mole fractions) and PCT Normalized B, Na, and Li Releases (g/m^2)

Comp.	1* WVDG-40	2 WVDG-46	3 FY92#5	4 FY92#6	5 FY92#7	6 FY92#9	7 FY92#10	8 FY92REF5
SiO_2	0.535544	0.513421	0.436609	0.526622	0.543849	0.516604	0.491458	0.491773
Al_2O_3	0.043326	0.047064	0.049811	0.033538	0.034635	0.033504	0.050969	0.045412
ZrO_2	0.001354	0.001168	0.007620	0.007538	0.007784	0.007530	0.007797	0.001864
ThO_2	0.011511	0.005608	0.007193	0.007115	0.007348	0.011846	0.012267	0.009679
Na_2O	0.113291	0.113924	0.100421	0.116704	0.067061	0.064870	0.067173	0.113741
K_2O	0.024411	0.024526	0.051954	0.051392	0.053073	0.023356	0.053162	0.024235
Li_2O	0.065300	0.065613	0.121404	0.054629	0.056416	0.119966	0.056511	0.065106
B_2O_3	0.078458	0.120428	0.106670	0.105515	0.108967	0.105407	0.160378	0.132917
Fe_2O_3	0.069725	0.044602	0.063696	0.042915	0.065068	0.062942	0.044393	0.054035
BaO	0.000473	0.000447	0.001206	0.001193	0.001232	0.001192	0.001234	0.000749
CaO	0.009313	0.008312	0.006088	0.006022	0.006219	0.006016	0.006230	0.008705
Ce_2O_3	0.000885	0.000737	0.000672	0.000665	0.000686	0.000664	0.000687	0.000334
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000192
Cr_2O_3	0.000382	0.000316	0.000655	0.000648	0.000669	0.000647	0.000670	0.000661
Cs_2O	0.000103	0.000097	0.000000	0.000000	0.000000	0.000000	0.000000	0.000204
CuO	0.000182	0.000172	0.000000	0.000000	0.000000	0.000000	0.000000	0.000271
La_2O_3	0.000045	0.000042	0.000000	0.000000	0.000000	0.000000	0.000000	0.000088
MgO	0.032036	0.028404	0.015707	0.015537	0.016046	0.015521	0.016072	0.015852
MnO	0.001001	0.015455	0.008222	0.008133	0.008400	0.008125	0.008414	0.008340
MoO_3	0.000101	0.000095	0.000000	0.000000	0.000000	0.000000	0.000000	0.000199
Nd_2O_3	0.000172	0.000143	0.000000	0.000000	0.000000	0.000000	0.000000	0.000299
NiO	0.001748	0.001468	0.002381	0.002355	0.002432	0.002352	0.002436	0.002403
P_2O_5	0.003066	0.002849	0.006013	0.005948	0.006143	0.005942	0.006153	0.011986
PdO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000176
Pr_6O_{11}	0.000014	0.000013	0.000000	0.000000	0.000000	0.000000	0.000000	0.000028
RhO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000106
RuO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000432
Sm_2O_3	0.000021	0.000020	0.000000	0.000000	0.000000	0.000000	0.000000	0.000062
SO_3	0.001178	0.001028	0.002044	0.002021	0.002088	0.002019	0.002091	0.002062
SrO	0.000070	0.000066	0.001716	0.001698	0.001753	0.001696	0.001756	0.000139
TiO_2	0.004449	0.003689	0.007122	0.007045	0.007276	0.007038	0.007288	0.007188
U_3O_8	0.001630	0.000093	0.000522	0.000517	0.000533	0.000516	0.000534	0.000523
Y_2O_3	0.000032	0.000030	0.000000	0.000000	0.000000	0.000000	0.000000	0.000064
ZnO	0.000178	0.000168	0.002273	0.002248	0.002322	0.002246	0.002325	0.000176
PCT B	0.306	0.373	0.694	0.278	0.211	0.262	0.822	0.196
PCT Na	0.290	0.300	0.529	0.267	0.208	0.196	0.569	0.256
PCT Li	0.305	0.318	0.584	0.357	0.264	0.295	0.711	0.275

* The glass numbers are those used in the reference from which the data were taken.

Table A.9. WVDP Glass Compositions (mole fractions) and PCT Normalized B, Na, and Li Releases (g/m^2) (continued)

Comp.	9* Ratio2	10 Ratio4	11 Ratio5	12 LoTh2	13 LoTh4	14 LoTh5	15 HiFe2	16 HiFe3
SiO_2	0.467398	0.507408	0.455155	0.493499	0.498396	0.494554	0.469548	0.460604
Al_2O_3	0.047106	0.039271	0.035947	0.042493	0.041431	0.038299	0.037635	0.038835
ZrO_2	0.007013	0.010832	0.005720	0.007644	0.006766	0.006651	0.006648	0.006485
ThO_2	0.003545	0.011440	0.007475	0.003699	0.004737	0.006477	0.008274	0.007836
Na_2O	0.102240	0.081605	0.102350	0.100185	0.099771	0.080481	0.102030	0.105904
K_2O	0.042045	0.041762	0.037413	0.033330	0.035405	0.033059	0.041196	0.043552
Li_2O	0.089163	0.096386	0.096710	0.091526	0.076731	0.077503	0.096194	0.101236
B_2O_3	0.113777	0.113012	0.147815	0.117252	0.137726	0.146677	0.113543	0.115087
Fe_2O_3	0.072418	0.044341	0.057290	0.056796	0.045684	0.061579	0.069749	0.065675
BaO	0.001221	0.001191	0.001195	0.001183	0.001178	0.001208	0.001219	0.001210
CaO	0.006163	0.006013	0.006033	0.005972	0.005947	0.006099	0.006151	0.006107
Ce_2O_3	0.000680	0.000663	0.000666	0.000659	0.000656	0.000673	0.000679	0.000674
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000663	0.000647	0.000649	0.000643	0.000640	0.000656	0.000662	0.000657
Cs_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
CuO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
MgO	0.015901	0.015512	0.015564	0.015406	0.015342	0.015735	0.015868	0.015755
MnO	0.008324	0.008120	0.008148	0.008065	0.008031	0.008237	0.008307	0.008247
MoO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Nd_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
NiO	0.002410	0.002351	0.002359	0.002335	0.002325	0.002385	0.002405	0.002388
P_2O_5	0.006088	0.005939	0.005959	0.005898	0.005874	0.006024	0.006075	0.006032
PdO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pr_6O_{11}	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RhO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RuO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SO_3	0.002069	0.002018	0.002025	0.002004	0.001996	0.002047	0.002064	0.002050
SrO	0.001737	0.001695	0.001701	0.001683	0.001676	0.001719	0.001734	0.001721
TiO_2	0.007210	0.007034	0.007057	0.006986	0.006957	0.007135	0.007195	0.007144
U_3O_8	0.000529	0.000516	0.000517	0.000512	0.000510	0.000523	0.000528	0.000524
Y_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
ZnO	0.002301	0.002244	0.002252	0.002229	0.002220	0.002277	0.002296	0.002279
PCT B	1.546	0.261	0.244	0.393	0.644	0.242	0.588	0.418
PCT Na	0.909	0.255	0.297	0.229	0.487	0.385	0.498	0.382
PCT Li	1.129	0.290	0.305	0.283	0.577	0.433	0.555	0.423

* The glass numbers are those used in the reference from which the data were taken.

Table A.9. WVDP Glass Compositions (mole fractions) and PCT Normalized B, Na, and Li Releases (g/m^2) (continued)

Comp.	17* HiFe4	18 PNL190	19 Alkali1	20 Alkali2	21 Alkali3	22 Alkali4	23 Alkali5	24 Alkali6
SiO_2	0.457673	0.465367	0.508815	0.460112	0.477124	0.512849	0.476404	0.480355
Al_2O_3	0.037883	0.033261	0.046069	0.041230	0.041893	0.044116	0.043052	0.045291
ZrO_2	0.005349	0.007302	0.008413	0.008327	0.008841	0.008796	0.007182	0.008089
ThO_2	0.008590	0.011796	0.010831	0.010848	0.008957	0.009927	0.010324	0.009369
Na_2O	0.094911	0.115019	0.085363	0.087370	0.094820	0.089148	0.091386	0.089663
K_2O	0.032730	0.050551	0.035674	0.034795	0.036521	0.033841	0.034575	0.038824
Li_2O	0.098431	0.118126	0.086136	0.097763	0.081547	0.082971	0.086482	0.091188
B_2O_3	0.149651	0.103392	0.107832	0.149425	0.136918	0.112944	0.147461	0.121539
Fe_2O_3	0.060359	0.042040	0.055964	0.055415	0.058343	0.051012	0.048769	0.060619
BaO	0.001202	0.001174	0.001212	0.001208	0.001215	0.001201	0.001201	0.001216
CaO	0.006066	0.005924	0.006120	0.006099	0.006134	0.006063	0.006060	0.006138
Ce_2O_3	0.000669	0.000654	0.000675	0.000673	0.000677	0.000669	0.000669	0.000677
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000653	0.000638	0.000659	0.000656	0.000660	0.000652	0.000652	0.000660
Cs_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
CuO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
MgO	0.015650	0.015283	0.015788	0.015734	0.015826	0.015642	0.015634	0.015834
MnO	0.008193	0.008000	0.008265	0.008236	0.008285	0.008188	0.008184	0.008289
MoO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Nd_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
NiO	0.002372	0.002316	0.002393	0.002385	0.002399	0.002371	0.002369	0.002400
P_2O_5	0.005992	0.005851	0.006044	0.006024	0.006059	0.005989	0.005985	0.006062
PdO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pr_6O_{11}	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RhO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RuO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SO_3	0.002036	0.001988	0.002054	0.002047	0.002059	0.002035	0.002034	0.002060
SrO	0.001710	0.001670	0.001725	0.001719	0.001729	0.001709	0.001708	0.001730
TiO_2	0.007096	0.006930	0.007159	0.007134	0.007176	0.007093	0.007089	0.007180
U_3O_8	0.000520	0.000508	0.000525	0.000523	0.000526	0.000520	0.000520	0.000526
Y_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
ZnO	0.002264	0.002211	0.002284	0.002276	0.002290	0.002263	0.002262	0.002291
PCT B	0.741	1.227	0.251	0.647	0.454	0.274	0.636	0.328
PCT Na	0.572	1.014	0.217	0.430	0.316	0.195	0.421	0.240
PCT Li	0.652	1.069	0.280	0.474	0.355	0.257	0.477	0.302

* The glass numbers are those used in the reference from which the data were taken.

Table A.9. WVDP Glass Compositions (mole fractions) and PCT Normalized B, Na, and Li Releases (g/m^2) (continued)

Comp.	25* Alkali7	26 Alkali8	27 Alkali9	28 Ref6Q2	29 FY93#1	30 FY93#2	31 FY93#3	32 FY93#4
SiO_2	0.461738	0.483394	0.499984	0.484195	0.481539	0.481008	0.402515	0.559838
Al_2O_3	0.040465	0.039194	0.046624	0.041776	0.055402	0.029330	0.051866	0.030436
ZrO_2	0.009237	0.008340	0.009370	0.007605	0.007849	0.007468	0.007348	0.007749
ThO_2	0.011127	0.010649	0.011310	0.009572	0.004939	0.004699	0.004624	0.004877
Na_2O	0.093542	0.103625	0.082796	0.091634	0.067617	0.115620	0.113765	0.066761
K_2O	0.040781	0.041668	0.038588	0.037683	0.024345	0.050914	0.050098	0.052836
Li_2O	0.095225	0.078810	0.081096	0.088142	0.056884	0.054122	0.117066	0.056164
B_2O_3	0.142031	0.128131	0.127970	0.131444	0.174278	0.165814	0.163154	0.095803
Fe_2O_3	0.051228	0.051390	0.047532	0.053436	0.070884	0.037497	0.036895	0.069987
BaO	0.001206	0.001210	0.001209	0.001204	0.001242	0.001182	0.001163	0.001227
CaO	0.006089	0.006108	0.006100	0.006076	0.006271	0.005967	0.005871	0.006192
Ce_2O_3	0.000672	0.000674	0.000673	0.000670	0.000692	0.000658	0.000648	0.000683
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000655	0.000657	0.000656	0.000654	0.000675	0.000642	0.000632	0.000666
Cs_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
CuO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
MgO	0.015708	0.015758	0.015738	0.015676	0.016179	0.015393	0.015146	0.015974
MnO	0.008223	0.008249	0.008239	0.008206	0.008469	0.008058	0.007929	0.008362
MoO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Nd_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
NiO	0.002381	0.002388	0.002385	0.002376	0.002452	0.002333	0.002296	0.002421
P_2O_5	0.006014	0.006033	0.006025	0.006002	0.006194	0.005893	0.005799	0.006116
PdO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pr_6O_{11}	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RhO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RuO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SO_3	0.002044	0.002050	0.002048	0.002040	0.002105	0.002003	0.001971	0.002078
SrO	0.001716	0.001722	0.001720	0.001713	0.001768	0.001682	0.001655	0.001745
TiO_2	0.007123	0.007145	0.007136	0.007108	0.007336	0.006980	0.006868	0.007243
U_3O_8	0.000522	0.000524	0.000523	0.000521	0.000538	0.000512	0.000504	0.000531
Y_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
ZnO	0.002273	0.002280	0.002277	0.002268	0.002341	0.002227	0.002191	0.002311
PCT B	0.889	0.468	0.284	0.415	0.544	4.044	3.266	0.239
PCT Na	0.567	0.350	0.208	0.317	0.328	2.426	1.897	0.190
PCT Li	0.586	0.412	0.271	0.353	0.504	2.702	2.265	0.250

* The glass numbers are those used in the reference from which the data were taken.

Table A.9. WVDP Glass Compositions (mole fractions) and PCT Normalized B, Na, and Li Releases (g/m^2) (continued)

Comp.	33* FY93#5	34 FY93#6	35 FY93#7	36 FY93#8	37 FY93#9	38 FY93#10	39 FY94#1	40 FY94#2
SiO_2	0.519219	0.528517	0.557559	0.432517	0.441461	0.521456	0.555001	0.521361
Al_2O_3	0.027934	0.050950	0.054619	0.031393	0.057586	0.028528	0.050695	0.052872
ZrO_2	0.007112	0.007218	0.007738	0.007993	0.008158	0.007263	0.004138	0.004316
ThO_2	0.004476	0.004542	0.014608	0.015090	0.015402	0.013713	0.012698	0.007532
Na_2O	0.061271	0.111756	0.066661	0.123754	0.126313	0.112458	0.094669	0.061121
K_2O	0.022061	0.022389	0.052757	0.024793	0.055623	0.022530	0.044493	0.045630
Li_2O	0.113312	0.097410	0.056080	0.057929	0.062440	0.115721	0.065453	0.097519
B_2O_3	0.157922	0.089234	0.095660	0.177051	0.100857	0.089795	0.090301	0.074192
Fe_2O_3	0.035712	0.036244	0.038854	0.072186	0.073679	0.036471	0.028913	0.079514
BaO	0.001126	0.001143	0.001225	0.001265	0.001291	0.001150	0.001184	0.001235
CaO	0.005683	0.005767	0.006182	0.006386	0.006518	0.005803	0.005979	0.006235
Ce_2O_3	0.000627	0.000636	0.000682	0.000705	0.000719	0.000640	0.000660	0.000688
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000612	0.000621	0.000665	0.000687	0.000701	0.000625	0.000643	0.000671
Cs_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
CuO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
MgO	0.014660	0.014879	0.015950	0.016476	0.016817	0.014972	0.015424	0.016087
MnO	0.007674	0.007789	0.008349	0.008625	0.008803	0.007838	0.008074	0.008421
MoO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Nd_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
NiO	0.002222	0.002255	0.002417	0.002497	0.002549	0.002269	0.002338	0.002438
P_2O_5	0.005613	0.005696	0.006106	0.006308	0.006438	0.005732	0.005905	0.006159
PdO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pr_6O_{11}	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RhO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RuO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SO_3	0.001907	0.001936	0.002075	0.002144	0.002188	0.001948	0.002007	0.002093
SrO	0.001602	0.001626	0.001743	0.001800	0.001837	0.001636	0.001685	0.001758
TiO_2	0.006647	0.006746	0.007232	0.007471	0.007625	0.006789	0.006994	0.007294
U_3O_8	0.000487	0.000495	0.000530	0.000548	0.000559	0.000498	0.000513	0.000535
Y_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
ZnO	0.002121	0.002153	0.002308	0.002384	0.002433	0.002166	0.002232	0.002328
PCT B	1.267	0.269	0.186	1.575	0.431	0.757	0.186	0.215
PCT Na	0.658	0.225	0.145	0.962	0.377	0.467	0.208	0.222
PCT Li	0.881	0.266	0.200	1.197	0.385	0.495	0.253	0.297

* The glass numbers are those used in the reference from which the data were taken.

Table A.9. WVDP Glass Compositions (mole fractions) and PCT Normalized B, Na, and Li Releases (g/m^2) (continued)

Comp.	41* FY94#3	42 FY94#4	43 FY94#5	44 FY94#6	45 FY94#7	46 FY94#8	47 FY94#9	48 FY94#10
SiO_2	0.433979	0.406858	0.534509	0.483946	0.510653	0.414041	0.492486	0.470732
Al_2O_3	0.039121	0.029883	0.036318	0.055976	0.043582	0.031117	0.032356	0.040420
ZrO_2	0.004175	0.004198	0.009453	0.011475	0.010533	0.011177	0.010477	0.003990
ThO_2	0.005338	0.002415	0.007905	0.014467	0.012555	0.003004	0.006519	0.009182
Na_2O	0.125077	0.104036	0.116235	0.071663	0.075110	0.099357	0.070816	0.084749
K_2O	0.034415	0.039868	0.047175	0.033007	0.029952	0.029089	0.048727	0.022377
Li_2O	0.066037	0.109079	0.100267	0.116435	0.056651	0.091700	0.081603	0.108175
B_2O_3	0.189197	0.174043	0.068568	0.075389	0.177606	0.186438	0.139071	0.180789
Fe_2O_3	0.048544	0.075209	0.027869	0.080798	0.029195	0.078704	0.062874	0.027874
BaO	0.001195	0.001202	0.001142	0.001255	0.001196	0.001223	0.001216	0.001142
CaO	0.006032	0.006065	0.005763	0.006336	0.006037	0.006172	0.006139	0.005764
Ce_2O_3	0.000666	0.000669	0.000636	0.000699	0.000666	0.000681	0.000677	0.000636
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000649	0.000653	0.000620	0.000682	0.000650	0.000664	0.000661	0.000620
Cs_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
CuO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
MgO	0.015562	0.015647	0.014867	0.016346	0.015575	0.015923	0.015837	0.014870
MnO	0.008146	0.008191	0.007783	0.008557	0.008153	0.008335	0.008290	0.007784
MoO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Nd_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
NiO	0.002359	0.002371	0.002253	0.002477	0.002361	0.002413	0.002400	0.002254
P_2O_5	0.005958	0.005990	0.005692	0.006258	0.005963	0.006096	0.006063	0.005693
PdO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pr_6O_{11}	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RhO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RuO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SO_3	0.002025	0.002036	0.001934	0.002127	0.002026	0.002072	0.002060	0.001935
SrO	0.001700	0.001710	0.001624	0.001786	0.001702	0.001740	0.001730	0.001625
TiO_2	0.007056	0.007095	0.006741	0.007412	0.007062	0.007220	0.007181	0.006743
U_3O_8	0.000517	0.000520	0.000494	0.000543	0.000518	0.000529	0.000527	0.000494
Y_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
ZnO	0.002252	0.002264	0.002151	0.002365	0.002253	0.002304	0.002291	0.002152
PCT B	4.057	3.336	0.453	0.288	1.047	2.242	0.435	3.385
PCT Na	2.553	2.296	0.495	0.266	0.693	1.565	0.368	2.151
PCT Li	3.559	2.605	0.532	0.364	0.949	1.920	0.447	2.885

* The glass numbers are those used in the reference from which the data were taken.

Table A.9. WVDP Glass Compositions (mole fractions) and PCT Normalized B, Na, and Li Releases (g/m^2) (continued)

Comp.	49* Sigma1	50 Sigma2	51 Sigma3	52 Sigma4	53 Sigma5	54 Sigma6	55 Sigma7	56 Sigma8
SiO_2	0.389960	0.392802	0.441782	0.403975	0.400893	0.417742	0.410534	0.425531
Al_2O_3	0.028809	0.029019	0.032613	0.032858	0.031049	0.031699	0.034272	0.032531
ZrO_2	0.004056	0.004086	0.004576	0.004495	0.004468	0.004576	0.004337	0.004711
ThO_2	0.002308	0.013478	0.010513	0.002590	0.002346	0.005730	0.002855	0.002617
Na_2O	0.121520	0.122406	0.127130	0.113627	0.116592	0.112061	0.118290	0.108148
K_2O	0.050010	0.050374	0.051417	0.046455	0.048951	0.047452	0.048009	0.046217
Li_2O	0.116861	0.117713	0.118539	0.114408	0.112854	0.110463	0.113504	0.112158
B_2O_3	0.183818	0.185157	0.079018	0.181692	0.177939	0.172859	0.167314	0.158814
Fe_2O_3	0.050080	0.032003	0.078901	0.047397	0.052060	0.044612	0.048270	0.056210
BaO	0.001161	0.001170	0.001226	0.001159	0.001167	0.001166	0.001162	0.001172
CaO	0.005861	0.005903	0.006187	0.005852	0.005891	0.005886	0.005865	0.005915
Ce_2O_3	0.000647	0.000651	0.000683	0.000646	0.000650	0.000649	0.000647	0.000653
CoO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Cr_2O_3	0.000631	0.000635	0.000666	0.000630	0.000634	0.000633	0.000631	0.000637
Cs_2O	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
CuO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
La_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
MgO	0.015120	0.015230	0.015963	0.015098	0.015197	0.015185	0.015130	0.015259
MnO	0.007915	0.007972	0.008356	0.007904	0.007955	0.007949	0.007920	0.007988
MoO_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Nd_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
NiO	0.002292	0.002308	0.002419	0.002288	0.002303	0.002301	0.002293	0.002313
P_2O_5	0.005788	0.005831	0.006111	0.005780	0.005818	0.005814	0.005793	0.005842
PdO	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pr_6O_{11}	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RhO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
RuO_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Sm_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
SO_3	0.001967	0.001981	0.002077	0.001964	0.001977	0.001976	0.001968	0.001985
SrO	0.001652	0.001664	0.001744	0.001650	0.001660	0.001659	0.001653	0.001667
TiO_2	0.006856	0.006906	0.007238	0.006846	0.006891	0.006885	0.006861	0.006919
U_3O_8	0.000503	0.000506	0.000531	0.000502	0.000505	0.000505	0.000503	0.000507
Y_2O_3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
ZnO	0.002188	0.002204	0.002310	0.002184	0.002199	0.002197	0.002189	0.002208
PCT B	6.609	10.278	7.742	4.655	5.268	4.921	4.429	3.407
PCT Na	4.920	7.965	5.429	3.551	3.930	3.683	3.326	2.559
PCT Li	5.312	7.535	4.071	3.839	4.262	3.969	3.545	2.730

* The glass numbers are those used in the reference from which the data were taken.

Table A.9. WVDP Glass Compositions (mole fractions) and PCT Normalized B, Na, and Li Releases (g/m^2) (continued)

Comp.	57* Sigma9	58 Sigma10
SiO_2	0.433440	0.439137
Al_2O_3	0.035418	0.034050
ZrO_2	0.004791	0.004677
ThO_2	0.011310	0.013149
Na_2O	0.110930	0.106428
K_2O	0.044973	0.045702
Li_2O	0.110395	0.109213
B_2O_3	0.154621	0.157584
Fe_2O_3	0.040792	0.036741
BaO	0.001178	0.001177
CaO	0.005944	0.005943
Ce_2O_3	0.000656	0.000656
CoO	0.000000	0.000000
Cr_2O_3	0.000640	0.000640
Cs_2O	0.000000	0.000000
CuO	0.000000	0.000000
La_2O_3	0.000000	0.000000
MgO	0.015335	0.015333
MnO	0.008028	0.008026
MoO_3	0.000000	0.000000
Nd_2O_3	0.000000	0.000000
NiO	0.002324	0.002324
P_2O_5	0.005871	0.005870
PdO	0.000000	0.000000
Pr_6O_{11}	0.000000	0.000000
RhO_2	0.000000	0.000000
RuO_2	0.000000	0.000000
Sm_2O_3	0.000000	0.000000
SO_3	0.001995	0.001995
SrO	0.001676	0.001675
TiO_2	0.006954	0.006952
U_3O_8	0.000510	0.000510
Y_2O_3	0.000000	0.000000
ZnO	0.002219	0.002218
PCT B	3.542	4.028
PCT Na	2.485	2.913
PCT Li	2.833	3.245

* The glass numbers are those used in the reference from which the data were taken.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2)

Comp.	HG-1-1	HG-1-2	HG-1-3	HG-2-1	HG-2-2	HG-2-3	HG-3-1	HG-3-2	HG-3-3	AH-165AL
Al_2O_3	0.0344	0.0318	0.0310	0.0319	0.0343	0.0336	0.0352	0.0359	0.0360	0.0848
CaO	0.0152	0.0121	0.0125	0.0123	0.0126	0.0125	0.0130	0.0134	0.0140	0.0059
Fe_2O_3	0.0522	0.0472	0.0465	0.0480	0.0513	0.0503	0.0502	0.0513	0.0496	0.0185
FeO	0.0004	0.0004	0.0013	0.0006	0.0006	0.0006	0.0046	0.0068	0.0093	0.0021
MgO	0.0246	0.0237	0.0237	0.0236	0.0218	0.0218	0.0217	0.0215	0.0217	0.0106
MnO	0.0197	0.0203	0.0200	0.0205	0.0220	0.0216	0.0223	0.0233	0.0224	0.0238
Na_2O	0.0954	0.0890	0.0903	0.0901	0.1070	0.1072	0.1042	0.1015	0.0993	0.1103
Li_2O	0.0953	0.0973	0.0981	0.0975	0.0945	0.0949	0.0933	0.0918	0.0923	0.0907
NiO	0.0074	0.0066	0.0063	0.0066	0.0066	0.0065	0.0068	0.0067	0.0067	0.0058
SiO_2	0.5601	0.5782	0.5803	0.5811	0.5712	0.5747	0.5680	0.5648	0.5643	0.5754
Cr_2O_3	0.0015	0.0014	0.0012	0.0014	0.0012	0.0013	0.0014	0.0012	0.0010	0.0000
B_2O_3	0.0650	0.0627	0.0632	0.0619	0.0557	0.0553	0.0565	0.0576	0.0586	0.0680
SrO	0.0001	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002	0.0000
ZrO_2	0.0008	0.0005	0.0000	0.0000	0.0011	0.0004	0.0009	0.0009	0.0008	0.0041
TiO_2	0.0037	0.0022	0.0021	0.0021	0.0018	0.0017	0.0018	0.0019	0.0020	0.0000
K_2O	0.0183	0.0205	0.0174	0.0165	0.0123	0.0122	0.0137	0.0152	0.0158	0.0000
Cs_2O	0.0002	0.0002	0.0002	0.0001	0.0001	0.0002	0.0001	0.0001	0.0000	0.0000
P_2O_5	0.0000	0.0002	0.0002	0.0002	0.0003	0.0000	0.0002	0.0001	0.0001	0.0000
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0005	0.0003	0.0003	0.0003	0.0004	0.0003	0.0003	0.0004	0.0004	0.0000
PbO	0.0003	0.0006	0.0005	0.0005	0.0007	0.0005	0.0007	0.0007	0.0006	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZnO	0.0025	0.0030	0.0029	0.0030	0.0032	0.0030	0.0035	0.0031	0.0034	0.0000
CuO	0.0026	0.0017	0.0017	0.0017	0.0012	0.0011	0.0014	0.0015	0.0015	0.0000
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.340	0.365	0.340	0.345	0.385	0.395	0.375	0.390	0.365	0.260
PCT Li	0.330	0.335	0.310	0.320	0.365	0.360	0.360	0.365	0.340	0.315
PCT Na	0.335	0.345	0.325	0.335	0.400	0.395	0.385	0.385	0.370	0.180

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	AH-165AV	AH-165FE	AH-131AL	AH-131AV	AH-131-FE	AH-168AV	AH-168FE	AH-200AL	AH-200AV	AH-200FE
Al_2O_3	0.0325	0.0090	0.0853	0.0280	0.0142	0.0357	0.0156	0.0870	0.0338	0.0135
CaO	0.0119	0.0161	0.0044	0.0088	0.0116	0.0079	0.0156	0.0064	0.0075	0.0109
Fe_2O_3	0.0444	0.0366	0.0185	0.0453	0.0307	0.0430	0.0380	0.0182	0.0482	0.0407
FeO	0.0042	0.0641	0.0008	0.0063	0.0789	0.0056	0.0559	0.0006	0.0036	0.0549
MgO	0.0105	0.0104	0.0221	0.0108	0.0105	0.0120	0.0114	0.0205	0.0207	0.0199
MnO	0.0232	0.0097	0.0228	0.0238	0.0084	0.0243	0.0089	0.0232	0.0241	0.0089
Na_2O	0.1030	0.1113	0.1466	0.1035	0.1132	0.1064	0.1126	0.1133	0.1058	0.1136
Li_2O	0.1076	0.0874	0.0882	0.0926	0.0874	0.0926	0.0891	0.0587	0.0602	0.0576
NiO	0.0087	0.0256	0.0054	0.0091	0.0221	0.0089	0.0244	0.0054	0.0092	0.0228
SiO_2	0.5896	0.5580	0.4976	0.5957	0.5506	0.5606	0.5193	0.5334	0.5530	0.5238
Cr_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
B_2O_3	0.0605	0.0674	0.1000	0.0710	0.0678	0.0994	0.1058	0.0970	0.0993	0.0963
SrO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZrO_2	0.0040	0.0044	0.0018	0.0046	0.0045	0.0037	0.0035	0.0002	0.0001	0.0001
TiO_2	0.0000	0.0000	0.0058	0.0005	0.0001	0.0000	0.0000	0.0141	0.0118	0.0148
K_2O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0219	0.0227	0.0222
Cs_2O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
La_2O_3	0.0000	0.0000	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CuO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.320	2.380	0.360	0.340	1.790	0.400	2.565	0.230	0.290	2.550
PCT Li	0.330	1.965	0.350	0.365	1.600	0.375	2.210	0.285	0.310	2.190
PCT Na	0.265	2.090	0.345	0.305	1.545	0.295	1.950	0.220	0.295	2.190

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	AH-202AL	AH-202AV	AH-202-FE	AH-2	AH-4	AH-5	AH-6	AH-7	AH-8	AH-9
Al_2O_3	0.0885	0.0318	0.0086	0.0431	0.0300	0.0356	0.0362	0.0412	0.0385	0.0396
CaO	0.0047	0.0084	0.0110	0.0077	0.0116	0.0078	0.0080	0.0076	0.0082	0.0082
Fe_2O_3	0.0175	0.0473	0.0387	0.0479	0.0449	0.0473	0.0490	0.0474	0.0485	0.0485
FeO	0.0008	0.0028	0.0561	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MgO	0.0206	0.0211	0.0201	0.0097	0.0118	0.0099	0.0099	0.0098	0.0199	0.0096
MnO	0.0230	0.0239	0.0086	0.0252	0.0195	0.0246	0.0254	0.0247	0.0252	0.0249
Na_2O	0.0768	0.0691	0.0789	0.1114	0.1041	0.0987	0.1124	0.0999	0.1052	0.0992
Li_2O	0.0908	0.0935	0.0917	0.0844	0.0895	0.0835	0.1019	0.0706	0.0709	0.0776
NiO	0.0054	0.0088	0.0235	0.0083	0.0085	0.0085	0.0083	0.0085	0.0087	0.0087
SiO_2	0.5659	0.5889	0.5614	0.4972	0.5807	0.5849	0.5222	0.5463	0.5447	0.5659
Cr_2O_3	0.0000	0.0000	0.0000	0.0001	0.0002	0.0000	0.0000	0.0000	0.0001	0.0001
B_2O_3	0.0692	0.0699	0.0653	0.1281	0.0662	0.0661	0.0889	0.1106	0.0969	0.0840
SrO	0.0000	0.0000	0.0000	0.0003	0.0003	0.0000	0.0003	0.0000	0.0003	0.0003
ZrO_2	0.0001	0.0001	0.0001	0.0034	0.0000	0.0001	0.0036	0.0001	0.0000	0.0000
TiO_2	0.0139	0.0112	0.0138	0.0109	0.0106	0.0109	0.0116	0.0108	0.0110	0.0111
K_2O	0.0229	0.0231	0.0223	0.0221	0.0219	0.0222	0.0221	0.0224	0.0218	0.0222
Cs_2O	0.0000	0.0000	0.0000	0.0001	0.0001	0.0000	0.0001	0.0000	0.0001	0.0001
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CuO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.175	0.260	1.580	0.475	0.265	0.210	0.345	0.220	0.250	0.220
PCT Li	0.240	0.295	1.275	0.475	0.305	0.260	0.365	0.245	0.275	0.255
PCT Na	0.145	0.255	1.355	0.435	0.315	0.245	0.350	0.225	0.245	0.230

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	AH-10	AH-11	AH-12	AH-13	AH-14	AH-15	AH-16	AH-17	SFRIT1	SFRIT2
Al_2O_3	0.0329	0.0373	0.0396	0.0437	0.0475	0.0465	0.0420	0.0371	0.0304	0.0304
CaO	0.0079	0.0077	0.0082	0.0153	0.0152	0.0156	0.0151	0.0077	0.0177	0.0177
Fe_2O_3	0.0462	0.0460	0.0485	0.0586	0.0595	0.0588	0.0565	0.0472	0.0600	0.0600
FeO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MgO	0.0180	0.0184	0.0096	0.0084	0.0090	0.0175	0.0167	0.0095	0.0141	0.0141
MnO	0.0246	0.0247	0.0249	0.0315	0.0322	0.0317	0.0306	0.0252	0.0184	0.0184
Na_2O	0.0720	0.0691	0.0992	0.0976	0.1077	0.1048	0.0711	0.0705	0.1254	0.1254
Li_2O	0.0971	0.0809	0.0776	0.0764	0.0902	0.0647	0.0916	0.1037	0.0733	0.0733
NiO	0.0084	0.0083	0.0087	0.0105	0.0103	0.0104	0.0099	0.0081	0.0100	0.0100
SiO_2	0.5892	0.5600	0.5660	0.5607	0.5098	0.5238	0.5630	0.5774	0.5376	0.5376
Cr_2O_3	0.0000	0.0001	0.0000	0.0000	0.0000	0.0001	0.0003	0.0004	0.0004	0.0004
B_2O_3	0.0712	0.1151	0.0840	0.0633	0.0810	0.0912	0.0697	0.0771	0.0824	0.0824
SrO	0.0003	0.0003	0.0003	0.0004	0.0004	0.0004	0.0005	0.0002	0.0000	0.0000
ZrO_2	0.0000	0.0000	0.0000	0.0001	0.0032	0.0000	0.0000	0.0035	0.0006	0.0006
TiO_2	0.0106	0.0108	0.0111	0.0111	0.0113	0.0116	0.0110	0.0108	0.0100	0.0100
K_2O	0.0214	0.0212	0.0222	0.0223	0.0224	0.0227	0.0219	0.0215	0.0193	0.0193
Cs_2O	0.0001	0.0001	0.0001	0.0001	0.0002	0.0001	0.0001	0.0001	0.0000	0.0000
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0004
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CuO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.215	0.235	0.425	0.215	0.260	0.215	0.210	0.180	0.375	0.365
PCT Li	0.260	0.285	0.305	0.260	0.290	0.240	0.240	0.225	0.345	0.350
PCT Na	0.215	0.225	0.365	0.235	0.305	0.225	0.220	0.185	0.355	0.350

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	SFRIT3	202P	202G	200R	NBS623	165CGW	ARM1-4/88	ARM1-5/89	ARM1-7/90	ARM1-12/90
Al_2O_3	0.0304	0.0274	0.0291	0.0311	0.0394	0.0264	0.0369	0.0369	0.0369	0.0369
CaO	0.0177	0.0141	0.0149	0.0180	0.0080	0.0176	0.0268	0.0268	0.0268	0.0268
Fe_2O_3	0.0600	0.0436	0.0487	0.0529	0.0000	0.0520	0.0000	0.0000	0.0000	0.0000
FeO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MgO	0.0141	0.0471	0.0508	0.0213	0.0000	0.0163	0.0000	0.0000	0.0000	0.0000
MnO	0.0184	0.0000	0.0000	0.0206	0.0000	0.0232	0.0000	0.0000	0.0000	0.0000
Na_2O	0.1254	0.0965	0.0855	0.1473	0.0659	0.1082	0.1051	0.1051	0.1051	0.1051
Li_2O	0.0733	0.0744	0.0811	0.0692	0.0000	0.1075	0.1145	0.1145	0.1145	0.1145
NiO	0.0100	0.0061	0.0058	0.0049	0.0000	0.0083	0.0000	0.0000	0.0000	0.0000
SiO_2	0.5376	0.5540	0.6000	0.5157	0.7754	0.5758	0.5213	0.5213	0.5213	0.5213
Cr_2O_3	0.0004	0.0003	0.0003	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
B_2O_3	0.0824	0.0803	0.0557	0.0934	0.0981	0.0619	0.1093	0.1093	0.1093	0.1093
SrO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0029	0.0029	0.0029	0.0029
ZrO_2	0.0006	0.0000	0.0000	0.0000	0.0000	0.0026	0.0098	0.0098	0.0098	0.0098
TiO_2	0.0100	0.0101	0.0055	0.0000	0.0000	0.0000	0.0271	0.0271	0.0271	0.0271
K_2O	0.0193	0.0395	0.0187	0.0255	0.0041	0.0000	0.0000	0.0000	0.0000	0.0000
Cs_2O	0.0000	0.0003	0.0001	0.0000	0.0000	0.0000	0.0028	0.0028	0.0028	0.0028
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0031	0.0031	0.0031	0.0031
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0119	0.0119	0.0119	0.0119
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0004	0.0008	0.0007	0.0000	0.0092	0.0000	0.0029	0.0029	0.0029	0.0029
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0056	0.0056	0.0056	0.0056
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0078	0.0078	0.0078	0.0078
ZnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0121	0.0121	0.0121	0.0121
CuO	0.0000	0.0054	0.0032	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.380	0.320	0.195	0.575	0.055	0.420	0.290	0.295	0.240	0.250
PCT Li	0.410	0.255	0.195	0.485	0.005	0.365	0.375	0.280	0.285	0.295
PCT Na	0.435	0.370	0.260	0.505	0.075	0.410	0.345	0.235	0.255	0.260

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	ARM1-5/91	ARM1-10/91	ARM1-10/92	ARM1-4/93	ARM1-6/93	ARM1-8/93	ARM1-12/91	TARM1-1/92	SSARM1-A	SSARM1-B
Al_2O_3	0.0369	0.0369	0.0369	0.0369	0.0369	0.0369	0.0369	0.0369	0.0369	0.0369
CaO	0.0268	0.0268	0.0268	0.0268	0.0268	0.0268	0.0268	0.0268	0.0268	0.0268
Fe_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
FeO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MgO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Na_2O	0.1051	0.1051	0.1051	0.1051	0.1051	0.1051	0.1051	0.1051	0.1051	0.1051
Li_2O	0.1145	0.1145	0.1145	0.1145	0.1145	0.1145	0.1145	0.1145	0.1145	0.1145
NiO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SiO_2	0.5213	0.5213	0.5213	0.5213	0.5213	0.5213	0.5213	0.5213	0.5213	0.5213
Cr_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
B_2O_3	0.1093	0.1093	0.1093	0.1093	0.1093	0.1093	0.1093	0.1093	0.1093	0.1093
SrO	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029
ZrO_2	0.0098	0.0098	0.0098	0.0098	0.0098	0.0098	0.0098	0.0098	0.0098	0.0098
TiO_2	0.0271	0.0271	0.0271	0.0271	0.0271	0.0271	0.0271	0.0271	0.0271	0.0271
K_2O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cs_2O	0.0028	0.0028	0.0028	0.0028	0.0028	0.0028	0.0028	0.0028	0.0028	0.0028
P_2O_5	0.0031	0.0031	0.0031	0.0031	0.0031	0.0031	0.0031	0.0031	0.0031	0.0031
Nd_2O_3	0.0119	0.0119	0.0119	0.0119	0.0119	0.0119	0.0119	0.0119	0.0119	0.0119
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0056	0.0056	0.0056	0.0056	0.0056	0.0056	0.0056	0.0056	0.0056	0.0056
MoO_3	0.0078	0.0078	0.0078	0.0078	0.0078	0.0078	0.0078	0.0078	0.0078	0.0078
ZnO	0.0121	0.0121	0.0121	0.0121	0.0121	0.0121	0.0121	0.0121	0.0121	0.0121
CuO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.270	0.255	0.220	0.240	0.235	0.205	0.255	0.245	0.265	0.270
PCT Li	0.315	0.300	0.250	0.290	0.260	0.235	0.300	0.300	0.315	0.320
PCT Na	0.270	0.270	0.225	0.250	0.240	0.215	0.255	0.265	0.275	0.280

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	EA1-7A	EA-1-7B	EA-2-7	EA-7	T-EA	SS-EA-19	SS-EA-15	SS-EA-1-7	SS-EA-2-7
Al_2O_3	0.0228	0.0228	0.0228	0.0228	0.0228	0.0228	0.0228	0.0228	0.0228
CaO	0.0125	0.0125	0.0125	0.0125	0.0125	0.0125	0.0125	0.0125	0.0125
Fe_2O_3	0.0290	0.0290	0.0290	0.0290	0.0290	0.0290	0.0290	0.0290	0.0290
FeO	0.0127	0.0127	0.0127	0.0127	0.0127	0.0127	0.0127	0.0127	0.0127
MgO	0.0268	0.0268	0.0268	0.0268	0.0268	0.0268	0.0268	0.0268	0.0268
MnO	0.0119	0.0119	0.0119	0.0119	0.0119	0.0119	0.0119	0.0119	0.0119
Na_2O	0.1702	0.1702	0.1702	0.1702	0.1702	0.1702	0.1702	0.1702	0.1702
Li_2O	0.0895	0.0895	0.0895	0.0895	0.0895	0.0895	0.0895	0.0895	0.0895
NiO	0.0048	0.0048	0.0048	0.0048	0.0048	0.0048	0.0048	0.0048	0.0048
SiO_2	0.5091	0.5091	0.5091	0.5091	0.5091	0.5091	0.5091	0.5091	0.5091
Cr_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
B_2O_3	0.1019	0.1019	0.1019	0.1019	0.1019	0.1019	0.1019	0.1019	0.1019
SrO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZrO_2	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023	0.0023
TiO_2	0.0055	0.0055	0.0055	0.0055	0.0055	0.0055	0.0055	0.0055	0.0055
K_2O	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003
Cs_2O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
La_2O_3	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008
BaO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CuO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	7.000	8.395	7.605	8.860	7.375	8.205	8.395	9.250	8.880
PCT Li	3.925	5.345	4.715	4.945	4.260	4.560	4.870	5.140	4.885
PCT Na	5.760	7.245	6.390	6.945	5.910	6.545	6.800	7.165	6.860

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	SRS-SEA-A	SRS-SEA-B	CUASEA-A	CUASEA-B	TDS131-EA	TDS131-SOP	BLEND1-7A	BLEND1-7B	BLEND1.6	BATCH1-7A
Al_2O_3	0.0228	0.0228	0.0228	0.0228	0.0371	0.0350	0.0266	0.0266	0.0266	0.0316
CaO	0.0125	0.0125	0.0125	0.0125	0.0108	0.0106	0.0120	0.0120	0.0120	0.0144
Fe_2O_3	0.0290	0.0290	0.0290	0.0290	0.0588	0.0462	0.0445	0.0445	0.0445	0.0531
FeO	0.0127	0.0127	0.0127	0.0127	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MgO	0.0268	0.0268	0.0268	0.0268	0.0249	0.0226	0.0228	0.0228	0.0228	0.0233
MnO	0.0119	0.0119	0.0119	0.0119	0.0293	0.0307	0.0154	0.0154	0.0154	0.0160
Na_2O	0.1702	0.1702	0.1702	0.1702	0.1546	0.1431	0.0960	0.0960	0.0960	0.0960
Li_2O	0.0895	0.0895	0.0895	0.0895	0.1061	0.0912	0.0969	0.0969	0.0969	0.0980
NiO	0.0048	0.0048	0.0048	0.0048	0.0127	0.0133	0.0078	0.0078	0.0078	0.0066
SiO_2	0.5091	0.5091	0.5091	0.5091	0.4348	0.4977	0.5630	0.5630	0.5630	0.5522
Cr_2O_3	0.0000	0.0000	0.0000	0.0000	0.0002	0.0005	0.0006	0.0006	0.0006	0.0005
B_2O_3	0.1019	0.1019	0.1019	0.1019	0.1197	0.1004	0.0754	0.0754	0.0754	0.0739
SrO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZrO_2	0.0023	0.0023	0.0023	0.0023	0.0023	0.0018	0.0007	0.0007	0.0007	0.0005
TiO_2	0.0055	0.0055	0.0055	0.0055	0.0076	0.0060	0.0073	0.0073	0.0073	0.0056
K_2O	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0255	0.0255	0.0255	0.0234
Cs_2O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002	0.0002	0.0002	0.0001
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0004	0.0004	0.0004	0.0003
La_2O_3	0.0008	0.0008	0.0008	0.0008	0.0007	0.0007	0.0000	0.0000	0.0000	0.0000
BaO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0008	0.0008	0.0006
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0007	0.0007	0.0007	0.0005
ZnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CuO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0036	0.0036	0.0036	0.0033
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	8.225	8.495	8.425	8.230	2.215	1.405	0.360	0.390	0.360	0.365
PCT Li	4.670	4.560	4.835	4.605	1.925	1.225	0.405	0.400	0.380	0.405
PCT Na	6.425	6.755	6.475	6.710	2.140	1.150	0.390	0.395	0.375	0.400

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	BATCH1-7B	BATCH1-1.6	BATCH2-7A	BATCH2-7B	BATCH2-1.6	BATCH3-7A	BATCH3-7B	BATCH3-1.6	BATCH4-7A	BATCH4-7B
Al_2O_3	0.0316	0.0316	0.0296	0.0296	0.0296	0.0220	0.0220	0.0220	0.0222	0.0222
CaO	0.0144	0.0144	0.0125	0.0125	0.0125	0.0115	0.0115	0.0115	0.0099	0.0099
Fe_2O_3	0.0531	0.0531	0.0453	0.0453	0.0453	0.0479	0.0479	0.0479	0.0484	0.0484
FeO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MgO	0.0233	0.0233	0.0229	0.0229	0.0229	0.0230	0.0230	0.0230	0.0234	0.0234
MnO	0.0160	0.0160	0.0129	0.0129	0.0129	0.0140	0.0140	0.0140	0.0236	0.0236
Na_2O	0.0960	0.0960	0.0967	0.0967	0.0967	0.0949	0.0949	0.0949	0.0975	0.0975
Li_2O	0.0980	0.0980	0.0980	0.0980	0.0980	0.0985	0.0985	0.0985	0.0947	0.0947
NiO	0.0066	0.0066	0.0078	0.0078	0.0078	0.0092	0.0092	0.0092	0.0094	0.0094
SiO_2	0.5522	0.5522	0.5645	0.5645	0.5645	0.5714	0.5714	0.5714	0.5499	0.5499
Cr_2O_3	0.0005	0.0005	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006
B_2O_3	0.0739	0.0739	0.0737	0.0737	0.0737	0.0721	0.0721	0.0721	0.0771	0.0771
SrO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZrO_2	0.0005	0.0005	0.0009	0.0009	0.0009	0.0006	0.0006	0.0006	0.0012	0.0012
TiO_2	0.0056	0.0056	0.0056	0.0056	0.0056	0.0056	0.0056	0.0056	0.0085	0.0085
K_2O	0.0234	0.0234	0.0234	0.0234	0.0234	0.0236	0.0236	0.0236	0.0270	0.0270
Cs_2O	0.0001	0.0001	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0002	0.0002
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nd_2O_3	0.0003	0.0003	0.0005	0.0005	0.0005	0.0003	0.0003	0.0003	0.0008	0.0008
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0006	0.0006	0.0007	0.0007	0.0007	0.0008	0.0008	0.0008	0.0011	0.0011
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0005	0.0005	0.0008	0.0008	0.0008	0.0005	0.0005	0.0005	0.0009	0.0009
ZnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CuO	0.0033	0.0033	0.0034	0.0034	0.0034	0.0033	0.0033	0.0033	0.0037	0.0037
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.365	0.355	0.330	0.335	0.320	0.430	0.445	0.425	0.485	0.450
PCT Li	0.380	0.380	0.385	0.360	0.355	0.450	0.425	0.425	0.500	0.445
PCT Na	0.375	0.370	0.365	0.345	0.335	0.445	0.425	0.415	0.500	0.435

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	BATCH4-1.6	HM-1-7A	HM-1-7B	HM-1-1.6	PUREX-1A	PUREX-1B	PUREX-1.6	PUREX-S1.6	PUREX-S4.0	PUREX-CUA
Al_2O_3	0.0222	0.0447	0.0447	0.0447	0.0196	0.0196	0.0196	0.0196	0.0196	0.0196
CaO	0.0099	0.0115	0.0115	0.0115	0.0130	0.0130	0.0130	0.0130	0.0130	0.0130
Fe_2O_3	0.0484	0.0311	0.0311	0.0311	0.0555	0.0555	0.0555	0.0555	0.0555	0.0555
FeO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MgO	0.0234	0.0236	0.0236	0.0236	0.0234	0.0234	0.0234	0.0234	0.0234	0.0234
MnO	0.0236	0.0158	0.0158	0.0158	0.0159	0.0159	0.0159	0.0159	0.0159	0.0159
Na_2O	0.0975	0.0881	0.0881	0.0881	0.1363	0.1363	0.1363	0.1363	0.1363	0.1363
Li_2O	0.0947	0.0986	0.0986	0.0986	0.0721	0.0721	0.0721	0.0721	0.0721	0.0721
NiO	0.0094	0.0035	0.0035	0.0035	0.0107	0.0107	0.0107	0.0107	0.0107	0.0107
SiO_2	0.5499	0.5925	0.5925	0.5925	0.5181	0.5181	0.5181	0.5181	0.5181	0.5181
Cr_2O_3	0.0006	0.0004	0.0004	0.0004	0.0007	0.0007	0.0007	0.0007	0.0007	0.0007
B_2O_3	0.0771	0.0644	0.0644	0.0644	0.0993	0.0993	0.0993	0.0993	0.0993	0.0993
SrO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZrO_2	0.0012	0.0017	0.0017	0.0017	0.0002	0.0002	0.0002	0.0002	0.0002	0.0002
TiO_2	0.0085	0.0045	0.0045	0.0045	0.0057	0.0057	0.0057	0.0057	0.0057	0.0057
K_2O	0.0270	0.0150	0.0150	0.0150	0.0242	0.0242	0.0242	0.0242	0.0242	0.0242
Cs_2O	0.0002	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nd_2O_3	0.0008	0.0010	0.0010	0.0010	0.0001	0.0001	0.0001	0.0001	0.0001	0.0001
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0011	0.0005	0.0005	0.0005	0.0009	0.0009	0.0009	0.0009	0.0009	0.0009
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0009	0.0010	0.0010	0.0010	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004
ZnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CuO	0.0037	0.0020	0.0020	0.0020	0.0035	0.0035	0.0035	0.0035	0.0035	0.0035
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.470	0.230	0.230	0.215	1.095	0.985	2.230	1.190	1.130	1.425
PCT Li	0.470	0.310	0.285	0.280	0.930	0.825	1.625	1.020	0.980	1.185
PCT Na	0.470	0.245	0.230	0.220	1.045	0.880	2.130	1.040	0.995	1.210

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	BND1-3457	BND1-3479	BND1-3498	BND1-3510	BND1-3526	BND2-3611	BND2-3622	BND2-3635	BND2-3654	BND2-3666
Al_2O_3	0.0346	0.0345	0.0346	0.0351	0.0332	0.0334	0.0323	0.0325	0.0317	0.0319
CaO	0.0131	0.0127	0.0130	0.0130	0.0127	0.0115	0.0107	0.0107	0.0104	0.0104
Fe_2O_3	0.0529	0.0520	0.0533	0.0541	0.0518	0.0502	0.0488	0.0476	0.0479	0.0483
FeO	0.0005	0.0015	0.0008	0.0008	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000
MgO	0.0212	0.0210	0.0208	0.0208	0.0207	0.0216	0.0214	0.0215	0.0213	0.0217
MnO	0.0199	0.0203	0.0211	0.0212	0.0206	0.0200	0.0199	0.0197	0.0199	0.0201
Na_2O	0.1083	0.1072	0.1165	0.1158	0.1167	0.1091	0.1093	0.1098	0.1122	0.1109
Li_2O	0.0939	0.0943	0.0930	0.0927	0.0937	0.0942	0.0950	0.0953	0.0945	0.0958
NiO	0.0074	0.0076	0.0082	0.0080	0.0086	0.0085	0.0084	0.0082	0.0085	0.0084
SiO_2	0.5590	0.5594	0.5476	0.5460	0.5474	0.5664	0.5684	0.5686	0.5677	0.5668
Cr_2O_3	0.0010	0.0010	0.0010	0.0010	0.0009	0.0011	0.0010	0.0010	0.0010	0.0011
B_2O_3	0.0661	0.0665	0.0670	0.0666	0.0686	0.0639	0.0652	0.0647	0.0646	0.0652
SrO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZrO_2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
TiO_2	0.0020	0.0019	0.0017	0.0016	0.0015	0.0014	0.0013	0.0014	0.0012	0.0012
K_2O	0.0178	0.0182	0.0193	0.0212	0.0207	0.0167	0.0166	0.0170	0.0172	0.0164
Cs_2O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CuO	0.0018	0.0015	0.0016	0.0016	0.0015	0.0014	0.0014	0.0014	0.0014	0.0014
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.300	0.290	0.315	0.340	0.335	0.305	0.305	0.305	0.300	0.300
PCT Li	0.335	0.320	0.350	0.370	0.370	0.335	0.330	0.325	0.325	0.325
PCT Na	0.325	0.315	0.335	0.365	0.360	0.335	0.330	0.330	0.320	0.320

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	BND2-3676	BND3-3768	BND3-3789	BND3-3793	BND3-3802	HM1-3824	HM1-3829	HM1-3851	HM1-3855	HM2-3979
Al_2O_3	0.0313	0.0323	0.0347	0.0362	0.0362	0.0363	0.0388	0.0393	0.0416	0.0475
CaO	0.0100	0.0106	0.0121	0.0130	0.0127	0.0108	0.0106	0.0107	0.0098	0.0086
Fe_2O_3	0.0473	0.0477	0.0513	0.0538	0.0537	0.0439	0.0444	0.0431	0.0396	0.0401
FeO	0.0000	0.0010	0.0010	0.0009	0.0023	0.0020	0.0017	0.0016	0.0019	0.0000
MgO	0.0215	0.0227	0.0231	0.0232	0.0233	0.0260	0.0262	0.0265	0.0262	0.0247
MnO	0.0196	0.0210	0.0230	0.0239	0.0239	0.0224	0.0236	0.0236	0.0242	0.0249
Na_2O	0.1103	0.1117	0.1125	0.1134	0.1095	0.1029	0.0989	0.1048	0.1052	0.1060
Li_2O	0.0963	0.0976	0.0957	0.0940	0.0941	0.0985	0.0983	0.0980	0.0986	0.0948
NiO	0.0083	0.0085	0.0088	0.0089	0.0087	0.0068	0.0068	0.0067	0.0059	0.0059
SiO_2	0.5696	0.5602	0.5481	0.5410	0.5439	0.5695	0.5727	0.5706	0.5737	0.5685
Cr_2O_3	0.0010	0.0013	0.0011	0.0011	0.0011	0.0010	0.0010	0.0010	0.0009	0.0021
B_2O_3	0.0656	0.0660	0.0675	0.0681	0.0677	0.0642	0.0628	0.0617	0.0607	0.0616
SrO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009
ZrO_2	0.0000	0.0003	0.0002	0.0002	0.0002	0.0001	0.0002	0.0002	0.0001	0.0004
TiO_2	0.0012	0.0011	0.0011	0.0010	0.0010	0.0007	0.0008	0.0007	0.0007	0.0007
K_2O	0.0161	0.0161	0.0176	0.0186	0.0193	0.0132	0.0116	0.0099	0.0094	0.0109
Cs_2O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0004	0.0005	0.0006	0.0006	0.0006	0.0004	0.0004	0.0004	0.0004	0.0004
PbO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0002
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZnO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008
CuO	0.0014	0.0016	0.0017	0.0019	0.0018	0.0012	0.0012	0.0012	0.0011	0.0011
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.295	0.300	0.315	0.315	0.350	0.295	0.285	0.260	0.265	0.265
PCT Li	0.320	0.320	0.330	0.330	0.355	0.315	0.315	0.300	0.300	0.305
PCT Na	0.315	0.330	0.350	0.355	0.385	0.310	0.305	0.275	0.275	0.270

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	HM2-4099	HM2-4120	HM3-4176	HM3-4225	HM3-4357	HM4-5260	HM4-5641	HM4-5748	PX1-4643	PX1-4726
Al_2O_3	0.0488	0.0471	0.0491	0.0548	0.0583	0.0333	0.0395	0.0352	0.0340	0.0313
CaO	0.0083	0.0080	0.0079	0.0086	0.0091	0.0057	0.0057	0.0056	0.0172	0.0172
Fe_2O_3	0.0401	0.0377	0.0385	0.0408	0.0427	0.0340	0.0320	0.0289	0.0436	0.0450
FeO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MgO	0.0243	0.0244	0.0238	0.0249	0.0256	0.0141	0.0168	0.0184	0.0239	0.0230
MnO	0.0251	0.0241	0.0233	0.0257	0.0271	0.0136	0.0150	0.0148	0.0289	0.0296
Na_2O	0.1083	0.1090	0.1129	0.1111	0.1065	0.0981	0.0963	0.0956	0.1039	0.1040
Li_2O	0.0943	0.0995	0.0900	0.0929	0.0922	0.0958	0.0929	0.0942	0.0948	0.0934
NiO	0.0057	0.0052	0.0050	0.0051	0.0053	0.0053	0.0084	0.0044	0.0141	0.0147
SiO_2	0.5639	0.5632	0.5685	0.5520	0.5480	0.5789	0.5779	0.5947	0.5412	0.5417
Cr_2O_3	0.0020	0.0017	0.0017	0.0017	0.0018	0.0019	0.0028	0.0016	0.0020	0.0023
B_2O_3	0.0619	0.0622	0.0600	0.0626	0.0630	0.0919	0.0849	0.0802	0.0693	0.0680
SrO	0.0010	0.0009	0.0009	0.0009	0.0010	0.0005	0.0005	0.0005	0.0002	0.0002
ZrO_2	0.0003	0.0004	0.0003	0.0003	0.0004	0.0062	0.0036	0.0023	0.0004	0.0004
TiO_2	0.0010	0.0008	0.0008	0.0008	0.0008	0.0020	0.0021	0.0020	0.0014	0.0030
K_2O	0.0125	0.0132	0.0149	0.0153	0.0157	0.0160	0.0184	0.0188	0.0202	0.0207
Cs_2O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0001
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0004	0.0004	0.0003	0.0004	0.0004	0.0002	0.0002	0.0002	0.0008	0.0008
PbO	0.0002	0.0002	0.0001	0.0001	0.0001	0.0003	0.0002	0.0001	0.0005	0.0005
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003	0.0002	0.0001	0.0000	0.0000
ZnO	0.0008	0.0007	0.0007	0.0007	0.0007	0.0009	0.0009	0.0008	0.0013	0.0014
CuO	0.0012	0.0011	0.0012	0.0013	0.0013	0.0008	0.0016	0.0015	0.0025	0.0026
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.275	0.265	0.280	0.275	0.255	0.375	0.265	0.350	0.360	0.355
PCT Li	0.315	0.310	0.325	0.320	0.295	0.380	0.285	0.355	0.390	0.380
PCT Na	0.280	0.270	0.265	0.260	0.265	0.320	0.260	0.325	0.365	0.360

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Table A.10. SRTC Homogeneous Glass Compositions (mole fractions) and PCT Normalized B, Li, and Na Releases (g/m^2) (continued)

Comp.	PX1-4776	PX2-4455	PX2-4509	PX2-4566	MG-9	MG-18	MG-25	MG-28
Al_2O_3	0.0274	0.0538	0.0446	0.0385	0.0012	0.0057	0.0876	0.1016
CaO	0.0152	0.0091	0.0133	0.0170	0.1001	0.1027	0.0370	0.0000
Fe_2O_3	0.0402	0.0384	0.0450	0.0448	0.0000	0.0000	0.0355	0.0496
FeO	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0111	0.0212
MgO	0.0235	0.0254	0.0252	0.0245	0.0000	0.0000	0.0000	0.0000
MnO	0.0257	0.0257	0.0280	0.0300	0.0000	0.0000	0.0000	0.0000
Na_2O	0.0993	0.1085	0.1007	0.1042	0.2543	0.2576	0.1720	0.1925
Li_2O	0.0968	0.0934	0.0944	0.0943	0.0000	0.0000	0.0000	0.0000
NiO	0.0135	0.0055	0.0103	0.0133	0.0000	0.0000	0.0000	0.0000
SiO_2	0.5619	0.5558	0.5458	0.5335	0.5953	0.4912	0.5212	0.5412
Cr_2O_3	0.0022	0.0017	0.0020	0.0020	0.0000	0.0000	0.0000	0.0000
B_2O_3	0.0671	0.0635	0.0675	0.0698	0.0491	0.1428	0.1357	0.0939
SrO	0.0001	0.0009	0.0005	0.0003	0.0000	0.0000	0.0000	0.0000
ZrO_2	0.0004	0.0003	0.0003	0.0004	0.0000	0.0000	0.0000	0.0000
TiO_2	0.0029	0.0008	0.0014	0.0018	0.0000	0.0000	0.0000	0.0000
K_2O	0.0189	0.0147	0.0172	0.0210	0.0000	0.0000	0.0000	0.0000
Cs_2O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
P_2O_5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Nd_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
La_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BaO	0.0007	0.0004	0.0006	0.0008	0.0000	0.0000	0.0000	0.0000
PbO	0.0005	0.0001	0.0003	0.0004	0.0000	0.0000	0.0000	0.0000
Ce_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MoO_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ZnO	0.0013	0.0008	0.0011	0.0012	0.0000	0.0000	0.0000	0.0000
CuO	0.0023	0.0013	0.0019	0.0023	0.0000	0.0000	0.0000	0.0000
Y_2O_3	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
PCT B	0.395	0.240	0.290	0.365	35.120	28.910	0.415	0.315
PCT Li	0.415	0.285	0.325	0.390	.	.	.	.
PCT Na	0.385	0.240	0.305	0.365	28.210	23.885	0.395	0.360

Note: Glass names are those in the reference from which the data were taken, except some names have been shortened.

Appendix B

Scatterplot Matrices

This appendix contains the scatterplot matrix for each data set described in Section 4. A scatterplot matrix in this appendix consists of a matrix of scatterplots of pairs of glass components for a given data set. Because individual plots in a scatterplot matrix get quite small for larger numbers of components, only those components included in the first-order mixture model for each data set are included in the scatterplot matrix.

Various features of a data set can adversely affect property models fitted to the data set. Such features that can be detected in a scatterplot are:

(1) A component being constant or nearly constant over a data set. This indicates that it is impossible to accurately estimate the component's coefficient in empirical mixture models.

(2) A correlation between pairs of components in a scatterplot, indicated by the points having a linear appearance. The stronger such a correlation, the more difficult (and eventually impossible) it is to separate the effects of the components on glass properties using the data set. Incorrect empirical model coefficients can result if pairwise component correlations are strong enough.

(3) Clustering of points or an uneven coverage of pairwise combinations of components. Clustering of points can indicate that the data set contains points with similar combinations of components in many compositions. An uneven coverage of pairwise combinations can indicate a lack of compositions in parts of the model domain. Both of these conditions can result in a poor basis for estimating the effects of the affected components on glass properties. However, an uneven coverage can be indicative of constraints imposed in collecting the data (e.g., avoiding compositions with low SiO_2 and low Al_2O_3).

The presence or absence of any such bothersome features is discussed for each data set in the corresponding subsection of Section 4.

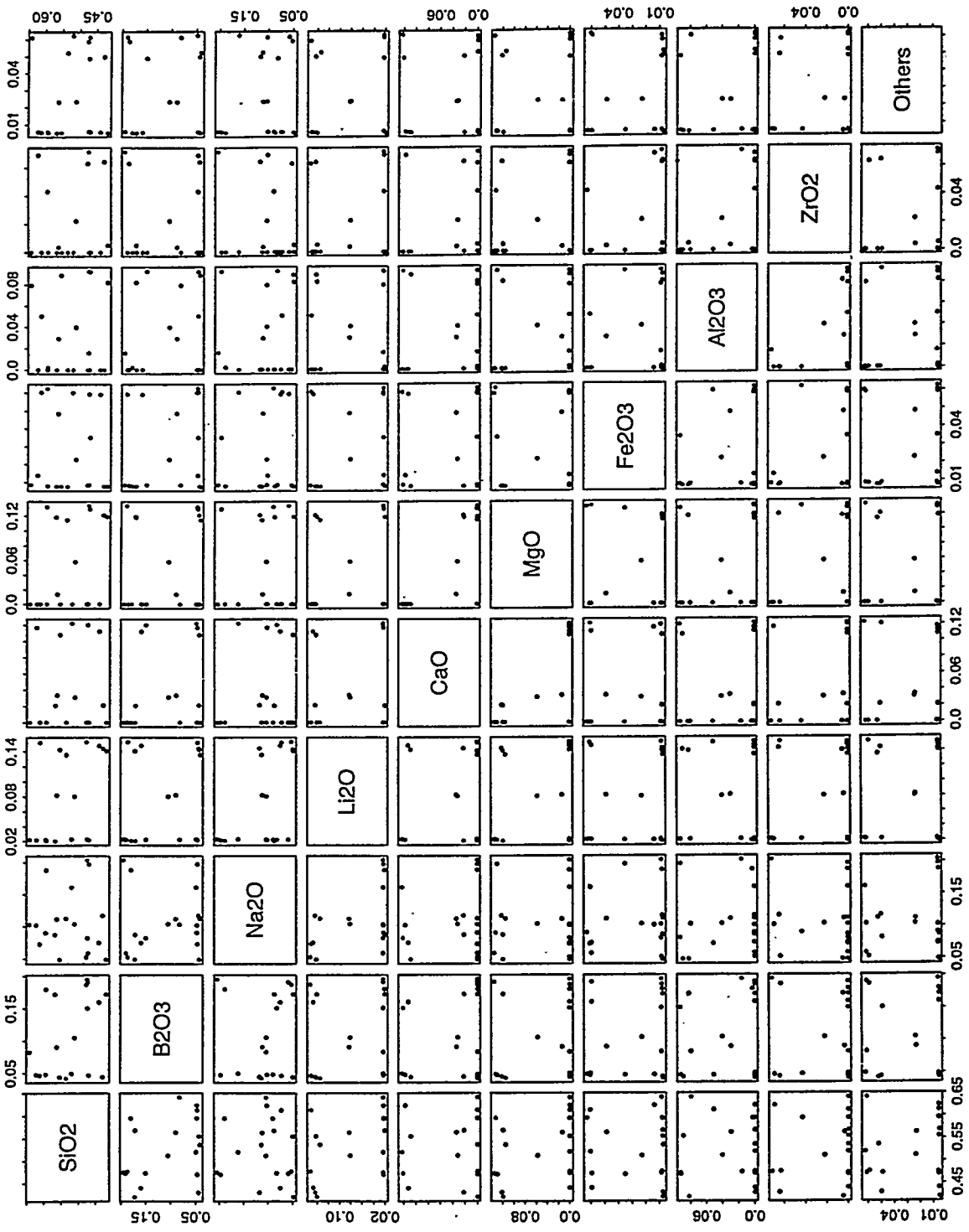

Figure B.1. Scatterplot Matrix of CVS-I Data Set Glass Compositions

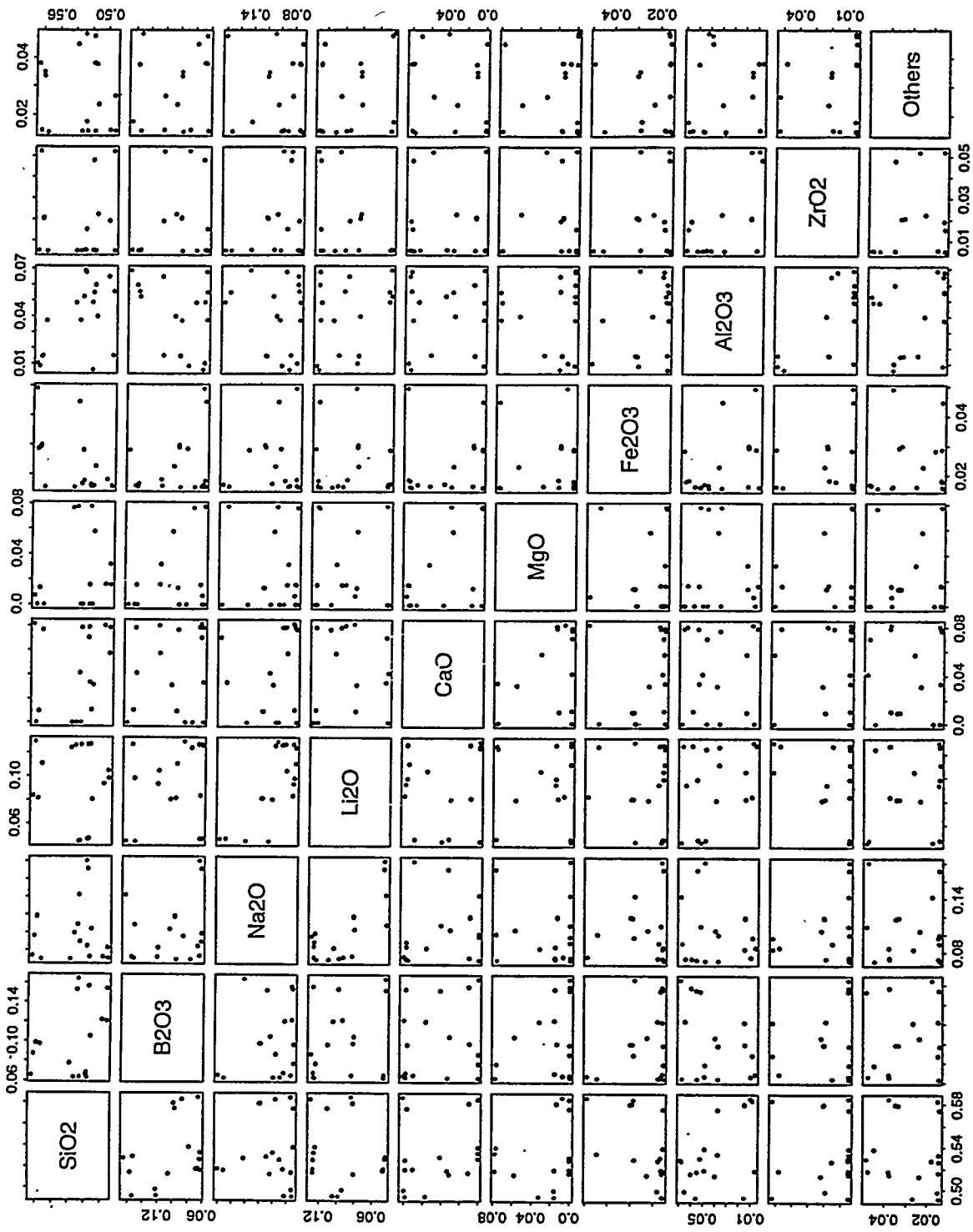

Figure B.2. Scatterplot Matrix of CVS-II Phase 1 Data Set Glass Compositions

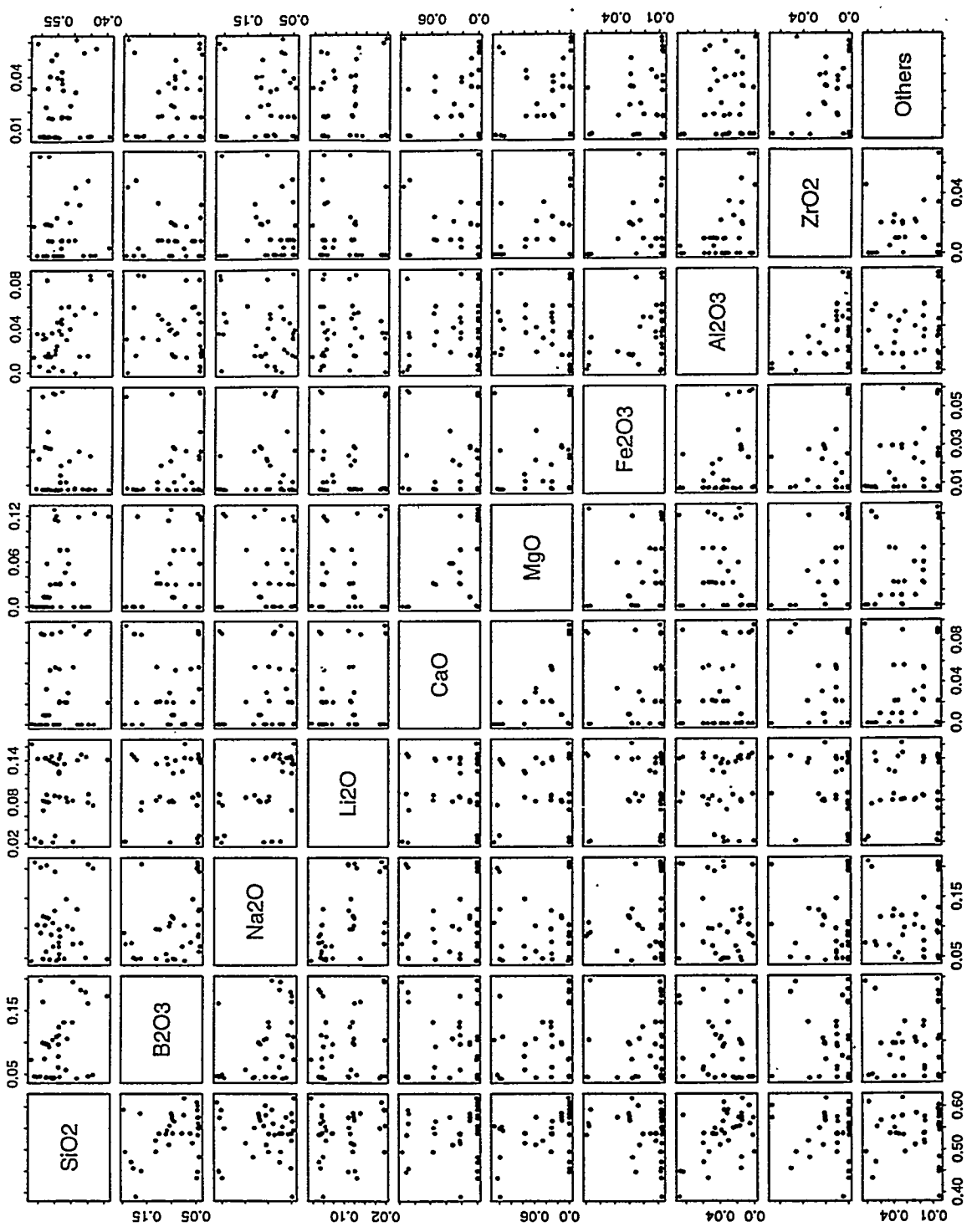

Figure B.3. Scatterplot Matrix of CVS-II Phase 2 Data Set Glass Compositions

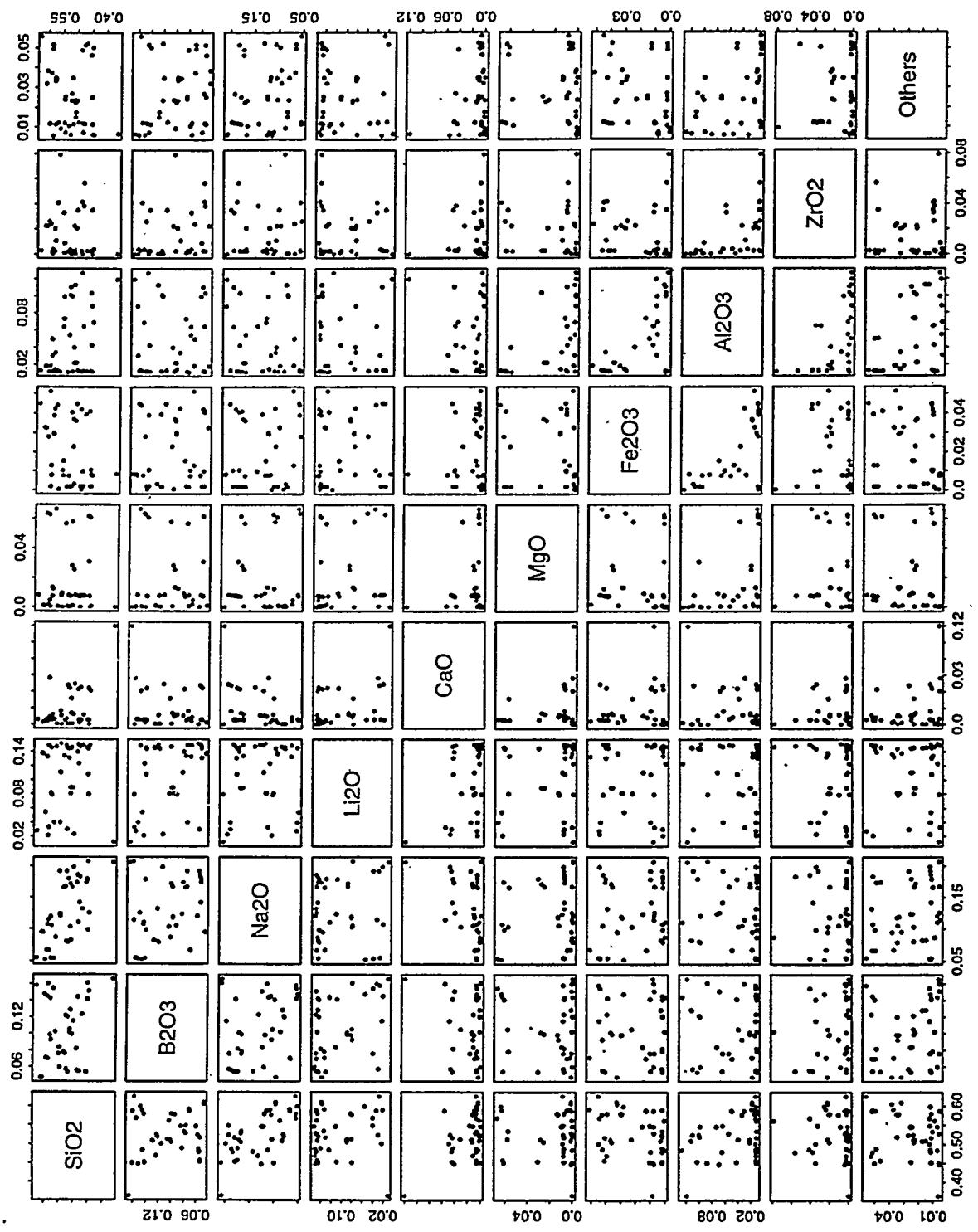

Figure B.4. Scatterplot Matrix of CVS-II Phase 3 Data Set Glass Compositions

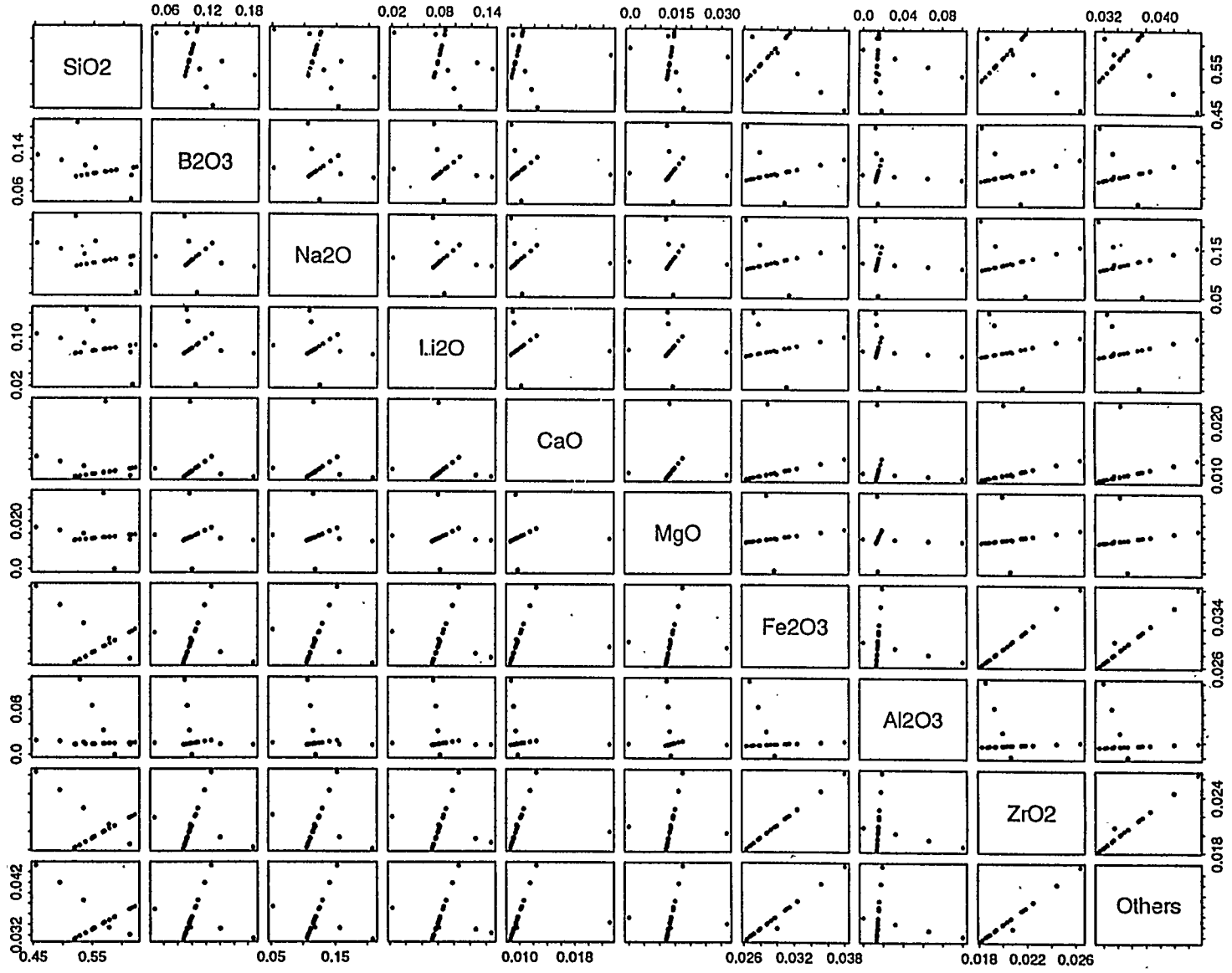

Figure B.5. Scatterplot Matrix of CVS-II Phase 4 Data Set Glass Compositions

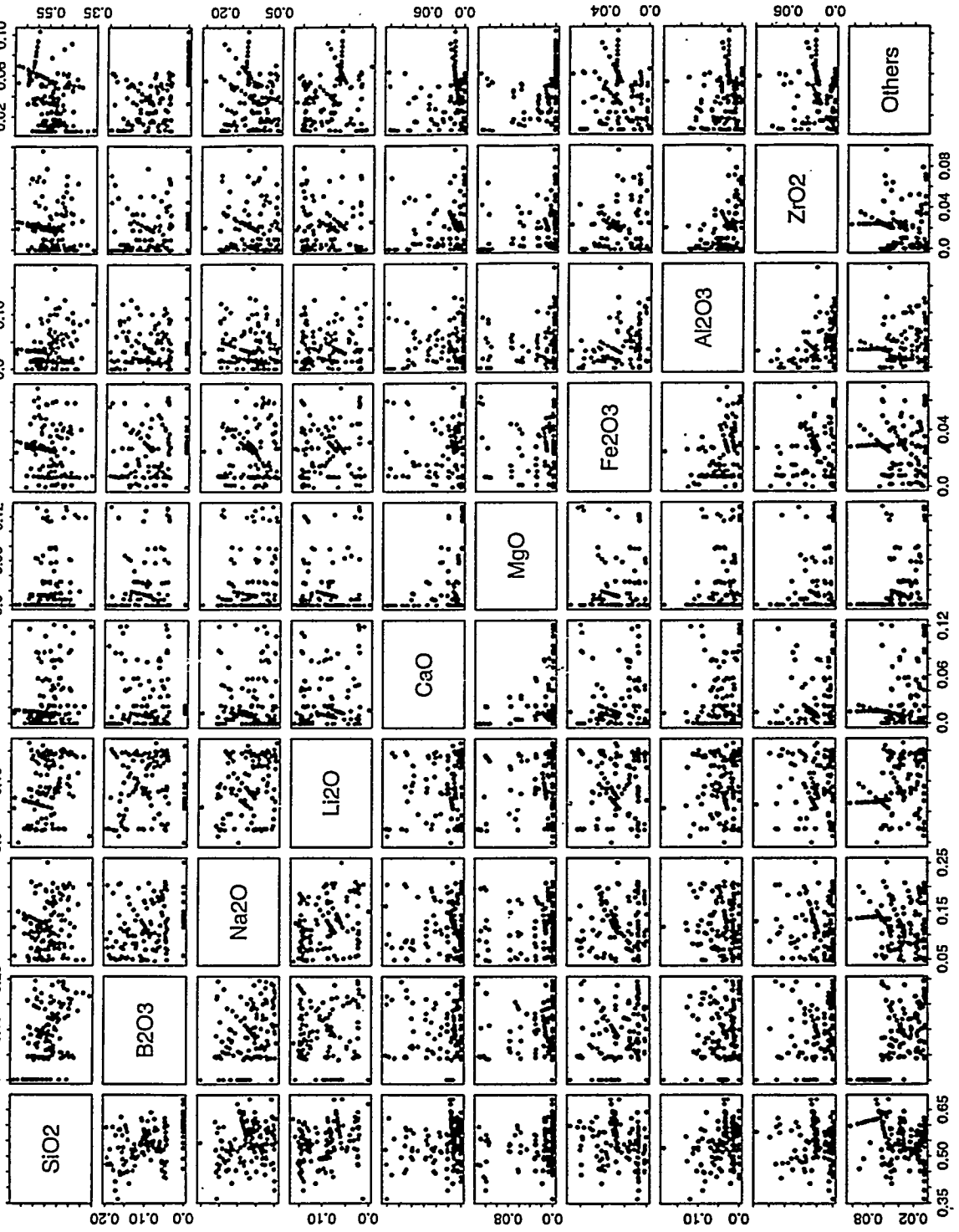

Figure B.6. Scatterplot Matrix of CVS-I and CVS-II Phases 1, 2, 3, and 4 Glass Compositions

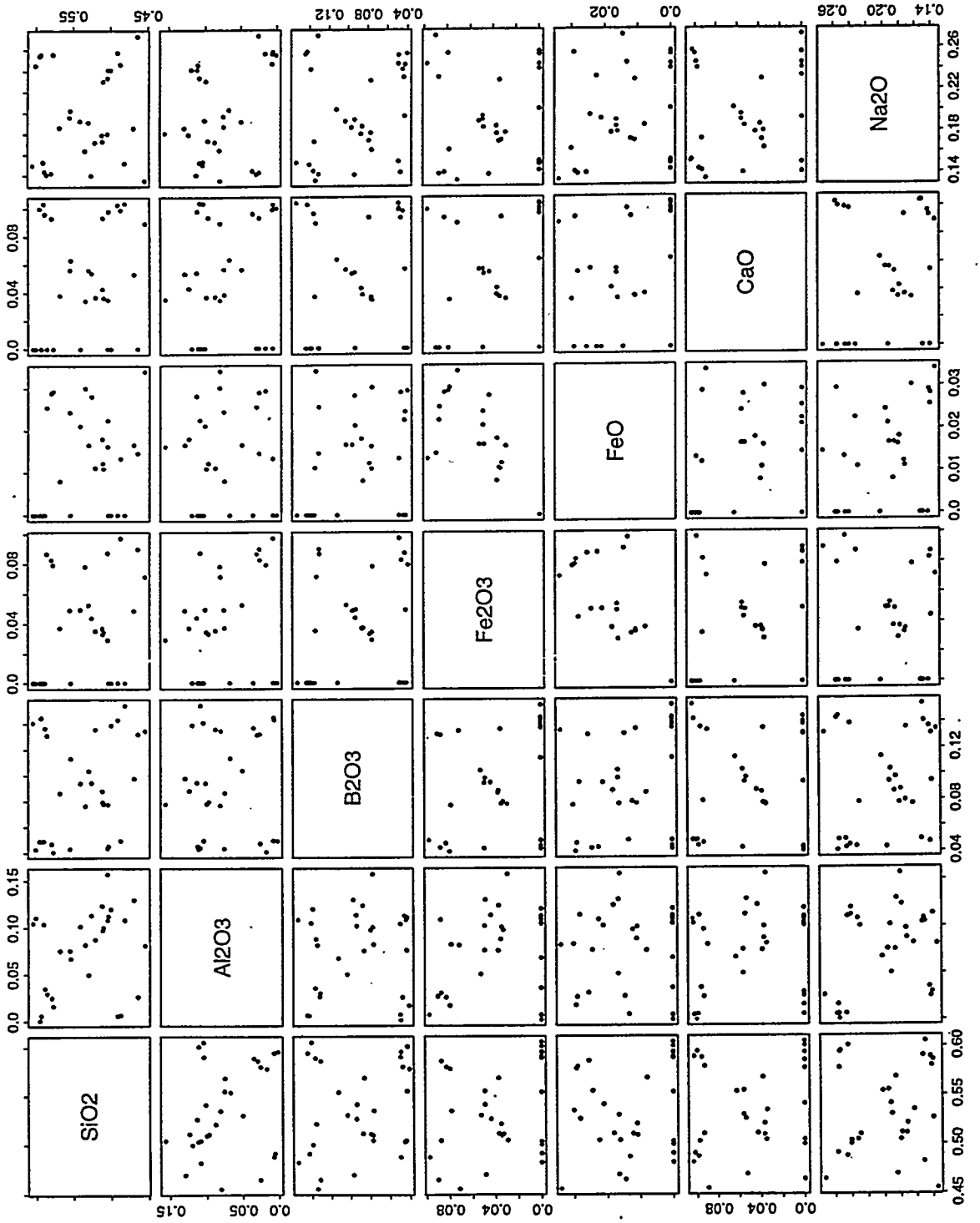

Figure B.7. Scatterplot Matrix of Ramsey Data Set Glass Compositions

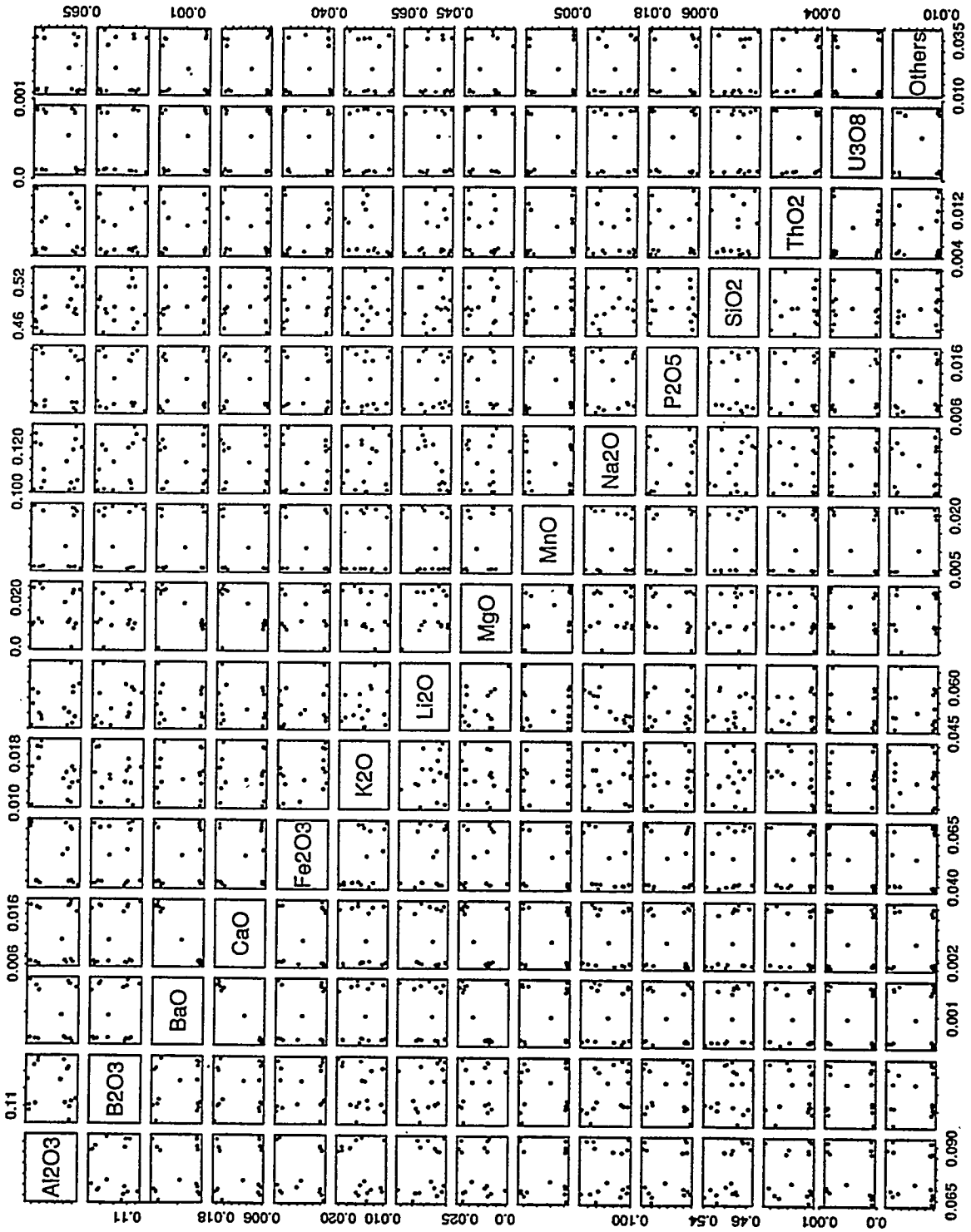

Figure B.8. Scatterplot Matrix of WV87 Data Set Glass Compositions

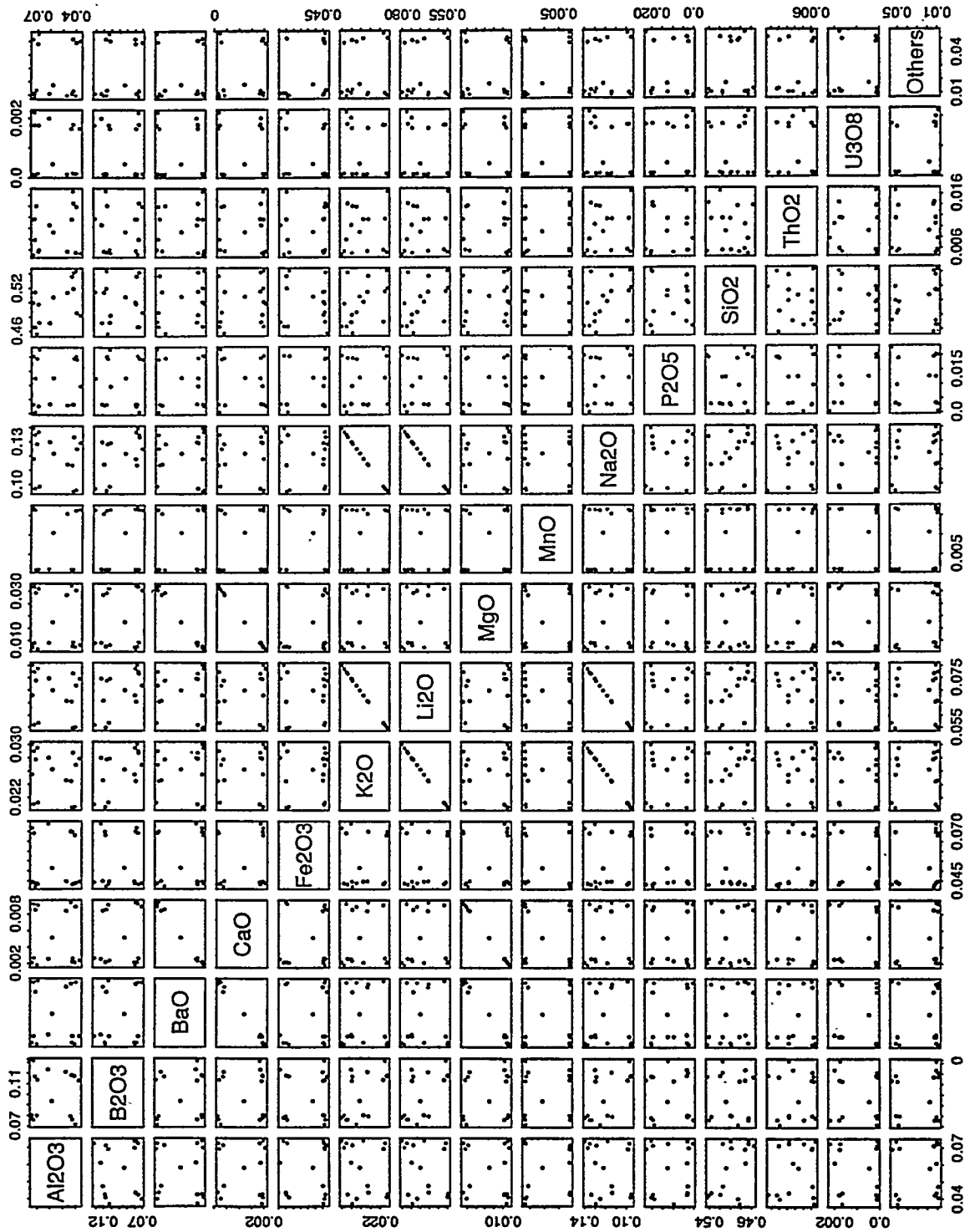

Figure B.9. Scatterplot Matrix of WV88 Data Set Glass Compositions

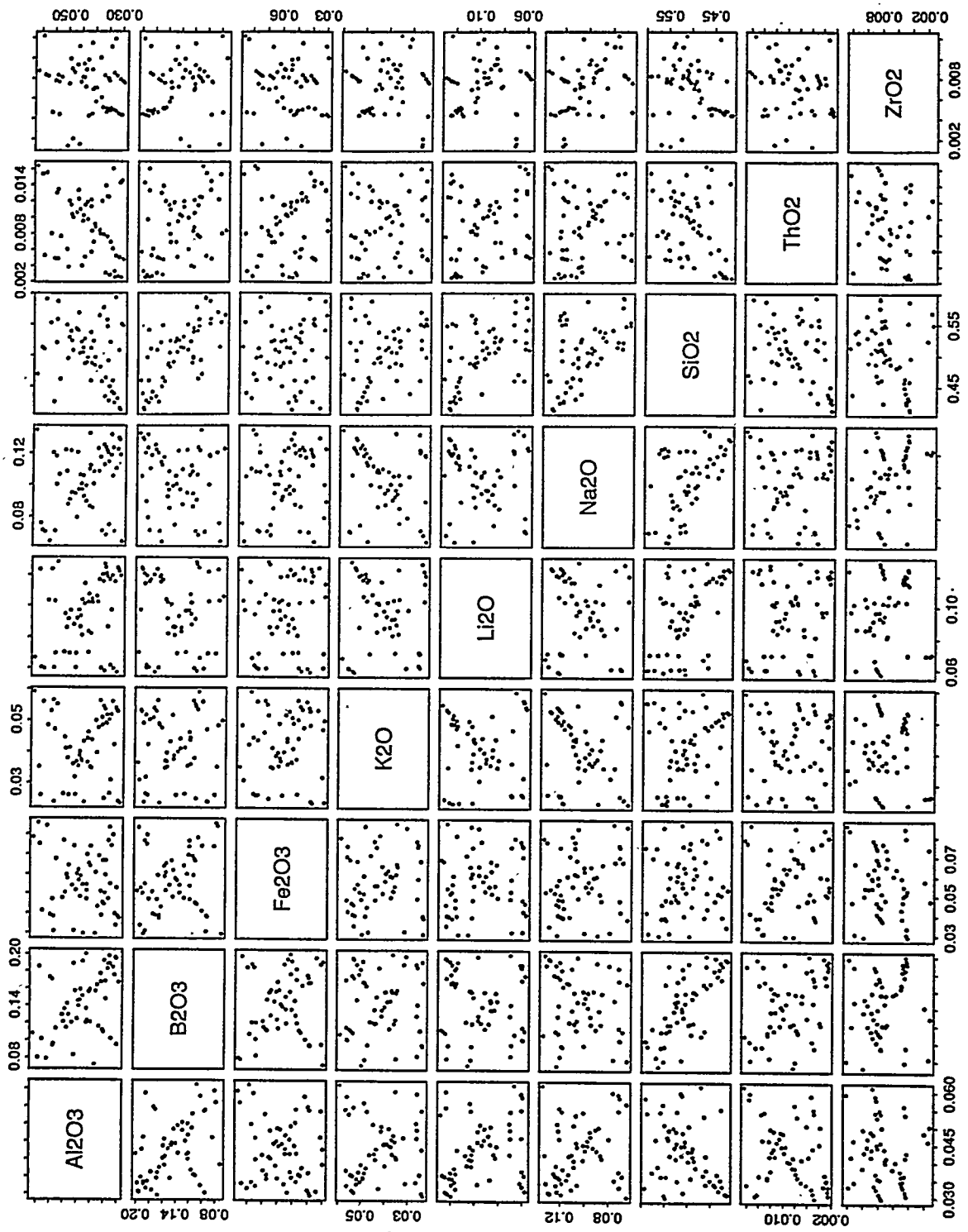

Figure B.10. Scatterplot Matrix of WVDP Data Set Glass Compositions

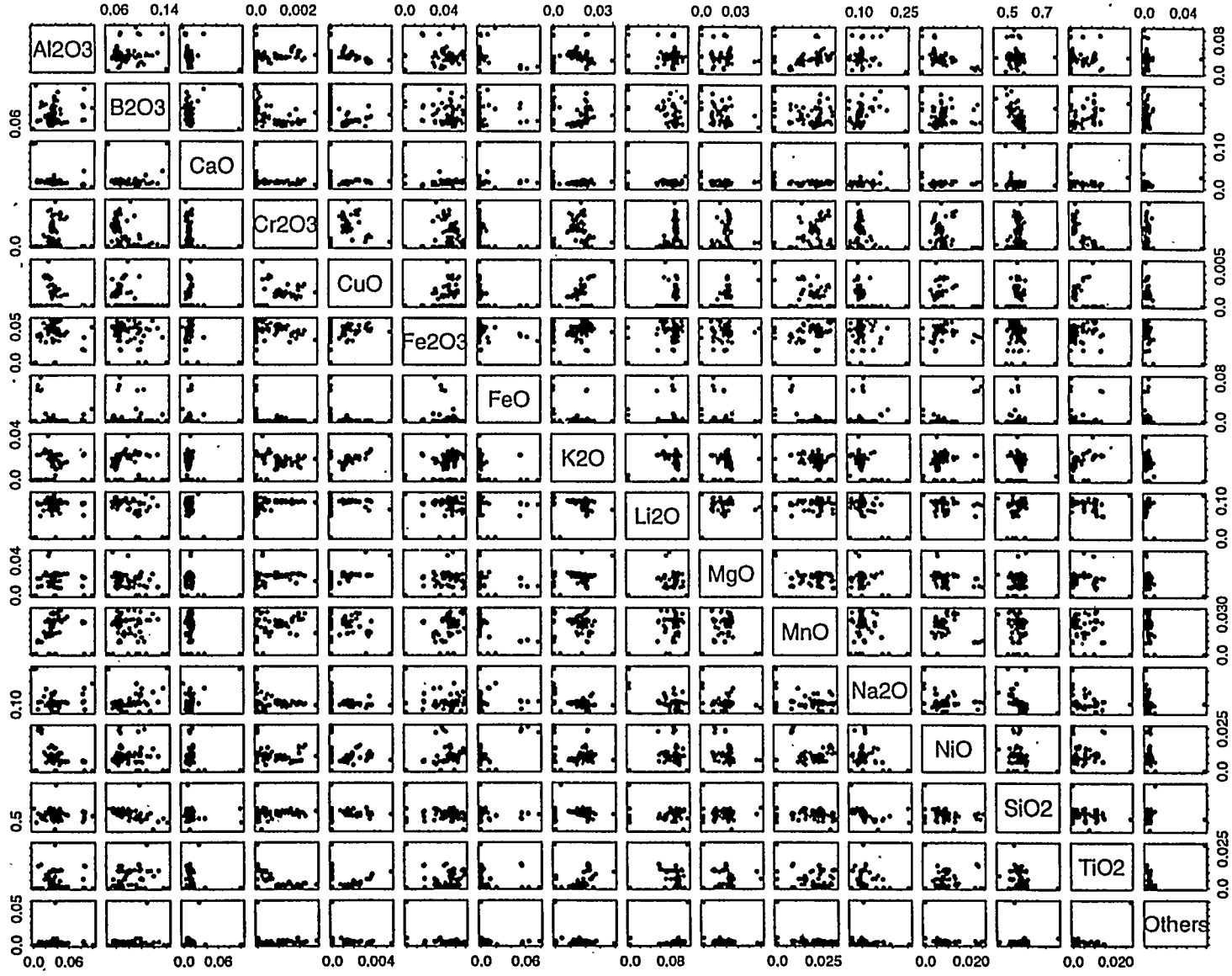

Figure B.11. Scatterplot Matrix of SRTC Homogeneous Data Set Glass Compositions (All 137 Observations)

Figure B.12. Scatterplot Matrix of SRTC Homogeneous Data Set Glass Compositions (118 Observations)

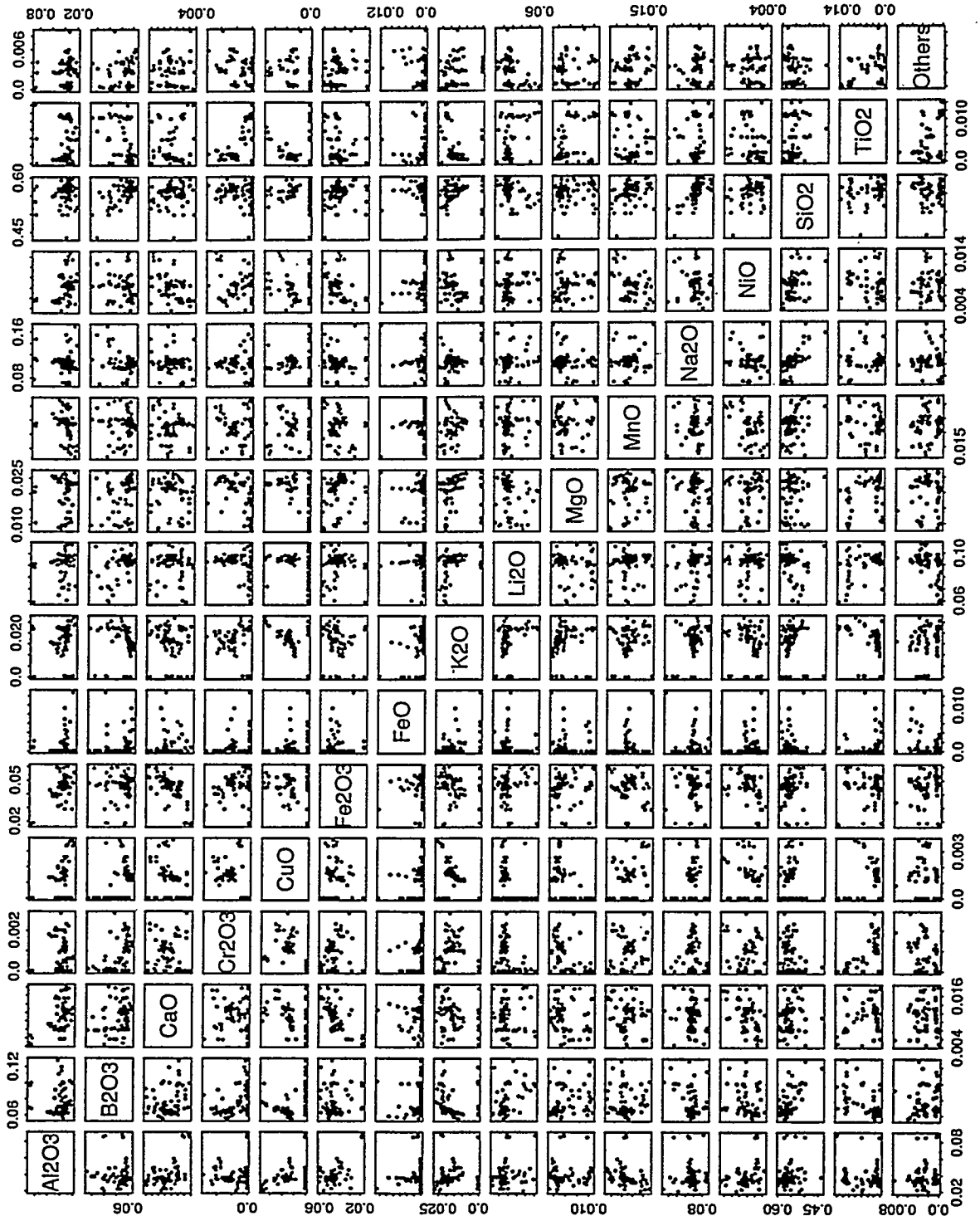

Figure B.13. Scatterplot Matrix of SRTC Homogeneous Data Set Glass Compositions (111 Observations)

Appendix C

Predicted Versus Measured Plots

This appendix contains the predicted versus measured ln(NR) plots for the free energy of hydration and first-order mixture models presented in Section 6. A predicted versus measured plot for a given model consists of a scatterplot of the ln(NR) values predicted by the model for each data point (on the y-axis) versus the measured ln(NR) values for each data point (on the x-axis). Included in each predicted versus measured plot is a 45° line that represents perfect prediction by the model. That is, if the model predicted the data perfectly, the predicted value would equal the measured value for each data point, and the plotted points would all fall on the 45° line.

Any tendency for points to fall more above the 45° line than below for a particular range of ln(NR) values indicates the model tends to overpredict for that range of values. Similarly, any tendency for points to fall more below the 45° line than above for a particular range of ln(NR) values indicates the model tends to underpredict for that range of values. Ideally, a model should yield unbiased predictions (i.e., not tend to overpredict or underpredict) over its whole range of applicability.

The imprecision of a model is indicated by the scatter of predicted versus measured points about the 45° line. A very tight scatter about the 45° line indicates the model's predictions are very precise (i.e., have low uncertainty). A very wide scatter about the 45° line indicates the model's predictions are not very precise (i.e., have high uncertainty). Ideally a model should yield very precise predictions.

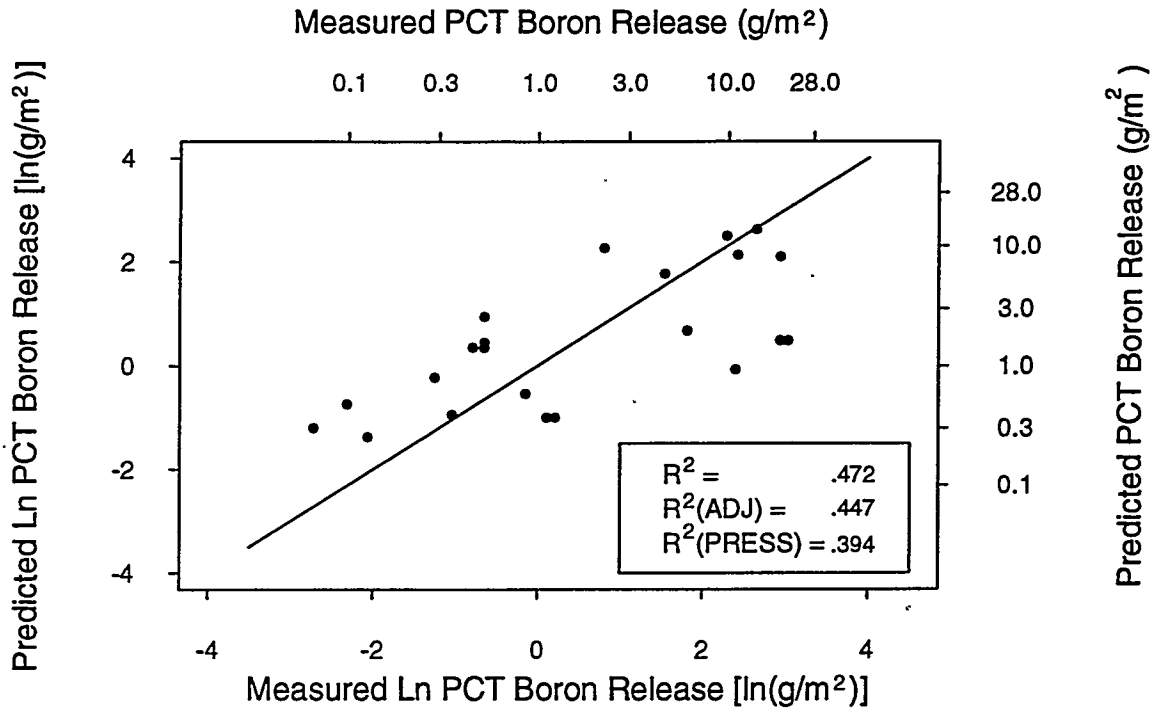

Figure C.1. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the CVS-I Data

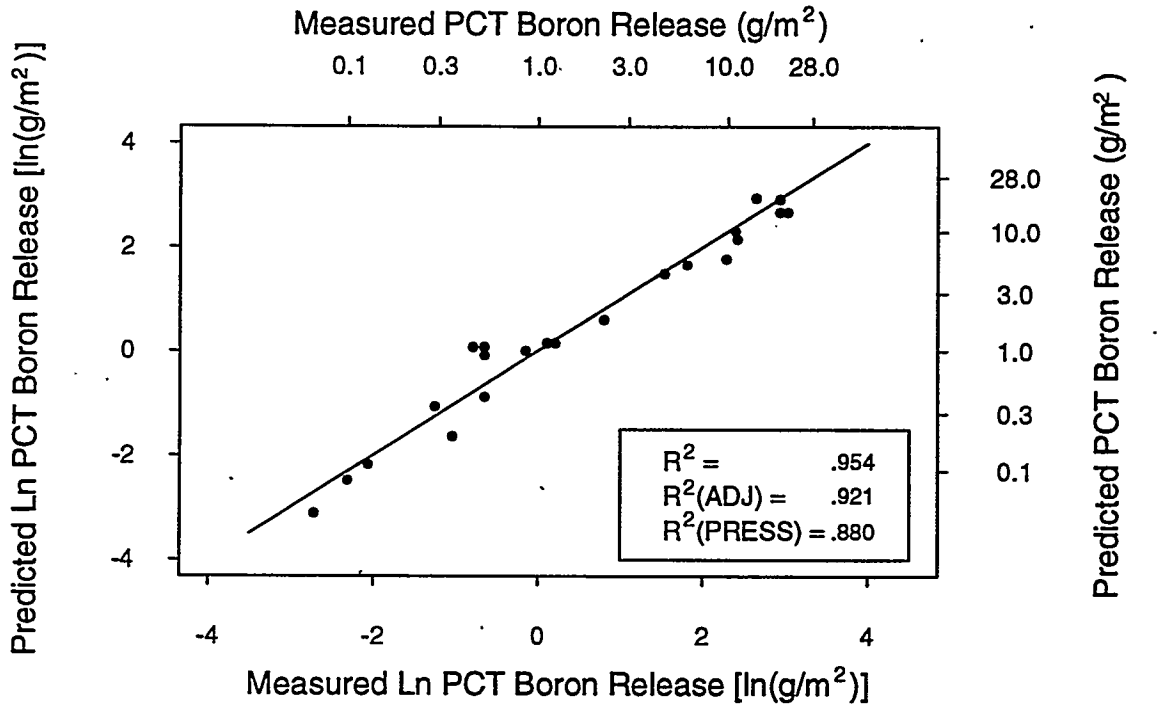

Figure C.2. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the CVS-I Data

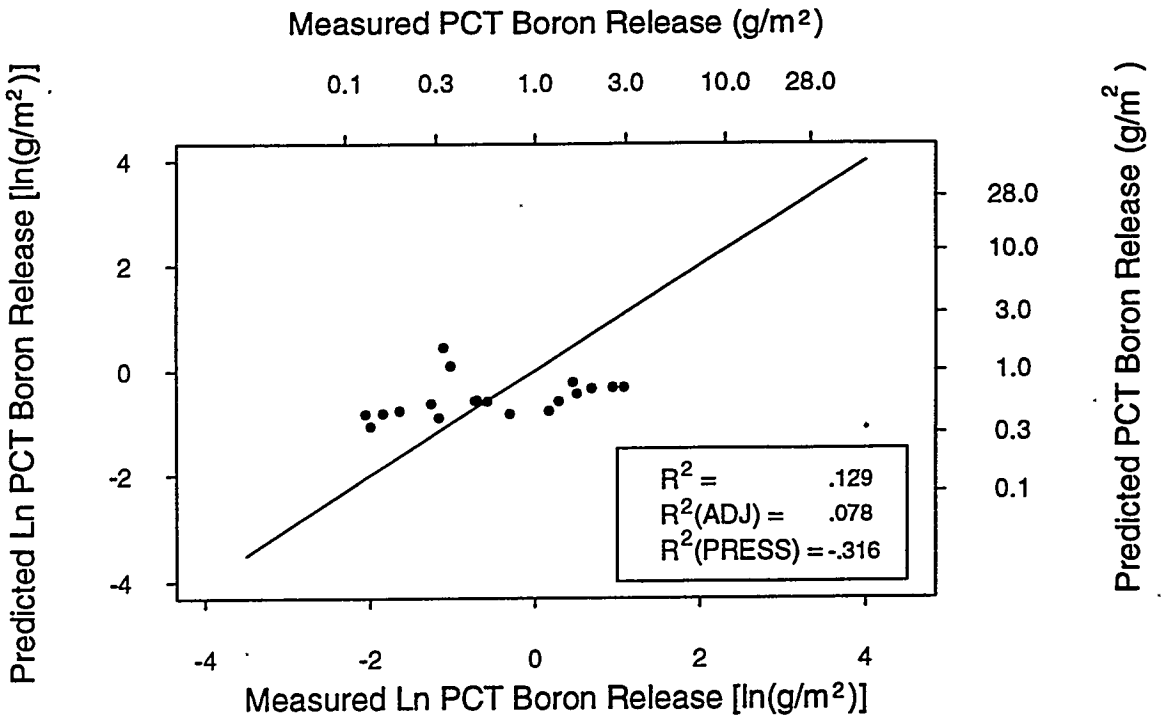

Figure C.3. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the CVS-II Phase 1 Data

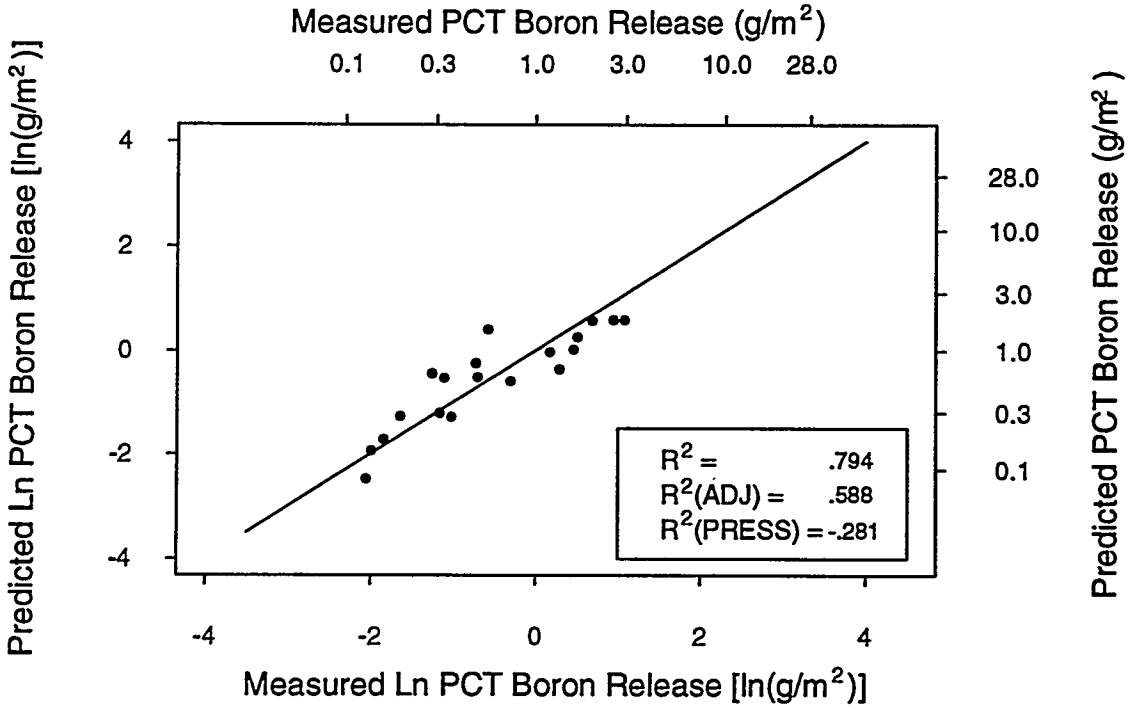

Figure C.4. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the CVS-II Phase 1 Data

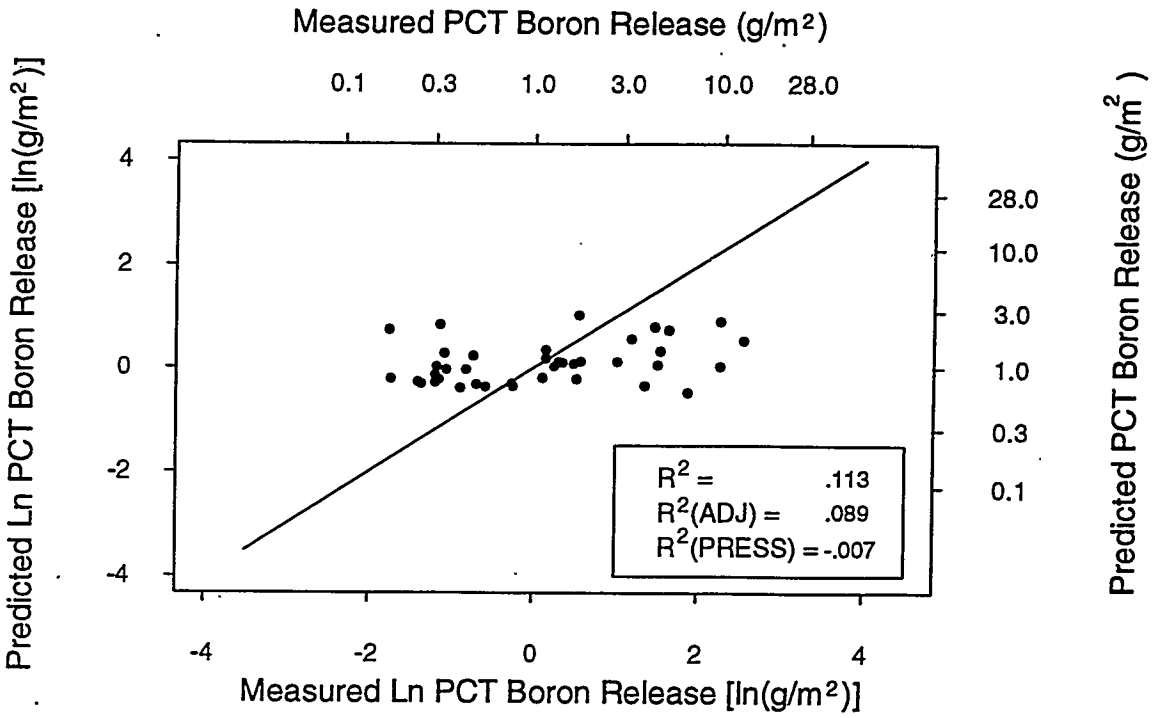

Figure C.5. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the CVS-II Phase 2 Data

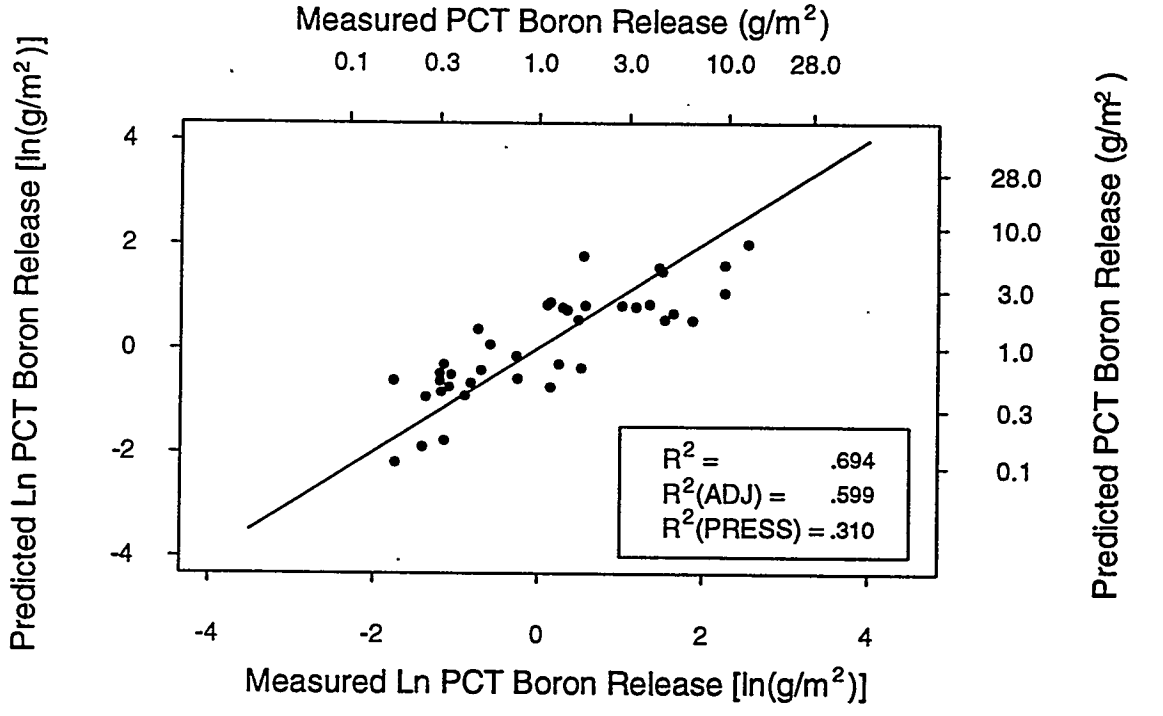

Figure C.6. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the CVS-II Phase 2 Data

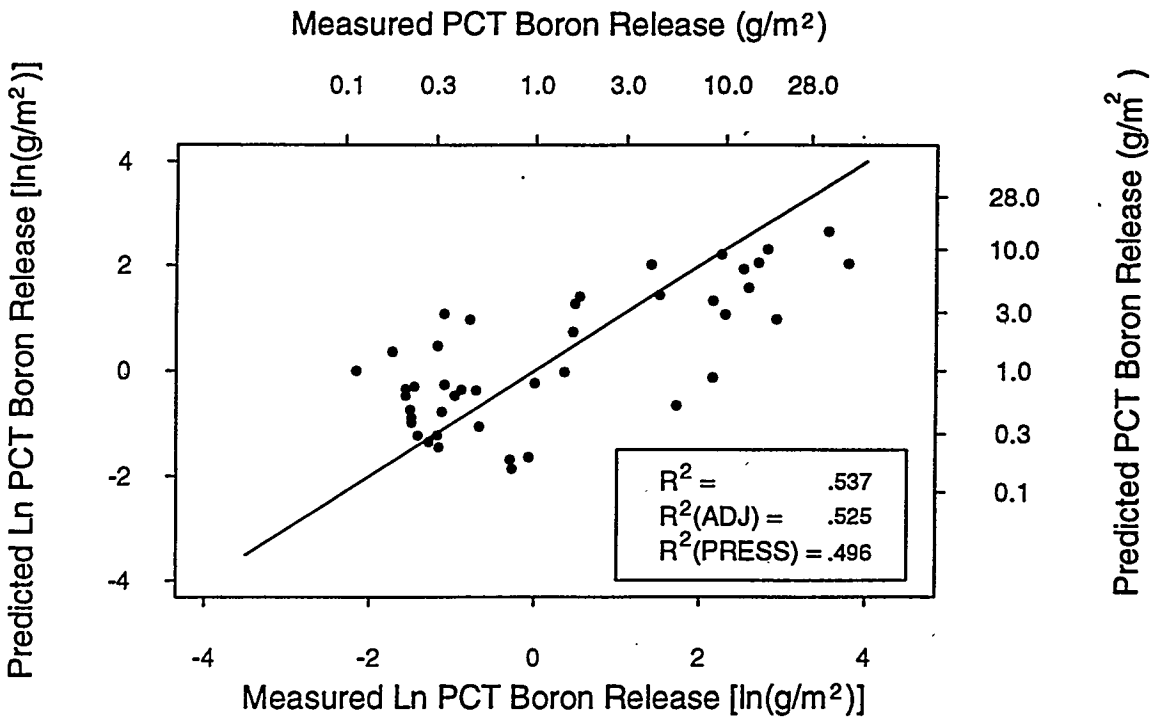

Figure C.7. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the CVS-II Phase 3 Data

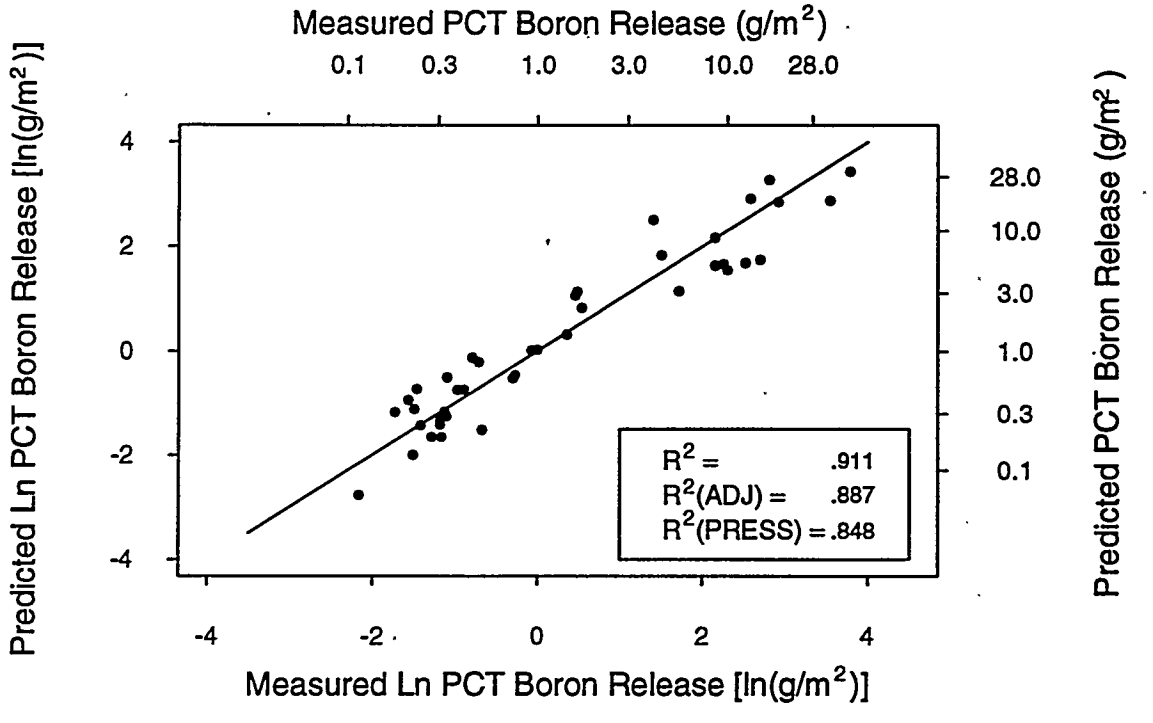

Figure C.8. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the CVS-II Phase 3 Data

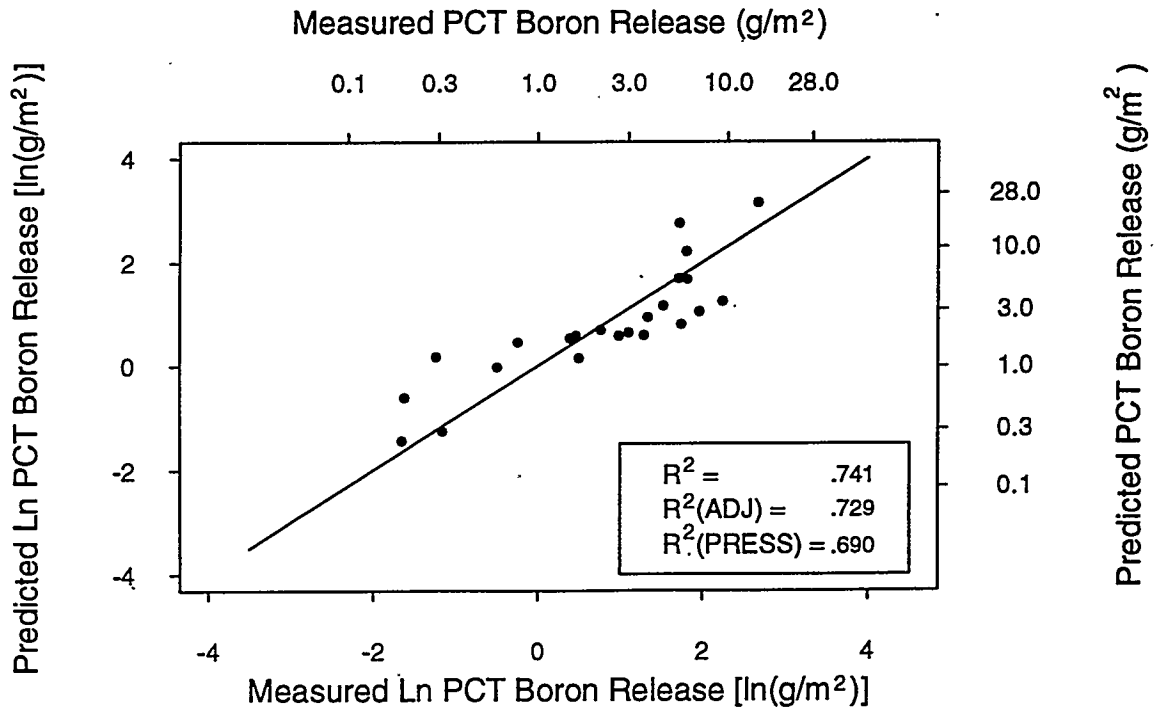

Figure C.9. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the CVS-II Phase 4 Data

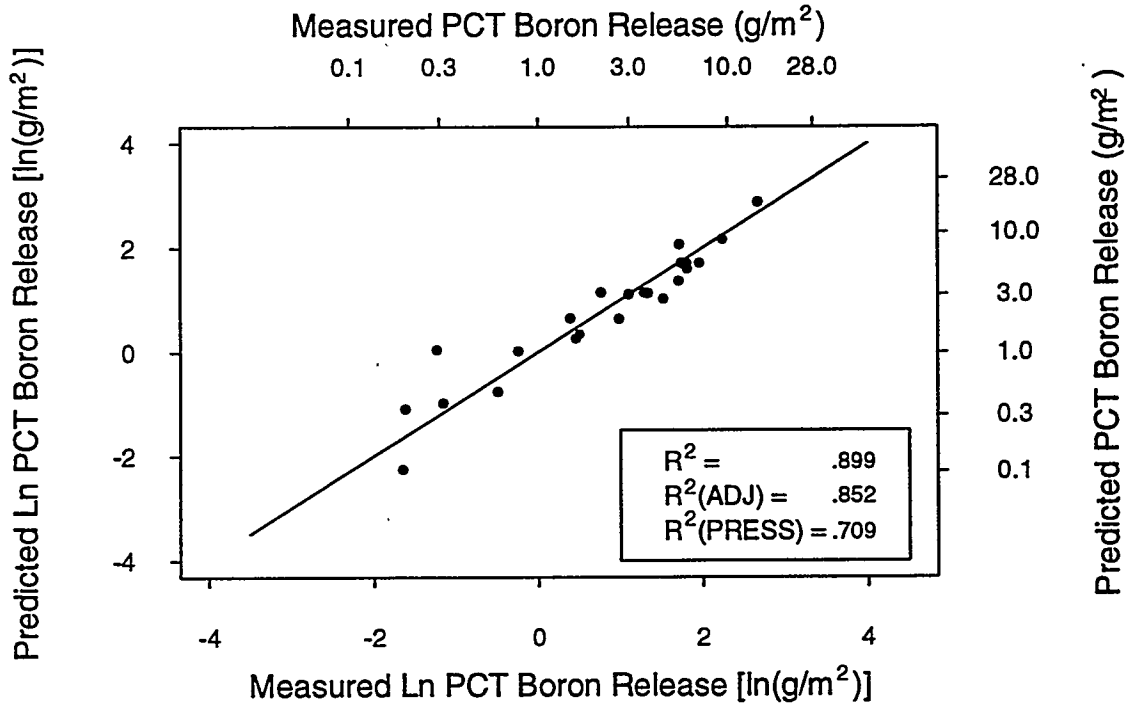

Figure C.10. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the CVS-II Phase 4 Data

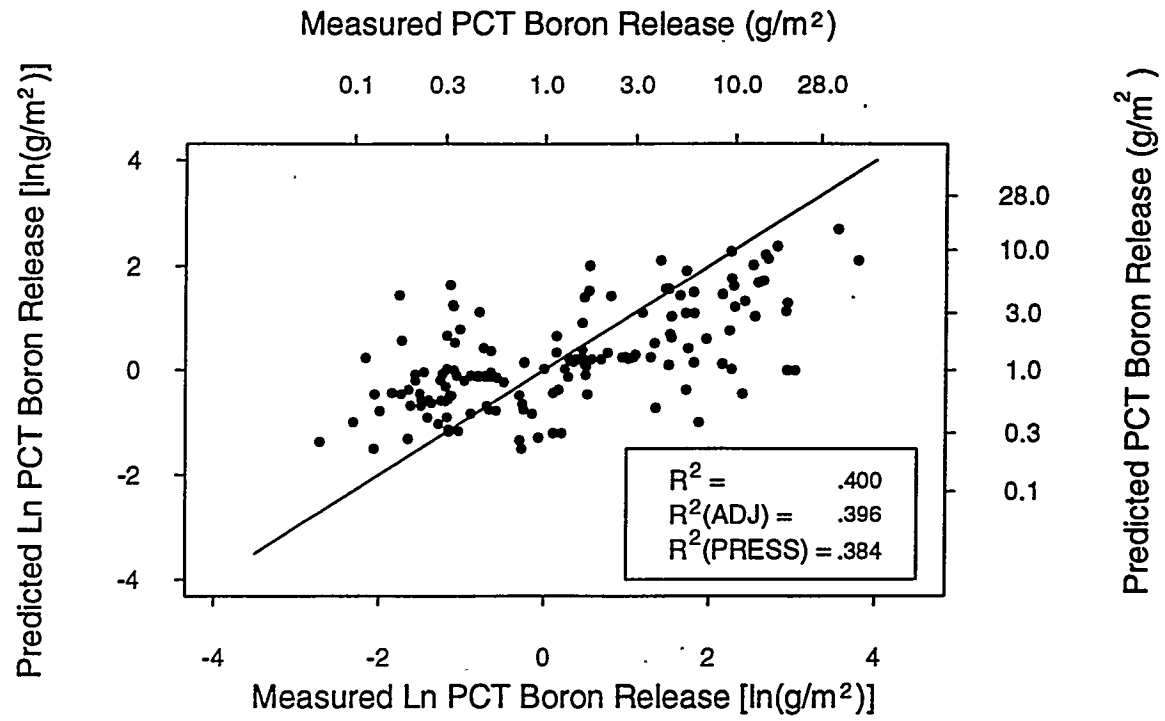

Figure C.11. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to All of the CVS Data

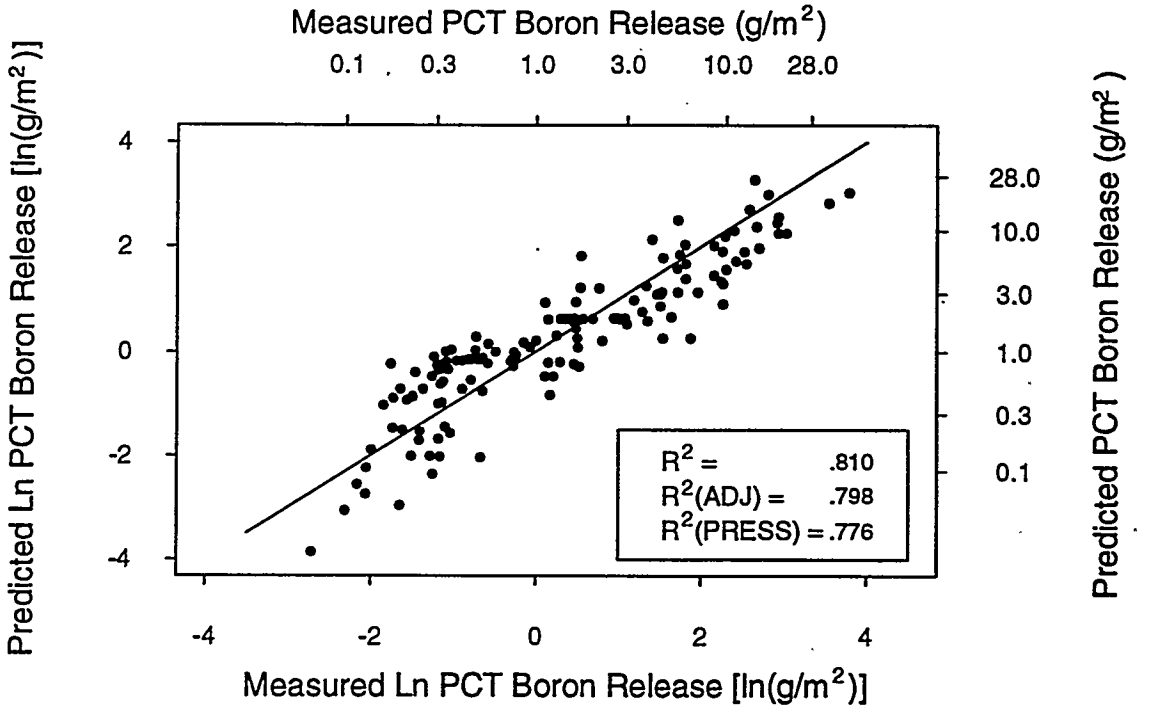

Figure C.12. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to All of the CVS Data

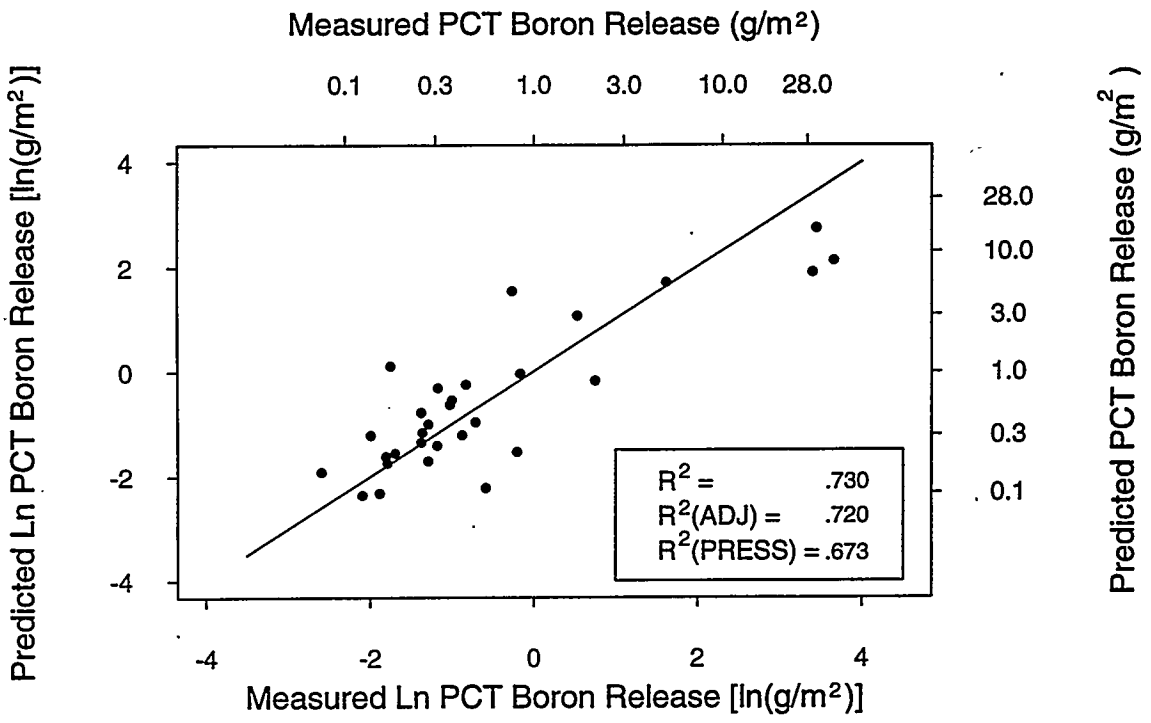

Figure C.13. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the Ramsey Data

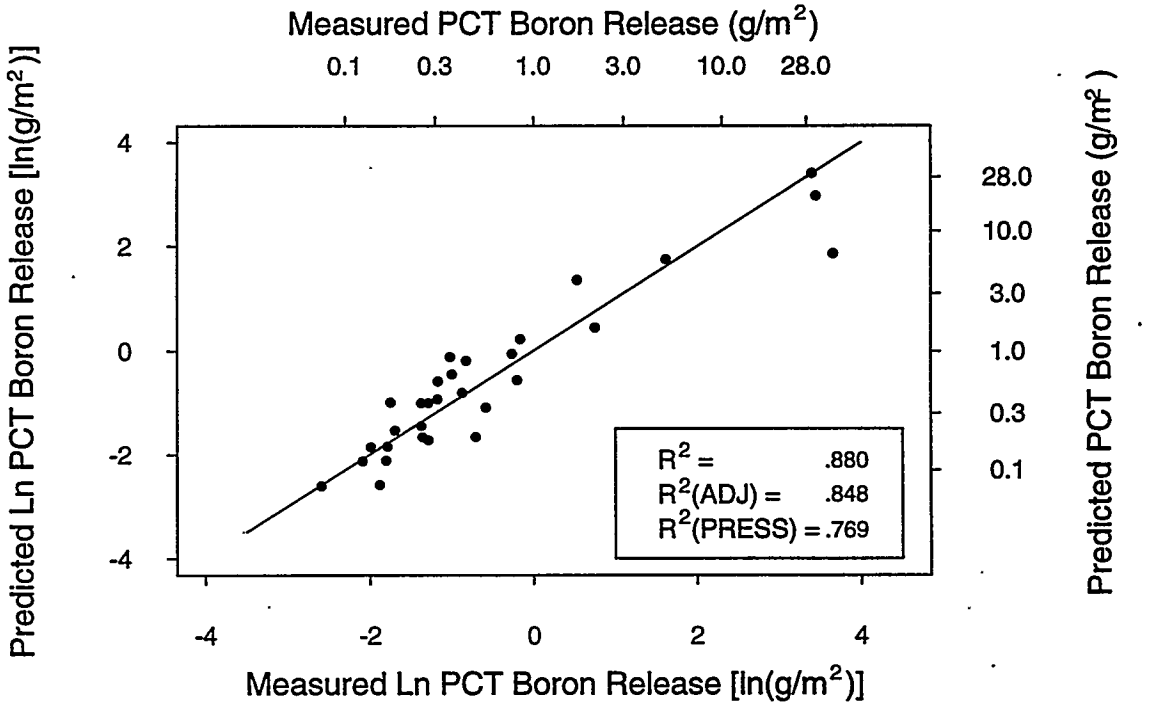

Figure C.14. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the Ramsey Data

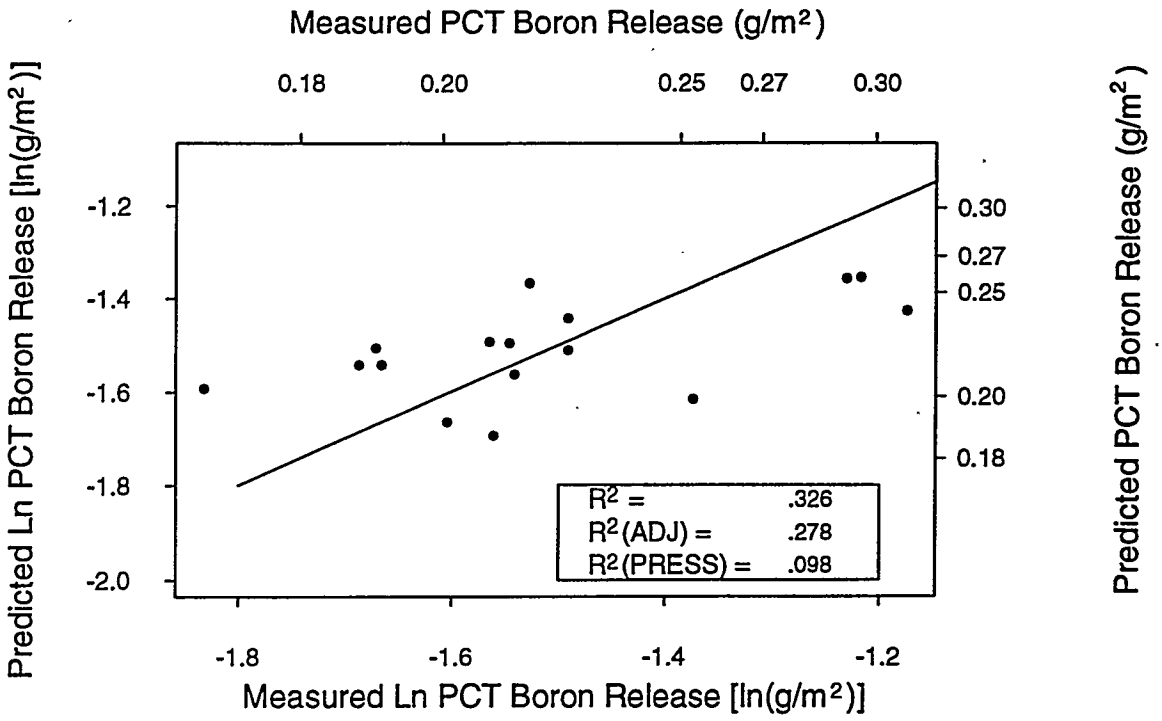

Figure C.15. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the WV87 Data

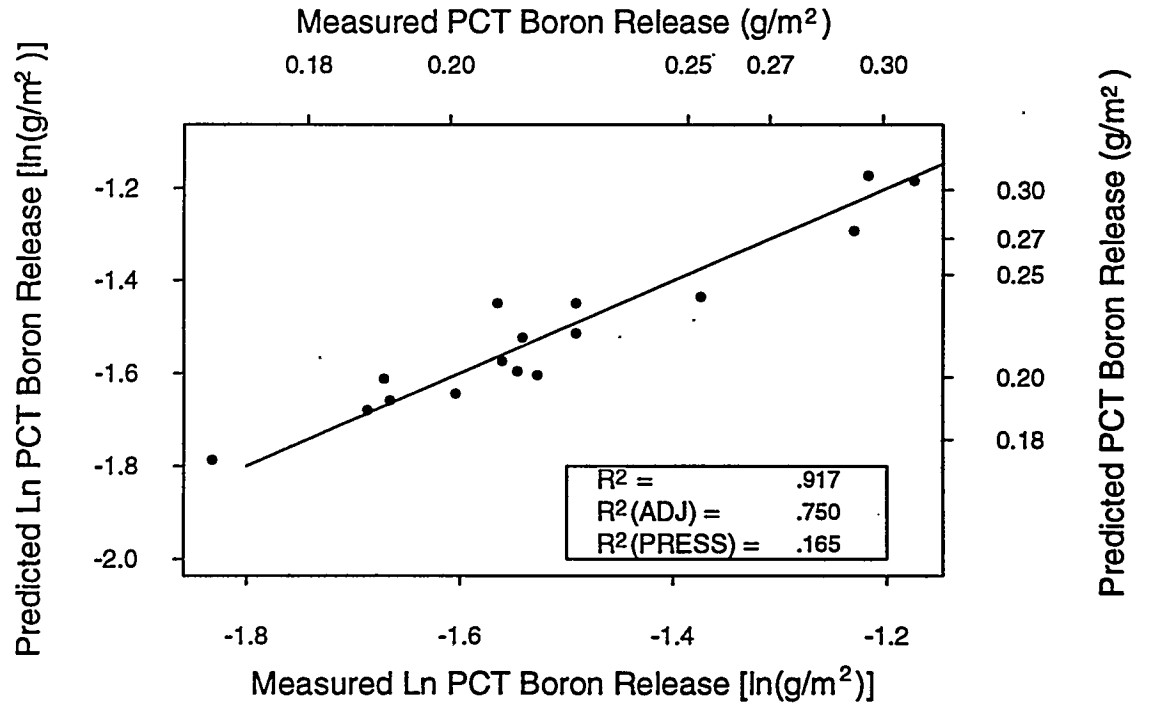

Figure C.16. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the WV87 Data

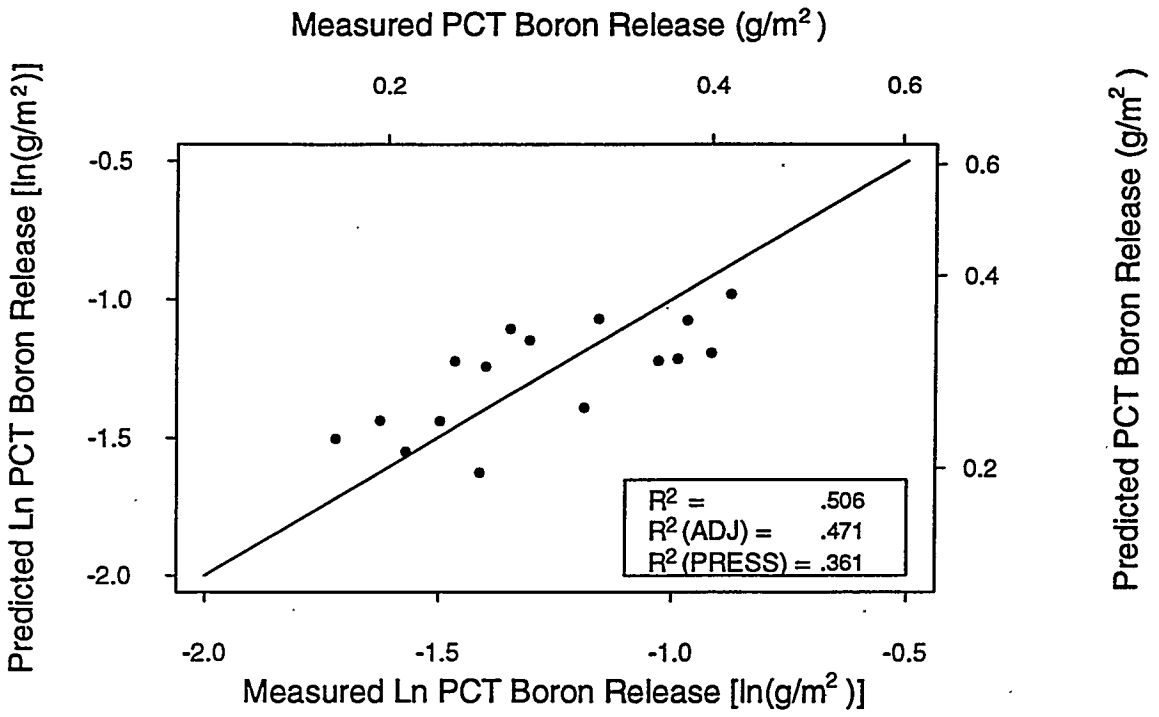

Figure C.17. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the WV88 Data

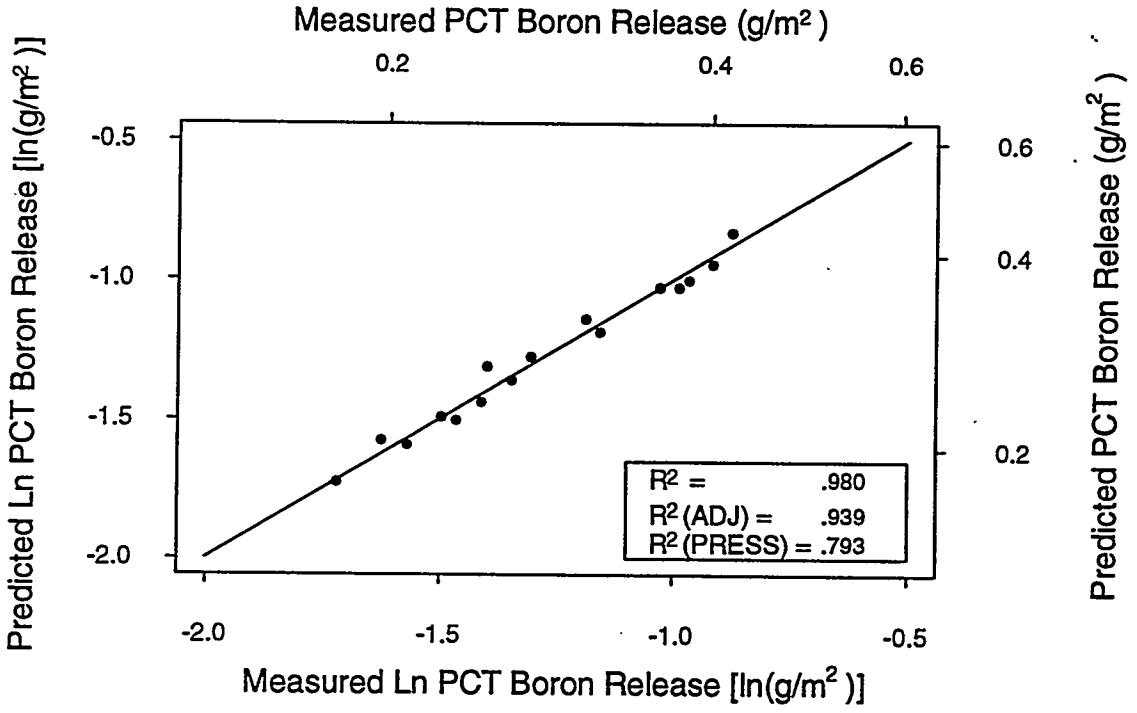

Figure C.18. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the WV88 Data

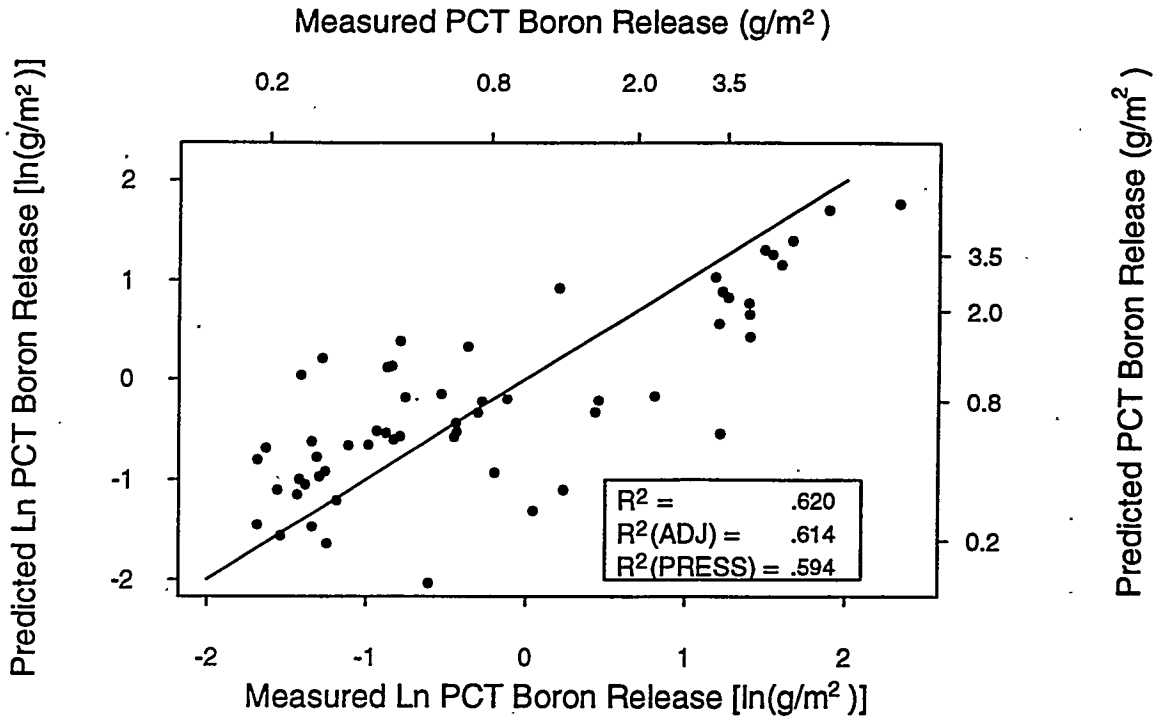

Figure C.19. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the WVDP Data

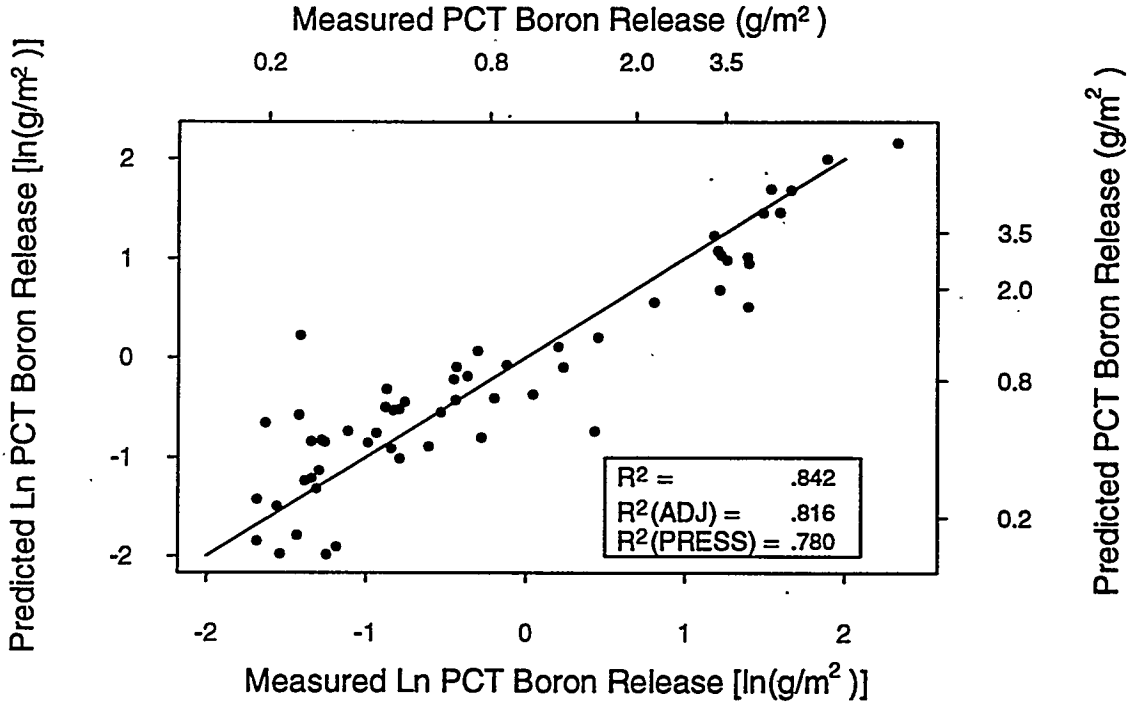

Figure C.20. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the WVDP Data

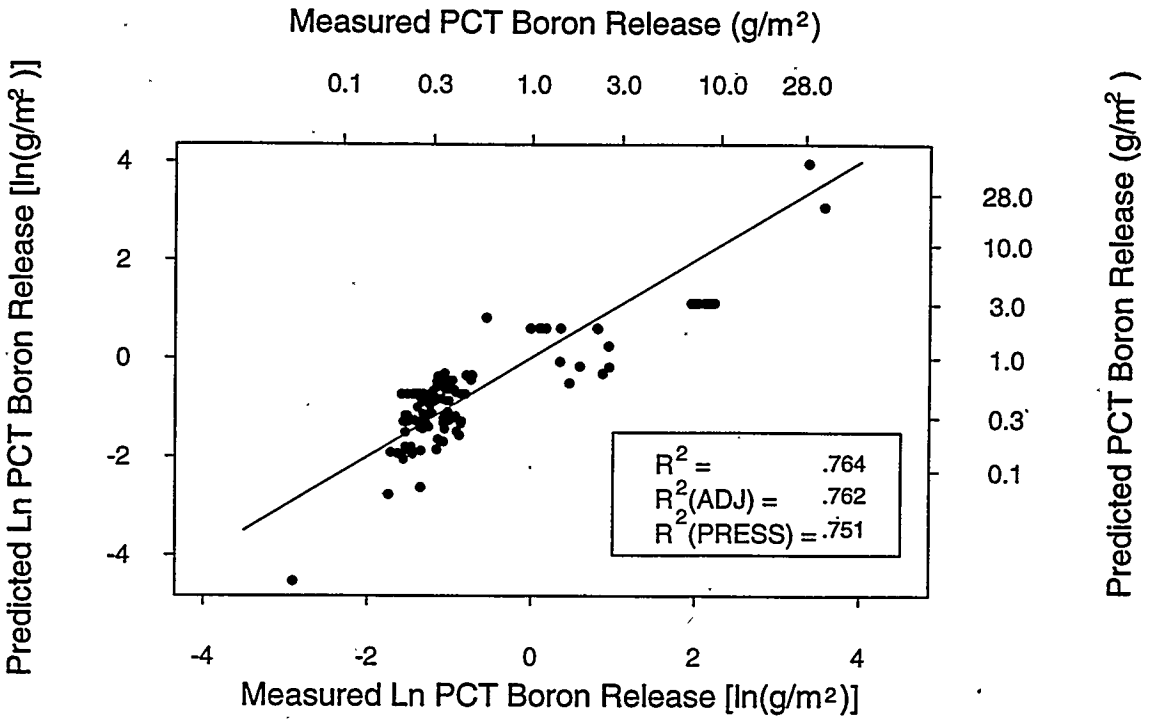

Figure C.21. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the SRTC Homogeneous Data (All 137 Observations)

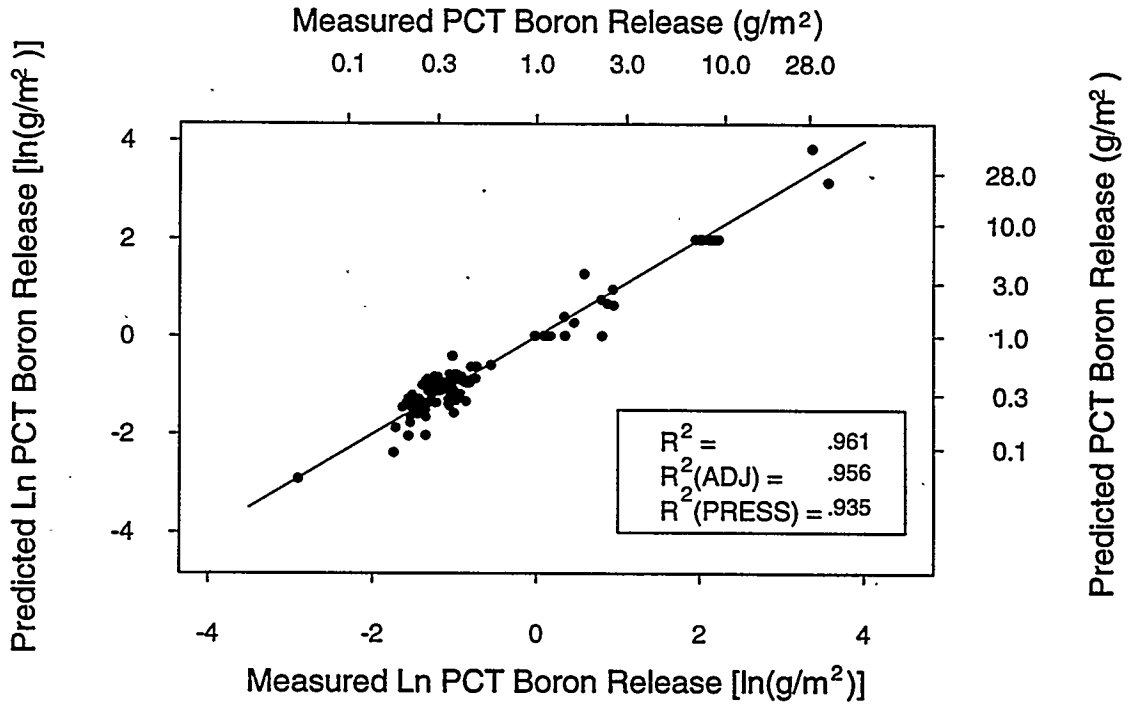

Figure C.22. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the SRTC Homogeneous Data (All 137 Observations)

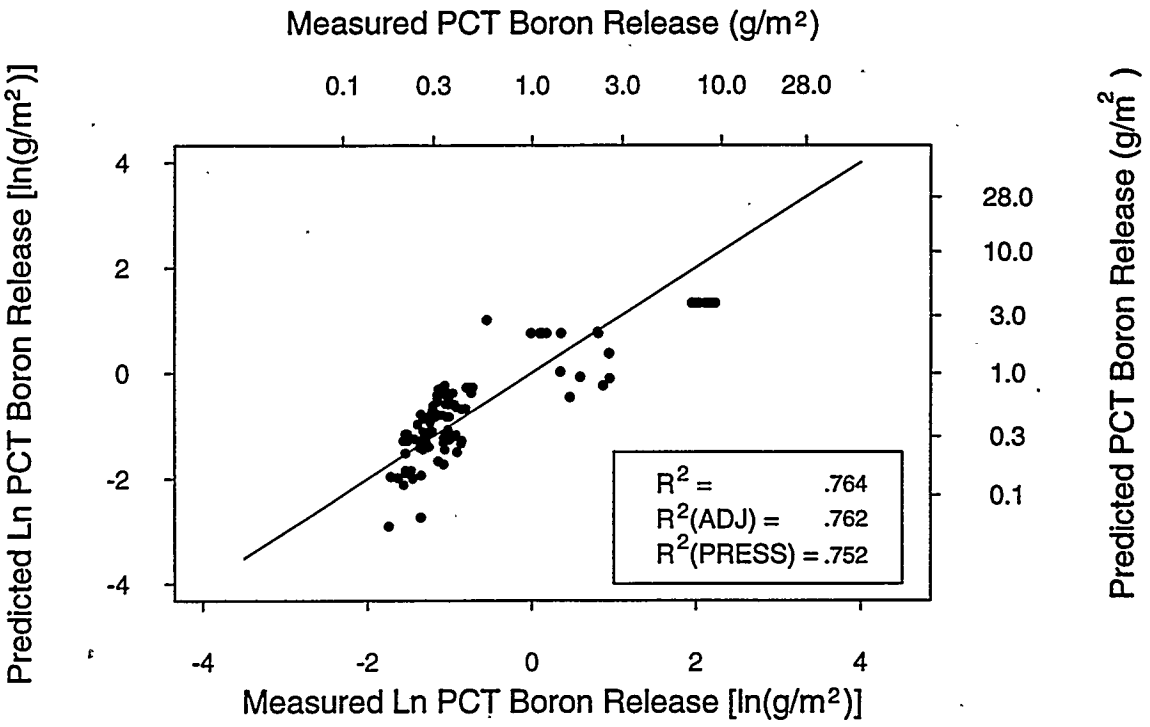

Figure C.23. Predicted Versus Measured Plot for the Free Energy of Hydration Model Fitted to the SRTC Homogeneous Data (118 Observations)

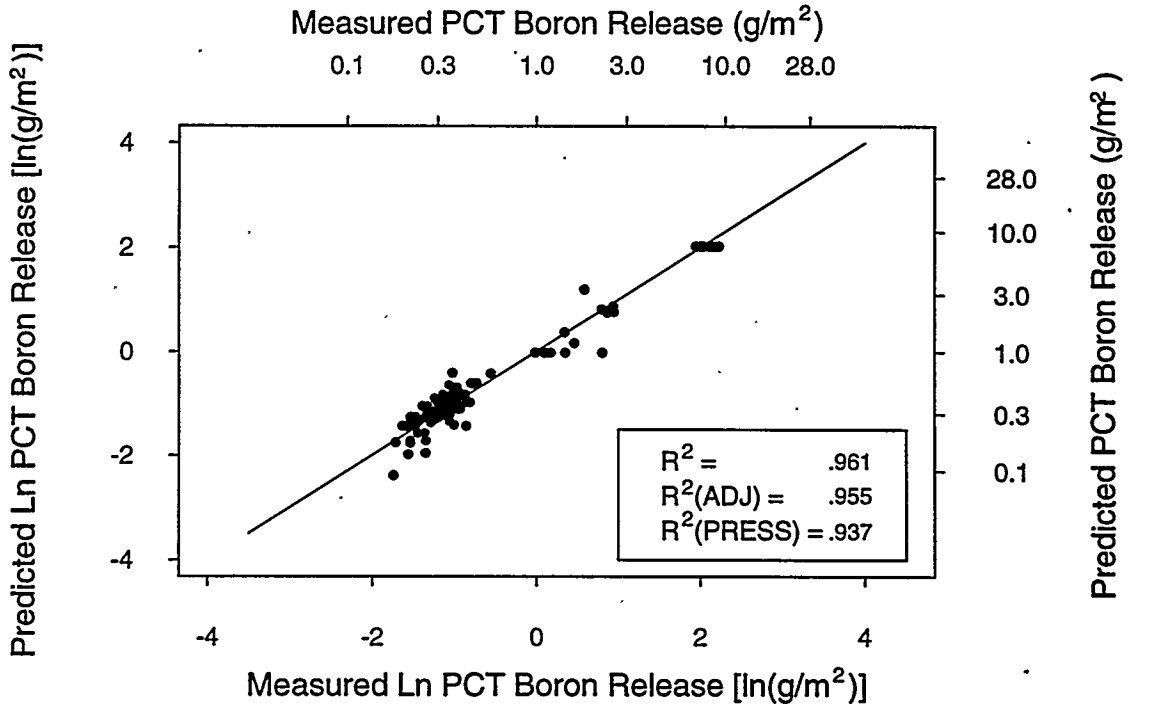

Figure C.24. Predicted Versus Measured Plot for the First-Order Mixture Model Fitted to the SRTC Homogeneous Data (118 Observations)

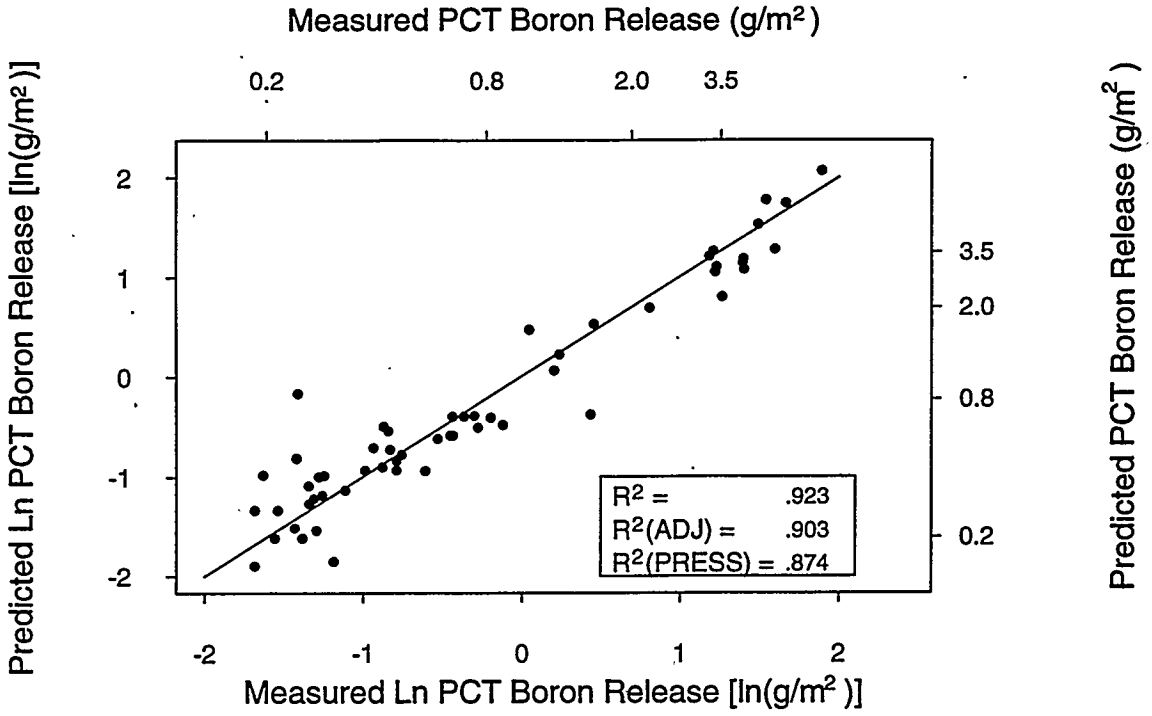

Figure C.25. Predicted Versus Measured Plot for the Reduced Second-Order Mixture Model Fitted to the WVDP Data

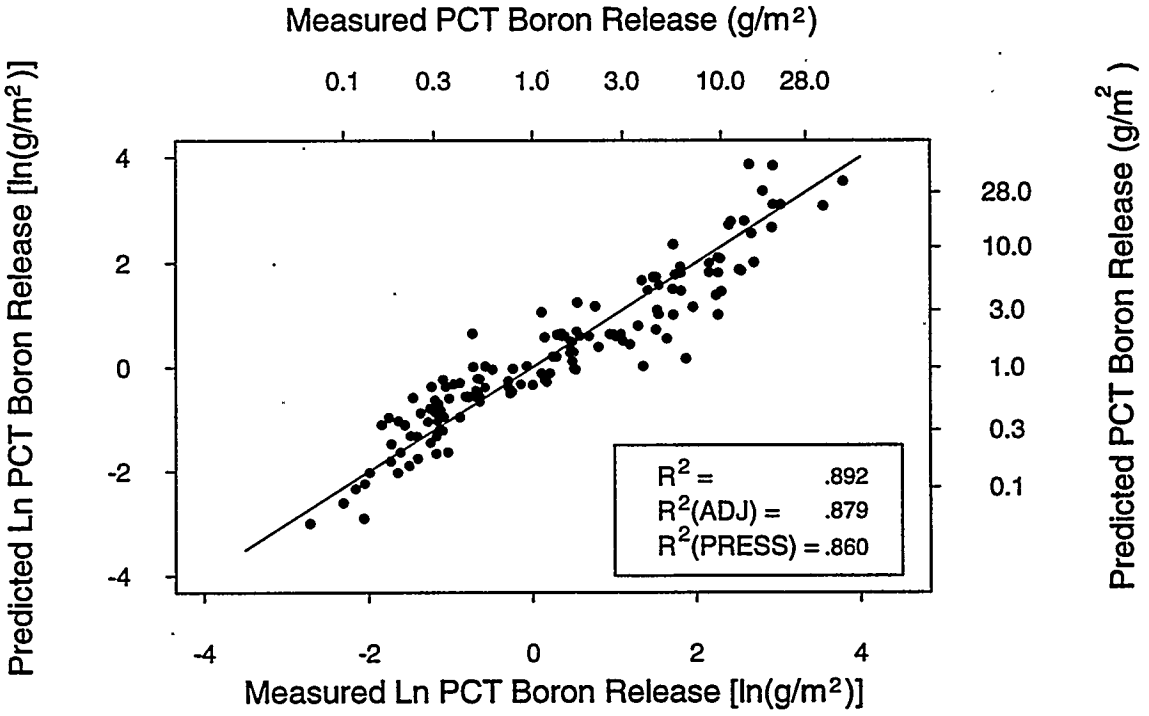

Figure C.26. Predicted Versus Measured Plot for the Reduced Second-Order Mixture Model Fitted to the CVS(all) Data

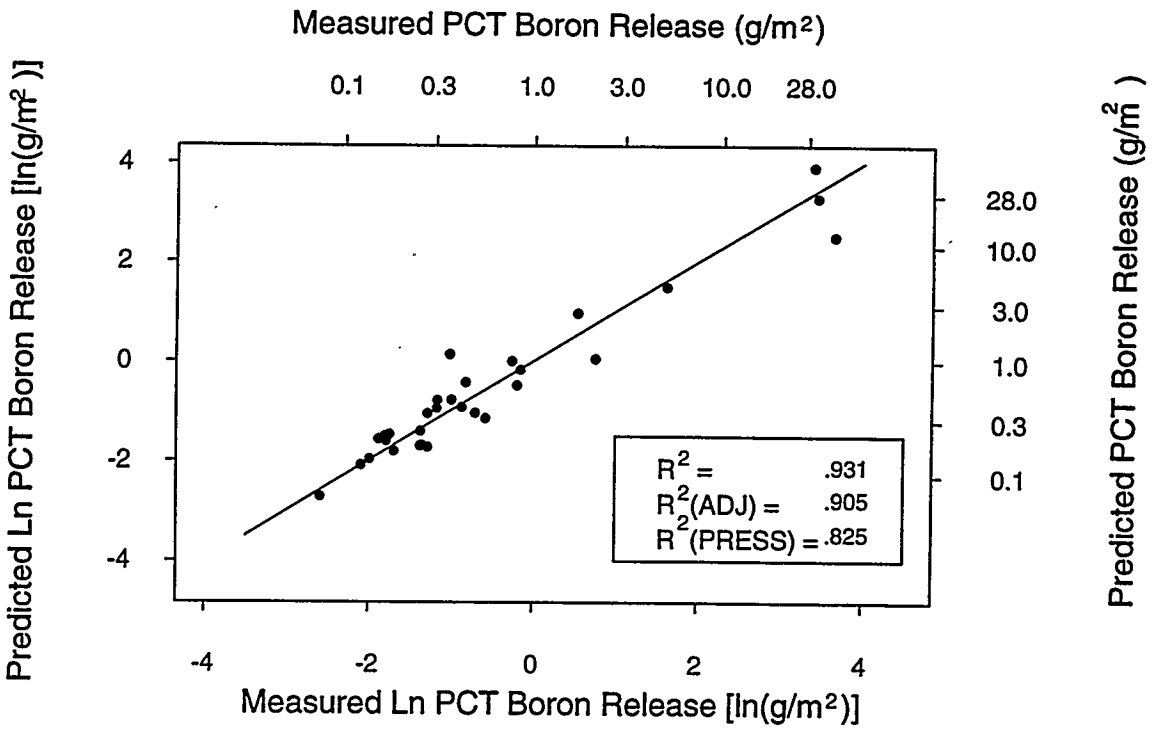

Figure C.27. Predicted Versus Measured Plot for the Reduced Second-Order Mixture Model Fitted to the Ramsey Data

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