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HIGH TEMPERATURE CHEMISTRY

Progress Report

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1972, November 1 to 1973, October 31

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DISCLAIMER

ABSTRACT

The education of graduate students and postdoctoral research associates in fields of interest to AEC continues, and the program is described. Three scientists have completed their education. One has gone to Los Alamos; one to International Nickel; one to Avila College. A faculty member on sabbatical leave from another university has joined the group.

For the titanium-oxygen system reasonably good values for D(TiO) and D(TiO_2) are available; the extent of fragmentation of TiO^+ and TiO_2^+ are known; the range of nonstoichiometry in Ti_3O_5 has been measured at high temperature; and the variation in the chemical potential of oxygen has been studied between Ti_2O_3 and TiO_2. The isomolecular exchange of sulfur between gaseous titanium and gadolinium has been measured mass spectrometrically, and the data are now being interpreted in the light of previous absolute vapor pressure measurements in titanium and gadolinium sulfides. Preliminary studies on the kinetics of vaporization of lithium fluoride were begun.

Into the nuclide mass spectrometer will soon be inserted an extension housing containing a mechanical neutral beam chopper and a retractable quadrupole mass spectrometer head. Signal-to-noise enhancement, establishment of extents of fragmentation, identification of neutral species through time-of-flight measurements, and mass calibration of the quadrupole are all planned.

INTRODUCTION

This Progress Report is divided into six parts which describe Education, Publications and Papers at Meetings, Research Progress Highlights, Space and Facilities, Level of Activity, and Miscellaneous.

EDUCATION

The education of graduate students, undergraduate students, and postdoctoral research associates in high temperature chemistry and associated fields of interest to the Atomic Energy Commission is one of the continuing and most important purposes of this contract. During the contract year three scientists have completed their education in high temperature chemistry and have taken permanent positions.

Dean E. Peterson, who was supported by the contract during his Ph.D. work, completed his degree in December and assumed a staff position at Los Alamos Scientific Laboratory where he is working with Dr. R. N. R. Mulford. That he was well educated in the field of high temperature chemistry and materials is revealed by the fact that within two or three weeks at Los Alamos he was actively engaged in activities associated with PuO_2, Ir, HfO_2, C, Al_2O_3, Ar, Si, Ge, Mo shoes, Ti screws, Ta cans, Co, $PuIr_2$, IrO_3, and IrO_2 as they are related to power sources and to safety matters in satellites.

Dr. Bruce R. Conard, who was a postdoctoral research associate under the contract, left near the end of December to join the International Nickel Company of Canada in Toronto. He began to put his education to work immediately to study phase diagrams of three- and four-component systems, to study mass spectrometrically the effluent gas from a metallurgical process, and to study mass spectrometrically fundamental systems in an effort to clarify predictions for metallurgical processes.

Dr. C. Larry Sullivan, who had been a postdoctoral research associate under the contract, departed in August to assume an assistant professorship of chemistry at Avila College in Kansas City, Missouri.

Dr. J. Edward Bennett, Professor of Chemistry at Arkansas State University, Jonesboro, Arkansas, has come to the University of Kansas on his sabbatical leave and will be associated with the high temperature group. His goals in coming to the University of Kansas include working with an active group in high temperature studies and working with small computers in laboratory experimentation.

Tables I, II, and III summarize the past and present educational products of the program. Table I gives in chronological order of graduation, the names, the dates, and the locations of the scientists who have completed education in high temperature chemistry at the University of Kansas. In Table II, the same information is given, but the names are arranged according to the type of installation. Table III gives the names of the people currently in high temperature research. The count now stands at twenty Ph.D.'s, eighteen postdoctoral research associates, and six masters. These scientists and their accomplishments attest to the educational value of the program.

About twenty-eight of the scientists more or less, some 63 percent, are currently engaged in high temperature research. Thirteen are in universities, two in colleges, seven in AEC laboratories, six in other research establishments, ten in industry, three in postdoctoral study, one in school, and two uncertain.

The accomplishments subsequent to their graduation of the people who have been educated under the program at the University of Kansas are the product of the individual efforts of the scientists so trained. The principal investigator takes considerable pride in the accomplishments of these men. Of the people whose names are listed in Table I and II, at least fourteen have substantial international reputations because of their research. We note again the accomplishments of the people in the AEC laboratories, Ackermann, Leitnaker, Smith, Hobrock, Unruh, Jackson, and Peterson, and in addition, Franzen, who is listed at Iowa State University and also in the Ames Laboratory. In the AEC laboratories at least five people, Leitnaker, Franzen, Smith, Unruh and Hobrock, have planning and supervisory responsibilities, and Ackermann is assuming an ever more important role at Argonne. One of the purposes of the contract is to aid in the training of scientists skilled in branches of chemistry of interest to the Atomic Energy Commission, and the presence of these men in the AEC program clearly demonstrates the accomplishments.

Report TID-26400, Atomic Energy Commission Research and Development Laboratories, A National Resource, published 1973, September, lists as multiprogram laboratories Argonne, Oak Ridge, Lawrence Livermore, Lawrence Berkeley, Brookhaven, Pacific Northwest and Los Alamos. Graduates from the program are in five of these seven laboratories. Of the specialized physical research laboratories, one of the graduates is at Ames; of the production, development and fabrication sites, one is at Savannah River; and of the weapons fabrication complex, one is at Mound Laboratories. Much of the work performed by these men is in the high temperature field, but the breadth of their education is revealed in part by the ability of some to work in other fields, notably analytical mass spectrometry and radiation monitoring.

The Midwest High Temperature Chemistry Conference was held at Northwestern University in June. This conference was inaugurated at the University of Kansas in 1965 and has been held in alternate years. Once again, much of the program was contributed by graduates from the program including Carlson, Wu, Milne, Greene, Wahlbeck, Edwards, Eick, Franzen, Lewis, Margrave, Cater, as well as the current group, Sullivan, Behrens, Huang, and Sheldon. Twenty-one of those attending have been or are associated with the program at the University of Kansas. The next one scheduled for 1975 is to be at the University of Toledo under the chairmanship of former postdoctoral research associate, Jimmie G. Edwards.

Table IV lists seventeen seminar talks of the University of more or less interest to people in the program. Of these, four were given by scientists who came especially to the high temperature group. Other scientists in the high temperature field who visited but did not give talks were Lin of Army Materials and Mechanics Research Center, J. R. McCreary of Argonne, J. Bloem of Amsterdam and Eindhoven, M. Lundberg of Stockholm, and F. T. Greene of Midwest Research Institute.

PUBLICATIONS AND PAPERS AT MEETINGS

The permanent, public record is contained in one published article on work supported largely by AROD, two articles accepted for publication and two submitted for publication, all detailed in Table V. A paper or two on the titanium-oxygen system, a paper on the hydrogen-boron-silicon system, and two papers on the rare earth-sulfur system are nearing completion.

Under the auspices of the National Science Foundation Dr. Gilles was one of eleven U.S. scientists participating in the United States - Japan Cooperative Science Program Seminar held at Ames Laboratory in June on "Thermodynamics and Phase Relations of Nuclear Materials."

Five invited talks and five contributed talks are described in Table VI.

RESEARCH HIGHLIGHTS

The completed work is described by the publications. Manuscripts submitted for publication and reprints have been submitted to the contracting office in the usual fashion; the contents of those appearing in journals will not be repeated here. The work will be described in the following categories: (A) vaporization behavior of refractory systems; (B) high molecular weight inorganic gaseous substances; (C) kinetics of high temperature vaporization reactions; and (D) phase studies.

(A) Vaporization Behavior of Refractory Systems. Three topics are described here. (1) In an effort to clarify vaporization phenomena of high temperature materials, Figure 1 has been prepared. It describes vaporization processes from the physical chemical point of view. The vaporization of the single condensed phase is classified according to its congruence, i.e., whether or not the product gas phase has the same overall composition as the condensed phase. For purposes of simplicity, not completeness, the single most important and usually the overwhelmingly predominant chemical reaction is classified next according to whether it produces only one, or more than one product. The classification next continues according to the molecularity of the products. Finally examples are given from high temperature vaporization studies. Two examples will illustrate the use of the chart. The solid La_2O_3 shown in the middle column of Figure 1 vaporizes by a congruent process yielding two gases, the element O(g) and the compound LaO(g). The solid Ti_4O_7 shown in the right-hand column vaporizes incongruently to give one principal gaseous product $TiO_2(g)$ and solid Ti_3O_5. Although the chart was not prepared for more complicated chemical systems, the right-hand column can be used for the vaporization of a mixture of condensed phases. For example, the solid mixture of Ti_4O_7 and Ti_3O_5 yields a gas, principally TiO_2, which does not have the same composition as either of the condensed phases or a mixture of them. By which of these several modes a particular substance vaporizes is determined largely, but not exclusively, by the stability of the gaseous compound.

(2) With Conard's departure, work on the titanium-oxygen system has been continued by Sheldon and by Bennett. The work as it stood about two months before Conard's departure is described in the previous report. The situation then and now is reasonably easily summarized. The congruently vaporizing solution lies in the Ti_3O_5 phase region; its range of homogeneity at temperature is under investigation; its gaseous products are TiO(g) and $TiO_2(g)$; their dissociation energies are those given by Hampson and Gilles as 157 and 312 kcal/mole; the recent value from Rome of 144 kcal/mole is believed surely to be incorrect, and the suspected source of error is their measurement of an ion ratio supposed to be O_2^+/O^+, and the contributions to the Ti^+ and the TiO^+ intensities arising from fragmentation amounts to about ten percent of the TiO^+ intensity, and to less than 5 percent of the TiO_2^+ intensity, respectively.

During the current year Conard performed a preliminary analysis of one of his experiments, and Sheldon and Bennett have pursued an analysis of Conard's other experiments. In order to clarify the extent of fragmentation of TiO_2^+ Conard studied the vaporization of TiO_2. This sample was used because it has a sufficiently high oxygen potential that the only source of TiO^+ is from fragmentation of TiO_2^+. Bennett has written a relatively simple computer program to retrieve Conard's data stored on the computer disc. From Conard's measurements taken early during the experiment, at which time the minimum amount of decomposition of TiO_2 to lower oxides would have occurred, Bennett finds that the TiO^+ intensity arising from fragmentation of TiO_2^+ at 70 eV is less than (2.5 ± 2.4) percent of the intensity of TiO_2^+ and may be zero. The uncertainty associated with this value arises because of the large background in the spectrum at mass 64. An oscillographic display of the data reveals a slight intensity above the background, a result which is confirmed by the numbers put out by the program.

A recent report by Hyde and coworkers in Perth, W.A., on the titanium-oxygen system at temperatures some 600° lower than those employed in the vaporization experiments at the University indicates that the extent of solid solubility in the Ti_3O_5 is negligible. At the higher temperatures, however, the evidence of appreciable solubility is incontrovertible. The data are the intensity ratio TiO_2^+/TiO^+ as a function of time. This ratio after correction for fragmentation is important because it is proportional to the oxygen potential in the sample. Hampson reported three such experiments, one starting on the metal-rich side and two starting on the oxygen-rich side of Ti_3O_5. Conard performed one experiment starting on the metal-rich side and another starting with TiO_2. All experiments show a change of the ratio with time indicating an approach to a congruently vaporizing solution in the Ti_3O_5 region.

Run S was interrupted by a tornado, and air got into the hot sample when the emergency line, to which the mechanical pump was attached, failed to operate. This accident provides the best data showing exactly what is occurring. Before the accident the metal-rich sample showed an increasing TiO_2^+/TiO^+ intensity ratio which leveled off indicating the achievement of congruence. Immediately after the resumption of heating following the accident the intensity ratio was much higher, corresponding to values characteristic of a solid mixture of Ti_3O_5 and Ti_4O_7. As heating proceeded the intensity ratio fell, just as it did in those experiments that were originally oxygen-rich. Ultimately the same intensity ratio was reached as had been achieved in the earlier part of the experiment. Thus in a single experiment equilibrium was approached from both sides.

Reasonably simple equations have been deduced whereby the compositions of the lower phase boundary, the congruently vaporizing solution, and the upper phase boundary for the Ti_3O_5 phase can be obtained from the loss of mass of the sample during the vaporization process and from instantaneous measurements of the intensities of TiO^+ and TiO_2^+ during the entire course of the vaporization.

The data from Runs K, LM, and N, have been used by Sheldon. The results indicate that from the metal-rich boundary to the congruently vaporizing solution the composition changes by about 0.02 in the O/Ti ratio, and a similar width of homogeneity exists on the oxygen-rich side between the upper phase boundary and the congruently vaporizing solution. The uncertainties in the numbers are considerably less than 0.01. The composition of the congruently vaporizing solution as revealed by experiments K and LM is 1.67 corresponding to stoichiometric Ti_3O_5; but for experiment N, which was nearly a duplicate of LM, it is 1.70.

In summary, we have reasonably good values for the dissociation energies of $TiO(g)$ and $TiO_2(g)$; we know the fragmentation contribution to the TiO^+ intensity; we have a less reliable value for the Ti^+/TiO^+ ratio coming from fragmentation of TiO; we know roughly the range of nonstoichiometry in Ti_3O_5 at temperature, although the composition of the congruently vaporizing solution is not yet fixed; we know the variation in the chemical potential of oxygen from Ti_2O_3 to Ti_4O_7; and we have some information on the chemical potential of oxygen in reduced TiO_2 samples.

(3) The work on the dissociation energies of gaseous diatomic sulfides being performed by Behrens has continued. Two mass spectrometric isomolecular exchange reaction experiments have been completed for the reaction,

$$GdS(g) + Ti(g) = Gd(g) + TiS(g).$$

The results are currently being evaluated. We have pointed out previously that this particular reaction is one of great importance, for it will be one of the very few to link absolute vapor pressure measurements and mass spectrometric isomolecular exchange reaction experiments. Absolute vapor pressure measurements were made on both GdS and TiS essentially in the same apparatus, and both gaseous molecules have been studied in the same mass spectrometer. Both TiS(s) and GdS(s) vaporize congruently to give a mixture of atoms and molecules. The attitude taken in the present work is to ascertain whether the equilibrium constant for the above reaction is consistent with equilibrium constants obtained for the individual dissociation reactions. A comparison of the equilibrium constants is a more direct way of studying the systematics of the chemistry than to compare the derived dissociation energies whose values depend so much on unknown electronic multiplicities. The experimental work is complete. The data analysis should be completed within about two months.

(B) High Molecular Weight Inorganic Gaseous Substances. Progress in this endeavor was limited to the preparation and submission of paper number COO-1140-208, "High Temperature Vaporization of Ternary Systems. I. Mass Spectrometry of Oxygen-Rich Vanadium-Tungsten-Oxygen Species," the first of several we hope to publish in this area.

(C) Kinetics of High Temperature Vaporization Reactions. The results that Peterson obtained on cuprous chloride in the vacuum balance and the mass spectrometer were summarized last year. These results are being prepared for publication. Sullivan undertook studies on the kinetics of vaporization of single crystals of lithium fluoride with the quadrupole mass spectrometer. He designed an X-Y table for the quadrupole mass spectrometer apparatus and arranged for its construction. He designed and had built a spherical cell for use with lithium fluoride. On rather short notice a teaching position became available at Avila College, a small liberal arts college in Kansas City. Sullivan decided that in view of the job situation he should take that position and was not able to complete the study.

Huang has been studying the kinetics of vaporization and plans to continue experiments with the quadrupole mass spectrometer.

(D) Phase Studies. The compositions of the lower phase boundary, the congruently vaporizing solution, and the upper phase boundary for the Ti_3O_5 phase have been mentioned previously. Behrens studied slightly the titanium-gadolinium-sulfur system so that he would know the phases present in his vaporization experiments.

SPACE, FACILITIES, AND COMPUTER PROGRAMS

Apparatus Modification and Improvements. At the beginning of the year the plan was to obtain a neutral beam modulation apparatus for the Nuclide mass spectrometer. It was to be used with the multichannel analyzer and the dedicated laboratory computer. Time-of-flight measurements could be made on neutral molecules arising in the studies of ternary gaseous oxides for identification purposes; it would be useful for measuring the extent of fragmentation of smaller molecules; also it would be useful for extracting small signals from large backgrounds. A separate plan was to modify the vacuum housing of the quadrupole mass spectrometer so that higher temperature systems could be studied with the fast scanning capabilities of the quadrupole instrument.

These two improvements have been combined in a creative way so that an even different type of experiment can be performed in addition to the ones that were originally contemplated. On order is the mechanical chopper and associated devices consisting of audio oscillator, power amplifier to power the motor, reference signal source and pickup, start-run voltage limiter, capacitors and switch for different frequency ranges, reference signal voltage supplies, motor reversing switch, three globe motors to cover the frequency range 41-666 rps, and connecting cables. Specifications were carefully written so that the chopper can be used either with a multichannel analyzer or with a lock-in amplifier, both of which are already available. Instead of modifying the housing for the quadrupole mass spectrometer as originally planned, we have designed and ordered parts for an extension housing to the Nuclide mass spectrometer. This housing will be inserted between the Knudsen cell housing and the ion source housing of the Nuclide mass spectrometer. Into this extension housing will go not only the modulation apparatus, but also a quadrupole mass spectrometer head. A bellows arrangment will enable the scientist to insert the ionization chamber of the quadrupole mass spectrometer into or withdraw it from the molecular beam.

This arrangement has a number of very great appealing features, for several modes of operation can occur. With the quadrupole removed from the beam, the Nuclide mass spectrometer can be operated in the conventional fashion with only a loss in intensity. With the quadrupole still withdrawn, phase sensitive detection can be used with the rotating slotted wheel and the beam modulation electronics, thus allowing a significant increase in the signal-to-noise ratio that will in all likelihood overcome a loss in intensity. Thirdly, again with the quadrupole head withdrawn, time-of-flight measurements can be made to identify neutral precursors of ions in complicated ternary oxide systems in which more than 60 different ions have been observed with masses ranging from 16 to nearly 1400. This same arrangement will be useful for fragmentation studies. Fourthly, with the quadrupole head inserted the desired rapid sweep capabilities of the quadrupole can be used for the higher temperature studies that are possible with the Nuclide Knudsen cell rather than with the existing lower temperature quadrupole crucible housing. The chopper can of course be used with the quadrupole in the fashion suggested above for the Nuclide. And finally, this arrangement of the apparatus which is available in no other place to our knowledge will enable the sensitivity of the quadrupole mass spectrometer to be obtained relative to that of the magnetic instrument. The loss of transmission with increasing mass of a quadrupole mass spectrometer has been recognized for several years, but definitive measurements have not been made. This calibration of the quadrupole will be one of the first experiments performed.

The use of the quadrupole will be especially effective in the study of high temperature systems that undergo reasonably rapid changes in chemistry. Whereas minutes are required to change the Nuclide magnet from one mass to another, only a hundred milliseconds is required for the quadrupole.

During the current year an X-Y table was designed and installed in the older quadrupole mass spectrometer crucible assembly.

During the contract year a digital voltmeter, whose cost was about $6,000, was made available to the high temperature group by the Department of Chemistry. It had been purchased for a faculty member who had resigned. It will be used with the quadrupole mass spectrometer.

The small Hewlett-Packard 2100A computer arrived on November 17. Part of its cost was provided under the contract. Software to enable it to operate in a multiprogramming mode was purchased with other funds. The real-time executive operating system is currently being tested. We should be able to control both the Nuclide and the quadrupole mass spectrometer from the computer and to take data from both concurrently. Alternatively, either could be run as a foreground job while the background is used for program development.

Computer Programs. In addition to the six major computer programs for on-line, real-time data acquisition and equipment control that were described last year, several other major programs have been written. One of the programs available last year was to measure, monitor, and record intensities of signals from the Nuclide mass spectrometer as a function of time. Another was to measure ionization efficiency curves. Another was to obtain shutter profiles. Another was a display program. Another read information from the multichannel analyzer into the computer for storage on the disc or magnetic tape. Sheldon has written five time-of-flight programs that have been prepared with two purposes in mind. They were used as an aid in designing the chopping assembly and the Nuclide extension housing. Secondly they will be used for comparing experimentally measured time-of-flight curves with computer predicted curves as an aid in identifying neutral precursors of ions observed with the mass spectrometers. He also wrote another program to help determine under what conditions the modulation of background gases may be a problem in modulated beam experiments. As has previously been mentioned, Bennett has prepared programs for retrieving data previously stored from Nuclide experiments. Huang has written two major programs. The first of these takes the scientist's input of mass numbers on the teletype and then causes the magnet of the Nuclide mass spectrometer to change until the desired ion is brought to focus, albeit slowly. This program uses the subroutine described last year to find the setting for maximum intensity, and to keep the mass spectrometer focussed. The other program was written to enable computer readings of the temperatures. Mr. Fast, supported by the Chemical Physics Trilevel Computer Network activity, redesigned the program running the Nuclide for measuring the intensity of an ion as a function of time to a greatly enhanced program to run the quadrupole mass spectrometer. Rinehart has written some display programs for high temperature data.

LEVEL OF ACTIVITY

The employment of personnel occurred at substantially the level specified in the revised budget. Considerable support to the program was provided by the arrival of Professor J. Edward Bennett of Arkansas State University who is spending his sabbatical year at the University. His base of operations is the high temperature laboratory. He is a splendid influence on the postdoctoral research associates and the graduate students. He participates actively in the group seminars, and he is a very welcome addition.

MISCELLANEOUS

Several activities at the national level may be mentioned. 1. Professor Gilles was recently elected to the Board of Trustees of Argonne Universities Association. 2. He served as Chairman of the Review Committee for the Division of Chemical Engineering of Argonne National Laboratory. 3. He serves on an Advisory Committee to the Argonne National Laboratory Center for Educational Affairs. 4. He continues to serve on the Editorial Board of *High Temperature Science*. 5. He serves on the National Research Council Committee on Computers in Chemistry. 6. He serves on the Editorial Board of *Advances in High Temperature*.

On the local level: 1. Professor Gilles was recently elected to the newly constituted Committee on Graduate Studies of the College of Liberal Arts and Sciences. He was elected by the committee to be its chairman. 2. He serves on the Board of Directors of the University of Kansas Center for Research, Inc. 3. He served on a Phi Beta Kappa election committee. 4. He served on the Faculty Selection Committee seeking a chairman for the Department of Mathematics. 5. Some of the high temperature work was featured in two places in the departmental brochure entitled, "Marks of Excellence." 6. His wife was elected President of the Board of Education of Unified School District No. 497 encompassing the Lawrence community and surrounding rural areas.

VAPORIZATION OF CONDENSED PHASES
CLASSIFICATION OF THE SINGLE MOST IMPORTANT REACTION

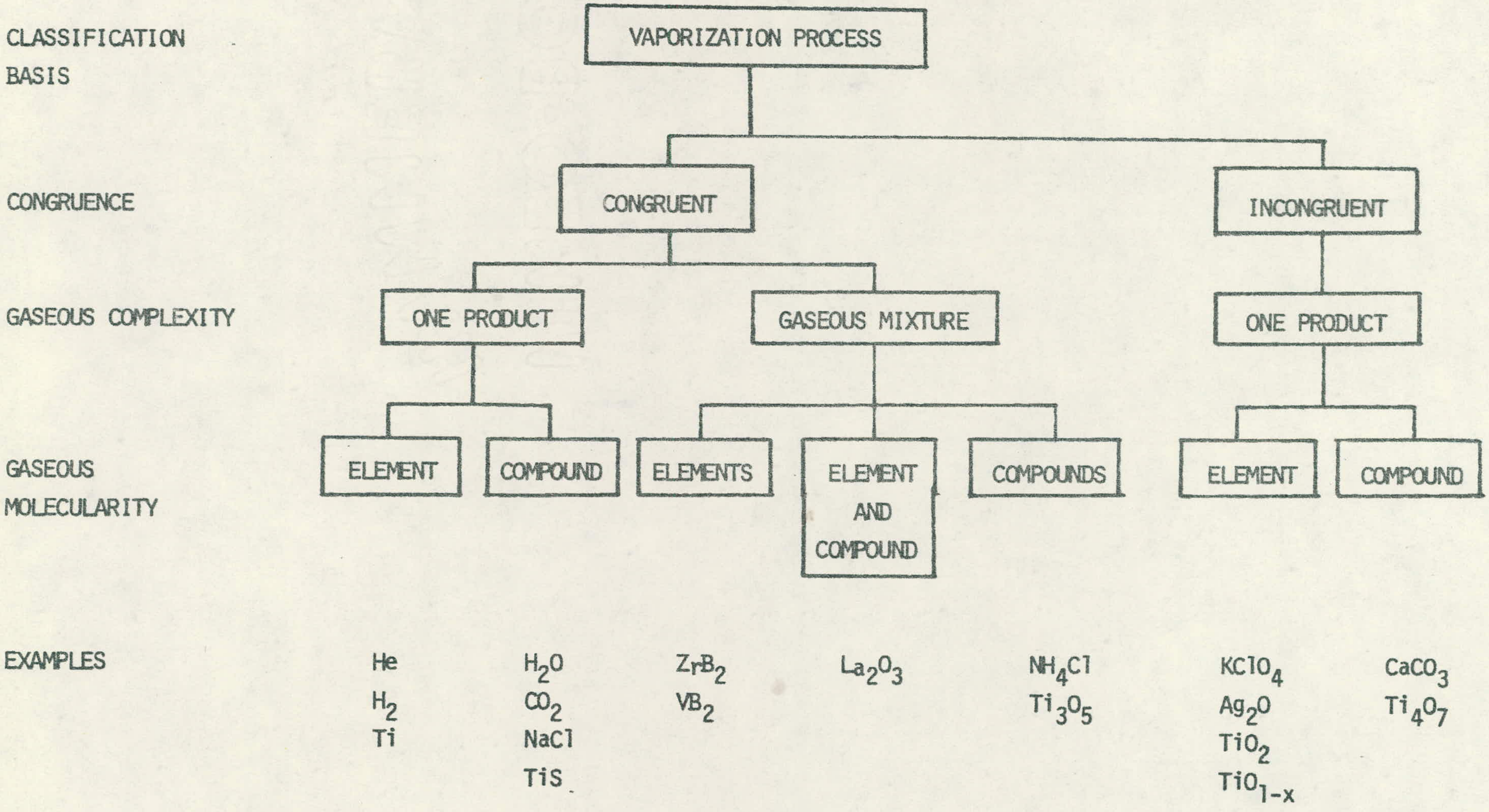

FIGURE 1

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TABLE I
Scientists Trained in High Temperature Chemistry at the University of Kansas

Name	Degree	Year	Present Location
Margrave, John L.	Ph.D.	1950	Department of Chemistry, Rice University
Pollock, Bernard D.	Ph.D.	1953	Explosives Laboratory, Picatinny Arsenal
Wheatley, Quentin D.	Ph.D.	1954	Electrochem., du Pont, Niagara Falls
Milne, Thomas A.	Ph.D.	1954	Physical Science Div., Midwest Research Inst.
Ackermann, Raymond J.	Ph.D.	1955	Chemistry Div., Argonne Nat'l. Laboratory
Robson, Harry E.	Ph.D.	1958	Esso Research Laboratories, Baton Rouge
Carlson, K. Douglas	Ph.D.	1960	Dept. of Chem., Case Western Reserve U.
Cater, E. David	Ph.D.	1960	Dept. of Chemistry, University of Iowa
Leitnaker, James M.	Ph.D.	1960	Metals & Ceramics, Oak Ridge Nat'l. Lab.
Plante, Ernest R.	Ph.D.	1960	U. S. National Bureau of Standards
Knarr, Warren A.	Ph.D.	1960	Pharmacy Student, University of Iowa
Franzen, Hugo F.	Ph.D.	1962	Dept. of Chem. & Ames Lab., Iowa State U.
Smith, P. Kent	Ph.D.	1964	Nuclear Mat. Div., Savannah River Lab, duPont.
Killingbeck, Stanley	Ph.D.	1964	Dept. of Chem., Central Missouri State
Lin, Sin-Shong	Ph.D.	1966	Army Mat. & Mechanics Res., Watertown, Mass.
Spear, Karl E.	Ph.D.	1967	Mat. Res. Lab & Mat. Sci. Dept., Penn State
Chen, Horng-yih	Ph.D.	1968	Central Res. Dept., du Pont, Wilmington, Del.
Nordine, Paul C.	Ph.D.	1970	Dept. of Chemical Engineering, Yale
Wu, Richard	Ph.D.	1971	Wright-Patterson Air Force Base
Peterson, Dean E.	Ph.D.	1972	CMB-5 Los Alamos Scientific Laboratory
Eick, Harry A.	Post Ph.D.	1958	Dept. of Chem.,Michigan State University
Wahlbeck, Phillip G.	Post Ph.D.	1960	Dept. of Chem., Wichita State University
Wall, John G. L.	Post Ph.D.	1960	Monsanto Chem. Ltd., Belgium
Westman, Sven	Post Ph.D.	1962	Inst. for Inorg. Chem., U of Stockholm
Greene, Frank T.	Post Ph.D.	1962	Physical Science Div., Midwest Research Inst.
Wang, Chih Chun	Post Ph.D.	1963	RCA Laboratories, Princeton, N. J.
Wiedemeier, Heribert	Post Ph.D.	1964	Dept. of Chem. Rensselaer Polytechnic Inst.
Lewis, Gordon	Post Ph.D.	1964	Dept. of Ceram. Eng., Univ. of Mo., Rolla
Hobrock, Don L.	Post Ph.D.	1965	Mound Laboratory, Miamisburg, Ohio
Edwards, Jimmie G.	Post Ph.D.	1967	Dept. of Chemistry, University of Toledo
Petzel, Thomas	Post Ph.D.	1967	Chem. Lab., Univ. of Freiburg, Germany
Bennett, Stephen L.	Post Ph.D.	1968	Dept. of Chem., Rice University
Bergner, Dieter	Post Ph.D.	1968	Farbwerke Hoechst, Frankfurt, Germany
Hampson, Peter J.	Post Ph.D.	1970	Cent. Elect. R. L., CEGB, Leatherhead, England
Mertin, Wilhelm	Post Ph.D.	1971	Inorg. Chem. Inst., U. of Giessen, Germany
Castles, Jeffrey R.	Post Ph.D.	1971	Melbourne, Australia
Conard, Bruce R.	Post Ph.D.	1972	International Nickel, Ltd., Ontario, Canada
Sullivan, C. Larry	Post Ph.D.	1973	Avila College, Kansas City, Missouri
Richardson, Paul J.	M.S.	1950	Lewis Res. Center, NASA, Sandusky, Ohio
Unruh, Carl M.	M.S.	1954	Battelle-Northwest, Richland, Washington
Jackson, Donald D.	M.S.	1958	Lawrence Radiation Lab., Livermore, Calif.
Ernick, Frederick	M.S.	1961	Silicon Transistor Corp., Garden City, N.Y.
Stone, G. Duane	M.S.	1962	Parlin Res. Lab., du Pont, Wilmington, Del.
rner, Donald W.	M.S.	1965	Uncertain

TABLE II

Distribution of Scientists Trained in High Temperature Chemistry at the University of Kansas

Type of Institution	People
Universities	Margrave, Carlson, Cater, Franzen, Spear, Eick, Wahlbeck, Westman, Wiedemeier, Lewis, Edwards, Petzel, Mertin
College	Killingbeck, Sullivan
AEC Laboratories	Ackermann, Leitnaker, Smith, Hobrock, Unruh, Jackson, Peterson
Research Establishments	
Army Materials & Mechanics Research	Lin
Midwest Research Institute	Milne, Greene
NASA	Richardson
National Bureau of Standards	Plante
Picatinny Arsenal	Pollock
Industry	Wheatley, Robson, Wall, Wang, Bergner, Hampson, Ernick, Stone, Chen, Conard
Postdoctoral Study	Bennett, Nordine, Wu
Student	Knarr
Uncertain	Werner, Castles

TABLE III

Scientists Currently in High Temperature Chemistry Research at the University of Kansas

Name	Degree	Year	Remarks
Sheldon, Robert	Ph.D.	1974	
Huang, John	Ph.D.	1975	
Rinehart, Gary	Ph.D.	1975	
Behrens, Robert G.	Post Ph.D.		Educated with Rosenblatt at Penn. State
Bennett, J. Edward	Sabbatical Leave Professor		Educated with Freeman at Oklahoma State

TABLE IV

Visitors at the University of Kansas
Of Interest to High Temperature Chemists
For the Period 1972, November 1, to 1973, October 31

No.	Visitor	Title of Talk	Date Visited
V-198	Prof. Gordon A. Gallup University of Nebraska Lincoln, Nebraska	"Recent Results in Ab Initio Valance Bonds Calculations"	72, Nov. 3
V-199	Dr. Gary Sigai Xerox Corporation Rochester, N. Y.	"Research at RPI"	72, Nov. 9
V-200	Prof. C. G. Enke Michigan State University East Lansing, Michigan	"Data Domains and Chemical Instrumentation"	72, Nov. 14
V-201	Dr. Arthur Breipohl Electrical Engineering University of Kansas Lawrence, Kansas	"The Energy Future"	72, Nov. 15
V-202	Prof. Phillip G. Wahlbeck Wichita State University Wichita, Kansas	"Failure of Isotropy"	72, Nov. 16
V-203	Mr. Tom Eagle Western Electric Company	"Process Control in Wafer Preparation for Semiconductor Devices."	72, Nov. 28
V-204	Dr. Bernard Abraham Argonne National Laboratory Argonne, Illinois	"Why and How of Ultrasonic Measurements"	72, Dec. 4
V-205	Dr. Dean E. Peterson Los Alamos Scientific Lab. Los Alamos, New Mexico	"High Temperature Chemistry in Isotopic Power Packages"	72, Dec. 5
V-206	Dr. Virgil Wallentine Kansas State University Manhattan, Kansas	"Process Control Languages"	72, Dec. 5
V-207	Prof. Charles L. Wilkins University of Nebraska Lincoln, Nebraska	"Computer Controlled Fourier Transform NMR"	73, Feb. 7

No.	Visitor	Title of Talk	Date Visited
V-208	Prof. J. W. Culvahouse University of Kansas Lawrence, Kansas	"The University of Kansas Chemical Physics Trilevel Computer Network"	73, Feb. 12
V-209	Prof. Richard B. Bernstein University of Wisconsin Madison, Wisconsin	"Energy Disposal and Energy Requirements of Chemical Reactions"	73, Feb. 13
V-210	Prof. Heribert Wiedemeier Rensselaer Polytechnic Inst. Troy, New York	"Sublimation and Condensation -- Crystal"	73, April 9
V-211	Prof. David Buckingham University of Cambridge Cambridge, England	"Molecules in Electric and Magnetic Fields"	73, April 13
V-212	Dr. Charles R. Morgan W. R. Grace & Company Clarksville, Maryland	"Photopolymerization"	73, April 14
V-123	Prof. Robert J. Friauf Department of Physics University of Kansas Lawrence, Kansas	"Application of Chi Square Tests to Analysis of Anomalous Ionic Conductivity in the Silver Halides"	73, Sept. 17
V-124	Dr. Charles Bender Lawrence Radiation Lab. Livermore, California	"*Ab Initio* Calculations of Potential Energy Surfaces, Including $H+F_2$ and CH_2+H_2 (singlet and triplet)."[2]	73, Oct. 18

TABLE V

Publications Resulting From
High Temperature Chemistry Research

Articles Published

A-81. "Electron Microscopy Studies of the Surface Structure of KCl Crystals Vaporized Under Near-Equilibrium Conditions." Jeffrey R. Castles and Paul W. Gilles. Reactivity of Solids, Chapman and Hall, London (1973), pp. 672-702.

Articles Accepted for Publication

COO-1140-204. "Rare Earth Sulfides at High Temperature. I. On the Existence of Equilibrium in Knudsen Cells." Richard L. C. Wu and Paul W. Gilles. J. Chem. Phys.

COO-1140-208. "High-Temperature Vaporization of Ternary Systems. I. Mass Spectrometry of Oxygen-Rich Vanadium-Tungsten-Oxygen Species." Stephen L. Bennett, Sin-Shong Lin, and Paul W. Gilles. J. Phys. Chem.

Articles Submitted

COO-1140-209. "Chemistry of Vaporization of Refractory Materials." Paul W. Gilles. J. Amer. Ceramic Soc.

COO-1140-210. "The Role of Vaporization Studies and Mass Spectrometry in the Thermodynamics and Phase Relations of Nuclear Materials." Paul W. Gilles. J. Nuclear Materials.

TABLE VI

Talks and Papers at Meetings

T-168 Kansas City Section of Association for Computer Machinery, Kansas City, Missouri. Invited talk -- "The Chemical Physics Trilevel Computer Network at the University of Kansas." 1973, January 17.

T-169 Department of Chemistry, Wichita State University, Wichita, Kansas. Invited talk -- "The Chemical Physics Trilevel Computer Network at the University of Kansas." 1973, March 28.

T-170 High Temperature Chemistry Symposium, American Ceramic Society Meeting, Cincinnati, Ohio. Invited talk -- "Chemistry of Vaporization of Refractory Materials." 1973, April 30.

T-171 Graduate Physics Colloquium, University of Kansas, Lawrence, Kansas. Invited talk -- "High Temperature Studies of the Titanium Oxides." 1973, May 7.

T-172 Mid West High Temperature Chemistry Conference, Northwestern University, Evanston, Illinois. "Time-of-Flighting Identity of Neutral Molecules." Robert I. Sheldon and Paul W. Gilles. 1973, June 25

T-173 Mid West High Temperature Chemistry Conference, Northwestern University, Evanston, Illinois. "Mass Spectrometric Studies of Transition and Rare Earth Sulfides." Robert G. Behrens and Paul W. Gilles. 1973, June 25.

T-174 Mid West High Temperature Chemistry Conference, Northwestern University, Evanston, Illinois. "Vaporization Kinetics of Lithium Halides." C. Larry Sullivan and Paul W. Gilles. 1973, June 26.

T-175 Mid West High Temperature Chemistry Conference, Northwestern University, Evanston, Illinois. "Computer-Assisted Automatic Pyrometric Temperature Measurements." Yun K. Huang and Paul W. Gilles. 1973, June 26.

T-176 Mid West High Temperature Chemistry Conference, Northwestern University, Evanston, Illinois. "University of Kansas Chemical Physics Trilevel Computer Network." 1973, June 26.

T-177 United States - Japan Cooperative Science Program Seminar, "Thermodynamics and Phase Relations of Nuclear Materials," Ames Laboratory, Iowa State University, Ames, Iowa. "The Role of Vaporization and Mass Spectrometry." 1973, July 9-12.