1 of 2

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**PHYSICAL AND CHEMICAL CHARACTERISTICS OF
FLUORINEL/SODIUM CALCINE GENERATED
DURING 30 CM PILOT-PLANT RUN 17**

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Summary

The 30 centimeter (cm) pilot plant calciner Run 17, of March 9, 1987, was performed to study the calcination of fluorinel-sodium blended waste blended at the ratio 3.5:1 fluorinel to sodium, respectively. The product of the run was analyzed by a variety of analytical techniques that included X-ray powder diffraction (XRD), inductively coupled plasma spectroscopy (ICP), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS) to deduce physical and chemical characteristics.

The analytical data, as well as data analyses and conclusions drawn from the data, are presented.

Table of Contents

Acknowledgements	i
Summary	ii
Table of Contents	iii
Table of Tables	v
Table of Figures	vi
Introduction	1
Background	3
Experimental Equipment and Techniques	7
X-Ray Powder Diffraction	7
Inductively Coupled Plasma Emission Spectroscopy, ICP	8
Scanning Electron Microscope Spectroscopy, SEM	9
X-Ray Physical Electron Spectroscopy, XPS	10
Analytical Methods Used to Determine Non-Metal	
Concentrations	11
Chloride	11
Fluoride	11
Nitrate	12
Sulfur	13
Results and Discussion	14
ICP and Non-Metal Determinations	14
X-Ray Powder Diffraction Results	16
SEM Results	19
XPS Data	43
F*A*C*T Program Data	48

Conclusions	52
Appendix A: Point by Point SEM Data for Particle 1	54
Appendix B: Point by Point SEM Data For Particle 2	60
Appendix C: Point by Point SEM Data For Particle 3	65
Appendix D: General Composition SEM Data For Small Particles	69
Appendix E: General Composition SEM Data For Medium Particles	76
Appendix F: General Composition SEM Data For Large Particles	82
Appendix G: XPS Raw Data	87
Appendix H: F*A*C*T EQUILIB Results	129
References	142

Table of Tables

Table I: Simulated Fluorinel Waste, Sodium Waste, and Blend Compositions	5
Table II: Element Concentrations in Run 17 Calcine	15
Table III: SEM Data: Elemental Weight Percents for Particle 1 From Point Analysis	23
Table IV: SEM Data: Weight Percent Elements in Particle 2 From Point Analysis	27
Table V: SEM Data: Weight Percent Elements in Particle 3 From Point Analysis	31
Table VI: SEM Data: Weight Percent Elements in Small Particle Size	34
Table VII: SEM Data: Weight Percent Elements in Medium Particle Size	35
Table VIII: SEM Data: Weight Percent Elements in Large Particle Size	36
Table IX: Atomic Concentrations of Elements Found in Calcine	45
Table X: Compounds Found By XPS Analysis That Are Most Likely To Be In Run 17 Calcine	47
Table XI: Products Resulting From F*A*C*T Program	49

Table of Figures

Figure 1: XRD Diffractogram for Run 17 Calcine	18
Figure 2: Particles Chosen for Point by Point Analysis . . .	20
Figure 3: Particle 1: Locations of Point Analyses	22
Figure 4: Particle 2: Locations of Point Analyses	26
Figure 5: Particle 3: Locations of Point Analyses	30
Figure 6: Particles Chosen for General Composition Determinations	33
Figure 7: X-Ray Mapping of Particle 1	38
Figure 8: X-Ray Mapping of Particle 1	39
Figure 9: X-Ray Mapping of Particle 2	40
Figure 10: X-Ray Mapping of Particle 2	41
Figure 11: X-Ray Mapping of Particle 3	42
Figure 12: ESCA Scan	44

Introduction

Most of the calcines generated in the Idaho Chemical Processing Plant (ICPP) pilot plants and the full-scale facility have never been thoroughly characterized. As a result, the distribution of crystalline and amorphous phases, and the chemical compositions of these phases in the calcine particles, are unknown. During many discussions of calcination, it has been generally assumed that all the non-volatile components of the aqueous calcine feed formed oxides in the solid calcine. It was important to test the reasonability of this assumption because the phase distribution and chemical composition of calcine is important input information for the design of future ICPP processes for calcine immobilization, and for the development of future calcination flowsheets.

Future processes necessary for calcine immobilization includes calcine grinding and transport. The distribution of compounds in the calcine must be known in order to determine calcine homogeneity. The homogeneity of calcine will influence grinding parameters; the less homogenous the calcine, the smaller it must be ground for the immobilization process. Particle size is important because it will impact the development of the processing equipment required for calcine immobilization.

Knowledge about the phase behavior of calcine is beneficial input data for waste form development and for deduction of the chemistry of the calcination process. Knowing the chemical forms of each species in the calcine could contribute to waste forms development, particularly to the understanding of the chemical reactions taking place during the formation of glass and glass-ceramic materials from admixtures of calcine and glass-forming materials. A knowledge of the chemistry that is occurring in the calcination process could also lead to the development of new calcination flowsheets needed for faster depletion of the sodium waste inventory and new calcination flowsheets that could result in greater waste volume reductions when the liquid waste is converted to the solid calcined product.

Background

High level radioactive liquid wastes (HLW) of various chemical compositions have been produced at the ICPP during the reprocessing of spent reactor fuels. The composition of the liquid waste is dependent on the fuel type. The classifications of liquid wastes, and the associated calcined products, include: aluminum HLW, which is calcined to produce alumina calcine; stainless steel HLW, which is calcined to produce stainless steel calcine; zirconium HLW, which is calcined to produce zirconia calcine or is blended with sodium waste and calcined to produce zirconia-sodium calcine; and fluorinel HLW, which calcined to produce fluorinel calcine or is blended with sodium waste and calcined to produce fluorinel-sodium calcine. These HLW solutions are the aqueous raffinates that were generated during the uranium recovery from the highly radioactive dissolver product solution and were stored in underground tanks prior to calcination. Sodium waste is generated during solvent clean-up and decontamination processes; it is segregated from other process solutions and is also stored in underground tanks prior to calcination.

During ICPP Pilot Plant Run 17, the 30 cm pilot-plant calciner was used to generate calcine, at temperatures near 500°C (773 K), from a non-radioactive blend of simulated fluorinel and sodium wastes; the blend ratio was 3.5:1 fluorinel to sodium,

respectively. Table I lists the compositions of the simulated wastes and the composition of the 3.5:1 blended feed. The non-radioactive product generated during Run 17 was generated to simulate the highly radioactive fluorinel/sodium calcine generated at the New Waste Calcine Facility (NWCF).^a Since the radionuclide content in the calcine is less than 1% by weight¹, this simulated calcine should be very representative of the highly radioactive product produced at NWCF.

Fluidized bed calcination at the NWCF is performed at temperatures near 773 K; amorphous and crystalline phases are formed in the calcine. XRD has historically been used to determine the compositions of the crystalline phases present in the calcine; however, quantitative analytical determinations of the amorphous phase composition has never been done. Consequently, little is known about the quantity and composition of the non-crystalline phases. ICP has been the preferred method for determination of the concentrations of cations in the calcine. The calcine was solubilized prior to the ICP analyses by digestion in an acidic solution. The ICP analyses do not identify the anions present in the analyzed solution so it has been assumed that the cations exist in the calcine as oxide phases. The possible presence of alloys or multiple metal complexes were not generally considered during routine analyses.

^a As of the end of 1986, 430 m³ of 3.5:1 (fluorinel:sodium) blend calcine was on inventory at the ICPP. See reference 1 at the end of this document.

Table I

Simulated Fluorinel Waste, Sodium Waste, and Blend Compositions

Component	Fluorinel Waste Composition (Molar)	Sodium Waste Composition (Molar)	3.5:1 Blend Composition (Molar)
Zr	0.33	*	0.25
Al	0.36	0.42	0.44
B	0.19	0.008	0.15
Ca	†	†	1.39
F	2.54	0.039	1.98
Na	*	1.39	0.31
K	*	0.22	0.049
Cd	0.11	*	0.086
H ⁺	1.44	1.81	1.61
SO ₄ ⁻²	0.07	0.065	0.069
NO ₃ ⁻	2.05	4.73	2.65
Cl	*	0.028	0.006

† added to feed after blending

* not in feed

The formation of compounds other than oxides could result in a more favorable greater waste volume reduction, when the liquid waste is converted to calcine, if these other phases had smaller molar volumes. As waste volume reduction values are used to determine calcine storage space currently being used (these numbers are compiled based on the formation of oxides), and to estimate future storage space requirements, it would be advantageous to have more information about the phase behavior of HLW calcines. With these uncertainties in mind, the product of

the 30 cm Run 17 has been selected for further study to identify its phase behavior.

Because of the need to identify the chemical composition of both phases, Run 17 calcine was further examined by Scanning Electron Microscope Spectroscopy (SEM) and X-Ray Photoelectron Spectroscopy (XPS).

Experimental Equipment and Techniques

Four analytical techniques were utilized to identify the composition of the phases, both crystalline and amorphous, present in a sample of Run 17 pilot plant calcine. The analytical techniques were selected based on availability and the type of information (quantitative identification of cations or anions, identification of crystalline and amorphous phase compositions, and physical characteristics of the multiphase calcine particles) desired.

X-Ray Powder Diffraction

X-Ray diffraction was used to determine the crystalline phases in the calcine particles. Calcine analyzed by this method was ground to a fine powder with an automated alumina grinding system for 30 minutes, resulting in particle sizes less than 0.0056 inches. This grinding system ensures particle uniformity and sample homogeneity. The finely ground calcine was analyzed on a Phillips XRG-3000 θ 2 θ (theta 2 theta) powder diffractometer with a scintillation detector. X-rays were produced by a tube with a copper target operated at 30 kV and 21 mA. The wavelength of the radiation was nominally 1.542 angstroms, that characteristic of Cu- α radiation, and was filtered through a nickel filter to remove beta radiation.

The signal from the sample was filtered with a graphite monochromator to prevent high backgrounds from x-ray fluorescence emissions. Reflection data were collected from 6° to 76° in 2θ . Detection limits for most crystalline compounds in the complex calcine matrix ranged from 2-5 wt%.

Since each crystalline phase possesses a unique powder diffraction pattern, the data obtained from Run 17 calcine was used as a "fingerprint" to identify the crystalline phases present in the material analyzed.

Inductively Coupled Plasma Emission Spectroscopy, ICP

ICP analyses were performed using a Jobin Yvon model 38 Spectrometer. The atomic emission spectrum of the sampled material was produced by an inductively coupled plasma torch utilizing Ar(g) as the cooling gas. The sample analyzed was prepared by dissolving a known mass of Run 17 calcine (approximately 0.1 gram) in enough 1 M HNO_3 to produce 100.00 mL of solution. The resulting solution was diluted with 1% HNO_3 (by volume) to bring the concentrations of the cations in the solution within the calibration range of the instrument. The cations were analyzed sequentially from duplicate aliquots of solution removed from the same sample.

Scanning Electron Microscope Spectroscopy, SEM

A random sample of Run 17 calcine particles was mounted in an epoxy resin under vacuum to remove all entrained "air" from the porous calcine and epoxy resin. This mount was allowed to cure overnight at room temperature. A thin wafer was cut from the mount to give a good cross section of the calcine particles. This wafer was ground (with silicon carbide papers at 240, 320, 400, and 600 grit and paraffin oil used as the lubricant) and polished (with an organic solvent in which the calcine is insoluble).

Final polishing was performed using 6-9 micron diamond suspensions in nylon cloth, followed by polishing with 1 micron diamond suspensions in synthetic rayon cloth. Samples were then mounted on a glass slide with the polished side down. The glass mounted sample was cut with a slow speed diamond saw to 30 microns. The "cut" or unpolished side of the glass mount was then polished as previously described. The resulting wafer had a thickness of 10 μm . The thin, mounted sample was analyzed with an Amray Model 1830 SEM equipped with a Kevex Delta 5 EDS system; the pressure in the sample chamber was near 10^{-6} mm Hg during each analysis.

Calcine homogeneity was determined by randomly selecting three calcine particles of different sizes, large ($>400 \mu\text{m}$), medium

(100 - 300 μm) and small ($< 100 \mu\text{m}$) for analyses. Points across the diameter of each particle were randomly selected and analyzed. The area of each point was approximately $2 \mu\text{m}^2$. Comparison of the compositions at various points on a single particle provides information pertaining to the homogeneity of that particle. These particles were then "mapped" to determine the elemental composition across the diameter of the particles. Mapping activities provide data that give the distributions of individual elements across the calcine particle.

Fifteen particles, ranging in size from large to small, were also analyzed to quantitatively determine the cross-section surface composition of each particle. These analyses were performed to identify possible relationships between particle size and chemical composition.

X-Ray Physical Electron Spectroscopy, XPS

Run 17 calcine was analyzed by XPS to determine the chemical composition of both amorphous and crystalline phases; an Esca Model 5300 X-ray spectrometer was used for the analyses. The calcine sample was prepared for analysis by grinding it to a fine powder with an alumina mortar and pestle. A portion of the ground material was then placed between two sheets of indium metal to immobilize the powder sample between the two sheets of indium foil. The "indium mount" was used because it would not

interfere with the detection of elements in the calcine as indium was not one of the elements present in the calcine sample.

Analytical Methods Used to Determine Non-Metal Concentrations

Chloride

Chloride concentration in the calcine was determined by X-ray fluorescence using a Phillips FW1404 X-ray spectrometer. A known amount of standard chloride solution (500 mls of 10 ug Cl/ml) was added to one sample of Run 17 calcine, an equal volume of water with no chloride was added to another sample of Run 17 calcine. The mixtures were dried at 65°C. This procedure was repeated for different known chloride additions. The calcine was finely ground with the same automated grinding system used for XRD analysis. Following chloride or water addition and grinding, 4 grams of each sample were pressed into a pellet using a 7 ton press. The pellets were then analyzed for chloride by X-ray Fluorescence Spectroscopy.

Fluoride

An Orion 94-09 Fluoride Ion Selective Electrode was used for fluoride determinations. Calcine sample preparations for fluoride determinations involved a calcine fusion with sodium hydroxide, followed by dissolution of the fused sample to form

aqueous solutions. The fusion converts the fluoride in the calcine, present as calcium fluoride, into buffer-soluble sodium fluoride. The fusion was performed by heating a mixture of known masses of sodium hydroxide and calcine, in a zirconium crucible, at temperatures less than 773 K.

Just as in the chloride analysis, the method of standard addition was used to determine the concentration of fluoride in calcine. The concentration of fluoride was then determined by comparing the electrode responses from the calcine-containing solutions to a standard titration curve (the titration curve for a sample containing only the standard-added amount of fluoride); the fluoride content of the calcine was computed from the difference. Other metal ions present in the solution are prevented from interfering with fluoride detection by buffering the samples to a pH of 7 using sodium citrate, sodium chloride, and triethanolamine.

Nitrate

Nitrate in the calcine was determined by the Kjeldahl method. The calcine was prepared for analysis by grinding it to a fine powder to insure wetting of the surface of the particles by the concentrated sodium hydroxide solution that was used to dissolve/leach the nitrate from the calcine. Nitrate in the sodium hydroxide media was reduced to ammonia with a Devarda's

alloy, with the composition 50% Cu, 45% Al, and 5% Zn. The ammonia was distilled into a boric acid solution and titrated with sulfuric acid to determine the amount of nitrogen present in the sample; the nitrate content was subsequently computed from the nitrogen result.

Sulfur

The calcine was prepared for analysis by first grinding it to a fine powder followed by heating 3 - 4 mg of ground sample to 1023 K, under a flowing gas stream, in the presence of vanadium pentoxide. Vanadium pentoxide acts as a catalyst that speeds the reduction of the condensed sulfur-containing species to $\text{SO}_2(\text{g})$. The volatilized sulfur-containing vapor was then swept over a hot bed of copper oxide to ensure complete conversion sulfur to $\text{SO}_2(\text{g})$. The $\text{SO}_2(\text{g})$ in the gas stream was coulometrically determined using a UIC Inc. Coulometer.

Results and Discussion

ICP and Non-Metal Determinations

Determinations of all metals known to be present in the calcine, except Sr, Hg, Na, and K, were performed by Inductively-Coupled Plasma Emission Spectroscopy. The Sr, Hg, Na, and K concentrations were determined by Atomic Emission Spectroscopy, fluoride was determined by fluoride ion specific electrode, chloride was determined by X-ray fluorescence, sulfur was determined by a colorimetric technique, and nitrate was determined by the Kjeldahl method. The results of these analyses, presented as elemental and ionic weight percents (w/o), are tabulated in Table II.

These results provide valuable insights toward understanding the gross composition of the calcine, however, they do not provide information regarding the phase composition of the calcine, nor do they contribute to determining the spatial distributions of these elements in the solid calcine particle.

ICP, AA, and anionic data are useful for identifying distinct phases when used in tandem with XRD and XPS results. XRD results can be used to identify the crystalline phases present in a sample; XPS results can be used to identify the bonding of elements present in a substance. Since the chemical matrix in

Table II**Element Concentrations in Run 17 Calcine**

Element	Wt % in Calcine
Al	5.61
B	0.96
Ca	24.9
Cd	4.63
Ce	<0.0069
Cr	0.99
Fe	0.33
Mn	0.088
Ni	0.11
Se	<0.24
Sr	0.064
Zr	13.1
Cs	<0.01
Hg	<0.0005
Na	3.5
K	0.80
Cl	2.45 ppm
F	17.3
S	1.07
NO _x	5.87

note: Remainder of mass balance is assumed to be oxygen

calcine is complex, XRD and XPS results identify a number of phases that may be present in the calcine. Consideration of ICP, AA, and anionic results in tandem with the XRD and XPS results can restrict the possible phases that may be present in the calcine; this type of analysis will be presented later in this report.

X-Ray Powder Diffraction Results

The X-ray diffraction data were collected as analog data, as a diffractogram (Figure 1), and as digital data that were stored in a computer disk file. The diffractogram is a plot of intensity (I) of X-rays, in counts-per-second (cps) as measured by the scintillation detector, versus the angle of reflection, 2θ , in degrees ($^{\circ}$). The digital data were compared to a computer database of X-ray diffraction data for a large number of crystalline phases, and the most likely matches with the data were identified.^b As a result of the database search/comparison activity, the crystalline phases identified, as those most likely present in the sample, were CaF_2 , CdS , ZrO_2 , and NaNO_3 ; less likely phases included $\text{Sr}_2\text{Zr}_2\text{O}_7$, $\text{Na}(\text{Ca},\text{Sr})_3\text{Al}_3\text{F}_{16}$, and $\text{Ca}_3(\text{OH})_2\text{Si}_3\text{O}_8$ (which could also be represented by the formula $\text{Ca}_3\text{Si}_3\text{O}_9 \cdot \text{H}_2\text{O}$).

^b The Fein/Marquardt Search Program includes diffraction patterns for all known inorganic crystalline phases.

Figure 1
XRD Diffractogram for Run 17 Calcine

Since the detection limit for XRD is approximately 5 w/o, and the ICP result showed only 0.064 wt % Sr in the calcine, the presence of the strontium compounds, $\text{NaSr}_3\text{Al}_3\text{F}_{16}$ and $\text{Sr}_3\text{Zr}_2\text{O}_7$, is precluded unless the sample was Sr-contaminated. As no likely method of Sr-contamination has been identified, it is assumed that these phases are not present in the calcine. Silicon analysis was not performed by ICP because of the inherent problems with its determination (high background levels and negative interferences caused by Si precipitation during sample preparation). As a consequence of this, and the fact that silicon is present in water and dust, it is possible that the calcine feed was Si-contaminated. It is likely, therefore, that the phases CaF_2 , CdS , ZrO_2 , NaNO_3 , $\text{NaCa}_3\text{Al}_3\text{F}_{16}$, and $\text{Ca}_3\text{Si}_3\text{O}_8(\text{OH})_2$ are present in Run 17 calcine.

XRD results, which are effective for identifying major phases but not quantities of each phase, can be used in conjunction with results of ICP and anionic analyses to provide an upper limit on the quantities of each major crystalline phase, neglecting the amorphous and minor crystalline phase portions. It is not possible to identify the minor phases because the X-ray powder diffraction method lacks sensitivity and the amorphous material in the calcine samples produces x-ray scattering of high amplitude that are quite broad and effectively mask the reflections from minor crystalline phases in the calcine. Because of the limitations of ICP, XRD and the techniques used to

determine the anions, SEM and XPS analyses were performed on samples of Run 17 calcine.

SEM Results

The calcine particles studied by SEM were randomly selected from the prepared sample. Figure 2, an image produced by backscattered 20 kV electrons that shows the particles sizes magnified by a factor of 50 (50X magnification), shows the three calcine particles, labelled 1, 2, and 3 that were selected for point by point analysis (analysis of a surface area of 2 um^2). The surface areas of particles, 1, 2, and 3 are approximately $2 \times 10^5 \text{ um}^2$, $3 \times 10^4 \text{ um}^2$, and $8 \times 10^3 \text{ um}^2$, respectively.

Figure 2. Particles Chosen for Point by Point Analysis

The points selected for point by point analysis of Particle 1 are shown in Figure 3. This figure shows Particle 1 magnified 200X and identifies the five points at which data were collected. The light grey areas of the image indicate crystalline material while the brighter areas of this picture are amorphous regions; this image shows clearly the phase non-homogeneity of the particle. The layered structure of the particle is an artifact of the calcination process. Growth of particles during calcination is a result of the deposition of material on the surface of the particle. Due to the kinetics of the deposition process, some of the layers are crystalline, while others are amorphous.

Table III contains point by point composition data for Particle 1; Appendix A contains the raw SEM data used to generate Table III. The data tabulated for the elements O, F, Na, Al, S, K, Ca, Cr, Mn, Zr, and Cd were collected at the five numbered points identified on Figure 2. There are distinct differences in the chemical compositions of each point. The point to point difference in composition is expected due to the considerations discussed in the preceding paragraph. The weight percent data in Table III were converted to moles and the molar quantities were used to determine the stoichiometry at each point.²

Figure 3. Points Analyzed on Particle Number 1

Table III

SEM Data
Elemental Weight Percents for Particle 1
From Point Analysis

Element	Point Number					
	1	2	3	4	5	Average Wt%
O	11.80	28.81	38.38	49.56	34.24	32.56 ± 13.88
F	41.23	28.86	16.15	15.69	32.95	26.98 ± 11.03
Na	*	1.84	*	2.53	*	0.87 ± 1.22
Al	1.51	2.05	13.50	9.44	8.32	6.96 ± 5.11
S	*	2.37	*	*	*	0.47 ± 1.06
K	0.31	0.33	*	*	*	0.13 ± 0.18
Ca	39.93	42.14	10.55	22.26	22.88	27.55 ± 13.28
Cr	0.13	0.30	0.43	*	0.58	0.29 ± 0.23
Mn	*	*	*	*	0.13	0.026 ± 0.058
Zr	4.85	2.88	24.62	14.57	19.09	13.20 ± 9.26
Cd	1.58	1.36	15.05	6.46	7.57	6.40 ± 5.59

¹ The raw data are tabulated in Appendix A.

² Precision of each measured weight percent value is about 2%; uncertainty of each measured weight percent value is about 10%.

* None Detected

The relative qualitative elemental abundances at point 1, in terms of decreasing mole quantities, are F, Ca, O, Al, Zr, Cd, K, and Cr. The calcium to fluoride ratio (Ca/F) of 0.46 is only slightly less than the value to be expected if all the fluorine were present as fluoride in $\text{CaF}_2(\text{s})$. It is supposed that the metals, other than calcium, are present primarily as oxides, although some crystalline fluorides and nitrates, as well as amorphous material, may also be present.

Point 2 of Particle 1 is located in a region of the particle that contains excess calcium as compared to the Ca/F ratio expected for CaF_2 . It is likely that some of the calcium in this region is present as CaO . The minor metals in this region are probably also present as crystalline oxides and nitrates and amorphous material.

The region in which point 3 is located is compositionally quite different from those containing points 1 and 2. This region (that which includes point 3) has considerable excess fluoride as compared to the Ca/F ratio of CaF_2 . It is most likely that all the calcium in this region is present as CaF_2 ; the remaining fluoride is distributed among the other metals as crystalline fluoride phases or amorphous materials.

Point 4, like point 2, has an excess of calcium compared to the Ca/F ratio of CaF_2 . The high concentrations of Al, Zr, and Cd in

this region, as compared to the three previously discussed points, suggests that these metals are present in crystalline and/or amorphous phases that probably do not contain much fluoride.

Point 5, like point 3, has an excess of fluoride compared to the Ca/F ratio of CaF_2 . It is most likely that all the calcium exist as CaF_2 ; the remaining fluoride is probably distributed between the Cd, Al, and Zr. The excess fluoride concentration at points 3 and 5 seem to be correlated with high zirconium concentrations. An actual correlation between high fluoride concentrations and high zirconium concentration has not been previously identified, but this result may indicate that the formation of ZrF_4 is favorable as compared to AlF_3 and CdF_2 .

Figure 4 is a picture of Particle 2 at 300X magnification. At high magnification, the distribution of the amorphous and crystalline phases is more pronounced than for the lower magnification image of Particle 1. Areas where point analysis were taken are also shown in this figure. Table IV lists the concentrations of the elements found at each point. As in the point analysis of Particle 1, points analyzed on Particle 2 differ considerably. Appendix B contains the raw SEM data used to generate Table IV.

Figure 4. Points Analyzed on Particle Number 2

Table IV
SEM Data
Weight Percent Elements in Particle 2
From Point Analysis

Element	Point Number				
	1	2	3	4	Average Wt%
O	54.82	*	54.62	19.55	32.25 ± 27.15
F	9.76	45.84	6.43	43.74	26.44 ± 21.25
Na	*	*	0.63	*	0.16 ± 0.31
Al	14.00	0.88	14.22	4.42	8.38 ± 6.77
S	*	*	*	*	0.00 ± 0.00
K	*	0.32	*	*	0.08 ± 0.16
Ca	13.17	44.74	18.27	38.84	28.76 ± 15.39
Cr	*	*	*	*	0.00 ± 0.00
Mn	0.24	*	*	*	0.06 ± 0.12
Zr	25.83	2.72	11.97	4.60	11.28 ± 10.49
Cd	11.21	1.32	12.52	3.18	7.06 ± 5.63

¹ The raw data are tabulated in Appendix B.

² Precision of each measured weight percent value is about 2%; uncertainty of each measured weight percent value is about 10%.

* None detected

Point 1 on Particle 2 has an excess of calcium as compared to the Ca/F ratio of CaF_2 . High aluminum and zirconium concentrations in the region might lead to a distribution of fluoride among these metals but it is more likely that these elements are present, in crystalline phases, as oxides, or as amorphous phases. Unlike points 3 and 5 of Particle 1, there is not an excess of fluoride with the high zirconium concentration, suggesting there is no correlation between excess fluoride with high zirconium concentrations. Because of the high concentrations of zirconium and aluminum, it is difficult to determine the extent of the metal-fluoride formation compared to the metal-oxide formation, but it is likely that most of the fluoride is present as crystalline CaF_2 .

Point 2 on this particle has a Ca/F ratio slightly less than that of CaF_2 . When the moles of excess fluoride are compared to the moles of aluminum, zirconium, and cadmium found in this region, there is stoichiometrically enough fluoride to form AlF_3 , ZrF_4 , and CdF_2 . The formation of these metal-fluoride compounds seems likely because of the lack of oxygen in the region.

Excess calcium, as compared to the Ca/F ratio of CaF_2 , is found at point 3. High concentrations of aluminum, zirconium, and cadmium are also present, leading to the conclusion that crystalline, oxide and/or nitrate phases, and/or amorphous phases are present in the region.

At point 4 there is excess fluoride as compared to the CaF_2 stoichiometry. This area most likely is CaF_2 , with minor concentrations of AlF_3 , ZrF_4 and/or CdF_2 . The hypothesized presence of these other metal-fluoride compounds is supported by the low concentration of oxygen, which means that oxide- and nitrate-containing phases are present only in small concentrations.

Figure 5 is a picture of Particle 3 at a magnification of 1000X. This particle has a higher density of the amorphous phase than the two larger particles, 1 and 2. If point 2 is representative of the amorphous areas, ZrO_2 could be the primary constituent in the amorphous phase, as could a nitrate-containing phase. Table V lists the concentrations of the elements found at each point. Appendix C contains the raw SEM data used to generate Table V.

Point 1 on Particle 3 contains very nearly stoichiometric amounts of fluoride and calcium as compared to the ideal composition of CaF_2 . The minor constituents of this region are most likely metal oxides or nitrates, crystalline or amorphous, present in very low concentrations, as indicated by the lack of oxygen in this region.

Point 2 is probably ZrO_2 , with a minor amounts of CaO , Al_2O_3 , and CdO , although nitrates might also be present. The relative stability of the crystalline nitrates, as compared to oxides,

Figure 5. Analyzed Particle Number 3

Table V
SEM Data
Weight Percent Elements in Particle 3
From Point Analysis

Element	Point Number			
	1	2	3	Average Wt%
O	7.91	49.54	50.88	36.11 ± 24.43
F	37.22	*	*	12.41 ± 21.49
Na	*	*	2.76	0.92 ± 1.59
Al	0.94	5.87	0.32	2.36 ± 3.01
S	*	*	4.15	1.38 ± 2.40
K	0.35	*	0.20	0.18 ± 0.18
Ca	43.00	10.80	21.18	24.99 ± 16.44
Cr	*	1.01	*	0.34 ± 0.58
Mn	*	*	*	0.00 ± 0.00
Zr	5.31	39.40	1.51	15.41 ± 20.87
Cd	1.87	7.38	0.63	3.29 ± 3.59

¹ The raw data are tabulated in Appendix C.

² Precision of each measured weight percent value is about 2%; uncertainty of each measured weight percent value is about 10%.

* None Detected

suggests that amorphous regions might be high in nitrate; no fluoride was detected in this region.

An evaluation of point 3 shows the multiphase character of this particle. This point is probably quite high in CaO, with minor amounts of Al_2O_3 and ZrO_2 , although it is not clear if these are amorphous or crystalline phases; it is also possible that nitrates might be present. The relatively high concentration of sulfur in this region indicates a great likelihood that CdS (found by XRD analysis), as well as sulfate phases that possibly include K_2SO_4 , are present. Excess sulfur would still exist if all the potassium and cadmium formed sulfur compounds, leading to the conclusion that other sulfate phases, such as CaSO_4 , are probably present.

From the point by point analyses done on Particles 1, 2, and 3 it is seen that the compositions differ across the cross-sectional surfaces of the sample particles. These results clearly indicate that the particles are inhomogeneous and multiphase in character. Analyses were performed on fifteen randomly chosen particles of different sizes to deduce any correlation between gross composition and particle size; Figure 6 is a photograph labelled to identify those particles analyzed.

Figure 6. Particles Chosen for General Analysis

Table VI
SEM Data
Weight Percent Elements in Small Particle Size

Element	Particle Number						
	3	8	10	11	12	13	Average Wt%
O	31.64	26.24	32.24	23.92	27.60	28.82	28.41 ± 3.19
F	25.21	32.27	22.74	26.36	26.92	24.59	26.35 ± 3.25
Na	1.59	0.97	1.17	0.34	0.14	0.59	0.80 ± 0.54
Al	5.14	3.67	4.90	5.69	6.06	6.09	5.26 ± 0.91
S	1.34	0.45	0.52	0.37	0.46	0.50	0.61 ± 0.36
K	*	0.26	*	*	*	*	0.043 ± 0.11
Ca	22.04	29.00	21.03	25.65	25.95	24.00	24.61 ± 2.90
Cr	1.28	*	1.25	0.17	0.16	0.28	0.52 ± 0.58
Mn	*	*	*	0.13	0.16	0.10	0.065 ± 0.074
Zr	13.56	9.66	12.47	14.49	14.15	15.10	13.24 ± 1.97
Cd	5.00	3.19	4.24	5.00	5.21	4.97	4.60 ± 0.77

¹ The raw data are tabulated in Appendix D.

² Precision of each measured weight percent value is about 2%; uncertainty of each measured weight percent value is about 10%.

* None Detected

Table VII
SEM Data
Weight Percent Elements in Medium Particle Size

Element	Particle Number					
	2	6	7	9	15	Average Wt%
O	30.51	30.38	29.22	30.84	29.66	30.12 ± 0.66
F	27.40	25.11	25.89	27.53	24.58	26.10 ± 1.33
Na	0.55	1.05	0.32	1.15	0.60	0.73 ± 0.35
Al	5.23	4.98	5.30	5.47	5.41	5.28 ± 0.19
S	0.50	0.26	0.31	0.42	0.57	0.41 ± 0.13
K	0.12	0.17	*	0.17	0.09	0.11 ± 0.07
Ca	24.90	22.03	25.16	25.04	24.88	24.40 ± 1.33
Cr	0.16	0.46	0.72	0.13	0.09	0.31 ± 0.27
Mn	*	*	0.09	*	0.05	0.028 ± 0.041
Zr	11.79	12.41	12.23	13.19	13.72	12.67 ± 0.77
Cd	5.31	3.13	5.04	5.07	5.17	4.74 ± 0.91

¹ The raw data are tabulated in Appendix E.

² Precision of each measured weight percent value is about 2%; uncertainty of each measured weight percent value is about 10%.

* None Detected

Table VIII
SEM Data
Weight Percent Elements in Large Particle Size

Element	Particle Number				
	1	4	5	14	Average Wt%
O	28.96	30.59	25.84	30.37	28.94 ± 2.19
F	28.44	26.00	26.63	28.56	27.41 ± 1.29
Na	1.67	0.62	0.21	0.65	0.79 ± 0.62
Al	6.09	6.27	4.97	5.59	5.73 ± 0.58
S	0.69	0.46	0.41	0.25	0.45 ± 0.18
K	0.11	*	0.14	0.23	0.12 ± 0.095
Ca	25.48	24.93	27.47	24.76	25.66 ± 1.25
Cr	1.33	0.07	0.18	0.48	0.52 ± 0.57
Mn	0.08	0.15	0.09	*	0.080 ± 0.062
Zr	11.28	14.52	11.55	14.08	12.86 ± 1.68
Cd	4.69	4.90	5.17	3.22	4.50 ± 0.87

¹ The raw data are tabulated in Appendix F.

² Precision of each measured weight percent value is about 2%; uncertainty of each measured weight percent value is about 10%.

* None Detected

The analyzed particles were grouped into three categories by their relative sizes: large, medium and small. Data from the analysis of each size particle was collated according to particle size. Tables VI-VIII list the results from the analyses of small, medium, and large particles, respectively. The raw SEM data used to generate Tables VI through VIII are found in Appendices D through F, respectively. As these results show, there is no correlation between the composition and size of these particles. Good compositional agreement for most elements is found between the SEMS results and the results obtained by other analytical techniques. Fluoride and sodium are exceptions, showing disagreement.

X-Ray mapping was also done on particles 1, 2, and 3. This mapping shows the distribution of the major elements throughout the individual particle. These maps are shown in Figures 7-11. X-Ray mapping data shows fairly even distribution of O, F, Al, Ca, Zr, and Cd throughout the particles. Chromium in particle 3 is seen to be unevenly distributed with heavy concentrations at the center and edges of the particle.

Figure 1. A R-17 Particle 1 200X

Figure 5. A Raman Map of Fluorine (F) and Zirconium (Zr).

Figure 9. X-Ray Mapping of Particle Number 2

Figure 10 X-Ray Mapping of Particle Number 2

Figure 11. A Rho Mapping of Particle Number 11

XPS Data

XPS analysis was performed to identify the chemical bonding of the metal atoms present in the calcine particles. Figure 12 is the XPS data obtained from an energy scan of the calcine. The x-axis represents the energy required to remove an electron from an atom in the sample, in electron volts (eV); the y-axis is a relative measure of the number of electrons ejected from the sample. Adjacent to each peak on the spectrum is a label that includes: the elemental symbol followed by an energy level/sublevel designation for the electron that would be ejected from an atom of that element, at the given binding energy. The specific amount of energy required to displace an electron (Binding Energy) from an atom is dependant on the chemical bonding of the atom. Because specific binding energies are associated with compounds, not elements, the chemical form of the elements in a sample may be identified by XPS analysis.

The calcine is a very complicated chemical matrix; subsequently, the spectrum exhibits broad energy peaks. These broad peaks make data interpretation very difficult because of the large number of compounds associated with a narrow range of binding energies. Small shifts in binding energy may also be caused by a large number of different elements and a rough-surfaced sample. As both of these attributes are exhibited by calcine, this adds even

Figure 12

ESCA Scan

ESCA SURVEY 12/1/92 ANGLE= 15 deg ACO TIME=59.64 min
 FILE: Brewer-1 Calcine run #17 from K. Brewer at CPP. as received.
 SCALE FACTOR= 1.913 k c/s. OFFSET= 0.460 k c/s PASS ENERGY= 89.450 eV Mg 400 N

greater uncertainty to the conclusions that may be drawn from these analytical results.

As seen on Figure 12, elements found in the calcine are: carbon, oxygen, fluoride, cadmium, calcium, zirconium, sodium, chloride, silicon, and aluminum. Some elements have more than one peak, suggesting that these elements are present in multiple chemical environments. Table IX shows the atomic percent of these elements in the calcine.

Table IX

Atomic Concentrations of Elements Found in Calcine

Element	Concentration Atomic %	Concentration Wt %
C	40.08	26.46
O	37.30	32.82
Na	7.55	9.54
F	3.92	4.11
Cd	0.62	3.84
Zr	1.33	6.66
Si	2.07	3.19
Al	3.23	4.80
Ca	3.91	8.61

The weight percents in Table IX differ significantly from the results of the ICP analyses. The discrepancy between these two methods can be attributed to the carbon and oxygen found by XPS, that was not detected by ICP because the technique cannot be used

to detect oxygen and carbon. It is not known if the carbon and oxygen results are representative of the samples or are artifacts of surface contamination on the calcine. Electron sputtering was not performed prior to XPS analysis to burn off the top layer of the calcine. Electron sputtering the surface of the calcine prior to analysis may elucidate the answers to these questions, and will be performed during future analyses.

Appendix G contains the raw data generated from the XPS analysis. Each element found will have two binding energy graphs, one graph was generated from multiplexing the data and the other is a gaussian fit. Multiplexing the data allows for easier interpretation of the data by accounting for all the possible interferences that might cause a shift in binding energy. The gaussian fit is done to check the reliability of multiplexing the data. A curve fit summary accompanies the curve fit graph of the peak. Following the curve fit summary is a list of possible compounds that include the element; these lists were produced by removing from the curve fit listing phases which were highly unlikely based on chemical knowledge and process conditions. The curve fit lists were further reduced by comparing the elements on this list to those found by ICP analysis (Table II) and the SEM (Tables III-VIII). Table X summarizes the data from XPS analysis. The listing includes a large number of silicious phases that are included even though it isn't very likely that large amounts of silicon were present in the calciner feed.

Table X

Compounds Found By XPS Analysis That Are Most Likely
To Be In Run 17 Calcine

Element	Compound
F	K_2SiF_6 , Na_2SiF_6 , CaF_2 *
Na	Na_2SiF_6 , NaCl, $NaAlSi_3O_8$ (Albite), Natrolite, Na_2O
Cd	CdS, CdO, CdF_2
Zr	ZrF_4 , K_2ZrF_6 , ZrO_2
Si	Al_2SiO_5 (Kyanite), $NaAlSi_3O_8$ (Albite), $AlSiO_5$ (Sillimanite), Natrolite
Al	Al_2O_3 , $NaAlSi_3O_8$ (Albite), Al_2SiO_5 (Kyanite), Bentonite
Ca	$Ca(NO_3)_2$, $CaSO_4$, CaF_2 , CaO, CaS, $CaCrO_4$, $CaCl_2$
C	Probably an Analytical Artifact
O	Na_2SiO_3 , $FeSO_4$, Cr_2SO_4 , $CaSO_4$, Al_2SiO_5 , SiO_2 , KNO_3 , $CaNO_3$, CO_2

* Major constituent

Minor constituents of the calcine were not detected, therefore,
no XPS data is available to deduce their composition.

F*A*C*T Program Data

In an attempt to further reduce the number of possible compounds formed during the calcination process, the Facility for the Analysis of Chemical Thermodynamics (F*A*C*T) EQUILIB code³ was used to determine which compounds would form at equilibrium conditions in the calciner operating conditions of 1 atm and 500°C. Calciner feed concentrations listed in Table I were used as input for the calculations into the program. In addition, fuel, oxygen and fluidizing air concentrations were also added. Chemically stated, the reactants going into the calciner were:

From a large list of possible products, the EQUILIB minimizes the Gibbs free energy of the system and predicts the equilibrium state of the chemical system. Table XI list the solid products and moles of each solid predicted from calculations using the composition shown in Eq. 1.

Table XI
Products Resulting From F*A*C*T Program

Product	Moles
CaF ₂	0.845
ZrO ₂	0.233
NaAlO ₂	0.218
(CdO) (Al ₂ O ₃)	0.081
(CaO) ₃ (B ₂ O ₃)	0.07
Na ₂ SO ₄	0.046
NaF	0.018
NaCl	0.01
Al ₂ O ₃	0.063

These results, computed assuming that no amorphous phases were formed, are in agreement with the results that would be expected. Calcium fluoride is the most thermodynamically stable fluoride-containing solid to be formed by the metals listed in Table XI,^{4,c} and as expected, CaF₂ is predicted to be the most abundant fluoride-containing crystalline phase. The relative stabilities of these crystalline phases also show NaF(s) to be more stable than the fluorides of Al, Zr, and Cd; the results predicted NaF(s) as the other, albeit minor, fluoride-containing

^c The standard Gibbs free energies of formation, from the constituent elements, for the metal-fluorides tabulated below are in kJ/gram-atom of fluoride at 800K: CaF₂, -544.67 kJ; ZrF₄, -411.45 kJ; AlF₃, -433.64 kJ; NaF, -491.96 kJ; and CdF₂, -282.10 kJ.

These data were computed from values in endnote 4 in the **References** section of the main body of this work.

crystalline phase. The oxides of zirconium, aluminum, and calcium are also quite stable^d and, as expected, ZrO_2 and Al_2O_3 are predicted. No CaO was predicted because the fluoride phase consumed most of the calcium and the remainder of the Ca is consumed by the formation of the $Ca_3B_2O_6$ phase; other mixed metal phases predicted are $NaAlO_2$ and $CdAl_2O_4$.

From the results tabulated in Table XI, it may be concluded that some of the important chemical reactions occurring during calcination may be:

Results from EQUILIB in many cases are in good agreement with the XRD analysis. XRD did identify CaF_2 and ZrO_2 as major crystalline structures in the calcine; however, the XRD analysis also found $NaNO_3$, which was not a predicted during the computational study. This discrepancy can be explained by addressing the kinetics of calcination chemistry.

^d The standard Gibbs free energies of formation, from the constituent elements, for the metal-oxides below are tabulated in kJ/gram-atom of oxygen at 800K: CaO , -551.59 kJ; ZrO_2 , -472.36 kJ; Al_2O_3 , -474.96 kJ; Na_2O , -308.12 kJ; and CdO , -178.40 kJ.

These data were computed from values in endnote 4 in the **References** section of the main body of this work.

The calcination process is most likely a dynamic, kinetically-controlled process. As the water in the feed evaporates, it is possible for nitrate to become trapped in the calcine particle. This could prevent the decomposition of alkali metal nitrates, even though 500°C is far above the normal decomposition temperatures of the nitrates of potassium and sodium, 334°C and 306°C, respectively.⁴

The computational results are also in good agreement with the SEM data. Areas with high concentrations of calcium and fluoride were found, as well as areas with high concentrations of calcium, aluminum, zirconium, and oxygen; it is likely that these are areas of calcium fluoride and of oxides phases, respectively.

XPS results are not in complete agreement with the XRD and computational results. The most glaring difference is the carbon detected during the XPS analyses. Carbonaceous phases were not identified during the XRD analyses, and because carbon was not identified as an element present during the computational work, no carbonaceous phases were predicted. The XPS results do, however, suggest the presence of a great number of sodium and aluminum phases. It is possible that these phases, which are compositionally quite similar, may have similar binding energies. This would make it difficult to distinguish the various sodium and aluminum compounds from one another.

Conclusions

The results of a variety of analyses, ICP, XRD, SEM, and XPS, and of equilibrium calculations on Run 17 pilot plant calcine have been performed in an attempt to characterize the physical and chemical nature of the calcine. The SEM results show that the calcine is inhomogeneous and multiphasic in chemical character. These results do suggest, however, that there is a correlation between gross composition and particle size, with compositional ranges for the major constituents of the calcine (F, Al, Ca, and Zr) deviating from 5 to 10 %; ranges of the minor constituents of the calcine can deviate up to 65 %.

Composition of the crystalline and amorphous phases of the calcine indicate that a large portion of the calcine is calcium fluoride, aluminum oxide, calcium oxide, and zirconium oxide. The computational results and XPS results indicate that most of the sodium is associated with the aluminum to form sodium aluminate. The SEM results also support this interpretation. Areas of pure aluminum oxide were not found; sodium was always detected with the aluminum, although there is no reason not to expect that some of this aluminum was present as Al_2O_3 and that some of the sodium present as NaF, NaCl, and NaSO_4 . Cadmium is most likely present as both CdO and CdS, although it is not possible to quantitatively determine the amounts of these phases because of the matrix effects associated with the analytical techniques

Additional analyses on Run 17 should be performed before quantitative concentrations of the compounds are reported. This may include microprobe analysis to determine boron concentrations and electron sputtering the calcine sample prior to XPS analysis.

Appendix A

Point by Point SEM Data for Particle 1

30-Nov-1992 13:12:57

R17FLNA-1-1

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION ± SIGMA	K-RATIO**
O KA	11.80	18.26	0.92	0.0627
F KA	41.23	53.76	0.49	0.7657
Al KA	1.51	1.38	0.04	0.0208
K KA	0.31	0.20	0.03	0.0075
Ca KA	39.93	24.67	0.12	0.7493
Cr KA	0.13	0.06	0.02	0.0037
Zr LA	4.85	1.32	0.07	0.1075
Cd LA	1.58	0.35	0.06	0.0215

TOTAL 101.34

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 13:17:08

R17FLNA-1-2

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	28.81	38.65	0.65	0.1616
F KA	28.86	32.60	0.42	0.4335
Na KA	1.84	1.72	0.07	0.0221
Al KA	2.05	1.63	0.04	0.0286
S KA	2.37	1.59	0.03	0.1008
K KA	0.33	0.18	0.03	0.0080
Ca KA	42.14	22.57	0.12	0.7870
Cr KA	0.30	0.12	0.03	0.0084
Zr LA	2.88	0.68	0.05	0.0638
Cd LA	1.36	0.26	0.06	0.0183

TOTAL 110.94

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
where R = reference(standard)/reference(sample)

30-Nov-1992 13:20:34

R17FLNA-1-3

Accelerating voltage 20.0 KeV
 Beam - sample incidence angle 90.0 degrees
 Xray emergence angle 35.0 degrees
 Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
 (ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION ± SIGMA	K-RATIO**
O KA	38.38	54.18	0.69	0.2462
F KA	16.15	19.20	0.32	0.2467
Al KA	13.50	11.30	0.09	0.1971
K KA	0.00	0.00	0.00	0.0000
Ca KA	10.55	5.95	0.07	0.1756
Cr KA	0.43	0.19	0.03	0.0127
Ni KA	0.16	0.06	0.03	0.0015
Zr LA	24.62	6.10	0.13	0.5115
Cd LA	15.05	3.02	0.11	0.1728
TOTAL	118.84			

ITERATIONS 4

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO × R
 where R = reference(standard)/reference(sample)

30-Nov-1992 13:26:28

R17FLNA-1-4

Accelerating voltage 20.0 KeV
 Beam - sample incidence angle 90.0 degrees
 Xray emergence angle 35.0 degrees
 Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
 (ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	49.56	60.08	0.75	0.3501
F KA	15.69	16.02	0.33	0.2171
Na KA	2.53	2.14	0.09	0.0325
Al KA	9.44	6.78	0.08	0.1360
K KA	0.00	0.00	0.00	0.0000
Ca KA	22.26	10.77	0.10	0.3901
Zr LA	14.57	3.10	0.10	0.3077
Cd LA	6.46	1.11	0.08	0.0786
TOTAL	120.51			

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 13:29:29

R17FLNA-1-5

Accelerating voltage 20.0 KeV
 Beam - sample incidence angle 90.0 degrees
 Xray emergence angle 35.0 degrees
 Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
 (ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	34.24	42.43	0.66	0.2269
F KA	32.95	34.39	0.43	0.5412
Al KA	8.32	6.11	0.07	0.1188
K KA	0.00	0.00	0.00	0.0000
Ca KA	22.88	11.32	0.10	0.3997
Cr KA	0.58	0.22	0.03	0.0170
Mn KA	0.13	0.05	0.02	0.0019
Zr LA	19.09	4.15	0.11	0.4084
Cd LA	7.57	1.34	0.08	0.0913

TOTAL 125.76

ITERATIONS 6

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

Appendix B

Point by Point SEM Data For Particle 2

30-Nov-1992 13:37:51

R17FLNA-2-1

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	54.82	66.21	0.82	0.3733
F KA	9.76	9.92	0.28	0.1324
Al KA	14.00	10.03	0.09	0.2084
K KA	0.00	0.00	0.00	0.0000
Ca KA	13.17	6.35	0.08	0.2212
Cr KA	0.00	0.00	0.00	0.0000
Mn KA	0.24	0.09	0.03	0.0037
Zr LA	25.83	5.47	0.14	0.5407
Cd LA	11.21	1.93	0.10	0.1286

TOTAL 129.03

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 13:41:57

R17FLNA-2-2

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
F KA	45.84	66.83	0.48	0.9606
Al KA	0.88	0.90	0.03	0.0120
K KA	0.32	0.23	0.03	0.0082
Ca KA	44.74	30.91	0.13	0.8534
Zr LA	2.72	0.83	0.06	0.0605
Cd LA	1.23	0.30	0.05	0.0172

TOTAL 95.73

ITERATIONS 3

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 13:49:28

R17FLNA-2-3

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	54.62	68.21	0.79	0.3857
F KA	6.43	6.76	0.22	0.0838
Na KA	0.63	0.54	0.06	0.0081
Al KA	14.22	10.53	0.09	0.2087
K KA	0.00	0.00	0.00	0.0000
Ca KA	18.27	9.11	0.09	0.3145
Zr LA	11.97	2.62	0.10	0.2456
Cd LA	12.52	2.23	0.10	0.1529
TOTAL	118.66			

ITERATIONS 4

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 13:54:42

R17FLNA-2-4

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	19.55	25.80	0.54	0.1174
F KA	43.74	48.61	0.48	0.8049
Al KA	4.42	3.46	0.06	0.0613
K KA	0.00	0.00	0.00	0.0000
Ca KA	38.84	20.46	0.12	0.7238
Zr LA	4.60	1.06	0.07	0.0998
Cd LA	3.18	0.60	0.05	0.0427
TOTAL	114.33			

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

Appendix C

Point by Point SEM Data For Particle 3

30-Nov-1992 14:03:35

R17FLNA-3-1

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	7.91	13.55	0.70	0.0370
F KA	37.22	53.68	0.47	0.6705
Al KA	0.94	0.96	0.03	0.0130
K KA	0.35	0.24	0.03	0.0085
Ca KA	43.00	29.40	0.13	0.8060
Ni KA	0.26	0.12	0.03	0.0023
Zr LA	5.31	1.60	0.07	0.1186
Cd LA	1.87	0.46	0.06	0.0254
TOTAL	96.86			

ITERATIONS 4

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 14:08:24

R17FLNA-3-2

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	49.54	75.29	0.85	0.2775
Al KA	5.82	5.24	0.06	0.0869
K KA	0.00	0.00	0.00	0.0000
Ca KA	10.80	6.55	0.07	0.1760
Cr KA	1.01	0.47	0.04	0.0296
Fe KA	0.62	0.27	0.04	0.0083
Ni KA	0.19	0.08	0.03	0.0017
Zr LA	39.40	10.50	0.16	0.8734
Cd LA	7.38	1.60	0.09	0.0791

TOTAL 114.76

ITERATIONS 6

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 14:12:13

R17FLNA-3-3

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	50.88	71.85	0.73	0.4995
Na KA	2.76	2.72	0.09	0.0310
Al KA	0.32	0.27	0.03	0.0043
S KA	4.15	2.93	0.04	0.1759
K KA	0.20	0.11	0.02	0.0046
Ca KA	21.18	11.94	0.09	0.4014
Cr KA	22.28	9.68	0.12	0.6560
Zr LA	1.51	0.37	0.05	0.0329
Cd LA	0.63	0.13	0.05	0.0084

TOTAL 103.91

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

Appendix D

General Composition SEM Data For Small Particles

30-Nov-1992 11:36:41

R17FLNA-3-G

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	31.64	45.21	0.64	0.2115
F KA	25.21	30.34	0.39	0.3922
Na KA	1.59	1.59	0.08	0.0195
Al KA	5.14	4.36	0.06	0.0727
S KA	1.34	0.95	0.03	0.0488
K KA	0.00	0.00	0.00	0.0000
Ca KA	22.04	12.57	0.09	0.3893
Cr KA	1.28	0.56	0.04	0.0373
Zr LA	13.56	3.40	0.10	0.2929
Cd LA	5.00	1.02	0.07	0.0611
TOTAL	106.80			

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO × R
where R = reference(standard)/reference(sample)

30-Nov-1992 12:13:21

R17FLNA-B-G

Accelerating voltage 20.0 KeV
 Beam - sample incidence angle 90.0 degrees
 Xray emergence angle 35.0 degrees
 Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
 (ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	26.24	37.31	0.60	0.1653
F KA	32.27	38.64	0.42	0.5376
Na KA	0.97	0.96	0.06	0.0116
Al KA	3.67	3.09	0.05	0.0513
S KA	0.45	0.32	0.02	0.0174
K KA	0.26	0.15	0.03	0.0060
Ca KA	29.00	16.46	0.10	0.5252
Zr LA	9.66	2.41	0.09	0.2107
Cd LA	3.19	0.65	0.07	0.0406
TOTAL	105.71			

ITERATIONS 6

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 12:21:58

R17FLNA-10-G

Accelerating voltage 20.0 KeV
 Beam - sample incidence angle 90.0 degrees
 Xray emergence angle 35.0 degrees
 Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
 (ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	32.24	48.16	0.63	0.2191
F KA	22.74	28.60	0.37	0.3427
Na KA	1.17	1.22	0.07	0.0143
Al KA	4.90	4.34	0.06	0.0694
S KA	0.52	0.39	0.02	0.0192
K KA	0.00	0.00	0.00	0.0000
Ca KA	21.03	12.54	0.09	0.3729
Cr KA	1.25	0.57	0.04	0.0362
Mn KA	0.00	0.00	0.00	0.0000
Zr LA	12.47	3.27	0.09	0.2693
Cd LA	4.24	0.90	0.06	0.0521

TOTAL 100.56

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 12:35:03

R17FLNA-11-G

Accelerating voltage 20.0 KeV
 Beam - sample incidence angle 90.0 degrees
 Xray emergence angle 35.0 degrees
 Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
 (ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	23.92	37.68	0.80	0.1392
F KA	26.36	34.96	0.42	0.4273
Na KA	0.34	0.38	0.05	0.0042
Al KA	5.69	5.31	0.06	0.0813
S KA	0.37	0.29	0.02	0.0131
K KA	0.00	0.00	0.00	0.0000
Ca KA	25.65	16.12	0.10	0.4529
Cr KA	0.17	0.08	0.02	0.0050
Mn KA	0.13	0.06	0.02	0.0020
Zr LA	14.49	4.00	0.10	0.3136
Cd LA	5.00	1.12	0.07	0.0611

TOTAL 102.12

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 12:39:10

R17FLNA-12-G

Accelerating voltage 20.0 KeV
 Beam - sample incidence angle 90.0 degrees
 Xray emergence angle 35.0 degrees
 Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
 (ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	27.60	40.66	0.88	0.1666
F KA	26.92	33.40	0.44	0.4294
Na KA	0.14	0.15	0.03	0.0017
Al KA	6.06	5.29	0.06	0.0867
S KA	0.46	0.34	0.02	0.0168
K KA	0.00	0.00	0.00	0.0000
Ca KA	25.95	15.26	0.10	0.4590
Cr KA	0.16	0.07	0.02	0.0048
Mn KA	0.16	0.07	0.03	0.0025
Zr LA	14.15	3.66	0.10	0.3058
Cd LA	5.21	1.09	0.07	0.0639

TOTAL 106.81

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 12:43:06

R17FLNA-13-G

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	29.82	43.95	0.86	0.1842
F KA	24.59	30.52	0.43	0.3834
Na KA	0.59	0.61	0.06	0.0073
Al KA	6.09	5.32	0.06	0.0872
S KA	0.50	0.37	0.03	0.0179
K KA	0.00	0.00	0.00	0.0000
Ca KA	24.00	14.12	0.10	0.4224
Cr KA	0.28	0.13	0.03	0.0081
Mn KA	0.10	0.04	0.02	0.0015
Zr LA	15.10	3.90	0.10	0.3261
Cd LA	4.97	1.04	0.07	0.0604

TOTAL 106.04

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

Appendix E

General Composition SEM Data For Medium Particles

30-Nov-1992 11:15:20

R17FLNA-2-G

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	30.51	43.47	0.62	0.1964
F KA	27.40	32.88	0.40	0.4349
Na KA	0.55	0.54	0.04	0.0066
Al KA	5.23	4.42	0.06	0.0741
S KA	0.50	0.35	0.02	0.0186
K KA	0.12	0.07	0.03	0.0027
Ca KA	24.90	14.16	0.10	0.4429
Cr KA	0.16	0.07	0.02	0.0045
Zr LA	11.79	2.95	0.09	0.2548
Cd LA	5.31	1.08	0.08	0.0661

TOTAL 106.47

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1972 12:00:53

R17FLNA-6-G

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	30.38	45.37	0.62	0.2049
F KA	25.11	31.58	0.40	0.3940
Na KA	1.05	1.09	0.06	0.0128
Al KA	4.98	4.41	0.06	0.0707
S KA	0.26	0.19	0.02	0.0094
Cl KA	0.17	0.11	0.02	0.0023
K KA	0.00	0.00	0.00	0.0000
Ca KA	22.03	13.13	0.09	0.3923
Cr KA	0.46	0.21	0.03	0.0132
Mn KA	0.00	0.00	0.00	0.0000
Zr LA	12.41	3.25	0.09	0.2683
Cd LA	3.13	0.66	0.06	0.0384
TOTAL	99.98			

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 12:06:09

R17FLNA-7-G

Accelerating voltage 20.0 KeV
 Beam - sample incidence angle 90.0 degrees
 Xray emergence angle 35.0 degrees
 Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
 (ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	29.22	43.16	0.87	0.1834
F KA	25.89	32.21	0.44	0.4026
Na KA	0.32	0.33	0.04	0.0038
Al KA	5.30	4.64	0.06	0.0752
S KA	0.31	0.23	0.02	0.0116
K KA	0.00	0.00	0.00	0.0000
Ca KA	25.16	14.84	0.10	0.4478
Cr KA	0.72	0.33	0.03	0.0210
Mn KA	0.09	0.04	0.02	0.0013
Zr LA	12.23	3.17	0.09	0.2644
Cd LA	5.04	1.06	0.07	0.0625

TOTAL 104.28

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 12:18:00

R17FLNA-9-G

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	30.84	43.13	0.64	0.1974
F KA	27.53	32.42	0.40	0.4391
Na KA	1.15	1.12	0.07	0.0140
Al KA	5.47	4.53	0.06	0.0775
S KA	0.42	0.29	0.01	0.0154
Cl KA	0.20	0.12	0.02	0.0028
K KA	0.17	0.10	0.03	0.0037
Ca KA	25.04	13.98	0.10	0.4440
Cr KA	0.13	0.05	0.02	0.0037
Zr LA	13.19	3.24	0.10	0.2851
Cd LA	5.07	1.01	0.08	0.0626

TOTAL 109.21

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 13:00:16

R17FLNA-15-G

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	29.66	43.98	0.89	0.1816
F KA	24.58	30.70	0.43	0.3818
Na KA	0.60	0.62	0.06	0.0073
Al KA	5.41	4.75	0.06	0.0772
S KA	0.57	0.42	0.02	0.0207
K KA	0.09	0.06	0.03	0.0021
Ca KA	24.88	14.72	0.10	0.4394
Cr KA	0.09	0.04	0.02	0.0025
Mn KA	0.11	0.05	0.02	0.0017
Zr LA	13.72	3.57	0.10	0.2972
Cd LA	5.17	1.09	0.08	0.0635

TOTAL 104.88

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
where R = reference(standard)/reference(sample)

Appendix F

General Composition SEM Data For Large Particles

30-Nov-1992 10:56:50

R17FLNA-1-G

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION ± SIGMA	K-RATIO**
O KA	28.96	40.61	1.66	0.1910
F KA	28.44	33.58	0.42	0.4578
Na KA	1.67	1.63	0.08	0.0203
Al KA	6.09	5.07	0.06	0.0857
S KA	0.69	0.48	0.03	0.0256
K KA	0.11	0.06	0.03	0.0024
Ca KA	25.48	14.26	0.10	0.4556
Cr KA	1.33	0.57	0.04	0.0385
Mn KA	0.08	0.03	0.02	0.0012
Zr LA	11.28	2.77	0.09	0.2415
Cd LA	4.69	0.94	0.08	0.0585

TOTAL 108.82

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
where R = reference(standard)/reference(sample)

30-Nov-1992 11:40:48

R17FLNA-4-G

Accelerating voltage 20.0 KeV
Beam - sample incidence angle 90.0 degrees
Xray emergence angle 35.0 degrees
Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
(ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION ± SIGMA	K-RATIO**
O KA	30.59	43.63	0.88	0.1914
F KA	26.00	31.23	0.45	0.4091
Na KA	0.62	0.61	0.06	0.0076
Al KA	6.27	5.30	0.06	0.0897
S KA	0.46	0.33	0.03	0.0167
K KA	0.00	0.00	0.00	0.0000
Ca KA	24.93	14.19	0.10	0.4404
Cr KA	0.07	0.03	0.01	0.0020
Mn KA	0.15	0.06	0.02	0.0022
Zr LA	14.52	3.63	0.10	0.3131
Cd LA	4.90	0.99	0.07	0.0599

TOTAL 108.51

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 11:56:02

R17FLNA-5-G

Accelerating voltage 20.0 KeV
 Beam - sample incidence angle 90.0 degrees
 Xray emergence angle 35.0 degrees
 Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
 (ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION 2 SIGMA	K-RATIO**
O KA	25.84	39.49	0.85	0.1524
F KA	26.63	34.28	0.44	0.4232
Na KA	0.21	0.22	0.03	0.0025
Al KA	4.97	4.50	0.06	0.0705
S KA	0.41	0.31	0.02	0.0153
K KA	0.14	0.09	0.03	0.0031
Ca KA	27.47	16.76	0.10	0.4897
Cr KA	0.18	0.08	0.02	0.0051
Mn KA	0.09	0.04	0.02	0.0013
Zr LA	11.55	3.10	0.09	0.2505
Cd LA	5.17	1.13	0.09	0.0647

TOTAL 102.66

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

30-Nov-1992 12:56:32

R17FLNA-14-G

Accelerating voltage 20.0 KeV
 Beam - sample incidence angle 90.0 degrees
 Xray emergence angle 35.0 degrees
 Xray - window incidence angle 0.0 degrees

QUANTITATIVE EDS RESULTS
 (ZAF CORRECTIONS VIA MAGIC V)

ELEMENT & LINE	WEIGHT PERCENT	ATOMIC PERCENT*	PRECISION ± SIGMA	K-RATIO**
O KA	30.37	42.55	0.85	0.1979
F KA	28.56	33.70	0.47	0.4568
Na KA	0.65	0.63	0.06	0.0079
Al KA	5.59	4.65	0.06	0.0798
S KA	0.25	0.18	0.02	0.0092
K KA	0.23	0.13	0.03	0.0050
Ca KA	24.76	13.85	0.10	0.4405
Cr KA	0.48	0.20	0.03	0.0138
Mn KA	0.00	0.00	0.00	0.0000
Zr LA	14.08	3.46	0.10	0.3047
Cd LA	3.22	0.64	0.07	0.0395

TOTAL 108.19

ITERATIONS 5

*NOTE: ATOMIC PERCENT is normalized to 100

**NOTE: K-RATIO = K-RATIO x R
 where R = reference(standard)/reference(sample)

Appendix G
XPS Raw Data

Atomic Concentration

a User Settings Previous New
 c Mode Area Height Baseline Linear Integrated
 f Regions 01 Na1 F1 Cd1 Zr1 Si1 Al1 Ca1

Element Name
 Massaged

Atomic Concentration Table

File: Brewer1
 Lens: Small Area Omni-Focus
 Calcine run #17 from K. Brewer at CPP. as received.

Element	Area (cts-eV/s)	Sensitivity Factor	Concentration (%)
Cl1s	8331	0.296	40.08
O1s	18624	0.711	37.30
Na1s	8931	1.685	7.55
F1s	2753	1.000	3.92
Cd3d5	1741	3.974	0.62
Zr3d	2399	2.576	1.33
Si2p	492	0.339	2.07
Al2p	530	0.234	3.23
Ca2p	5038	1.833	3.91

2 of 2

ESCA MULTIPLEX 12/2/92 EL=F1 REG 4 ANGLE= 15 deg ACO TIME=18.50 min
FILE: Brewer2 Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.110 k c/s, OFFSET= 4.610 k c/s PASS ENERGY= 71.550 eV Mg 400 M

Curve Fit

	a	b	c	d
Area	2169	Position	Height	% Gauss
1	686.29	931	2.00	80

Curve Fit Summary

Filename: Brewer2

Region: 4

Comment: Calcine run #17 from K. Brewer at CPP. as received.

Goodness of Fit: 1.025

Number of Completed Iterations: 4

Band No.	Peak Pos.	Delta	Height	FWHM	Gauss	%	Area	% of Total Area
1	686.29	0.00	931	2.00	80		2169	100.00

Chemical State Identification
 Element Name **F1** Type **Photoelectron** Anode **Mg** Anode Energy (eV) **1253.6**
a Identification Energy (eV) **686.30** **b** Identification Range (eV) **2.5**
c State Selection 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 686.60	KSbF6	11 685.90	CuF2
2 686.60	NH3BF3	12 685.80	Ph3POBF3
3 686.60	K2SiF6	13 685.80	BeF2
4 686.60	EtNH2BF3	14 685.75	MgF2
5 686.40	Na2SiF6	15 685.70	MgF2
6 686.30	AlF3.3H2O	16 685.70	K3RhF6
7 686.00	Na2SiF6	17 685.70	Ph3POBF3
8 686.00	HgF2	18 685.70	NaBeF3
9 685.90	CsF	19 685.60	Na2TaF7
10 685.90	Na2GeF6	20 685.60	UO2F2

ESCA MULTIPLEX 12/2/92 EL=Na1 REG 3 ANGLE= 15 deg ACO TIME=18.50 min

FILE: Brewer2 Calcine run #17 from K. Brewer at CPP. as received.

SCALE FACTOR= 0.301 k c/s, OFFSET= 12.075 k c/s PASS ENERGY= 71.550 eV Mg 400 W

Curve Fit Summary

Filename: Brewer2

Region: 3

Comment: Calcine run #17 from K. Brewer at CPP. as received.

Goodness of Fit: 1.122

Number of Completed Iterations: 10

Band No.	Peak Pos.	Band for		Separ.	Height	FWHM	%		Band for		%		%	
		Delta	Sep.				Gauss	Area	Area	Ratio	Area	Ratio	Total	Area
2	1073.26	0.72	0		1113	2.00	80	0	2595		41.97			
1	1072.54	0.00	0		1539	2.00	80	0	3588		58.03			

ESCA CURVE FIT 12/2/92 ANGLE= 15 deg ACO TIME=18.50 min
FILE: Curve_Fit Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.247 k c/s, OFFSET= 0.000 k c/s PASS ENERGY= 71.550 eV Mg 400 W

Element Name **Na1** Type **Photoelectron** Anode **Mg** Anode Energy (eV) **1253.6**
 Identification Energy (eV) **1073.30** b Identification Range (eV) **2.5**
 State Selection **1** 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 1072.70	NaBF4	11 1072.10	Na2SiF6
2 1072.55	Mol Sieve Y	12 1072.00	NaH2PO4
3 1072.50	Na2O	13 1072.00	Na2WO4
4 1072.50	NaCl	14 1071.90	Na2TaF7
5 1072.40	NaCrO2	15 1071.90	NaBeF3
6 1072.37	Natrolite	16 1071.90	Na2IrCl6
7 1072.30	NaCl	17 1071.82	Mol Sieve A
8 1072.27	Mol Sieve X	18 1071.80	NaCl
9 1072.23	NaAlSi3O8, albite	19 1071.80	Na
10 1072.20	p-(NaOCOCMe=CH2)	20 1071.80	Na2BeF4

Element Name **NaI** Type **Photoelectron** Anode **Mg** Anode Energy (eV) **1253.6**
 Identification Energy (eV) **1072.50** Identification Range (eV) **2.5**
 State Selection 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 1072.70	NaBF4	11 1072.10	Na2SiF6
2 1072.55	Mol Sieve Y	12 1072.00	NaH2PO4
3 1072.50	Na2O	13 1072.00	Na2WO4
4 1072.50	NaCl	14 1071.90	Na2TaF7
5 1072.40	NaCrO2	15 1071.90	NaBeF3
6 1072.37	NaFrolite	16 1071.90	Na2IrCl6
7 1072.30	NaCl	17 1071.82	Mol Sieve A
8 1072.27	Mol Sieve X	18 1071.80	NaCl
9 1072.23	NaAlSi3O8, albite	19 1071.80	Na
10 1072.20	p-(NaOCCOCMe=CH2)	20 1071.80	Na2BeF4

ESCA MULTIPLEX 12/2/92 EL=Cd1 REG 5 ANGLE= 15 deg ACO TIME=33.50 min
FILE: Brewer2 Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.049 k c/s, OFFSET= 1.918 k c/s PASS ENERGY= 71.550 eV Mg 400 H

ESCA CURVE FIT 12/2/92 ANGLE= 15 deg ACQ TIME=33.50 min
FILE: Curve_Fit Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.036 k c/s. OFFSET= 0.000 k c/s PASS ENERGY= 71.550 eV Mg 400 W

Curve Fit Summary

Filename: Brewer2

Region: 5

Comment: Calcine run #17 from K. Brewer at CPP. as received.

Goodness of Fit: 2.946

Number of Completed Iterations: 8

				Band				Band							
Band	Peak	Delta	Band	for	Height	FWHM	%	Band	for	Area	%	Area	Ratio	Area	%
No.	Pos.		Sep.				Gauss								of
2	412.74	6.80	1		244	1.84	80	1		0.67		523		39.98	
1	405.94	0.00	0		338	2.00	81	0				785		60.02	

Element Name **Cd1** Type **Chemical State Identification**
 Identification Energy (eV) **405.90** Anode **Mg** Anode Energy (eV) **1253.6**
 State Selection **1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16** Identification Range (eV) **2.5**

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 406.10	CdCl2	11 405.00	Cd(OH)2
2 406.00	CdBr2	12 404.92	Cd996Sn4
3 405.90	C12Cd(Ph3P)3	13 404.90	CdTe
4 405.90	CdF2	14 404.70	CdRh204
5 405.40	CdI2	15 404.60	Hg.8Cd.2Te
6 405.30	CdS	16 403.60	CdO2
7 405.30	CdSe		
8 405.20	CdO		
9 405.10	CdCO3		
10 405.00	Cd		

ESCA MULTIPLEX 12/2/92 EL=Zr1 REG 6 ANGLE= 15 deg ACO TIME=18.50 min
FILE: Brewer2 Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.057 k c/s, OFFSET= 0.875 k c/s PASS ENERGY= 71.550 eV Mg 400 M

Curve Fit Summary

Filename: Brewer2

Region: 6

Comment: Calcine run #17 from K. Brewer at CPP. as received.

Goodness of Fit: 2.332

Number of Completed Iterations: 6

Band No.	Band for			Band for Area		% of	
	Peak Pos.	Delta Sep.	Separ.	Height	FWHM	Gauss	Total Area
2	185.24	2.33	1	359	1.89	100	39.99
1	182.91	0.00	0	531	1.76	81	60.01
							Area 723
							Area 1085

ESCA CURVE FIT 12/2/92 ANGLE= 15 deg ACO TIME=18.50 min
FILE: Curve_Fit Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.054 k c/s, OFFSET= 0.000 k c/s PASS ENERGY= 71.550 eV Mg 400 W

Element Name **Zr** Type **Photoelectron** Anode **Mg** Anode Energy (eV) **1253.6**
 Identification Energy (eV) **182.90** Identification Range (eV) **2.5**
 State Selection **1 2 3 4 5 6 7**

Binding Energy	Chemical State Name
1 185.30	ZrF5
2 184.70	KZrF5.H2O
3 184.20	K2ZrF6
4 183.70	K3ZrF7
5 183.00	C12Zr(OH)2(CH3CHNH2)2C
6 182.90	Br2Zr(OH)2(CH3CHNH2)2C
7 182.20	ZrO2

ESCA MULTIPLEX 12/2/92 EL=Si1 REG 7 ANGLE= 15 deg ACD TIME=18.50 min

FILE: Brewer2 Calcine run #17 from K. Brewer at CPP. as received.

SCALE FACTOR= 0.023 k c/s, OFFSET= 0.863 k c/s PASS ENERGY= 71.550 eV Mg 400 W

ESCA CURVE FIT 12/2/92 ANGLE= 15 deg ACD TIME=18.50 min
FILE: Curve_Fit Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.019 k c/s, OFFSET= 0.000 k c/s PASS ENERGY= 71.550 eV Mg 400 W

Curve Fit Summary

Filename: Brewer2

Region: 7

Comment: Calcine run #17 from K. Brewer at CPP. as received.

Goodness of Fit: 0.883

Number of Completed Iterations: 7

		%		% of	
Band	Peak			Total	
No.	Pos.	Delta	Height	FWHM	Gauss Area
1	102.44	0.00	179	1.84	80 382 100.00

Chemical State Identification

Element Name **Sil** Type **Photoelectron** Anode **Mg** Anode Energy (eV) **1253.6**
 Identification Energy (eV) **102.40** Identification Range (eV) **2.5**
 State Selection 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 102.88	Pyrophyllite	11 102.60	Al2SiO5, sillimanite
2 102.84	Mol Sieve Y	12 102.46	LiAlSi2O6, spodumene
3 102.80	Al2SiO5, kyanite	13 102.40	p-Methylsil. (linear)
4 102.80	Mol Sieve Y, Ca form	14 102.36	Mollastonii, Ca3Si3O9
5 102.75	Mol Sieve Y	15 102.36	Mica, Muscovite
6 102.74	p-Phenylsil. (resin)	16 102.22	Natrolite
7 102.65	Kaolinite	17 102.16	Mol Sieve X
8 102.65	Mol Sieve X, Ca form	18 102.15	Mol Sieve X
9 102.64	AlSiO5, sillimanite	19 102.10	Et2SiCl2
10 102.63	NaAlSi3O8, albite	20 101.96	Zn4Si2O7(OH)2.2H2O

ESCA MULTIPLEX 12/2/92 EL=011 REG 8 ANGLE= 15 deg ACO TIME=23.50 min
FILE: Brewer2 Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.021 k c/s. OFFSET= 0.781 k c/s PASS ENERGY= 71.550 eV Mg 400 M

ESCA CURVE FIT 12/2/92 ANGLE= 15 deg ADO TIME=23.50 min
FILE: Curve_Fit Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.014 k c/s, OFFSET= 0.000 k c/s PASS ENERGY= 71.550 eV Mg 400 W

Curve Fit Summary

Filename: Brewer2

Region: 8

Comment: Calcine run #17 from K. Brewer at CPP. as received.

Goodness of Fit: 0.628

Number of Completed Iterations: 3

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Band No.	Peak Pos.	Delta	Height	FWHM	% of	
					Gauss	Total
1	75.04	0.00	123	2.24	73	Area 331 100.00

Chemical State Identification									
Element Name	HLI Type	Photoelectron		Anode	Mg	Anode Energy (eV)		1253.6	
Identification Energy (eV)	75.00	6	Identification Range (eV)		2.5				
State Selection	1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20								

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 75.60	LiAlH4	11 74.70	MgAl2O4
2 75.20	AlBr3	12 74.64	Al2SiO5, sillimanite
3 75.00	Bentonite	13 74.60	Al2S3
4 74.95	Hydroxysodalite	14 74.60	AlI3
5 74.82	H Zeolon	15 74.59	Kaolinite
6 74.80	Al2SiO5, mullite	16 74.40	AlN
7 74.71	Pyrophyllite	17 74.34	Albite, NaAlSi3O8
8 74.70	Al2SiO5, kyanite	18 74.32	Spodumene
9 74.70	Al2O3	19 74.30	Al2(MO4)3
10 74.70	AlCl3	20 74.30	Al2O3

ESCA MULTIPLEX 12/2/92 EL=Ca1 REG 9 ANGLE= 15 deg ACQ TIME=26.83 min
FILE: Brewer2 Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.096 k c/s, OFFSET= 1.820 k c/s PASS ENERGY= 71.550 eV Mg 400 W

ESCA CURVE FIT 12/2/92 ANGLE= 15 deg ACQ TIME=26.83 min
FILE: Curve_Fit Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.090 k c/s, OFFSET= 0.000 k c/s PASS ENERGY= 71.550 eV Mg 400 W

Curve Fit Summary

Filename: Brewer2

Region: 9

Comment: Calcine run #17 from K. Brewer at CPP. as received.

Goodness of Fit: 25.876

Number of Completed Iterations: 10

Band No.	Peak Pos.	Delta	Band for Sep.	Separ.	Height	FWHM	% Gauss	Band for Area	Area	% of Total Area
4	353.29	4.64	3	3.55	204	1.70	83	3	400	11.31
2	352.20	3.55	1	3.55	349	1.91	80	1	778	22.00
3	349.74	1.09	0		392	1.78	84	0	802	22.67
1	348.65	0.00	0		691	1.93	80	0	1557	44.02

Element Name **Ca** Type **Photoelectron** Anode **Mg** Anode Energy (eV) **1253.6**
 Identification Energy (eV) **348.70** Identification Range (eV) **2.5**
 State Selection **1** 2 3 4 5 6 7 8 9 10 11 12 13 14

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 348.70	Ca(NO3)2	11 346.65	CaO
2 348.30	CaCl2	12 346.50	CaMO4
3 348.00	CaSO4	13 346.45	CaS
4 347.80	CaF2	14 346.30	CaCrO4
5 347.30	CaO		
6 347.20	CaMoO4		
7 347.04	Ca3Si3O9		
8 346.90	CaCO3		
9 346.80	Ca		
10 346.70	CaH2		

ESCA MULTIPLEX 12/2/92 EL=C1 REG 1 ANGLE= 15 deg ACO TIME=6.55 min
FILE: Brewer2 Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.267 k c/s, OFFSET= 1.402 k c/s PASS ENERGY= 71.550 eV Mg 400 M

ESCA CURVE FIT 12/2/92 ANGLE= 15 deg ACO TIME=6.55 min
FILE: Curve_Fit Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.241 k c/s, OFFSET= 0.000 k c/s PASS ENERGY= 71.550 eV Mg 400 W

Curve Fit Summary

Filename: Brewer2

Region: 1

Comment: Calcine run #17 from K. Brewer at CPP. as received.

Goodness of Fit: 1.578

Number of Completed Iterations: 10

Band No.	Peak Pos.	Delta	Sep.	Height	FWHM	% Gauss	Band for Area		% of Total Area
							Area	Ratio	
2	286.29	1.49	0	897	2.00	80	0	0	34.97
1	284.81	0.00	0	2183	1.62	94	0	0	65.03

Element Name **Cl** Type **Chemical State Identification**
 Identification Energy (eV) **284.80** Anode **Mg** Anode Energy (eV) **1253.6**
 State Selection 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 285.50	K4V(CN)6	11 284.80	(C*HCOH)3
2 285.50	C5H5N	12 284.70	C6H5C*H3
3 285.40	Ph4PBr	13 284.70	Benzene
4 285.40	PhCN	14 284.60	PhNH2
5 285.30	PhNO2	15 284.60	Ph3PO
6 285.20	Cyclohexane	16 284.58	Ph4Sn
7 285.10	C6H5CH3 (C*CH3)	17 284.50	Fe(C5H5)2
8 285.10	C6H5Br	18 284.40	Cr(C6H6)2
9 285.00	C6H5CH3 (C*-H)	19 284.30	Graphite
10 284.90	Ph3P	20 284.00	K3Mn(CN)6

Element Name **Cl** Type **Photoelectron** Anode **Mg** Anode Energy (eV) **1253.6**
a Identification Energy (eV) **286.30** Identification Range (eV) **2.5**
c State Selection 1 2 3 4 5 6 7 8 9 10 11 **12** 13 14 15 16 17 18 19 20

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 286.80	EtNH2BF3	11 286.30	Triazole
2 286.70	Inositol	12 286.30	p(CH2=CHCl)
3 286.70	O(C*H2COOH)2	13 286.30	CH3C*H2OH
4 286.60	(CHC*OH)3	14 286.20	NaCN
5 286.50	(CH3C*H2)2O	15 286.10	CH3C*H2Cl
6 286.40	Hydroquinone	16 286.10	KCN
7 286.40	p(C*H3OCOCH=CH2)	17 286.10	C6HCl5
8 286.40	NC*N=C(NH2)2	18 285.95	Cr(acac)3
9 286.30	p(CH2=CHOH)	19 285.90	K3Co(CN)6
10 286.30	C*H3CN	20 285.70	C6H5Cl (C*H)

ESCA MULTIPLEX 12/2/92 EL=01 REG 2 ANGLE= 15 deg ADO TIME=7.05 min
FILE: Brewer2 Calcine run #17 from K. Brewer at CPP. as received.
SCALE FACTOR= 0.391 k c/s. OFFSET= 3.267 k c/s PASS ENERGY= 71.550 eV Mg 400 W

ESCA CURVE F11 12/2/92 ANGLE= 15 deg ACO TIME=7.05 min
 FILE: Curve_Fit Calcine run #17 from K. Brewer at CPP. as received.
 SCALE FACTOR= 0.358 k c/s. OFFSET= 0.000 k c/s PASS ENERGY= 71.550 eV Mg 400 M

Fillenane: Brewer2

Region: 2

Comment: Calcine run #17 from K. Brewer at CPP. as received.

Goodness of Fit: 1.237

Number of Completed Iterations: 10

Band No.	Peak Pos.	Band for		Separ.	Height	FWHM	%		Band for Area	Area	%	
		Delta	Sep.				Gauss	Area Ratio			Total	Area
1	533.42	2.91	0		2041	2.23	62	0		5737	41.76	
2	532.13	1.62	0		2270	2.19	100	0		5292	38.52	
3	530.51	0.00	0		987	2.39	83	0		2710	19.72	

Element Name **01** Type **01** Chemical State Identification
 Identification Energy (eV) **530.50** Anode **W2** Anode Energy (eV) **2253.0**
 State Selection 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 530.60	Na2SiO3.5H2O	11 530.50	SrO
2 530.60	Ag2CO3	12 530.50	V2O3
3 530.60	Nb2O5	13 530.40	HF02
4 530.60	SnO2	14 530.40	ZnO
5 530.60	Nd2O3	15 530.40	W02
6 530.60	W03	16 530.40	MoO3
7 530.60	CaMoO4	17 530.40	K3PO4
8 530.50	Cs2O4	18 530.40	UO2
9 530.50	In2O3	19 530.40	Na3PO4
10 530.50	V2O5	20 530.40	Rh2O3

Element Name **01** Type **01** Chemical State Identification
 Photoelectron Anode **Mg** Anode Energy (eV) **1253.6**
 Identification Energy (eV) **532.10** Identification Range (eV) **2.5**
 State Selection 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 532.40	FeS04	11 532.00	Al2(W04)3
2 532.30	KCl03	12 532.00	CaS04
3 532.30	NiSi03	13 532.00	MgSi0*3.2H20
4 532.20	PhCONH2	14 531.90	Re03
5 532.20	KCl04	15 531.90	Ni2Si04
6 532.20	p-Benzoquinone	16 531.88	Al2Si05, sillimanite
7 532.20	P205(bridging 0)	17 531.82	Ag203, alpha
8 532.10	Cr2(S04)3	18 531.80	In(OH)3
9 532.10	Mg0	19 531.80	Na2S203
10 532.10	NiS04	20 531.80	KOH

Element Name **01** Type **Photoelectron** Anode **Mg** Anode Energy (eV) **1253.6**
a **533.40** **b** Identification Range (eV) **2.5**
c State Selection 1 2 3 4 **5** 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

Chemical State Identification

Binding Energy	Chemical State Name	Binding Energy	Chemical State Name
1 533.60	P205(non-bridging O)	11 533.00	Ba(NO3)2
2 533.60	Ca(NO3)2	12 532.90	Na4P207(non-bridg O)
3 533.50	Hydroquinone	13 532.90	SiO2, Vycor
4 533.40	NaPO3(non-bridgin O)	14 532.84	SiO2, gel
5 533.40	LiClO4	15 532.80	AlPO4
6 533.20	SiO2, alpha quartz	16 532.80	MgSiO3.2H2O*
7 533.20	H2O	17 532.80	RbClO4
8 533.00	B2O3	18 532.80	NaOH
9 533.00	NaClO4	19 532.74	Methylsilicone resin
10 533.00	SiO2	20 532.70	KN03

Appendix H
F*A*C*T EQUILIB Results

The following pages contain all of the output generated by the F*A*C*T EQUILIB code. It is operated as follows: (1) the reactants are specified, (2) the temperature and pressure are specified, (3) the species, solutions, and/or phases to be considered in the free energy minimization calculation are specified from the database listing, and (4) the free energy minimization is performed.

**** ENTER REACTANTS (/H)
OR PRESS <RETURN> FOR
55.405H2O+4.558N*O3+.01CL+.046S+.092O2+1.648H+.081CD+.338NA+

CONTINUE THE REACTION
1.709F+1.055CA+.14B+.393AL+.233ZR+

CONTINUE THE REACTION
13.102 + 52.4N2 + 2.1C + 4.2H =

ENTER FINAL STATES (/H)
OR PRESS <RETURN> FOR

T PROD P PROD V PROD DELTA H DELTA V DELTA G DELTA S DELTA U DELTA A
(K) (ATM) (L) <---- requires "TH" option from OPTION MENU ----->

773. 1.

1 - 338 GASES
339 - 451 LIQUIDS
452 - 640 AQUEOUS
641 - 830 SOLIDS
831 - 832 SOLN-SLAG slag - Quasichemical model for molten oxides
833 - 835 SOLN-SALT salt - molten salt solution

ENTER THE CODE SELECTION (/H) (enter "LIST" to list species, "EG" for examples)
OR PRESS <RETURN> FOR

list

LIST: (HELP ALL G LIQ AQ S SOLN PRIV 2-11 LOC)
ENTER LIST COMMAND (H FOR HELP)
OR PRESS <RETURN> TO CONTINUE

all

#	SPECIES	LAST CALCULATED VALUE	PHASE	CP RANGE
1	H		G1 Gas	298 - 6000 K
2	H2		G1 Gas	298 - 3000 K
3	B		G1 Gas	295 - 300 K
4	B2		G1 Gas	298 - 6000 K
5	BH		G1 Gas	298 - 1500 K
6	BH2		G1 Gas	298 - 6000 K
7	BH3		G1 Gas	298 - 6000 K
8	B2H6		G1 Gas	298 - 1500 K
9	B5H9		G1 Gas	298 - 6000 K
10	B10H14		G1 Gas	298 - 6000 K
11	C		G1 Gas	298 - 4500 K
12	C2		G1 Gas	298 - 4000 K
13	C3		G1 Gas	298 - 6000 K
14	C4		G1 Gas	298 - 6000 K
15	C5		G1 Gas	298 - 6000 K
16	CH		G1 Gas	298 - 6000 K
17	CH2		G1 Gas	298 - 2000 K
18	CH3		G1 Gas	298 - 2000 K
19	CH4		G1 Gas	298 - 2000 K
20	C2H		G1 Gas	298 - 6000 K
21	C2H2		G1 Gas	298 - 2000 K
22	C2H3		G1 Gas	298 - 1500 K
23	C2H4		G1 Gas	298 - 1200 K
24	C2H5		G1 Gas	298 - 298 K
25	C2H6		G1 Gas	295 - 300 K
26	BC		G1 Gas	298 - 6000 K
27	N	0.9465E-29	G1 Gas	298 - 2500 K
28	N2	0.4185	G1 Gas	298 - 2500 K
29	N3	0.1929E-31	G1 Gas	298 - 6000 K
30	NH	0.3038E-31	G1 Gas	298 - 6000 K
31	NH2	0.7836E-27	G1 Gas	298 - 6000 K
32	NH3	0.5863E-23	G1 Gas	298 - 2000 K
33	N2H2	0.5976E-34	G1 Gas	298 - 6000 K

34	N2H4		G1 Gas	298	-	1500	K
35	BN		G1 Gas	295	-	300	K
36	B3H6N3		G1 Gas	298	-	6000	K
37	CN		G1 Gas	298	-	2000	K
38	C2N		G1 Gas	298	-	6000	K
39	CN2		G1 Gas	298	-	6000	K
40	C2N2		G1 Gas	298	-	2000	K
41	C4N2		G1 Gas	298	-	6000	K
42	HCN		G1 Gas	298	-	2000	K
43	CH3NH2		G1 Gas	295	-	300	K
44	CH3NC		G1 Methyliso.	295	-	300	K
45	CH3NC		G2 Acetonit.	295	-	300	K
46	C2H5N		G1 Ethylenimi	298	-	1000	K
47	(CH3)2NH		G1 Gas	295	-	300	K
48	CH3N2H3		G1 Gas	295	-	300	K
49	(CH3)2N2H2		G1 1,1-Di.	298	-	298	K
50	(CH3)2N2H2		G2 1,2-Di.	298	-	298	K
51	O	0.7254E-14	G1 Gas	298	-	3000	K
52	O2	0.1190	G1 Gas	298	-	3000	K
53	O3	0.2291E-14	G1 Gas	298	-	2000	K
54	OH	0.6166E-09	G1 Gas	298	-	6000	K
55	H2O	0.4464	G1 Steam	298	-	2500	K
56	H02	0.2638E-11	G1 Gas	298	-	6000	K
57	H2O2	0.5946E-11	G1 Gas	298	-	1500	K
58	BO		G1 Gas	298	-	6000	K
59	B2O		G1 Gas	298	-	6000	K
60	B02		G1 Gas	298	-	6000	K
61	B2O2		G1 Gas	298	-	6000	K
62	B2O3		G1 Gas	295	-	300	K
63	BOH		G1 Gas	298	-	6000	K
64	HBO2		G1 Gas	298	-	2000	K
65	B(OH)2		G1 Gas	298	-	6000	K
66	B3H3O3		G1 Gas	298	-	6000	K
67	B3H3O6		G1 Gas	298	-	6000	K
68	CO	0.1278E-15	G1 Gas	298	-	2500	K
69	CO2	0.1607E-01	G1 Gas	298	-	2500	K
70	C3O2		G1 Gas	298	-	6000	K
71	HCO	0.2820E-31	G1 Gas	298	-	2000	K
72	CH2O	0.4701E-35	G1 Gas	298	-	2000	K
73	CH3OH		G1 Gas	298	-	1000	K
74	CH2CO		G1 Gas	295	-	300	K
75	C2H4O		G1 Ethyl-Ox.	298	-	6000	K
76	C2H4O		G2 Acetal.	295	-	300	K
77	CH3CH2OH		G1 Gas	298	-	1500	K
78	CH3CH2OH		G2 (c*h3)2o	295	-	300	K
79	HCOOH	0.7448E-23	G1 Gas	298	-	1500	K
80	CH3COOH		G1 Gas	295	-	300	K
81	B(OCH3)		G1 Gas	295	-	300	K
82	(CH3)2O(B2H6)2		G1 Gas	298	-	1000	K
83	BH(OCH3)2		G1 Gas	295	-	300	K
84	NO	0.7947E-06	G1 Gas	298	-	3000	K
85	N2O	0.5227E-10	G1 Gas	298	-	6000	K
86	NO2	0.2488E-06	G1 Gas	298	-	3000	K
87	NO3	0.4920E-14	G1 Gas	298	-	6000	K
88	N2O3	0.5102E-17	G1 Gas	298	-	6000	K
89	N2O4	0.4353E-18	G1 Gas	298	-	6000	K
90	N2O5	0.9782E-22	G1 Gas	298	-	2000	K
91	HNO	0.2359E-16	G1 Gas	298	-	6000	K
92	N2H5OH		G1 Gas	298	-	1000	K
93	HNO2	0.9203E-09	G1 Gas.cis	298	-	6000	K
94	HNO2	0.1278E-08	G2 Gas.trans	298	-	6000	K
95	HNO3	0.7638E-10	G1 Gas	298	-	6000	K
96	CNO		G1 Gas	298	-	6000	K
97	CHNO	0.1033E-29	G1 Gas	298	-	6000	K
98	CH3NO2		G1 Gas	295	-	300	K
99	CH3NO3		G1 Gas	298	-	298	K
100	CH3CH2ONO2		G1 Gas	298	-	1000	K
101	F		G1 Gas	298	-	2000	K
102	F2	0.2257E-33	G1 Gas	298	-	2000	K
103	HF	0.1083E-04	G1 Gas	298	-	2500	K
104	BF		G1 Gas	298	-	2000	K
105	BF2		G1 Gas	298	-	2000	K
106	BF3		G1 Gas	298	-	2000	K
107	B2F4		G1 Gas	298	-	6000	K
108	BHF2		G1 Gas	298	-	6000	K
109	CF		G1 Gas	298	-	2000	K
110	CF2		G1 Gas	298	-	2000	K

111	C2F2		G1 Gas	298	- 6000	K
112	CF3		G1 Gas	298	- 6000	K
113	CF4		G1 Gas	298	- 6000	K
114	C2F4		G1 Gas	298	- 6000	K
115	C2F6		G1 Gas	298	- 6000	K
116	C6F6		G1 Hexafluoro	298	- 1000	K
117	C4F8		G1 Octafluoro	298	- 1000	K
118	CHF		G1 Gas	298	- 6000	K
119	CH3F		G1 Gas	298	- 6000	K
120	C2HF		G1 Gas	298	- 6000	K
121	C2FH5		G1 Fluoroetha	298	- 1000	K
122	CH2F2		G1 Gas	298	- 6000	K
123	CH2CF2		G1 Gas	295	- 300	K
124	CH3CHF2		G1 Gas	295	- 300	K
125	CHF3		G1 Gas	298	- 6000	K
126	C2F3H		G1 Trifluoroe	298	- 1000	K
127	CH3CF3		G1 Gas	295	- 300	K
128	NF	0.1312E-32	G1 Gas	298	- 6000	K
129	NF2		G1 Gas	298	- 6000	K
130	NF3		G1 Gas	298	- 6000	K
131	N2F4		G1 Gas	298	- 6000	K
132	CNF		G1 Gas	298	- 6000	K
133	C2NF3		G1 Gas	298	- 6000	K
134	OF	0.1080E-23	G1 Gas	298	- 6000	K
135	O2F	0.8619E-21	G1 Gas	298	- 6000	K
136	F2O	0.1230E-35	G1 Gas	298	- 2000	K
137	HO F	0.1330E-19	G1 Gas	298	- 6000	K
138	BO F		G1 Gas	298	- 6000	K
139	BO F2		G1 Gas	298	- 6000	K
140	B3O3F3		G1 Gas	298	- 6000	K
141	B2OF4		G1 Gas	298	- 6000	K
142	B3H2O3F		G1 Gas	298	- 6000	K
143	B(OH)F2		G1 Gas	209	- 6000	K
144	B3HO3F2		G1 Gas	298	- 6000	K
145	CO F	0.4182E-31	G1 Gas	298	- 2000	K
146	CO F2	0.2283E-21	G1 Gas	298	- 2000	K
147	CO F4		G1 Gas	298	- 6000	K
148	CHFO	0.1025E-27	G1 Gas	298	- 6000	K
149	(CH3)2O(BF3)		G1 Gas	298	- 1000	K
150	NO F	0.1770E-15	G1 Gas	298	- 1500	K
151	NO2F	0.8521E-18	G1 Gas	298	- 6000	K
152	NO F3		G1 Gas	298	- 6000	K
153	Na	0.1628E-18	G1 Gas	298	- 2000	K
154	Na2	0.3984E-36	G1 Gas	298	- 2000	K
155	NaH	0.3636E-28	G1 Gas	298	- 2000	K
156	NaCN		G1 Gas	298	- 2000	K
157	Na2(CN)2		G1 Gas	298	- 2000	K
158	NaO	0.8980E-19	G1 Gas	298	- 2200	K
159	Na2O2H2	0.4007E-14	G1 Gas	298	- 6000	K
160	NaBO2	0.2035E-12	G1 Gas	298	- 2000	K
161	NaF	0.3114E-10	G1 Gas	298	- 2500	K
162	Na2F2	0.1207E-11	G1 Gas	298	- 2000	K
163	Al		G1 Gas	2767	- 3200	K
164	Al2		G1 Gas	295	- 300	K
165	AlH		G1 Gas	298	- 6000	K
166	Al(BH4)3		G1 Gas	298	- 1000	K
167	AlC		G1 Gas	298	- 6000	K
168	AlO		G1 Gas	298	- 2000	K
169	AlO2		G1 Gas	298	- 2000	K
170	Al2O		G1 Gas	298	- 6000	K
171	Al2O2		G1 Gas	298	- 2000	K
172	AlOH		G1 Gas	209	- 6000	K
173	AlO2H		G1 Gas	298	- 6000	K
174	AlBO2		G1 Gas	298	- 6000	K
175	AlF		G1 Gas	298	- 2000	K
176	AlF2		G1 Gas	298	- 2000	K
177	AlF3		G1 Gas	298	- 2000	K
178	Al2F6		G1 Gas	298	- 6000	K
179	AlOF		G1 Gas	298	- 2500	K
180	AlOF2		G1 Gas	298	- 6000	K
181	NaAlF4		G1 Gas	298	- 6000	K
182	S		G1 Gas	298	- 2000	K
183	S2		G1 Gas	298	- 2000	K
184	S3		G1 Gas	298	- 2000	K
185	S4		G1 Gas	298	- 2000	K
186	S5		G1 Gas	298	- 2000	K
187	S6		G1 Gas	298	- 2000	K

188	S7		Q1 Gas	298	-	2000	K
189	S8		Q1 Gas	298	-	2000	K
190	SH		Q1 Gas	298	-	6000	K
191	H2S		Q1 Gas	298	-	1800	K
192	H2S2		Q1 Gas	298	-	1000	K
193	BS		Q1 Gas	298	-	6000	K
194	BS2		Q1 Gas	298	-	298	K
195	B2S2		Q1 Gas	298	-	1000	K
196	B2S3		Q1 Gas	298	-	2000	K
197	B4S6		Q1 Gas	298	-	1000	K
198	BHS		Q1 Gas	298	-	6000	K
199	CS		Q1 Gas	298	-	2000	K
200	CS2		Q1 Gas	298	-	2000	K
201	CH3SH		Q1 Gas	295	-	300	K
202	C2H4S		Q1 Gas	295	-	300	K
203	(CH3)2S		Q1 Gas	295	-	300	K
204	(CH3)2S		Q2 Ethaneth.	295	-	300	K
205	CH3SCH3		Q1 Gas	295	-	300	K
206	(CH3)2S(BH3)		Q1 Gas	298	-	1000	K
207	SN		Q1 Gas	298	-	2000	K
208	HCNS		Q1 Gas	295	-	300	K
209	CH3NCS		Q1 Gas	295	-	300	K
210	SO	0.1667E-34	Q1 Gas	298	-	2000	K
211	SO2	0.1686E-18	Q1 Gas	298	-	1800	K
212	SO3	0.3436E-17	Q1 Gas	298	-	2000	K
213	S2O		Q1 Gas	298	-	2000	K
214	H2SO4	0.1089E-18	Q1 Gas	298	-	2000	K
215	COS		Q1 Gas	298	-	1800	K
216	C2H4OS		Q1 Thioacetic	298	-	1000	K
217	(CH3)2SO		Q1 Gas	295	-	300	K
218	(CH3)2SO2		Q1 Gas	295	-	300	K
219	SF		Q1 Gas	298	-	6000	K
220	SF2		Q1 Gas	298	-	6000	K
221	SF3		Q1 Gas	298	-	6000	K
222	SF4		Q1 Gas	298	-	6000	K
223	SF5		Q1 Gas	298	-	6000	K
224	SF6		Q1 Gas	298	-	2000	K
225	S2F2		Q1 Df.sulfane	298	-	6000	K
226	S2F2		Q2 Thionyl.f	298	-	6000	K
227	S2F10		Q1 Gas	298	-	2000	K
228	SOF2		Q1 Gas	298	-	2200	K
229	SO2F2	0.1044E-22	Q1 Gas	298	-	2000	K
230	HSO3F	0.2375E-23	Q1 Gas	298	-	6000	K
231	AlS		Q1 Gas	298	-	2000	K
232	Al2S		Q1 Gas	298	-	400	K
233	Al2S2		Q1 Gas	298	-	1000	K
234	Cl	0.1714E-11	Q1 Gas	298	-	3000	K
235	Cl2	0.1254E-12	Q1 Gas	298	-	3000	K
236	HCl	0.2369E-06	Q1 Gas	298	-	2000	K
237	BCl		Q1 Gas	298	-	2000	K
238	BCl2		Q1 Gas	298	-	2000	K
239	BCl3	0.4741E-34	Q1 Gas	298	-	2000	K
240	B2Cl4		Q1 Gas	298	-	6000	K
241	BHCl2		Q1 Gas	298	-	6000	K
242	CCl		Q1 Gas	298	-	6000	K
243	CCl2		Q1 Gas	298	-	2000	K
244	C2Cl2		Q1 Gas	298	-	6000	K
245	CCl3		Q1 Gas	298	-	2000	K
246	CCl4		Q1 Gas	298	-	2000	K
247	C2Cl4		Q1 Gas	298	-	2000	K
248	C2Cl6		Q1 Gas	298	-	2000	K
249	C6Cl6		Q1 Hexachloro	298	-	1000	K
250	CHCl		Q1 Gas	298	-	6000	K
251	CH3Cl		Q1 Gas	298	-	6000	K
252	C2HCl		Q1 Gas	298	-	6000	K
253	CH2CHCl		Q1 Gas	295	-	300	K
254	C2H5Cl		Q1 Gas	295	-	300	K
255	CH2Cl2		Q1 Gas	298	-	6000	K
256	CH2CCl2		Q1 Gas	295	-	300	K
257	CH2CCl2		Q2 Cis-1,2	295	-	300	K
258	CH2CCl2		Q3 Trans-1,2	295	-	300	K
259	CH3CHCl2		Q1 Gas	295	-	300	K
260	CH3CHCl2		Q2 Gas	295	-	300	K
261	CHCl3		Q1 Gas	298	-	6000	K
262	CHClCCl2		Q1 Gas	295	-	300	K
263	CHCl2CH2Cl		Q1 Gas	295	-	300	K
264	CHCl2CHCl2		Q1 Gas	295	-	300	K

265	C2Cl5H	G1 Pentachlor	298	-	1000	K
266	CNCl	G1 Gas	298	-	6000	K
267	ClO	0.8209E-13 G1 Gas	298	-	2000	K
268	O2Cl	0.2698E-17 G1 Gas	298	-	6000	K
269	Cl2O	0.5114E-22 G1 Gas	298	-	2000	K
270	HOCl	0.1180E-09 G1 Gas	298	-	6000	K
271	BOCl	0.6150E-24 G1 Gas	298	-	2000	K
272	B3O3Cl3	G1 Gas	298	-	6000	K
273	COCl	0.1917E-27 G1 Gas	298	-	2000	K
274	COCl2	0.2857E-28 G1 Gas	298	-	2000	K
275	CH3COCl	G1 Gas	295	-	300	K
276	(CH3)2OHC1	G1 Gas	298	-	1000	K
277	NOCl	0.7196E-13 G1 Gas	298	-	2000	K
278	NO2Cl	0.1769E-15 G1 Gas	298	-	2000	K
279	ClF	0.3038E-19 G1 Gas	298	-	2000	K
280	ClF3	G1 Gas	298	-	2000	K
281	ClF5	G1 Gas	298	-	6000	K
282	(ClF3)2	G1 Gas	298	-	1000	K
283	HClF4	G1 Gas	298	-	1000	K
284	BClF	G1 Gas	298	-	6000	K
285	BClF2	0.4840E-22 G1 Gas	298	-	6000	K
286	BCl2F	0.9314E-28 G1 Gas	298	-	6000	K
287	CClF3	G1 Gas	298	-	6000	K
288	CF2CFCl	G1 Gas	295	-	300	K
289	CCl2F2	G1 Gas	298	-	6000	K
290	CCl3F	G1 Gas	298	-	6000	K
291	CCl3CF2Cl	G1 Gas	295	-	300	K
292	CH2ClF	G1 Gas	298	-	6000	K
293	CHClF2	G1 Gas	298	-	6000	K
294	CF2CHCl	G1 Gas	295	-	300	K
295	CHCl2F	G1 Gas	298	-	6000	K
296	O3ClF	G1 Gas	298	-	6000	K
297	COClF	G1 Gas	298	-	6000	K
298	NaCl	G1 Gas	298	-	2000	K
299	Na2Cl2	G1 Gas	298	-	2000	K
300	AlCl	G1 Gas	298	-	2000	K
301	AlCl2	G1 Gas	298	-	2000	K
302	AlCl3	G1 Gas	298	-	2000	K
303	Al2Cl6	G1 Gas	298	-	2000	K
304	AlOCl	G1 Gas	298	-	2000	K
305	AlClF	G1 Gas	298	-	6000	K
306	AlClF2	G1 Gas	298	-	6000	K
307	AlCl2F	G1 Gas	298	-	6000	K
308	SCl	G1 Gas	298	-	2000	K
309	SCl2	G1 Gas	298	-	2000	K
310	S2Cl2	G1 Gas	411	-	1000	K
311	SOCl2	G1 Gas	298	-	1100	K
312	SO2Cl2	G1 Gas	298	-	500	K
313	SF5Cl	G1 Gas	295	-	300	K
314	SO2ClF	0.2014E-32 G1 Gas	298	-	6000	K
315	Ca	G1 Gas	1757	-	2800	K
316	Ca2	G1 Gas	298	-	6000	K
317	CaH	G1 Gas	298	-	2000	K
318	Ca(OH)	G1 Gas	298	-	6000	K
319	CaF	G1 Gas	298	-	6000	K
320	CaF2	G1 Gas	295	-	300	K
321	CaS	G1 Gas	298	-	2000	K
322	CaCl	G1 Gas	298	-	6000	K
323	CaCl2	G1 Gas	295	-	300	K
324	Zr	G1 Gas	295	-	300	K
325	ZrH	G1 Gas	298	-	2000	K
326	ZrO	G1 Gas	298	-	2500	K
327	ZrF	G1 Gas	298	-	2000	K
328	ZrF2	G1 Gas	2529	-	3000	K
329	ZrF3	G1 Gas	1468	-	2000	K
330	ZrF4	G1 Gas	1179	-	2000	K
331	ZrS	G1 Gas	298	-	2000	K
332	ZrCl	G1 Gas	298	-	2000	K
333	ZrCl2	G1 Gas	1565	-	2000	K
334	ZrCl3	G1 Gas	1046	-	2000	K
335	ZrCl4	G1 Gas	607	-	2000	K
336	Cd	0.2389E-13 G1 Gas	1040	-	1200	K
337	Cd(CH3)2	G1 Gas	298	-	1000	K
338	CdS	0.5748E-29 G1 Gas	298	-	2000	K
339	B	L1 Liquid	2450	-	3697	K
340	B4C	L1 Liquid	2743	-	3500	K

341	N2H4	L1	Liquid	295	-	300	K
342	NN3	L1	Liquid	298	-	298	K
343	B3H6N3	L1	Liquid	298	-	310	K
344	HCN	L1	Liquid	295	-	300	K
345	CH3NH2	L1	Liquid	298	-	310	K
346	CH3NC	L1	Methyliso.	298	-	310	K
347	CH3NC	L2	Acetonit.	295	-	300	K
348	(CH3)2NH	L1	Liquid	295	-	300	K
349	CH3N2H3	L1	Liquid	295	-	300	K
350	(CH3)2N2H2	L1	1,1-Di.	295	-	300	K
351	(CH3)2N2H2	L2	1,2-Di	295	-	300	K
352	H2O2	L1	Liquid	298	-	431	K
353	B2O3	L1	Amorphous	298	-	2316	K
354	CH3OH	L1	Liquid	298	-	338	K
355	C2H4O	L1	Ethyl-Ox.	295	-	300	K
356	C2H4O	L2	Acetal.	298	-	310	K
357	CH3CH2OH	L1	Liquid	298	-	352	K
358	HCOOH	L1	Liquid	298	-	374	K
359	CH3COOH	L1	Liquid	295	-	300	K
360	(CH2OH)2	L1	Liquid	295	-	300	K
361	BH(OCH3)2	L1	Liquid	298	-	310	K
362	N2O4	L1	Liquid	295	-	300	K
363	NH4OH	L1	Liquid	295	-	300	K
364	(NH4)2O	L1	Liquid	295	-	300	K
365	HNO3	L1	Liquid	295	-	300	K
366	CH3NO2	L1	Liquid	295	-	300	K
367	CH3NO3	L1	Liquid	295	-	300	K
368	CH3CH2ONO2	L1	Liquid	295	-	300	K
369	Na	L1	Liquid	371	-	1156	K
370	C2Na2	L1	Liquid	546	-	1100	K
371	NaCN	L1	Liquid	835	-	1803	K
372	Na2O	L1	Liquid	1405	-	2223	K
373	NaOH	L1	Liquid	593	-	1663	K
374	NaBO2	L1	Liquid	1239	-	2000	K
375	(Na2O)(B2O3)2	L1	Liquid	1016	-	2000	K
376	Na2CO3	L1	Liquid	1123	-	2000	K
377	NaNO2	L1	Liquid	557	-	800	K
378	NaNO3	L1	Liquid	579	-	700	K
379	NaF	L1	Liquid	1269	-	1983	K
380	Al	L1	Liquid	933	-	2767	K
381	Al(BH4)3	L1	Liquid	295	-	300	K
382	Al2O3	L1	Liquid	2327	-	3500	K
383	Na3AlF6	L1	Liquid	1285	-	2500	K
384	S	L1	Liquid	388	-	718	K
385	H2S2	L1	Liquid	240	-	313	K
386	B2S3	L1	Liquid	836	-	1100	K
387	CS2	L1	Liquid	298	-	319	K
388	CH3SH	L1	Liquid	295	-	300	K
389	C2H4S	L1	Liquid	298	-	310	K
390	(CH3)2S	L1	Liquid	295	-	300	K
391	(CH3)2S	L2	Ethaneth.	295	-	300	K
392	CH3SCH3	L1	Liquid	295	-	300	K
393	H2CS3	L1	Liquid	298	-	331	K
394	(CH3)2S(BH3)	L1	Liquid	298	-	310	K
395	SO3	L1	Liquid	298	-	310	K
396	H2SO4	L1	Liquid	298	-	553	K
397	H2SO4(H2O)	L1	Liquid	295	-	300	K
398	H2SO4(H2O)2	L1	Liquid	295	-	300	K
399	H2SO4(H2O)3	L1	Liquid	295	-	300	K
400	H2SO4(H2O)4	L1	Liquid	295	-	300	K
401	(H2SO4)2(H2O)13	L1	Liquid	295	-	300	K
402	(CH3)2SO	L1	Liquid	295	-	300	K
403	SF6	L1	Liquid	298	-	310	K
404	S2F10	L1	Liquid	298	-	298	K
405	NaS	L1	Liquid	753	-	1500	K
406	Na2S	L1	Liquid	1251	-	2200	K
407	NaS2	L1	Liquid	458	-	1000	K
408	Na2S3	L1	Liquid	1026	-	1000	K
409	Na2SO3	L1	Liquid	1000	-	2000	K
410	Na2SO4	L1	Liquid	1157	-	2000	K
411	Al2S3	L1	Liquid	1370	-	1800	K
412	BCl3	L1	Liquid	295	-	300	K
413	B2Cl4	L1	Liquid	295	-	300	K
414	CCl4	L1	Liquid	298	-	350	K
415	C2Cl4	L1	Liquid	295	-	300	K
416	C2H5Cl	L1	Liquid	295	-	300	K
417	CH2Cl2	L1	Liquid	295	-	300	K

0.3162E-16

418	CH2CCl2	L1 Liquid	295	-	300	K
419	CH2CCl2	L2 Cis-1,2	295	-	300	K
420	CH2CCl2	L3 Trans-1,2	295	-	300	K
421	CH3CHCl2	L1 Liquid	295	-	300	K
422	CH3CHCl2	L2 Liquid	295	-	300	K
423	CHCl3	L1 Liquid	295	-	300	K
424	CHClCCl2	L1 Liquid	295	-	300	K
425	CHCl2CH2Cl	L1 Liquid	298	-	298	K
426	CHCl2CHCl2	L1 Liquid	295	-	300	K
427	CH3COCl	L1 Liquid	295	-	300	K
428	CCl3F	L1 Liquid	295	-	300	K
429	NaCl	L1 Liquid	1074	-	1768	K
430	SiCl2	L1 Liquid	298	-	411	K
431	Ca	L1 Liquid	1112	-	1757	K
432	CaO	L1 Liquid	2888	-	3500	K
433	(CaO)(B2O3)	L1 Liquid	1433	-	2000	K
434	(CaO)(B2O3)2	L1 Liquid	1263	-	2000	K
435	(CaO)2(B2O3)	L1 Liquid	1583	-	2000	K
436	(CaO)3(B2O3)	L1 Liquid	1763	-	2000	K
437	CaF2	L1 Liquid	1691	-	1800	K
438	CaAl2	L1 Liquid	1353	-	1800	K
439	CaAl4	L1 Liquid	1050	-	1700	K
440	CaCl2	L1 Liquid	1045	-	2273	K
441	Zr	L1 Liquid	2125	-	4777	K
442	ZrB2	L1 Liquid	3323	-	4466	K
443	ZrN	L1 Liquid	3223	-	3500	K
444	ZrO2	L1 Liquid	2950	-	4548	K
445	ZrF2	L1 Liquid	1175	-	2529	K
446	ZrCl2	L1 Liquid	1000	-	1565	K
447	Cd	L1 Liquid	594	-	1040	K
448	Cd(CH3)2	L1 Liquid	295	-	300	K
449	NaCd2	L1 Liquid	655	-	900	K
450	CdCl2	L1 Liquid	841	-	1234	K
451	H2O	L1 Water	273	-	374	K
641	B	S1 Solid	298	-	2450	K
642	B10H14	S1 Solid	295	-	300	K
643	C	S1 Graphite	298	-	4073	K
644	C	S2 Diamond	298	-	1200	K
645	B4C	S1 Solid	298	-	2743	K
646	NH4N3	S1 Solid	298	-	298	K
647	BN	S1 Solid	298	-	1200	K
648	CNH(NH2)(NHCN)	S1 Solid	295	-	300	K
649	H2O	S1 Ice	250	-	273	K
650	B2O3	S1 Solid	298	-	723	K
651	HBO2	S1 Solid	298	-	509	K
652	HBO2	S2 Monoclinic	298	-	310	K
653	HBO2	S3 Orthorhom.	298	-	310	K
654	H3BO3	S1 Solid	298	-	444	K
655	N2O5	S1 Solid	295	-	300	K
656	NH4NO3	S1 Solid	295	-	300	K
657	CO(NH2)2	S1 Solid	295	-	300	K
658	NH2CH2COOH	S1 Solid	295	-	300	K
659	NH2COONH4	S1 Solid	298	-	298	K
660	NH4HCO3	S1 Solid	298	-	310	K
661	NH4F	S1 Solid	295	-	300	K
662	NH5F2	S1 Solid	295	-	300	K
663	Na	S1 Solid	298	-	371	K
664	NaH	S1 Solid	298	-	700	K
665	C2Na2	S1 Solid	298	-	546	K
666	NaCN	S1 Solid	298	-	835	K
667	NaO2	S1 Solid	298	-	825	K
668	Na2O	S1 Solid-C	298	-	1023	K
669	Na2O	S2 Solid-B	1023	-	1243	K
670	Na2O	S3 Solid-A	1243	-	1405	K
671	Na2O2	S1 Solid-A	298	-	785	K
672	Na2O2	S2 Solid-B	785	-	948	K
673	NaOH	S1 Solid-A	298	-	568	K
674	NaOH	S2 Solid-B	568	-	593	K
675	NaBO2	S1 Solid	298	-	1239	K
676	(Na2O)(B2O3)2	S1 Solid	298	-	1016	K
677	(Na2O)(B2O3)3	S1 Solid	298	-	1039	K
678	Na2CO3	S1 Solid-A	298	-	723	K
679	Na2CO3	S2 Solid-B	723	-	1123	K
680	NaHCO3	S1 Solid	298	-	500	K
681	NaNO2	S1 Alpha	298	-	434	K
682	NaNO2	S2 Beta	434	-	557	K

683	NaNO3		81	Solid	298	-	579	K
684	NaF	1.000	81	Villiaumite	298	-	1269	K
685	Al		81	Solid	298	-	933	K
686	AlH3		81	Solid(hex)	298	-	400	K
687	AlB2		81	Solid	298	-	1300	K
688	AlB12		81	Solid	298	-	2473	K
689	Al4C3		81	Solid	298	-	1800	K
690	AlN	0.1220E-31	81	Solid	298	-	2000	K
691	Al2O3	1.000	81	Corundum	298	-	2327	K
692	Al(OH)3		81	Solid	298	-	700	K
693	Al2O3(H2O)		81	Diaspore	298	-	500	K
694	Al2O3(H2O)		82	Boehmite	295	-	300	K
695	Al2O3(H2O)3		81	Gibbsite	298	-	500	K
696	(Al2O3)2(B2O3)	0.1429E-03	81	Solid	298	-	1308	K
697	(Al2O3)9(B2O3)2	0.4759E-03	81	Solid	298	-	1600	K
698	Al(NO3)3(H2O)6		81	Solid	295	-	300	K
699	AlF3		81	Solid-A	298	-	728	K
700	AlF3	0.1470E-09	82	Solid-B	728	-	1949	K
701	NaAlO2		81	Solid-A	298	-	740	K
702	NaAlO2	1.000	82	Solid-B	740	-	1800	K
703	AlCH2NaO5		81	Dawsonite	298	-	500	K
704	Na3AlF6	0.3047E-03	81	A-Cryolite	298	-	838	K
705	Na3AlF6		82	B-Cryolite	838	-	1153	K
706	Na3AlF6		83	C-Cryolite	1153	-	1285	K
707	S		81	Rhombic	298	-	368	K
708	S		82	Monoclinic	368	-	388	K
709	S82		81	Solid	298	-	310	K
710	S283		81	Solid	298	-	836	K
711	NH4HS		81	Solid	298	-	310	K
712	SO3		81	Solid	298	-	298	K
713	(CH3)2SO2		81	Solid	298	-	298	K
714	(NH4)2(SO4)		81	Muscovite	298	-	600	K
715	(NH4)2SO4(NH3)3		81	Solid	298	-	310	K
716	NH2CH2CH2SO3H		81	Solid	295	-	300	K
717	Na8		81	Solid	298	-	733	K
718	Na28		81	Solid	298	-	1251	K
719	Na82		81	Solid	298	-	458	K
720	Na282		81	Solid	298	-	310	K
721	Na283		81	Solid	298	-	626	K
722	Na284		81	Solid	298	-	310	K
723	Na28O3	0.1025E-14	81	Solid	298	-	1000	K
724	Na28O4		81	Thénardite	298	-	522	K
725	Na28O4	1.000	82	Solid-B	522	-	980	K
726	Na28O4		83	Solid-C	980	-	1157	K
727	Al8		81	Solid	298	-	310	K
728	Al283		81	Solid	298	-	1370	K
729	Al2(SO4)3		81	Solid	298	-	1100	K
730	Al2(SO4)3(H2O)6		81	Solid	295	-	300	K
731	NH4Al(SO4)2		81	Solid	295	-	300	K
732	NH4Al(SO4)2(H2O)12		81	Tschernig.	295	-	300	K
733	(NH4)2O(Al2O3)3(SO3)4(H2O)6		81	Solid	295	-	300	K
734	NH4Cl		81	Solid-A	298	-	458	K
735	NH4Cl		82	Solid-B	458	-	793	K
736	CH3NH3Cl		81	Solid	295	-	300	K
737	NH4ClO4		81	Solid	298	-	513	K
738	NaCl	1.000	81	Halite	298	-	1074	K
739	NaClO4	0.7733E-21	81	Solid-A	298	-	581	K
740	NaClO4		82	Solid-B	581	-	735	K
741	AlCl3		81	Solid	298	-	454	K
742	AlOCl		81	Solid	298	-	700	K
743	AlCl3(H2O)6		81	Solid	298	-	400	K
744	NaAlCl4		81	Solid	298	-	424	K
745	Na3AlCl6	0.3488E-28	81	Solid	298	-	780	K
746	Ca		81	Solid-A	298	-	720	K
747	Ca		82	Solid-B	720	-	1112	K
748	CaH2		81	Solid	298	-	1053	K
749	CaC2		81	Solid-A	298	-	720	K
750	CaC2		82	Solid-B	720	-	1275	K
751	Ca3N2		81	Solid	298	-	1468	K
752	CaO	0.1218E-02	81	Lime	298	-	2858	K
753	CaO2		81	Solid	298	-	427	K
754	Ca(OH)2	0.7331E-03	81	Solid	298	-	1000	K
755	(CaO)(B2O3)	0.1120E-02	81	Solid	298	-	1433	K
756	(CaO)(B2O3)2	0.3626E-09	81	Solid	298	-	1263	K
757	(CaO)2(B2O3)	0.8299E-01	81	Solid-A	298	-	804	K
758	(CaO)2(B2O3)	0.8082E-01	82	Solid-B	804	-	1583	K
759	(CaO)3(B2O3)	1.000	81	Solid	298	-	1763	K

760	CaCO3	0.7509E-01	81	Aragonite	298	- 1200 K
761	CaCO3	0.7822E-01	82	Calcite	298	- 1200 K
762	CaC2O4(H2O)		81	Solid	295	- 300 K
763	Ca(NO3)2	0.3257E-13	81	Solid	298	- 834 K
764	Ca(NO3)2(H2O)2		81	Solid	298	- 310 K
765	Ca(NO3)2(H2O)3		81	Solid	298	- 310 K
766	Ca(NO3)2(H2O)4		81	Solid	298	- 310 K
767	CaF2	1.000	81	Fluorite	298	- 1424 K
768	CaF2		82	Solid-B	1424	- 1691 K
769	CaAl2		81	Solid	298	- 1353 K
770	CaAl4		81	Solid	298	- 1050 K
771	(CaO)(Al2O3)	0.1392	81	Solid	298	- 1878 K
772	(CaO)(Al2O3)2	0.3145	81	Solid	298	- 2023 K
773	(CaO)3(Al2O3)	0.2882E-06	81	Solid	298	- 1808 K
774	(CaO)12(Al2O3)7	0.2044E-21	81	Solid	298	- 1800 K
775	(CaO)3(Al2O3)(H2O)6		81	Solid	298	- 700 K
776	(CaO)4(Al2O3)(H2O)13		81	Solid	298	- 500 K
777	Ca8		81	Oldhamite	298	- 2000 K
778	CaSO3	0.8391E-15	81	Solid	298	- 1000 K
779	CaSO4	0.1120E-02	81	Anhydrite	298	- 1200 K
780	CaSO4		82	Solid-Alpha	295	- 300 K
781	CaSO4		83	Solid-Beta	295	- 300 K
782	CaSO3(H2O)2		81	Solid	295	- 300 K
783	CaSO4(H2O)2	0.1353E-10	81	Gypsum	298	- 800 K
784	(CaSO4)2(H2O)	0.6060E-10	81	Solid	298	- 800 K
785	(CaSO4)2(H2O)		82	Solid-Beta	295	- 300 K
786	CaCl2		81	Solid	298	- 1045 K
787	CaOCl2		81	Solid	298	- 500 K
788	Ca(ClO4)2(H2O)4		81	Solid	298	- 310 K
789	Zr		81	Solid-A	298	- 1135 K
790	Zr		82	Solid-B	1135	- 2125 K
791	ZrH2		81	Solid	295	- 300 K
792	ZrB2		81	Solid	298	- 3323 K
793	ZrC		81	Solid	298	- 3500 K
794	ZrC4		81	Solid	298	- 550 K
795	ZrN		81	Solid	298	- 3225 K
796	ZrO2	1.000	81	Solid-A	298	- 1478 K
797	ZrO2	0.5793	82	Solid-B	1478	- 2950 K
798	ZrF2		81	Solid	298	- 1175 K
799	ZrF3	0.8885E-32	81	Solid	298	- 1468 K
800	ZrF4	0.9958E-19	81	Solid-A	298	- 723 K
801	ZrF4	0.9962E-19	82	Solid-B	723	- 1179 K
802	ZrB2		81	Solid	298	- 1823 K
803	ZrB3		81	Solid	298	- 310 K
804	Zr2B3		81	Solid	298	- 310 K
805	ZrCl2		81	Solid	298	- 1000 K
806	ZrCl3		81	Solid	298	- 1046 K
807	ZrCl4		81	Solid	298	- 607 K
808	(CaO)(ZrO2)	0.3437	81	Solid	298	- 2613 K
809	Cd		81	Solid	298	- 594 K
810	CdO		81	Solid	298	- 1500 K
811	Cd(OH)2		81	Solid	298	- 310 K
812	Cd(SO2)2		81	Solid	298	- 310 K
813	CdCO3		81	Solid	298	- 560 K
814	CdC2O4(H2O)3		81	Solid	298	- 310 K
815	CdF2	0.7450E-07	81	Solid	298	- 1345 K
816	NaCd2		81	Solid	298	- 655 K
817	(CdO)(Al2O3)	1.000	81	Solid	298	- 1200 K
818	Cd8		81	Greenoc. te	298	- 1300 K
819	CdSO4	0.3025E-08	81	Solid	298	- 1273 K
820	CdSO4(H2O)		81	Solid	295	- 300 K
821	Cd3SO4(OH)4		81	Solid	298	- 310 K
822	(CdSO4)2Cd(OH)2		81	Solid	298	- 310 K
823	(CdSO4)3(H2O)8		81	Solid	295	- 300 K
824	CdCl2	0.3337E-06	81	Solid	298	- 841 K
825	CdCl2(NH3)2		81	Solid	298	- 310 K
826	CdCl2(NH3)4		81	Solid	298	- 310 K
827	CdCl2(NH3)6		81	Solid	298	- 310 K
828	Cd(OH)Cl		81	Solid	298	- 310 K
829	CdCl2(H2O)		81	Solid	298	- 310 K
830	(CdCl2)2(H2O)5		81	Solid	298	- 298 K

LIST: (HELP ALL G LIG AG 8 SOLN PRIV 2-11 LOC)
 ENTER LIST COMMAND (H FOR HELP)
 OR PRESS <RETURN> TO CONTINUE

/11-23,26-34,36-42,46,51-57,68-73,75,77,79,82,84-97,102,103,109-122,

CONTINUE THE SELECTION
128-137, 145-162, 182-192, 207, 210-216, 219-230, 234-252, 261, 265-274,

CONTINUE THE SELECTION
276-287, 308-311, 314, 331, 332, 334, 336-338/369, 384, 447/641, 643, 647, 666, 668,

CONTINUE THE SELECTION
671, 675, 676, 679, 684, 685, 687-691, 696, 697, 700, 702, 704, 710, 718, 723, 725,

CONTINUE THE SELECTION
728, 729, 738, 739, 745, 747, 750, 751, 752, 754-761, 763, 767, 769-774, 777-779,

CONTINUE THE SELECTION
783, 784, 789, 792, 793, 795-802, 805, 806, 808, 815, 817-819, 824

PRESS <RETURN> WHEN READY FOR OUTPUT
OR ENTER OPTION(S), OR ENTER "O" FOR OPTIONS MENU
(enter /C to go to command mode)

55.405H2O+4.558NO3+.01Cl+.046S+.092O2+1.648H+.081Cd+.338Na+

1.709F+1.055Ca+.14B+.393Al+.2332r+

13.102 + 52.4N2 + 2.1C + 4.2H =

130.65	mol	(	0.44644	H2O	
		+	0.41851	N2	
		+	0.11896	O2	
		+	0.16073E-01	CO2	
		+	0.10825E-04	HF	
		+	0.79473E-06	NO	
		+	0.24880E-06	NO2	
		+	0.23689E-06	HCl	
		+	0.12777E-08	HNO2	
		+	0.92026E-09	HNO2	
		+	0.61662E-09	OH	
		+	0.11802E-09	HNO3	
		+	0.76379E-10	HNO3	
		+	0.52267E-10	H2O	
		+	0.31145E-10	NaF	
		+	0.59464E-11	H2O2	
		+	0.26382E-11	NO2	
		+	0.17138E-11	Cl	
		+	0.12068E-11	Na2F2	
		+	0.20347E-12	NaBO2	
		+	0.12538E-12	Cl2	
		+	0.82094E-13	ClO	
		+	0.71959E-13	NOCl	
		+	0.23888E-13	Cd	
		+	0.72540E-14	O	
		+	0.49198E-14	NO3	
		+	0.40067E-14	Na2O2H2	
		+	0.22906E-14	O3	
		+	0.17702E-15	NOF	
		+	0.17693E-15	NO2Cl	
		+	0.12784E-15	CO	
		+	0.23587E-16	HNO	
		+	0.51015E-17	H2O3	
		+	0.34360E-17	SO3	
		+	0.26980E-17	O2Cl	
		+	0.85210E-18	NO2F	
		+	0.43527E-18	H2O4	
		+	0.16858E-18	SO2	
		+	0.16279E-18	Na	
		+	0.10894E-18	H2SO4	
		+	0.89799E-19	NaO	
		+	0.30380E-19	ClF	
		+	0.13304E-19	NOF)	
		(	773.00 K, 1.0000	atm, gas)	
+ 0.00000E+00	mol	(	0.12320E-11	Cd	
		+	0.31623E-16	Na)	
		(	773.00 K, 1.0000	atm, liquid, a=0.12321E-11)	
		+	0.84500	mol CaF2	

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( 773.00 K, 1.0000 atm, S1, a= 1.0000 )
+ 0.23300 mol ZrO2
( 773.00 K, 1.0000 atm, S1, a= 1.0000 )
+ 0.21844 mol NaAlO2
( 773.00 K, 1.0000 atm, S2, a= 1.0000 )
+ 0.81000E-01 mol (CdO)(Al2O3)
( 773.00 K, 1.0000 atm, S1, a= 1.0000 )
+ 0.70000E-01 mol (CaO)3(B2O3)
( 773.00 K, 1.0000 atm, S1, a= 1.0000 )
+ 0.46000E-01 mol Na2SO4
( 773.00 K, 1.0000 atm, S2, a= 1.0000 )
+ 0.17587E-01 mol NaF
( 773.00 K, 1.0000 atm, S1, a= 1.0000 )
+ 0.99690E-02 mol NaCl
( 773.00 K, 1.0000 atm, S1, a= 1.0000 )
+ 0.62778E-02 mol Al2O3
( 773.00 K, 1.0000 atm, S1, a= 1.0000 )
+ 0.00000E+00 mol Na2CO3
( 773.00 K, 1.0000 atm, S2, a=0.62746 )
+ 0.00000E+00 mol ZrO2
( 773.00 K, 1.0000 atm, S2, a=0.57931 ) X
+ 0.00000E+00 mol (CaO)(ZrO2)
( 773.00 K, 1.0000 atm, S1, a=0.34374 )
+ 0.00000E+00 mol (CaO)(Al2O3)2
( 773.00 K, 1.0000 atm, S1, a=0.31452 )
+ 0.00000E+00 mol (CaO)(Al2O3)
( 773.00 K, 1.0000 atm, S1, a=0.13923 )
+ 0.00000E+00 mol NaBO2
( 773.00 K, 1.0000 atm, S1, a=0.11172 )
+ 0.00000E+00 mol (CaO)2(B2O3)
( 773.00 K, 1.0000 atm, S1, a=0.82986E-01)
+ 0.00000E+00 mol (CaO)2(B2O3)
( 773.00 K, 1.0000 atm, S2, a=0.80822E-01) X
+ 0.00000E+00 mol CaCO3
( 773.00 K, 1.0000 atm, S2, a=0.78219E-01)
+ 0.00000E+00 mol CaCO3
( 773.00 K, 1.0000 atm, S1, a=0.75091E-01)
+ 0.00000E+00 mol CaO
( 773.00 K, 1.0000 atm, S1, a=0.12180E-02)
+ 0.00000E+00 mol (CaO)(B2O3)
( 773.00 K, 1.0000 atm, S1, a=0.11200E-02)
+ 0.00000E+00 mol CaSO4
( 773.00 K, 1.0000 atm, S1, a=0.11199E-02)
+ 0.00000E+00 mol Ca(OH)2
( 773.00 K, 1.0000 atm, S1, a=0.73312E-03)
+ 0.00000E+00 mol Na3AlF6
( 773.00 K, 1.0000 atm, S1, a=0.30467E-03)
+ 0.00000E+00 mol (Al2O3)2(B2O3)
( 773.00 K, 1.0000 atm, S1, a=0.14294E-03)
+ 0.00000E+00 mol (Al2O3)9(B2O3)2
( 773.00 K, 1.0000 atm, S1, a=0.47594E-05)

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+ 0.00000E+00 mol CdCl2
( 773.00 K, 1.0000 atm, S1, a=0.33374E-06)
+ 0.00000E+00 mol (CaO)3(Al2O3)
( 773.00 K, 1.0000 atm, S1, a=0.28816E-06)
+ 0.00000E+00 mol CdF2
( 773.00 K, 1.0000 atm, S1, a=0.74499E-07)
+ 0.00000E+00 mol (Na2O)(B2O3)2
( 773.00 K, 1.0000 atm, S1, a=0.10063E-07)
+ 0.00000E+00 mol CdSO4
( 773.00 K, 1.0000 atm, S1, a=0.30248E-08)
+ 0.00000E+00 mol (CaO)(B2O3)2
( 773.00 K, 1.0000 atm, S1, a=0.36264E-09)
+ 0.00000E+00 mol AlF3
( 773.00 K, 1.0000 atm, S2, a=0.14701E-09)
+ 0.00000E+00 mol (CaSO4)2(H2O)
( 773.00 K, 1.0000 atm, S1, a=0.60599E-10)
+ 0.00000E+00 mol Na2O2
( 773.00 K, 1.0000 atm, S1, a=0.24979E-10)
+ 0.00000E+00 mol CaSO4(H2O)2
( 773.00 K, 1.0000 atm, S1, a=0.13535E-10)
+ 0.00000E+00 mol Na2O
( 773.00 K, 1.0000 atm, S1, a=0.44225E-12)
+ 0.00000E+00 mol Ca(NO3)2
( 773.00 K, 1.0000 atm, S1, a=0.32570E-13)
+ 0.00000E+00 mol Na2SO3
( 773.00 K, 1.0000 atm, S1, a=0.10252E-14)
+ 0.00000E+00 mol CaSO3
( 773.00 K, 1.0000 atm, S1, a=0.83912E-15)
+ 0.00000E+00 mol ZrF4
( 773.00 K, 1.0000 atm, S2, a=0.99620E-19)
+ 0.00000E+00 mol ZrF4
( 773.00 K, 1.0000 atm, S1, a=0.99576E-19) X

```

The cutoff concentration has been specified to 1.000E-20

Data on 3 product species identified with "X" have not been extrapolated in computing the phase assemblage

Data on 1 product species identified with "T" have been extrapolated

Press <CR> or enter C for chemical capacitance table or enter help

References

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3. G. F. Kessinger, Verification of Thermodynamic Codes REACT and EQUILIB for the Study of Non-aqueous Inorganic Systems, WINCO-1105, September, 1992.
4. Ihsan Barin in collaboration with F. Sauert, E. Schultze-Rhonhof, and W. S. Sheng, Thermochemical Data of Pure Substances, VCH Publishers, New York, 1989.

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