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WATEQ3 - A GEOCHEMICAL MODEL WITH URANIUM ADDED

by James W. Ball, Everett A. Jenne and Mark W. Cantrell

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WATEQ3 - A GEOCHEMICAL MODEL WITH URANIUM ADDED

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ABSTRACT

The addition of uranium to the 1979 WATEQ2 chemical model has resulted in a larger version known as WATEQ3. This larger version of the model was tested against a second model and the computer codes were corrected until each model performed the calculations accurately and produced virtually identical results. Thermodynamic data from the 1978 compilation of Donald Langmuir were used in the input data base. This report makes available the computer code and the data base used, together with a description of the changes made.

INTRODUCTION

Many present and potential problems exist involving contamination of potable waters with uranium (U) from mines, tailings piles, and nuclear wastes. It is important in the assessment of some of these problems to be able to calculate the distribution of dissolved U among its various complexed and uncomplexed species, including valence forms. This in turn may lead to an understanding of the sorption potential, and hence mobility, of U solute species. Calculations yielding the activity of the dissolved uncomplexed species are necessary to evaluate solubility limitations, and are most reliably done with a geochemical model containing all major cations and anions as well as any minor ones that may affect U speciation. It is also important that the thermodynamic data base be documented and readily accessible (Ball and others, 1979; 1980) and tested by application to natural waters (Jenne and Truesdell, 1973; Nordstrom and Jenne, 1977; Jenne and others, 1980). Small departures from equilibrium

solubility may be evaluated using appropriate sensitivity analyses (Jenne and Truesdell, 1973; Jenne and others, 1978; Nordstrom and others, 1979), to determine if the departures from equilibrium could be the result of errors in or omissions of analytical or thermodynamic data (Jenne and others, 1980). As an example of a sensitivity analysis, the concentration of an individual input constituent might be varied and the effect of the change on the resulting computed solubility observed.

Thermochemical data at the standard reference state of 25°C and 1 bar pressure for U were taken from the recent evaluation of Langmuir (1978). THERMO2, a modification of THERMO (Nathenson, 1973), a thermodynamic model designed to compute log K of reaction (log K_r) values using entropy (S) and enthalpy (ΔH) data was used initially to obtain the log K_r values of U species and minerals for WATEQ3. Inconsistencies were found between the log K_r computed from solubility measurements and log K_r computed from ΔH and S data (Table 1). Log K_r values derived from solubility measurements are considered to be more meaningful in studies of the natural environment than those derived from ΔH and S values; therefore, the former were selected.

Table 1. List of thermochemical values calculated by THERMO2 for addition to WATEQ3.

Reaction Number	Species or Solid	ΔH_r	Log K_r from ΔH-$T\Delta S$	Log K_r from solubility measurements
544	kU +3	24.400	-5.384	-8.796[1]
553	U409 (c)	-101.235	3.080	-3.384
554	U308 (c)	-116.020	34.589	21.107
565	kUSO4 +2	3.700	5.046	5.461
566	kU(SO4)2 aq	7.600	9.290	9.749
570	kU(HPO4)4 -4	-26.500	88.483	88.031
573	kU02 +	-3.300	6.178	2.785
597	(U02)3(PO4)2	94.900	-129.134	-49.037

[1]Underlined values are those used in WATEQ3.

Procedures were coded for the speciation of U solutes and calculation of the activity products of U solid phases. These procedures were inserted into WATEQ3 along with temperature corrections to the log K_r values and calculations of pe for the oxidation of U^{4+} to UO_2^{2+}.

The model with the added U was tested by comparing output data with data obtained using a U-speciation-solubility model (TEK-U)[2] written by F. J. Pearson (U.S. Geological Survey, Reston, Va.) for Tektronix 4050-series desktop computers. The TEK-U program was modified for the present study so that the two outputs could be directly compared.

Geochemical models must continuously evolve to provide new kinds of information and take advantage of new analytical capabilities. Since the WATEQ2 model was published (Ball and others, 1979), additions and refinements beyond the addition of U to the model have also been made.

RESULTS AND DISCUSSION

Testing of the Model

Modeling of the two test data sets used previously for an intermodel comparison by Nordstrom and others (1979) established that the computation of non-uranium solutes or solids was not affected by the addition of U to the model. A test data set from Potter and others (1979), number USBM-1, was next modeled with WATEQ3. The output activities for the major ion species and the U concentration from this data set were used as input to TEK-U. Errors found in the respective computer codes were corrected. Results of calculations in both programs for U solutes and solids were compared and the differences in output data between the two models were resolved.

The differences between the two models were found to result from different mass-balance calculation methods. Two of the aqueous U species in the models are polynuclear (2 or 3 U atoms in the complex). These require special consideration as their calculation is difficult in a noniterative model such as TEK-U. Pearson treated the reactions for these two species by dividing the formulas by 2 and 3, respectively, the number of U atoms in each complex. This worked satisfactorily, as long as one remembered that the resultant molalities were the square root and cube root, respectively, of the true values; to obtain the true concentrations of these species, the results had to be squared and cubed, respectively.

When the values of the polynuclear species were squared and cubed, a true mass balance no longer occurred and the concentrations of all other species were underestimated by a percentage which was dependent upon the fraction of the total U speciated into these two polynuclear forms. In the USBM-1 test set used (Potter and others, 1979), the underestimation was about 6.2 percent for all nonpolynuclear species. For some

2/ Presently with INTERA Environmental Consultants, Houston, TX

purposes this may not be a significant error; however, it was a major discrepancy in contrast to models such as WATEQ3 which test for mass balance to ±0.1 percent. Therefore, we modified the TEK-U model to obtain a more accurate speciation to further verify the WATEQ3 calculations.

A noniterative approach to a similar problem with the earlier WATEQ2 was used for the HF_2^- complexation reaction (D. K. Nordstrom, oral commun., 1976). The square root of $M_{HF_2^-}$ was used to compute the $M_{HF_2^-}$ fraction for substitution into the mass balance equation which computed the molality of F^- (M_{F^-}). Squaring the resulting $\sqrt{M_{HF_2^-}}$ obtained by multiplying the fraction $\sqrt{M_{HF_2^-}}/a_{F^-}$ by $a_{F^-}^2$ yielded an initial estimate for $M_{HF_2^-}$. This estimate of $M_{HF_2^-}$ was subsequently recalculated in the F^- ion mass balance section, so the square root calculation served its purpose of increasing the accuracy of the initial estimate of a_{F^-} without affecting the accuracy of the model's final output. There was no comparable recalculation of $a_U{}^{4+}$, $M_{(UO_2)_2(OH)_2^{2+}}$ or $M_{(UO_2)_3(OH)_5^+}$ in TEK-U; therefore, the mass-balance calculation remained inaccurate due to use of the square root and cube root terms. A further difficulty in TEK-U was that the square root of gamma, the activity coefficient, was not used, and the true molalities were not calculated so that the model produced $M_{1/2(UO_2)_2(OH)_2^{2+}}$ and $M_{1/3(UO_2)_3(OH)_5^+}$. This problem did not exist in WATEQ2 because roots were not used in final calculations involving the polynuclear species.

The problems resulting from the speciation of U into polynuclear complexes in TEK-U were solved by modifying it to calculate the distribution of aqueous species a second time, using a more accurate method of calculation of the polynuclear species on the second iteration. The square root and cube root forms of calculation for the polynuclear species are retained for the first iteration only, and $a_U{}^{4+}$, a quantity known only after completion of the first iteration, is used for the second iteration. The thermochemical data were altered to represent the true composition of the species, and the calculations in the TEK-U model were altered so that applicable roots of the equilibrium constants and activity coefficients were used for the first iteration. The reactions used in TEK-U follow:

1st iteration:

$$\frac{\sqrt{m_{(UO_2)_2(OH)_2^{2+}}}}{a_{U^{4+}}} = \frac{a_{H_2O}^3}{\sqrt{K_t}\ a_{H^+}^5\ a_{e^-}^2\ \sqrt{\gamma_{(UO_2)_2(OH)_2^{2+}}}}$$

and

$$\frac{\sqrt[3]{m_{(UO_2)_3(OH)_5^+}}}{a_{U^{4+}}} = \frac{\sqrt[3]{a_{H_2O}^{11}}}{\sqrt[3]{K_t\ a_{H^+}^{17}\ a_{e^-}^2}\ \sqrt[3]{\gamma_{(UO_2)_3(OH)_5^+}}}$$

2nd iteration:

$$\frac{m_{(UO_2)_2(OH)_2^{2+}}}{a_{U^{4+}}} = \frac{a_{H_2O}^6\ a_{U^{4+}}}{K_t\ a_{H^+}^{10}\ a_{e^-}^4\ \gamma_{(UO_2)_2(OH)_2^{2+}}}$$

and

$$\frac{m_{(UO_2)_3(OH)_5^+}}{a_{U^{4+}}} = \frac{a_{H_2O}^{11}\ a_{U^{4+}}^2}{K_t\ a_{H^+}^{17}\ a_{e^-}^6\ \gamma_{(UO_2)_3(OH)_5^+}}$$

With this modification to the form of the calculations in TEK-U, the two models yield comparable results using the same thermodynamic data base. Even though two different methods of calculation are used, similar distributions of aqueous species are obtained, increasing our confidence in the correctness of the models and their computer codes.

In WATEQ3 the U polynuclear species are ignored in the first iteration of the U section. As they are quantitatively minor species, the accuracy of the mass balance calculation is not impaired. The HF_2^- species, by contrast, may constitute a major proportion of the total F^- and therefore must be included in the initial mass balance calculation.

The present model is, of course, still limited by the selection of the elements considered. For example, V, an element frequently associated with U in nature, is not in WATEQ3. The absence of V prevents the calculation of solubility indices for carnotite ($K_2(UO_2)_2(VO_4)_2$) and tyuyamunite ($Ca(UO_2)_2(VO_4)_2$).

Other Additions to the Model

Calculations for the association of aqueous NaF^{o} were added because we have used a Na-bearing decomplexing agent in the ion-specific electrode method for F analysis. In a 2 *M* NaCl solution containing 0.1 mg L^{-1} of F, 10.9 percent of the F is computed by WATEQ3 to be present as the NaF^{o} complex.

The dissolution reaction for $Ba_3(AsO_4)_2$ has also been added to WATEQ3 following the suggestion of Steven Lindberg (Oak Ridge National Laboratory, oral commun., 1979) that this mineral might limit the concentration of As in the leachates of ash which has resulted from coal combustion. However, using the thermochemical data given in the compilation of Sillen (1964), $Ba_3(AsO_4)_2$ computes to be grossly oversaturated in a number of geothermal water analyses. Thus, it appears unlikely that the precipitation of this solid will limit As concentrations in fly ash leachates.

WATEQ2 DOCUMENTATION ERRORS

To date, only one minor error has been found in the WATEQ2 model (Ball and others, 1979). Line ERRC 370 should read: ERR(106)=SQRT((3*RSD(7))**2+(2*RSD(44))**2);. However, six problems in the documentation (Ball and others, 1980) have been brought to our attention by colleagues. The temperature dependence of log K_r given for aragonite in reaction 21 is not included in the model, and is in the documentation in terms of temperature in degrees Celsius rather than in kelvins. The kelvin temperature expression is:

$$\log K_r = -10.21 + 0.0217T - 5.17 \times 10^{-5}T^2.$$

Second, a minus sign is missing from the first term of the temperature dependence on the log K_r equation of reaction 35 for $H_2CO_3^{o}$ aq which should read:

$$\log K_r = -14.8435 + 0.032786T + 3404.71/T.$$

Reaction 127 is reversed in the documentation relative to the way it is written in the model. For reaction 158, the analytical expression should read:

$$\log K_r = -5.4 + 1.52\ pH.$$

Reaction 194 is in error and should read:

$$MnHPO_4 \rightleftarrows Mn^{2+} + HPO_4^{2-}.$$

Finally, the log K_r values for reactions 510 to 512 and 514 to 517 are from Zirino and Yamamoto (1972) not Mattigod and Sposito (1977).

THERMOCHEMICAL DATA

The computer code reaction number, the reaction itself, the selected ΔH_r and log K_r values, analytical expressions of the temperature dependence of log K_r, and the sources of the thermochemical data for U are given in Table 2. Appendix I gives a listing of the computer code, and Appendix II gives the results of the WATEQ3 run of test case USBM-1 (Potter and others, 1979).

TABLE 2. Thermochemical data used for the reactions included in WATEQ3

I	Page2	Reaction	ΔH_r (kcal mol^{-1})	Source	Log K_r	Source
538	kpe(H2S/S)	$S_s + 2H^+ + 2e^- \langle=\rangle H_2S^o$	-9.5	NBS 270-3	4.882	NBS 270-3
539	kpe(S/SO4)	$SO_4^{2-} + 8H^+ + 6e^- \langle=\rangle S_s + 4H_2O$	-55.94	NBS 270-3	35.754	NBS 270-3
540	kNaF aq	$Na^+ + F^- \langle=\rangle NaF^o$	-	-	-0.956	Miller and Kester, 1976
541	Ba3(AsO4)2	$Ba_3(AsO_4)_2 \langle=\rangle 3Ba^{2+} + 2AsO_4^{3-}$	9.5	NBS 270-3, 270-6[1/]	-50.11	Sillen, 1964
542	kU +4	$UO_2^{2+} + 4H^+ + 2e^- \langle=\rangle U^{4+} + 2H_2O$	-34.43	Langmuir, 1978[2/]	9.216	Langmuir, 1978[2/]
543	blank					
544	kU +3	$U^{4+} + e^- \langle=\rangle U^{3+}$	24.4		-8.796	
545	kUOH +3	$U^{4+} + H_2O \langle=\rangle UOH^{3+} + H^+$	11.715		-0.656	
			$\log K_r = -9.16+0.0285T$			
546	kU(OH)2 +2	$U^{4+} + 2H_2O \langle=\rangle U(OH)_2^{2+} + 2H^+$	17.73		-2.27	
547	kU(OH)3 +	$U^{4+} + 3H_2O \langle=\rangle U(OH)_3^+ + 3H^+$	22.645		-4.935	
548	kU(OH)4 aq	$U^{4+} + 4H_2O \langle=\rangle U(OH)_4^o + 4H^+$	24.76		-8.498	
549	kU(OH)5 -	$U^{4+} + 5H_2O \langle=\rangle U(OH)_5^- + 5H^+$	27.575		-13.12	
550	kU6(OH)15 +9	$6U^{4+} + 15H_2O \langle=\rangle U_6(OH)_{15}^{9+} + 15H^+$	-		-17.229	
551	Uraninite	$UO_2 + 4H^+ \langle=\rangle U^{4+} + 2H_2O$	-18.63		-4.7	
552	UO2 (a)	$UO_2 + 4H^+ \langle=\rangle U^{4+} + 2H_2O$	-		0.934	
553	U4O9 (c)	$U_4O_9 + 18H^+ + 2e^- \langle=\rangle 4U^{4+} + 9H_2O$	-101.235		-3.384	
554	U3O8 (c)	$U_3O_8 + 16H^+ + 4e^- \langle=\rangle 3U^{4+} + 8H_2O$	-116.02		21.107	
555	Coffinite	$USiO_4 + 4H^+ \langle=\rangle U^{4+} + H_4SiO_4^o$	-11.6		-9.396	
556	kUF +3	$U^{4+} + F^- \langle=\rangle UF^{3+}$	5.05		8.659	
557	kUF2 +2	$U^{4+} + 2F^- \langle=\rangle UF_2^{2+}$	7.2		14.457	
558	kUF3 +	$U^{4+} + 3F^- \langle=\rangle UF_3^+$	7.15		19.115	

559	kUF4 aq	$U^{4+} + 4F^- \leftrightarrows UF_4^o$	4.6	23.64
560	kUF5 -	$U^{4+} + 5F^- \leftrightarrows UF_5^-$	4.85	25.238
561	kUF6 -2	$U^{4+} + 6F^- \leftrightarrows UF_6^{2-}$	3.3	27.718
562	UF4 (c)	$UF_4 \leftrightarrows U^{4+} + 4F^-$	-18.9	-18.606
563	UF4, 2.5H2O (c)	$UF_4 \cdot 2.5H_2O \leftrightarrows U^{4+} + 4F^- + 2.5H_2O$	-0.588	-27.57
564	kUCl +3	$U^{4+} + Cl^- \leftrightarrows UCl^{3+}$	9.933	1.338
565	kUSO4 +2	$U^{4+} + SO_4^{2-} \leftrightarrows USO_4^{2+}$	3.7	5.461
566	kU(SO4)2 aq	$U^{4+} + 2SO_4^{2-} \leftrightarrows U(SO_4)_2^o$	7.6	9.749
567	kUHPO4 +2	$U^{4+} + PO_4^{3-} + H^+ \leftrightarrows UHPO_4^{2+}$	7.5	24.443
568	kU(HPO4)2 aq	$U^{4+} + 2PO_4^{3-} + 2H^+ \leftrightarrows U(HPO_4)_2^o$	1.7	46.833
569	kU(HPO4)3 -2	$U^{4+} + 3PO_4^{3-} + 3H^+ \leftrightarrows U(HPO_4)_3^{2-}$	-7.8	67.564
570	kU(HPO4)4 -4	$U^{4+} + 4PO_4^{3-} + 4H^+ \leftrightarrows U(HPO_4)_4^{4-}$	-26.5	88.483
571	U(HPO4)2,4H2O	$U(HPO_4)_2 \cdot 4H_2O \leftrightarrows U^{4+} + 2PO_4^{3-} + 2H^+ + 4H_2O$	3.84	-51.584
572	Ningyoite	$CaU(PO_4)_2 \cdot 2H_2O \leftrightarrows U^{4+} + Ca^{2+} + 2PO_4^{3-} + 2H_2O$	-2.27	-53.906
573	kUO2 +	$UO_2^{2+} + e^- \leftrightarrows UO_2^+$	-3.3	2.785
574	kUO2OH +	$UO_2^{2+} + H_2O \leftrightarrows UO_2OH^+ + H^+$	11.015	-5.672
575	k(UO2)2(OH)2 +2	$2UO_2^{2+} + 2H_2O \leftrightarrows (UO_2)_2(OH)_2^{2+} + 2H^+$	10.23	-5.645
576	k(UO2)3(OH)5 +	$3UO_2^{2+} + 5H_2O \leftrightarrows (UO_2)_3(OH)_5^+ + 5H^+$	25.075	-15.593
577	UO3 (c)	$UO_3 + 2H^+ \leftrightarrows UO_2^{2+} + H_2O$	-19.315	7.719
578	Gummite	$UO_3 + 2H^+ \leftrightarrows UO_2^{2+} + H_2O$	-23.015	10.403
579	B-UO2(OH)2 (c)	$UO_2(OH)_2 + 2H^+ \leftrightarrows UO_2^{2+} + 2H_2O$	-13.73	5.544
580	Schoepite	$UO_2(OH)_2 \cdot H_2O + 2H^+ \leftrightarrows UO_2^{2+} + 3H_2O$	-12.045	5.404
581	kUO2CO3 aq	$UO_2^{2+} + CO_3^{2-} \leftrightarrows UO_2CO_3^o$	0.84	10.071

$\log K_r = -9.56+0.03434T+2809/T$

TABLE 2. Thermochemical data used for the reactions included in WATEQ3(Continued):

I	Page2	Reaction	ΔH_r (kcal mol^{-1})	Source	Log K_r	Source
582	kUO2(CO3)2 -2	$UO_2^{2+} + 2CO_3^{2-} \leftrightarrows UO_2(CO_3)_2^{2-}$	3.48		17.008	
		$\log K_r = 14.14+0.0096T$				
583	kUO2(CO3)3 -4	$UO_2^{2+} + 3CO_3^{2-} \leftrightarrows UO_2(CO_3)_3^{4-}$	-8.78		21.384	
		$\log K_r = 27.84-0.0216T$				
584	Rutherfordine	$UO_2CO_3 \leftrightarrows UO_2^{2+} + CO_3^{2-}$	-1.44		-14.439	
		$\log K_r = 4.54-0.03318T-2716/T$				
585	kUO2F +	$UO_2^{2+} + F^- \leftrightarrows UO_2F^+$	-0.45		5.105	
586	kUO2F2 aq	$UO_2^{2+} + 2F^- \leftrightarrows UO_2F_2^o$	-0.90		8.92	
587	kUO2F3 -	$UO_2^{2+} + 3F^- \leftrightarrows UO_2F_3^-$	-0.85		11.364	
588	kUO2F4 -2	$UO_2^{2+} + 4F^- \leftrightarrows UO_2F_4^{2-}$	-1.10		12.607	
589	kUO2Cl +	$UO_2^{2+} + Cl^- \leftrightarrows UO_2Cl^+$	1.233		0.22	
590	kUO2SO4 aq	$UO_2^{2+} + SO_4^{2-} \leftrightarrows UO_2SO_4^o$	5.10		2.709	
		$\log K_r = 11.384-0.07088T+1.40277x10^{-4}T^2$				
591	kUO2(SO4)2 -2	$UO_2^{2+} + 2SO_4^{2-} \leftrightarrows UO_2(SO_4)_2^{2-}$	6.10		4.183	
		$\log K_r = 12.130-0.068297T+1.3987x10^{-4}T^2$				
592	kUO2HPO4 aq	$UO_2^{2+} + PO_4^{3-} + H^+ \leftrightarrows UO_2HPO_4^o$	-2.1		20.814	
593	kUO2(HPO4)2 -2	$UO_2^{2+} + 2PO_4^{3-} + 2H^+ \leftrightarrows UO_2(HPO_4)_2^{2-}$	-11.8		43.441	
594	kUO2H2PO4 +	$UO_2^{2+} + PO_4^{3-} + 2H^+ \leftrightarrows UO_2H_2PO_4^+$	-3.70		22.643	
595	kUO2(H2PO4)2 aq	$UO_2^{2+} + 2PO_4^{3-} + 4H^+ \leftrightarrows UO_2(H_2PO_4)_2^o$	-16.5		44.70	
596	kUO2(H2PO4)3 -	$UO_2^{2+} + 3PO_4^{3-} + 6H^+ \leftrightarrows UO_2(H_2PO_4)_3^-$	-28.6		66.245	
597	(UO2)3(PO4)2 (c)	$(UO_2)_3(PO_4)_2 \leftrightarrows 3UO_2^{2+} + 2PO_4^{3-}$	94.9		-49.037	
598	H-Autunite	$H_2(UO_2)_2(PO_4)_2 \leftrightarrows 2H^+ + 2UO_2^{2+} + 2PO_4^{3-}$	-3.6		-47.931	

599	Na-Autunite	$Na_2(UO_2)_2(PO_4)_2 \leftrightarrows 2Na^+ + 2UO_2^{2+} + 2PO_4^{3-}$	-0.46	-47.409
600	K-Autunite	$K_2(UO_2)_2(PO_4)_2 \leftrightarrows 2K^+ + 2UO_2^{2+} + 2PO_4^{3-}$	5.86	-48.244
601	Uramphite	$(NH_4)_2(UO_2)_2(PO_4)_2 \leftrightarrows 2UO_2^{2+} + 2NH_4^+ + 2PO_4^{3-}$	9.70	-51.749
602	Saleeite	$Mg(UO_2)_2(PO_4)_2 \leftrightarrows 2UO_2^{2+} + Mg^{2+} + 2PO_4^{3-}$	-20.18	-43.646
603	Autunite	$Ca(UO_2)_2(PO_4)_2 \leftrightarrows 2UO_2^{2+} + Ca^{2+} + 2PO_4^{3-}$	-14.34	-43.927
604	Sr-Autunite	$Sr(UO_2)_2(PO_4)_2 \leftrightarrows 2UO_2^{2+} + Sr^{2+} + 2PO_4^{3-}$	-13.05	-44.457
605	Uranocircite	$Ba(UO_2)_2(PO_4)_2 \leftrightarrows 2UO_2^{2+} + Ba^{2+} + 2PO_4^{3-}$	-10.10	-44.631
606	Bassetite	$Fe(UO_2)_2(PO_4)_2 \leftrightarrows 2UO_2^{2+} + Fe^{2+} + 2PO_4^{3-}$	-19.9	-44.485
607	Torbernite	$Cu(UO_2)_2(PO_4)_2 \leftrightarrows 2UO_2^{2+} + Cu^{2+} + 2PO_4^{3-}$	-15.9	-45.279
608	Przhevalskite	$Pb(UO_2)_2(PO_4)_2 \leftrightarrows 2UO_2^{2+} + Pb^{2+} + 2PO_4^{3-}$	-11.0	-44.365
609	kUO2H3SiO4 +	$UO_2^{2+} + H_4SiO_4^o \leftrightarrows UO_2SiO(OH)_3^+ + H^+$	-	-2.4
610	Uranophane	$Ca(UO_2)_2(SiO_3OH)_2 + 6H^+ \leftrightarrows 2UO_2^{2+} + Ca^{2+} + 2H_4SiO_4^o$	-	17.489

1/ Data for $Ba_3(AsO_4)_2$ and Ba^{2+} from Parker and others (1971). Data for AsO_4^{3-} from Wagman and others (1968).

2/ All data for reactions 542 through 610 are from Langmuir(1978).

PROGRAM OPERATION

This version of the WATEQ model was developed on the Menlo Park, Calif., Multics computer system of the U.S. Geological Survey. Data are input from a user segment stored online in card-image form analogous to the card-input scheme discussed in Ball and others (1980). The following additional input parameters are available:

cunits(298)	U total
cunits(299)	U4+ tot
cunits(341)	U6+ tot.

The term "tot" after U4+ and U6+ signifies that the quantity is the total U in the specified valence state, not the quantity of free aqueous U^{4+} or U^{6+} species.

The output of the model is placed in an online segment which the user may request to be printed by a high-speed printer, printed at a remote terminal, deleted, etc. The form of the output is identical to that of the WATEQ2 of Ball and others (1980), with the exception of the addition of U solutes and solids and U^{4+}/U^{6+} redox potential calculations, polynuclear Fe species conversion to log form, the NaF^{o} complexation reaction and formation of the $Ba_3(AsO_4)_2$ solid.

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SUMMARY

Procedures for calculation of the activity of U solute forms and the activity products of U solids have been added to the WATEQ2 computerized chemical model resulting in the WATEQ3 version. The model with U added and its computer code were evaluated by comparing program output to that of a second model available to the authors for the calculation of U speciation and degree of saturation with U solid phases. During testing, several alterations were made to both the WATEQ3 model and the second model and their respective computer codes. Upon completion they calculated nearly identical results.

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Appendix I. Program Listing

```
wateq3: proc;
  dcl (intable,prep,set,maj_el,tr_el,sums,solutes,ratio,apcalc,errcalc,u_el,
       outpnch,phases)entry options(variable),(d,e,g,h,iter,prnt,punch,ehopt)fixed
       bin(31)ext,rbit bit(1)ext,table1 file record sequential env(stringvalue),
       semicln char(1)ext;
       dcl vline char(80) varying,
        flend bit(1)ext,
       sysin file record sequential env(stringvalue),
           line char(80),
           io entry options(variable);
  dcl outprint ext file constant,pchflg bit(1)init("0"b);
call ic ("attach","outprint","vfile_","wateq3.output");
       call io ("attach","table1","record_stream_","-target","vfile_",
                "table1");
       open file(table1) input;
call io("attach","sysin","record_stream_","-target","vfile_",
       "wateq3.data"); open file(sysin) input;
   read file(table1) into (vline);
   line=vline;
   get string(line)edit(semicln,d,e,g)(a(1),x(2),f(3),x(2),f(3),x(2),f(3));
  close file(table1);
  call io ("detach","table1");
   begin;
    dcl page1(0:d)char(8),page2(0:e)char(12),
       (nmbr,anal(0:d),index(0:g),index2(0:d),z(0:d))fixed bin(31),
       (alfa(0:d),analmi(0:d),ap(0:e),cunits(0:d),dh(0:e),dha(0:d),
       err(0:e),errt(0:e),gamma(0:d),gfw(0:d),kt(0:e),logkt(0:e),
       logkto(0:e),maxkto(0:e),mi(0:d),minkto(0:e),sigma(0:d),v(0:d))
       float dec(20);
  nmbr=0;
  call intable(page1,page2,index,z,dha,gfw,v,dh,logkto,maxkto,minkto,
                errt,index2,nmbr);
  if nmbr^=0 then go to quit;
  sigma=0;  nmbr=0;
  next_data:
  nmbr=nmbr+1;
  call prep(anal,z,analmi,cunits,dh,errt,gfw,logkto,mi,sigma,v);
  if flend="1"b then do;  goto quit; end;
  call set(dh,gamma,kt,logkt,logkto,mi);
    iter = 0; rbit = "1"b;  alfa=0;
    do while (rbit); iter = iter + 1;
      call maj_el(alfa,cunits,dha,gamma,kt,mi,z);
      call tr_el(alfa,gamma,kt,logkt,mi);
      call u_el(alfa,gamma,kt,logkt,mi);
      call sums(alfa,gamma,kt,logkt,mi);
      end;
   call solutes(anal,z,page1,alfa,analmi,cunits,gamma,gfw,kt,mi,logkt,
                index2,sigma,err);
   if prnt ^= 1 & prnt ^= 3 then
       call ratio(page1,alfa,cunits,z,analmi);
   if prnt^=2 & prnt^=3 | punch=0 then do;
     call apcalc(ap,alfa,gamma,mi);
     err=2e7;
     call errcalc(cunits,sigma,err);
     if punch=0 then do;  call outprch(alfa,ap,cunits,logkt);
       pchflg="1"b;  end;
     if prnt^=2 & prnt^=3 then
     call phases(page2,index,ap,dh,logkt,maxkto,minkto,err,errt);  end;
   go to next_data;
   end;
```

```
quit:  call io("close","outprint");
       call io("detach","outprint");
       if pchflg then do;
       call io("close","syspnch");
       call io("detach","syspnch");  end;
       end wateq3;
```

```
intable: proc(page1,page2,index,z,dha,qfw,v,dh,logkto,maxkto,minkto,
              errt,index2,nmbr);
        dcl (d,e,g,h,prnt,punch,short)fixed bin(31)ext,(onchar,onsource)
         builtin,page1(*)char(8),page2(*)char(12),
         (i,j,k,n,nmbr,index(*),index2(*),z(*))fixed bin(31),
         (c,f,r,sigmado,sigmaeh,sigmah)float dec(20)ext,
         (dha(*),qfw(*),v(*),dh(*),logkto(*),maxkto(*),minkto(*),
          errt(*))float dec(20);
 dcl qtemp fixed bin(31);
dcl (endfile,endpage,conversion)condition,
    outprint  external file constant,
    (table1,table2) file record sequential env(stringvalue),
    (table3,table4) file,
    vline char(80) varying,
    line char(80),
    io entry options(variable);
 call io ("attach","table1","record_stream_","-target","vfile_",
          "table1");
 call io ("attach","table2","record_stream_","-target","vfile_",
          "table2");
 call io ("attach","table3","vfile_","table3");
call io ("attach","table4","vfile_","table4");
 open file(table1) input;
  open file(table3) input;
  open file(table4) input;
open file(table2) input;
open file(outprint) print;
  on endfile(table1) begin;
    put file(outprint)page list("program table #1 input incomplete. run terminated");
    call outtable;  nmbr=1;  go to finish;  end;
  on endfile(table2) begin;
    put file(outprint)page list("program table #2 input incomplete. run terminated");
    call outtable;  nmbr=1;  go to finish;  end;
      on conversion begin;
      put file (outprint) edit ("input conversion error in i= ",i,
      "onchar=",onchar,"onsource=",onsource)
        (skip (5) ,a,x(3),f(3),2(x(3),a,x(2),a)); nmbr=1;  go to finish;  end;
      v,qfw,z,dha=1.0
      logkto,minkto,maxkto,dh=1.0;  errt=0.1;
/* dummy out first record of table1 since it has already been read*/
  read file(table1) into(vline);
    do n = 0 to d;
     read file(table1) into(vline);
     line=vline;
      get string(line) edit(i,page1(i),z(i),qfw(i),dha(i))
          (col(1),f(4),x(1),a(8),f(3),f(9,4),f(4,1));
        end;
      do n = 0 to e;
      read file(table2) into (vline);
      line=vline;
      get string(line) edit(i,page2(i),dh(i),logkto(i),minkto(i),
        maxkto(i),errt(i) )(col(1),f(4),x(1),a(12),
        4 f(9,3),f(5,2));
       end;
      index=0;  i=0;  do while(index(i)<999);  i=i+1;
        get file(table3)list(index(i));  end;  qtemp=i-1;
      index2=0;  i=0;  do while(index2(i)<999);  i=i+1;
           get file(table4)list(index2(i));  end;  h=i-1;
  do i=0 to d;  v(i)=max(1,abs(z(i)));  end;
```

```
 prnt,punch,ehopt=0;  sigmajo,sigmaeh,sigmaph=0e0;
 c=2.302585093;      f=23.0603;  r=1.98719e-3;
 call outtable;

outtable:  proc  ;
    dcl coef(1:24,0:5) float(16) init
       (12,  13.543,    -.0401,    -3000,     0,          0,
        13,  6.368,     -.016346, -3405.,    0,          0,
        14,  39.478,    -.065927, -12355.1, 0,          0,
        24,  .684,      .0051295, 0,          0,          0,
        25,  28.6059,   .012078,  1573.21,  0,          0,
        26,  .6322,     -.001225, -2835.76, 0,          0,
        35,  -14.8435,  .032786,  3404.71,  0,          0,
        62,  109.25,    .0024,    3120.98,  -4.9e-7,    -2038.47,
        68,  -6.498,    .02379,   2902.39,  0,          0,
        72,  3.106,     0.0,      -673.6,   0,          0,
        73,  .991,      .00667,   0,          0,          0,
        74,  2.319,     -.011056, 0,          2.29812e-5,0,
        77,  -2.95,     .0133,    0,          0,          0,
        78,  -27.393,   .05617,   4114,     0,          0,
        89,  -5.3505,   .0183412, 557.2461, 0,          0,
        91,  11.17,     -.02386,  -3279,     0,          0,
        220, 2.497,     0.0,      3833,     0,          0,
        545, -9.16,     .0285,    0,          0,          0,
        581, -9.56,     .03434,   +2809,     0,          0,
        582, 14.14,     +.0096,   0,          0,          0,
        583, 27.84,     -.0216,   0,          0,          0,
        584, 4.54,      -.03318,  -2716,     0,          0,
        590, 11.384,    -.07088,  0,          1.40277e-4,0,
        591, 12.130,    -.068297, 0,          1.3987e-4,0);
      dcl head1 char(84)init("  i    page2              dh       maxkto     minkto     logkto      error "),
          head2 char(46)init("i   page1      z  dha      qfw"),
          line char(131),
          line1 char(26)def(line)pos(1),
          line2 char(10)def(line)pos(27),
          line3 char(10)def(line)pos(37),
          line4 char(10)def(line)pos(47),
          line5 char(8)def(line)pos(58),
          line6 char(39)def(line)pos(77),
          line7 char(1)def(line)pos(57);
      on endpage(outprint)begin;
          put file(outprint)page list(head1);
          if i<d+1 then put file(outprint)edit(head2)(a);
          put file(outprint)skip;  end;
      i=0;  signal endpage(outprint);
 do i=0 to e;
   line=" ";
   put string(line1)edit(i,page2(i),dh(i))(f(3),x(2),a(12),f(9,3));
   if maxkto(i)^=0e0 then put string(line2)edit(maxkto(i))(f(10,3));
   if minkto(i)^=0e0 then put string(line3)edit(minkto(i))(f(10,3));
   put string(line4)edit(logkto(i))(f(10,3));
   if errt(i)>0e0 then put string(line5)edit(errt(i))(f(8,2));
   if i<(d+1) then put string(line6)edit(i,page1(i),z(i),dha(i),qfw(i))
   (f(10),x(2),a,f(4),f(5,1),f(10,4));
   do n=1 to 24;
     if i=coef(n,0) then do;  put string(line7)edit("*")(a(1));  n=51;
         end;  end;
   put file(outprint)list(line);
   end;
   put file(outprint)skip(2)edit("""*"" denotes that an analytical expression for kt has been used",
```

```
 "Summary of analytical expressions of the form  log k = a+b*t+c/t+d*t**2+e/t**2",
"    i  react prod          a            b            c           d            e")
(a,page,a,skip(2),a);
     do k=1 to 24;
       i=coef(k,0);
       put file(outprint)skip edit(i,page2(i))(f(4),x(2),a);
       n=7;  do j=1 to 3;  n=n+12;
       if coef(k,j)^=0 then put file(outprint)edit(coef(k,j))(col(n),f(12,4));  end;
       n=44;  do j=4,5;  n=n+12;
       if coef(k,j)^=0 then put file(outprint)edit(coef(k,j))(col(n),e(12,4));  end;
       end;
     put file(outprint)page   list("reference numbers for all possible numbered input constituents:");
     put file(outprint)skip(2)list("number    constituent  z");
     do i = 0 to 8,13,16,17,34,38,44,48,50,61,80,84,86,87,89,94,96,97,
             109,130,145,160,182,202,204,212,249,261,262,284,285,298,299,341;
       put file(outprint)skip edit(i,page1(i),z(i))(f(4),x(10),a(8),f(2));  end;
   end outtable;
finish:
g=gtemp;
close file(table1);
close file(table2);
close file(table3);
close file(table4);
call io ("detach","table1");
call io ("detach","table2");
call io ("detach","table3");
call io ("detach","table4");
  end intable;
```

```
prep: proc(anal,z,analmi,cunits,dh,errt,gfw,logkto,mi,sigma,v);
dcl long char(1400)var ext,card(0:20)char(80)ext,flag char(3)var ext,
    semicln char(1)ext,(fulflag,humflag)bit(1)ext,
    (coralk,d,ehopt,empox,istdata,prnt,punch)fixed bin(31)ext,
    (i,n,anal(*),z(*))fixed bin(31),
    (onchar,oncode,onloc,onsource)builtin,
    (a,b,c,c1,ag,as,cd,co,cr,cu,hg,mo,ni,pb,zn,dens,diff,dox,ehas,
    ehdo,ehdo2,ehfe,ehm,ehn,ehno2,ehpt,ehs,ehso4,ehss,ehu,epman,epmcat,f,
    musave,pe,peas,pedo,pedo2,pefe,pen,peno2,pept,pes,peso4,pess,peu,pn,
    r,sigmado,sigmaeh,sigmaph,t,temp)float dec(20) ext,
    (s1,s2,s3,analmi(*),cunits(*),dh(*),errt(*),gfw(*),logkto(*),
     mi(*),sigma(*),v(*))float dec(20) ;
  dcl flend bit(1) init("0"b) ext;
   card(0)="zzz";
 dcl (outprint) external file constant,
     sysin file record sequential env(stringvalue),
     vline char(80) varying,
     line char(80),
     (conversion,endfile,error) condition,
     io entry options(variable);
 on conversion begin;
   put file(outprint) edit("input conversion error")(page,a)
                         ("onsource=",onsource,"onchar=",onchar)
                         (2(x(2),2 a))
                         ((card(i) do i = 1 to n))(skip,a);
   go to start;     end;
 on endfile (sysin) begin;
   close file(sysin);
call io("detach","sysin"); flend ="1"b;  goto quit; end;
  start:  cunits,mi,anal=0;  coralk=0;  empox=0;
   fulflag,humflag="0"b;
  ehas,ehfe,ehdo,ehdo2,ehn,ehno2,ehs,ehso4,ehss,ehu=9.9; analmi=1.0;
  peas,pedo,pedo2,pefe,pen,peno2,pept,pes,peso4,pess,peu=1e2;  dox=-1;
   dens=1;  n=0;  ag,as,cd,co,cr,cu,hg,mo,ni,pb,zn=0;
   do while(card(n)^=" ");  n=n+1;
   read file(sysin) into(vline);
  line=vline;
     get string(line) edit (card(n))(a(80));  end;  n=n-1;
   put file(outprint)page; do i=1 to n; put file(outprint)skip edit(card(i))(a); end;
   put file(outprint)skip(2);
   get string(card(1))edit(istdata)(x(79),f(1));  long="";
   if istdata<2 then do;
     put file(outprint)edit("istdata value not given on card 1 of:") (page,a)
           ((card(i) do i=1 to n)) (skip,a);
     go to start; end;
   do i=3 to istdata; long=long||card(i); end;
   long=long||(17)" 1e38 ";
   get string(long) list(temp,ph,ehm,flag,(cunits(i)
                do i = 0,1,2,3,4,5,6,16,13,17,34,38,36,44,50,61,64));
   if cunits(84)>1.0e+35 then do;
    put file(outprint)edit("insufficient number of input data items in the ",
              "following set:") (page,2 a)
              ((card(i) do i=1 to n)) (skip,a);
     go to start; end;
   long="";
   do i=istdata+1 to n; long=long||card(i); end;
   long=long||semicln;
   if n>istdata then get string(long) data;
   t = temp + 273.16e0;
```

```
      if cunits(130)=0 then cunits(130)=cu;
      if cunits(145)=0 then cunits(145)=zn;
      if cunits(160)=0 then cunits(160)=cd;
      if cunits(182)=0 then cunits(182)=pb;
      if cunits(204)=0 then cunits(204)=ni;
      if cunits(212)=0 then cunits(212)=ag;
      if cunits(249)=0 then cunits(249)=as;
      do i=0 to d;
      if cunits(i)<0e0 then do; anal(i)=1; cunits(i)=0e0; end; end;
      ehpt=ehm;  if ehm>9e0 then pept=1e2;  else pept=ehm/(c*r*t/f);
      if cunits(284) > 0e0 & gfw(284)=650 then do;
        fulflag="1"b;  put file(outprint) skip(2)list("no gfw input with conc value for fulvic acid.  Results will be flagged with asteri
sks to signify that they are purely qualitative.");  end;
      if cunits(285) > 0e0 & gfw(285)=2000 then do;
        humflag="1"b;  put file(outprint)skip(2)list("no gfw input with conc value for humic acid.  Results will be flagged with asterisk
s to signify that they are purely qualitative.");  end;
      put file(outprint)edit("Iter","s1-analCO3","s2-analSO4","s3-analF","s4-analPO4",
       "s5-analCl","s6-analH2S","s7-analFulv","s8-analHum")(skip(2),x(1),
       a,x(4),a,x(6),a,2(x(7),a),x(6),a,x(7),a,x(5),a,x(6),a);

  /* calculation of analyzed molality */
      if flag="meq/l" then do; cunits=cunits*gfw/v; flag="mg/l"; end;
      if flag="mg/l" then do;
        cunits=cunits/dens;  flag="ppm";  end;
      c1=0;
      do i=0 to d;   c1=c1+cunits(i);  end;
      if flag="ppm" then do;
      mi=cunits*(1/(1-1e-6*c1))/(1e3*gfw);  end;
      else if flag="mol" then do;  mi=cunits;
           cunits=mi*1e3*gfw*(1-1e-6*c1);  end;
      analmi=mi;  epmcat, epman = 0e0;

  /* calculation of cation-anion balance */
      mi(63)=1e1**-ph;
      mi(26)=1e1**(ph-14);
      do i = 0 to d;
        if z(i)>0 then epmcat = epmcat + z(i) * mi(i);
                  else epman = epman-z(i)*mi(i); end;
      diff=0e0;
      if epman+epmcat^=0 then diff=abs(2*(epman-epmcat)/(epman+epmcat));
      if diff>.3 then do;
        put file(outprint)skip(2)edit("Error in input charge balance greater than 30 percent.  ",
    "Check input data.")(2 a)
                  ("Anal epmcat =",1e3*epmcat,"Anal epman =",1e3*epman)
                  (skip(1),a,f(10,4),x(3),a,f(10,4));
        end;

  /* temp. affects on debye-huckel solvent constants */
      s1=374.11e0-temp; s2=s1**.333333e0;
      s3=sqrt((1e0+.1342489e0*s2-3.946263e-3*s1)/
              (3.1975e0-.3151548e0*s2-1.203374e-3*s1+7.48908e-13*s1**4));
      if t < 373.16e0
        then c1=87.74e0-temp*(temp*(1.41e-6*temp-9.398e-4)+.4008e0);
        else c1=5321e0/t+233.76e0-t*(t*(8.292e-7*t-1.417e-3)+.9297e0);
      c1=sqrt(c1*t);
      a = 18246e2 * s3 / c1**3;  b = 50.29 * s3 / c1;
quit: end prep;
```

```
set: proc(dh,gamma,kt,logkt,logkto,mi);
  dcl (e,empox,coralk)fixed bin(31)ext,i fixed bin(31),
      (agtot,altot,analco3,astotal,as3tot,as5tot,batot,btot,c,
      catot,cdtot,cltot,co2tit,cstot,cutot,f,fetotal,fe2tot,
      fe3tot,ftot,fulvtot,hco3tot,humtot,h2stot,ktot,kw,litot,mgtot,
      mntot,natot,nh4tot,nitot,no2tot,pbtot,ph,ptot,r,sitot,so4tot,
      srtot,t,tenph,zntot,utotal,u4tot,u6tot)float dec(20) ext,
      (c1,dh(*),gamma(*),kt(*),logkt(*),logkto(*),mi(*))float dec(21) ;
  kt=1e-37;  logkt=1.0;  gamma=1.0;
/* initialize starting values for iterative loop and constant gammas */
          analco3,co2tit = mi(6) + 2*mi(17);  sitot = mi(34);
   if coralk=2 then co2tit=mi(6)+mi(17)+mi(85);
   catot = mi(0);   mgtot = mi(1);   natot = mi(2);
   ktot = mi(3);   so4tot = mi(5);  fetotal = mi(16);
   fe2tot=mi(7);  fe3tot=mi(8);  no2tot=mi(202);  agtot=mi(212);
   ptot,mi(46) = mi(44);   altot = mi(50);   ftot = mi(51);
   btot = mi(86);  litot= mi(80);  nh4tot = mi(38);  h2stot = mi(13);
   srtot = mi(87);  batot = mi(89);  nitot = mi(204);  cstot = mi(48);
   cltot = mi(4);  hco3tot = mi(6);  pbtot = mi(182);
   mntot=mi(109);  cutot=mi(130);  zntot=mi(145);  cdtot=mi(160);
   as3tot = mi(261);  as5tot = mi(262);  astotal = mi(249);
   fulvtot=mi(284);  humtot=mi(285); utotal=mi(298); u4tot=mi(299); u6tot=mi(341);
   mi(249),mi(261),mi(262)=0e0;  mi(34)=0e0;  mi(16),mi(86)=0e0;
   mi(298),mi(299),mi(341)=0e0; tenph=1e1**ph;

/* vant hoff eqn. for effect of t on k */
   c1=(298.16e0-t)/(298.16e0*t*c*r);
   logkt=logkto-dh*c1;
   do i=0 to e;
   if abs(logkt(i)) < 38 then kt(i)=1e1**logkt(i);
   end;

/* analytical exprs. for effect of t on k */
   kw = kt(152);
   c1 = log10(t);
   kt(12) = 1e1 ** (13.543-.0401*t-3e3/t);
   kt(13) = 1e1 ** (6.368e0-1.6346e-2*t-3405.7e0/t);
   kt(14) = 1e1 ** (39.478e0-6.5927e-2*t-12355.1e0/t);
   kt(21) = 1e1 ** (-8.15-6.35e-3*t-5.42e-5*t*t);
   kt(24) = 1e1 ** (.684+.0051*t);
   kt(25) = kw*1e1**(1573.21e0/t+28.6059e0+1.2078e-2*t-13.2248e0*c1);
   kt(26) = 1e1 ** (0.6322e0-1.225e-3*t-2835.76e0/t);
   kt(35) = 1e1 ** (-14.8435+.032786*t+3404.71/t);
   kt(62)  = 1e1 **  (109.25+.0124*t-3120.98/t-(16.34*log(t))
                     -2088.47/(t*t)-4.9e-7*t*t-(298.4/sqrt(t)));
   kt(68) = 1e1 ** (-6.498+.02379*t+2902.39/t);
   kt(72) = 1e1 ** (3.106e0-673.6e0/t);
   kt(73) = 1e1 ** (.991+.00567*t);
   kt(74) = 1e1 ** (2.319-.011056*t+2.29312e-5*t*t);
   kt(77) = 1e1 ** (-2.95+.0133*t);
   kt(78) = 1e1 ** (-27.393+.05617*t+4114/t);
   kt(89) = 1e1 ** (+557.2467e0/t-5.3505e0+0.0183412e0*t);
   kt(91) = 1e1 ** (-3279.0e0/t+11.17e0-0.02386e0*t);
   kt(157) = 1e1 ** (-5.7e0+1.68e0*ph);
   kt(158) = 1e1 ** (-5.4e0+1.52e0*ph);
   kt(220) = 1e1 ** (2.497e0-3833/t);
   kt(545) = 1e1 ** (-9.16+.0235*t);
   kt(581) = 1e1 ** (-9.56+.03434*t+2809/t);
   kt(582) = 1e1 ** (14.14+.0096*t);
```

```
kt(583) = 1e1 ** (27.84-.0215*t);
kt(584) = 1e1 ** (4.54-.03313*t-2716/t);
kt(590) = 1e1 ** (11.384-.07088*t+1.40277*1e-4*t*t);
kt(591) = 1e1 ** (12.130-.063297*t+1.3987*1e-4*t*t);
do i=12,13,14,24,25,26,35,62,68,72,73,74,77,78,89,91,157,158,220,545,581 to 584, 590,591;
  logkt(i)=log10(kt(i));  end;
end set;
```

```
 maj_el: proc(alfa,cunits,dha,gamma,kt,mi,z);
   dcl (d,ehopt,empox,iter,coralk)fixed bin(31)ext,(1,z(*))fixed bin(31),
       (a,ah2o,altot,b,batot,btot,c,carbonc,catot,co2tit,
        co3calc,cstot,dox,dum1,endo,ehdo,ehdo2,ehfe,ehm,ehpt,f,fetotal,fe2tot,
        fe3tot,ftot,fulvtot,hco3tot,humtot,h2stot,ktot,kw,lh2o,litot,
        matot,mu,muhalf,natot,nh4tot,no2tot,pe,pedo,pedo2,pefe,pept,ph,
        ptot,r,sitot,so4tot,srtot,t,tenmpe,tenph)float dec(20) ext,
        (c1,c2,c3,c4,alfa(*),cunits(*),dha(*),gamma(*),kt(*),mi(*))
        float dec(20) ;
/* calc. of total molality & ah2o */
      c1=0e0; do i=0 to 15,17 to 33, 35 to 64,66 to 68,72 to 82,84,
       85,87 to 248,250 to 260,263 to 297,301 to d;
        c1 = c1 + mi(i);  end;
      ah2o=1e0-1.7e-2*c1;
 if ah2o>0e0 then lh2o=log10(ah2o);
  else lh2o=0;

/* calc. of activity coefficients */
      mu=0e0; do i=0 to 15,17 to 33, 35 to 64,66 to 68,72 to 82,84,
       85,87 to 248,250 to 260,263 to d;
      if mi(i) > 1e-38 then
      mu=mu+0.5e0*mi(i)*z(i)*z(i);   end;  muhalf=sqrt(mu);
      c1 = -a * 4e0 * muhalf;
      gamma(0)=1e1 **(c1/(1e0+b*5e0*muhalf)+0.165 * mu);
      gamma(1) = 1e1 ** (c1/(1e0+b*5.5*muhalf)+0.2 * mu);
      gamma(2) = 1e1  ** (-a*muhalf/(1e0+b*4e0*muhalf)+0.175*mu);
      gamma(3), gamma(4) = 1e1  ** (-a * muhalf / (1e0 + b * 3.5
                                  * muhalf) + 0.015 * mu);
     gamma(5) = 1e1 ** (c1/(1e0+b*5e0*muhalf)-0.04 *mu);
      do i=7 to d;  /* Davies equation for most activity coeffs */
        if z(i) = 0 then gamma(i) = 1e1**(1e-1 * mu);   else do;
        c2 = -a * z(i) * z(i) * (muhalf / (1 + muhalf) - 0.3 * mu);
        if abs(c2) < 38 then gamma(i) = 1e1 ** c2;  else gamma(i) = 0;
        end;  end;
    /* Debye-Huckel eqn for polysulfide species(dha from Cloke,1963) */
      do i = 6,17,259,260,263 to 270;  /* and carbonates */
        if dha(i) > 0e0 then gamma(i) = 1e1 ** (-a * z(i) * z(i) *
                          muhalf / (1e0 + dha(i) * b * muhalf));  end;
    gamma(85)=1e1**(mu*(170.01/t-.8798+.0013935*t)+mu*mu*(28.91/t-.2108+.0003641*t));
  do i=0 to d; if gamma(i)<1e-38 then gamma(i)=1e0;
               end;

/* calc of minor anion activities */
      do i=84,96,97,202;  alfa(i)=mi(i)*gamma(i);  end;

/* calc. of pe & ehdo */
      if dox > 0e0 then do;
      pedo= -(log10(kt(136))+ph+0.5*lh2o-0.25*log10(dox/32e3));
      pedo2=-(log10(kt(151))+ph+0.5*lh2o-0.25*log10(dox/32e3));
      ehdo=pedo*c*r*t/f;  ehdo2=pedo2*c*r*t/f;  end;
      pe=pept;  if ehpt>9e0 then if dox>0e0 then do;     pe=pedo;
      if empox=1 then pe=pedo2;  end;
   if pe > 38.0 then pe=38.;
     tenmpe=1e1**(-pe);

/* activities of oh & h+ species */
      alfa(26)=ah2o*kw*tenph;
      mi(26) = alfa(26) / gamma(26);
      alfa(63)=1e1**(-ph);
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```
      mi(63)=1e0/(tenph*gamma(63));

   if iter = 1 then do;
/* initial co2 species */
   if coralk^=2 then do;
     c1=2e0*tenph/(kt(68)*gamma(17));
     mi(6)=co2tit/(1e0 + gamma(6)*c1);
     alfa(6)=mi(6)*gamma(6);
     c2=kt(35)/(tenph*gamma(85));
     mi(17)=c1*alfa(6)/2e0;
     mi(85)=c2*alfa(6);
     do i=17,85;  alfa(i)=mi(i)*gamma(i);  end;  end;
   else do;
     mi(6)=co2tit/(1e0 + gamma(6)*((kt(35)/(tenph*gamma(85)))+tenph/
          (kt(68)*gamma(17))));
     alfa(6)=mi(6)*gamma(6);
     mi(17)=alfa(6)*tenph/(gamma(17)*kt(68));
     mi(85)=alfa(6)*kt(35)/(tenph*gamma(85));
     do i=17,85;  alfa(i)=mi(i)*gamma(i);  end;  end;

/* initial sulfate species */
   if so4tot > 0e0 then do;
     mi(62)=kt(89)/(tenph*gamma(62));
     mi(5)=so4tot/(1e0 + gamma(5)*mi(62));
     alfa(5),c1=mi(5)*gamma(5);
       mi(62)=c1*mi(62);  alfa(62)=mi(62)*gamma(62);
     end;

/* initial fluoride species */
   if ftot > 0e0 then do;
       mi(125)=kt(202)/(tenph*gamma(125));
       mi(126)=kt(203)*mi(61)*gamma(61)/(tenph*gamma(125));
       mi(296)=kt(537)*mi(61)*gamma(61)/(tenph**2*gamma(296));
       mi(61)=ftot/(1+gamma(61)*(mi(125)+mi(126)+mi(296)));
       alfa(61),c1=mi(61)*gamma(61);
       do i=125,126,296;  mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);  end;
       end;

/* initial phosphate species */
   if ptot > 0e0 then do;
     mi(46)=kt(15)/(tenph*gamma(46));
     mi(47)=kt(16)/(tenph**2*gamma(47));
     mi(44)=ptot/(1e0 + gamma(44)*(mi(46)+mi(47)));
     alfa(44),c1=mi(44)*gamma(44);
     do i=46,47;  mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);  end;
     end;

/* initial chloride */
     alfa(4)=mi(4)*gamma(4);

/* initial sulfide species */
   if h2stot > 0e0 then do;
     mi(13)=1/(kt(91)*tenph*gamma(13));
     mi(67)=kt(92)*tenph/gamma(67);
     mi(263)=kt(502)*tenph/gamma(263);
     mi(264)=kt(503)*tenph/gamma(264);
     mi(265)=kt(504)*tenph/gamma(265);
     mi(266)=kt(505)*tenph/gamma(266);
     mi(267)=kt(506)*tenph/gamma(267);
     mi(66)=h2stot/(1e0 + gamma(66)*(mi(13)+mi(67)+mi(263)+mi(264)+
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```
            mi(265)+mi(266)+mi(267)));
      alfa(66),c1=mi(66)*gamma(66);
      do i=13,67,263 to 267;  mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);
      end;  end;

/* initial organic ligands */
   if fulvtot > 0e0 then do;
      mi(285)=kt(523)/(tenph*gamma(286));
      mi(284)=fulvtot/(1 + gamma(284)*mi(286));
      alfa(284),c1=mi(284)*gamma(284);
      mi(286)=c1*mi(286);  alfa(285)=mi(286)*gamma(286);  end;

   if humtot > 0e0 then do;
      mi(287)=kt(524)/(tenph*gamma(287));
      mi(285)=humtot/(1 + gamma(285)*mi(287));
      alfa(285),c1=mi(285)*gamma(285);
      mi(287)=c1*mi(287);  alfa(287)=mi(287)*gamma(287);  end;
   end;
   else do i = 4,5,6,17,44,46,47,61,66,284,285;
          alfa(i)=mi(i)*gamma(i);  end;

/* silica species */
       c1 = kt(13) * tenph   /  gamma(24);
       c2 = kt(14) * tenph**2 / gamma(25);
       if alfa(61)>0e0 then
       dum1=log10(kt(201))+6*log10(alfa(61))-(log10(gamma(124))+4*ph+4*lh2o);
       else dum1=100;
       if abs(dum1)<38 then c3=1e1**dum1;
       else c3=0e0;
      if iter>1 then do;
        if alfa(300)>1e-38 then
          c4=kt(609)*alfa(300)*tenph/gamma(340);
        else c4=0;
        end;
     else c4=0;
       mi(23) = sitot / (1e0 + gamma(23) * (c1 + c2 + c3 + c4));
       alfa(23) = mi(23) * gamma(23);
       mi(24) = alfa(23) * c1;   mi(25) = alfa(23) * c2;
       mi(124)=alfa(23)*c3; mi(340)=alfa(23)*c4;
       alfa(24)=mi(24)*gamma(24); alfa(25)=mi(25)*gamma(25);
       alfa(124)=mi(124)*gamma(124); alfa(340)=mi(340)*gamma(340);

/* boron species */
    if btot > 0e0 then do;
       mi(36)=kt(25)*tenph/gamma(36);
       mi(101)=kt(161)*alfa(61)/gamma(101);
       mi(102)=kt(162)*alfa(61)**2/(gamma(102)*alfa(26));
       mi(103)=kt(163)*alfa(61)**3/(gamma(103)*alfa(26)**2);
       mi(104)=kt(164)*alfa(61)**4/(gamma(104)*alfa(26)**3);
       mi(35)=btot/(1+gamma(35)*(mi(36)+mi(101)+mi(102)+
              mi(103)+mi(104)));
       alfa(35),c1=mi(35)*gamma(35);
       do i=36,101 to 104;  mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);
          end;  end;

/* nitrogen species */
       c1=tenph*kt(26)/gamma(37);
       c2=alfa(5)*kt(131)/gamma(91);
       mi(38)=nh4tot/(1e0+gamma(38)*(c1+c2));
       alfa(38)=mi(38)*gamma(38);
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      mi(37)=alfa(38)*c1; alfa(37)=mi(37)*gamma(37);
      mi(91)=alfa(38)*c2; alfa(91)=mi(91)*gamma(91);

/* mg species */
      mi(18)=alfa(26)*kt(24)/gamma(18);
      mi(19)=alfa(61)*kt(22)/gamma(19);
      mi(20)=alfa(17)*kt(73)/gamma(20);
      mi(21)=alfa(6)*kt(74)/gamma(21);
      mi(22)=alfa(5)*kt(75)/gamma(22);
      mi(39)=alfa(44)*kt(123)/gamma(39);
      mi(40)=alfa(47)*kt(124)/gamma(40);
      mi(72)=alfa(46)*kt(33)/gamma(72);
      mi(1)=mgtot/(1e0+gamma(1)*(mi(18)+mi(19)+mi(20)+mi(21)+mi(22)
            +mi(39)+mi(40)+mi(72)));
      alfa(1),c1=mi(1)*gamma(1);
      do i=18 to 22,39,40,72; mi(i)=c1*mi(i);
        alfa(i)=mi(i)*gamma(i); end;

/* ca species */
      mi(28)=alfa(26)*kt(76)/gamma(28);
      mi(29)=alfa(6)*kt(77)/gamma(29);
      mi(30)=alfa(17)*kt(78)/gamma(30);
      mi(31)=alfa(5)*kt(23)/gamma(31);
      mi(73)=alfa(46)*kt(34)/gamma(73);
      mi(74)=alfa(44)*kt(121)/gamma(74);
      mi(75)=alfa(47)*kt(122)/gamma(75);
      mi(100)=alfa(61)*kt(160)/gamma(100);
      mi(0)=catot/(1e0+gamma(0)*(mi(28)+mi(29)+mi(30)+mi(31)
            +mi(73)+mi(74)+mi(75)+mi(100)));
      alfa(0),c1=mi(0)*gamma(0);
      do i=28 to 31,73,74,75,100; mi(i)=c1*mi(i);
        alfa(i)=mi(i)*gamma(i); end;

/* na species */
      mi(41)=alfa(17)*kt(69)/gamma(41);
      mi(42)=alfa(6)*kt(70)/gamma(42);
      mi(43)=alfa(5)*kt(71)/gamma(43);
      mi(49)=alfa(46)*kt(30)/gamma(49);
      mi(297)=alfa(61)*kt(540)/gamma(297);
      mi(2)=natot/(1e0+gamma(2)*(mi(41)+mi(42)+mi(43)+mi(49)
            +mi(297)));
      alfa(2),c1=mi(2)*gamma(2);
      do i=41,42,43,49,297;  mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);
        end;

/* k species */
      mi(45)=alfa(5)*kt(72)/gamma(45);
      mi(60)=alfa(46)*kt(32)/gamma(60);
      mi(3)=ktot/(1e0+gamma(3)*(mi(45)+mi(60)));
      alfa(3),c1=mi(3)*gamma(3);
      do i=45,60;  mi(i)=c1*mi(i); alfa(i)=mi(i)*gamma(i); end;

/* al species */
    if altot > 0 then do;
      mi(51)=ah2o*tenph*kt(80)/gamma(51);
      mi(52)=(ah2o*tenph)**2*kt(81)/gamma(52);
      mi(53)=(ah2o*tenph)**4*kt(82)/gamma(53);
      mi(54)=alfa(61)*kt(83)/gamma(54);
      mi(55)=alfa(61)**2*kt(84)/gamma(55);
      mi(56)=alfa(61)**3*kt(85)/gamma(56);
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      mi(57)=alfa(61)**4*kt(86)/gamma(57);
      mi(58)=alfa(5)*kt(87)/gamma(58);
      mi(59)=alfa(5)**2*kt(88)/gamma(59);
      mi(181)=kt(336)*(ah2o*tenph)**3/gamma(181);
      mi(50)=altot/(1e0+gamma(50)*(mi(51)+mi(52)+mi(53)+mi(54)+mi(55)
             +mi(56)+mi(57)+mi(58)+mi(59)+mi(181)));
      alfa(50),c1=mi(50)*gamma(50);
      do i=51 to 59,181; mi(i)=c1*mi(i); alfa(i)=mi(i)*gamma(i); end;
      end;  else do i=51 to 59,181;  mi(i)=0e0;  end;
/* fe species */
   if fe2tot + fe3tot > 0 | ehm < 9.9 & fetotal > 0e0 then do;
/* fe +2 species */
      mi(10)=kt(2)*ah2o*tenph/gamma(10);
      mi(11)=kt(3)*ah2o**3*tenph**3/gamma(11);
      mi(33)=kt(8)*alfa(5)/gamma(33);
      mi(64)=kt(120)*alfa(47)/gamma(64);
      mi(79)=kt(105)*(ah2o*tenph)**2/gamma(79);
      mi(99)=kt(138)*alfa(46)/gamma(99);
      mi(247)=kt(476)*alfa(66)**2/gamma(247);
      mi(248)=kt(477)*alfa(66)**3/gamma(248);
/* fe +3 species */
      mi(9)=kt(1)*ah2o*tenph/gamma(9);
      mi(12)=kt(139)*alfa(46)/gamma(12);
      mi(14)=kt(4)*alfa(5)/gamma(14);
      mi(15)=kt(5)*alfa(4)/gamma(15);
      mi(27)=kt(6)*alfa(4)**2/gamma(27);
      mi(32)=kt(7)*alfa(4)**3/gamma(32);
      mi(76)=kt(102)*(ah2o*tenph)**2/gamma(76);
      mi(77)=kt(103)*(ah2o*tenph)**3/gamma(77);
      mi(78)=kt(104)*(ah2o*tenph)**4/gamma(78);
      mi(98)=kt(156)*alfa(47)/gamma(98);
      mi(105)=alfa(61)*kt(165)/gamma(105);
      mi(106)=alfa(61)**2*kt(166)/gamma(106);
      mi(107)=alfa(61)**3*kt(167)/gamma(107);
      mi(108)=kt(333)*alfa(5)**2/gamma(108);
      if mi(8) > 1e-38 then do;
      c2=log10(kt(334))+2*(lh2o+ph)+log10(mi(8))+log10(gamma(8))
            -log10(gamma(179));
      if abs(c2) < 36 then mi(179)=10**c2;  else mi(179)=0e0;
      c3=log10(kt(335))+4*(lh2o+ph)+2*(log10(mi(8))
            +log10(gamma(8)))-log10(gamma(180));
      if abs(c3) < 36 then mi(180)=10**c3;  else mi(180)=0e0;
        end;
      mi(288)=kt(525)*alfa(284)/gamma(288);
      mi(289)=kt(526)*alfa(285)/gamma(289);
   if fe2tot + fe3tot > 0e0 then call split_iron;
   else do;
      mi(8)=1e0/gamma(8);
      c1=kt(0)/tenmpe;
      do i=8,9,12,14,15,27,32,76,77,78,98,105 to 108,288,289;
        mi(i)=c1*mi(i);  end;
      if mi(7) > 1e-38 then do;
      c2=log10(kt(334))+2*log10(c1)+2*(lh2o+ph)+log10(mi(7))
            +log10(gamma(7))-log10(gamma(179));
      if abs(c2) < 36 then mi(179)=10**c2;  else mi(179)=0e0;
      c3=log10(kt(335))+3*log10(c1)+4*(lh2o+ph)+2*log10(mi(7))
            +2*log10(gamma(7))-log10(gamma(180));
      if abs(c3) < 36 then mi(180)=10**c3;  else mi(180)=0e0;
        end;
      mi(7)=fetotal/(1e0+gamma(7)*(mi(8)+mi(9)+mi(10)+mi(11)+mi(12)+
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            mi(14)+mi(15)+mi(27)+mi(32)+mi(33)+mi(64)+mi(76)+mi(77)+
            mi(78)+mi(79)+mi(98)+mi(99)+mi(105)+mi(106)+mi(107)+
            mi(108)+2*mi(179)+3*mi(180)+mi(247)+mi(248)+mi(288)+
            mi(289)));
        alfa(7),c1=mi(7)*gamma(7);
        do i = 8 to 12,14,15,27,32,33,64,76 to 79,98,99,105 to 108,
            179,180,247,248,288,289;
          mi(i)=c1*mi(i);  end;  alfa(8)=mi(8)*gamma(8);  end;
        do i = 9 to 12,14,15,27,32,33,64,76 to 79,98,99,105 to 108,
            179,180,247,248,288,289;  alfa(i)=mi(i)*gamma(i);  end;
  end; else do i = 7 to 12,14,15,27,32,33,64,76 to 79,98,99,105 to 108,
             179,180,247,248,288,289;
        mi(i)=0e0; end;
      if alfa(7)*alfa(8)>0 then do;
        pefe=-log10(kt(0)*alfa(7)/alfa(8));
        ehfe=pefe*c*r*t/f;
        if cunits(7)*cunits(8)>0 then
        if ehpt>9e0 | ehopt^=0 then do;  ehm=enfe;  pe=pefe;
            tenmpe=1e1**(-pe); end;
        end;

/* li, sr, ba, cs, rb species */
      c2 = kt(126) * alfa(5)/gamma(82);
      mi(80) = litot/(1e0+gamma(80)*c2);
      alfa(80) = mi(80)*gamma(80);
      mi(82)=c2 * alfa(80);
      c1=kt(129) * alfa(26)/gamma(88);
      mi(87) = srtot/(1e0+gamma(87)*c1);
      mi(88) = gamma(87)*mi(87)*c1;
      c1=kt(130)*alfa(26)/gamma(90);
      mi(89)=batot/(1e0+gamma(89)*c1);
      mi(90)=gamma(89)*mi(89)*c1;
      do i=48,82,87 to 90,94; alfa(i) = mi(i) * gamma(i); end;

split_iron:  proc ;
/* fe +2 species */
        mi(7)=fe2tot/(1 + gamma(7)*(mi(10)+mi(11)+mi(33)+mi(64)+mi(77)
            +mi(99)+mi(247)+mi(248)));
        alfa(7),c1=mi(7)*gamma(7);
        do i=10,11,33,64,79,99,247,248;
          mi(i)=c1*mi(i);  end;
/* fe +3 species */
        mi(8)=fe3tot/(1 + gamma(8)*(mi(9)+mi(12)+mi(14)+mi(15)+mi(27)
            +mi(32)+mi(76)+mi(77)+mi(78)+mi(98)+mi(105)+mi(106)
            +mi(107)+mi(108)+2*mi(179)+3*mi(180)+mi(288)+mi(289)));
        alfa(8),c1=mi(8)*gamma(8);
        do i=9,12,14,15,27,32,76,77,78,98,105 to 108,179,180,288,289;
          mi(i)=c1*mi(i);  end;
  end split_iron;
 end maj_el;
```

```
 tr_el: proc(alfa,gamma,kt,logkt,mi);
   dcl (agtot,ah2o,astotal,as3tot,as5tot,cdtot,cutot,ehm,lh2o,mntot,
        nitot,obtot,pe,ph,tenmpe,tenph,zntot)float dec(20) ext,
        (c1,alfa(*),gamma(*),kt(*),
        logkt(*),mi(*),xmi120,xmi121,xmi178)float dec(20) ,i fixed bin(31);

/* mn species */
  if mntot>0 then do;
/* mn +2 species */
    mi(111)=kt(170)*alfa(4)/gamma(111);
    mi(112)=kt(171)*alfa(4)**2/gamma(112);
    mi(113)=kt(172)*alfa(4)**3/gamma(113);
    mi(114)=kt(173)*ah2o*tenph/gamma(114);
    mi(115)=kt(174)*(ah2o*tenph)**3/gamma(115);
    mi(116)=kt(175)*alfa(61)/gamma(116);
    mi(117)=kt(176)*alfa(5)/gamma(117);
    mi(118)=kt(177)*alfa(84)**2/gamma(118);
    mi(119)=kt(178)*alfa(6)/gamma(119);
    if ehm<9.9 then do;
/* mn +3, +6, +7 species */
      mi(110)=kt(169)/(gamma(110)*tenmpe);
      xmi120=logkt(179)+4*lh2o-(log10(gamma(120))-8*ph-5*pe);
      if xmi120 > -35 then mi(120)=10**xmi120;  else mi(120)=0;
      xmi121=logkt(180)+4*lh2o-(log10(gamma(121))-8*ph-4*pe);
      if xmi121 > -35 then mi(121)=10**xmi121;  else mi(121)=0;  end;
    mi(109)=mntot/(1+gamma(109)*(mi(110)+mi(111)+mi(112)+mi(113)+
            mi(114)+mi(115)+mi(116)+mi(117)+mi(118)+mi(119)+mi(120)
            +mi(121)));
    alfa(109),c1=mi(109)*gamma(109);
    do i=110 to 121;
      mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);  end;  end;
  else do i=109 to 121;  mi(i)=0e0;  end;

/* cu species */
  if cutot > 0 then do;
    if ehm < 9.9 then do;
/* cu +1 species */
      mi(127)=kt(208)*tenmpe/gamma(127);
      mi(128)=kt(206)*alfa(4)**2*termpe/gamma(128);
      mi(129)=kt(207)*alfa(4)**3*tenmpe/gamma(129);
      mi(259)=kt(485)*(alfa(66)*tenph)**2*tenmpe/gamma(259);
      mi(260)=kt(486)*(alfa(66)*tenph)**2*tenmpe/gamma(260);  end;
/* cu +2 species */
    mi(131)=kt(209)*alfa(17)/gamma(131);
    mi(132)=kt(210)*alfa(17)**2/gamma(132);
    mi(133)=kt(211)*alfa(4)/gamma(133);
    mi(134)=kt(212)*alfa(4)**2/gamma(134);
    mi(135)=kt(213)*alfa(4)**3/gamma(135);
    mi(136)=kt(214)*alfa(4)**4/gamma(136);
    mi(137)=kt(215)*alfa(61)/gamma(137);
    mi(138)=kt(216)*ah2o*tenph/gamma(138);
    mi(139)=kt(217)*(ah2o*tenph)**2/gamma(139);
    mi(140)=kt(218)*(ah2o*tenph)**3/gamma(140);
    c1=logkt(219)+4*(lh2o+ph)-log10(gamma(141));
    if abs(c1)<38 then mi(141)=10**c1;
    mi(142)=kt(220)*mi(130)*gamma(130)*(ah2o*tenph)**2/gamma(142);
    mi(143)=kt(221)*alfa(5)/gamma(143);
    mi(144)=kt(222)*alfa(66)**3/gamma(144);
    mi(271)=kt(510)*alfa(6)/gamma(271);
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      mi(290)=kt(527)*alfa(284)/gamma(290);
      mi(291)=kt(528)*alfa(285)/gamma(291);
      mi(130)=cutot/(1+gamma(130)*(mi(127)+mi(128)+mi(129)+mi(131)
              +mi(132)+mi(133)+mi(134)+mi(135)+mi(136)+mi(137)
              +mi(138)+mi(139)+mi(140)+mi(141)+2*mi(142)+mi(143)
              +mi(144)+mi(259)+mi(260)+mi(271)+mi(290)+mi(291)));
      alfa(130),c1=mi(130)*gamma(130);
      do i=127 to 129,131 to 144,259,260,271,290,291;  mi(i)=c1*mi(i);
        alfa(i)=mi(i)*gamma(i);  end;
    end; else do i = 127 to 144,259,260,271,290,291;  mi(i)=0e0;  end;

  /* zn species */
    if zntot>0 then do;
      mi(146)=kt(251)*alfa(4)/gamma(146);
      mi(147)=kt(252)*alfa(4)**2/gamma(147);
      mi(148)=kt(253)*alfa(4)**3/gamma(148);
      mi(149)=kt(254)*alfa(4)**4/gamma(149);
      mi(150)=kt(255)*alfa(61)/gamma(150);
      mi(151)=kt(256)*ah2o*tenph/gamma(151);
      mi(152)=kt(257)*(ah2o*tenph)**2/gamma(152);
      mi(153)=kt(258)*(ah2o*tenph)**3/gamma(153);
      c1=logkt(259)+4*(lh2o+ph)-log10(gamma(154));
      if abs(c1)<38 then mi(154)=10**c1;
      mi(155)=kt(260)*ah2o*tenph*alfa(4)/gamma(155);
      mi(156)=kt(261)*alfa(66)**2/gamma(156);
      mi(157)=kt(262)*alfa(66)**3/gamma(157);
      mi(158)=kt(263)*alfa(5)/gamma(158);
      mi(159)=kt(264)*alfa(5)**2/gamma(159);
      mi(229)=kt(447)*alfa(97)/gamma(229);
      mi(230)=kt(448)*alfa(97)**2/gamma(230);
      mi(231)=kt(449)*alfa(96)/gamma(231);
      mi(232)=kt(450)*alfa(96)**2/gamma(232);
      mi(272)=kt(511)*alfa(6)/gamma(272);
      mi(273)=kt(512)*alfa(17)/gamma(273);
      mi(274)=kt(513)*alfa(17)**2/gamma(274);
      mi(145)=zntot/(1+gamma(145)*(mi(146)+mi(147)+mi(148)+mi(149)+
              mi(150)+mi(151)+mi(152)+mi(153)+mi(154)+mi(155)+mi(156)
              +mi(157)+mi(158)+mi(159)+mi(229)+mi(230)+mi(231)
              +mi(232)+mi(272)+mi(273)+mi(274)));
      alfa(145),c1=mi(145)*gamma(145);
      do i=146 to 159,229 to 232,272 to 274;   mi(i)=c1*mi(i);
        alfa(i)=mi(i)*gamma(i);  end;
   end;  else do i = 145 to 159,229 to 232,272 to 274;  mi(i)=0e0;  end;

  /* cd species */
    if cdtot > 0 then do;
      mi(161)=kt(294)*alfa(4)/gamma(161);
      mi(162)=kt(295)*alfa(4)**2/gamma(162);
      mi(163)=kt(296)*alfa(4)**3/gamma(163);
      mi(164)=kt(297)*alfa(61)/gamma(164);
      mi(165)=kt(298)*alfa(61)**2/gamma(165);
      mi(166)=kt(299)*alfa(17)**3/gamma(166);
      mi(167)=kt(300)*ah2o*tenph/gamma(167);
      mi(168)=kt(301)*(ah2o*tenph)**2/gamma(168);
      mi(169)=kt(302)*(ah2o*tenph)**3/gamma(169);
      c1=logkt(303)+4*(lh2o+ph)-log10(gamma(170));
      if abs(c1)<38 then mi(170)=10**c1;
      mi(171)=kt(304)*mi(160)*gamma(160)*ah2o*tenph/gamma(171);
      mi(172)=kt(305)*ah2o*tenph*alfa(4)/gamma(172);
      mi(173)=kt(306)*alfa(84)/gamma(173);
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      mi(174)=kt(307)*alfa(5)/gamma(174);
      mi(175)=kt(308)*alfa(66)/gamma(175);
      mi(176)=kt(309)*alfa(66)**2/gamma(176);
      mi(177)=kt(310)*alfa(66)**3/gamma(177);
      if alfa(66)>0e0 then do;
      xmi178=logkt(311)+4e0*log10(alfa(66))-log10(gamma(178));
      if xmi178 > -35 then mi(178)=10**xmi178;  else mi(178)=0e0;  end;
      mi(233)=kt(451)*alfa(97)/gamma(233);
      mi(234)=kt(452)*alfa(97)**2/gamma(234);
      mi(235)=kt(453)*alfa(96)/gamma(235);
      mi(236)=kt(454)*alfa(96)**2/gamma(236);
      mi(275)=kt(514)*alfa(6)/gamma(275);
      mi(276)=kt(515)*alfa(17)/gamma(276);
      mi(277)=kt(516)*alfa(5)**2/gamma(277);
      mi(292)=kt(529)*alfa(284)/gamma(292);
      mi(293)=kt(530)*alfa(285)/gamma(293);
      mi(160)=cdtot/(1+gamma(160)*(mi(161)+mi(162)+mi(163)+mi(164)+
              mi(165)+mi(166)+mi(167)+mi(168)+mi(169)+mi(170)+2*mi(171)
              +mi(172)+mi(173)+mi(174)+mi(175)+mi(176)+mi(177)+
              mi(178)+mi(233)+mi(234)+mi(235)+mi(236)+mi(275)+mi(276)+
              mi(277)+mi(292)+mi(293)));
      alfa(160),c1=mi(160)*gamma(160);
      do i=161 to 178,233 to 236,275 to 277,292,293;  mi(i)=c1*mi(i);
        alfa(i)=mi(i)*gamma(i);  end;
      end;  else do i=160 to 178,233 to 236,275 to 277,292,293;
                  mi(i)=0e0;  end;

  /* pb species */
    if pbtot > 0 then do;
      mi(183)=kt(341)*alfa(4)/gamma(183);
      mi(184)=kt(342)*alfa(4)**2/gamma(184);
      mi(185)=kt(343)*alfa(4)**3/gamma(185);
      mi(186)=kt(344)*alfa(4)**4/gamma(186);
      mi(187)=kt(345)*alfa(17)**2/gamma(187);
      mi(188)=kt(346)*alfa(61)/gamma(188);
      mi(189)=kt(347)*alfa(61)**2/gamma(189);
      mi(190)=kt(348)*alfa(61)**3/gamma(190);
      mi(191)=kt(349)*alfa(61)**4/gamma(191);
      mi(192)=kt(350)*ah2o*tenph/gamma(192);
      mi(193)=kt(351)*(ah2o*tenph)**2/gamma(193);
      mi(194)=kt(352)*(ah2o*tenph)**3/gamma(194);
      mi(195)=kt(353)*ah2o*tenph*mi(182)*gamma(182)/gamma(195);
      mi(196)=kt(354)*alfa(84)/gamma(196);
      mi(197)=kt(355)*alfa(5)/gamma(197);
      mi(198)=kt(356)*alfa(66)**2/gamma(198);
      mi(199)=kt(357)*alfa(66)**3/gamma(199);
      mi(200)=0e0;
      if mi(182)>1e-38 then do;
        c1=logkt(358)+2*(log10(mi(182))+log10(gamma(182)))+4*(lh2o+ph)-log10(gamma(200));
        if abs(c1)<38 then mi(200)=10**c1;  end;
      mi(237)=kt(455)*alfa(97)/gamma(237);
      mi(238)=kt(456)*alfa(97)**2/gamma(238);
      mi(239)=kt(457)*alfa(96)/gamma(239);
      mi(240)=kt(458)*alfa(96)**2/gamma(240);
      mi(241)=kt(468)*alfa(17)/gamma(241);
      c1=logkt(469)+4*(lh2o+ph)-log10(gamma(242));
      if abs(c1)<38 then mi(242)=10**c1;
      mi(243)=kt(470)*alfa(5)**2/gamma(243);
      mi(278)=kt(517)*alfa(6)/gamma(278);
      mi(182)=pbtot/(1+gamma(182)*(mi(183)+mi(184)+mi(185)+mi(186)+
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          mi(187)+mi(188)+mi(189)+mi(190)+mi(191)+mi(192)+mi(193)+
          mi(194)+2*mi(195)+mi(196)+mi(197)+mi(198)+mi(199)+2*mi(200)+
          mi(237)+mi(238)+mi(239)+mi(240)+mi(241)+mi(242)+
          mi(243)+mi(278)));
      alfa(182),c1=mi(182)*gamma(182);
      do i=183 to 200,237 to 243,279;  mi(i)=c1*mi(i);
        alfa(i)=mi(i)*gamma(i);  end;
      end;  else do i=182 to 200,237 to 243,278;  mi(i)=0;  end;

    /* ni species */
      if nitot >0 then do;
        mi(205)=kt(403)*alfa(97)/gamma(205);
        mi(206)=kt(404)*alfa(4)/gamma(206);
        mi(207)=kt(405)*alfa(61)/gamma(207);
        mi(208)=kt(406)*ah2o*tenph/gamma(208);
        mi(209)=kt(407)*(ah2o*tenph)**2/gamma(209);
        mi(210)=kt(408)*(ah2o*tenph)**3/gamma(210);
        mi(211)=kt(409)*alfa(5)/gamma(211);
        mi(279)=kt(518)*alfa(4)**2/gamma(279);
        mi(280)=kt(519)*alfa(6)/gamma(280);
        mi(281)=kt(520)*alfa(17)/gamma(281);
        mi(282)=kt(521)*alfa(17)**2/gamma(282);
        mi(283)=kt(522)*alfa(5)**2/gamma(283);
        mi(204)=nitot/(1+gamma(204)*(mi(205)+mi(206)+mi(207)+mi(208)+
              mi(209)+mi(210)+mi(211)+mi(279)+mi(280)+mi(281)+mi(282)+
              mi(283)));
        alfa(204),c1=mi(204)*gamma(204);
        do i=205 to 211,279 to 283;  mi(i)=c1*mi(i);
          alfa(i)=mi(i)*gamma(i);  end;
        end;  else do i=204 to 211,279 to 283;  mi(i)=0e0;  end;

    /* ag species */
      if agtot > 0 then do;
        mi(213)=kt(421)*alfa(97)/gamma(213);
        mi(214)=kt(422)*alfa(97)**2/gamma(214);
        mi(215)=kt(423)*alfa(4)/gamma(215);
        mi(216)=kt(424)*alfa(4)**2/gamma(216);
        mi(217)=kt(425)*alfa(4)**3/gamma(217);
        mi(218)=kt(426)*alfa(4)**4/gamma(218);
        mi(219)=kt(427)*alfa(61)/gamma(219);
        mi(220)=kt(428)*alfa(66)/gamma(220);
        mi(221)=kt(429)*alfa(66)**2/gamma(221);
        mi(222)=kt(430)*alfa(96)/gamma(222);
        mi(223)=kt(431)*alfa(96)**2/gamma(223);
        mi(224)=kt(432)*ah2o*tenph/gamma(224);
        mi(225)=kt(433)*(ah2o*tenph)**2/gamma(225);
        mi(226)=kt(434)*alfa(5)/gamma(226);
        mi(227)=kt(435)*alfa(84)/gamma(227);
        mi(228)=kt(436)*alfa(202)**2/gamma(228);
        mi(244)=kt(473)*alfa(97)**3/gamma(244);
        mi(245)=kt(474)*alfa(96)**3/gamma(245);
        mi(246)=kt(475)*alfa(96)**4/gamma(246);
        mi(268)=kt(507)*(alfa(66)*tenph)**2/gamma(268);
        mi(269)=kt(508)*(alfa(66)*tenph)**2/gamma(269);
        mi(270)=kt(509)*alfa(66)**2*tenph/gamma(270);
        mi(294)=kt(531)*alfa(284)/gamma(294);
        mi(295)=kt(532)*alfa(285)/gamma(295);
        mi(212)=agtot/(1+gamma(212)*(mi(213)+mi(214)+mi(215)+mi(216)+
                mi(217)+mi(218)+mi(219)+mi(220)+mi(221)+mi(222)+mi(223)+
                mi(224)+mi(225)+mi(226)+mi(227)+mi(228)+mi(244)+mi(245)+
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            mi(245)+mi(268)+mi(269)+mi(270)+mi(294)+mi(295)));
    alfa(212),c1=mi(212)*gamma(212);
    do i=213 to 228,244 to 246,268 to 270,294,295;  mi(i)=c1*mi(i);
      alfa(i)=mi(i)*gamma(i);  end;
    end;  else do i=212 to 228,244 to 246,268 to 270,294,295;
                mi(i)=0e0;  end;

/* as species */
  if as3tot + as5tot > 0e0 | ehm < 9.9 & astotal > 0e0 then do;
    mi(251)=kt(478)*tenph/gamma(251);
    mi(252)=kt(479)*tenph**2/gamma(252);
    mi(253)=kt(480)*tenph**3/gamma(253);
    mi(254)=kt(481)/(tenph*gamma(254));
    mi(256)=kt(482)*tenph/gamma(256);
    mi(257)=kt(483)*tenph**2/gamma(257);
    mi(258)=kt(484)*tenph**3/gamma(258);
    if as3tot + as5tot > 0e0 then call split_arsenic;
    else do;
      mi(255)=1e0/gamma(255);
      c1=kt(487)*ah2o*tenph**2/tenmpe**2;
      do i=255 to 258;  mi(i)=c1*mi(i);  end;
      mi(250)=astotal/(1e0 + gamma(250)*(mi(251)+mi(252)+mi(253)+
              mi(254)+mi(255)+mi(256)+mi(257)+mi(258)));
      alfa(250),c1=mi(250)*gamma(250);
      do i=251 to 258;  mi(i)=c1*mi(i);  end;
      alfa(255)=mi(255)*gamma(255);
      end;
    do i=251 to 254, 256 to 258;  alfa(i)=mi(i)*gamma(i);  end;  end;
    else do i = 250 to 258;  mi(i) = 0e0;  end;

 split_arsenic:  proc ;
/* as +3 species */
   mi(250)=as3tot/(1e0 + gamma(250)*(mi(251)+mi(252)+mi(253)+mi(254)));
   alfa(250),c1=mi(250)*gamma(250);
   do i=251 to 254;  mi(i)=c1*mi(i);  end;
/* as +5 species */
   mi(255)=as5tot/(1e0 + gamma(255)*(mi(256)+mi(257)+mi(258)));
   alfa(255),c1=mi(255)*gamma(255);
   do i=256 to 258;  mi(i)=c1*mi(i);  end;
 end split_arsenic;
  end tr_el;
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u_el:  proc(alfa,gamma,kt,logkt,mi);
   dcl  (utotal,u4tot,u6tot,an2o,tenph,tenmpe,ehm,peu,ehu,c,r,t,f,lh2o,ph)float dec(21) ext,
        (c1,alfa(*),gamma(*),kt(*),logkt(*),mi(*))float dec(20),
        utemp(301:340) float dec(20),
        (xa4,xa5,xa17,xa44,xa51,xa300) float dec(20),
        i fixed bin(31);

 /**  URANIUM MASS ACTION AND MASS BALANCE **/
 if u4tot+u6tot>0  | ehm<9.9 & utotal >0e0
   then do;
     /*U+4 species*/
     utemp(301)=logkt(544)+log10(termpe)-log10(gamma(301));
     utemp(302)=logkt(545)+lh2o+ph-log10(gamma(302));
     utemp(303)=logkt(546)+2*(lh2o+ph)-log10(gamma(303));
     utemp(304)=logkt(547)+3*(lh2o+ph)-log10(gamma(304));
     utemp(305)=logkt(548)+4*(lh2o+ph)-log10(gamma(305));
     utemp(306)=logkt(549)+5*(lh2o+ph)-log10(gamma(306));

     if mi(299)*gamma(299)>1e-38 then do;
     utemp(307)=logkt(550)+15*(ph+lh2o)+5*log10(mi(299)*gamma(299))-log10(gamma(307));
     end; else utemp(307)=39;

     if alfa(61)>1e-38 then do;
        xa61=log10(alfa(61));
     utemp(308)=logkt(556)+xa61-log10(gamma(308));
     utemp(309)=logkt(557)+2*xa61-log10(gamma(309));
     utemp(310)=logkt(558)+3*xa61-log10(gamma(310));
     utemp(311)=logkt(559)+4*xa61-log10(gamma(311));
     utemp(312)=logkt(560)+5*xa61-log10(gamma(312));
     utemp(313)=logkt(561)+6*xa61-log10(gamma(313));
     end; else do i=308 to 313; utemp(i)=39; end;

     if alfa(4)>1e-38 then do;
        xa4=log10(alfa(4));
     utemp(314)=logkt(564)+xa4-log10(gamma(314));
     end; else utemp(314)=39;

     if alfa(5)>1e-38 then do;
        xa5=log10(alfa(5));
     utemp(315)=logkt(565)+xa5-log10(gamma(315));
     utemp(316)=logkt(566)+2*xa5-log10(gamma(316));
     end; else do i=315,316; utemp(i)=39; end;

     if alfa(44)>1e-38 then do;
        xa44=log10(alfa(44));
     utemp(317)=logkt(567)+xa44-ph-log10(gamma(317));
     utemp(318)=logkt(568)+2*(xa44-ph)-log10(gamma(318));
     utemp(319)=logkt(569)+3*(xa44-ph)-log10(gamma(319));
     utemp(320)=logkt(570)+4*(xa44-ph)-log10(gamma(320));
     end; else do i=317 to 320; utemp(i)=39; end;

     /*U+6 species*/
     utemp(321)=logkt(573)+log10(termpe)-log10(gamma(321));
     utemp(322)=logkt(574)+lh2o+ph-log10(gamma(322));

     if mi(300)*gamma(300)>1e-38 then do;
        xa300=log10(mi(300)*gamma(300));
     utemp(323)=logkt(575)+xa300+2*(lh2o+ph)-log10(gamma(323));
     utemp(324)=logkt(576)+2*xa300+5*(lh2o+ph)-log10(gamma(324));
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end; else do i=323,324; utemp(i)=39; end;

if alfa(17)>1e-38 then do;
   xa17=log10(alfa(17));
utemp(325)=logkt(581)+xa17-log10(gamma(325));
utemp(326)=logkt(582)+2*xa17-log10(gamma(326));
utemp(327)=logkt(583)+3*xa17-log10(gamma(327));
end; else do i=325 to 327; utemp(i)=39; end;

if alfa(61)>1e-38 then do;
   xa61=log10(alfa(61));
utemp(328)=logkt(585)+xa61-log10(gamma(328));
utemp(329)=logkt(586)+2*xa61-log10(gamma(329));
utemp(330)=logkt(587)+3*xa61-log10(gamma(330));
utemp(331)=logkt(588)+4*xa61-log10(gamma(331));
end; else do i=328 to 331; utemp(i)=39; end;

if alfa(4)>1e-38 then do;
   xa4=log10(alfa(4));
utemp(332)=logkt(589)+xa4-log10(gamma(332));
end; else utemp(322)=39;

if alfa(5)>1e-38 then do;
   xa5=log10(alfa(5));
utemp(333)=logkt(590)+xa5-log10(gamma(333));
utemp(334)=logkt(591)+2*xa5-log10(gamma(334));
end; else do i=333,334; utemp(i)=39; end;

if alfa(44)>1e-38 then do;
   xa44=log10(alfa(44));
utemp(335)=logkt(592)+xa44-oh-log10(gamma(335));
utemp(336)=logkt(593)+2*(xa44-ph)-log10(gamma(336));
utemp(337)=logkt(594)+xa44-2*ph-log10(gamma(337));
utemp(338)=logkt(595)+2*(xa44-ph-ph)-log10(gamma(338));
utemp(339)=logkt(596)+3*(xa44-ph-ph)-log10(gamma(339));
end; else do i=335 to 339; utemp(i)=39; end;

if alfa(24)>1e-38 then do;
utemp(340)=logkt(609)+log10(alfa(23))+ph-log10(gamma(340));
end; else utemp(340)=39;

do i=301 to 340;
   if abs(utemp(i))<38 then mi(i)=1e1**utemp(i); else mi(i)=0;
end;

if u4tot+u6tot > 0e0
  then do;
    mi(299)=u4tot/(1+gamma(299)*(mi(301)+mi(302)+mi(303)+mi(304)+
                                 mi(305)+mi(306)+6*mi(307)+mi(308)+
                                 mi(309)+mi(310)+mi(311)+mi(312)+
                                 mi(313)+mi(314)+mi(315)+mi(316)+
                                 mi(317)+mi(318)+mi(319)+mi(320)));
    alfa(299),c1=mi(299)*gamma(299);
    do i=301 to 320;
         mi(i)=c1*mi(i);
    end;
    mi(300)=u6tot/(1+gamma(300)*(mi(321)+mi(322)+2*mi(323)+3*mi(324)+
                                 mi(325)+mi(326)+mi(327)+mi(328)+
                                 mi(329)+mi(330)+mi(331)+mi(332)+
                                 mi(333)+mi(334)+mi(335)+mi(336)+
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                                        mi(337)+mi(338)+mi(339)+mi(340)));
          alfa(300),c1=mi(300)*gamma(300);
          do i=321 to 340;
            mi(i)=c1*mi(i);
          end;
         end;
        else do;
          /* if utot but u4tot and u6tot not specified */
          mi(299)=1e0/gamma(299);
          c1=kt(542)*tenmpe**2/(an2o**2*tenph**4);
          do i=299,301 to 320;
            mi(i)=c1*mi(i);
          end;
            c1=0;
            do i=299,301 to 340;
              c1=c1+mi(i);
            end;
            c1=c1+5*mi(307)+mi(323)+2*mi(324);
            mi(300)=utotal/(1e0+gamma(300)*c1);
          alfa(300),c1=mi(300)*gamma(300);
          do i=299,301 to 340;
            mi(i)=mi(i)*c1;
          end;
          alfa(299)=mi(299)*gamma(299);
        end;
        do i=301 to 340; alfa(i)=mi(i)*gamma(i); end;
         if alfa(299)>1e-38 & alfa(300)>1e-38 then do;
              peu=-.5*(-logkt(542)+log10(alfa(299))+2*ln2o-log10(alfa(300))+4*ph);
              ehu=peu*c*r*t/f;
            end;
    end;
    else do i=299 to 340;
           mi(i)=0e0;
         end;
enc u_el;
```

```
 sums: proc(alfa,gamma,kt,logkt,mi);
 dcl(d,coralk,iter)fixed bin(31)ext,(c1,c2,c3,s2,s3,s4,s5,s6,s7,s8,alfa(*),
     gamma(*),kt(*),logkt(*),mi(*))float dec(20) ,rbit bit(1)ext,(ah2o,analco3,btot,
     carbonc,cltot,co2tit,ftot,fulvtot,humtot,h2stot,noncarb,ptot,
     so4tot,s1,tenph,ph)float dec(20) ext,i fixed bin(31);
dcl outprint external file constant;
/* summation of anion species */
    if coralk=2 then
      s1 = mi(6) + mi(17) + mi(20) + mi(21) + mi(29)
           + mi(30) + mi(41) + mi(42) + mi(85) + mi(119) +
           mi(131) + 2*mi(132) + 3*mi(166) + 2*mi(187) + mi(241)
           + mi(271) + mi(272) + mi(273) + 2*mi(274) + mi(275) +
           mi(276) + mi(278) + mi(280) + mi(281) + 2*mi(282) +
           mi(325)+2*mi(326)+3*mi(327);
    else
      s1 = mi(6) + 2*mi(17) + 2*mi(20) + mi(21) + mi(29)
           + 2*mi(30) + 2*mi(41) + mi(42)              + mi(119) +
           2*mi(131) + 4*mi(132) + 6*mi(166) + 4*mi(187) + 2*mi(241) +
           mi(271) + mi(272) + 2*mi(273) + 4*mi(274) + mi(275) +
           2*mi(276) + mi(278) + mi(280) + 2*mi(281) + 4*mi(282)+
           2*mi(325)+4*mi(326)+6*mi(327);
      s2 = mi(5) + mi(14) + mi(22) + mi(31) + mi(43) + mi(45) +
           mi(58) +2e0* mi(59) + mi(62) + mi(82) + mi(91) +
           mi(33) + mi(117) + mi(143) + mi(158) + 2*mi(159) +
           mi(174) + 2*mi(108) + mi(197) + mi(211) + mi(226) +
           2*mi(243) + 2*mi(277) + 2*mi(283)+
           mi(315)+2*mi(316)+mi(333)+2*mi(334);
      s3 = mi(61)+mi(54)+2*mi(55)+3*mi(56)+4*mi(57)+mi(19)+mi(100)
           +mi(101)+2*mi(102)+3*mi(103)+4*mi(104)+mi(105)+2*mi(106)+
           3*mi(107)+mi(116)          +6*mi(124)+mi(125)+2*mi(126)+
           mi(137)+mi(150)+mi(164)+2*mi(165)+mi(188)+2*mi(189)+
           3*mi(190)+4*mi(191)+mi(207)+mi(219)+2*mi(296)+mi(297);
           s3=s3+mi(308)+2*mi(309)+3*mi(310)+4*mi(311)+5*mi(312)+6*mi(313)+
           mi(328)+2*mi(329)+3*mi(330)+4*mi(331);
      s4 = mi(44) + mi(46) + mi(47) + mi(49) + mi(60) + mi(72) +
           mi(73) + mi(74) + mi(75) + mi(39) + mi(40) + mi(12) +
           mi(64) + mi(98) + mi(99)+
           mi(317)+2*mi(318)+3*mi(319)+4*mi(320)+
           mi(335)+2*mi(336)+mi(337)+2*mi(338)+3*mi(339);
      s5 = mi(4) + mi(15) + 2*mi(27) + 3*mi(32) +
                   2*mi(128) + 3 *mi(129) + mi(133) + 2*mi(134) +
           3*mi(135) + 4*mi(136) + mi(146) + 2*mi(147) + 3*mi(148) +
           4*mi(149) + mi(155) + mi(161) + 2*mi(162) + 3*mi(163) ;
           s5=s5+mi(172) + mi(183) + 2*mi(184) + 3*mi(185) + 4*mi(186)
           + mi(111) + 2*mi(112) + 3*mi(113) + mi(206) + mi(215) +
           2*mi(216) + 3*mi(217) + 4*mi(218) + 2*mi(279)+mi(314)+mi(332);
      s6 = mi(13)+mi(66)+mi(67)+2*mi(247)+3*mi(248)+3*mi(144)+2*mi(156)
           +3*mi(157)+mi(175)+2*mi(176)+3*mi(177)+4*mi(178)+2*mi(198)
           +3*mi(199)+mi(220)+2*mi(221)+2*mi(259)+2*mi(260)+
           mi(263)+mi(264)+mi(265)+mi(266)+mi(267)+2*mi(268)+
           2*mi(269)+2*mi(270);
      s7 = mi(284)+mi(286)+mi(283)+mi(290)+mi(292)+mi(294);
      s8 = mi(285)+mi(287)+mi(289)+mi(291)+mi(293)+mi(295);

/* anion mass balance calculations */
/* mass balance on carbon */
  if co2tit > 0e0 then do;
   mi(6)=kt(68)/(tenph*gamma(6));
   mi(20)=kt(73)*alfa(1)/gamma(20);
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    mi(21)=kt(74)*kt(68)*alfa(1)/(tenph*gamma(21));
    mi(29)=kt(77)*kt(68)*alfa(0)/(tenph*gamma(29));
    mi(30)=kt(78)*alfa(0)/gamma(30);
    mi(41)=kt(69)*alfa(2)/gamma(41);
    mi(42)=kt(70)*kt(68)*alfa(2)/(tenph*gamma(42));
    mi(85)=kt(35)*kt(68)/(tenph**2*gamma(85));
    mi(119)=kt(178)*kt(68)*alfa(109)/(tenph*gamma(119));
    mi(131)=kt(209)*alfa(130)/gamma(131);
    mi(132)=kt(210)*alfa(130)*alfa(17)/gamma(132);
    mi(166)=kt(299)*alfa(160)*alfa(17)**2/gamma(166);
    mi(187)=kt(345)*alfa(182)*alfa(17)/gamma(187);
    mi(241)=kt(468)*alfa(182)/gamma(241);
    mi(271)=kt(510)*kt(68)*alfa(130)/(tenph*gamma(271));
    mi(272)=kt(511)*kt(68)*alfa(145)/(tenph*gamma(272));
    mi(273)=kt(512)*alfa(145)/gamma(273);
    mi(274)=kt(513)*alfa(145)*alfa(17)/gamma(274);
    mi(275)=kt(514)*kt(68)*alfa(150)/(tenph*gamma(275));
    mi(276)=kt(515)*alfa(160)/gamma(276);
    mi(278)=kt(517)*kt(68)*alfa(132)/(tenph*gamma(278));
    mi(280)=kt(519)*kt(68)*alfa(204)/(tenph*gamma(280));
    mi(281)=kt(520)*alfa(204)/gamma(281);
    mi(282)=kt(521)*alfa(204)*alfa(17)/gamma(282);
     if alfa(300)>1e-38 then do;
       c1=log10(alfa(300));c2=log10(alfa(17));
       c3=logkt(581)+c1-log10(gamma(325));
       if abs(c3)<38 then mi(325)=10**c3; else mi(325)=0;
       c3=logkt(582)+c1+c2-log10(gamma(326));
       if abs(c3)<38 then mi(326)=10**c3; else mi(326)=0;
       c3=logkt(583)+c1+c2+c2-log10(gamma(327));
       if abs(c3)<38 then mi(327)=10**c3; else mi(327)=0;
     end; else do i=325 to 327; mi(i)=0; end;
    if coralk=2 then
    mi(17)=analco3/(1e0 + gamma(17)*(mi(6)+mi(20)+mi(21)+mi(29)+
           mi(30)+mi(41)+mi(42)+mi(85)+mi(119)+mi(131)+2*mi(132)+
           3*mi(166)+2*mi(187)+mi(241)+mi(271)+mi(272)+mi(273)+2*mi(274)
           +mi(275)+mi(276)+mi(273)+mi(280)+mi(281)+2*mi(282)+
           mi(325)+2*mi(326)+3*mi(327)));
    else do;  noncarb=mi(24)+2*mi(25)+mi(26)+mi(36)+2*mi(44)+mi(46)
       +mi(53)+mi(66)+2*mi(67);
             if coralk=0 then analcc3 = co2tit - noncarb;
    mi(17)=analco3/(2e0 + gamma(17)*(mi(6)+2*mi(20)+mi(21)+mi(29)+
           2*mi(30)+2*mi(41)+mi(42)+mi(119)+2*mi(131)+4*mi(132)+
           6*mi(166)+4*mi(187)+2*mi(241)+mi(271)+mi(272)+2*mi(273)+
           4*mi(274)+mi(275)+2*mi(276)+mi(278)+mi(280)+2*mi(281)+
           4*mi(282)+2*mi(325)+4*mi(326)+6*mi(327)));
    end;
    alfa(17),c1=mi(17)*gamma(17);
    do i=6,20,21,29,30,41,42,85,119,131,132,166,187,241,271 to 276,278,
      280 to 282,325 to 327;  mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);  end;
    end;

/* mass balance on sulfate */
  if so4tot > 0e0 then do;
     mi(14)=kt(4)*alfa(8)/gamma(14);
     mi(22)=kt(75)*alfa(1)/gamma(22);
     mi(31)=kt(23)*alfa(0)/gamma(31);
     mi(33)=kt(8)*alfa(7)/gamma(33);
     mi(43)=kt(71)*alfa(2)/gamma(43);
     mi(45)=kt(72)*alfa(3)/gamma(45);
     mi(58)=kt(87)*alfa(50)/gamma(58);
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      mi(59)=kt(88)*alfa(50)*alfa(5)/gamma(59);
      mi(62)=kt(89)/(tenph*gamma(62));
      mi(82)=kt(126)*alfa(80)/gamma(82);
      mi(91)=kt(131)*alfa(38)/gamma(91);
      mi(108)=kt(333)*alfa(8)*alfa(5)/gamma(108);
      mi(117)=kt(176)*alfa(109)/gamma(117);
      mi(143)=kt(221)*alfa(130)/gamma(143);
      mi(158)=kt(263)*alfa(145)/gamma(158);
      mi(159)=kt(264)*alfa(145)*alfa(5)/gamma(159);
      mi(174)=kt(307)*alfa(160)/gamma(174);
      mi(197)=kt(355)*alfa(182)/gamma(197);
      mi(211)=kt(409)*alfa(204)/gamma(211);
      mi(226)=kt(434)*alfa(212)/gamma(226);
      mi(243)=kt(470)*alfa(182)*alfa(5)/gamma(243);
      mi(277)=kt(516)*alfa(160)*alfa(5)/gamma(277);
      mi(283)=kt(522)*alfa(204)*alfa(5)/gamma(283);
      if alfa(299)>1e-38 then do; c1=log10(alfa(299)); c2=log10(alfa(5));
        c3=logkt(565)+c1-log10(gamma(315));
        if abs(c3)<38 then mi(315)=10**c3; else mi(315)=0;
        c3=logkt(566)+c1+c2-log10(gamma(316));
        if abs(c3)<38 then mi(316)=10**c3; else mi(316)=0;
      end; else do i=315,316; mi(i)=0; end;
      if alfa(300)>1e-38 then do c1=log10(alfa(300)); c2=log10(alfa(5));
        c3=logkt(590)+c1-log10(gamma(333));
        if abs(c3)<38 then mi(333)=10**c3; else mi(333)=0;
        c3=logkt(591)+c1+c2-log10(gamma(334));
        if abs(c3)<38 then mi(334)=10**c3; else mi(334)=0;
      end; else do i=333,334; mi(i)=0; end;
      mi(5)=so4tot/(1e0 + gamma(5)*(mi(14)+mi(22)+mi(31)+mi(33)+mi(43)+
            mi(45)+mi(58)+2*mi(59)+mi(62)+mi(82)+mi(91)+2*mi(108)+
            mi(117)+mi(143)+mi(158)+2*mi(159)+mi(174)+mi(197)+mi(211)+
            mi(226)+2*mi(243)+2*mi(277)+2*mi(283)+mi(315)+2*mi(316)+mi(333)+2*mi(334)));
      alfa(5),c1=mi(5)*gamma(5);
      do i=14,22,31,33,43,45,58,59,62,82,91,108,117,143,158,159,174,
           197,211,226,243,277,283,315,316,333,334;
        mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);  end;
      end;

  /* mass balance on fluoride */
    if ftot > 0e0 then do;
      mi(19)=kt(22)*alfa(1)/gamma(19);
      mi(54)=kt(83)*alfa(50)/gamma(54);
      mi(55)=kt(84)*alfa(50)*alfa(61)/gamma(55);
      mi(56)=kt(85)*alfa(50)*alfa(61)**2/gamma(56);
      mi(57)=kt(86)*alfa(50)*alfa(61)**3/gamma(57);
      mi(100)=kt(160)*alfa(0)/gamma(100);
      mi(101)=kt(161)*alfa(35)/gamma(101);
      mi(102)=kt(162)*alfa(35)*alfa(61)/(alfa(26)*gamma(102));
      mi(103)=kt(163)*alfa(35)*alfa(61)**2/(alfa(26)**2*gamma(103));
      mi(104)=kt(164)*alfa(35)*alfa(61)**3/(alfa(26)**3*gamma(104));
      mi(105)=kt(165)*alfa(8)/gamma(105);
      mi(106)=kt(166)*alfa(8)*alfa(61)/gamma(106);
      mi(107)=kt(167)*alfa(8)*alfa(61)**2/gamma(107);
      mi(116)=kt(175)*alfa(109)/gamma(116);
      mi(124)=kt(201)*alfa(23)*alfa(61)**5/((tenph*ah2o)**4*gamma(124));
      mi(125)=kt(202)/(tenph*gamma(125));
      mi(126)=kt(203)*alfa(61)/(tenph*gamma(126));
      mi(137)=kt(215)*alfa(130)/gamma(137);
      mi(150)=kt(255)*alfa(145)/gamma(150);
      mi(164)=kt(297)*alfa(160)/gamma(164);
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      mi(165)=kt(298)*alfa(160)*alfa(61)/gamma(165);
      mi(188)=kt(346)*alfa(182)/gamma(188);
      mi(189)=kt(347)*alfa(182)*alfa(61)/gamma(189);
      mi(190)=kt(348)*alfa(182)*alfa(61)**2/gamma(190);
      mi(191)=kt(349)*alfa(182)*alfa(61)**3/gamma(191);
      mi(207)=kt(405)*alfa(204)/gamma(207);
      mi(219)=kt(427)*alfa(212)/gamma(219);
      mi(296)=kt(537)*alfa(61)/(tenph**2*gamma(296));
      mi(297)=kt(540)*alfa(2)/gamma(297);
      if alfa(299)>1e-38 then do; c1=log10(alfa(299)); c2=log10(alfa(61));
        c3=logkt(556)+c1-log10(gamma(308));
        if abs(c3)<38 then mi(308)=10**c3; else mi(308)=0;
        c3=logkt(557)+c1+c2-log10(gamma(309));
        if abs(c3)<38 then mi(309)=10**c3; else mi(309)=0;
        c3=logkt(558)+c1+2*c2-log10(gamma(310));
        if abs(c3)<38 then mi(310)=10**c3; else mi(310)=0;
        c3=logkt(559)+c1+3*c2-log10(gamma(311));
        if abs(c3)<38 then mi(311)=10**c3; else mi(311)=0;
        c3=logkt(560)+c1+4*c2-log10(gamma(312));
        if abs(c3)<38 then mi(312)=10**c3; else mi(312)=0;
        c3=logkt(561)+c1+5*c2-log10(gamma(313));
        if abs(c3)<38 then mi(313)=10**c3; else mi(313)=0;
      end; else do i=308 to 313; mi(i)=0; end;
      if alfa(300)>1e-38 then do; c1=log10(alfa(300)); c2=log10(alfa(61));
        c3=logkt(585)+c1-log10(gamma(328));
        if abs(c3)<38 then mi(328)=10**c3; else mi(328)=0;
        c3=logkt(586)+c1+c2-log10(gamma(329));
        if abs(c3)<38 then mi(329)=10**c3; else mi(329)=0;
        c3=logkt(587)+c1+2*c2-log10(gamma(330));
        if abs(c3)<38 then mi(330)=10**c3; else mi(330)=0;
        c3=logkt(588)+c1+3*c2-log10(gamma(331));
        if abs(c3)<38 then mi(331)=10**c3; else mi(331)=0;
      end; else do i=328 to 331; mi(i)=0; end;
      c1=mi(19)+mi(54)+2*mi(55)+3*mi(56)+
              4*mi(57)+mi(100)+mi(101)+2*mi(102)+3*mi(103)+4*mi(104)+
              mi(105)+2*mi(106)+3*mi(107)+mi(116)+6*mi(124)+mi(125)+
              2*mi(126)+mi(137)+mi(150)+mi(164)+2*mi(165)+mi(188);
             c1=c1+2*mi(189)+3*mi(190)+4*mi(191)+mi(207)+mi(219)+2*mi(296)
              +mi(297)+mi(308)+2*mi(309)+3*mi(310)+4*mi(311)+5*mi(312)+
              6*mi(313)+mi(328)+2*mi(329)+3*mi(330)+4*mi(331);
       mi(61)=ftot/(1e0+gamma(61)*c1);
      alfa(61)=c1=mi(61)*gamma(61);
      do i=19,54 to 57,100 to 107,116,124 to 126,137,150,164,165,188 to
           191,207,219,296,297,308 to 313, 328 to 331;  mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);
           end;  end;

/* mass balance on phosphate */
    if ptot > 0e0 then do;
      mi(12)=kt(139)*kt(15)*alfa(8)/(tenph*gamma(12));
      mi(39)=kt(123)*alfa(1)/gamma(39);
      mi(40)=kt(124)*kt(16)*alfa(1)/(tenph**2*gamma(40));
      mi(46)=kt(15)/(tenph*gamma(46));
      mi(47)=kt(16)/(tenph**2*gamma(47));
      mi(49)=kt(30)*kt(15)*alfa(2)/(tenph*gamma(49));
      mi(60)=kt(32)*kt(15)*alfa(3)/(tenph*gamma(60));
      mi(64)=kt(120)*kt(16)*alfa(7)/(tenph**2*gamma(64));
      mi(72)=kt(33)*kt(15)*alfa(1)/(tenph*gamma(72));
      mi(73)=kt(34)*kt(15)*alfa(0)/(tenph*gamma(73));
      mi(74)=kt(121)*alfa(0)/gamma(74);
      mi(75)=kt(122)*kt(16)*alfa(0)/(tenph**2*gamma(75));
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      mi(98)=kt(156)*kt(16)*alfa(8)/(tenph**2*gamma(98));
      mi(99)=kt(138)*kt(15)*alfa(7)/(tenph*gamma(99));
       if alfa(299)>1e-38 then do; c1=log10(alfa(299)); c2=log10(alfa(44));
         c3=logkt(567)+c1-ph-log10(gamma(317));
         if abs(c3)<38 then mi(317)=10**c3; else mi(317)=0;
         c3=logkt(568)+c1+c2-2*ph-log10(gamma(318));
         if abs(c3)<38 then mi(318)=10**c3; else mi(318)=0;
         c3=logkt(569)+c1+2*c2-3*ph-log10(gamma(319));
         if abs(c3)<38 then mi(319)=10**c3; else mi(319)=0;
         c3=logkt(570)+c1+3*c2-4*ph-log10(gamma(320));
         if abs(c3)<38 then mi(320)=10**c3; else mi(320)=0;
       end; else do i=317 to 320; mi(i)=0; end;
   if alfa(300)>1e-38 then do; c1=log10(alfa(300)); c2=log10(alfa(44));
         c3=logkt(592)+c1-ph-log10(gamma(335));
         if abs(c3)<38 then mi(335)=10**c3; else mi(335)=0;
         c3=logkt(593)+c1+c2-2*ph-log10(gamma(336));
         if abs(c3)<38 then mi(336)=10**c3; else mi(336)=0;
         c3=logkt(594)+c1-2*ph-log10(gamma(337));
         if abs(c3)<38 then mi(337)=10**c3; else mi(337)=0;
         c3=logkt(595)+c1+c2-4*ph-log10(gamma(338));
         if abs(c3)<38 then mi(338)=10**c3; else mi(338)=0;
         c3=logkt(596)+c1+2*c2-6*ph-log10(gamma(339));
         if abs(c3)<38 then mi(339)=10**c3; else mi(339)=0;
       end; else do i=335 to 339; mi(i)=0; end;
      mi(44)=ptot/(1e0 + gamma(44)*(mi(12)+mi(39)+mi(40)+mi(46)+mi(47)+
             mi(49)+mi(60)+mi(64)+mi(72)+mi(73)+mi(74)+mi(75)+mi(98)+
             mi(99)+mi(317)+2*mi(318)+3*mi(319)+4*mi(320)+mi(335)+2*mi(336)+
             mi(337)+2*mi(338)+3*mi(339)));
      alfa(44),c1=mi(44)*gamma(44);
      do i=12,39,40,46,47,49,60,64,72 to 75,98,99,317 to 320,335 to 339;  mi(i)=c1*mi(i);
        alfa(i)=mi(i)*gamma(i);  end;
      end;

    /* mass balance on chloride */
      if cltot > 0e0 then do;
       mi(15)=kt(5)*alfa(8)/gamma(15);
       mi(27)=kt(6)*alfa(8)*alfa(4)/gamma(27);
       mi(32)=kt(7)*alfa(8)*alfa(4)**2/gamma(32);
       mi(111)=kt(170)*alfa(109)/gamma(111);
       mi(112)=kt(171)*alfa(109)*alfa(4)/gamma(112);
       mi(113)=kt(172)*alfa(109)*alfa(4)**2/gamma(113);
       mi(128)=(kt(206)/kt(208))*alfa(127)*alfa(4)/gamma(128);
       mi(129)=(kt(207)/kt(208))*alfa(127)*alfa(4)**2/gamma(129);
       mi(133)=kt(211)*alfa(130)/gamma(133);
       mi(134)=kt(212)*alfa(130)*alfa(4)/gamma(134);
       mi(135)=kt(213)*alfa(130)*alfa(4)**2/gamma(135);
       mi(136)=kt(214)*alfa(130)*alfa(4)**3/gamma(136);
       mi(146)=kt(251)*alfa(145)/gamma(146);
       mi(147)=kt(252)*alfa(145)*alfa(4)/gamma(147);
       mi(148)=kt(253)*alfa(145)*alfa(4)**2/gamma(148);
       mi(149)=kt(254)*alfa(145)*alfa(4)**3/gamma(149);
       mi(155)=kt(260)*alfa(145)*ah2o*tenph/gamma(155);
       mi(161)=kt(294)*alfa(160)/gamma(161);
       mi(162)=kt(295)*alfa(160)*alfa(4)/gamma(162);
       mi(163)=kt(296)*alfa(160)*alfa(4)**2/gamma(163);
       mi(172)=kt(305)*alfa(160)*ah2o*tenph/gamma(172);
       mi(183)=kt(341)*alfa(182)/gamma(183);
       mi(184)=kt(342)*alfa(182)*alfa(4)/gamma(184);
       mi(185)=kt(343)*alfa(182)*alfa(4)**2/gamma(185);
       mi(186)=kt(344)*alfa(182)*alfa(4)**3/gamma(186);
```

```
      mi(205)=kt(404)*alfa(204)/gamma(206);
      mi(215)=kt(423)*alfa(212)/gamma(215);
      mi(216)=kt(424)*alfa(212)*alfa(4)/gamma(216);
      mi(217)=kt(425)*alfa(212)*alfa(4)**2/gamma(217);
      mi(218)=kt(426)*alfa(212)*alfa(4)**3/gamma(218);
      mi(279)=kt(518)*alfa(204)*alfa(4)/gamma(279);
      if alfa(299)>1e-38 then do;
        c1=logkt(564)+log10(alfa(299))-log10(gamma(314));
        if abs(c1)<38 then mi(314)=10**c1; else mi(314)=0;
      end; else mi(314)=0;
      if alfa(300)>1e-38 then do;
        c1=logkt(539)+log10(alfa(300))-log10(gamma(332));
        if abs(c1)<38 then mi(332)=10**c1; else mi(332)=0;
      end; else mi(332)=0;
      c1=0;
      do i=15,111,133,146,155,161,172,183,206,215,314,332;
        c1=c1+mi(i);  end;
      do i=27,112,128,134,147,162,184,216,279;
        c1=c1+2*mi(i);  end;
      do i=32,113,129,135,148,163,185,217;
        c1=c1+3*mi(i);  end;
      do i=136,149,186,218;
        c1=c1+4*mi(i);  end;
      mi(4)=cltot/(1e0 + gamma(4)*c1);
      alfa(4),c1=mi(4)*gamma(4);
      do i=15,27,32,111 to 113,128,129,133 to 136,146 to 149,
           155,161 to 163,172,183 to 186,206,215 to 218,279,314,332;
        mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);  end;  end;

/* mass balance on sulfide */
  if h2stot > 0e0 then do;
    mi(13)=1/(kt(91)*tenph*gamma(13));
    mi(67)=kt(92)*tenph/gamma(67);
    mi(247)=kt(476)*alfa(7)*alfa(66)/gamma(247);
    mi(248)=kt(477)*alfa(7)*alfa(66)**2/gamma(248);
    mi(144)=kt(222)*alfa(130)*alfa(66)**2/gamma(144);
    mi(156)=kt(261)*alfa(145)*alfa(66)/gamma(156);
    mi(157)=kt(262)*alfa(145)*alfa(66)**2/gamma(157);
    mi(175)=kt(308)*alfa(160)/gamma(175);
    mi(176)=kt(309)*alfa(160)*alfa(66)/gamma(176);
    mi(177)=kt(310)*alfa(160)*alfa(66)**2/gamma(177);
    mi(178)=kt(311)*alfa(160)*alfa(66)**3/gamma(178);
    mi(198)=kt(356)*alfa(182)*alfa(66)/gamma(198);
    mi(199)=kt(357)*alfa(182)*alfa(66)**2/gamma(199);
    mi(220)=kt(428)*alfa(212)/gamma(220);
    mi(221)=kt(429)*alfa(212)*alfa(66)/gamma(221);
    mi(259)=kt(485)*alfa(127)*alfa(66)*tenph**2/gamma(259)/kt(205);
    mi(260)=kt(486)*alfa(127)*alfa(66)*tenph**2/gamma(260)/kt(208);
    mi(263)=kt(502)*tenph/gamma(263);
    mi(264)=kt(503)*tenph/gamma(264);
    mi(265)=kt(504)*tenph/gamma(265);
    mi(266)=kt(505)*tenph/gamma(266);
    mi(267)=kt(506)*tenph/gamma(267);
    mi(268)=kt(507)*alfa(212)*alfa(66)*tenph**2/gamma(268);
    mi(269)=kt(508)*alfa(212)*alfa(66)*tenph**2/gamma(269);
    mi(270)=kt(509)*alfa(212)*alfa(66)*tenph/gamma(270);
    mi(66)=h2stot/(1+gamma(66)*(mi(13)+mi(67)+2*mi(247)+3*mi(248)+
           3*mi(144)+2*mi(156)+3*mi(157)+mi(175)+2*mi(176)+3*mi(177)+
           4*mi(178)+2*mi(198)+3*mi(199)+mi(220)+2*mi(221)+2*mi(259)+
           2*mi(260)+mi(263)+mi(264)+mi(265)+mi(266)+mi(267)+
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```
            2*mi(268)+2*mi(269)+2*mi(270)));
      alfa(56),c1=mi(66)*gamma(66);
      do i=13,67,247,248,144,156,157,175 to 178,198,199,220,221,259,261,
           263 to 270;
        mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);  end;
      end;

  /* mass balance on fulvate */
    if fulvtot > 0e0 then do;
      mi(286)=kt(523)/(tenph*gamma(286));
      mi(288)=kt(525)*alfa(8)/gamma(288);
      mi(290)=kt(527)*alfa(130)/gamma(290);
      mi(292)=kt(529)*alfa(160)/gamma(292);
      mi(294)=kt(531)*alfa(212)/gamma(294);
      mi(284)=fulvtot/(1 + gamma(234)*(mi(286)+mi(288)+mi(290)+mi(292)+
              mi(294)));
      alfa(284),c1=mi(284)*gamma(234);
      do i=286 to 294 by 2;  mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);
        end;  end;

  /* mass balance on humate */
    if humtot > 0e0 then do;
      mi(287)=kt(524)/(tenph*gamma(287));
      mi(289)=kt(526)*alfa(8)/gamma(289);
      mi(291)=kt(528)*alfa(130)/gamma(291);
      mi(293)=kt(530)*alfa(160)/gamma(293);
      mi(295)=kt(532)*alfa(212)/gamma(295);
      mi(285)=humtot/(1 + gamma(285)*(mi(287)+mi(289)+mi(291)+mi(293)+
              mi(295)));
      alfa(285),c1=mi(285)*gamma(235);
      do i=287 to 295 by 2;  mi(i)=c1*mi(i);  alfa(i)=mi(i)*gamma(i);
        end;  end;

  /* iterative tests */
        rbit = "0"b;
        if abs(s1 - analco3) > 1e-3  * analco3 then rbit = "1"b;
        if abs(s2 - so4tot) > 1e-3  * so4tot then rbit = "1"b;
        if abs(s3 - ftot) > 1e-3  * ftot then rbit = "1"b;
        if abs(s4 - ptot) > 1e-3  * ptot then rbit = "1"b;
        if abs(s5 - cltot) > 1e-3  * cltot then rbit = "1"b;
        if abs(s6 - h2stot) > 1e-3  * h2stot then rbit = "1"b;
        if abs(s7 - fulvtot) > 1e-3 * fulvtot then rbit = "1"b;
        if abs(s8 - humtot) > 1e-3 * humtot then rbit = "1"b;
       put file(outprint)edit(iter,s1-analco3,s2-so4tot,s3-ftot,s4-ptot,s5-cltot,
              s6-h2stot,s7-fulvtot,s8-humtot)
          (skip,f(4),8 e(16,6));

  /* iteration monitor */
        if iter = 40 then do;  rbit = "0"b;
         put file(outprint)page list((131)"*");
       put file(outprint)skip(3)list("Convergence not reached in 40 iterations.  calculation terminated.  Print of calculations follows
or checking only.");
         put file(outprint)skip(3)list((131)"*");  end;
        if iter < 2 then rbit = "1"b;
    end sums;
```

```
   solutes: proc(anal,z,page1,alfa,analmi,cunits,gamma,gfw,kt,mi,logkt,
                 index2,sigma,err);
   dcl eherr entry options(variable);
   dcl (endpage,conv) condition,
       j fixed bin;
   dcl outprint external file constant;
   dcl long char(6),card(0:20)char(80)ext,flag char(8)var ext,
         head char(130)init("  I  Species          Anal ppm       Calc ppm  Anal molal   Calc molal     Activity      Act coeff  -log Act"
),
        (d,e,h,ehopt)fixed bin(31)ext,(i,n,anal(*),index2(*),z(*))
        fixed bin(31),page1(*)char(8),date builtin,
        (an2o,c,cond,diff,dischg,doc,dox,ehas,ehdo,ehfe2,ehfe,ehn,ehno2,
         enpt,ehs,ehu,epman,epmcat,f,fetotal,hco3tot,indate,itds,
         lh2o,mu,muhalf,noncarb,pco2,pe,peas,pedo,pedo2,pefe,pen,peno2,
         pept,pes,peu,ph,r,salin,sigmaeh,sl,t,tds,temp,tenph,time)
         float dec(20) ext,
         (carbonic,concalc,c1,c2,sigmape,alfa(*),analmi(*),cunits(*),
         err(*),gamma(*),gfw(*),kt(*),mi(*),logkt(*),sigma(*))float dec(20) ;
    on conv begin;
      put file(outprint) skip(5)edit("conversion error occurred while attempting to read",
" card 2.  check formatting of the card.  read commamd aborted.")(2 a);
      go to skip_read;  end;
     cond,itds,indate,dischg,doc,salin,time=0e0;
     get string(card(2))edit(cond,itds,indate,dischg,doc,salin,time)
         (f(5,0),f(6,0),f(7,0),4 f(8,0));  skip_read:
       c2=0; do n=0 to d;  c2=c2+analmi(n)*gfw(n)*1e3; end;
       c2=c2*1e6/(c2+1e6);
   call conductance_test;
/* auxiliary pe calculations */
    sigmape=sigmaeh*f/(c*r*t);
    if alfa(5)*alfa(13) > 0e0 then do;
    pes=0.125*log10(kt(90))+0.125*log10(alfa(5))-1.25*ph
           -0.125*log10(alfa(13))-0.5*lh2o;
    ehs=pes*c*r*t/f;  end;
    if alfa(38)*alfa(84)>0e0 then do;
    pen=(-logkt(127)+log10(alfa(84))-10e0*ph-log10(alfa(38))-3e0*lh2o)
           /8e0;
    ehn=pen*c*r*t/f;  end;
    if alfa(202)*alfa(84)>0e0 then do;
    peno2=(logkt(400)+log10(alfa(84))-log10(alfa(202))-lh2o-2*ph)/2;
    ehno2=peno2*c*r*t/f;  end;
    if alfa(250)*alfa(255) > 0e0 then do;
    peas=(log10(alfa(255)/alfa(250))-logkt(487)-lh2o)/2e0-ph;
    ehas=peas*c*r*t/f;  end;
    call eherr(cunits,sigma,err);

/* print of input */
    long=date;
   put file(outprint) page edit(card(1),"Date = ") (a(80),x(2),a)
                ((substr(long,n,2),"/" do n=3,5),substr(long,1,2))(a);
    put file(outprint) skip edit(card(2))(a(80));
    put file(outprint) skip;
    if dox > 0e0 then put file(outprint) edit("DOX = ",dox)(x(5),a,f(12,4));
    if doc > 0e0 then put file(outprint) edit("DOC = ",doc)(x(10),a,f(8,1));
    if itds > 0e0 then put file(outprint) skip edit("Input TDS = ",itds)(a,f(8,1));
    put file(outprint) skip edit("Anal cond = ",cond)(a,f(8,1))
                ("Calc cond = ",concalc)(x(6),a,f(10,1));
    if flag = "meq" then put file(outprint) edit ("Data in meq/l") (x(5),a);
    else if flag="mol" then put file(outprint) edit("Data in moles") (x(5),a);
```

```
     if cunits(7)*cunits(8)>0 then if ehpt>9e0 | ehopt^=0 then
     put file(outprint) skip list("***** Eh and pe calculated from iron 2/3 activity ratio have been substituted for input Eh data *****
*");
    put file(outprint) edit      ("Anal epmcat =",1e3*epmcat,"Anal epman =",1e3*epman)
                  (skip(1),a,f(10,4),x(3),a,f(10,4))
                  ("Percent difference in input cation/anion balance =",
                   diff*1e2)(x(3),a,f(8,4));

 /* recalculation of cation-anion balance */
     epmcat, epman = 0e0;
               do i=0 to 15,17 to 33, 35 to 68,72 to 82,84,
        85,87 to d;  if mi(i)>1e-38 then do;
       if z(i)>0 then epmcat = epmcat + z(i) * mi(i);
       else epman = epman-z(i)*mi(i); end;  end;
    put file(outprint) edit      ("Calc epmcat =",1e3*epmcat,"Calc epman =",1e3*epman)
                  (skip(1),a,f(10,4),x(3),a,f(10,4));

 /* calc. of po2 & pch4 */
       if abs(pe) < 19e0 then do;
     c1 = log10(kt(93)) + ph + pe + 0.5*lh2o;
if abs(c1) < 9e0 then alfa(69)=1e1 **(4e0*c1);
else alfa(69)= 0e0;
       if alfa(6) > 0e0  then do;
             c1=(log10(kt(94)) -8e0*pe -9e0*ph -3e0*lh2o
                  +log10(alfa(6)));
        if abs(c1) <38.0 then alfa(70)=1e1**c1;
         else alfa(70)=0.; end; end;

     pco2=0e0; if alfa(85)>0e0 then
       pco2=1e1**(log10(alfa(85))-2385.73e0/t-1.5264e-2*t+14.0184e0+
                 mu*(0.119-8.33e-4*temp+6.66e-6*temp**2));
       noncarb=mi(24)+2*mi(25)+mi(26)+mi(36)+2*mi(44)+mi(46)
       +mi(53)+mi(66)+2*mi(67)+mi(81);
       carbonic=mi(6)+2*mi(17);
       s1 = mi(6) + mi(17) + mi(20) + mi(21) + mi(29)
            + mi(30) + mi(41) + mi(42) + mi(85) + mi(117) +
            mi(131) + 2*mi(132) + 3*mi(166) + 2*mi(187) + mi(241);
       tds=0; do i= 0 to d;
       tds=tds+analmi(i)*qfw(i)*1e3*(1-1e-6*c2);  end;
     if abs(pe) > 19e0 then pe = 99.9999;

 /* print of solute data */
     put file(outprint) skip(2)edit("Sato","calc")(x(34),a(4),col(82),a(4))
        ("Input sigma   Fe3/Fe2 sigma   H2O2/O2 sigma   NO3/NO2 sigma",
"   NO3/NH4 sigma   H2O2/O2 sigma   SO4/S= sigma   As5/As3 sigma")
     (skip,x(3),2 a)
         ((30) "- ","Eh",(30) " -")(skip,x(3),3 a);
     put file(outprint) skip edit(ehpt,sigmaeh,ehfe,ehjo,ehno2,ehn,ehjo2,ehs,ehas)
      (f(8,3),f(6,3),f(10,3),2 f(16,3),f(15,3),f(16,3),f(15,3),f(16,3));
     put file(outprint) skip(0)edit((err(i) do i=9 to 15))(col(15),3 f(16,3),2(f(15,3),f(16,3)));
     put file(outprint) skip(2)edit((30) "- ","pE",(30) " -")(x(3),3 a);
     put file(outprint) skip edit(pept,sigmape,pefe,pejo,peno2,pen,pejo2,pes,peas)
      (f(8,3),f(6,3),f(10,3),2 f(16,3),f(15,3),f(16,3),f(15,3),f(16,3));
     put file(outprint) skip(0)edit((err(i) do i=0 to 6))(col(15),3 f(16,3),2(f(15,3),
         f(16,3)));
     put file(outprint)skip(2)edit("L4/U6     sigma")(x(3),a);
     put file(outprint)edit((30) "- ","Eh",(30) " -")(skip,x(3),3 a);
     put file(outprint)edit(eh)(skip,f(8,3));
     put file(outprint)edit((30) "- ","pE",(30) " -")(skip(2),x(3),3 a);
     put file(outprint)edit(pe)(skip,f(8,3));
```

```
   put file(outprint) edit("T","pH","Tds ppm","Ionic str","pO2 atm",
"pCO2 atm","pCH4 atm","CO2 tot","uncom CO2","ppm uncom CO2","ncrb alk","aH2O")
   (skip(2),x(4),a,x(6),a,x(4),a,x(2),a,5(x(3),a),x(2),a,x(3),a,x(5),a));
   put file(outprint) edit(temp,ph,tds,mu,alfa(69),pco2,alfa(70),s1,carbonic,4.4e4*carbonic,
noncarb,ah2o)(skip,f(7,2),f(8,3),f(9,1),f(10,5),3 e(11,2),f(10,5)
   ,e(11,2), e(13,2),e(14,2),f(11,4));
     put file(outprint) skip(2)list(head);
       c2=0; do n=0 to d;  c2=c2+mi(r)*gfw(n)*1e3; end;
       c2=c2*1e6/(c2+1e6);
    do n=1 to h;  i=index2(n);
      if mi(i) > 0e0 | analmi(i) > 0e0 | anal(i)=1 then call print;
      end;

print:  proc ;
       dcl line char(130)init(" "),
           line1 char(16)def(line)pos(1),
           line2 char(16)def(line)pos(17),
           line3 char(13)def(line)pos(33),
           line4 char(11)def(line)pos(46),
           line5 char(13)def(line)pos(57),
           line6 char(25)def(line)pos(70),
           line7 char(11)def(line)pos(95),
           (fulflag,humflag)bit(1)ext,stars char(2)init("  ");
       on endpage(outprint)begin;
        put file(outprint) page list(card(1));
         put file(outprint) skip(2)list(head);  put file(outprint)skip;  end;
       if alfa(i)>1e-38 then c1=-log10(alfa(i)); else c1=0e0;
       if fulflag then do j=284 to 294 by 2;  if i=j then stars="**";
          end;
       if humflag then do j=285 to 295 by 2;  if i=j then stars="**";
          end;
       put string(line1)edit(i,stars,page1(i),z(i))
             (f(3),a(2),a(8),f(3));
       s1=cunits(i);
       if s1>0e0 & s1<1e-2 then put string(line2)edit(s1)(f(16,6));
       else if anal(i)=1 | s1>0e0 then put string(line2)edit(s1)
                                          (f(13,3));
       s1=mi(i)*gfw(i)*1e3*(1-1e-6*c2);
       if s1>0e0 then if s1<1e-2 ther
       put string(line3)edit(s1)(f(13,6));
       else if s1>0e0 then put string(line3)edit(s1)(f(10,3));
       if analmi(i)>0e0 then
       put string(line4)edit(analmi(i))(e(11,3));
       if mi(i)>0e0 then put string(line5)edit(mi(i)) (e(13,3));
       if alfa(i)>0e0 then put string(line6)edit(alfa(i),gamma(i))
                                  (e(13,3),f(12,4));
       if c1>0e0 then put string(line7)edit(c1)(f(11,3));
       put file(outprint) list(line);
       end print;

  conductance_test:  proc  ;
   dcl(norm,lambda)float dec(20) ,lzero(10)float dec(20) init(59.5,53,50.1,73.5,
      76.35,80,44.5,71.46,349.8,198.3),x(10)float dec(20) init(115.1,109.2,
      41.3,47.1,47.8,133.9,40.5,46.7,110.42,75.73),conv(10)float dec(20)
      init(4.99e-5,8.226e-5,4.35e-5,2.557e-5,2.821e-5,2.082e-5,
      1.639e-5,1.613e-5,99.209e-5,5.38e-5);
   do i=26,63;  cunits(i)=mi(i)*1e3*gfw(i)*(1-1e-6*c2);  end;
   c1=0e0;  n=0;  do i=0 to 6,84,63,26;  n=n+1;
     lambda=lzero(n)-x(n)*muhalf/(1e0+muhalf);
     norm=cunits(i)*conv(n);  c1=c1+lambda*norm;  end;
```

```
   concalc=1e3*c1;
   cunits(26),cunits(63)=0e0;
   end conductance_test;

   if ehpt>9e0 then pept=999;
   if cunits(7)*cunits(8)<=0 then pefe=999;
    if pe >9e1 then  pe = 2e1;
/* conversion of alfa and cunits to log form for ap calcs & punching
   deleted for examination of Runnels' problem on 9-30-80 by JWB
    Then restored temporarily on 10-28-80 by JWB */
    do i=0 to 10,13,16,17,23,26,34,35,38,39,44,46,48,50,51,53,61,66,67,
         80,84,86,87,89,94,96,97,101,106,108 to 110,114,127,130,138,
         145,151,160,167,182,192,202,204,208,212,224,249,250,255,259,
         261,262,298,299,300,25;
      if alfa(i)>1e-38 then alfa(i)=log10(alfa(i));
      else alfa(i)=-2e4;
      if cunits(i)>0e0 then cunits(i)=log10(cunits(i));
      else cunits(i)=-2e4; end;
   end solutes;
```

```
ratio: proc(page1,alfa,cunits,z,analmi);
 dcl outprint external file constant;
 dcl (i,z(*))fixed bin(31),page1(*)char(8),(cltot,co2tit,ph)
     float dec(20) ext,(alfa(*),cunits(*),analmi(*))float dec(20) ;
/* calculation of molar concentration ratios and log activity ratios*/
 put file(outprint) page    edit("mole ratios from analytical molality")(a)
         ("log activity ratios")(col(83),a);
 do i=0,1,2,3,50,5;
 put file(outprint) skip edit("Cl/",page1(i),"=")(a(3),a(4),a(1));
 if analmi(i)>0e0 then put file(outprint) edit(cltot/analmi(i))(x(2),e(11,4));
 if i ^= 5 then do;
 put file(outprint) edit("log",page1(i),"/H",z(i),"=")
              (col(83),a,x(1),a(2),a(2),f(1),a);
 if alfa(i)>-1e3 then put file(outprint) edit(z(i)*ph+alfa(i))(f(11,4));
 end; end;
 if(alfa(0)+alfa(1)) >-1e4 then
 put file(outprint) edit("log Ca/Mg=",alfa(0)-alfa(1))(col(83),a,f(11,4));
 put file(outprint) skip edit("Cl/HCO3=")(a);
 if co2tit>0e0 then put file(outprint) edit(cltot/co2tit)(x(2),e(11,4));
 put file(outprint) edit("log Na/K =")(col(33),a);
 if(alfa(2)+alfa(3)) >-1e4 then put file(outprint) edit(alfa(2)-alfa(3))(f(11,4));
 put file(outprint) skip edit("Ca/Mg  =")(a);
 if analmi(1)>0e0 then put file(outprint) edit(analmi(0)/analmi(1))(x(2),e(11,4));
put file(outprint) edit("log Ca/K2=")(col(83),a);
if(alfa(0)+alfa(3)) > -1e4 then put file(outprint) edit(alfa(0)-2*alfa(3))(f(11,4));
 put file(outprint) skip edit("Na/K   =")(a);
 if analmi(3)>0e0 then put file(outprint) edit(analmi(2)/analmi(3))(x(2),e(11,4));
put file(outprint) edit("log diss Fe/H2=")(col(78),a);
if analmi(7) >-2e4 then put file(outprint) edit(2*ph+analmi(7))(f(11,4));
   end ratio;
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apcalc: proc(ap,alfa,gamma,mi);
  dcl (c1,ap(*),alfa(*),gamma(*),mi(*))float dec(20) ,
      (lh2o,pe,peas,ph)float dec(20) ext,i fixed bin(31);
/* calc. of ion activity products (in terms of logs) */
    ap=2e4;
    ap(9)=alfa(7)+alfa(17);
    ap(10)=alfa(1)+alfa(17);
    ap(11)=alfa(0)+ap(10)+alfa(17);
    ap(12),ap(21)=alfa(0)+alfa(17);
    ap(17)=alfa(0)+alfa(5);
    ap(18)=ap(17)+2e0*lh2o;
    ap(19)=alfa(1)+2e0*alfa(26);
    ap(20)=3e0*alfa(1)+2e0*alfa(23)+6e0*alfa(26)-5e0*lh2o;
    ap(27)=2e0*alfa(1)+alfa(23)+4e0*(alfa(26)-lh2o);
    ap(28)=alfa(0)+alfa(1)+2e0*alfa(23)+4e0*alfa(26)-5e0*lh2o;
    ap(29)=alfa(1)+alfa(23)+2e0*alfa(26)-3e0*lh2o;
    ap(31)=2e0*alfa(0)+5e0*alfa(1)+8e0*alfa(23)+14e0*alfa(26)
          -22e0*lh2o;
    ap(36),ap(153)=2e0*alfa(1)+3e0*alfa(23)+4e0*alfa(26)-4.5e0*lh2o;
    ap(37)=3e0*alfa(1)+4e0*alfa(23)+6e0*alfa(26)-1e1*lh2o;
    ap(38)=5e0*alfa(1)+4e0*alfa(17)+2e0*alfa(26)+4e0*lh2o;
    ap(39)=alfa(3)+alfa(53)+3e0*alfa(23)-8e0*lh2o;
    ap(40)=ap(39)-alfa(3)+alfa(2);
    ap(41)=alfa(0)+2e0*(alfa(53)+alfa(23))-8e0*lh2o;
    ap(42)=alfa(2)+alfa(53)+2e0*alfa(23)-5e0*lh2o;
    ap(43)=alfa(3)+3e0*(alfa(53)+alfa(23))-2e0*ph-12e0*lh2o;
    ap(44)=alfa(3)+alfa(53)+3e0*(alfa(1)+alfa(23))+6e0*ph
          -4e0*lh2o;
    ap(45)=.6e0*alfa(3)+.25e0*alfa(1)+2.3e0*alfa(53)+3.5e0*alfa(23)-
          1.2e0*ph-11.2e0*lh2o;
    ap(46),ap(47)=2e0*(alfa(53)+alfa(23)-ph       )-7e0*lh2o;
    if (mi(1)+mi(2)+mi(3))=0e0 then c1=2e4; else
    c1=log10(sqrt(mi(1)*gamma(1))+mi(2)*gamma(2)+mi(3)*gamma(3));
    ap(48) = .33e0*c1+2.33e0*alfa(53)+3.67e0*alfa(23)-2e0*ph-12e0*lh2o;
    ap(49)=5e0*alfa(1)+2e0*alfa(53)+3e0*alfa(23)+8e0*alfa(26)-1e1*lh2o;
    ap(50)=alfa(3)+3e0*alfa(50)+6e0*alfa(26)+2e0*alfa(5);
    ap(51)=alfa(50)+3e0*(lh2o+ph);
    ap(52),ap(154)=alfa(50)+3e0*alfa(26)-lh2o;
    ap(53)=2e0*alfa(53)+4e0*alfa(23)-2e0*ph-12.0*lh2o;
    ap(54)=.5e0*(alfa(2)+alfa(3))+alfa(53)+3e0*alfa(23)-7e0*lh2o;
    ap(55) = alfa(2)+alfa(53)+3.5e0*alfa(23)-6e0*lh2o;
    if (mi(2)+mi(3))^=0e0 then  do;
    ap(56)=.5e0*log10(mi(2)*gamma(2)+mi(3)*gamma(3))+alfa(53)
      +5e0*alfa(23)-8.5e0*lh2o;
    ap(57)=.5e0*log10(mi(2)*gamma(2)+mi(3)*gamma(3))+alfa(53)
      +4.5e0*alfa(23)-8e0*lh2o;  end;
    ap(58)=alfa(2)+alfa(6);
    ap(59)=3e0*alfa(2)+alfa(6)+alfa(17)+2e0*lh2o;
    ap(61)=2e0*alfa(2)+alfa(17)+lh2o;
    ap(60)=ap(61)+9e0*lh2o;
    ap(62)=alfa(0)+2e0*alfa(61);
    ap(63) = .167e0*alfa(0)+2.33e0*alfa(53)+3.67e0*alfa(23)
              -2e0*ph-12e0*lh2o;
    ap(64)=alfa(2)+alfa(4);
    ap(65)=2e0*alfa(2)+alfa(5);
    ap(66)=ap(65)+1e1*lh2o;
    ap(67),ap(119)=alfa(7)+alfa(66)+ph;
    ap(95)=5e0*alfa(0)+3e0*alfa(46)+4e0*ph+lh2o;
    ap(96)=5e0*alfa(0)+3e0*alfa(46)+5e0*ph+alfa(61);
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ap(98)=alfa(3)+7e0*alfa(23)+ph       -9e0*lh2o;
ap(97),ap(99),ap(100),ap(101),ap(395)=alfa(23)-2e0*lh2o;
ap(106)=3e0*alfa(7)+2e0*alfa(44)+9e0*lh2o;
ap(107)=2e0*alfa(8)+alfa(7)+4e0*lh2o+3e0*ph;
ap(108),ap(109)=2e0*alfa(8)+3e0*lh2o+6e0*ph;
ap(110)=alfa(8)+3e0*ph+2e0*lh2o;
ap(111)=3e0*alfa(7)+2e0*alfa(23)+6e0*ph+lh2o;
ap(112)=alfa(8)+3e0*(lh2o+ph);
ap(113)=ap(44)+3e0*(alfa(7)-alfa(1));
ap(114)=alfa(7)+2e0*(alfa(66)+pe+ph);
c1=log10(mi(2)*gamma(2)+mi(3)*gamma(3)+mi(63)*gamma(63));
ap(115)=0.83e0*c1+0.29e0*alfa(1)+.23e0*alfa(3)+1.58e0*alfa(53)
        +3.93e0*alfa(23)-1e1*lh2o;
ap(116)=0.83e0*c1+.45e0*alfa(1)+.34e0*alfa(8)+1.47e0*alfa(53)+
        3.82e0*alfa(23)-9.2*lh2o+.76e0*ph;
ap(117)=3e0*alfa(1)+alfa(0)+4e0*alfa(17);
ap(118)=2e0*alfa(8)+alfa(7)+4e0*(alfa(66)+ph);
ap(128)=alfa(0)+2e0*alfa(53)+4e0*alfa(23)-8e0*lh2o;
ap(134)=2e0*alfa(110)+3e0*alfa(5);
ap(140)=alfa(50)+3e0*alfa(26);
ap(141)=2e0*(alfa(0)+alfa(53)+ph       )+3e0*alfa(23)-6e0*lh2o;
ap(142)=alfa(87)+alfa(17);
ap(143)=alfa(87)+alfa(5);
ap(144)=alfa(89)+alfa(5);
ap(145)=alfa(89)+alfa(17);
ap(146)=alfa(8)+alfa(44)+2e0*lh2o;
ap(147)=2e0*alfa(0)+4e0*alfa(53)+8e0*alfa(23)-17e0*lh2o;
ap(149)=alfa(1)+alfa(17)+3e0*lh2o;
ap(150)=2e0*alfa(0)+alfa(17)+2e0*ph+5e0*lh2o;
ap(155)=ap(128)-2e0*lh2o;
c1=1.24e0-0.135e0*ph;
ap(157),ap(158)=(1e0-c1)*alfa(50)+c1*alfa(23)+(3e0-3e0*c1)*ph;
ap(181)=alfa(8)+0.3*alfa(4)+2.7*(lh2o+ph);
ap(182)=alfa(109)+alfa(5);
ap(183),ap(184),ap(185)=alfa(110)+2*lh2o+4*ph+pe;
ap(186)=2*alfa(110)+3*lh2o+6*ph;
ap(187)=3*alfa(109)+4*lh2o+8*ph+2*pe;
ap(188)=alfa(109)+2*(lh2o+ph);
ap(189)=alfa(110)+2*lh2o+3*ph;
ap(190)=alfa(109)+alfa(17);
ap(191)=alfa(109)+2*alfa(4)+4*lh2o;
ap(192)=alfa(109)+alfa(66)+ph;
ap(193)=3*alfa(109)+2*alfa(44);
ap(194)=alfa(109)+alfa(46);
ap(195)=16*alfa(110)+.8*alfa(3)+17*lh2o+34*ph-7.4*alfa(109);
ap(196)=14*alfa(110)+.57*alfa(7)+.82*alfa(89)+16*lh2o+32*ph
        -6.41*alfa(109);
ap(197)=14*alfa(110)+.78*alfa(89)+.19*alfa(0)+.03*alfa(3)
        +18.485*lh2o+31.97*ph-6*alfa(109);
ap(198)=10*alfa(110)+.393*alfa(0)+.473*alfa(1)+14*lh2o+24*ph
        -3.866*alfa(109);
ap(199)=20*alfa(110)+2*alfa(30)+3*alfa(50)+49*lh2o+70*ph
        -8*alfa(109);
ap(200)=8*alfa(110)+.44*alfa(0)+12*lh2o+16*ph-3.44*alfa(109);
ap(204)=3*alfa(8)+2*alfa(5)+alfa(2)+6*(lh2o+ph);
ap(205)=3*alfa(8)+2*alfa(5)+alfa(3)+6*(lh2o+ph);
ap(223)=alfa(127)-pe;
ap(224)=alfa(127)+alfa(4);
ap(225)=alfa(127)+alfa(61);
ap(226)=2*alfa(127)+lh2o+2*ph;
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ap(227)=2*alfa(127)+alfa(66)+ph;
ap(228)=2*alfa(127)+alfa(5);
ap(229)=alfa(127)+alfa(8)+2*lh2c+4*ph;
ap(230)=alfa(130)+2*alfa(4);
ap(231)=alfa(130)+alfa(17);
ap(232)=alfa(130)+2*alfa(61);
ap(233)=alfa(130)+2*alfa(61)+2*lh2o;
ap(234)=alfa(130)+2*lh2o+2*ph;
ap(235)=2*alfa(130)+2*lh2o+alfa(6)+3*oh;
ap(236)=3*alfa(130)+2*lh2o+2*alfa(6)+4*ph;
ap(237)=2*alfa(130)+3*lh2o+alfa(4)+3*oh;
ap(238)=2*alfa(130)+3*lh2o+alfa(34)+3*ph;
ap(239)=3*alfa(130)+4*lh2o+alfa(5)+4*oh;
ap(240)=4*alfa(130)+6*lh2o+alfa(5)+6*oh;
ap(241)=4*alfa(130)+7*lh2o+alfa(5)+6*oh;
ap(242)=alfa(130)+lh2o+2*oh;
ap(243)=2*alfa(130)+lh2o+alfa(5);
ap(244)=3*alfa(130)+2*alfa(44);
ap(245)=3*alfa(130)+2*alfa(44)+3*lh2o;
ap(246)=alfa(130)+alfa(66)+on;
ap(247)=alfa(130)+alfa(5);
ap(248)=alfa(130)+alfa(5)+5*lh2c;
ap(249)=alfa(130)+2*alfa(8)+4*lh2o+8*oh;
ap(250)=alfa(130)+alfa(7)+2*(alfa(66)+ph);
ap(265)=alfa(145)-2*pe;
ap(266)=alfa(145)+2*alfa(35)+2*ph-2*lh2o;
ap(267)=alfa(145)+2*alfa(4);
ap(268)=alfa(145)+alfa(17);
ap(269)=alfa(145)+alfa(17)+lh2o;
ap(270)=alfa(145)+2*alfa(61);
ap(271),ap(272),ap(273),ap(274),ap(275)=alfa(145)+2*(lh2o+ph);
ap(276)=2*alfa(145)+3*(lh2o+oh)+alfa(4);
ap(277)=5*alfa(145)+8*(lh2o+ph)+2*alfa(4);
ap(278)=2*alfa(145)+2*(lh2o+oh)+alfa(5);
ap(279)=4*alfa(145)+6*(lh2o+oh)+alfa(5);
ap(280)=alfa(145)+2*alfa(84)+6*lh2o;
ap(281),ap(282)=alfa(145)+lh2o+2*oh;
ap(283)=3*alfa(145)+2*alfa(5)+lh2o+2*oh;
ap(284)=3*alfa(145)+2*alfa(44)+4*lh2o;
ap(285),ap(286),ap(287)=alfa(145)+alfa(66)+ph;
ap(288)=alfa(145)+alfa(23)+2*oh-lh2o;
ap(289)=2*alfa(145)+alfa(23)+4*ph;
ap(290)=alfa(145)+alfa(5);
ap(291)=alfa(145)+alfa(5)+lh2o;
ap(292)=alfa(145)+alfa(5)+6*lh2c;
ap(293)=alfa(145)+alfa(5)+7*lh2c;
ap(312),ap(313)=alfa(160)-2*pe;
ap(314)=alfa(160)+2*alfa(35)+2*ph-2*lh2o;
ap(315)=alfa(160)+alfa(17);
ap(316)=alfa(160)+2*alfa(4);
ap(317)=ap(316)+lh2c;
ap(318)=ap(316)+2.5*lh2o;
ap(319)=alfa(160)+2*alfa(61);
ap(320),ap(321)=alfa(160)+2*(lh2o+ph);
ap(322)=alfa(160)+lh2o+ph+alfa(4);
ap(323)=3*alfa(160)+4*(lh2o+oh)+alfa(5);
ap(324)=3*alfa(160)+2*(lh2o+oh)+2*alfa(5);
ap(325)=4*alfa(160)+6*(lh2o+oh)+alfa(5);
ap(326)=alfa(160)+lh2o+2*oh;
ap(327)=3*alfa(160)+2*alfa(44);
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ap(328)=alfa(160)+alfa(23)+2*ph-lh2o;
ap(329)=alfa(160)+alfa(5);
ap(330)=ap(329)+lh2o;
ap(331)=ap(329)+lh2o*8/3;
ap(332)=alfa(160)+alfa(66)+ph;
ap(337)=alfa(8)*3+alfa(5)*2+ph*5+lh2o*7;
ap(338)=alfa(3)+alfa(50)+alfa(5)*2+lh2o*12;
ap(339)=alfa(7)+alfa(5)+lh2o*7;
ap(340)=alfa(1)+alfa(5)+lh2o*7;
ap(359)=alfa(145)+2*alfa(8)+4*lh2o+8*ph;
ap(360)=alfa(182)-2*pe;
ap(361)=alfa(182)+2*alfa(35)+2*ph-2*lh2o;
ap(362)=alfa(182)+2*alfa(4);
ap(363)=alfa(182)+alfa(4)+alfa(61);
ap(364)=alfa(182)*2+alfa(4)*2+alfa(17);
ap(365)=alfa(182)+alfa(17);
ap(366)=alfa(182)+alfa(61)*2;
ap(367),ap(368)=alfa(182)+lh2o+2*ph;
ap(369)=alfa(182)+lh2o*4/3+2*ph;
ap(370)=alfa(182)*2+lh2o+alfa(17)+2*ph;
ap(371)=alfa(182)*2+lh2o+alfa(5)+2*ph;
ap(372)=alfa(182)*3+lh2o*2+alfa(5)+4*ph;
ap(373)=alfa(182)*4+lh2o*3+alfa(5)+6*ph;
ap(374)=alfa(182)+alfa(46);
ap(375)=alfa(182)*3+alfa(46)*2+2*ph;
ap(376)=alfa(182)*5+alfa(44)*3+alfa(4);
ap(377)=alfa(182)*5+alfa(44)*3+lh2o+ph;
ap(378)=alfa(182)*3+2*lh2o+alfa(17)+4*ph;
ap(379)=alfa(182)+3*alfa(50)+2*alfa(44)+5*ph+6*lh2o;
ap(380)=alfa(182)+3*alfa(50)+alfa(44)+6*(lh2o+ph)+alfa(5);
ap(381)=alfa(182)*2+alfa(130)+alfa(44)+3*ph+6*lh2o;
ap(382)=alfa(182)+alfa(23)-lh2o+2*ph;
ap(383)=alfa(182)*2+alfa(23)+4*ph;
ap(384)=alfa(182)+alfa(5);
ap(385)=alfa(182)+alfa(66)+ph;
ap(386)=alfa(182)+2*lh2o+4*ph+2*pe;
ap(387)=alfa(182)*2+lh2o*3+6*ph+2*pe;
ap(388)=alfa(182)*3+lh2o*4+8*ph+2*pe;
ap(389)=alfa(182)+(lh2o+ph)*2;
ap(390)=alfa(182)+lh2o+ph+alfa(4);
ap(391)=alfa(182)*2+(lh2o+ph)*3+alfa(4);
ap(392)=alfa(182)*3+(lh2o+ph)*2+alfa(17)*2;
ap(393)=alfa(182)*2+lh2o*3+4*ph;
ap(394)=alfa(182)*4+lh2o*6+6*ph+alfa(5);
ap(396)=9.496*alfa(0)+0.35*alfa(2)+0.144*alfa(1)+4.8*alfa(44)
      +1.2*alfa(17)+2.48*alfa(61);
ap(398)=alfa(89)+2*alfa(61);
ap(399)=alfa(87)+2*alfa(61);
ap(401)=2*alfa(8)+3*alfa(5);
ap(402)=alfa(67)+2*pe;
ap(410)=alfa(204)+alfa(17);
ap(411)=alfa(204)+2*(lh2o+ph);
ap(412)=4*alfa(204)+6*(lh2o+ph)+alfa(5);
ap(413)=alfa(204)+lh2o+2*ph;
ap(414)=3*alfa(204)+2*alfa(44);
ap(415)=alfa(204)+alfa(66)+ph;
ap(416)=alfa(204)+alfa(5)+6*lh2o;
ap(417)=ap(416)+lh2o;
ap(418)=2*alfa(204)+alfa(23)+4*ph;
ap(419)=2*alfa(8)+alfa(7)+8*(lh2o+ph);
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ap(420)=alfa(130)+alfa(23)+2*ph;
ap(437)=alfa(212)-pe;
ap(438)=alfa(212)+alfa(97);
ap(439)=alfa(212)+alfa(4);
ap(440)=2*alfa(212)+alfa(17);
ap(441)=alfa(212)+alfa(61)+4*lh2o;
ap(442)=alfa(212)+alfa(96);
ap(443)=2*alfa(212)+lh2o+2*ph;
ap(444)=3*alfa(212)+alfa(44);
ap(445)=2*alfa(212)+alfa(66)+ph;
ap(446)=2*alfa(212)+alfa(5);
ap(459)=alfa(127)+alfa(97);
ap(460)=alfa(127)+alfa(96);
ap(461)=alfa(145)+2*alfa(97)+2*lh2o;
ap(462)=alfa(145)+2*alfa(96);
ap(463)=alfa(160)+2*alfa(97)+4*lh2o;
ap(464)=alfa(160)+2*alfa(96);
ap(465)=alfa(182)+2*alfa(97);
ap(466)=alfa(182)+alfa(97)+alfa(61);
ap(467)=alfa(182)+2*alfa(96);
ap(471)=alfa(50)+alfa(5)+lh2o+ph;
ap(472)=4*alfa(50)+alfa(5)+10*(lh2o+ph);
ap(488)=2*alfa(255)-3*lh2o;
ap(489)=alfa(50)+alfa(258)+2*lh2o;
ap(541)=3*alfa(89)+2*alfa(253);
ap(490)=3*alfa(0)+2*alfa(258)+4*lh2o;
ap(491)=3*alfa(130)+2*alfa(258)+6*lh2o;
ap(492)=alfa(8)+alfa(258)+2*lh2o;
ap(493)=3*alfa(109)+2*alfa(258)+3*lh2o;
ap(494)=3*alfa(204)+2*alfa(258)+3*lh2o;
ap(495)=3*alfa(182)+2*alfa(258);
ap(496)=3*alfa(145)+2*alfa(258)+2.5*lh2o;
ap(497),ap(498)=4*alfa(250)-5*lh2o;
ap(499)=alfa(250)+3*alfa(96)-3*(lh2o+ph);
ap(500)=2*alfa(250)+3*alfa(66)-3*ph-6*lh2o;
ap(501)=alfa(250)+alfa(66)-3*lh2o-2*ph-peas;
ap(533)=0.9*alfa(130)+0.2*alfa(127)+alfa(66)+ph;
ap(534)=0.6*alfa(130)+0.8*alfa(127)+alfa(66)+ph;
ap(535)=.25*alfa(130)+1.5*alfa(127)+alfa(66)+ph;
ap(536)=.066*alfa(130)+1.868*alfa(127)+alfa(66)+ph;
ap(551)=alfa(299)+2*lh2o+4*ph;
ap(552)=alfa(299)+2*lh2o+4*ph;
ap(553)=4*alfa(299)+9*lh2o+13*ph+2*pe;
ap(554)=3*alfa(299)+8*lh2o+16*ph+4*pe;
ap(555)=alfa(299)+4*ph+alfa(23);
ap(562)=alfa(299)+4*alfa(61);
ap(563)=ap(562)+2.5*lh2o;
ap(571)=alfa(299)+2*alfa(44)+4*lh2o-2*ph;
ap(572)=alfa(299)+2*alfa(44)+2*lh2o+alfa(0);
ap(577)=alfa(300)+lh2o+2*ph;
ap(578)=alfa(300)+lh2o+2*ph;
ap(579)=alfa(300)+2*lh2o+2*ph;
ap(580)=alfa(300)+3*lh2o+2*ph;
ap(584)=alfa(300)+alfa(17);
ap(597)=3*alfa(300)+2*alfa(44);
ap(598)=2*alfa(300)+2*alfa(44)-2*ph;
ap(599)=2*alfa(300)+2*alfa(44)+2*alfa(2);
ap(600)=2*alfa(300)+2*alfa(44)+2*alfa(3);
ap(601)=2*alfa(300)+2*alfa(44)+2*alfa(38);
ap(602)=2*alfa(300)+2*alfa(44)+alfa(1);
```

```
 ap(603)=2*alfa(300)+2*alfa(44)+alfa(0);
 ap(604)=2*alfa(300)+2*alfa(44)+alfa(97);
 ap(605)=2*alfa(300)+2*alfa(44)+alfa(89);
 ap(606)=2*alfa(300)+2*alfa(44)+alfa(7);
 ap(607)=2*alfa(300)+2*alfa(44)+alfa(130);
 ap(608)=2*alfa(300)+2*alfa(44)+alfa(182);
 ap(610)=2*alfa(300)+alfa(0)+2*alfa(23)+6*ah;
 if abs(pe)>19e0 then do i=114,134,183 to 187,189,195 to 200,223 to 229,
   265,312,313,360,386 to 389,402,437,459,460,533 to 536,553,554;
 ap(i)=2e4; end;
end apcalc;
```

```
  outpnch: proc(alfa,ap,cunits,logkt);
   dcl syspnch file;
  open file(syspnch) title("vfile_ syspnch") stream print output linesize(80);
   dcl card(0:20)char(80)ext,(i,n)fixed bin(31),
       (ah2o,as,co,cr,hg,mo,pe,pn,temp)float dec(20) ext,
        (c3,alfa(*),ap(*),cunits(*),logkt(*),lp(600))float dec(20) ;
dcl (pefe,peno2,pept) float dec(20) ext;
  /***  convert values of alpha and cunits to log form for eqplot    ***
   ***  punchout by inserting page1 reference numbers into cards     ***
   ***  5080 and 5090 at end of procedure solutes.                   **/
/* duplicate descriptor cards */
    put file(syspnch) edit(card(1))(col(1),a(80));
    put file(syspnch) edit(card(2))(col(1),a(80));
/* log activity values for solute constituents */
   n=0; do i=0 to 10,17,23,26,35,38,44,46,48,50,51,61,67,80,84,87,89,
        94,96,97,101,106,108,109,114,130,138,145,151,160,167,182,192,
        204,208,212,224,250,255,258;
    n=n+1;  if alfa(i)> -1e2 & alfa(i)<1e3 then lp(n)=alfa(i);
    else lp(n)=999; end;
/* log(ap) and log(ap/k) for mineral phases */
    do i=10,11,12,17,18,36,40,43,45,46,48,49,51,54,62,63,95,96,97,99,
    100,106,110,111,112,114,119,128,140,155,157,158,159,47,50,52,65,66,
    107,108,109,113,115,184,185,190,193,194,195,198,199,204,205,239,
    240,242,248,288,289,292,293,330,331,337,338,339,341,365,376,389,
    396,401,411,419,437,445,472,500,501;
    n=n+1; if ap(i)>-1e3 & ap(i)<1e3 then lp(n)=ap(i); else lp(n)=999;
    n=n+1; c3=ap(i)-logkt(i); if c3>-1e2 & c3<1e3 then lp(n)=c3;
       else lp(n)=999;  end;
/* log concentration of major constituents */
        do i=0 to 8,13,16,17,34,38,44,48,50,61,80,84,86,87,89,94,96,97,
             202;
    n=n+1;  if cunits(i)> -1e2 & cunits(i)<1e3 then lp(n)=cunits(i);
    else lp(n)=999; end;
/* log concentration(ug/l)of trace elements */
    do i=212,249,261,262,160;
 n=n+1; if cunits(i)>-1e2 & cunits(i)<1e3 then lp(n)=cunits(i)+3;
           else lp(n)=999;  end;
   n=n+1;  if co>0 then lp(n)=log10(co*1e3);  else lp(n)=999;
   n=n+1;  if cr>0 then lp(n)=log10(cr*1e3);  else lp(n)=999;
 n=n+1; if cunits(130)>-1e2 & cunits(130)<1e3 then lp(n)=cunits(130)+3;
           else lp(n)=999;
   n=n+1;  if hg>0 then lp(n)=log10(hg*1e3);  else lp(n)=999;
 n=n+1; if cunits(109)>-1e2 & cunits(109)<1e3 then lp(n)=cunits(109)+3;
           else lp(n)=999;
   n=n+1;  if mo>0 then lp(n)=log10(mo*1e3);  else lp(n)=999;
    do i=204,182,145;
 n=n+1; if cunits(i)>-1e2 & cunits(i)<1e3 then lp(n)=cunits(i)+3;
           else lp(n)=999;  end;
   if pept>19 then pept=999;  if pefe>19 then pefe=999;
   if peno2>19 then peno2=999;
/* punch out the array lp with all selected values in sequence */
    put file(syspnch) edit(temp,ph,pept,pefe,peno2,ah2o,
        (lp(i) do i=1 to n))
    (col(1),600 f(8,3));
/* blank dataset separator card */
    put file(syspnch)edit((80) " ")(col(1),80 a(1));
     end outpnch;
```

```
errcalc: proc(cunits,sigma,err);
  dcl d fixed bin(31)ext,i fixed bin(31),
      (c1,rsd0,cunits(*),sigma(*),err(*),rsd(0:d))float dec(20) ,
       (c,dox,f,ehm,ph,sigmado,sigmaph,sigmaeh,r,t)float dec(20) ext;
  rsd=2e7;
  do i=0 to 8,13,16,17,26,34,38,44,48,50,61,63,71,80,84,86,87,89,94,
       96,97,109,130,145,160,182,202,204,212,249,251,262;
      if abs(cunits(i)) < 39e0 then c1=1e1**cunits(i);
      else c1=0.0;
    if c1*sigma(i)>0 then rsd(i)=sigma(i)/c1/c;
    end;
  if rsd(17)>1e7 then rsd(17)=rsd(6);
  if rsd(8)>1e7 then rsd(8)=rsd(7)*2;
  err(9)=sqrt((rsd(7))**2+(rsd(17))**2);
  err(10)=sqrt((rsd(1))**2+(rsd(17))**2);
  err(11)=sqrt((rsd(0))**2+(rsd(1))**2+(2*rsd(17))**2);
  err(12),err(21)=sqrt((rsd(0))**2+(rsd(17))**2);
  err(17),err(18)=sqrt((rsd(0))**2+(rsd(5))**2);
  err(36),err(153)=sqrt((2*rsd(1))**2+(3*rsd(34))**2+
                   (4*sigmaph)**2);
  err(40)=sqrt(rsd(2)**2+rsd(50)**2+(3*rsd(34))**2);
  err(41)=sqrt(rsd(0)**2+(2*rsd(50))**2+(2*rsd(34))**2);
  err(45)=sqrt((.6*rsd(3))**2+(.25*rsd(1))**2+(2.3*rsd(50))**2
         +(3.5*rsd(34))**2+(1.2*sigmaph)**2);
  err(46),err(47)=sqrt((2*rsd(50))**2+(2*rsd(34))**2+(2*sigmaph)
                  **2);
  err(51),err(140),err(168)=sqrt((rsd(50))**2+(3*sigmaph)**2);
  err(54)=sqrt((.5*(rsd(2)+rsd(3)))**2+(rsd(50))**2+(3*rsd(34))
         **2);
  err(62)=sqrt((rsd(0))**2+(2*rsd(61))**2);
  err(63)=sqrt((.167*rsd(0))**2+(2.33*rsd(50))**2
         +(3.67*rsd(34))**2+(2*sigmaph)**2);
  err(67),err(119)=sqrt((rsd(7))**2+(rsd(13))**2);
  err(95)=sqrt((5*rsd(0))**2+(3*rsc(44))**2+(4*sigmaph)**2);
  do i=97,99,100,101,395;      /*sio2*/
    err(i)=rsd(34);  end;
  err(106)=sqrt((3*rsd(7))**2+(2*rsd(44))**2);
  err(112)=sqrt((rsd(8))**2+(3*sigmaph)**2);
  err(115)=sqrt((.277*rsd(2))**2+(.277*rsd(3))**2
          +(.277*sigmaph)**2+(.29*rsd(1))**2+(.23*rsd(8))**2
          +(1.58*rsd(50))**2+(3.93*rsd(34))**2);
  err(116)=sqrt((.277*rsd(2))**2+(.277*rsd(3))**2
          +(.277*sigmaph)**2+(.45*rsd(1))**2+(.34*rsd(8))**2
          +(1.47*rsd(50))**2+(3.82*rsd(34))**2+(.76*sigmaph)**2);
  err(117)=sqrt((3*rsd(1))**2+(rsd(0))**2+(4*rsd(17))**2);
  err(142)=sqrt(rsd(87)**2 + rsd(17)**2);
  err(143)=sqrt(rsd(87)**2 + rsd(5)**2);
  err(144)=sqrt(rsd(89)**2 + rsd(5)**2);
  err(145)=sqrt(rsd(89)**2 + rsd(17)**2);
  err(147)=sqrt((2*rsd(0))**2+(4*rsd(50))**2+(8*rsd(34))**2);
  c1=1.24-.135*ph;
  err(157),err(158)=sqrt(((1-c1)*rsd(50))**2+(c1*rsd(34))**2
                    +((3-3*c1)*sigmaph)**2);
  err(204)=sqrt((rsd(2))**2+(2*rsd(5))**2+(3*rsd(8))**2
          +(6*sigmaph)**2);
  err(205)=sqrt((rsd(3))**2+(2*rsd(5))**2+(3*rsd(8))**2
          +(6*sigmaph)**2);
  err(230)=sqrt((rsd(130))**2+(2*rsd(4))**2);
  err(235)=sqrt((2*rsd(130))**2+(rsd(6))**2+(3*sigmaph)**2);
```

```
 err(236)=sqrt((3*rsd(130))**2+(2*rsd(6))**2+(4*sigmaph)**2);
 err(242)=sqrt((rsd(130))**2+(2*sigmaph)**2);
 err(268),err(269)=sqrt((rsd(145))**2+(rsd(17))**2);
 err(288)=sqrt((rsd(145))**2+(rsd(34))**2+(2*sigmaph)**2);
 err(315)=sqrt((rsd(160))**2+(rsd(17))**2);
 err(339)=sqrt((rsd(7))**2+(rsd(5))**2);
 err(365)=sqrt((rsd(182))**2+(rsd(17))**2);
 err(374)=sqrt((rsd(182))**2+(rsd(44))**2);
 err(376)=sqrt((5*rsd(182))**2+(3*rsd(44))**2+rsd(4)**2);
 err(379)=sqrt((rsd(182))**2+(3*rsd(50))**2+(2*rsd(44))**2+
         (5*sigmaph)**2);
 err(419)=sqrt((2*rsd(8))**2+(rsd(7))**2+2*(2*rsd(8))*(rsd(7)
          )+(8*sigmaph)**2);
 err(471)=sqrt((rsd(50))**2+(rsd(5))**2+sigmaph**2);
 err(472)=sqrt((4*rsd(50))**2+(rsd(5))**2+(10*sigmaph)**2);
 return;

eherr: entry(cunits,sigma,err);
  rsd=2e7;  do i = 5,7,8,13,38,34,202,261,262;
    if cunits(i)*sigma(i) > 0 then rsd(i)=sigma(i)/cunits(i)/c;  end;
  if sigmado*dox > 0 then rsddo=sigmado/dox/c;  else rsddo=2e7;
  err(0)=sqrt(rsd(7)**2 + rsd(8)**2);
  err(1),err(4)=sqrt(sigmaph**2 + rsddo**2);
  err(2)=sqrt(sigmaph**2+(.5*rsd(84))**2+(.5*rsd(202))**2);
  err(3)=sqrt((1.125*sigmaph)**2+(.125*rsd(84))**2+
         (.125*rsd(38))**2);
  err(5)=sqrt((1.125*sigmaph)**2+(.125*rsd(5))**2+(.125*rsd(13))**2);
  err(6)=sqrt(rsd(261)**2+rsd(262)**2+(2*sigmaph)**2);
  err(7)=sqrt(.5*rsd(13)**2+sigmaph**2);
  err(8)=sqrt((rsd(5)/6)**2+(sigmaph/.75)**2);
  do i=0 to 8;  if abs(err(i))>1e2 then err(i)=0e0;
                err(i+9)=err(i)*c*r*t/f;  end;
 end errcalc;
```

```
phases: proc(page2,index,ap,dh,lockt,maxkto,minkto,err,errt);
 dcl card(0:20)char(80)ext,page2(*)char(12),q fixed bin(31)ext,
     (i,n,index(*))fixed bin(31),head char(130)
  init("    phase            log ap/kt    sigma(a)    sigma(t) log ap/minkt log ap/maxkt    log ap      log kt     log minkt  log maxkt"),
     (c,r,t)float dec(20) ext,(c1,c2,s1,s2,ap(*),dh(*),lockt(*),maxkto(*),
      minkto(*),err(*),errt(*))float dec(20) ;
  dcl outprint external file constant;
  dcl endpage condition;
  on endpage(outprint)begin;
  put file(outprint) page list(card(1));
  put file(outprint) skip(2)list(head);
put file(outprint) skip;
  end;
  signal endpage(outprint);
  c1=(298.16e0-t)/(298.16e0*t*c*r);
  do n=1 to q;  i=index(n);
    c2=ap(i);
    if abs(c2)<5e2 then call print2;  end;

 print2:  proc;
 dcl line char(130)init(" "),
     line1 char(16)def(line)pos(1),
     line2 char(11)def(line)pos(98),
     line3 char(11)def(line)pos(51),
     line4 char(11)def(line)pos(109),
     line5 char(12)def(line)pos(63),
     line6 char(11)def(line)pos(87),
     line7 char(12)def(line)pos(17),
     line8 char(11)def(line)pos(76),
     line9 char(11)def(line)pos(29),
     line10 char(11)def(line)pos(40);
    put string(line1)edit(i,page2(i))(f(3),x(1),a(12));
  if minkto(i)^=0e0 then do;
  s1=minkto(i)-dh(i)*c1;
  s2=c2-s1;
    put string(line2)edit(s1)(f(11,3));
    put string(line3)edit(s2)(f(11,3));  end;
  if maxkto(i)^=0e0 then do;
  s1=maxkto(i)-dh(i)*c1;
  s2=c2-s1;
    put string(line4)edit(s1)(f(11,3));
    put string(line5)edit(s2)(f(12,3));  end;
  if lockt(i)^=0e0 then do;
  put string(line6)edit(lockt(i))(f(11,3));
  put string(line7)edit(c2-lockt(i))(f(12,3));  end;
          put string(line8)edit (c2) (f(11,3));
  if err(i)<5e2 then put string(line9)edit(err(i))(f(11,3));
  if errt(i)>0e0 then put string(line10)edit(errt(i))(f(11,3));
  put file(outprint) list(line);
   end print2;

   end phases;
```

Appendix II. Test Case

i	name?	dh	maxkto	minkto	logkto	error
0	kFe +3	10.000			-13.032	
1	kFeOH +2	10.400			-2.190	0.02
2	kFeOH +	13.200			-9.500	0.10
3	kFeOH3 -	30.300			-31.000	1.50
4	kFeSO4 +	3.910			3.920	
5	kFeCl +2	5.600			1.480	
6	kFeCl2 +	0.000			2.130	
7	kFeCl3aq	0.000			1.130	
8	kFeSO4aq	3.230			2.250	
9	Siderite	-5.328		-12.104	-10.550	
10	Magnesite	-6.169	-7.779	-8.279	-8.029	
11	Dolomite	-8.290			-17.000	
12	Calcite	-2.585		-8.560	-8.475*	0.01
13	kH3SiO4-	8.935			-9.930*	
14	kH2SiO4=	29.714			-21.619*	
15	kHPO4 -2	-3.530			12.346	
16	kH2PO4 -	-4.520			19.553	
17	Anhydrite	-3.769			-4.637	
18	Gypsum	0.261			-4.600	
19	Brucite	0.850			-11.204	
20	Chrysotile	27.585			-51.800	
21	Aragonite	-2.615			-8.360	0.04
22	kMgF+	4.674			1.820	
23	kCaSO4 aq	1.470			2.309	
24	kMgOH +	2.590			2.206*	0.05
25	kH3BO3 aq	3.224			-9.240*	
26	kNH3 aq	12.480			-9.252*	
27	Forsterite	4.870			-27.694	
28	Diopside	21.100			-36.106	
29	Clinoenstite	6.675	-16.364	-17.024	-16.658	
30	kNaHPO4-	0.000			0.290	
31	Tremolite	90.215			-139.426	
32	kKHPO4 -	0.000			0.290	
33	kMgHPO4 aq	3.300			2.870	
34	kCaHPO4 aq	3.300			2.739	
35	kH2CO3 aq	-2.247			6.351*	0.01
36	Sepiolite(c)	26.532			-40.079	
37	Talc	45.065	-60.900	-65.000	-60.933	
38	Hydrmagnesit	-25.520			-36.762	
39	Adularia	30.820			-20.573	
40	Albite	25.896			-18.002	
41	Anorthite	11.580			-19.714	
42	Analcime	18.206			-12.701	
43	Kmica	67.860			-49.102	
44	Phlogopite	-42.300			43.300	3.00
45	Illite	54.684			-40.267	
46	Kaolinite	49.150	-35.320	-37.800	-36.921	
47	Halloysite	44.680			-32.830	
48	Beidellite	60.355			-45.272	
49	Chlorite	54.760			-89.563	
50	Alunite	29.820			-95.334	
51	Gibbsite (c)	-22.800	9.440	8.437	8.770	1.20
52	Boehmite	11.905		-33.929	-33.416	
53	Pyrophyllite	0.000	-46.480	-51.610	-48.314	
54	Phillipsite	0.000			-19.874	
55	Erionite	0.000			0.000	
56	Clinoptilolt	0.000			0.000	
57	Mordenite	0.000			0.000	
58	Wahcolite	3.720			-0.548	

i	name1	z	dha	gfw
0	Ca	2	6.0	40.0800
1	Mg	2	6.5	24.3120
2	Na	1	4.0	22.9898
3	K	1	3.0	39.1020
4	Cl	-1	3.0	35.4530
5	SO4	-2	4.0	96.0616
6	HCO3	-1	5.4	61.0173
7	Fe	2	6.0	55.8470
8	Fe	3	9.0	55.8470
9	FeOH	2	5.0	72.8544
10	FeOH	1	5.0	72.8544
11	Fe(OH)3	-1	5.0	106.8691
12	FeHPO4	1	5.4	151.8264
13	H2S aq	0	0.0	34.0799
14	FeSO4	1	5.0	151.9086
15	FeCl	2	5.0	91.3000
16	Fe total	2	0.0	55.8470
17	CO3	-2	5.4	60.0094
18	MgOH	1	6.5	41.3194
19	MgF	1	4.5	43.3104
20	MgCO3 aq	0	0.0	84.3214
21	MgHCO3	1	4.0	85.3293
22	MgSO4 aq	0	0.0	120.3736
23	H4SiO4aq	0	0.0	96.1155
24	H3SiO4	-1	4.0	95.1075
25	H2SiO4	-2	5.4	94.0995
26	OH	-1	3.5	17.0074
27	FeCl2	1	5.0	126.7530
28	CaOH	1	6.0	57.0874
29	CaHCO3	1	6.0	101.0973
30	CaCO3 aq	0	0.0	100.0894
31	CaSO4 aq	0	0.0	136.1416
32	FeCl3 aq	0	0.0	162.2060
33	FeSO4 aq	0	0.0	151.9086
34	SiO2 tot	0	0.0	60.0848
35	H3BO3 aq	0	0.0	61.8331
36	H2BO3	-1	2.5	60.8251
37	NH3 aq	0	0.0	17.0306
38	NH4	1	2.5	18.0386
39	MgPO4	-1	5.4	119.2834
40	MgH2PO4	1	5.4	121.2993
41	NaCO3	-1	5.4	82.9992
42	NaHCO3aq	0	0.0	84.0071
43	NaSO4	-1	5.4	119.0514
44	PO4	-3	5.0	94.9714
45	KSO4	-1	5.4	135.1636
46	HPO4	-2	5.0	95.9794
47	H2PO4	-1	5.4	96.9873
48	Cs	1	0.0	132.9050
49	NaHPO4	-1	5.4	118.9692
50	Al	3	9.0	26.9815
51	AlOH	2	5.4	43.9889
52	Al(OH)2	1	5.4	60.9962
53	Al(OH)4	-1	4.5	95.0110
54	AlF	2	5.4	45.9799
55	AlF2	1	5.4	64.9783
56	AlF3 aq	0	0.0	83.9767
57	AlF4	-1	4.5	102.9751
58	AlSO4	1	4.5	123.0431

i	page2	dh	maxkto	minkto	logkto	error
59	Trona	-18.000			-0.795	
60	Natron	15.745			-1.311	
61	Thermonatr	-2.802			0.125	
62	Fluorite	4.710			-10.960*	
63	Montmoril Ca	58.373			-45.027	
64	Halite	0.918			1.582	
65	Thenardite	-0.572			-0.179	
66	Mirabilite	13.987			-1.114	
67	Mackinawite	0.000			-4.648	
68	kHCO3 -	-3.617			10.330*	0.01
69	kNaCO3 -	8.911			1.268	
70	kNaHCO3 aq	0.000			-0.250	
71	kNaSO4 -	1.120			0.700	0.05
72	kKSO4 -	2.250			0.850*	0.05
73	kMgCO3 aq	2.020			2.980*	0.03
74	kMgHCO3 +	1.190			1.070*	0.03
75	kMgSO4 aq	1.400			2.250	0.02
76	kCaOH +	1.190			1.400	
77	kCaHCO3+	5.410			1.000*	0.05
78	kCaCO3 aq	4.030			3.150*	0.08
79	blank	0.000			0.000	
80	kAlOH +2	11.900			-4.990	0.02
81	kAl(OH)2 +	0.000			-10.100	0.20
82	kAlOH4 -	44.060			-23.000	0.30
83	kAlF +2	0.000			7.010	
84	kAlF2 +	20.000			12.750	
85	kAlF3 aq	2.500			17.020	
86	kAlF4 -	0.000			19.720	
87	kAlSO4 +	2.150			3.020	
88	kAlSO42-	2.840			4.920	
89	kHSO4 -	4.910			1.987*	
90	kpescalc	-65.440			40.644	
91	kH2S aq	5.300			-6.994*	
92	kHS -	12.100			-12.918	
93	koxy	34.157			-20.730	
94	kCH4	-57.435			30.741	
95	Hydroxyapati	-36.155	3.240	-5.950	-3.421	
96	Fluorapatite	-20.070		-25.243	-17.600	
97	Chalcedony	4.615			-3.523	
98	Magadiite	0.000			-14.300	
99	Cristobalite	5.500			-3.587	
100	SiO2 (a,L)	4.440			-3.018	
101	Quartz	6.220			-4.006	
102	kFeOH2 +	0.000			-5.670	0.10
103	kFeOH3 aq	0.000			-13.600	
104	kFeOH4 -	0.000			-21.600	0.20
105	kFeOH2 aq	28.565			-20.570	1.00
106	Vivianite	0.000			-36.000	
107	Magnetite	-50.460	6.525	3.367	3.737	
108	Hematite	-30.845			-4.008	
109	Maghemite	0.000			6.385	
110	Goethite	-14.480			0.500	0.80
111	Greenalite	0.000			20.810	
112	Ferrihydrite	0.000	4.296	1.557	4.891	
113	Annite	62.480			-35.645	
114	Pyrite	11.300			-18.479	
115	Montmoril BF	0.000			-34.913	
116	Montmoril AB	0.000			-29.633	
117	Huntite	-25.760			-29.968	

i	page1	z	dha	dfw
59	Al(SO4)2	-1	4.5	219.1047
60	KHPO4	-1	5.4	135.0814
61	F	-1	3.5	18.9964
62	HSO4	-1	4.5	97.0696
63	H	1	9.0	1.0080
64	FeH2PO4	1	5.4	152.8343
65	H2S calc	0	0.0	34.0799
66	HS	-1	3.5	33.0720
67	S	-2	5.0	32.0640
68	blank	0	0.0	1.0000
69	pO2	0	0.0	31.9988
70	pCH4	0	0.0	16.0430
71	AH2O	0	0.0	18.0153
72	MgHPO4aq	0	0.0	120.2914
73	CaHPO4aq	0	0.0	136.0594
74	CaPO4	-1	5.4	135.0514
75	CaH2PO4	1	5.4	137.0673
76	Fe(OH)2	1	5.4	89.8617
77	Fe(OH)3	0	0.0	106.8691
78	Fe(OH)4	-1	5.4	123.8765
79	Fe(OH)2	0	0.0	89.8617
80	Li	1	6.0	6.9390
81	blank	0	0.0	1.0000
82	LiSO4	-1	5.0	103.0006
83	NH4calc	1	2.5	18.0386
84	NO3	-1	3.0	62.0049
85	H2CO3 aq	0	0.0	62.0253
86	B tot	0	0.0	10.8110
87	Sr	2	5.0	87.6200
88	SrOH	1	5.0	104.6274
89	Ba	2	5.0	137.3400
90	BaOH	1	5.0	154.3474
91	NH4SO4	-1	5.0	114.1002
92	blank	0	0.0	1.0000
93	blank	0	0.0	1.0000
94	Rb	1	0.0	85.4700
95	blank	0	0.0	1.0000
96	I	-1	0.0	126.9044
97	Br	-1	4.0	79.9040
98	FeH2PO4	2	5.4	152.8343
99	FeHPO4aq	0	0.0	151.8264
100	CaF	1	5.0	59.0784
101	BF(OH)3	-1	2.5	80.8315
102	BF2(OH)2	-1	2.5	82.8225
103	BF3OH	-1	2.5	84.8136
104	BF4	-1	2.5	86.8046
105	FeF	2	5.0	74.8454
106	FeF2	1	5.0	93.8438
107	FeF3 aq	0	0.0	112.8422
108	Fe(SO4)2	-1	0.0	247.9702
109	Mn	2	6.0	54.9380
110	Mn	3	9.0	54.9380
111	MnCl	1	5.0	90.3910
112	MnCl2 aq	0	0.0	125.8440
113	MnCl3	-1	5.0	161.2970
114	MnOH	1	5.0	71.9454
115	Mn(OH)3	-1	5.0	105.9601
116	MnF	1	5.0	73.9364
117	MnSO4 aq	0	0.0	150.9996

i	page1	dh	maxkto	minkto	logkto	error
118	Greigite	0.000			-45.035	
119	FeS ppt	0.000			-3.915	
120	kFeH2PO4 +	0.000			2.700	
121	kCaPO4 -	3.100			6.459	
122	kCaH2PO4 +	3.400			1.408	
123	kMgPO4 -	3.100			6.539	
124	kMgH2PO4 +	3.400			1.513	
125	blank	0.000			0.000	
126	kLiSO4 -	0.000			0.640	
127	kNH4/NO3	187.055			-119.077	
128	Laumontite	39.610			-30.960	
129	kSrOH +	1.150			0.820	
130	kBaOH +	1.750			0.640	
131	kNH4SO4-	0.000			1.110	
132	blank	0.000			0.000	
133	blank	0.000			0.000	
134	Mn2(SO4)3	-39.060			-5.711	
135	blank	0.000			0.000	
136	kO2 Sato	0.000			-11.385	
137	kH2CO3 aq	-5.000			-1.452	
138	kFeHPO4 aq	0.000			3.600	
139	kFeHPO4 +	5.760			5.430	
140	AlOH3 (a)	12.990		-32.300	-31.611	
141	Prehnite	10.390			-11.695	
142	Strontianite	-0.690		-11.789	-9.250	
143	Celestite	-0.470	-6.349		-6.465	
144	Barite	6.280	-9.773		-9.976	
145	Witherite	0.360		-13.335	-8.585	
146	Strengite	-2.030	-26.235	-29.123	-26.400	
147	Leonhardite	90.070			-69.756	
148	blank	0.000			0.000	
149	Nesquehonite	-5.789	-4.546	-5.133	-5.621	
150	Artinite	-28.742			9.600	
151	kO2 calc	33.457			-21.495	
152	kw	13.345			-13.997	
153	Sepiolite(a)	0.000			-37.212	
154	Diaspore	15.405			-35.121	
155	Wairkite	26.140			-26.708	
156	kFeH2PO4	0.000			5.430	
157	Allophane(a)	0.000			6.060	
158	Allophane(F)	0.000			5.240	
159	blank	0.000			0.000	
160	kCaF +	3.798			0.940	
161	kBF(OH)3 -	1.850			-0.400	
162	kBF2(OH)2 -	14.980			-6.370	
163	kBF3OH -	25.110			-14.330	
164	kBF4 -	38.240			-21.720	
165	kFeF +2	2.700			6.200	
166	kFeF2 +	4.800			10.800	
167	kFeF3 aq	5.400			14.000	
168	blank	0.000			0.000	
169	kMn +3	25.760			-25.507	
170	kMnCl +	0.000			0.607	
171	kMnCl2 aq	0.000			0.041	
172	kMnCl3 -	0.000			-0.305	
173	kMnOH +	14.400			-10.590	0.04
174	kMn(OH)3	0.000			-34.800	
175	kMnF +	0.000			0.850	
176	kMnSO4 aq	2.170		1.708	2.260	

i	page1	z	dha	gfw
118	Mn(NO3)2	0	0.0	178.9478
119	MnHCO3	1	5.0	115.9553
120	MnO4	-1	3.0	118.9356
121	MnO4	-2	5.0	118.9356
122	blank	0	0.0	1.0000
123	blank	0	0.0	1.0000
124	SiF6	-2	5.0	142.0764
125	HF aq	0	0.0	20.0064
126	HF2	-1	3.5	39.0048
127	Cu	1	2.5	63.5460
128	CuCl2	-1	4.0	134.4520
129	CuCl3	-2	5.0	169.9050
130	Cu	2	6.0	63.5460
131	CuCO3 aq	0	0.0	123.5554
132	Cu(CO3)2	-2	0.0	183.5647
133	CuCl	1	4.0	98.9990
134	CuCl2 aq	0	0.0	134.4520
135	CuCl3	-1	4.0	169.9050
136	CuCl4	-2	5.0	205.3580
137	CuF	1	0.0	82.5444
138	CuOH	1	4.0	80.5534
139	Cu(OH)2	0	0.0	97.5607
140	Cu(OH)3	-1	0.0	114.5681
141	Cu(OH)4	-2	0.0	131.5751
142	Cu2(OH)2	2	0.0	161.1067
143	CuSO4 aq	0	0.0	159.6076
144	Cu(HS)3	-1	0.0	162.7619
145	Zn	2	6.0	65.3700
146	ZnCl	1	4.0	100.8230
147	ZnCl2 aq	0	0.0	136.2760
148	ZnCl3	-1	4.0	171.7290
149	ZnCl4	-2	5.0	207.1820
150	ZnF	1	0.0	84.3684
151	ZnOH	1	0.0	82.3774
152	Zn(OH)2	0	0.0	99.3847
153	Zn(OH)3	-1	0.0	116.3921
154	Zn(OH)4	-2	0.0	133.3995
155	ZnOHCl aq	0	0.0	117.8304
156	Zn(HS)2	0	0.0	131.5139
157	Zn(HS)3	-1	0.0	164.5859
158	ZnSO4 aq	0	0.0	161.4316
159	Zn(SO4)2	-2	0.0	257.4932
160	Cd	2	0.0	112.4000
161	CdCl	1	0.0	147.8530
162	CdCl2 aq	0	0.0	183.3060
163	CdCl3	-1	0.0	218.7590
164	CdF	1	0.0	131.3984
165	CdF2 aq	0	0.0	150.3968
166	Cd(CO3)3	-4	0.0	292.4281
167	CdOH	1	0.0	129.4074
168	Cd(OH)2	0	0.0	146.4147
169	Cd(OH)3	-1	0.0	163.4221
170	Cd(OH)4	-2	0.0	180.4295
171	Cd2OH	3	0.0	241.8074
172	CdOHCl aq	0	0.0	164.8604
173	CdNO3	1	0.0	174.4049
174	CdSO4 aq	0	0.0	208.4616
175	CdHS	1	0.0	145.4720
176	Cd(HS)2	0	0.0	178.5439

i	pagel	dh	maxkto	minkto	logkto	error
177	kMn(NO3)2 aq	-0.396			0.600	
178	kMnHCO3 +	0.000			1.270	
179	kMnO4 -	176.620			-127.824	
180	kMnO4 -2	150.020			-118.440	
181	FeOH)2.7Cl.3	0.000			-3.040	
182	MnSO4	-15.480			2.669	
183	Pyrolusite	-29.180	16.138		15.861	
184	Birnessite	0.000			18.091	
185	Nsutite	0.000			17.504	
186	Bixbyite	-15.245	-0.430	-2.226	-0.611	
187	Hausmannite	-80.140			61.540	
188	Pyrocroite	-22.590	15.381		15.088	
189	Manganite	0.000			-0.238	
190	Rhodochrosit	-2.079	-9.993	-11.019	-10.419	
191	MnCl2, 4H2O	17.380			2.710	
192	Mns Green	-5.790			3.800	
193	Mn3(PO4)2	2.120			-23.927	
194	MnHPO4	0.000			-12.947	
195	a-Cryptomeln	0.000			0.000	
196	Hollandite	0.000			0.000	
197	Psilomelane	0.000			0.000	
198	Todorokite	0.000			0.000	
199	Lithiophorit	0.000			0.000	
200	Rancieite	0.000			0.000	
201	kSiF6 -2	-16.260			30.180	
202	kHF aq	3.460			3.169	0.01
203	kHF2 -	4.550			3.749	0.06
204	Jarosite Na	-36.180			-11.200	1.00
205	Jarosite K	-31.280	-12.500		-14.800	1.10
206	kCuCl2 -	1.230		7.268	8.220	
207	kCuCl3 2-	1.910	8.508	6.899	8.420	
208	kCu 2+	1.650		2.590	2.720	
209	kCuCO3 aq	0.000	6.910	6.340	6.730	0.05
210	kCu(CO3)2 2-	0.000	10.010		9.830	0.04
211	kCuCl +	8.650	0.950	0.010	0.430	
212	kCuCl2 aq	10.560		-1.000	0.160	
213	kCuCl3 -	13.690	-1.600	-2.700	-2.290	
214	kCuCl4 2-	17.780	-3.600	-5.200	-4.590	
215	kCuF +	1.620	1.300	1.230	1.250	
216	kCuOH +	0.000	-7.418		-8.000	
217	kCu(OH)2 aq	0.000			-13.660	
218	kCu(OH)3 -	0.000	-26.378	-26.948	-26.900	
219	kCu(OH)4 2-	0.000		-40.058	-39.600	
220	kCu2(OH)2 2+	17.539	-10.378	-10.548	-10.359*	
221	kCuSO4 aq	1.220	2.522	2.152	2.310	
222	kCu(HS)3 -	0.000			25.900	
223	Cu metal	17.130	-8.300		-8.760	
224	Nantokite	9.980	-6.530		-6.760	
225	CuF	-12.370			7.080	
226	Cuprite	6.245	-0.700	-1.870	-1.550	
227	Chalcocite	49.350	-30.900	-34.920	-34.619	0.16
228	Cu2SO4	-4.560			-1.950	
229	Cuprousferit	-3.800	-6.330		-8.920	
230	Melanothalli	-12.320	4.450		3.730	
231	CuCO3	0.000	-9.610	-9.650	-9.630	
232	CuF2	-13.320			-0.620	
233	CuF2, 2H2O	-3.650			-4.550	
234	Cu(OH)2	-15.250	9.200		8.640	
235	Malachite	-19.760	5.360	4.500	5.150	0.08

i	pagel	z	dha	dfw
177	Cd(HS)3	-1	0.0	211.6159
178	Cd(HS)4	-2	0.0	244.6879
179	Fe2(OH)2	4	0.0	145.7087
180	Fe3(OH)4	5	0.0	235.5705
181	Al(OH)3	0	0.0	78.0036
182	Pb	2	0.0	207.1900
183	PbCl	1	0.0	242.6430
184	PbCl2 aq	0	0.0	278.0960
185	PbCl3	-1	0.0	313.5490
186	PbCl4	-2	0.0	349.0020
187	Pb(CO3)2	-2	0.0	327.2087
188	PbF	1	0.0	226.1884
189	PbF2 aq	0	0.0	245.1868
190	PbF3	-1	0.0	264.1852
191	PbF4	-2	0.0	283.1836
192	PbOH	1	0.0	224.1974
193	Pb(OH)2	0	0.0	241.2047
194	Pb(OH)3	-1	0.0	258.2121
195	Pb2OH	3	0.0	431.3874
196	PbNO3	1	0.0	269.1949
197	PbSO4 aq	0	0.0	303.2516
198	Pb(HS)2	0	0.0	273.3339
199	Pb(HS)3	-1	0.0	306.4059
200	Pb3(OH)4	2	0.0	689.5995
201	HPbO2	-1	0.0	240.1968
202	NO2	-1	0.0	46.0055
203	blank	0	0.0	1.0000
204	Ni	2	0.0	58.7100
205	NiBr	1	0.0	138.6140
206	NiCl	1	0.0	94.1630
207	NiF	1	0.0	77.7084
208	NiOH	1	0.0	75.7174
209	Ni(OH)2	0	0.0	92.7247
210	Ni(OH)3	-1	0.0	109.7321
211	NiSO4 aq	0	0.0	154.7716
212	Ag	1	0.0	107.8680
213	AgBr aq	0	0.0	187.7720
214	AgBr2	-1	0.0	267.6760
215	AgCl aq	0	0.0	143.3210
216	AgCl2	-1	0.0	178.7740
217	AgCl3	-2	0.0	214.2270
218	AgCl4	-3	0.0	249.6800
219	AgF aq	0	0.0	126.8664
220	AgHS aq	0	0.0	140.9400
221	Ag(HS)2	-1	0.0	174.0119
222	AgI aq	0	0.0	234.7724
223	AgI2	-1	0.0	361.6768
224	AgOH aq	0	0.0	124.8754
225	Ag(OH)2	-1	0.0	141.8827
226	AgSO4	-1	0.0	203.9296
227	AgNO3 aq	0	0.0	169.8729
228	Ag(NO2)2	-1	0.0	199.8790
229	ZnBr	1	0.0	145.2740
230	ZnBr2 aq	0	0.0	225.1780
231	ZnI	1	0.0	192.2744
232	ZnI2 aq	0	0.0	319.1788
233	CdBr	1	0.0	192.3040
234	CdBr2 aq	0	0.0	272.2080
235	CdI	1	0.0	239.3044

i	page2	ah	maxkto	minkto	logkto	error
236	Azurite	-30.870		1.130	3.751	0.09
237	Atacamite	-18.690	7.490	7.240	7.340	
238	Cu2(OH)3NO3	-17.350	9.310		9.240	
239	Antlerite	0.000	8.900		8.220	
240	Brochantite	0.000	15.500	15.150	15.340	1.16
241	Langite	-39.610	17.400		16.790	
242	Tenorite	-15.240	7.890	7.350	7.620	
243	CuOCuSO4	-35.575			11.550	
244	Cu3(PO4)2	0.000	-36.900		-36.850	
245	Cu3(PO4)2,3w	0.000			-35.120	
246	Covellite	24.010	-22.170		-23.033	0.11
247	CuSO4	-18.140	3.420	2.550	3.010	
248	Chalcanthite	1.440	-2.135	-2.960	-2.640	
249	Cupricferrit	-38.690		5.350	5.680	
250	Chalcopyrite	35.480	-30.790		-35.270	
251	kZnCl +	7.790			0.430	
252	kZnCl2 aq	8.500			0.450	
253	kZnCl3 -	9.560			0.500	
254	kZnCl4 2-	10.960			0.200	
255	kZnF +	2.220			1.150	
256	kZnOH +	13.400			-8.960	0.05
257	kZn(OH)2 aq	0.000			-16.900	
258	kZn(OH)3 -	0.000			-28.400	0.20
259	kZn(OH)4 2-	0.000			-41.200	0.10
260	kZnOHCl aq	0.000			-7.430	
261	kZn(HS)2 aq	0.000			14.940	
262	kZn(HS)3 -	0.000			16.100	
263	kZnSO4 aq	1.360			2.370	
264	kZn(SO4)2 2-	0.000			3.280	
265	Zn metal	-36.780	25.790		25.757	
266	Zn(BO2)2	0.000			8.290	
267	ZnCl2	-17.480	7.060		7.030	
268	Smithsonite	-4.360	-9.320	-10.810	-10.000	
269	ZnCO3, 1H2O	0.000			-10.260	
270	ZnF2	-13.080	-1.080		-1.520	
271	Zn(OH)2 (a)	0.000	12.430	12.260	12.450	
272	Zn(OH)2 (c)	0.000			12.200	
273	Zn(OH)2 (b)	0.000	11.890	11.320	11.750	0.02
274	Zn(OH)2 (g)	0.000	11.340	11.190	11.710	
275	Zn(OH)2 (e)	0.000	11.620	10.950	11.500	0.03
276	Zn2(OH)3Cl	0.000			15.200	
277	Zn5(OH)8Cl	0.000			38.500	
278	Zn2(OH)2SO4	0.000			7.500	
279	Zn4(OH)6SO4	0.000			28.400	
280	ZnNO3)2,6H2O	5.510			3.440	
281	ZnO(active)	0.000	11.860	11.570	11.310	
282	Zincite	-21.860	11.540	10.990	11.140	
283	Zn3O(SO4)2	-62.000			19.020	
284	Zn3(PO4)2,4w	0.000			-32.040	
285	Zns (a)	3.670			-9.052	
286	Sphalerite	3.250	-5.952	-13.212	-11.618	
287	Wurtzite	5.060	-8.552	-10.182	-9.682	
288	ZnSiO3	-18.270			2.930	
289	Willemite	-33.370		13.350	15.330	
290	Zincosite	-19.200	3.930		3.010	
291	ZnSO4, 1H2O	-10.640	-0.500		-0.570	
292	Bianchite	-0.160	-1.120		-1.765	
293	Goslarite	3.300	-1.870		-1.960	
294	kCdCl +	0.590		1.370	1.930	0.03

i	page1	z	ahа	gfw
236	CuI2 aq	0	0.0	366.2088
237	PbBr	1	0.0	287.0940
238	PbBr2 aq	0	0.0	366.9980
239	PbI	1	0.0	334.0944
240	PbI2 aq	0	0.0	460.9988
241	PbCO3 aq	0	0.0	267.1994
242	Pb(OH)4	-2	0.0	275.2195
243	Pb(SO4)2	-2	0.0	399.3132
244	AgBr3	-2	0.0	347.5800
245	AgI3	-2	0.0	488.5812
246	AgI4	-3	0.0	615.4856
247	Fe(HS)2	0	0.0	121.9909
248	Fe(HS)3	-1	0.0	155.0629
249	As total	0	0.0	74.9216
250	H3AsO3aq	0	0.0	125.9437
251	H2AsO3	-1	0.0	124.9357
252	HAsO3	-2	0.0	123.9278
253	AsO3	-3	0.0	122.9198
254	H4AsO3	1	0.0	126.9517
255	H3AsO4aq	0	0.0	141.9431
256	H2AsO4	-1	0.0	140.9351
257	HAsO4	-2	0.0	139.9272
258	AsO4	-3	0.0	138.9192
259	Cu(S4)2	-3	23.0	320.0580
260	CuS4S5	-3	25.0	352.1220
261	As3 tot	0	0.0	74.9216
262	As5 tot	0	0.0	74.9216
263	S2	-2	6.5	64.1280
264	S3	-2	8.0	96.1920
265	S4	-2	10.0	128.2560
266	S5	-2	12.0	160.3200
267	S6	-2	14.0	192.3840
268	Ag(S4)2	-3	22.0	364.3800
269	AgS4S5	-3	24.0	396.4440
270	Ag(HS)S4	-2	15.0	269.1960
271	CuHCO3	1	0.0	124.5633
272	ZnHCO3	1	0.0	126.3573
273	ZnCO3	0	0.0	125.3794
274	Zn(CO3)2	-2	0.0	185.3587
275	CdHCO3	1	0.0	173.4173
276	CdCO3	0	0.0	172.4094
277	Cd(SO4)2	-2	0.0	208.4616
278	PbHCO3	1	0.0	268.2073
279	NiCl2	0	0.0	129.6160
280	NiHCO3	1	0.0	119.7273
281	NiCO3	0	0.0	118.7194
282	Ni(CO3)2	-2	0.0	178.7287
283	Ni(SO4)2	-2	0.0	250.8332
284	fulvate	-2	0.0	650.0000
285	Humate	-2	0.0	2000.0000
286	Hfulvate	-1	0.0	651.0080
287	H Humate	-1	0.0	2001.0080
288	Fefulvat	1	0.0	705.8470
289	Fehumate	1	0.0	2055.8470
290	Cufulvat	0	0.0	713.5460
291	Cuhumate	0	0.0	2063.5460
292	Cdfulvat	0	0.0	762.4000
293	Cdhumate	0	0.0	2112.4000
294	Agfulvat	-1	0.0	757.8680

i	page2	dh	maxkto	minkto	logkto	error
295	kCdCl2 aq	1.240		2.210	2.600	0.10
296	kCdCl3 -	3.900	3.400	2.110	2.400	0.10
297	kCdF +	0.000			1.100	
298	kCdF2 aq	0.000			1.500	
299	kCd(CO3)3 4-	0.000	6.240		6.220	
300	kCdOH +	13.100	-7.530		-10.080	0.10
301	kCd(OH)2 aq	0.000	-18.540		-20.350	0.20
302	kCd(OH)3 -	0.000	-32.320		-33.300	
303	kCd(OH)4 2-	0.000	-46.750		-47.350	0.10
304	kCd2OH 3+	10.900			-9.390	0.05
305	kCdOHCl aq	4.355	-8.150		-7.404	
306	kCdNO3 +	-5.200		-0.320	0.400	
307	kCdSO4 aq	1.080		2.030	2.460	
308	kCdHS +	0.000			10.170	
309	kCd(HS)2 aq	0.000			16.530	
310	kCd(HS)3 -	0.000			18.710	
311	kCd(HS)4 2-	0.000			20.900	
312	Cd metal	-18.000	13.640		13.490	
313	Gamma Cd	-18.140			13.590	
314	Cd(BO2)2	0.000			9.840	
315	Otavite	-0.580	-11.210	-13.810	-13.740	
316	CdCl2	-4.470	-0.470		-0.680	
317	CdCl2, 1H2O	-1.820			-1.710	
318	CdCl2,2.5H2O	1.710			-1.940	
319	CdF2	-9.720			-2.980	
320	Cd(OH)2 (a)	-20.770	14.300	13.610	13.730	
321	Cd(OH)2 (c)	0.000			13.650	0.04
322	CdOHCl	-7.407		3.300	3.520	
323	Cd3(OH)4SO4	0.000			22.560	
324	Cd3OH2(SO4)2	0.000			6.710	
325	Cd4(OH)6SO4	0.000			28.400	
326	Monteponite	-24.760	15.740		15.120	
327	Cd3(PO4)2	0.000			-32.600	
328	CdSiO3	-16.630		7.960	9.060	
329	CdSO4	-14.740	-0.050	-0.130	-0.100	
330	CdSO4, 1H2O	-7.520	-1.630	-1.680	-1.657	
331	CdSO4,2.7H2O	-4.300	-1.860	-1.890	-1.873	
332	Greenockite	16.360	-13.112		-15.930	
333	kFe(SO4)2 -	4.600	5.425	5.398	5.420	
334	kFe2(OH)2 4+	13.500			-2.950	0.05
335	kFe3(OH)4 5+	14.300			-6.300	0.10
336	kAl(OH)3 aq	0.000			-16.000	
337	Jarosite H	-55.150			-12.100	
338	Alum k	7.220			-5.170	
339	Melanterite	2.860			-2.470	
340	Epsomite	2.820			-2.140	
341	kPbCl +	4.380	1.750	1.100	1.600	
342	kPbCl2 aq	1.080		1.780	1.800	
343	kPbCl3 -	2.170		1.400	1.700	
344	kPbCl4 2-	3.530		0.810	1.360	
345	kPb(CO3)2 2-	0.000		8.230	10.640	
346	kPbF +	0.000	1.300		1.250	
347	kPbF2 aq	0.000	3.500	2.270	2.560	
348	kPbF3 -	0.000	3.450		3.420	
349	kPbF4 2-	0.000			3.100	
350	kPbOH +	0.000	-6.170		-7.710	0.10
351	kPb(OH)2 aq	0.000		-17.170	-17.120	0.10
352	kPb(OH)3 -	0.000	-28.050	-28.100	-28.060	0.05
353	kPb2OH 3+	0.000			-6.360	0.10

i	page1	z	dha	gfw
295	Agnunate	-1	0.0	2107.8680
296	H2F2 aq	0	0.0	40.0127
297	NaF aq	0	0.0	41.9882
298	U total	0	0.0	238.0290
299	U	4	0.0	238.0290
300	UO2	2	0.0	270.0278
301	U	3	0.0	238.0290
302	UOH	3	0.0	255.0364
303	U(OH)2	2	0.0	272.0437
304	U(OH)3	1	0.0	289.0511
305	U(OH)4	0	0.0	306.0585
306	U(OH)5	-1	0.0	323.0659
307	U6(OH)15	9	0.0	1683.2846
308	UF	3	0.0	257.0274
309	UF2	2	0.0	276.0258
310	UF3	2	0.0	295.0242
311	UF4	0	0.0	314.0226
312	UF5	-1	0.0	333.0210
313	UF6	-2	0.0	352.0194
314	UCL	3	0.0	273.4820
315	USO4	2	0.0	334.0906
316	U(SO4)2	0	0.0	430.1522
317	UHPO4	2	0.0	334.0084
318	U(HPO4)2	0	0.0	429.9877
319	U(HPO4)3	-2	0.0	525.9671
320	U(HPO4)4	-4	0.0	621.9465
321	UO2	1	0.0	270.0278
322	UO2OH	1	0.0	287.0352
323	UO2)2OH2	2	0.0	574.0703
324	UO2)3OH5	1	0.0	895.1203
325	UO2CO3	0	0.0	330.0372
326	UO2CO3)2	-2	0.0	390.0465
327	UO2CO3)3	-4	0.0	450.0559
328	UO2F	1	0.0	289.0262
329	UO2F2	0	0.0	308.0246
330	UO2F3	-1	0.0	327.0230
331	UO2F4	-2	0.0	346.0214
332	UO2CL	1	0.0	305.4808
333	UO2SO4	0	0.0	366.0894
334	UO2SO4)2	-2	0.0	462.1510
335	UO2HPO4	0	0.0	366.0072
336	UO2HPO42	-2	0.0	461.9865
337	UO2H2PO4	1	0.0	367.0151
338	U2H2P4,2	0	0.0	464.0025
339	U2H2P4,3	-1	0.0	560.9898
340	UH3SiO4	1	0.0	365.1353
341	U+6 tot	2	0.0	238.0290

i	page2	dh	maxkto	minkto	logkto	error
354	kPbNO3 +	0.000		1.070	1.170	0.02
355	kPbSO4 aq	0.000	3.200	2.620	2.750	0.10
356	kPb(HS)2 aq	0.000			15.270	
357	kPb(HS)3 -	0.000			16.570	
358	kPb3(OH)4 2+	26.500			-23.830	0.20
359	Franklinite	-53.140			6.845	
360	Pb metal	0.400	4.310	4.070	4.270	
361	Pb(BO2)2	-5.800			7.610	
362	Cotunnite	5.600	-4.670	-4.976	-4.770	
363	Matlockite	7.950	-8.500		-9.430	
364	Phosgenite	0.000		-19.940	-19.810	
365	Cerrusite	4.860	-12.330	-13.440	-13.130	
366	PbF2	-0.700		-7.570	-7.440	
367	Massicot	-16.780		12.790	12.910	
368	Litharge	-16.380	13.070	12.640	12.720	
369	PbO, .3H2O	0.000			12.990	
370	Pb2OCO3	-11.460		-0.780	-0.530	
371	Larnakite	-6.440		-6.300	-0.280	
372	Pb3O2SO4	-20.750			10.400	
373	Pb4O3SO4	-35.070			22.100	
374	PbHPO4	7.040	-9.200	-15.630	-11.460	
375	Pb3(PO4)2	-1.670	-17.380	-30.030	-19.670	
376	Clpyromorph	0.000	-34.510		-84.430	
377	Hxypyromorph	0.000			-62.790	
378	Pb3O2CO3	-26.430			11.020	
379	Plumbgummite	0.000			-32.790	
380	Hinsdalite	0.000			-2.500	
381	Tsumebite	0.000			-9.790	
382	PbSiO3	-9.260	7.640	6.120	7.320	
383	Pb2SiO4	-26.000	20.500	19.220	19.760	
384	Anglesite	2.150		-7.970	-7.790	0.02
385	Galena	19.400	-13.682	-16.452	-15.132	
386	Plattnerite	-70.730		49.000	49.300	
387	Pb2O3	0.000			61.040	
388	Minium	-102.760		70.800	73.690	
389	Pb(OH)2 (c)	-13.990	13.630		8.150	
390	Laurionite	0.000		0.175	0.623	
391	Pb2(OH)3Cl	0.000			8.723	
392	Hydcerrusite	0.000			-17.460	
393	Pb2O(OH)2	0.000	27.100		26.200	
394	Pb4(OH)6SO4	0.000			21.100	
395	SiO2 (a,M)	3.910			-2.710	
396	FCO3apatite	39.390			-114.400	
397	blank	0.000			0.000	
398	BaF2	1.000	-4.550	-6.740	-5.760	
399	SrF2	1.250		-9.120	-8.540	
400	kNO3/NO2	-43.760		28.300	28.570	
401	Fe2(SO4)3	-59.120		-0.650	3.580	
402	Sulfur	7.900		-16.100	-15.625	
403	kNiBr +	0.000			0.500	
404	kNiCl +	0.000			0.430	
405	kNiF +	0.000			1.300	
406	kNiOH +	12.420		-10.920	-9.250	0.03
407	kNi(OH)2 aq	0.000			-19.000	1.00
408	kNi(OH)3 -	0.000			-30.000	0.50
409	kNiSO4 aq	1.520	2.320		2.290	
410	NiCO3	-2.940			-6.840	
411	Ni(OH)2	30.450	13.590	10.590	10.800	0.10
412	Ni4(OH)6SO4	0.000			32.000	

i	page2	dh	maxkto	minkto	logkto	error
413	Bunsenite	-25.920	12.330		12.450	
414	Ni3(PO4)2	0.000			-31.300	
415	Millerite	2.500		-8.132	-8.142	
416	Retgersite	1.100			-2.040	
417	Morenosite	2.940			-2.361	
418	Ni2Si04	-33.360			14.541	
419	Fe3(OH)8	0.000	24.105	17.112	20.222	
420	Dioptase	-8.960			6.500	
421	kAgBr aq	0.000			4.240	
422	kAg3r2 -	0.000			7.280	
423	kAgCl aq	-2.680			3.271	
424	kAgCl2 -	-3.930			5.270	
425	kAgCl3 2-	0.000			5.290	
426	kAgCl4 3-	0.000			5.510	
427	kAgF aq	-2.830			0.350	
428	kAgHS aq	0.000			14.050	
429	kAg(HS)2 -	0.000			18.451	
430	kAgI aq	0.000			6.600	
431	kAgI2 -	0.000			10.680	
432	kAgOH aq	0.000			-12.000	0.30
433	kAg(OH)2 -	0.000			-24.000	0.05
434	kAgSO4 -	1.490			1.290	
435	kAgNO3 aq	0.000			-0.290	
436	kAg(NO2)2 -	0.000			2.220	
437	Ag metal	25.234			-13.510	
438	Bromyrite	20.170			-12.270	
439	Cerargyrite	15.652			-9.750	
440	Ag2CO3	9.530			-11.070	
441	AgF, 4H2O	4.270			0.550	
442	Iodyrite	26.820			-16.070	
443	Ag2O	-10.430			12.580	0.10
444	Ag3PO4	0.000			-17.550	
445	Acanthite	53.300			-36.050	
446	Ag2SO4	4.250			-4.920	
447	kZnBr +	0.000			-0.580	
448	kZnBr2 aq	0.000			-0.980	
449	kZnI +	0.000	-2.200		-2.910	
450	kZnI2 aq	0.000	-0.600		-1.690	
451	kCdBr +	-0.810			2.170	
452	kCdBr2 aq	0.000			2.900	
453	kCdI +	-2.370	2.700		2.150	
454	kCdI2 aq	0.000	3.800		3.590	
455	kPbBr +	2.880	1.300		1.770	0.10
456	kPbBr2 aq	0.000	3.000		1.440	
457	kPbI +	0.000	2.000		1.940	
458	kPbI2 aq	0.000	3.700		3.200	
459	CuBr	13.080			-8.210	
460	CuI	20.140			-11.890	
461	ZnBr2, 2H2O	-7.510			5.210	
462	ZnI2	-13.440			7.230	
463	CdBr2, 4H2O	7.230			-2.420	
464	CdI2	4.080			-3.610	
465	PbBr2	8.100	-4.410	-5.340	-5.180	
466	PbBrF	0.000			-8.420	
467	PbI2	15.160			-8.070	
468	kPbCO3 aq	0.000			7.240	
469	kPb(OH)4 2-	0.000			-39.700	
470	kPb(SO4)2 2-	0.000			3.470	
471	AlOHSO4	0.000	-3.170	-3.390	-3.230	

i	page?	dh	maxkto	minkto	logkto	error
472	Al4(OH)10SO4	0.000			22.700	
473	kAgBr3 2-	0.000			8.710	
474	kAgI3 2-	-27.030			13.370	
475	kAgI4 3-	0.000			14.080	
476	kFe(HS)2 aq	0.000			8.950	
477	kFe(HS)3 -	0.000			10.987	
478	kH2AsO3 -	6.560	-9.180	-9.294	-9.223	
479	kHAsO3 2-	14.200			-21.330	
480	kAsO3 3-	20.250			-34.744	
481	kH4AsO3 +	0.000		-2.650	-0.305	
482	kH2AsO4 -	-1.690	-2.199	-3.592	-2.243	
483	kHAsO4 2-	-0.920		-10.848	-9.001	
484	kAsO4 3-	3.430		-23.309	-20.597	
485	kCu(S4)2 3-	0.000			6.169	
486	kCuS4S5 3-	0.000			5.382	
487	kAs3->As5	30.015	-18.704	-19.825	-19.444	
488	As2O5	-5.405	9.478		6.699	
489	AlAsO4, 2H2O	0.000			-15.837	
490	Ca3AsO4)2,4w	0.000			-18.905	
491	Cu3AsO4)2,6w	0.000			-35.123	
492	FeAsO4, 2H2O	0.000			-20.249	
493	Mn3AsO4)2,8w	0.000			-28.707	
494	Ni3AsO4)2,8w	0.000			-25.511	
495	Pb3(AsO4)2	0.000			-35.403	
496	Zn3AsO422.5w	0.000			-27.546	
497	Arsenolite	14.330	-2.728	-2.859	-2.801	
498	Claudetite	13.290	-3.021		-3.065	
499	AsI3	1.875			4.155	
500	Orpiment	82.890	-46.004		-60.971	
501	Realgar	30.545		-26.574	-19.747	
502	kS2 2-	11.400	-11.816		-14.528	
503	kS3 2-	10.400	-10.790	-13.355	-13.242	
504	kS4 2-	9.700		-12.109	-9.829	
505	kS5 2-	9.300	-9.265		-9.595	
506	kS6 2-	0.000			-9.881	
507	kAg(S4)2 3-	0.000			0.991	
508	kAgS4S5 3-	0.000			0.680	
509	kAg(HS)S4 2-	0.000			10.431	
510	kCuHCO3 +	0.000			2.700	
511	kZnHCO3 +	0.000			2.100	
512	kZnCO3 aq	0.000			5.300	
513	kZn(CO3)2 2-	0.000			9.630	
514	kCdHCO3 +	0.000			2.100	
515	kCdCO3 aq	0.000			5.400	
516	kCd(SO4)2 2-	0.000			3.500	
517	kPbHCO3 +	0.000			2.900	
518	kNiCl2 aq	0.000			0.960	
519	kNiHCO3 +	0.000			2.140	
520	kNiCO3 aq	0.000			6.870	
521	kNi(CO3)2 2-	0.000			10.110	
522	kNi(SO4)2 2-	0.000			1.020	
523	kH fulvate	0.000			4.270	
524	kh humate	0.000			4.270	
525	kFe fulvate	0.000			9.400	
526	kFe humate	0.000			9.400	
527	kCu fulvate	0.000			6.200	
528	kCu humate	0.000			6.200	
529	kCd fulvate	0.000			3.500	
530	kCd humate	0.000			3.500	

i	name?	dh	maxkto	minkto	logkto	error
531	kAg fulvate	0.000			2.400	
532	kAg humate	0.000			2.400	
533	Blaublei I	0.000			-24.162	0.15
534	Blaublei II	0.000			-27.279	0.15
535	Anilite	43.535			-31.873	0.15
536	Djurleite	47.881			-33.970	0.15
537	kH2F2 aq	0.000			6.768	
538	kpe(H2S/S)	-9.500			4.832	
539	kpe(S/SO4)	-55.940			35.754	
540	kNaF aq	0.000			-0.932	0.05
541	Ba3(AsO4)2	9.500			-50.110	
542	kU +4	-34.430			9.216	
543	blank	0.000			0.000	
544	kU +3	24.400	-5.384		-8.796	
545	kUOH +3	11.715			-0.656*	
546	kU(OH)2 +2	17.730			-2.270	
547	kU(OH)3 +	22.645			-4.935	
548	kU(OH)4 aq	24.760			-8.493	
549	kU(OH)5 -	27.575			-13.120	
550	kU6(OH)15 +9	0.000			-17.229	
551	Uraninite	-18.630			-4.700	
552	UO2 (a)	0.000			0.934	
553	U409 (c)	-101.235	3.180		-3.384	
554	U308 (c)	-116.020	34.589		21.107	
555	Coffinite	-11.600			-9.396	
556	kUF +3	5.050			8.569	
557	kUF2 +2	7.200			14.457	
558	kUF3 +	7.150			19.115	
559	kUF4 aq	4.600			23.640	
560	kUF5 -	4.850			25.238	
561	kUF6 -2	3.300			27.718	
562	UF4 (c)	-18.900			-18.606	
563	UF4,2.5H2O	-0.588			-27.570	
564	kUCl +3	9.933			1.338	
565	kUSO4 +2	3.700		5.046	5.461	
566	kU(SO4)2 aq	7.600		9.290	9.749	
567	kUHPO4 +2	7.500			24.443	
568	kU(HPO4)2 aq	1.700			46.833	
569	kU(HPO4)3 -2	-7.800			67.564	
570	kU(HPO4)4 -4	-26.500			88.493	
571	U(HPO4)2, 4w	3.840			-51.584	
572	Ningyoite	-2.270			-53.906	
573	kUO2 +	-3.300	6.178		2.795	
574	kUO2OH +	11.015			-5.672	
575	k(UO2)2(OH)2	10.230			-5.645	
576	k(UO2)3(OH)5	25.075			-15.593	
577	UO3 (c)	-19.315			7.719	
578	Gummite	-23.015			10.403	
579	B-UO2(OH)2	-13.730			5.544	
580	Schoepite	-12.045			5.404	
581	kUO2CO3 aq	0.840			10.071*	
582	kUO2(CO3)2-2	3.480			17.008*	
583	kUO2(CO3)3-4	-8.780			21.384*	
584	Rutherfordin	-1.440			-14.439*	
585	kUO2F +	-0.450			5.105	
586	kUO2F2 aq	-0.900			8.921	
587	kUO2F3 -	-0.850			11.364	
588	kUO2F4 -2	-1.100			12.607	
589	kUO2Cl +	1.233			0.220	

i	page'	dh	maxkto	minkto	logkto	error
590	kU02S)4 aq	5.100			2.709*	
591	kU02(SO4)2-2	6.100			4.183*	
592	kU02HP04 aq	-2.100			20.514	
593	kU02(H2P04)2=	-11.800			43.441	
594	kU02H2P04 +	-3.700			22.643	
595	kU02H2P04)2	-16.500			44.700	
596	kU02H2P04)3-	-28.600			66.245	
597	(U02)3(P04)2	94.900		-129.134	-49.137	
598	H-Autunite	-3.600			-47.931	
599	Na-Autunite	-0.460			-47.409	
600	K-Autunite	5.860			-48.244	
601	Uramphite	9.700			-51.749	
602	Saleeite	-20.180			-43.646	
603	Autunite	-14.340			-43.927	
604	Sr-Autunite	-13.050			-44.457	
605	Uranocircite	-10.100			-44.631	
606	Bassetite	-19.900			-44.435	
607	Torbernite	-15.900			-45.279	
608	Przhevalskit	-11.000			-44.365	
609	kU02H3Si04 +	0.000			-2.403	
610	Uranophane	0.000			17.489	

"*" denotes that an analytical expression for kt has been used

summary of analytical expressions of the form log k = a+b*t+c/t+d*t**2+e/t**2

i	react prod	a	b	c	d	e
12	Calcite	13.5430	-0.0401	-3000.0000		
13	kH3SiO4-	6.3680	-0.0163	-3405.0000		
14	kH2SiO4=	39.4780	-0.0659	-12355.1000		
24	kMgOH +	0.6840	0.0051			
25	kH3BO3 aq	28.6059	0.0121	1573.2100		
26	kNH3 aq	0.6322	-0.0012	-2835.7600		
35	kH2CO3 aq	-14.8435	0.0328	3404.7100		
62	Fluorite	109.2500	0.0024	3120.9800	-4.9000e-007	-2.0885e+003
68	kHCO3 -	-6.4980	0.0238	2902.3900		
72	kKSO4 -	3.1060		-873.6000		
73	kMgCO3 aq	0.9910	0.0067			
74	kMgHCO3 +	2.3190	-0.0111		2.2981e-005	
77	kCaHCO3+	-2.9500	0.0133			
78	kCaCO3 aq	-27.3930	0.0562	4114.0000		
89	kHSO4 -	-5.3505	0.0183	557.2461		
91	kH2S aq	11.1700	-0.0239	-3279.0000		
220	kCu2(OH)2 2+	2.4970		3833.0000		
545	kUOH +3	-9.1600	0.0285			
581	kUO2CO3 aq	-9.5600	0.0343	2809.0000		
582	kUO2(CO3)2-2	14.1400	0.0096			
583	kUO2(CO3)3-4	27.8400	-0.0216			
584	Rutherfordin	4.5400	-0.0332	-2716.0000		
590	kUO2SO4 aq	11.3840	-0.0709		1.4028e-004	
591	kUO2(SO4)2-2	12.1300	-0.0683		1.3987e-004	

reference numbers for all possible numbered input constituents:

number	constituent	z
0	Ca	2
1	Mg	2
2	Na	1
3	K	1
4	Cl	-1
5	SO4	-2
6	HCO3	-1
7	Fe	2
8	Fe	3
13	H2S aq	0
16	Fe total	2
17	CO3	-2
34	SiO2 tot	0
38	NH4	1
44	PO4	-3
48	Cs	1
50	Al	3
61	F	-1
80	Li	1
84	NO3	-1
86	B tot	0
87	Sr	2
89	Ba	2
94	Rb	1
96	I	-1
97	Br	-1
109	Mn	2
130	Cu	2
145	Zn	2
160	Cd	2
182	Pb	2
202	NO2	-1
204	Ni	2
212	Ag	1
249	As total	0
261	As3 tot	0
262	As5 tot	0
284	fulvate	-2
285	Humate	-2
298	U total	0
299	U	4
341	U+6 tot	2

```
USBM-1  table  Potter etal  Report 79,1144                                    5
   0      0       0        0        0        0        0        0
 24.5 6.90 -.131 "mg/l"
48.6 5.4 153 11.9 94 65 328 .12 0 0
38 .1 1.1 .05 .003 .55 0
cunits(298)=.01
```

Iter	s1-analCO3	s2-analSO4	s3-analF	s4-analPO4	s5-analCl	s6-analH2S	s7-analFulv	s8-analHum
1	7.017144e-005	9.005902e-005	4.665110e-007	7.894116e-008	5.790300e-018	0.000000e+000	0.000000e+000	0.000000e+000
2	6.869322e-007	1.365688e-006	4.907626e-009	1.231736e-009	2.030000e-020	0.000000e+000	0.000000e+000	0.000000e+000
3	-7.415233e-009	-2.289755e-008	-4.151741e-011	-2.474102e-011	1.400000e-021	0.000000e+000	0.000000e+000	0.000000e+000

0 0 0 0 0 0 0 0

Anal cond = 0.0 Calc cond = 963.4
Anal epmcat = 9.8465 Anal epman = 9.4179 Percent difference in input cation/anion balance = 4.4499
Calc epmcat = 9.6297 Calc epman = 9.2004

Input	sigma	Fe3/Fe2	sigma	Sato H202/02	sigma	NO3/NO2	sigma	NO3/NH4	sigma	calc H202/02	sigma	SO4/S=	sigma	As5/As3	sigma
								Eh							
-0.131	0.000	-0.131	0.000	9.900	0.000	9.900	0.000	9.900	0.000	9.900	0.000	9.900	0.000	9.900	0.000
								pE							
-2.218	0.000	-2.218	0.000	100.000	0.000	100.000	0.000	100.000	0.000	100.000	0.000	100.000	0.000	100.000	0.000

U4/U6	sigma
Eh	
-0.131	
pE	
-2.218	

T	pH	Tds ppm	Ionic str	pO2 atm	pCO2 atm	pCH4 atm	CO2 tot	uncom CO2	ppm uncom CO2	ncrb alk	aH2O
24.50	6.900	745.8	0.01133	0.00e+000	3.93e-002	1.36e-016	0.00673	5.31e-003	2.34e+002	1.48e-006	0.9997

I	Species		Anal ppm	Calc ppm	Anal molal	Calc molal	Activity	Act coeff	-log Act
298	U total	0	0.010		4.204e-008				
299	U	4		0.000000		9.453e-029	1.650e-029	0.1746	28.782
301	U	3		0.000000		1.086e-035	4.069e-036	0.3746	35.390
302	UOH	3		0.000000		7.364e-023	2.759e-023	0.3746	22.559
303	U(OH)2	2		0.000000		8.222e-018	5.314e-018	0.6464	17.275
304	U(OH)3	1		0.000000		1.004e-013	9.000e-014	0.8967	13.046
305	U(OH)4	0		0.000059		1.938e-010	1.943e-010	1.0026	9.711
306	U(OH)5	-1		0.013		4.077e-008	3.655e-008	0.8967	7.437
308	UF	3		0.000000		4.114e-025	1.541e-025	0.3746	24.812
309	UF2	2		0.000000		4.680e-024	3.025e-024	0.6464	23.519
310	UF3	2		0.000000		5.443e-024	3.518e-024	0.6464	23.454
311	UF4	0		0.000000		3.026e-024	3.034e-024	1.0026	23.518
312	UF5	-1		0.000000		3.424e-027	3.070e-027	0.8967	26.513
313	UF6	-2		0.000000		3.682e-029	2.380e-029	0.6464	28.623
314	UCL	3		0.000000		2.215e-030	8.297e-031	0.3746	30.081
315	USO4	2		0.000000		2.842e-027	1.837e-027	0.6464	26.736
316	U(SO4)2	0		0.000000		1.369e-026	1.372e-026	1.0026	25.863
317	UHPO4	2		0.000000		3.709e-024	2.397e-024	0.6464	23.620
318	U(HPO4)2	0		0.000000		3.191e-021	3.200e-021	1.0026	20.495
319	U(HPO4)3	-2		0.000000		1.464e-019	9.463e-020	0.6464	19.024
320	U(HPO4)4	-4		0.000000		2.537e-017	4.429e-018	0.1746	17.354
321	UO2	1		0.000041		1.504e-010	1.349e-010	0.8967	9.870
300	UO2	2		0.000000		2.053e-015	1.327e-015	0.6464	14.877
322	UO2OH	1		0.000000		2.424e-014	2.174e-014	0.8967	13.663
323	UO2)2OH2	2		0.000000		3.778e-022	2.442e-022	0.6464	21.612
324	UO2)3OH5	1		0.000000		1.955e-026	1.753e-026	0.8967	25.756
325	UO2CO3	0		0.000010		2.919e-011	2.927e-011	1.0026	10.534
326	UO2CO3)2	-2		0.000246		6.305e-010	4.075e-010	0.6464	9.390
327	UO2CO3)3	-4		0.000048		1.062e-010	1.854e-011	0.1746	10.732
328	UO2F	1		0.000000		4.823e-015	4.325e-015	0.8967	14.364
329	UO2F2	0		0.000000		7.209e-016	7.228e-016	1.0026	15.141
330	UO2F3	-1		0.000000		5.726e-018	5.134e-018	0.8967	17.290
331	UO2F4	-2		0.000000		3.555e-021	2.298e-021	0.6464	20.639
332	UO2Cl	1		0.000000		5.812e-018	5.211e-018	0.8967	17.283

I	Species		Anal ppm	Calc ppm	Anal molal	Calc molal	Activity	Act coeff	-log Act
333	UO2SO4	0		0.000000		2.670e-016	2.477e-016	1.0026	15.572
334	UO2(SO4)2	-2		0.000000		4.354e-018	3.137e-018	0.6464	17.503
335	UO2HPO4	0		0.000000		4.643e-014	4.655e-014	1.0026	13.332
336	UO2HPO42	-2		0.000077		1.677e-010	1.084e-010	0.6464	9.965
337	UO2H2PO4	1		0.000000		4.428e-019	3.971e-019	0.8967	18.401
338	U2H2P4,2	0		0.000000		3.153e-023	3.161e-023	1.0026	22.500
339	U2H2P4,3	-1		0.000000		8.617e-028	7.727e-028	0.8967	27.112
340	UH3SiO4	1		0.000000		2.967e-014	2.660e-014	0.8967	13.575
0	Ca	2	48.600	44.618	1.213e-003	1.114e-003	7.308e-004	0.6559	3.136
28	CaOH	1		0.000090		1.571e-009	1.409e-009	0.8967	8.851
31	CaSO4 aq	0		7.828		5.755e-005	5.770e-005	1.0026	4.239
29	CaHCO3	1		4.012		3.972e-005	3.561e-005	0.8967	4.448
30	CaCO3 aq	0		0.180		1.800e-006	1.805e-006	1.0026	5.744
100	CaF	1		0.011		1.795e-007	1.609e-007	0.8967	6.793
75	CaH2PO4	1		0.000690		5.035e-009	4.515e-009	0.8967	8.345
73	CaHPO4aq	0		0.006453		4.747e-008	4.759e-008	1.0026	7.322
74	CaPO4	-1		0.000133		9.881e-010	8.860e-010	0.8967	9.053
1	Mg	2	5.400	4.960	2.223e-004	2.042e-004	1.349e-004	0.6607	3.870
18	MgOH	1		0.000076		1.844e-009	1.654e-009	0.8967	8.782
22	MgSO4 aq	0		1.115		9.274e-006	9.299e-006	1.0026	5.032
21	MgHCO3	1		0.710		8.328e-006	7.467e-006	0.8967	5.127
20	MgCO3 aq	0		0.019		2.240e-007	2.245e-007	1.0026	6.649
19	MgF	1		0.011		2.507e-007	2.248e-007	0.8967	6.648
40	MgH2PO4	1		0.000143		1.184e-009	1.061e-009	0.8967	8.974
72	MgHPO4aq	0		0.001424		1.185e-008	1.186e-008	1.0026	7.925
39	MgPO4	-1		0.000029		2.460e-010	2.206e-010	0.8967	9.656
2	Na	1	153.000	152.315	6.660e-003	6.631e-003	5.953e-003	0.8978	2.225
43	NaSO4	-1		1.536		1.291e-005	1.157e-005	0.8967	4.936
42	NaHCO3aq	0		1.338		1.594e-005	1.598e-005	1.0026	4.796
41	NaCO3	-1		0.017		2.109e-007	1.891e-007	0.8967	6.723
297	NaF aq	0		0.000745		1.775e-008	1.779e-008	1.0026	7.750
49	NaHPO4	-1		0.000184		1.552e-009	1.392e-009	0.8967	8.856
3	K	1	11.900	11.867	3.046e-004	3.037e-004	2.718e-004	0.8949	3.566
45	KSO4	-1		0.111		8.218e-007	7.369e-007	0.8967	6.133
60	KHPO4	-1		0.000010		7.086e-011	6.354e-011	0.8967	10.197
63	H	1		0.000141		1.404e-007	1.259e-007	0.8967	6.900
26	OH	-1		0.001459		8.586e-008	7.699e-008	0.8967	7.114
17	CO3	-2		0.161		2.677e-006	1.758e-006	0.6564	5.755
6	HCO3	-1	328.000	323.373	5.380e-003	5.304e-003	4.774e-003	0.9001	2.321
85	H2CO3 aq	0		83.896		1.354e-003	1.358e-003	1.0028	2.867
5	SO4	-2	65.000	57.250	6.772e-004	5.965e-004	3.892e-004	0.6524	3.410
62	HSO4	-1		0.000507		5.231e-009	4.690e-009	0.8967	8.329
61	F	-1	0.550	0.541	2.897e-005	2.850e-005	2.556e-005	0.8967	4.592
125	HF aq	0		0.000094		4.689e-009	4.702e-009	1.0026	8.328
126	HF2	-1		0.000000		5.079e-013	4.554e-013	0.8967	12.342
296	H2F2 aq	0		0.000000		6.052e-017	6.068e-017	1.0026	16.217
4	Cl	-1	94.000	93.990	2.653e-003	2.653e-003	2.374e-003	0.8949	2.624
44	PO4	-3	0.050	0.000000	5.269e-007	1.134e-012	4.250e-013	0.3746	12.372
46	HPO4	-2		0.018		1.855e-007	1.199e-007	0.6464	6.921
47	H2PO4	-1		0.026		2.719e-007	2.438e-007	0.8967	6.613
34	SiO2 tot	0	38.000		6.329e-004				
23	H4SiO4aq	0		60.719		5.323e-004	6.339e-004	1.0026	3.198
24	H3SiO4	-1		0.061		6.451e-007	5.784e-007	0.8967	6.238
25	H2SiO4	-2		0.000001		1.375e-011	8.887e-012	0.6464	11.051
124	SiF6	-2		0.000000		1.089e-028	7.042e-029	0.6464	28.152
86	B tot	0	1.100		1.018e-004				
35	H3BO3 aq	0		6.259		1.013e-004	1.016e-004	1.0026	3.993

I	Species		Anal ppm	Calc ppm	Anal molal	Calc molal	Activity	Act coeff	-log Act
36	H2BO3	-1		0.031		5.159e-007	4.626e-007	0.8967	6.335
101	BF(OH)3	-1		0.000093		1.147e-009	1.026e-009	0.8967	8.988
102	BF2(OH)2	-1		0.000000		3.929e-013	3.523e-013	0.8967	12.453
103	BF3OH	-1		0.000000		1.390e-018	1.246e-018	0.8967	17.904
104	BF4	-1		0.000000		1.811e-023	1.623e-023	0.8967	22.790
37	NH3 aq	0		0.000366		2.150e-008	2.156e-008	1.0026	7.666
38	NH4	1	0.100	0.099	5.548e-006	5.499e-006	4.930e-006	0.8967	5.307
91	NH4SO4	-1		0.003143		2.757e-008	2.472e-008	0.8967	7.607
50	Al	3	0.003000	0.000000	1.113e-007	2.946e-012	1.104e-012	0.3746	11.957
51	AlOH	2		0.000006		1.341e-010	8.671e-011	0.6464	10.062
52	Al(OH)2	1		0.000376		6.165e-009	5.528e-009	0.8967	8.257
181	Al(OH)3	0		0.004296		5.512e-008	5.526e-008	1.0026	7.258
53	Al(OH)4	-1		0.004100		4.319e-008	3.873e-008	0.8967	7.412
54	AlF	2		0.000021		4.465e-010	2.886e-010	0.6464	9.540
55	AlF2	1		0.000277		4.272e-009	3.830e-009	0.8967	8.417
56	AlF3 aq	0		0.000160		1.911e-009	1.916e-009	1.0026	8.718
57	AlF4	-1		0.000003		2.756e-011	2.471e-011	0.8967	10.607
58	AlSO4	1		0.000000		4.986e-013	4.470e-013	0.8967	12.350
59	Al(SO4)2	-1		0.000000		1.538e-014	1.379e-014	0.8967	13.860
16	Fe total	2	0.120		2.150e-006				
7	Fe	2		0.115		2.055e-006	1.328e-006	0.6464	5.877
10	FeOH	1		0.000261		3.584e-009	3.213e-009	0.8967	8.493
79	Fe(OH)2	0		0.000030		2.074e-013	2.079e-013	1.0026	12.682
11	Fe(OH)3	-1		0.000000		6.807e-017	6.104e-017	0.8967	16.214
33	FeSO4 aq	0		0.014		9.086e-008	9.109e-008	1.0026	7.041
99	FeHPO4aq	0		0.000096		6.323e-010	6.340e-010	1.0026	9.198
64	FeH2PO4	1		0.000028		1.810e-010	1.623e-010	0.8967	9.790
8	Fe	3		0.000000		1.938e-021	7.261e-022	0.3746	21.139
9	FeOH	2		0.000000		5.592e-017	3.615e-017	0.6464	16.442
76	Fe(OH)2	1		0.000000		1.092e-013	9.789e-014	0.8967	13.009
77	Fe(OH)3	0		0.000000		9.109e-015	9.133e-015	1.0026	14.039
78	Fe(OH)4	-1		0.000000		8.088e-016	7.252e-016	0.8967	15.140
179	Fe2(OH)2	4		0.000000		2.056e-031	3.590e-032	0.1746	31.445
180	Fe3(OH)4	5		0.000000		1.120e-041	7.325e-043	0.0654	
14	FeSO4	1		0.000000		2.592e-021	2.325e-021	0.8967	20.634
108	Fe(SO4)2	-1		0.000000		3.184e-023	2.855e-023	0.8967	22.544
15	FeCl	2		0.000000		7.928e-023	5.125e-023	0.6464	22.290
27	FeCl2	1		0.000000		6.159e-025	5.522e-025	0.8967	24.258
32	FeCl3 aq	0		0.000000		1.308e-028	1.311e-028	1.0026	27.882
105	FeF	2		0.000000		4.516e-020	2.919e-020	0.6464	19.535
106	FeF2	1		0.000000		3.292e-020	2.952e-020	0.8967	19.530
107	FeF3 aq	0		0.000000		1.191e-021	1.194e-021	1.0026	20.923
12	FeHPO4	1		0.000000		2.571e-023	2.305e-023	0.8967	22.637
98	FeH2PO4	2		0.000000		7.371e-023	4.764e-023	0.6464	22.322

mole ratios from analytical molality

Cl/Ca	=	2.1865e+000
Cl/Mg	=	1.1937e+001
Cl/Na	=	3.9840e-001
Cl/K	=	8.7122e+000
Cl/Al	=	2.3846e+004
Cl/SO4	=	3.9184e+000
Cl/HCO3	=	4.9324e-001
Ca/Mg	=	5.4593e+000
Na/K	=	2.1868e+001

log activity ratios

log Ca/H2	=	10.6638
log Mg/H2	=	9.9300
log Na/H1	=	4.6746
log K /H1	=	3.3343
log Al/H3	=	8.7428
log Ca/Mg	=	0.7338
log Na/K	=	1.3405
log Ca/K2	=	5.9953
log diss Fe/H2	=	13.8000

	phase	log ap/kt	sigma(a)	sigma(t)	log ap/minkt	log ap/maxkt	log ap	log kt	log minkt	log maxkt
551	Uraninite	3.494					-1.183	-4.677		
552	UO2 (a)	-2.117					-1.183	0.934		
553	U409 (c)	7.892				1.429	4.633	-3.259		3.205
554	U308 (c)	-6.070				-12.552	15.180	21.250		34.732
555	Coffinite	5.001					-4.380	-9.382		
562	UF4 (c)	-28.570					-47.152	-18.583		
563	UF4,2.5H2O	-19.583					-47.153	-27.569		
571	U(HPO4)2, 4w	-15.737					-67.326	-51.589		
572	Ningyoite	-2.759					-56.662	-53.903		
577	UO3 (c)	-8.820					-1.077	7.743		
578	Gummite	-11.509					-1.077	10.431		
579	B-UO2(OH)2	-6.638					-1.077	5.561		
580	Schoepite	-6.496					-1.078	5.419		
584	Rutherfordin	-6.171					-20.632	-14.461		
597	(UO2)3(PO4)2	-20.221			59.876		-69.374	-49.154	-129.251	
598	H-Autunite	-20.371					-68.297	-47.927		
599	Na-Autunite	-11.539					-58.948	-47.408		
600	K-Autunite	-13.378					-61.629	-48.251		
601	Uramphite	-13.351					-65.112	-51.761		
602	Saleeite	-14.746					-58.367	-43.621		
603	Autunite	-13.724					-57.634	-43.909		
606	Bassetite	-15.914					-60.374	-44.460		
610	Uranophane	-15.375					2.114	17.489		
39	Adularia	0.040					-20.570	-20.611		
40	Albite	-1.196					-19.230	-18.034		
140	AlOH3 (a)	-1.671			-0.982		-33.298	-31.627	-32.316	
471	AlOHSO4	-5.237			-5.077	-5.397	-8.467	-3.230	-3.390	-3.070
472	Al4(OH)10SO4	-4.940					17.760	22.700		
157	Allophane(a)	-0.833					5.059	5.892		
158	Allophane(F)	-0.029					5.059	5.088		
338	Alum k	-17.165					-22.344	-5.179		
50	Alunite	-3.568					-88.938	-85.371		
42	Analcime	-3.309					-16.032	-12.723		
17	Anhydrite	-1.914					-6.546	-4.632		
113	Annite	88.921					3.199	-85.722		
41	Anorthite	-4.627					-24.355	-19.728		
21	Aragonite	-0.534		0.040			-8.891	-8.357		
150	Artinite	-7.864					1.772	9.635		
48	Beidellite	1.965					-43.382	-45.346		
52	Boehmite	0.133			0.646		-33.298	-33.431	-33.944	
19	Brucite	-6.892					-18.097	-11.205		
12	Calcite	-0.420		0.010	-0.334		-8.891	-8.472	-8.557	
97	Chalcedony	0.331					-3.198	-3.529		
49	Chlorite	-11.045					-100.675	-89.630		
20	Chrysotile	-8.853					-60.687	-51.834		
29	Clinoenstite	-4.628			-4.262	-4.922	-21.295	-16.666	-17.032	-16.372
56	Clinoptilolt						-24.504			
99	Cristobalite	0.396					-3.198	-3.594		
154	Diaspore	1.842					-33.293	-35.140		
28	Diopside	-5.724					-41.856	-36.132		
11	Dolomite	-1.527					-18.516	-16.990		
340	Epsomite	-5.137					-7.281	-2.143		
55	Erionite						-20.829			
112	Ferrihydrite	-5.330			-1.926	-5.455	-0.459	4.891	1.557	4.996
419	Fe3(OH)8	-13.178			-10.068	-17.061	7.044	20.222	17.112	24.105
181	FeOH)2.7Cl.3	-0.257					-3.297	-3.040		
401	Fe2(SO4)3	-56.160			-51.930		-52.508	3.655	-0.577	