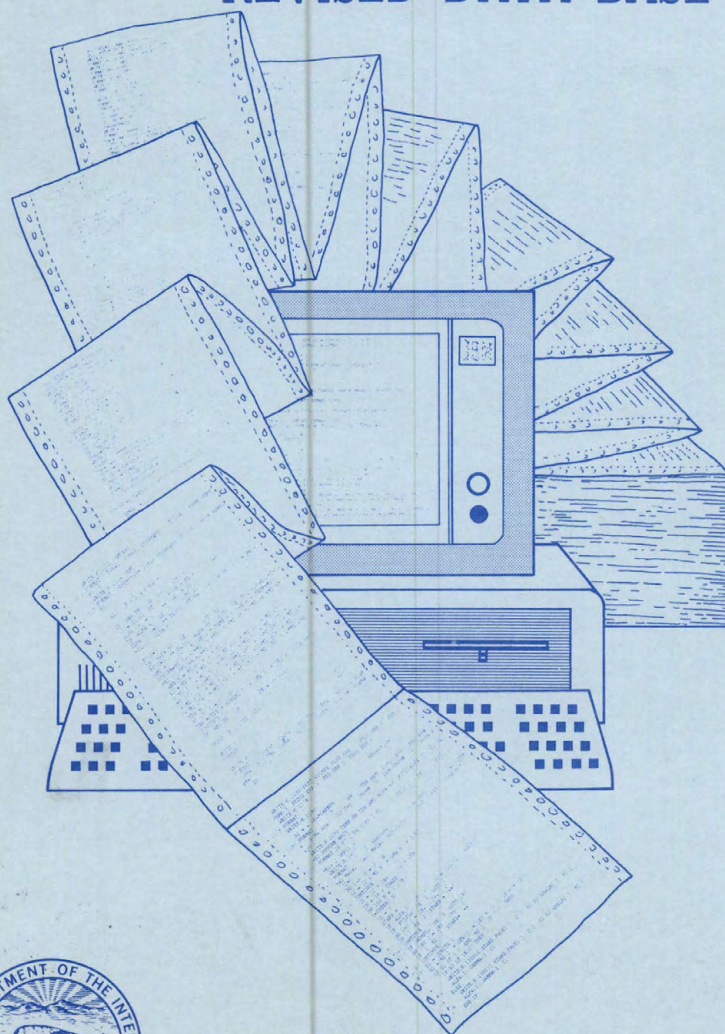


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WATEQ4F--

A PERSONAL COMPUTER FORTRAN TRANSLATION  
OF THE  
GEOCHEMICAL MODEL WATEQ2  
WITH  
REVISED DATA BASE



U.S. GEOLOGICAL SURVEY

Open-File Report 87-50





WATEQ4F--A PERSONAL COMPUTER FORTRAN TRANSLATION OF THE  
GEOCHEMICAL MODEL WATEQ2 WITH REVISED DATA BASE

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U.S. GEOLOGICAL SURVEY

Open-File Report 87-50



Menlo Park, California

1987

DEPARTMENT OF THE INTERIOR  
DONALD PAUL HODEL, Secretary  
U.S. GEOLOGICAL SURVEY  
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## CONVERSION FACTORS AND ABBREVIATIONS

Metric (International system) units are used in this report. For readers who prefer inch-pound units, the conversion factors for the terms used in this report are listed below.

| <u>Multiply metric units</u>        | <u>By</u>                | <u>To obtain inch-pound units</u> |
|-------------------------------------|--------------------------|-----------------------------------|
| cal (calorie)                       | 0.003968                 | Btu (British thermal unit)        |
| cm <sup>2</sup> (square centimeter) | 0.1550                   | in <sup>2</sup> (square inch)     |
| L (liter)                           | 0.2642                   | gal (gallon)                      |
| mg (milligram)                      | 3.520 X 10 <sup>-5</sup> | oz (ounce)                        |

### Explanation of abbreviations:

°C (degrees Celsius)  
 cu ft sec<sup>-1</sup> (cubic feet per second)  
 kcal (kilocalories)  
 mg L<sup>-1</sup> (milligrams per liter)  
 mol (molar, moles per liter)  
 μS (microSiemens, reciprocal megohms)



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ABSTRACT

A FORTRAN 77 version of the PL/1 computer program for the geochemical model WATEQ2, which computes major and trace element speciation and mineral saturation for natural waters, has been developed. The code (WATEQ4F) has been adapted to execute on an IBM PC<sup>1</sup> or compatible microcomputer. Two versions of the code are available, one operating with IBM Professional FORTRAN and an 8087 or 80287 numeric coprocessor, and one which operates without a numeric coprocessor using Microsoft FORTRAN 77. The calculation procedure is identical to WATEQ2, which has been installed on many mainframes and minicomputers. Limited data base revisions include the addition of the following ion pairs:  $\text{AlHSO}_4^{2+}$ ,  $\text{BaSO}_4^0$ ,  $\text{CaHSO}_4^+$ ,  $\text{FeHSO}_4^+$ ,  $\text{FeHSO}_4^{2+}$ ,  $\text{NaF}^0$ ,  $\text{SrCO}_3^0$ , and  $\text{SrHCO}_3^+$ . This report provides the reactions and references for the data base revisions, instructions for program operation, and an explanation of the input and output files. Attachments contain sample output from three water analyses used as test cases and the complete FORTRAN source listing. U.S. Geological Survey geochemical simulation program PHREEQE and mass balance program BALANCE also have been adapted to execute on an IBM PC or compatible microcomputer with a numeric coprocessor and the IBM Professional FORTRAN compiler.

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<sup>1</sup>The use of trade, brand or product names in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.





## INTRODUCTION

The original computer program, WATEQ (Truesdell and Jones, 1974) written in PL/1 and designed for aqueous speciation calculations of natural waters, has been translated into FORTRAN IV (WATEQF, Plummer and others, 1976), trace elements have been added (WATEQ2, Ball and others, 1979, 1980), uranium species added (WATEQ3, Ball and others, 1981), and additional recommendations for the data base have been made, primarily on the aqueous aluminum species and forms of gibbsite (Nordstrom and others, 1984). This report describes a FORTRAN 77 version of WATEQ2 that has been adapted for operation on a personal microcomputer with math coprocessor and Professional FORTRAN compiler, and is named WATEQ4F. This program is intended to be used with the reports of Ball and others (1979, 1980) as a source of program documentation, except for the source listing, which is included in this report. Additional changes to the data base have been included and the printed output has been upgraded to be displayed in upper/lower case. The original translation of WATEQ2 into FORTRAN 77 was made by Zachmann and Baethge (written commun., January, 1985).

The geochemical simulation program PHREEQE (Parkhurst and others, 1980) and the mass balance program BALANCE (Parkhurst and others, 1982) have been similarly adapted for execution on an IBM Personal Computer. The reader is referred to the reports of Parkhurst and others (1980, 1982) for full instructions on the operation of PHREEQE and BALANCE. Otherwise, similarly to WATEQ4F, the requirements are a suitably configured IBM PC or compatible with math coprocessor, the PHREEQE or BALANCE program, and, if recompilation is desired, the IBM Professional FORTRAN compiler.

## THERMODYNAMIC DATA

The number assigned to the specific chemical reaction used in the computer code, the reaction, selected enthalpy ( $\Delta H_r^\circ$ ) and equilibrium reaction constant ( $\log K_r$ ) values, and the sources of the thermodynamic data are given in Table 1. Reactions not shown in Table 1 are unchanged from their coding in WATEQ2 (Ball and others, 1980). The barium hydrolysis reaction has been rewritten in terms of  $H^+$  and  $H_2O$ , from  $OH^-$ . The most precise and internally consistent sets of data available for the solubility product constants and ion association constants in the  $CaCO_3$ - $CO_2$ - $H_2O$  system and in the  $SrCO_3$ - $CO_2$ - $H_2O$  system are those of Plummer and Busenberg (1982) and Busenberg and others (1984), respectively. These data are included in WATEQ4F. Thermodynamic data revisions for gypsum, talc, sepiolite, muscovite, and chlorite were made but the use of ion activity product (IAP) calculations for the silicate minerals is rather controversial at this time. Bisulfate ion association constants are given or estimated for  $Fe^{2+}$ ,  $Fe^{3+}$ ,  $Ca^{2+}$ , and  $Al^{3+}$  because of their importance in very acid waters such as some mine waters issuing from oxidizing ore deposits.

Table 1. Additional and Revised Thermodynamic Data

$\Delta H_r^\circ$  is enthalpy of reaction;  $\log K_r^\circ$  is equilibrium constant for the reaction;  
 $\text{kcal mol}^{-1}$  is kilocalories per mole;  $1\sigma$  is the uncertainty in the listed value.

| I <sup>6</sup> | Species<br>Name                    | Reaction                                                                                                                                                           | $\Delta H_r^\circ$<br>(kcal mol <sup>-1</sup> ) | Source           | $\log K_r^\circ \pm 1\sigma$ | Source           |
|----------------|------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|------------------|------------------------------|------------------|
| 12             | Calcite                            | $\text{CaCO}_3 = \text{Ca}^{2+} + \text{CO}_3^{2-}$                                                                                                                | -2.585 <sup>2</sup>                             | 1                | -8.48±0.02                   | 1                |
|                |                                    | $\log K_r = -171.9065 - 0.077993T + 2839.319/T + 71.595\log_{10}T$                                                                                                 |                                                 |                  |                              |                  |
| 18             | Gypsum                             | $\text{CaSO}_4 = \text{Ca}^{2+} + \text{SO}_4^{2-}$                                                                                                                | 0.27                                            | 18               | -4.60±0.02                   | 2, 13, 14, 15    |
| 21             | Aragonite                          | $\text{CaCO}_3 = \text{Ca}^{2+} + \text{CO}_3^{2-}$                                                                                                                | -2.615 <sup>2</sup>                             | 1                | -8.34±0.02                   | 1                |
|                |                                    | $\log K_r = -171.9773 - 0.077993T + 2903.293/T + 71.595\log_{10}T$                                                                                                 |                                                 |                  |                              |                  |
| 35             | kH <sub>2</sub> CO <sub>3</sub> aq | $\text{HCO}_3^- + \text{H}^+ = \text{H}_2\text{CO}_3^0$                                                                                                            | -2.247 <sup>2</sup>                             | 1                | 6.351                        | 1                |
|                |                                    | $\log K_r = 356.3094 + 0.0609196T - 21834.37/T - 126.8339\log_{10}T + 1684915/T^2$                                                                                 |                                                 |                  |                              |                  |
| 36             | Sepiolite(c)                       | $\text{Mg}_2\text{Si}_3\text{O}_{7.5}(\text{OH}) \cdot 3\text{H}_2\text{O} + 0.5\text{H}_2\text{O} + 4\text{H}^+ = 2\text{Mg}^{2+} + 3\text{H}_4\text{SiO}_4^0$    | -26.486                                         | 3                | 15.364                       | 3                |
| 37             | Talc                               | $\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2 + 4\text{H}_2\text{O} + 6\text{H}^+ = 3\text{Mg}^{2+} + 4\text{H}_4\text{SiO}_4^0$                               | -46.352                                         | 4                | 21.399                       | 4                |
| 43             | Kmica                              | $\text{KAl}_3\text{Si}_3\text{O}_{10}(\text{OH})_2 + 10\text{H}^+ = \text{K}^+ + 3\text{Al}^{3+} + 3\text{H}_4\text{SiO}_4^0$                                      | -59.376                                         | 4                | 12.703                       | 4                |
| 49             | Chlorite 14A                       | $\text{Mg}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_8 + 6\text{H}_2\text{O} + 16\text{H}^+ = 5\text{Mg}^{2+} + 2\text{Al}^{3+} + 3\text{H}_4\text{SiO}_4^0$ | -151.494                                        | 5                | 68.380±6.0                   | 5                |
| 68             | kHCO <sub>3</sub> -                | $\text{H}^+ + \text{CO}_3^{2-} = \text{HCO}_3^-$                                                                                                                   | -3.167 <sup>2</sup>                             | 1                | 10.330                       | 1                |
|                |                                    | $\log K_r = 107.8871 + 0.03252849T - 5151.79/T - 38.92561\log_{10}T + 563713.9/T^2$                                                                                |                                                 |                  |                              |                  |
| 77             | kCaHCO <sub>3</sub> +              | $\text{Ca}^{2+} + \text{HCO}_3^- = \text{CaHCO}_3^+$                                                                                                               | 5.410 <sup>2</sup>                              | 1                | 1.11±0.07                    | 1                |
|                |                                    | $\log K_r = 1209.12 + 0.31294T - 34765.05/T - 478.782\log_{10}T$                                                                                                   |                                                 |                  |                              |                  |
| 78             | kCaCO <sub>3</sub> aq              | $\text{Ca}^{2+} + \text{CO}_3^{2-} = \text{CaCO}_3^0$                                                                                                              | 4.030 <sup>2</sup>                              | 1                | 3.22±0.14                    | 1                |
|                |                                    | $\log K_r = -1228.732 - 0.299444T + 35512.75/T + 485.818\log_{10}T$                                                                                                |                                                 |                  |                              |                  |
| 79             | kSrHCO <sub>3</sub> +              | $\text{Sr}^{2+} + \text{HCO}_3^- = \text{SrHCO}_3^+$                                                                                                               | 6.047 <sup>2</sup>                              | 6                | 1.18                         | 6                |
|                |                                    | $\log K_r = -3.248 + 0.014867T$                                                                                                                                    |                                                 |                  |                              |                  |
| 125            | Chlorite 7A                        | $\text{Mg}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_8 + 6\text{H}_2\text{O} + 16\text{H}^+ = 5\text{Mg}^{2+} + 2\text{Al}^{3+} + 3\text{H}_4\text{SiO}_4^0$ | -155.261                                        | 5                | 71.752±6.0                   | 5                |
| 130            | kBaOH +                            | $\text{Ba}^{2+} + \text{H}_2\text{O} = \text{BaOH}^+ + \text{H}^+$                                                                                                 | 15.095                                          | --- <sup>1</sup> | -13.357                      | --- <sup>1</sup> |
| 135            | kSrCO <sub>3</sub> aq              | $\text{Sr}^{2+} + \text{CO}_3^{2-} = \text{SrCO}_3^0$                                                                                                              | 5.217 <sup>2</sup>                              | 6                | 2.81                         | 6                |
|                |                                    | $\log K_r = -1.019 + 0.012826T$                                                                                                                                    |                                                 |                  |                              |                  |
| 142            | Strontianite                       | $\text{SrCO}_3 = \text{Sr}^{2+} + \text{CO}_3^{2-}$                                                                                                                | -0.401 <sup>2</sup>                             | 6                | -9.271±0.02                  | 6                |
|                |                                    | $\log K_r = 155.0305 - 7239.594/T - 56.58638\log_{10}T$                                                                                                            |                                                 |                  |                              |                  |
| 148            | kFeHSO <sub>4</sub> +              | $\text{Fe}^{2+} + \text{HSO}_4^- = \text{FeHSO}_4^+$                                                                                                               | --- <sup>4</sup>                                | --- <sup>4</sup> | 1.08                         | 7                |
| 153            | Sepiolite(a)                       | $\text{Mg}_2\text{Si}_3\text{O}_{7.5}(\text{OH}) \cdot 3\text{H}_2\text{O} + 0.5\text{H}_2\text{O} + 4\text{H}^+ = 2\text{Mg}^{2+} + 3\text{H}_4\text{SiO}_4^0$    | --- <sup>4</sup>                                | --- <sup>4</sup> | 18.66                        | 8                |
| 159            | kFeHSO <sub>4</sub> + 2            | $\text{Fe}^{3+} + \text{HSO}_4^- = \text{FeHSO}_4^{2+}$                                                                                                            | --- <sup>4</sup>                                | --- <sup>4</sup> | 2.48                         | 7, 16            |
| 168            | kCaHSO <sub>4</sub> +              | $\text{Ca}^{2+} + \text{HSO}_4^- = \text{CaHSO}_4^+$                                                                                                               | --- <sup>4</sup>                                | --- <sup>4</sup> | 1.08                         | --- <sup>5</sup> |

Table 1. Additional and Revised Thermodynamic Data (continued)

| I <sup>6</sup> | Species<br>Name                                  | Reaction                                                                                               | $\Delta H_f^\circ$<br>(kcal mol <sup>-1</sup> ) | Source           | Log K <sub>r</sub> <sup>o</sup> ± 1σ | Source           |
|----------------|--------------------------------------------------|--------------------------------------------------------------------------------------------------------|-------------------------------------------------|------------------|--------------------------------------|------------------|
| 397            | kAlHSO <sub>4</sub> +2                           | Al <sup>3+</sup> + HSO <sub>4</sub> <sup>-</sup> = AlHSO <sub>4</sub> <sup>2+</sup>                    | --- <sup>4</sup>                                | --- <sup>4</sup> | 0.46                                 | 17               |
| 538            | Blank                                            | --- <sup>3</sup>                                                                                       | --- <sup>3</sup>                                | --- <sup>3</sup> | --- <sup>3</sup>                     | --- <sup>3</sup> |
| 539            | Blank                                            | --- <sup>3</sup>                                                                                       | --- <sup>3</sup>                                | --- <sup>3</sup> | --- <sup>3</sup>                     | --- <sup>3</sup> |
| 540            | kNaF aq                                          | Na <sup>+</sup> + F <sup>-</sup> = NaF <sup>o</sup>                                                    | --- <sup>4</sup>                                | --- <sup>4</sup> | -0.932                               | 9                |
| 541            | Ba <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub> | Ba <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub> = 3Ba <sup>2+</sup> + 2AsO <sub>4</sub> <sup>3-</sup> | 9.5                                             | 10,11            | -50.11                               | 12               |
| 542            | Blank                                            | --- <sup>3</sup>                                                                                       | --- <sup>3</sup>                                | --- <sup>3</sup> | --- <sup>3</sup>                     | --- <sup>3</sup> |
| 543            | kBaSO <sub>4</sub> aq                            | Ba <sup>2+</sup> + SO <sub>4</sub> <sup>2-</sup> = BaSO <sub>4</sub> <sup>o</sup>                      | --- <sup>4</sup>                                | --- <sup>4</sup> | 2.7                                  | 2                |

Footnotes to Table 1

<sup>1</sup>Reaction rewritten to be in terms of H<sup>+</sup> and H<sub>2</sub>O.

<sup>2</sup>Enthalpy derived from the temperature variation of log K using the vant Hoff relation.

<sup>3</sup>Not presently used.

<sup>4</sup>No thermodynamic data are presently available.

<sup>5</sup>Assumes that divalent metal bisulfate ion pair stability constants are approximately equivalent (see Mattigod and Sposito, 1977). No reliable data exist.

<sup>6</sup>Reaction number.

Data sources for Table 1

1. Plummer and Busenberg (1982)
2. Smith and Martell (1976)
3. Helgeson and Kirkham (1974)
4. Robie and others (1978)
5. Helgeson and others (1978)
6. Busenberg and others (1984)
7. Mattigod and Sposito (1977)
8. Wollast and others (1968)
9. Miller and Kester (1976)
10. Wagman and others (1968)
11. Parker and others (1971)
12. Sillen and Martell (1964)
13. Nordstrom and Munoz (1986), p. 372-374
14. Pitzer (1979)
15. Bennett and Adams (1972)
16. Sykes (1957)
17. Akitt and others (1969)
18. Marshall and Slusher (1966)



## PROGRAM OPERATION

The program is written in FORTRAN 77, and requires a numeric coprocessor and IBM Personal Computer Professional FORTRAN, Version 1.00 or later, by Ryan-McFarland Corporation. The minimum configuration required is an IBM PC or full compatible with a numeric coprocessor and at least 512K bytes of random access memory (RAM) and a 5M byte or larger hard disk. For linking of the object code, the IBM Personal Computer Linker supplied with Professional FORTRAN is required. It was found by experiment that a substitute Microsoft linker produced an object code that would not execute. The program described in this report has been compiled, linked, and executed correctly on an IBM PC/AT with 640K of RAM, an 80287 numeric coprocessor, and a 20MB hard disk; it also has been compiled, linked, and executed correctly on an AT&T 6300 with 640K RAM, an 8087 numeric coprocessor, and a 20MB hard disk.

The executable code occupies about 232K of disk storage. The test cases were solved on the PC/AT in an average time of less than 20 seconds each, including output of the results to a disk file. This should represent an upper limit of execution time, since particularly the first test case contains a fairly comprehensive array of constituents and output options. The size of the output file is quite variable, depending upon the complexity of the input and the print options selected, but will occupy approximately 25-50K of disk storage per data set. The calculations done on the PC are virtually identical to those done by the same code on the U.S. Geological Survey Prime 850 minicomputer, exhibiting minor variations in the fifth decimal place or so for a small minority of numbers.

### Input

The data base for the calculation of mineral and solute reactions and their accompanying thermodynamic data is read initially, from four separate files, named TABLE1, TABLE2, TABLE3, and TABLE4. This change facilitates future expansion of the data base, in that species merely need to be appended to their respective file, rather than the file having to be expanded in the middle for insertion of data.

User-supplied input of water analyses to WATEQ4F is read from a disk file that must be named WATEQ4F.DAT. The input format has been modified extensively to conform to constraints in the FORTRAN language, as compared to PL/1. To facilitate preparation of input data sets, a separate computer program (WQ4FINPT--An interactive computer program for constructing input data sets to the geochemical modeling program WATEQ4F) has been written by Ball, J. W. (written commun., 1987). The number of records per input data set is not fixed.

The description of the input variables is the same as for WATEQ2, found in Ball and others, 1980. A list of all the optional analytical input constituents and their assigned reference numbers is in Table 2. The required input is as follows:

| Record                         | Variable Name       | Variable                                                                                                            | FORTTRAN Format | Comments                                |
|--------------------------------|---------------------|---------------------------------------------------------------------------------------------------------------------|-----------------|-----------------------------------------|
| 1                              | CHECK               | start-of-data-set record                                                                                            | A4              | four asterisks                          |
| 2                              | CARD1               | sample description                                                                                                  | A80             |                                         |
| 3                              | CARD2               | Physical parameters carried through to plot program:                                                                |                 |                                         |
|                                |                     | conductivity                                                                                                        | F5.0            | $\mu\text{S cm}^{-2}$ at 25°C           |
|                                |                     | total dissolved solids                                                                                              | F6.0,1X         | parts per million                       |
|                                |                     | date, year, month, day                                                                                              | F6.0            | yymmdd                                  |
|                                |                     | discharge                                                                                                           | F8.0            | $\text{cu ft sec}^{-1}$                 |
|                                |                     | dissolved organic carbon                                                                                            | F8.0            | $\text{mg L}^{-1}$                      |
|                                |                     | salinity                                                                                                            | F8.0            | parts per thousand                      |
|                                |                     | time, day.hour                                                                                                      | F8.0            | dd.hhhh                                 |
| 4                              |                     | dummy record                                                                                                        | A80             | ignored by program                      |
| 5                              | TEMP                | temperature                                                                                                         | F8.2,1X         | °C                                      |
|                                | PH                  | pH, measured in field                                                                                               | F8.2,1X         |                                         |
|                                | EHM                 | Eh, measured in field                                                                                               | F8.2,1X         | volts <sub>1</sub>                      |
|                                | DOC                 | dissolved organic carbon                                                                                            | F8.2,1X         | $\text{mg L}^{-1}$                      |
|                                | DOX                 | dissolved oxygen                                                                                                    | F8.2,1X         | $\text{mg L}^{-1}$                      |
|                                | CORALC              | alkalinity correction flag                                                                                          | F8.2,1X         | 0, 1 or 2                               |
| 6                              |                     | dummy record                                                                                                        | A80             | ignored by program                      |
| 7                              | FLG                 | units in which remaining concentrations are expressed                                                               | A4              | options: MQ/L, MG/L, PPM, MOL           |
|                                | DENS                | density                                                                                                             | F11.5           |                                         |
|                                | PRNT                | print option                                                                                                        | I6              | 0, 1, 2, or 3                           |
|                                | PUNCH               | punch option                                                                                                        | I6              | 0 or 1                                  |
|                                | EHOPT               | Eh option                                                                                                           | I6              | 0 or 1                                  |
| 8                              |                     | dummy record                                                                                                        | A80             | ignored by program                      |
| 9                              | EMPOX               | dissolved oxygen treatment                                                                                          | I8              | 0 or 1                                  |
|                                | ITDS                | analytical TDS                                                                                                      | F8.2,1X         | parts per million                       |
|                                | COND                | specific conductance                                                                                                | F8.2,1X         | $\mu\text{S cm}^{-2}$ at 25°C           |
|                                | SIGMDO              | dissolved oxygen sigma                                                                                              | F12.4           |                                         |
|                                | SIGMEH              | Eh sigma                                                                                                            | F12.4           |                                         |
|                                | SIGMPH              | pH sigma                                                                                                            | F12.4           |                                         |
| 10                             |                     | dummy record                                                                                                        | A80             | ignored by program                      |
| 11                             | CUNITS(I)           | Ca, Mg, Na, K, Cl, SO <sub>4</sub>                                                                                  | 6F12.4          | in FLG units                            |
| 12                             |                     | dummy record                                                                                                        | A80             | ignored by program                      |
| 13                             | CUNITS(I)           | HCO <sub>3</sub> , Fe <sub>tot</sub> , H <sub>2</sub> S, CO <sub>3</sub> , SiO <sub>2</sub> , NH <sub>4</sub>       | 6F12.4          | in FLG units                            |
| 14                             |                     | dummy record                                                                                                        | A80             | ignored by program                      |
| 15                             | CUNITS(I)           | B <sub>tot</sub> , PO <sub>4</sub> , Al, F, NO <sub>3</sub>                                                         | 5F12.4          | in FLG units                            |
| 16                             |                     | dummy record                                                                                                        | A80             | ignored by program                      |
| 17 to n-1, where               |                     | additional concentration values, sigma values, or replacement log <sub>10</sub> K <sub>r</sub> <sup>o</sup> values: |                 |                                         |
| n=# of records in the data set | WORD                | record type identifier                                                                                              | A4,1X           | 'CUN ', 'SIGM', 'LOKT'                  |
|                                | J                   | subscript                                                                                                           | I3,1X           | 0 to 543                                |
|                                | CUNITS(J)           | concentration, sigma, or log <sub>10</sub> K <sub>r</sub> <sup>o</sup> values                                       | F12.5           | numerical value for referenced quantity |
|                                | SIGMA(J), LOGKTO(J) |                                                                                                                     |                 |                                         |
| n                              |                     | blank-final record in a data set                                                                                    |                 | REQUIRED                                |

Table 2. Reference Numbers for Optional Analytical Input Constituents

| Number | Constituent | Ionic Charge | Number | Constituent         | Ionic Charge |
|--------|-------------|--------------|--------|---------------------|--------------|
| 7      | Fe          | 2            | 145    | Zn                  | 2            |
| 8      | Fe          | 3            | 160    | Cd                  | 2            |
| 48     | Cs          | 1            | 182    | Pb                  | 2            |
| 80     | Li          | 1            | 202    | NO <sub>2</sub>     | -1           |
| 87     | Sr          | 2            | 204    | Ni                  | 2            |
| 89     | Ba          | 2            | 212    | Ag                  | 1            |
| 94     | Rb          | 1            | 249    | As total            | 0            |
| 96     | I           | -1           | 261    | As <sup>3</sup> tot | 0            |
| 97     | Br          | -1           | 262    | As <sup>5</sup> tot | 0            |
| 109    | Mn          | 2            | 284    | Fulvate             | -2           |
| 130    | Cu          | 2            | 285    | Humate              | -2           |
|        |             |              | 298    | Se Total            | 0            |

### Output

The following information is initially output by WATEQ4F: the permanent data base is written in tabular form, followed by a table of the analytical expressions for the temperature dependence of selected equilibrium constants, and by a listing of the names and reference numbers of all possible analytical input constituents. This information is written into a separate file, named TABLES.OUT, on the default disk drive, for later printing at the user's convenience.

For the water analysis data, output is placed in a disk file named WATEQ4F.OUT. First, a listing of the input data is written, which includes the species name, index number, and input concentration of each species, as well as the values of all other parameters entered. Results of the anion mass balance calculations follow in the form: CO<sub>2</sub>, SO<sub>4</sub>, F, PO<sub>4</sub>, Cl, H<sub>2</sub>S, fulvic, and humic. When mass balance convergence to within 0.1 percent is obtained (or 40 iterations have been done), a table of distribution of aqueous species is written. If convergence to 0.1 percent or better is not obtained after 40 iterations, a warning message is printed and execution continues as though convergence were obtained. Both the sums of analytical and calculated equivalents per million cation and anion values, and analytical and calculated specific conductance are listed for comparison. The percent differences in the input and calculated charge balances are computed and displayed. The total (based on the input data) and the effective (calculated after speciation) ionic strengths are displayed for comparison. Numerous input and calculated solution parameters are also listed, including temperature, pH, and Eh and pE calculated using various redox couples. The concentration of each aqueous species with a value greater than zero is listed in parts per million, molality, and activity, as well as the individual ion activity coefficient used and the negative log activity of each species. This is followed by a table of analytical molality ratios and log activity ratios. A table follows of the mineral equilibrium calculations, printed in the following order: the reaction number, the name of the solid phase, the computed saturation index

( $\log_{10}(\text{IAP}/K)$ ), the analytical propagated standard deviation in the  $\log_{10}$  of the activity product, the uncertainty in the  $\log_{10}$  of the equilibrium constant, the maximum and minimum saturation indices ( $\log_{10}(\text{IAP}/\text{MaxKT})$  and  $\log_{10}(\text{IAP}/\text{MinKT})$ ) which are computed using alternate literature values for the equilibrium constants, the  $\log_{10}(\text{AP})$ ,  $\log_{10}(\text{KT})$ ,  $\log_{10}(\text{MinKT})$ , and  $\log_{10}(\text{MaxKT})$ . This information is listed for each solid phase for which an activity product has been calculated. All the above is written to disk for subsequent printing at the user's convenience.

#### TEST CASES AND PROGRAM LISTING

Attachment A contains a listing of the output from WATEQ4F of calculations for the same three test cases appearing in Ball and others (1980), the first two of which also appear in Nordstrom and others (1979). Test case 1 is a seawater analysis, which contains concentrations for virtually every species available for consideration by WATEQ4F, and is of relatively high (0.7) ionic strength. Test case 2 is a surface water analysis and is much more dilute, but also contains a fairly complete array of analytical values. These two test cases are described in more detail by Nordstrom and others (1979). Test case 3 is the analysis of an acidic volcanic condensate, and is a demonstration of extremes of high ionic strength (1.4) and very low pH (0.3) at which the model can still be solved.

Attachment B gives a listing of the FORTRAN source code.

#### PROGRAM PHREEQE

PHREEQE (Parkhurst and others, 1980) is a FORTRAN 77 computer program designed to model geochemical reactions, and is, like WATEQ4F, based on an ion pairing aqueous model. This program can calculate pH, redox potential, and mass transfer as a function of reaction progress, and can calculate the composition of solutions in equilibrium with multiple phases. PHREEQE is an attractive alternative tool for the interpretation and investigation of geochemical processes, and was well-suited to adaptation for execution on a microcomputer. Thus, PHREEQE was modified to be run on an IBM PC or compatible with an 8087 or 80287 numeric coprocessor, using the report of Parkhurst and others (1980) as a source of program documentation and running instructions.

#### PROGRAM BALANCE

PC BALANCE is a FORTRAN 77 computer program adapted from the mainframe version of BALANCE (Parkhurst and others, 1982). BALANCE calculates the mass transfer (amounts of solid or gaseous phases entering or leaving the aqueous phase) necessary to account for the observed change in composition between two solutions. The program can also help to define and quantify chemical reactions that take place between groundwater and minerals. BALANCE is also particularly well-suited for execution on a microcomputer. Program documentation and running instructions can be found in Parkhurst and others (1982).

## SUMMARY

The WATEQ2 geochemical model by Ball and others, the PHREEQE geochemical reaction simulation program by Parkhurst and others, and the BALANCE mass transfer calculation program by Parkhurst and others have been translated into IBM Professional FORTRAN, and adapted for operation on an IBM or compatible personal microcomputer with an 8087 math coprocessor. This WATEQ version is called WATEQ4F. The codes are known to execute correctly on an IBM PC/AT with 20MB hard disk and 640K RAM, and on an identically configured AT&T 6300, Zenith XT-compatible, or Stanford turbo-XT clone. For WATEQ4F, the data base and computer code have been revised from WATEQ2, and several changes in the output, primarily of a cosmetic nature, have been made. WATEQ4F, PC PHREEQE and PC BALANCE are available by contacting the senior author.



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Attachment A. Test cases

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```

0      0 000000      0      0 35.147      0
      TEMP      =      25.000000
      PH      =      8.220000
      EHM      =      0.500000
      DOC      =      0.000000
      DOX      =      6.600000
      CORALC    =      0.000000
      FLG      =      PPM
      DENS      =      1.023360
      PRNT      =      0
      PUNCH      =      1
      EHPT      =      0
      EMPOX      =      0
      ITDS      =      0.000000
      COND      =      0.000000
      SIGMDO     =      0.000000
      SIGMEH     =      0.000000
      SIGMPH     =      0.000000

```

| Species  | Index No | Input Concentration |
|----------|----------|---------------------|
| Ca       | : 0 :    | 412.30000000        |
| Mg       | : 1 :    | 1291.80000000       |
| Na       | : 2 :    | 10768.00000000      |
| K        | : 3 :    | 399.10000000        |
| Cl       | : 4 :    | 19353.00000000      |
| SO4      | : 5 :    | 2712.00000000       |
| HCO3     | : 6 :    | 141.68200000        |
| Fe total | : 16 :   | 0.00200000          |
| H2S aq   | : 13 :   | 0.00000000          |
| CO3      | : 17 :   | 0.00000000          |
| SiO2 tot | : 34 :   | 4.28000000          |
| NH4      | : 38 :   | 0.29000000          |
| B tot    | : 86 :   | 4.45000000          |
| PO4      | : 44 :   | 0.06000000          |
| Al       | : 50 :   | 0.00200000          |
| F        | : 61 :   | 1.39000000          |
| NO3      | : 84 :   | 0.29000000          |
| Cs       | : 48 :   | 0.00040000          |
| Li       | : 80 :   | 0.18100000          |
| Sr       | : 87 :   | 8.14000000          |
| Ba       | : 89 :   | 0.02000000          |
| Rb       | : 94 :   | 0.11700000          |
| I        | : 96 :   | 0.06200000          |
| Br       | : 97 :   | 67.30000000         |
| Mn       | : 109 :  | 0.00020000          |
| Cu       | : 130 :  | 0.00070000          |
| Zn       | : 145 :  | 0.00490000          |
| Cd       | : 160 :  | 0.00010000          |
| Pb       | : 182 :  | 0.00005000          |
| NO2      | : 202 :  | 0.02000000          |
| Ni       | : 204 :  | 0.00170000          |
| Ag       | : 212 :  | 0.00004000          |
| As total | : 249 :  | 0.00400000          |

DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data

A5

0 0 000000 0 0 35.147 0

| ITER | S1-AnalCO3    | S2-AnalSO4    | S3-AnalF      | S4-AnalPO4   | S5-AnalCL     | S6-AnalH2S   | S7-AnalFULV  | S8-AnalHUM   |
|------|---------------|---------------|---------------|--------------|---------------|--------------|--------------|--------------|
| 1    | 1.187580E-03  | 2.371452E-02  | 6.770372E-05  | 3.128672E-06 | 3.194115E-08  | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 2    | 6.155865E-05  | 1.231458E-03  | 3.007505E-06  | 2.486154E-08 | 6.792302E-09  | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 3    | -8.660313E-07 | -6.992563E-05 | 2.075554E-07  | 6.378900E-09 | 6.350011E-10  | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 4    | -4.268398E-07 | -1.129203E-05 | -6.697297E-09 | 1.994747E-10 | -3.997035E-11 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |

DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data A5 Date = 9/12/86 9:56

0 0 000000 0 0 35.147 0  
 DOX = 6.6000 DOC = 0.0 INPUT TDS = 0.0  
 Anal Cond = 0.0 Calc Cond = 46744.4  
 Anal EPMCAT = 627.7348 Anal EPMAN = 627.6592 Percent difference in input cation/anion balance = 0.0120  
 Calc EPMCAT = 606.1146 Calc EPMAN = 606.0351 Percent difference in calc cation/anion balance = 0.0131  
 Total Ionic Strength (T.I.S.) from input data = 0.72279  
 Effective Ionic Strength (E.I.S.) from speciation = 0.67994

| Sato  |       |         |       | Calc    |       |         |       |         |       |         |       |         |       |         |       |
|-------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|
| Input | Sigma | Fe3/Fe2 | Sigma | H2O2/O2 | Sigma | NO3/NO2 | Sigma | NO3/NH4 | Sigma | H2O2/O2 | Sigma | SO4/S=  | Sigma | As5/As3 | Sigma |
| 0.500 | 0.000 | 0.500   | 0.000 | 0.133   | 0.000 | 0.390   | 0.000 | 0.269   | 0.000 | 0.731   | 0.000 | 9.900   | 0.000 | 0.500   | 0.000 |
| pE    |       |         |       |         |       |         |       |         |       |         |       |         |       |         |       |
| 8.451 | 0.000 | 8.451   | 0.000 | 2.248   | 0.000 | 6.585   | 0.000 | 4.551   | 0.000 | 12.358  | 0.000 | 100.000 | 0.000 | 8.451   | 0.000 |

| Effective |       |         |           |          |          |          |         |           |               |          |        |
|-----------|-------|---------|-----------|----------|----------|----------|---------|-----------|---------------|----------|--------|
| T         | pH    | TDS ppm | Ionic Str | pO2 Atm  | pCO2 Atm | pCH4 Atm | CO2 Tot | Uncom CO2 | ppm Uncom CO2 | Nerb Alk | aH2O   |
| 25.00     | 8.220 | 35164.5 | 0.67994   | 3.54E-17 | 4.66E-04 | 1.50-114 | 0.00214 | 1.56E-03  | 6.87E+01      | 6.03E-05 | 0.9805 |

| I   | Species  | Anal ppm | Calc ppm  | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|----------|----------|-----------|------------|------------|-----------|-----------|----------|
| 0   | Ca       | 2        | 412.300   | 365.108    | 1.066E-02  | 9.442E-03 | 0.2493    | 2.628    |
| 28  | CaOH     | 1        |           | 0.007143   |            | 1.297E-07 | 9.688E-08 | 0.7470   |
| 31  | CaSO4 aq | 0        |           | 151.476    |            | 1.153E-03 | 1.349E-03 | 1.1695   |
| 81  | CaHSO4   | 1        |           | 0.000008   |            | 6.232E-11 | 4.655E-11 | 0.7470   |
| 29  | CaHCO3   | 1        |           | 3.928      |            | 4.027E-05 | 3.008E-05 | 0.7470   |
| 30  | CaCO3 aq | 0        |           | 2.540      |            | 2.630E-05 | 3.076E-05 | 1.1695   |
| 100 | CaF      | 1        |           | 0.045      |            | 7.879E-07 | 5.886E-07 | 0.7470   |
| 75  | CaH2PO4  | 1        |           | 0.000033   |            | 2.506E-10 | 1.872E-10 | 0.7470   |
| 73  | CaHPO4aq | 0        |           | 0.004640   |            | 3.535E-08 | 4.134E-08 | 1.1695   |
| 74  | CaPO4    | -1       |           | 0.002831   |            | 2.173E-08 | 1.623E-08 | 0.7470   |
| 1   | Mg       | 2        | 1291.800  | 1142.861   | 5.507E-02  | 4.872E-02 | 1.403E-02 | 0.2880   |
| 18  | MgOH     | 1        |           | 0.197      |            | 4.931E-06 | 3.683E-06 | 0.7470   |
| 22  | MgSO4 aq | 0        |           | 697.090    |            | 6.002E-03 | 7.019E-03 | 1.1695   |
| 21  | MgHCO3   | 1        |           | 18.023     |            | 2.189E-04 | 1.635E-04 | 0.7470   |
| 20  | MgCO3 aq | 0        |           | 7.268      |            | 8.934E-05 | 1.045E-04 | 1.1695   |
| 19  | MgF      | 1        |           | 1.489      |            | 3.563E-05 | 2.662E-05 | 0.7470   |
| 40  | MgH2PO4  | 1        |           | 0.000223   |            | 1.903E-09 | 1.422E-09 | 0.7470   |
| 72  | MgHPO4aq | 0        |           | 0.033      |            | 2.849E-07 | 3.332E-07 | 1.1695   |
| 39  | MgPO4    | -1       |           | 0.020      |            | 1.748E-07 | 1.305E-07 | 0.7470   |
| 2   | Na       | 1        | 10768.000 | 10621.356  | 4.855E-01  | 4.788E-01 | 3.381E-01 | 0.7061   |
| 43  | NaSO4    | -1       |           | 732.899    |            | 6.381E-03 | 4.766E-03 | 0.7470   |
| 42  | NaHCO3aq | 0        |           | 13.205     |            | 1.629E-04 | 1.905E-04 | 1.1695   |
| 41  | NaCO3    | -1       |           | 5.240      |            | 6.544E-05 | 4.889E-05 | 0.7470   |
| 49  | NaHPO4   | -1       |           | 0.003245   |            | 2.827E-08 | 2.112E-08 | 0.7470   |
| 297 | NaF aq   | 0        |           | 0.039      |            | 9.707E-07 | 1.135E-06 | 1.1695   |
| 3   | K        | 1        | 399.100   | 392.634    | 1.058E-02  | 1.041E-02 | 6.477E-03 | 0.6223   |
| 45  | KSO4     | -1       |           | 22.350     |            | 1.714E-04 | 1.280E-04 | 0.7470   |
| 60  | KHPO4    | -1       |           | 0.000071   |            | 5.415E-10 | 4.045E-10 | 0.7470   |
| 63  | H        | 1        |           | 0.000008   |            | 7.989E-09 | 6.026E-09 | 0.7542   |
| 26  | OH       | -1       |           | 0.036      |            | 2.193E-06 | 1.639E-06 | 0.7470   |
| 17  | CO3      | -2       |           | 2.182      |            | 3.768E-05 | 7.801E-06 | 0.2070   |
| 6   | HCO3     | -1       | 141.682   | 87.456     | 2.407E-03  | 1.486E-03 | 1.002E-03 | 0.6745   |
| 85  | H2CO3 aq | 0        |           | 0.692      |            | 1.157E-05 | 1.357E-05 | 1.1733   |
| 5   | SO4      | -2       | 2712.000  | 1441.459   | 2.926E-02  | 1.555E-02 | 2.813E-03 | 0.1809   |
| 62  | HSO4     | -1       |           | 0.000206   |            | 2.202E-09 | 1.645E-09 | 0.7470   |
| 61  | F        | -1       | 1.390     | 0.704      | 7.583E-05  | 3.843E-05 | 2.871E-05 | 0.7470   |
| 125 | HF aq    | 0        |           | 0.000004   |            | 2.183E-10 | 2.553E-10 | 1.1695   |
| 126 | HF2      | -1       |           | 0.000000   |            | 3.730E-14 | 2.786E-14 | 0.7470   |

## DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data

A5

| I   | Species  |    | Anal ppm  | Calc ppm  | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|----------|----|-----------|-----------|------------|------------|-----------|-----------|----------|
| 296 | H2F2 aq  | 0  |           | 0.000000  |            | 1.500E-19  | 1.754E-19 | 1.1695    | 18.756   |
| 4   | Cl       | -1 | 19353.000 | 19352.848 | 5.658E-01  | 5.658E-01  | 3.521E-01 | 0.6223    | 0.453    |
| 97  | Br       | -1 | 67.300    | 67.299    | 8.730E-04  | 8.730E-04  | 6.521E-04 | 0.7470    | 3.186    |
| 96  | I        | -1 | 0.062     | 0.062     | 5.064E-07  | 5.064E-07  | 3.783E-07 | 0.7470    | 6.422    |
| 44  | PO4      | -3 | 0.060000  | 0.000003  | 6.548E-07  | 3.308E-11  | 2.397E-12 | 0.0725    | 11.620   |
| 46  | HPO4     | -2 |           | 0.009525  |            | 1.029E-07  | 3.203E-08 | 0.3114    | 7.494    |
| 47  | H2PO4    | -1 |           | 0.000389  |            | 4.162E-09  | 3.109E-09 | 0.7470    | 8.507    |
| 34  | SiO2 tot | 0  | 4.280     |           | 7.383E-05  |            |           |           |          |
| 23  | H4SiO4aq | 0  |           | 6.643     |            | 7.163E-05  | 8.378E-05 | 1.1695    | 4.077    |
| 24  | H3SiO4   | -1 |           | 0.201     |            | 2.193E-06  | 1.638E-06 | 0.7470    | 5.786    |
| 25  | H2SiO4   | -2 |           | 0.000163  |            | 1.791E-09  | 5.578E-10 | 0.3114    | 9.253    |
| 124 | SiF6     | -2 |           | 0.000000  |            | 3.250E-34  | 1.012E-34 | 0.3114    | 33.995   |
| 86  | B tot    | 0  | 4.450     |           | 4.266E-04  |            |           |           |          |
| 35  | H3BO3 aq | 0  |           | 22.125    |            | 3.709E-04  | 4.337E-04 | 1.1695    | 3.363    |
| 36  | H2BO3    | -1 |           | 3.272     |            | 5.575E-05  | 4.165E-05 | 0.7470    | 4.380    |
| 101 | BF(OH)3  | -1 |           | 0.000518  |            | 6.636E-09  | 4.957E-09 | 0.7470    | 8.305    |
| 102 | BF2(OH)2 | -1 |           | 0.000000  |            | 1.246E-13  | 9.306E-14 | 0.7470    | 13.031   |
| 103 | BF3OH    | -1 |           | 0.000000  |            | 2.393E-20  | 1.788E-20 | 0.7470    | 19.748   |
| 104 | BF4      | -1 |           | 0.000000  |            | 1.708E-26  | 1.276E-26 | 0.7470    | 25.894   |
| 202 | NO2      | -1 | 0.020     | 0.020     | 4.506E-07  | 4.506E-07  | 3.366E-07 | 0.7470    | 6.473    |
| 84  | NO3      | -1 | 0.290     | 0.290     | 4.848E-06  | 4.848E-06  | 3.621E-06 | 0.7470    | 5.441    |
| 37  | NH3 aq   | 0  |           | 0.015     |            | 9.185E-07  | 1.074E-06 | 1.1695    | 5.969    |
| 38  | NH4      | 1  | 0.290     | 0.264     | 1.666E-05  | 1.519E-05  | 1.135E-05 | 0.7470    | 4.945    |
| 91  | NH4SO4   | -1 |           | 0.061     |            | 5.506E-07  | 4.113E-07 | 0.7470    | 6.386    |
| 50  | Al       | 3  | 0.002000  | 0.000000  | 7.683E-08  | 1.087E-16  | 7.874E-18 | 0.0725    | 17.104   |
| 51  | AlOH     | 2  |           | 0.000000  |            | 4.210E-14  | 1.311E-14 | 0.3114    | 13.882   |
| 52  | Al(OH)2  | 1  |           | 0.000001  |            | 2.217E-11  | 1.656E-11 | 0.7470    | 10.781   |
| 181 | Al(OH)3  | 0  |           | 0.000218  |            | 2.901E-09  | 3.393E-09 | 1.1695    | 8.469    |
| 53  | Al(OH)4  | -1 |           | 0.006775  |            | 7.390E-08  | 5.521E-08 | 0.7470    | 7.258    |
| 54  | AlF      | 2  |           | 0.000000  |            | 7.428E-15  | 2.313E-15 | 0.3114    | 14.636   |
| 55  | AlF2     | 1  |           | 0.000000  |            | 4.885E-14  | 3.649E-14 | 0.7470    | 13.438   |
| 56  | AlF3 aq  | 0  |           | 0.000000  |            | 1.668E-14  | 1.951E-14 | 1.1695    | 13.710   |
| 57  | AlF4     | -1 |           | 0.000000  |            | 3.757E-16  | 2.807E-16 | 0.7470    | 15.552   |
| 58  | AlSO4    | 1  |           | 0.000000  |            | 3.104E-17  | 2.319E-17 | 0.7470    | 16.635   |
| 59  | Al(SO4)2 | -1 |           | 0.000000  |            | 6.933E-18  | 5.179E-18 | 0.7470    | 17.286   |
| 203 | AlHSO4   | 2  |           | 0.000000  |            | 1.200E-25  | 3.736E-26 | 0.3114    | 25.428   |
| 16  | Fe total | 2  | 0.002000  |           | 3.712E-08  |            |           |           |          |
| 7   | Fe       | 2  |           | 0.000000  |            | 1.123E-14  | 3.497E-15 | 0.3114    | 14.456   |
| 10  | FeOH     | 1  |           | 0.000000  |            | 2.409E-16  | 1.799E-16 | 0.7470    | 15.745   |
| 79  | Fe(OH)2  | 0  |           | 0.000000  |            | 2.131E-19  | 2.492E-19 | 1.1695    | 18.603   |
| 11  | Fe(OH)3  | -1 |           | 0.000000  |            | 2.017E-21  | 1.507E-21 | 0.7470    | 20.822   |
| 33  | FeSO4 aq | 0  |           | 0.000000  |            | 1.496E-15  | 1.749E-15 | 1.1695    | 14.757   |
| 122 | FeHSO4   | 1  |           | 0.000000  |            | 9.258E-23  | 6.916E-23 | 0.7470    | 22.160   |
| 99  | FeHPO4aq | 0  |           | 0.000000  |            | 3.813E-19  | 4.459E-19 | 1.1695    | 18.351   |
| 64  | FeH2PO4  | 1  |           | 0.000000  |            | 7.293E-21  | 5.448E-21 | 0.7470    | 20.264   |
| 8   | Fe       | 3  |           | 0.000000  |            | 1.268E-18  | 9.185E-20 | 0.0725    | 19.037   |
| 9   | FeOH     | 2  |           | 0.000000  |            | 3.099E-13  | 9.650E-14 | 0.3114    | 13.015   |
| 76  | Fe(OH)2  | 1  |           | 0.000604  |            | 6.961E-09  | 5.200E-09 | 0.7470    | 8.284    |
| 77  | Fe(OH)3  | 0  |           | 0.000877  |            | 8.501E-09  | 9.941E-09 | 1.1695    | 8.003    |
| 78  | Fe(OH)4  | -1 |           | 0.002588  |            | 2.166E-08  | 1.618E-08 | 0.7470    | 7.791    |
| 179 | Fe2(OH)2 | 4  |           | 0.000000  |            | 2.666E-23  | 2.507E-25 | 0.0094    | 24.601   |
| 180 | Fe3(OH)4 | 5  |           | 0.000000  |            | 3.998E-28  | 2.725E-31 | 0.0007    | 30.565   |
| 14  | FeSO4    | 1  |           | 0.000000  |            | 2.877E-18  | 2.149E-18 | 0.7470    | 17.668   |
| 108 | Fe(SO4)2 | -1 |           | 0.000000  |            | 2.558E-19  | 1.911E-19 | 0.7470    | 18.719   |
| 123 | FeHSO4   | 2  |           | 0.000000  |            | 1.465E-25  | 4.563E-26 | 0.3114    | 25.341   |
| 15  | FeCl     | 2  |           | 0.000000  |            | 3.136E-18  | 9.767E-19 | 0.3114    | 18.010   |
| 27  | FeCl2    | 1  |           | 0.000000  |            | 2.056E-18  | 1.536E-18 | 0.7470    | 17.814   |

## DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data

A5

| I   | Species   | Anal ppm | Calc ppm | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|-----------|----------|----------|------------|------------|-----------|-----------|----------|
| 32  | FeCl3 aq  | 0        | 0.000000 |            | 4.625E-20  | 5.408E-20 | 1.1695    | 19.267   |
| 105 | FeF       | 2        | 0.000000 |            | 1.342E-17  | 4.179E-18 | 0.3114    | 17.379   |
| 106 | FeF2      | 1        | 0.000000 |            | 6.394E-18  | 4.776E-18 | 0.7470    | 17.321   |
| 107 | FeF3 aq   | 0        | 0.000000 |            | 1.858E-19  | 2.173E-19 | 1.1695    | 18.663   |
| 12  | FeHPO4    | 1        | 0.000000 |            | 1.060E-21  | 7.919E-22 | 0.7470    | 21.101   |
| 98  | FeH2PO4   | 2        | 0.000000 |            | 2.468E-22  | 7.686E-23 | 0.3114    | 22.114   |
| 109 | Mn        | 2        | 0.000112 | 3.773E-09  | 2.114E-09  | 6.583E-10 | 0.3114    | 9.182    |
| 119 | MnHCO3    | 1        | 0.000002 |            | 1.644E-11  | 1.228E-11 | 0.7470    | 10.911   |
| 111 | MnCl      | 1        | 0.000109 |            | 1.255E-09  | 9.377E-10 | 0.7470    | 9.028    |
| 112 | MnCl2 aq  | 0        | 0.000009 |            | 7.669E-11  | 8.969E-11 | 1.1695    | 10.047   |
| 113 | MnCl3     | -1       | 0.000003 |            | 1.906E-11  | 1.424E-11 | 0.7470    | 10.847   |
| 116 | MnF       | 1        | 0.000000 |            | 1.791E-13  | 1.338E-13 | 0.7470    | 12.874   |
| 114 | MnOH      | 1        | 0.000000 |            | 3.686E-12  | 2.753E-12 | 0.7470    | 11.560   |
| 115 | Mn(OH)3   | -1       | 0.000000 |            | 6.018E-20  | 4.496E-20 | 0.7470    | 19.347   |
| 118 | Mn(NO3)2  | 0        | 0.000000 |            | 2.939E-20  | 3.437E-20 | 1.1695    | 19.464   |
| 117 | MnSO4 aq  | 0        | 0.000042 |            | 2.881E-10  | 3.369E-10 | 1.1695    | 9.472    |
| 110 | Mn        | 3        | 0.000000 |            | 7.995E-26  | 5.792E-27 | 0.0725    | 26.237   |
| 121 | MnO4      | -2       | 0.000000 |            | 2.610E-28  | 8.128E-29 | 0.3114    | 28.090   |
| 120 | MnO4      | -1       | 0.000000 |            | 1.271E-29  | 9.493E-30 | 0.7470    | 29.023   |
| 127 | Cu        | 1        | 0.000000 |            | 5.472E-17  | 4.088E-17 | 0.7470    | 16.389   |
| 128 | CuCl2     | -1       | 0.000000 |            | 2.145E-12  | 1.602E-12 | 0.7470    | 11.795   |
| 129 | CuCl3     | -2       | 0.000000 |            | 2.871E-12  | 8.942E-13 | 0.3114    | 12.049   |
| 130 | Cu        | 2        | 0.000004 | 1.142E-08  | 7.072E-11  | 2.202E-11 | 0.3114    | 10.657   |
| 271 | CuHCO3    | 1        | 0.000002 |            | 1.481E-11  | 1.106E-11 | 0.7470    | 10.956   |
| 131 | CuCO3 aq  | 0        | 0.000094 |            | 7.889E-10  | 9.226E-10 | 1.1695    | 9.035    |
| 132 | Cu(CO3)2  | -2       | 0.000005 |            | 2.908E-11  | 9.056E-12 | 0.3114    | 11.043   |
| 133 | CuCl      | 1        | 0.000003 |            | 2.794E-11  | 2.087E-11 | 0.7470    | 10.680   |
| 134 | CuCl2 aq  | 0        | 0.000000 |            | 3.375E-12  | 3.947E-12 | 1.1695    | 11.404   |
| 135 | CuCl3     | -1       | 0.000000 |            | 6.600E-15  | 4.930E-15 | 0.7470    | 14.307   |
| 136 | CuCl4     | -2       | 0.000000 |            | 2.794E-17  | 8.700E-18 | 0.3114    | 17.060   |
| 137 | CuF       | 1        | 0.000000 |            | 1.540E-14  | 1.151E-14 | 0.7470    | 13.939   |
| 138 | CuOH      | 1        | 0.000004 |            | 4.797E-11  | 3.584E-11 | 0.7470    | 10.446   |
| 139 | Cu(OH)2   | 0        | 0.000981 |            | 1.042E-08  | 1.218E-08 | 1.1695    | 7.914    |
| 140 | Cu(OH)3   | -1       | 0.000000 |            | 1.599E-13  | 1.195E-13 | 0.7470    | 12.923   |
| 141 | Cu(OH)4   | -2       | 0.000000 |            | 1.246E-17  | 3.879E-18 | 0.3114    | 17.411   |
| 142 | Cu2(OH)2  | 2        | 0.000000 |            | 1.807E-15  | 5.629E-16 | 0.3114    | 15.250   |
| 143 | CuSO4 aq  | 0        | 0.000002 |            | 1.082E-11  | 1.265E-11 | 1.1695    | 10.898   |
| 145 | Zn        | 2        | 0.001553 | 7.769E-08  | 2.462E-08  | 7.668E-09 | 0.3114    | 8.115    |
| 272 | ZnHCO3    | 1        | 0.000158 |            | 1.295E-09  | 9.673E-10 | 0.7470    | 9.014    |
| 273 | ZnCO3     | 0        | 0.001234 |            | 1.020E-08  | 1.193E-08 | 1.1695    | 7.923    |
| 274 | Zn(CO3)2  | -2       | 0.001142 |            | 6.388E-09  | 1.989E-09 | 0.3114    | 8.701    |
| 146 | ZnCl      | 1        | 0.000946 |            | 9.727E-09  | 7.266E-09 | 0.7470    | 8.139    |
| 147 | ZnCl2 aq  | 0        | 0.000301 |            | 2.291E-09  | 2.679E-09 | 1.1695    | 8.572    |
| 148 | ZnCl3     | -1       | 0.000235 |            | 1.417E-09  | 1.058E-09 | 0.7470    | 8.975    |
| 149 | ZnCl4     | -2       | 0.000120 |            | 5.997E-10  | 1.868E-10 | 0.3114    | 9.729    |
| 150 | ZnF       | 1        | 0.000000 |            | 4.162E-12  | 3.109E-12 | 0.7470    | 11.507   |
| 151 | ZnOH      | 1        | 0.000146 |            | 1.831E-09  | 1.368E-09 | 0.7470    | 8.864    |
| 152 | Zn(OH)2   | 0        | 0.000210 |            | 2.186E-09  | 2.556E-09 | 1.1695    | 8.592    |
| 153 | Zn(OH)3   | -1       | 0.000000 |            | 1.761E-12  | 1.315E-12 | 0.7470    | 11.881   |
| 154 | Zn(OH)4   | -2       | 0.000000 |            | 1.089E-16  | 3.392E-17 | 0.3114    | 16.470   |
| 155 | ZnOHCl aq | 0        | 0.001414 |            | 1.244E-08  | 1.455E-08 | 1.1695    | 7.837    |
| 158 | ZnSO4 aq  | 0        | 0.000673 |            | 4.323E-09  | 5.056E-09 | 1.1695    | 8.296    |
| 159 | Zn(SO4)2  | -2       | 0.000092 |            | 3.710E-10  | 1.155E-10 | 0.3114    | 9.937    |
| 229 | ZnBr      | 1        | 0.000000 |            | 1.761E-12  | 1.315E-12 | 0.7470    | 11.881   |
| 230 | ZnBr2 aq  | 0        | 0.000000 |            | 2.920E-16  | 3.414E-16 | 1.1695    | 15.467   |
| 231 | ZnI       | 1        | 0.000000 |            | 4.777E-18  | 3.568E-18 | 0.7470    | 17.448   |
| 232 | ZnI2 aq   | 0        | 0.000000 |            | 1.915E-23  | 2.240E-23 | 1.1695    | 22.650   |

## DK Nordstrom Test Data - Test Case #1 - Seawater rerun with new data

A5

| I   | Species   | Anal ppm | Calc ppm | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|-----------|----------|----------|------------|------------|-----------|-----------|----------|
| 160 | Cd        | 2        | 0.000100 | 9.221E-10  | 2.697E-11  | 8.398E-12 | 0.3114    | 11.076   |
| 166 | Cd(CO3)3  | -4       | 0.000000 |            | 7.027E-19  | 6.610E-21 | 0.0094    | 20.180   |
| 275 | CdHCO3    | 1        | 0.000000 |            | 1.418E-12  | 1.059E-12 | 0.7470    | 11.975   |
| 276 | CdCO3     | 0        | 0.000002 |            | 1.407E-11  | 1.646E-11 | 1.1695    | 10.784   |
| 161 | CdCl      | 1        | 0.000054 |            | 3.780E-10  | 2.824E-10 | 0.7470    | 9.549    |
| 162 | CdCl2 aq  | 0        | 0.000063 |            | 3.544E-10  | 4.145E-10 | 1.1695    | 9.382    |
| 163 | CdCl3     | -1       | 0.000026 |            | 1.233E-10  | 9.208E-11 | 0.7470    | 10.036   |
| 164 | CdF       | 1        | 0.000000 |            | 4.063E-15  | 3.035E-15 | 0.7470    | 14.518   |
| 165 | CdF2 aq   | 0        | 0.000000 |            | 1.872E-19  | 2.189E-19 | 1.1695    | 18.660   |
| 167 | CdOH      | 1        | 0.000000 |            | 1.522E-13  | 1.137E-13 | 0.7470    | 12.944   |
| 168 | Cd(OH)2   | 0        | 0.000000 |            | 8.494E-16  | 9.933E-16 | 1.1695    | 15.003   |
| 169 | Cd(OH)3   | -1       | 0.000000 |            | 2.428E-20  | 1.814E-20 | 0.7470    | 19.741   |
| 170 | Cd(OH)4   | -2       | 0.000000 |            | 8.446E-26  | 2.630E-26 | 0.3114    | 25.580   |
| 171 | Cd2OH     | 3        | 0.000000 |            | 6.454E-23  | 4.676E-24 | 0.0725    | 23.330   |
| 172 | CdOHCl aq | 0        | 0.000003 |            | 1.623E-11  | 1.898E-11 | 1.1695    | 10.722   |
| 173 | CdNO3     | 1        | 0.000000 |            | 1.023E-16  | 7.639E-17 | 0.7470    | 16.117   |
| 174 | CdSO4 aq  | 0        | 0.000001 |            | 5.825E-12  | 6.813E-12 | 1.1695    | 11.167   |
| 277 | Cd(SO4)2  | -2       | 0.000000 |            | 6.744E-13  | 2.100E-13 | 0.3114    | 12.678   |
| 233 | CdBr      | 1        | 0.000000 |            | 1.084E-12  | 8.101E-13 | 0.7470    | 12.091   |
| 234 | CdBr2 aq  | 0        | 0.000000 |            | 2.426E-15  | 2.837E-15 | 1.1695    | 14.547   |
| 235 | CdI       | 1        | 0.000000 |            | 6.007E-16  | 4.487E-16 | 0.7470    | 15.348   |
| 236 | CdI2 aq   | 0        | 0.000000 |            | 3.998E-21  | 4.675E-21 | 1.1695    | 20.330   |
| 182 | Pb        | 2        | 0.000050 | 2.501E-10  | 4.894E-12  | 1.524E-12 | 0.3114    | 11.817   |
| 278 | PbHCO3    | 1        | 0.000000 |            | 1.624E-12  | 1.213E-12 | 0.7470    | 11.916   |
| 241 | PbCO3 aq  | 0        | 0.000046 |            | 1.766E-10  | 2.066E-10 | 1.1695    | 9.685    |
| 187 | Pb(CO3)2  | -2       | 0.000004 |            | 1.299E-11  | 4.046E-12 | 0.3114    | 11.393   |
| 183 | PbCl      | 1        | 0.000007 |            | 2.860E-11  | 2.136E-11 | 0.7470    | 10.670   |
| 184 | PbCl2 aq  | 0        | 0.000003 |            | 1.019E-11  | 1.192E-11 | 1.1695    | 10.924   |
| 185 | PbCl3     | -1       | 0.000001 |            | 4.463E-12  | 3.334E-12 | 0.7470    | 11.477   |
| 186 | PbCl4     | -2       | 0.000001 |            | 1.804E-12  | 5.618E-13 | 0.3114    | 12.250   |
| 188 | PbF       | 1        | 0.000000 |            | 1.042E-15  | 7.781E-16 | 0.7470    | 15.109   |
| 189 | PbF2 aq   | 0        | 0.000000 |            | 3.899E-19  | 4.560E-19 | 1.1695    | 18.341   |
| 190 | PbF3      | -1       | 0.000000 |            | 1.270E-22  | 9.484E-23 | 0.7470    | 22.023   |
| 191 | PbF4      | -2       | 0.000000 |            | 4.184E-27  | 1.303E-27 | 0.3114    | 26.885   |
| 192 | PbOH      | 1        | 0.000001 |            | 6.473E-12  | 4.835E-12 | 0.7470    | 11.316   |
| 193 | Pb(OH)2   | 0        | 0.000000 |            | 2.618E-13  | 3.061E-13 | 1.1695    | 12.514   |
| 194 | Pb(OH)3   | -1       | 0.000000 |            | 7.656E-16  | 5.719E-16 | 0.7470    | 15.243   |
| 242 | Pb(OH)4   | -2       | 0.000000 |            | 6.846E-19  | 2.132E-19 | 0.3114    | 18.671   |
| 195 | Pb2OH     | 3        | 0.000000 |            | 2.283E-21  | 1.654E-22 | 0.0725    | 21.781   |
| 200 | Pb3(OH)4  | 2        | 0.000000 |            | 1.056E-26  | 3.289E-27 | 0.3114    | 26.483   |
| 196 | PbNO3     | 1        | 0.000000 |            | 1.093E-16  | 8.163E-17 | 0.7470    | 16.088   |
| 197 | PbSO4 aq  | 0        | 0.000001 |            | 2.061E-12  | 2.411E-12 | 1.1695    | 11.618   |
| 243 | Pb(SO4)2  | -2       | 0.000000 |            | 1.142E-13  | 3.557E-14 | 0.3114    | 13.449   |
| 237 | PbBr      | 1        | 0.000000 |            | 7.834E-14  | 5.852E-14 | 0.7470    | 13.233   |
| 238 | PbBr2 aq  | 0        | 0.000000 |            | 1.526E-17  | 1.785E-17 | 1.1695    | 16.748   |
| 239 | PbI       | 1        | 0.000000 |            | 6.721E-17  | 5.021E-17 | 0.7470    | 16.299   |
| 240 | PbI2 aq   | 0        | 0.000000 |            | 2.955E-22  | 3.456E-22 | 1.1695    | 21.461   |
| 204 | Ni        | 2        | 0.001700 | 3.001E-08  | 1.662E-09  | 5.175E-10 | 0.3114    | 9.286    |
| 205 | NiBr      | 1        | 0.000000 |            | 1.429E-12  | 1.067E-12 | 0.7470    | 11.972   |
| 280 | NiHCO3    | 1        | 0.000011 |            | 9.582E-11  | 7.158E-11 | 0.7470    | 10.145   |
| 281 | NiCO3     | 0        | 0.002931 |            | 2.559E-08  | 2.993E-08 | 1.1695    | 7.524    |
| 282 | Ni(CO3)2  | -2       | 0.000225 |            | 1.302E-09  | 4.055E-10 | 0.3114    | 9.392    |
| 206 | NiCl      | 1        | 0.000056 |            | 6.127E-10  | 4.577E-10 | 0.7470    | 9.339    |
| 279 | NiCl2     | 0        | 0.000063 |            | 5.003E-10  | 5.851E-10 | 1.1695    | 9.233    |
| 207 | NiF       | 1        | 0.000000 |            | 3.968E-13  | 2.965E-13 | 0.7470    | 12.528   |
| 208 | NiOH      | 1        | 0.000001 |            | 1.556E-11  | 1.162E-11 | 0.7470    | 10.935   |
| 209 | Ni(OH)2   | 0        | 0.000000 |            | 1.172E-12  | 1.370E-12 | 1.1695    | 11.863   |



| I   | Species     | Anal ppm | Calc ppm | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|-------------|----------|----------|------------|------------|-----------|-----------|----------|
| 210 | Ni(OH)3 -1  |          | 0.000000 |            | 2.985E-15  | 2.230E-15 | 0.7470    | 14.652   |
| 211 | NiSO4 aq 0  |          | 0.000036 |            | 2.427E-10  | 2.838E-10 | 1.1695    | 9.547    |
| 283 | Ni(SO4)2 -2 |          | 0.000000 |            | 1.376E-13  | 4.286E-14 | 0.3114    | 13.368   |
| 212 | Ag 1        | 0.000040 | 0.000000 | 3.843E-10  | 4.037E-15  | 3.015E-15 | 0.7470    | 14.521   |
| 213 | AgBr aq 0   |          | 0.000000 |            | 2.922E-14  | 3.417E-14 | 1.1695    | 13.466   |
| 214 | AgBr2 -1    |          | 0.000000 |            | 3.271E-14  | 2.444E-14 | 0.7470    | 13.612   |
| 244 | AgBr3 -2    |          | 0.000000 |            | 1.377E-15  | 4.289E-16 | 0.3114    | 15.368   |
| 215 | AgCl aq 0   |          | 0.000000 |            | 1.691E-12  | 1.977E-12 | 1.1695    | 11.704   |
| 216 | AgCl2 -1    |          | 0.000016 |            | 9.318E-11  | 6.961E-11 | 0.7470    | 10.157   |
| 217 | AgCl3 -2    |          | 0.000017 |            | 8.241E-11  | 2.566E-11 | 0.3114    | 10.591   |
| 218 | AgCl4 -3    |          | 0.000050 |            | 2.070E-10  | 1.500E-11 | 0.0725    | 10.824   |
| 219 | AgF aq 0    |          | 0.000000 |            | 1.696E-19  | 1.983E-19 | 1.1695    | 18.703   |
| 222 | AgI aq 0    |          | 0.000000 |            | 3.883E-15  | 4.541E-15 | 1.1695    | 14.343   |
| 223 | AgI2 -1     |          | 0.000000 |            | 2.765E-17  | 2.065E-17 | 0.7470    | 16.685   |
| 245 | AgI3 -2     |          | 0.000000 |            | 1.229E-20  | 3.826E-21 | 0.3114    | 20.417   |
| 246 | AgI4 -3     |          | 0.000000 |            | 1.024E-25  | 7.423E-27 | 0.0725    | 26.129   |
| 224 | AgOH aq 0   |          | 0.000000 |            | 4.196E-19  | 4.907E-19 | 1.1695    | 18.309   |
| 225 | Ag(OH)2 -1  |          | 0.000000 |            | 1.069E-22  | 7.985E-23 | 0.7470    | 22.098   |
| 226 | AgSO4 -1    |          | 0.000000 |            | 2.214E-16  | 1.654E-16 | 0.7470    | 15.782   |
| 227 | AgNO3 aq 0  |          | 0.000000 |            | 4.789E-21  | 5.600E-21 | 1.1695    | 20.252   |
| 228 | Ag(NO2)2 -1 |          | 0.000000 |            | 7.590E-26  | 5.670E-26 | 0.7470    | 25.246   |
| 249 | As total 0  | 0.004000 |          | 5.533E-08  |            |           |           |          |
| 254 | H4AsO3 1    |          | 0.000000 |            | 3.175E-38  | 2.372E-38 | 0.7470    | 37.625   |
| 250 | H3AsO3aq 0  |          | 0.000000 |            | 6.793E-30  | 7.944E-30 | 1.1695    | 29.100   |
| 251 | H2AsO3 -1   |          | 0.000000 |            | 1.044E-30  | 7.799E-31 | 0.7470    | 30.108   |
| 252 | HAsO3 -2    |          | 0.000000 |            | 3.286E-34  | 1.023E-34 | 0.3114    | 33.990   |
| 253 | AsO3 -3     |          | 0.000000 |            | 9.037E-39  | 6.547E-40 | 0.0725    | 39.184   |
| 255 | H3AsO4aq 0  |          | 0.000000 |            | 5.277E-16  | 6.171E-16 | 1.1695    | 15.210   |
| 256 | H2AsO4 -1   |          | 0.000107 |            | 7.835E-10  | 5.853E-10 | 0.7470    | 9.233    |
| 257 | HAsO4 -2    |          | 0.007351 |            | 5.445E-08  | 1.696E-08 | 0.3114    | 7.771    |
| 258 | AsO4 -3     |          | 0.000013 |            | 9.848E-11  | 7.135E-12 | 0.0725    | 11.147   |
| 80  | Li 1        | 0.181    | 0.179    | 2.704E-05  | 2.671E-05  | 1.995E-05 | 0.7470    | 4.700    |
| 82  | LiSO4 -1    |          | 0.033    |            | 3.279E-07  | 2.450E-07 | 0.7470    | 6.611    |
| 87  | Sr 2        | 8.140    | 8.074    | 9.629E-05  | 9.550E-05  | 2.331E-05 | 0.2441    | 4.632    |
| 88  | SrOH 1      |          | 0.000038 |            | 3.810E-10  | 2.524E-10 | 0.6624    | 9.598    |
| 68  | SrHCO3 1    |          | 0.076    |            | 5.299E-07  | 3.575E-07 | 0.6745    | 6.447    |
| 95  | SrCO3 aq 0  |          | 0.036    |            | 2.540E-07  | 1.161E-07 | 0.4571    | 6.935    |
| 89  | Ba 2        | 0.020    | 0.015    | 1.509E-07  | 1.097E-07  | 3.418E-08 | 0.3114    | 7.466    |
| 90  | BaOH 1      |          | 0.000000 |            | 3.272E-13  | 2.445E-13 | 0.7470    | 12.612   |
| 201 | BaSO4 aq 0  |          | 0.009278 |            | 4.120E-08  | 4.818E-08 | 1.1695    | 7.317    |
| 48  | Cs 1        | 0.000400 | 0.000400 | 3.119E-09  | 3.119E-09  | 2.330E-09 | 0.7470    | 8.633    |
| 94  | Rb 1        | 0.117    | 0.117    | 1.419E-06  | 1.419E-06  | 1.060E-06 | 0.7470    | 5.975    |

## Mole ratios from analytical molality - Log activity ratios

|         |   |            |                |     |   |         |
|---------|---|------------|----------------|-----|---|---------|
| Cl/Ca   | = | 5.3065E+01 | Log Ca         | /H2 | = | 13.8118 |
| Cl/Mg   | = | 1.0274E+01 | Log Mg         | /H2 | = | 14.5872 |
| Cl/Na   | = | 1.1655E+00 | Log Na         | /H1 | = | 7.7491  |
| Cl/K    | = | 5.3483E+01 | Log K          | /H1 | = | 6.0314  |
| Cl/Al   | = | 7.3643E+06 | Log Al         | /H3 | = | 7.5562  |
| Cl/Fe   | = | 0.0000E-01 | Log Fe         | /H2 | = | 1.9837  |
| Cl/SO4  | = | 1.9336E+01 | Log Ca/Mg      |     | = | -0.7754 |
| Cl/HCO3 | = | 2.3509E+02 | LOG NA/K       |     | = | 1.7177  |
| Ca/Mg   | = | 1.9360E-01 | Log Ca/K2      |     | = | 1.7491  |
| Na/K    | = | 4.5890E+01 | Log Diss Fe/H2 |     | = | 16.4400 |

| Phase            | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP  | Log KT   | Log MinKT | Log MaxKT |
|------------------|-----------|----------|----------|--------------|--------------|---------|----------|-----------|-----------|
| 39 Adularia      | -1.036    | 0.000    | 0.000    | 0.000        | 0.000        | -21.609 | -20.573  | 0.000     | 0.000     |
| 40 Albite        | -1.889    | 0.000    | 0.000    | 0.000        | 0.000        | -19.891 | -18.002  | 0.000     | 0.000     |
| 140 AlOH3 (a)    | -2.849    | 0.000    | 0.000    | -2.160       | 0.000        | -34.460 | -31.611  | -32.300   | 0.000     |
| 471 AlOHSO4      | -8.213    | 0.000    | 0.000    | -8.053       | -8.373       | -11.443 | -3.230   | -3.390    | -3.070    |
| 472 Al4(OH)10SO4 | -11.552   | 0.000    | 0.000    | 0.000        | 0.000        | 11.148  | 22.700   | 0.000     | 0.000     |
| 157 Allophane(a) | -2.069    | 0.000    | 0.000    | 0.000        | 0.000        | 6.040   | 8.110    | 0.000     | 0.000     |
| 158 Allophane(F) | -1.054    | 0.000    | 0.000    | 0.000        | 0.000        | 6.040   | 7.094    | 0.000     | 0.000     |
| 338 Alum k       | -19.327   | 0.000    | 0.000    | 0.000        | 0.000        | -24.497 | -5.170   | 0.000     | 0.000     |
| 50 Alunite       | -7.981    | 0.000    | 0.000    | 0.000        | 0.000        | -93.315 | -85.334  | 0.000     | 0.000     |
| 42 Analcime      | -3.139    | 0.000    | 0.000    | 0.000        | 0.000        | -15.840 | -12.701  | 0.000     | 0.000     |
| 17 Anhydrite     | -0.542    | 0.000    | 0.000    | 0.000        | 0.000        | -5.179  | -4.637   | 0.000     | 0.000     |
| 113 Annite       | 20.684    | 0.000    | 0.000    | 0.000        | 0.000        | -64.961 | -85.645  | 0.000     | 0.000     |
| 41 Anorthite     | -5.516    | 0.000    | 0.000    | 0.000        | 0.000        | -25.230 | -19.714  | 0.000     | 0.000     |
| 21 Aragonite     | 0.600     | 0.000    | 0.020    | 0.000        | 0.000        | -7.736  | -8.336   | 0.000     | 0.000     |
| 150 Artinite     | -3.567    | 0.000    | 0.000    | 0.000        | 0.000        | 6.033   | 9.600    | 0.000     | 0.000     |
| 398 BaF2         | -10.790   | 0.000    | 0.000    | -9.810       | -11.900      | -16.550 | -5.760   | -6.740    | -4.650    |
| 144 Barite       | -0.041    | 0.000    | 0.000    | 0.000        | -0.244       | -10.017 | -9.976   | 0.000     | -9.773    |
| 48 Beidellite    | -3.049    | 0.000    | 0.000    | 0.000        | 0.000        | -48.321 | -45.272  | 0.000     | 0.000     |
| 52 Boehmite      | -1.036    | 0.000    | 0.000    | -0.523       | 0.000        | -34.452 | -33.416  | -33.929   | 0.000     |
| 19 Brucite       | -2.220    | 0.000    | 0.000    | 0.000        | 0.000        | -13.424 | -11.204  | 0.000     | 0.000     |
| 12 Calcite       | 0.744     | 0.000    | 0.020    | 0.824        | 0.000        | -7.736  | -8.480   | -8.560    | 0.000     |
| 143 Celestite    | -0.718    | 0.000    | 0.000    | 0.000        | -0.834       | -7.183  | -6.465   | 0.000     | -6.349    |
| 97 Chalcedony    | -0.537    | 0.000    | 0.000    | 0.000        | 0.000        | -4.060  | -3.523   | 0.000     | 0.000     |
| 49 Chlorite 14A  | 7.386     | 0.000    | 6.000    | 12.661       | -1.338       | 75.766  | 68.380   | 63.105    | 77.104    |
| 125 Chlorite 7A  | 4.014     | 0.000    | 6.000    | 0.000        | 0.000        | 75.766  | 71.752   | 0.000     | 0.000     |
| 20 Chrysotile    | 3.417     | 0.000    | 0.000    | 0.000        | 0.000        | -48.383 | -51.800  | 0.000     | 0.000     |
| 29 Clinoenstite  | -0.817    | 0.000    | 0.000    | -0.451       | -1.111       | -17.475 | -16.658  | -17.024   | -16.364   |
| 56 Clinoptilolt  | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -27.801 | 0.000    | 0.000     | 0.000     |
| 99 Cristobalite  | -0.473    | 0.000    | 0.000    | 0.000        | 0.000        | -4.060  | -3.587   | 0.000     | 0.000     |
| 154 Diaspore     | 0.669     | 0.000    | 0.000    | 0.000        | 0.000        | -34.452 | -35.121  | 0.000     | 0.000     |
| 28 Diopside      | 0.380     | 0.000    | 0.000    | 0.000        | 0.000        | -35.726 | -36.106  | 0.000     | 0.000     |
| 11 Dolomite      | 2.303     | 0.000    | 0.000    | 0.000        | 0.000        | -14.697 | -17.000  | 0.000     | 0.000     |
| 340 Epsomite     | -2.324    | 0.000    | 0.000    | 0.000        | 0.000        | -4.464  | -2.140   | 0.000     | 0.000     |
| 55 Erionite      | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -21.947 | 0.000    | 0.000     | 0.000     |
| 112 Ferrihydrite | 0.706     | 0.000    | 0.000    | 4.040        | 0.601        | 5.597   | 4.891    | 1.557     | 4.996     |
| 419 Fe3(OH)8     | -7.061    | 0.000    | 0.000    | -3.951       | -10.944      | 13.161  | 20.222   | 17.112    | 24.105    |
| 181 FeOH)2.7Cl.3 | 6.038     | 0.000    | 0.000    | 0.000        | 0.000        | 2.998   | -3.040   | 0.000     | 0.000     |
| 401 Fe2(SO4)3    | -49.306   | 0.000    | 0.000    | -45.076      | 0.000        | -45.726 | 3.580    | -0.650    | 0.000     |
| 396 FCO3apatite  | 15.834    | 0.000    | 0.000    | 0.000        | 0.000        | -98.566 | -114.400 | 0.000     | 0.000     |
| 96 Fluorapatite  | 2.094     | 0.000    | 0.000    | 9.737        | 0.000        | -15.506 | -17.600  | -25.243   | 0.000     |
| 62 Fluorite      | -0.763    | 0.000    | 0.000    | 0.000        | 0.000        | -11.712 | -10.949  | 0.000     | 0.000     |
| 27 Forsterite    | -3.197    | 0.000    | 0.000    | 0.000        | 0.000        | -30.891 | -27.694  | 0.000     | 0.000     |
| 51 Gibbsite (c)  | -1.239    | 0.000    | 0.200    | -0.956       | -1.909       | 7.531   | 8.770    | 8.487     | 9.440     |
| 110 Goethite     | 5.106     | 0.000    | 0.800    | 0.000        | 0.000        | 5.606   | 0.500    | 0.000     | 0.000     |
| 111 Greenalite   | -23.021   | 0.000    | 0.000    | 0.000        | 0.000        | -2.211  | 20.810   | 0.000     | 0.000     |
| 18 Gypsum        | -0.596    | 0.000    | 0.000    | 0.000        | 0.000        | -5.196  | -4.600   | 0.000     | 0.000     |
| 64 Halite        | -2.506    | 0.000    | 0.000    | 0.000        | 0.000        | -0.924  | 1.582    | 0.000     | 0.000     |
| 47 Halloysite    | -6.220    | 0.000    | 0.000    | 0.000        | 0.000        | -39.050 | -32.830  | 0.000     | 0.000     |
| 108 Hematite     | 15.229    | 0.000    | 0.000    | 0.000        | 0.000        | 11.221  | -4.008   | 0.000     | 0.000     |
| 117 Huntite      | 1.350     | 0.000    | 0.000    | 0.000        | 0.000        | -28.618 | -29.968  | 0.000     | 0.000     |
| 38 Hydrmagnesit  | -4.539    | 0.000    | 0.000    | 0.000        | 0.000        | -41.301 | -36.762  | 0.000     | 0.000     |
| 95 Hydroxyapati  | 0.668     | 0.000    | 0.000    | 3.197        | -5.993       | -2.753  | -3.421   | -5.950    | 3.240     |
| 45 Illite        | -2.240    | 0.000    | 0.000    | 0.000        | 0.000        | -42.507 | -40.267  | 0.000     | 0.000     |
| 204 Jarosite Na  | -2.215    | 0.000    | 1.000    | 0.000        | 0.000        | -13.415 | -11.200  | 0.000     | 0.000     |
| 205 Jarosite K   | -0.332    | 0.000    | 1.100    | 0.000        | -2.632       | -15.132 | -14.800  | 0.000     | -12.500   |
| 337 Jarosite H   | -9.072    | 0.000    | 0.000    | 0.000        | 0.000        | -21.172 | -12.100  | 0.000     | 0.000     |
| 46 Kaolinite     | -2.129    | 0.000    | 0.000    | -1.250       | -3.230       | -39.050 | -36.921  | -37.800   | -35.820   |

| Phase             | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP   | Log KT   | Log MinKT | Log MaxKT |
|-------------------|-----------|----------|----------|--------------|--------------|----------|----------|-----------|-----------|
| 43 Kmica          | 3.766     | 0.000    | 1.300    | 5.164        | 2.087        | 16.469   | 12.703   | 11.305    | 14.382    |
| 128 Laumontite    | -2.423    | 0.000    | 0.000    | 0.000        | 0.000        | -33.383  | -30.960  | 0.000     | 0.000     |
| 147 Leonhardite   | 2.998     | 0.000    | 0.000    | 0.000        | 0.000        | -66.758  | -69.756  | 0.000     | 0.000     |
| 98 Magadiite      | -8.130    | 0.000    | 0.000    | 0.000        | 0.000        | -22.430  | -14.300  | 0.000     | 0.000     |
| 109 Maghemite     | 4.835     | 0.000    | 0.000    | 0.000        | 0.000        | 11.221   | 6.386    | 0.000     | 0.000     |
| 10 Magnesite      | 1.068     | 0.000    | 0.000    | 1.318        | 0.818        | -6.961   | -8.029   | -8.279    | -7.779    |
| 107 Magnetite     | 9.459     | 0.000    | 0.000    | 9.829        | 6.601        | 13.196   | 3.737    | 3.367     | 6.595     |
| 339 Melanterite   | -14.597   | 0.000    | 0.000    | 0.000        | 0.000        | -17.067  | -2.470   | 0.000     | 0.000     |
| 63 Montmoril Ca   | -3.623    | 0.000    | 0.000    | 0.000        | 0.000        | -48.650  | -45.027  | 0.000     | 0.000     |
| 115 Montmoril BF  | 2.209     | 0.000    | 0.000    | 0.000        | 0.000        | -32.704  | -34.913  | 0.000     | 0.000     |
| 116 Montmoril AB  | 2.081     | 0.000    | 0.000    | 0.000        | 0.000        | -27.607  | -29.688  | 0.000     | 0.000     |
| 57 Mordenite      | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -25.767  | 0.000    | 0.000     | 0.000     |
| 66 Mirabilite     | -2.464    | 0.000    | 0.000    | 0.000        | 0.000        | -3.578   | -1.114   | 0.000     | 0.000     |
| 58 Nahcolite      | -2.922    | 0.000    | 0.000    | 0.000        | 0.000        | -3.470   | -0.548   | 0.000     | 0.000     |
| 60 Natron         | -4.824    | 0.000    | 0.000    | 0.000        | 0.000        | -6.135   | -1.311   | 0.000     | 0.000     |
| 149 Nesquehonite  | -1.365    | 0.000    | 0.000    | -1.853       | -2.440       | -6.986   | -5.621   | -5.133    | -4.546    |
| 54 Phillipsite    | -0.885    | 0.000    | 0.000    | 0.000        | 0.000        | -20.759  | -19.874  | 0.000     | 0.000     |
| 44 Phlogopite     | -21.182   | 0.000    | 3.000    | 0.000        | 0.000        | 22.118   | 43.300   | 0.000     | 0.000     |
| 141 Prehnite      | -3.800    | 0.000    | 0.000    | 0.000        | 0.000        | -15.495  | -11.695  | 0.000     | 0.000     |
| 53 Pyrophyllite   | 1.153     | 0.000    | 0.000    | 4.449        | -0.681       | -47.161  | -48.314  | -51.610   | -46.480   |
| 101 Quartz        | -0.054    | 0.000    | 0.000    | 0.000        | 0.000        | -4.060   | -4.006   | 0.000     | 0.000     |
| 36 Sepiolite(c)   | 1.584     | 0.000    | 0.000    | 0.000        | 0.000        | 16.948   | 15.364   | 0.000     | 0.000     |
| 153 Sepiolite(a)  | -1.712    | 0.000    | 0.000    | 0.000        | 0.000        | 16.948   | 18.660   | 0.000     | 0.000     |
| 9 Siderite        | -9.014    | 0.000    | 0.000    | -7.460       | 0.000        | -19.564  | -10.550  | -12.104   | 0.000     |
| 100 SiO2 (a,L)    | -1.042    | 0.000    | 0.000    | 0.000        | 0.000        | -4.060   | -3.018   | 0.000     | 0.000     |
| 395 SiO2 (a,M)    | -1.350    | 0.000    | 0.000    | 0.000        | 0.000        | -4.060   | -2.710   | 0.000     | 0.000     |
| 399 SrF2          | -5.176    | 0.000    | 0.000    | -4.596       | 0.000        | -13.716  | -8.540   | -9.120    | 0.000     |
| 146 Strengite     | -4.274    | 0.000    | 0.000    | -1.551       | -4.439       | -30.674  | -26.400  | -29.123   | -26.235   |
| 142 Strontianite  | -0.470    | 0.000    | 0.000    | 2.049        | 0.000        | -9.740   | -9.271   | -11.789   | 0.000     |
| 37 Talc           | 6.089     | 0.000    | 2.000    | 8.257        | 4.341        | 27.488   | 21.399   | 19.231    | 23.147    |
| 65 Thenardite     | -3.314    | 0.000    | 0.000    | 0.000        | 0.000        | -3.493   | -0.179   | 0.000     | 0.000     |
| 61 Thermonatr     | -6.183    | 0.000    | 0.000    | 0.000        | 0.000        | -6.058   | 0.125    | 0.000     | 0.000     |
| 31 Tremolite      | 11.481    | 0.000    | 0.000    | 0.000        | 0.000        | -127.945 | -139.426 | 0.000     | 0.000     |
| 59 Trona          | -8.742    | 0.000    | 0.000    | 0.000        | 0.000        | -9.537   | -0.795   | 0.000     | 0.000     |
| 106 Vivianite     | -30.678   | 0.000    | 0.000    | 0.000        | 0.000        | -66.678  | -36.000  | 0.000     | 0.000     |
| 155 Wairkite      | -6.658    | 0.000    | 0.000    | 0.000        | 0.000        | -33.366  | -26.708  | 0.000     | 0.000     |
| 145 Witherite     | -3.989    | 0.000    | 0.000    | 0.761        | 0.000        | -12.574  | -8.585   | -13.335   | 0.000     |
| 183 Pyrolusite    | -0.784    | 0.000    | 0.000    | 0.000        | -0.961       | 15.077   | 15.861   | 0.000     | 16.038    |
| 184 Birnessite    | -3.014    | 0.000    | 0.000    | 0.000        | 0.000        | 15.077   | 18.091   | 0.000     | 0.000     |
| 185 Nsutite       | -2.427    | 0.000    | 0.000    | 0.000        | 0.000        | 15.077   | 17.504   | 0.000     | 0.000     |
| 186 Bixbyite      | -2.569    | 0.000    | 0.000    | -0.954       | -2.750       | -3.180   | -0.611   | -2.226    | -0.430    |
| 187 Hausmannite   | -6.456    | 0.000    | 0.000    | 0.000        | 0.000        | 55.084   | 61.540   | 0.000     | 0.000     |
| 188 Pyrochroite   | -7.847    | 0.000    | 0.000    | 0.000        | -8.140       | 7.241    | 15.088   | 0.000     | 15.381    |
| 189 Manganite     | -1.356    | 0.000    | 0.000    | 0.000        | 0.000        | -1.594   | -0.238   | 0.000     | 0.000     |
| 190 Rhodochrosit  | -3.879    | 0.000    | 0.000    | -3.270       | -4.296       | -14.289  | -10.410  | -11.019   | -9.993    |
| 191 MnCl2, 4H2O   | -12.832   | 0.000    | 0.000    | 0.000        | 0.000        | -10.122  | 2.710    | 0.000     | 0.000     |
| 182 MnSO4         | -14.401   | 0.000    | 0.000    | 0.000        | 0.000        | -11.732  | 2.669    | 0.000     | 0.000     |
| 134 Mn2(SO4)3     | -54.416   | 0.000    | 0.000    | 0.000        | 0.000        | -60.127  | -5.711   | 0.000     | 0.000     |
| 193 Mn3(PO4)2     | -26.959   | 0.000    | 0.000    | 0.000        | 0.000        | -50.786  | -23.827  | 0.000     | 0.000     |
| 194 MnHPO4        | -3.729    | 0.000    | 0.000    | 0.000        | 0.000        | -16.676  | -12.947  | 0.000     | 0.000     |
| 195 a-Cryptomelnl | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -74.267  | 0.000    | 0.000     | 0.000     |
| 196 Hollandite    | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -59.925  | 0.000    | 0.000     | 0.000     |
| 197 Psilomelane   | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -55.984  | 0.000    | 0.000     | 0.000     |
| 198 Todorokite    | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -31.624  | 0.000    | 0.000     | 0.000     |
| 199 Lithiophorit  | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -22.540  | 0.000    | 0.000     | 0.000     |
| 200 Rancieite     | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -31.611  | 0.000    | 0.000     | 0.000     |
| 223 Cu metal      | -16.080   | 0.000    | 0.000    | 0.000        | -16.040      | -24.840  | -8.760   | 0.000     | -8.800    |

| Phase                                                    | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP  | Log KT  | Log MinKT | Log MaxKT |
|----------------------------------------------------------|-----------|----------|----------|--------------|--------------|---------|---------|-----------|-----------|
| 224 Nantokite                                            | -10.082   | 0.000    | 0.000    | 0.000        | -10.212      | -16.842 | -6.760  | 0.000     | -6.630    |
| 225 CuF                                                  | -28.011   | 0.000    | 0.000    | 0.000        | 0.000        | -20.931 | 7.080   | 0.000     | 0.000     |
| 226 Cuprite                                              | -14.796   | 0.000    | 0.000    | -14.476      | -15.646      | -16.346 | -1.550  | -1.870    | -0.700    |
| 228 Cu <sub>2</sub> SO <sub>4</sub>                      | -33.378   | 0.000    | 0.000    | 0.000        | 0.000        | -35.328 | -1.950  | 0.000     | 0.000     |
| 229 Cuprousferit                                         | 6.357     | 0.000    | 0.000    | 0.000        | 4.317        | -2.563  | -8.920  | 0.000     | -6.880    |
| 230 Melanothalli                                         | -15.294   | 0.000    | 0.000    | 0.000        | -16.014      | -11.564 | 3.730   | 0.000     | 4.450     |
| 231 CuCO <sub>3</sub>                                    | -6.135    | 0.000    | 0.000    | -6.115       | -6.155       | -15.765 | -9.630  | -9.650    | -9.610    |
| 232 CuF <sub>2</sub>                                     | -19.121   | 0.000    | 0.000    | 0.000        | 0.000        | -19.741 | -0.620  | 0.000     | 0.000     |
| 233 CuF <sub>2</sub> , 2H <sub>2</sub> O                 | -15.208   | 0.000    | 0.000    | 0.000        | 0.000        | -19.758 | -4.550  | 0.000     | 0.000     |
| 234 Cu(OH) <sub>2</sub>                                  | -2.874    | 0.000    | 0.000    | 0.000        | -3.434       | 5.766   | 8.640   | 0.000     | 9.200     |
| 235 Malachite                                            | -4.820    | 0.000    | 0.080    | -4.170       | -5.030       | 0.330   | 5.150   | 4.500     | 5.360     |
| 236 Azurite                                              | -8.857    | 0.000    | 0.090    | -6.287       | 0.000        | -5.107  | 3.750   | 1.180     | 0.000     |
| 237 Atacamite                                            | -4.473    | 0.000    | 0.000    | -4.373       | -4.623       | 2.867   | 7.340   | 7.240     | 7.490     |
| 238 Cu <sub>2</sub> (OH) <sub>3</sub> NO <sub>3</sub>    | -11.361   | 0.000    | 0.000    | 0.000        | -11.431      | -2.121  | 9.240   | 0.000     | 9.310     |
| 239 Antlerite                                            | -9.966    | 0.000    | 0.000    | 0.000        | -10.576      | -1.676  | 8.290   | 0.000     | 8.900     |
| 240 Brochantite                                          | -11.251   | 0.000    | 0.160    | -11.061      | -11.411      | 4.089   | 15.340  | 15.150    | 15.500    |
| 241 Langite                                              | -12.709   | 0.000    | 0.000    | 0.000        | -13.319      | 4.081   | 16.790  | 0.000     | 17.400    |
| 242 Tenorite                                             | -1.846    | 0.000    | 0.000    | -1.576       | -2.116       | 5.774   | 7.620   | 7.350     | 7.890     |
| 243 CuOCuSO <sub>4</sub>                                 | -35.404   | 0.000    | 0.000    | 0.000        | 0.000        | -23.874 | 11.530  | 0.000     | 0.000     |
| 244 Cu <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>      | -18.362   | 0.000    | 0.000    | 0.000        | -18.312      | -55.212 | -36.850 | 0.000     | -36.900   |
| 245 Cu <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> , 3w | -20.118   | 0.000    | 0.000    | 0.000        | 0.000        | -55.238 | -35.120 | 0.000     | 0.000     |
| 247 CuSO <sub>4</sub>                                    | -16.218   | 0.000    | 0.000    | -15.858      | -16.628      | -13.208 | 3.010   | 2.650     | 3.420     |
| 248 Chalcantite                                          | -10.611   | 0.000    | 0.000    | -10.291      | -11.116      | -13.251 | -2.640  | -2.960    | -2.135    |
| 420 Dioptase                                             | -4.794    | 0.000    | 0.000    | 0.000        | 0.000        | 1.706   | 6.500   | 0.000     | 0.000     |
| 249 Cupricferrit                                         | 11.115    | 0.000    | 0.000    | 11.645       | 0.000        | 16.995  | 5.880   | 5.350     | 0.000     |
| 459 CuBr                                                 | -11.364   | 0.000    | 0.000    | 0.000        | 0.000        | -19.574 | -8.210  | 0.000     | 0.000     |
| 460 CuI                                                  | -10.921   | 0.000    | 0.000    | 0.000        | 0.000        | -22.811 | -11.890 | 0.000     | 0.000     |
| 265 Zn metal                                             | -50.775   | 0.000    | 0.000    | 0.000        | -50.808      | -25.018 | 25.757  | 0.000     | 25.790    |
| 266 Zn(BO <sub>2</sub> ) <sub>2</sub>                    | -6.674    | 0.000    | 0.000    | 0.000        | 0.000        | 1.616   | 8.290   | 0.000     | 0.000     |
| 267 ZnCl <sub>2</sub>                                    | -16.052   | 0.000    | 0.000    | 0.000        | -16.082      | -9.022  | 7.030   | 0.000     | 7.060     |
| 268 Smithsonite                                          | -3.223    | 0.000    | 0.000    | -2.413       | -3.403       | -13.223 | -10.000 | -10.810   | -9.820    |
| 269 ZnCO <sub>3</sub> , 1H <sub>2</sub> O                | -2.972    | 0.000    | 0.000    | 0.000        | 0.000        | -13.232 | -10.260 | 0.000     | 0.000     |
| 270 ZnF <sub>2</sub>                                     | -15.679   | 0.000    | 0.000    | 0.000        | -16.119      | -17.199 | -1.520  | 0.000     | -1.080    |
| 271 Zn(OH) <sub>2</sub> (a)                              | -4.142    | 0.000    | 0.000    | -3.952       | -4.172       | 8.308   | 12.450  | 12.260    | 12.480    |
| 272 Zn(OH) <sub>2</sub> (c)                              | -3.892    | 0.000    | 0.000    | 0.000        | 0.000        | 8.308   | 12.200  | 0.000     | 0.000     |
| 273 Zn(OH) <sub>2</sub> (b)                              | -3.442    | 0.000    | 0.020    | -3.012       | -3.582       | 8.308   | 11.750  | 11.320    | 11.890    |
| 274 Zn(OH) <sub>2</sub> (g)                              | -3.402    | 0.000    | 0.000    | -2.882       | -3.532       | 8.308   | 11.710  | 11.190    | 11.840    |
| 275 Zn(OH) <sub>2</sub> (e)                              | -3.192    | 0.000    | 0.030    | -2.642       | -3.312       | 8.308   | 11.500  | 10.950    | 11.620    |
| 276 Zn <sub>2</sub> (OH) <sub>3</sub> Cl                 | -7.250    | 0.000    | 0.000    | 0.000        | 0.000        | 7.950   | 15.200  | 0.000     | 0.000     |
| 277 Zn <sub>5</sub> (OH) <sub>8</sub> Cl                 | -14.292   | 0.000    | 0.000    | 0.000        | 0.000        | 24.208  | 38.500  | 0.000     | 0.000     |
| 278 Zn <sub>2</sub> (OH) <sub>2</sub> SO <sub>4</sub>    | -9.859    | 0.000    | 0.000    | 0.000        | 0.000        | -2.359  | 7.500   | 0.000     | 0.000     |
| 279 Zn <sub>4</sub> (OH) <sub>6</sub> SO <sub>4</sub>    | -14.144   | 0.000    | 0.000    | 0.000        | 0.000        | 14.256  | 28.400  | 0.000     | 0.000     |
| 280 ZnNO <sub>3</sub> ) <sub>2</sub> , 6H <sub>2</sub> O | -22.489   | 0.000    | 0.000    | 0.000        | 0.000        | -19.049 | 3.440   | 0.000     | 0.000     |
| 281 ZnO(active)                                          | -2.994    | 0.000    | 0.000    | -3.254       | -3.544       | 8.316   | 11.310  | 11.570    | 11.860    |
| 282 Zincite                                              | -2.824    | 0.000    | 0.000    | -2.674       | -3.224       | 8.316   | 11.140  | 10.990    | 11.540    |
| 283 Zn <sub>3</sub> O(SO <sub>4</sub> ) <sub>2</sub>     | -32.036   | 0.000    | 0.000    | 0.000        | 0.000        | -13.016 | 19.020  | 0.000     | 0.000     |
| 284 Zn <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> , 4w | -15.581   | 0.000    | 0.000    | 0.000        | 0.000        | -47.621 | -32.040 | 0.000     | 0.000     |
| 288 ZnSiO <sub>3</sub>                                   | 1.326     | 0.000    | 0.000    | 0.000        | 0.000        | 4.256   | 2.930   | 0.000     | 0.000     |
| 289 Willemite                                            | -2.758    | 0.000    | 0.000    | -0.778       | 0.000        | 12.572  | 15.330  | 13.350    | 0.000     |
| 290 Zincosite                                            | -13.676   | 0.000    | 0.000    | 0.000        | -14.596      | -10.666 | 3.010   | 0.000     | 3.930     |
| 291 ZnSO <sub>4</sub> , 1H <sub>2</sub> O                | -10.105   | 0.000    | 0.000    | 0.000        | -10.175      | -10.675 | -0.570  | 0.000     | -0.500    |
| 292 Bianchite                                            | -8.952    | 0.000    | 0.000    | 0.000        | -9.697       | -10.717 | -1.765  | 0.000     | -1.020    |
| 293 Goslarite                                            | -8.766    | 0.000    | 0.000    | 0.000        | -8.856       | -10.726 | -1.960  | 0.000     | -1.870    |
| 461 ZnBr <sub>2</sub> , 2H <sub>2</sub> O                | -19.714   | 0.000    | 0.000    | 0.000        | 0.000        | -14.504 | 5.210   | 0.000     | 0.000     |
| 462 ZnI <sub>2</sub>                                     | -28.190   | 0.000    | 0.000    | 0.000        | 0.000        | -20.960 | 7.230   | 0.000     | 0.000     |
| 312 Cd metal                                             | -41.469   | 0.000    | 0.000    | 0.000        | -41.619      | -27.979 | 13.490  | 0.000     | 13.640    |
| 313 Gamma Cd                                             | -41.569   | 0.000    | 0.000    | 0.000        | 0.000        | -27.979 | 13.590  | 0.000     | 0.000     |



| Phase             | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP  | Log KT  | Log MinKT | Log MaxKT |
|-------------------|-----------|----------|----------|--------------|--------------|---------|---------|-----------|-----------|
| 314 Cd(BO2)2      | -11.184   | 0.000    | 0.000    | 0.000        | 0.000        | -1.344  | 9.840   | 0.000     | 0.000     |
| 315 Otavite       | -2.444    | 0.000    | 0.000    | -2.374       | -4.974       | -16.184 | -13.740 | -13.810   | -11.210   |
| 316 CdCl2         | -11.302   | 0.000    | 0.000    | 0.000        | -11.512      | -11.982 | -0.680  | 0.000     | -0.470    |
| 317 CdCl2, 1H2O   | -10.281   | 0.000    | 0.000    | 0.000        | 0.000        | -11.991 | -1.710  | 0.000     | 0.000     |
| 318 CdCl2, 2.5H2O | -10.064   | 0.000    | 0.000    | 0.000        | 0.000        | -12.004 | -1.940  | 0.000     | 0.000     |
| 319 CdF2          | -17.180   | 0.000    | 0.000    | 0.000        | 0.000        | -20.160 | -2.980  | 0.000     | 0.000     |
| 320 Cd(OH)2 (a)   | -8.383    | 0.000    | 0.000    | -8.263       | -8.953       | 5.347   | 13.730  | 13.610    | 14.300    |
| 321 Cd(OH)2 (c)   | -8.303    | 0.000    | 0.040    | 0.000        | 0.000        | 5.347   | 13.650  | 0.000     | 0.000     |
| 322 CdOHC1        | -6.838    | 0.000    | 0.000    | -6.618       | 0.000        | -3.318  | 3.520   | 3.300     | 0.000     |
| 323 Cd3(OH)4SO4   | -25.492   | 0.000    | 0.000    | 0.000        | 0.000        | -2.932  | 22.560  | 0.000     | 0.000     |
| 324 Cd3OH2(SO4)2  | -28.616   | 0.000    | 0.000    | 0.000        | 0.000        | -21.906 | 6.710   | 0.000     | 0.000     |
| 325 Cd4(OH)6SO4   | -25.985   | 0.000    | 0.000    | 0.000        | 0.000        | 2.415   | 28.400  | 0.000     | 0.000     |
| 326 Montepsonite  | -9.764    | 0.000    | 0.000    | 0.000        | -10.384      | 5.356   | 15.120  | 0.000     | 15.740    |
| 327 Cd3(PO4)2     | -23.868   | 0.000    | 0.000    | 0.000        | 0.000        | -56.468 | -32.600 | 0.000     | 0.000     |
| 328 CdSiO3        | -7.764    | 0.000    | 0.000    | -6.664       | 0.000        | 1.296   | 9.060   | 7.960     | 0.000     |
| 329 CdSO4         | -13.527   | 0.000    | 0.000    | -13.497      | -13.577      | -13.627 | -0.100  | -0.130    | -0.050    |
| 330 CdSO4, 1H2O   | -11.978   | 0.000    | 0.000    | -11.955      | -12.005      | -13.635 | -1.657  | -1.680    | -1.630    |
| 331 CdSO4, 2.7H2O | -11.776   | 0.000    | 0.000    | -11.759      | -11.789      | -13.649 | -1.873  | -1.890    | -1.860    |
| 463 CdBr2, 4H2O   | -15.061   | 0.000    | 0.000    | 0.000        | 0.000        | -17.481 | -2.420  | 0.000     | 0.000     |
| 464 CdI2          | -20.310   | 0.000    | 0.000    | 0.000        | 0.000        | -23.920 | -3.610  | 0.000     | 0.000     |
| 360 Pb metal      | -32.990   | 0.000    | 0.000    | -32.790      | -33.030      | -28.720 | 4.270   | 4.070     | 4.310     |
| 361 Pb(BO2)2      | -9.696    | 0.000    | 0.000    | 0.000        | 0.000        | -2.086  | 7.610   | 0.000     | 0.000     |
| 362 Cotunnite     | -7.954    | 0.000    | 0.000    | -7.748       | -8.054       | -12.724 | -4.770  | -4.976    | -4.670    |
| 363 Matlockite    | -7.382    | 0.000    | 0.000    | 0.000        | -8.212       | -16.812 | -9.430  | 0.000     | -8.600    |
| 364 Phosgenite    | -9.839    | 0.000    | 0.000    | -9.709       | 0.000        | -29.649 | -19.810 | -19.940   | 0.000     |
| 365 Cerrusite     | -3.795    | 0.000    | 0.000    | -3.485       | -4.095       | -16.925 | -13.130 | -13.440   | -12.830   |
| 366 PbF2          | -13.461   | 0.000    | 0.000    | -13.331      | 0.000        | -20.901 | -7.440  | -7.570    | 0.000     |
| 367 Massicot      | -8.296    | 0.000    | 0.000    | -8.176       | 0.000        | 4.614   | 12.910  | 12.790    | 0.000     |
| 368 Litharge      | -8.106    | 0.000    | 0.000    | -8.026       | -8.456       | 4.614   | 12.720  | 12.640    | 13.070    |
| 369 PbO, .3H2O    | -8.368    | 0.000    | 0.000    | 0.000        | 0.000        | 4.612   | 12.980  | 0.000     | 0.000     |
| 370 Pb2OCO3       | -11.810   | 0.000    | 0.000    | -11.530      | 0.000        | -12.310 | -0.500  | -0.780    | 0.000     |
| 371 Larnakite     | -9.473    | 0.000    | 0.000    | -3.453       | 0.000        | -9.753  | -0.280  | -6.300    | 0.000     |
| 372 Pb3O2SO4      | -15.539   | 0.000    | 0.000    | 0.000        | 0.000        | -5.139  | 10.400  | 0.000     | 0.000     |
| 373 Pb4O3SO4      | -22.625   | 0.000    | 0.000    | 0.000        | 0.000        | -0.525  | 22.100  | 0.000     | 0.000     |
| 374 PbHPO4        | -7.851    | 0.000    | 0.000    | -3.681       | -9.411       | -19.311 | -11.460 | -15.630   | -9.900    |
| 375 Pb3(PO4)2     | -14.330   | 0.000    | 0.000    | -3.970       | -16.620      | -34.000 | -19.670 | -30.030   | -17.380   |
| 376 Clpyromorph   | -9.970    | 0.000    | 0.000    | 0.000        | -59.890      | -94.400 | -84.430 | 0.000     | -34.510   |
| 377 Hxypyromorph  | -22.945   | 0.000    | 0.000    | 0.000        | 0.000        | -85.735 | -62.790 | 0.000     | 0.000     |
| 378 Pb3O2CO3      | -18.716   | 0.000    | 0.000    | 0.000        | 0.000        | -7.696  | 11.020  | 0.000     | 0.000     |
| 379 Plumbgummite  | -12.531   | 0.000    | 0.000    | 0.000        | 0.000        | -45.321 | -32.790 | 0.000     | 0.000     |
| 380 Hinsdalite    | -25.531   | 0.000    | 0.000    | 0.000        | 0.000        | -28.031 | -2.500  | 0.000     | 0.000     |
| 381 Tsumebite     | -11.513   | 0.000    | 0.000    | 0.000        | 0.000        | -21.303 | -9.790  | 0.000     | 0.000     |
| 382 PbSiO3        | -6.765    | 0.000    | 0.000    | -5.565       | -7.085       | 0.555   | 7.320   | 6.120     | 7.640     |
| 383 Pb2SiO4       | -14.591   | 0.000    | 0.000    | -14.051      | -15.331      | 5.169   | 19.760  | 19.220    | 20.500    |
| 384 Anglesite     | -6.578    | 0.000    | 0.020    | -6.498       | 0.000        | -14.368 | -7.790  | -7.870    | 0.000     |
| 386 Plattnerite   | -11.351   | 0.000    | 0.000    | -11.051      | 0.000        | 37.949  | 49.300  | 49.000    | 0.000     |
| 387 Pb2O3         | -18.477   | 0.000    | 0.000    | 0.000        | 0.000        | 42.563  | 61.040  | 0.000     | 0.000     |
| 388 Minium        | -26.512   | 0.000    | 0.000    | -23.622      | 0.000        | 47.178  | 73.690  | 70.800    | 0.000     |
| 389 Pb(OH)2 (c)   | -3.544    | 0.000    | 0.000    | 0.000        | -9.024       | 4.606   | 8.150   | 0.000     | 13.630    |
| 390 Laurionite    | -4.682    | 0.000    | 0.000    | -4.234       | 0.000        | -4.059  | 0.623   | 0.175     | 0.000     |
| 391 Pb2(OH)3Cl    | -8.246    | 0.000    | 0.000    | 0.000        | 0.000        | 0.547   | 8.793   | 0.000     | 0.000     |
| 392 Hydcerussite  | -11.784   | 0.000    | 0.000    | 0.000        | 0.000        | -29.244 | -17.460 | 0.000     | 0.000     |
| 393 Pb2O(OH)2     | -16.980   | 0.000    | 0.000    | 0.000        | -17.880      | 9.220   | 26.200  | 0.000     | 27.100    |
| 465 PbBr2         | -13.008   | 0.000    | 0.000    | -12.848      | -13.778      | -18.188 | -5.180  | -5.340    | -4.410    |
| 466 PbBrF         | -11.055   | 0.000    | 0.000    | 0.000        | 0.000        | -19.545 | -8.490  | 0.000     | 0.000     |
| 467 PbI2          | -16.591   | 0.000    | 0.000    | 0.000        | 0.000        | -24.661 | -8.070  | 0.000     | 0.000     |
| 394 Pb4(OH)6SO4   | -21.650   | 0.000    | 0.000    | 0.000        | 0.000        | -0.550  | 21.100  | 0.000     | 0.000     |



| Phase             | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP   | Log KT  | Log MinKT | Log MaxKT |
|-------------------|-----------|----------|----------|--------------|--------------|----------|---------|-----------|-----------|
| 410 NiCO3         | -7.554    | 0.000    | 0.000    | 0.000        | 0.000        | -14.394  | -6.840  | 0.000     | 0.000     |
| 411 Ni(OH)2       | -3.663    | 0.000    | 0.100    | -3.453       | -6.163       | 7.137    | 10.800  | 10.590    | 13.300    |
| 412 Ni4(OH)6SO4   | -22.426   | 0.000    | 0.000    | 0.000        | 0.000        | 9.574    | 32.000  | 0.000     | 0.000     |
| 413 Bunsenite     | -5.305    | 0.000    | 0.000    | 0.000        | -5.245       | 7.145    | 12.450  | 0.000     | 12.390    |
| 414 Ni3(PO4)2     | -19.799   | 0.000    | 0.000    | 0.000        | 0.000        | -51.099  | -31.300 | 0.000     | 0.000     |
| 416 Retgersite    | -9.848    | 0.000    | 0.000    | 0.000        | 0.000        | -11.888  | -2.040  | 0.000     | 0.000     |
| 417 Morenosite    | -9.537    | 0.000    | 0.000    | 0.000        | 0.000        | -11.897  | -2.360  | 0.000     | 0.000     |
| 418 Ni2SiO4       | -4.309    | 0.000    | 0.000    | 0.000        | 0.000        | 10.231   | 14.540  | 0.000     | 0.000     |
| 437 Ag metal      | -9.462    | 0.000    | 0.000    | 0.000        | 0.000        | -22.972  | -13.510 | 0.000     | 0.000     |
| 438 Bromyrite     | -5.436    | 0.000    | 0.000    | 0.000        | 0.000        | -17.706  | -12.270 | 0.000     | 0.000     |
| 439 Cerargyrite   | -5.224    | 0.000    | 0.000    | 0.000        | 0.000        | -14.974  | -9.750  | 0.000     | 0.000     |
| 440 Ag2CO3        | -23.079   | 0.000    | 0.000    | 0.000        | 0.000        | -34.149  | -11.070 | 0.000     | 0.000     |
| 441 AgF, 4H2O     | -19.647   | 0.000    | 0.000    | 0.000        | 0.000        | -19.097  | 0.550   | 0.000     | 0.000     |
| 442 Iodyrite      | -4.873    | 0.000    | 0.000    | 0.000        | 0.000        | -20.943  | -16.070 | 0.000     | 0.000     |
| 443 Ag2O          | -25.190   | 0.000    | 0.100    | 0.000        | 0.000        | -12.610  | 12.580  | 0.000     | 0.000     |
| 444 Ag3PO4        | -37.632   | 0.000    | 0.000    | 0.000        | 0.000        | -55.182  | -17.550 | 0.000     | 0.000     |
| 446 Ag2SO4        | -26.672   | 0.000    | 0.000    | 0.000        | 0.000        | -31.592  | -4.920  | 0.000     | 0.000     |
| 488 As2O5         | -37.093   | 0.000    | 0.000    | 0.000        | -39.872      | -30.394  | 6.699   | 0.000     | 9.478     |
| 489 AlAsO4, 2H2O  | -12.431   | 0.000    | 0.000    | 0.000        | 0.000        | -28.268  | -15.837 | 0.000     | 0.000     |
| 541 Ba3(AsO4)2    | 5.418     | 0.000    | 0.000    | 0.000        | 0.000        | -44.692  | -50.110 | 0.000     | 0.000     |
| 490 Ca3AsO4)2, 4w | -11.307   | 0.000    | 0.000    | 0.000        | 0.000        | -30.212  | -18.905 | 0.000     | 0.000     |
| 491 Cu3AsO4)2, 6w | -19.193   | 0.000    | 0.000    | 0.000        | 0.000        | -54.316  | -35.123 | 0.000     | 0.000     |
| 492 FeAsO4, 2H2O  | -9.952    | 0.000    | 0.000    | 0.000        | 0.000        | -30.201  | -20.249 | 0.000     | 0.000     |
| 493 Mn3AsO4)2, 8w | -21.199   | 0.000    | 0.000    | 0.000        | 0.000        | -49.906  | -28.707 | 0.000     | 0.000     |
| 494 Ni3AsO4)2, 8w | -24.709   | 0.000    | 0.000    | 0.000        | 0.000        | -50.220  | -25.511 | 0.000     | 0.000     |
| 495 Pb3(AsO4)2    | -22.341   | 0.000    | 0.000    | 0.000        | 0.000        | -57.744  | -35.403 | 0.000     | 0.000     |
| 496 Zn3AsO4)2, 5w | -19.115   | 0.000    | 0.000    | 0.000        | 0.000        | -46.661  | -27.546 | 0.000     | 0.000     |
| 497 Arsenolite    | -113.548  | 0.000    | 0.000    | -113.490     | -113.621     | -116.349 | -2.801  | -2.859    | -2.728    |
| 498 Claudetite    | -113.284  | 0.000    | 0.000    | 0.000        | -113.328     | -116.349 | -3.065  | 0.000     | -3.021    |
| 499 AsI3          | -77.156   | 0.000    | 0.000    | 0.000        | 0.000        | -73.001  | 4.155   | 0.000     | 0.000     |

## DK Nordstrom Test Data - Test Case #2 - Surface Water

B5

|     |        |        |   |     |      |            |
|-----|--------|--------|---|-----|------|------------|
| 162 | 0      | 000000 | 0 | 2.5 | .13  | 0          |
|     | TEMP   | =      |   |     |      | 9.500000   |
|     | PH     | =      |   |     |      | 8.010000   |
|     | EHM    | =      |   |     |      | 0.440000   |
|     | DOC    | =      |   |     |      | 2.500000   |
|     | DOX    | =      |   |     |      | 10.940000  |
|     | CORALC | =      |   |     |      | 0.000000   |
|     | FLG    | =      |   |     | MG/L |            |
|     | DENS   | =      |   |     |      | 1.000000   |
|     | PRNT   | =      |   |     |      | 0          |
|     | PUNCH  | =      |   |     |      | 1          |
|     | EHOPT  | =      |   |     |      | 0          |
|     | EMPOX  | =      |   |     |      | 0          |
|     | ITDS   | =      |   |     |      | 0.000000   |
|     | COND   | =      |   |     |      | 162.000000 |
|     | SIGMDO | =      |   |     |      | 0.000000   |
|     | SIGMEH | =      |   |     |      | 0.000000   |
|     | SIGMPH | =      |   |     |      | 0.000000   |

| Species  | Index No | Input Concentration |
|----------|----------|---------------------|
| Ca       | : 0 :    | 12.20000000         |
| Mg       | : 1 :    | 7.50000000          |
| Na       | : 2 :    | 12.00000000         |
| K        | : 3 :    | 1.40000000          |
| Cl       | : 4 :    | 9.90000000          |
| SO4      | : 5 :    | 7.70000000          |
| HCO3     | : 6 :    | 75.20000000         |
| Fe total | : 16 :   | 0.01570000          |
| H2S aq   | : 13 :   | 0.00200000          |
| CO3      | : 17 :   | -1.00000000         |
| SiO2 tot | : 34 :   | 18.23000000         |
| NH4      | : 38 :   | 0.14400000          |
| B tot    | : 86 :   | 0.05000000          |
| PO4      | : 44 :   | 0.21000000          |
| Al       | : 50 :   | 0.00500000          |
| F        | : 61 :   | 0.10000000          |
| NO3      | : 84 :   | 0.89800000          |
| Fe       | : 7 :    | 0.01500000          |
| I        | : 96 :   | 0.00180000          |
| Br       | : 97 :   | 0.00600000          |
| Mn       | : 109 :  | 0.00440000          |
| Cu       | : 130 :  | 0.00050000          |
| Zn       | : 145 :  | 0.00049000          |
| Cd       | : 160 :  | 0.00010000          |
| Pb       | : 182 :  | 0.00003000          |
| NO2      | : 202 :  | 0.01900000          |
| Ni       | : 204 :  | 0.00180000          |
| Ag       | : 212 :  | 0.00004000          |
| As total | : 249 :  | 0.00200000          |

DK Nordstrom Test Data - Test Case #2 - Surface Water  
 162 0 000000 0 2.5 .13 0

B5

| ITER | S1-AnalCO3    | S2-AnalSO4    | S3-AnalF      | S4-AnalPO4    | S5-AnalCL    | S6-AnalH2S   | S7-AnalFULV  | S8-AnalHUM   |
|------|---------------|---------------|---------------|---------------|--------------|--------------|--------------|--------------|
| 1    | 1.439877E-05  | 5.445961E-06  | 6.342457E-08  | 4.338450E-07  | 7.406713E-11 | 3.106519E-08 | 0.000000E-01 | 0.000000E-01 |
| 2    | -2.993668E-07 | 2.296506E-08  | 1.635463E-10  | 1.780145E-09  | 9.711089E-13 | 6.417580E-09 | 0.000000E-01 | 0.000000E-01 |
| 3    | -4.810908E-09 | -3.771400E-10 | -2.186377E-12 | -2.991892E-11 | 1.538320E-13 | 1.389986E-09 | 0.000000E-01 | 0.000000E-01 |
| 4    | -6.067123E-10 | -4.612625E-12 | -3.300897E-14 | -3.786088E-13 | 3.273629E-14 | 2.931040E-10 | 0.000000E-01 | 0.000000E-01 |
| 5    | -1.305103E-10 | -6.477745E-14 | -7.097161E-16 | -6.037996E-15 | 6.881107E-15 | 6.126896E-11 | 0.000000E-01 | 0.000000E-01 |
| 6    | -2.719809E-11 | 9.952080E-14  | 5.355476E-16  | 2.740897E-15  | 1.436729E-15 | 1.278118E-11 | 0.000000E-01 | 0.000000E-01 |

## DK Nordstrom Test Data - Test Case #2 - Surface Water

B5

Date = 9/12/86 9:57

162 0 000000 0 2.5 .13 0  
 DOX = 10.9400 DOC = 2.5 INPUT TDS = 0.0  
 Anal Cond = 162.0 Calc Cond = 176.3  
 Anal EPMCAT = 1.7932 Anal EPMAN = 1.6994 Percent difference in input cation/anion balance = 5.3686  
 Calc EPMCAT = 1.7714 Calc EPMAN = 1.6742 Percent difference in calc cation/anion balance = 5.6438  
 Total Ionic Strength (T.I.S.) from input data = 0.00245  
 Effective Ionic Strength (E.I.S.) from speciation = 0.00240

| Sato  |       |         |       | Calc    |       |         |       |         |       |         |       |        |       |         |       |
|-------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|--------|-------|---------|-------|
| Input | Sigma | Fe3/Fe2 | Sigma | H2O2/O2 | Sigma | NO3/NO2 | Sigma | NO3/NH4 | Sigma | H2O2/O2 | Sigma | SO4/S= | Sigma | As5/As3 | Sigma |
| 0.440 | 0.000 | 0.073   | 0.000 | 0.141   | 0.000 | 0.445   | 0.000 | 0.328   | 0.000 | 0.783   | 0.000 | -0.229 | 0.000 | 0.440   | 0.000 |
| pE    |       |         |       |         |       |         |       |         |       |         |       |        |       |         |       |
| 7.845 | 0.000 | 1.302   | 0.000 | 2.508   | 0.000 | 7.927   | 0.000 | 5.845   | 0.000 | 13.963  | 0.000 | -4.080 | 0.000 | 7.845   | 0.000 |

| Effective |       |         |           |          |          |          |         |           |               |          |        |
|-----------|-------|---------|-----------|----------|----------|----------|---------|-----------|---------------|----------|--------|
| T         | pH    | TDS ppm | Ionic Str | pO2 Atm  | pCO2 Atm | pCH4 Atm | CO2 Tot | Uncom CO2 | ppm Uncom CO2 | Ncrb Alk | aH2O   |
| 9.50      | 8.010 | 145.6   | 0.00240   | 6.44E-26 | 6.05E-04 | 1.82-105 | 0.00126 | 1.22E-03  | 5.36E+01      | 3.82E-06 | 0.9999 |

| I   | Species  | Anal ppm | Calc ppm | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|----------|----------|----------|------------|------------|-----------|-----------|----------|
| 0   | Ca       | 2        | 11.931   | 3.044E-04  | 2.977E-04  | 2.419E-04 | 0.8126    | 3.616    |
| 28  | CaOH     | 1        | 0.000098 |            | 1.719E-09  | 1.631E-09 | 0.9486    | 8.788    |
| 31  | CaSO4 aq | 0        | 0.356    |            | 2.619E-06  | 2.620E-06 | 1.0006    | 5.582    |
| 81  | CaHSO4   | 1        | 0.000000 |            | 1.166E-13  | 1.106E-13 | 0.9486    | 12.956   |
| 29  | CaHCO3   | 1        | 0.271    |            | 2.683E-06  | 2.545E-06 | 0.9486    | 5.594    |
| 30  | CaCO3 aq | 0        | 0.124    |            | 1.238E-06  | 1.238E-06 | 1.0006    | 5.907    |
| 100 | CaF      | 1        | 0.000456 |            | 7.712E-09  | 7.315E-09 | 0.9486    | 8.136    |
| 75  | CaH2PO4  | 1        | 0.000147 |            | 1.071E-09  | 1.016E-09 | 0.9486    | 8.993    |
| 73  | CaHPO4aq | 0        | 0.017    |            | 1.274E-07  | 1.274E-07 | 1.0006    | 6.895    |
| 74  | CaPO4    | -1       | 0.003227 |            | 2.390E-08  | 2.267E-08 | 0.9486    | 7.645    |
| 1   | Mg       | 2        | 7.342    | 3.085E-04  | 3.020E-04  | 2.459E-04 | 0.8140    | 3.609    |
| 18  | MgOH     | 1        | 0.000428 |            | 1.037E-08  | 9.836E-09 | 0.9486    | 8.007    |
| 22  | MgSO4 aq | 0        | 0.281    |            | 2.338E-06  | 2.340E-06 | 1.0006    | 5.631    |
| 21  | MgHCO3   | 1        | 0.272    |            | 3.189E-06  | 3.025E-06 | 0.9486    | 5.519    |
| 20  | MgCO3 aq | 0        | 0.059    |            | 6.963E-07  | 6.967E-07 | 1.0006    | 6.157    |
| 19  | MgF      | 1        | 0.002374 |            | 5.482E-08  | 5.200E-08 | 0.9486    | 7.284    |
| 40  | MgH2PO4  | 1        | 0.000168 |            | 1.387E-09  | 1.315E-09 | 0.9486    | 8.881    |
| 72  | MgHPO4aq | 0        | 0.021    |            | 1.750E-07  | 1.751E-07 | 1.0006    | 6.757    |
| 39  | MgPO4    | -1       | 0.003907 |            | 3.276E-08  | 3.107E-08 | 0.9486    | 7.508    |
| 2   | Na       | 1        | 11.989   | 5.220E-04  | 5.216E-04  | 4.949E-04 | 0.9489    | 3.305    |
| 43  | NaSO4    | -1       | 0.017    |            | 1.436E-07  | 1.362E-07 | 0.9486    | 6.866    |
| 42  | NaHCO3aq | 0        | 0.027    |            | 3.194E-07  | 3.196E-07 | 1.0006    | 6.495    |
| 41  | NaCO3    | -1       | 0.001325 |            | 1.597E-08  | 1.515E-08 | 0.9486    | 7.820    |
| 49  | NaHPO4   | -1       | 0.000158 |            | 1.326E-09  | 1.258E-09 | 0.9486    | 8.900    |
| 297 | NaF aq   | 0        | 0.000012 |            | 2.854E-10  | 2.856E-10 | 1.0006    | 9.544    |
| 3   | K        | 1        | 1.400    | 3.581E-05  | 3.580E-05  | 3.394E-05 | 0.9482    | 4.469    |
| 45  | KSO4     | -1       | 0.001556 |            | 1.152E-08  | 1.092E-08 | 0.9486    | 7.962    |
| 60  | KHPO4    | -1       | 0.000012 |            | 9.096E-11  | 8.628E-11 | 0.9486    | 10.064   |
| 63  | H        | 1        | 0.000010 |            | 1.027E-08  | 9.772E-09 | 0.9520    | 8.010    |
| 26  | OH       | -1       | 0.005371 |            | 3.159E-07  | 2.996E-07 | 0.9486    | 6.523    |
| 17  | CO3      | -2       | 0.278    |            | 4.634E-06  | 3.767E-06 | 0.8129    | 5.424    |
| 6   | HCO3     | -1       | 75.200   | 1.233E-03  | 1.209E-03  | 1.148E-03 | 0.9495    | 2.940    |
| 85  | H2CO3 aq | 0        | 2.044    |            | 3.296E-05  | 3.298E-05 | 1.0006    | 4.482    |
| 5   | SO4      | -2       | 7.700    | 8.017E-05  | 7.505E-05  | 6.091E-05 | 0.8117    | 4.215    |
| 62  | HSO4     | -1       | 0.000004 |            | 4.008E-11  | 3.802E-11 | 0.9486    | 10.420   |
| 61  | F        | -1       | 0.100    | 5.264E-06  | 5.201E-06  | 4.934E-06 | 0.9486    | 5.307    |
| 125 | HF aq    | 0        | 0.000001 |            | 5.163E-11  | 5.166E-11 | 1.0006    | 10.287   |
| 126 | HF2      | -1       | 0.000000 |            | 9.235E-16  | 8.760E-16 | 0.9486    | 15.058   |

## DK Nordstrom Test Data - Test Case #2 - Surface Water

B5

| I   | Species     | Anal ppm | Calc ppm | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|-------------|----------|----------|------------|------------|-----------|-----------|----------|
| 296 | H2F2 aq 0   |          | 0.000000 |            | 1.362E-20  | 1.363E-20 | 1.0006    | 19.866   |
| 4   | Cl -1       | 9.900    | 9.900    | 2.793E-04  | 2.793E-04  | 2.648E-04 | 0.9482    | 3.577    |
| 97  | Br -1       | 0.006000 | 0.006000 | 7.510E-08  | 7.510E-08  | 7.124E-08 | 0.9486    | 7.147    |
| 96  | I -1        | 0.001800 | 0.001800 | 1.419E-08  | 1.419E-08  | 1.346E-08 | 0.9486    | 7.871    |
| 44  | PO4 -3      | 0.210000 | 0.000007 | 2.212E-06  | 6.978E-11  | 4.338E-11 | 0.6217    | 10.363   |
| 46  | HPO4 -2     |          | 0.155    |            | 1.610E-06  | 1.304E-06 | 0.8096    | 5.885    |
| 47  | H2PO4 -1    |          | 0.023    |            | 2.371E-07  | 2.249E-07 | 0.9486    | 6.648    |
| 34  | SiO2 tot 0  | 18.230   |          | 3.034E-04  |            |           |           |          |
| 23  | H4SiO4 aq 0 |          | 29.005   |            | 3.018E-04  | 3.020E-04 | 1.0006    | 3.520    |
| 24  | H3SiO4 -1   |          | 0.155    |            | 1.626E-06  | 1.542E-06 | 0.9486    | 5.812    |
| 25  | H2SiO4 -2   |          | 0.000005 |            | 5.305E-11  | 4.295E-11 | 0.8096    | 10.367   |
| 124 | SiF6 -2     |          | 0.000000 |            | 3.346E-37  | 2.709E-37 | 0.8096    | 36.567   |
| 13  | H2S aq 0    | 0.002000 | 0.000135 | 5.869E-08  | 3.965E-09  | 3.967E-09 | 1.0006    | 8.402    |
| 66  | HS -1       |          | 0.000946 |            | 2.862E-08  | 2.715E-08 | 0.9486    | 7.566    |
| 67  | S -2        |          | 0.000000 |            | 1.352E-13  | 1.095E-13 | 0.8096    | 12.961   |
| 263 | S2 -2       |          | 0.000000 |            | 3.516E-15  | 2.867E-15 | 0.8155    | 14.543   |
| 264 | S3 -2       |          | 0.000000 |            | 6.766E-14  | 5.542E-14 | 0.8191    | 13.256   |
| 265 | S4 -2       |          | 0.000026 |            | 2.038E-10  | 1.678E-10 | 0.8236    | 9.775    |
| 266 | S5 -2       |          | 0.000058 |            | 3.605E-10  | 2.985E-10 | 0.8279    | 9.525    |
| 267 | S6 -2       |          | 0.000084 |            | 4.391E-10  | 3.654E-10 | 0.8320    | 9.437    |
| 86  | B tot 0     | 0.050    |          | 4.626E-06  |            |           |           |          |
| 35  | H3BO3 aq 0  |          | 0.273    |            | 4.420E-06  | 4.422E-06 | 1.0006    | 5.354    |
| 36  | H2BO3 -1    |          | 0.013    |            | 2.057E-07  | 1.952E-07 | 0.9486    | 6.710    |
| 101 | BF(OH)3 -1  |          | 0.000001 |            | 7.716E-12  | 7.319E-12 | 0.9486    | 11.136   |
| 102 | BF2(OH)2 -1 |          | 0.000000 |            | 4.039E-17  | 3.831E-17 | 0.9486    | 16.417   |
| 103 | BF3OH -1    |          | 0.000000 |            | 2.856E-24  | 2.709E-24 | 0.9486    | 23.567   |
| 104 | BF4 -1      |          | 0.000000 |            | 5.683E-31  | 5.390E-31 | 0.9486    | 30.268   |
| 202 | NO2 -1      | 0.019    | 0.019    | 4.131E-07  | 4.131E-07  | 3.918E-07 | 0.9486    | 6.407    |
| 84  | NO3 -1      | 0.898    | 0.898    | 1.448E-05  | 1.448E-05  | 1.374E-05 | 0.9486    | 4.862    |
| 37  | NH3 aq 0    |          | 0.002322 |            | 1.364E-07  | 1.365E-07 | 1.0006    | 6.865    |
| 38  | NH4 1       | 0.144    | 0.141    | 7.984E-06  | 7.842E-06  | 7.438E-06 | 0.9486    | 5.129    |
| 91  | NH4SO4 -1   |          | 0.000702 |            | 6.153E-09  | 5.837E-09 | 0.9486    | 8.234    |
| 50  | Al 3        | 0.005000 | 0.000000 | 1.853E-07  | 2.338E-15  | 1.453E-15 | 0.6217    | 14.838   |
| 51  | AlOH 2      |          | 0.000000 |            | 6.248E-13  | 5.058E-13 | 0.8096    | 12.296   |
| 52  | Al(OH)2 1   |          | 0.000078 |            | 1.274E-09  | 1.209E-09 | 0.9486    | 8.918    |
| 181 | Al(OH)3 0   |          | 0.012    |            | 1.556E-07  | 1.557E-07 | 1.0006    | 6.808    |
| 53  | Al(OH)4 -1  |          | 0.002704 |            | 2.846E-08  | 2.700E-08 | 0.9486    | 7.569    |
| 54  | AlF 2       |          | 0.000000 |            | 9.063E-14  | 7.337E-14 | 0.8096    | 13.134   |
| 55  | AlF2 1      |          | 0.000000 |            | 3.294E-14  | 3.125E-14 | 0.9486    | 13.505   |
| 56  | AlF3 aq 0   |          | 0.000000 |            | 1.449E-14  | 1.450E-14 | 1.0006    | 13.839   |
| 57  | AlF4 -1     |          | 0.000000 |            | 4.765E-17  | 4.519E-17 | 0.9486    | 16.345   |
| 58  | AlSO4 1     |          | 0.000000 |            | 8.009E-17  | 7.597E-17 | 0.9486    | 16.119   |
| 59  | Al(SO4)2 -1 |          | 0.000000 |            | 3.635E-19  | 3.448E-19 | 0.9486    | 18.462   |
| 203 | AlHSO4 2    |          | 0.000000 |            | 1.968E-25  | 1.593E-25 | 0.8096    | 24.798   |
| 7   | Fe 2        | 0.015    | 0.015    | 2.686E-07  | 2.636E-07  | 2.134E-07 | 0.8096    | 6.671    |
| 10  | FeOH 1      |          | 0.000156 |            | 2.146E-09  | 2.035E-09 | 0.9486    | 8.691    |
| 79  | Fe(OH)2 0   |          | 0.000000 |            | 4.274E-13  | 4.276E-13 | 1.0006    | 12.369   |
| 11  | Fe(OH)3 -1  |          | 0.000000 |            | 1.460E-15  | 1.385E-15 | 0.9486    | 14.859   |
| 247 | Fe(HS)2 0   |          | 0.000000 |            | 1.401E-13  | 1.402E-13 | 1.0006    | 12.853   |
| 248 | Fe(HS)3 -1  |          | 0.000000 |            | 4.370E-19  | 4.145E-19 | 0.9486    | 18.382   |
| 33  | FeSO4 aq 0  |          | 0.000260 |            | 1.714E-09  | 1.715E-09 | 1.0006    | 8.766    |
| 122 | FeHSO4 1    |          | 0.000000 |            | 1.028E-16  | 9.755E-17 | 0.9486    | 16.011   |
| 99  | FeHPO4 aq 0 |          | 0.000168 |            | 1.107E-09  | 1.108E-09 | 1.0006    | 8.956    |
| 64  | FeH2PO4 1   |          | 0.000004 |            | 2.536E-11  | 2.406E-11 | 0.9486    | 10.619   |
| 8   | Fe 3        | 0.000700 | 0.000000 | 1.254E-08  | 2.536E-19  | 1.576E-19 | 0.6217    | 18.802   |
| 9   | FeOH 2      |          | 0.000000 |            | 4.913E-14  | 3.978E-14 | 0.8096    | 13.400   |
| 76  | Fe(OH)2 1   |          | 0.000334 |            | 3.720E-09  | 3.529E-09 | 0.9486    | 8.452    |

## DK Nordstrom Test Data - Test Case #2 - Surface Water

B5

| I   | Species  | Anal ppm | Calc ppm | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|----------|----------|----------|------------|------------|-----------|-----------|----------|
| 77  | Fe(OH)3  | 0        | 0.000453 |            | 4.240E-09  | 4.242E-09 | 1.0006    | 8.372    |
| 78  | Fe(OH)4  | -1       | 0.000567 |            | 4.576E-09  | 4.341E-09 | 0.9486    | 8.362    |
| 179 | Fe2(OH)2 | 4        | 0.000000 |            | 1.948E-25  | 8.368E-26 | 0.4295    | 25.077   |
| 180 | Fe3(OH)4 | 5        | 0.000000 |            | 2.146E-31  | 5.729E-32 | 0.2670    | 31.242   |
| 14  | FeSO4    | 1        | 0.000000 |            | 5.863E-20  | 5.562E-20 | 0.9486    | 19.255   |
| 108 | Fe(SO4)2 | -1       | 0.000000 |            | 1.060E-22  | 1.005E-22 | 0.9486    | 21.998   |
| 123 | FeHSO4   | 2        | 0.000000 |            | 2.236E-27  | 1.810E-27 | 0.8096    | 26.742   |
| 15  | FeCl     | 2        | 0.000000 |            | 9.274E-22  | 7.508E-22 | 0.8096    | 21.124   |
| 27  | FeCl2    | 1        | 0.000000 |            | 1.572E-24  | 1.491E-24 | 0.9486    | 23.826   |
| 32  | FeCl3 aq | 0        | 0.000000 |            | 3.947E-29  | 3.949E-29 | 1.0006    | 28.404   |
| 105 | FeF      | 2        | 0.000000 |            | 1.186E-18  | 9.601E-19 | 0.8096    | 18.018   |
| 106 | FeF2     | 1        | 0.000000 |            | 1.637E-19  | 1.553E-19 | 0.9486    | 18.809   |
| 107 | FeF3 aq  | 0        | 0.000000 |            | 1.148E-21  | 1.149E-21 | 1.0006    | 20.940   |
| 12  | FeHPO4   | 1        | 0.000000 |            | 3.422E-20  | 3.246E-20 | 0.9486    | 19.489   |
| 98  | FeH2PO4  | 2        | 0.000000 |            | 1.179E-20  | 9.542E-21 | 0.8096    | 20.020   |
| 109 | Mn       | 2        | 0.004284 | 8.010E-08  | 7.799E-08  | 6.313E-08 | 0.8096    | 7.200    |
| 119 | MnHCO3   | 1        | 0.000165 |            | 1.423E-09  | 1.350E-09 | 0.9486    | 8.870    |
| 111 | MnCl     | 1        | 0.000006 |            | 7.131E-11  | 6.764E-11 | 0.9486    | 10.170   |
| 112 | MnCl2 aq | 0        | 0.000000 |            | 4.863E-15  | 4.866E-15 | 1.0006    | 14.313   |
| 113 | MnCl3    | -1       | 0.000000 |            | 6.124E-19  | 5.809E-19 | 0.9486    | 18.236   |
| 116 | MnF      | 1        | 0.000000 |            | 2.325E-12  | 2.205E-12 | 0.9486    | 11.657   |
| 114 | MnOH     | 1        | 0.000003 |            | 4.617E-11  | 4.380E-11 | 0.9486    | 10.359   |
| 115 | Mn(OH)3  | -1       | 0.000000 |            | 1.130E-18  | 1.072E-18 | 0.9486    | 17.970   |
| 118 | Mn(NO3)2 | 0        | 0.000000 |            | 4.919E-17  | 4.922E-17 | 1.0006    | 16.308   |
| 117 | MnSO4 aq | 0        | 0.000086 |            | 5.722E-10  | 5.725E-10 | 1.0006    | 9.242    |
| 110 | Mn       | 3        | 0.000000 |            | 2.039E-26  | 1.268E-26 | 0.6217    | 25.897   |
| 121 | MnO4     | -2       | 0.000000 |            | 7.628E-37  | 6.175E-37 | 0.8096    | 36.209   |
| 120 | MnO4     | -1       | 0.000000 |            | 1.605E-39  | 1.523E-39 | 0.9486    | 38.817   |
| 127 | Cu       | 1        | 0.000000 |            | 2.783E-17  | 2.640E-17 | 0.9486    | 16.578   |
| 128 | CuCl2    | -1       | 0.000000 |            | 6.416E-19  | 6.086E-19 | 0.9486    | 18.216   |
| 129 | CuCl3    | -2       | 0.000000 |            | 2.963E-22  | 2.399E-22 | 0.8096    | 21.620   |
| 130 | Cu       | 2        | 0.000000 | 7.869E-09  | 5.067E-12  | 4.102E-12 | 0.8096    | 11.387   |
| 271 | CuHCO3   | 1        | 0.000000 |            | 2.489E-12  | 2.361E-12 | 0.9486    | 11.627   |
| 131 | CuCO3 aq | 0        | 0.000010 |            | 8.294E-11  | 8.298E-11 | 1.0006    | 10.081   |
| 132 | Cu(CO3)2 | -2       | 0.000000 |            | 4.861E-13  | 3.935E-13 | 0.8096    | 12.405   |
| 133 | CuCl     | 1        | 0.000000 |            | 1.384E-15  | 1.313E-15 | 0.9486    | 14.882   |
| 134 | CuCl2 aq | 0        | 0.000000 |            | 1.564E-19  | 1.565E-19 | 1.0006    | 18.806   |
| 135 | CuCl3    | -1       | 0.000000 |            | 1.160E-25  | 1.100E-25 | 0.9486    | 24.958   |
| 136 | CuCl4    | -2       | 0.000000 |            | 1.236E-31  | 1.000E-31 | 0.8096    | 31.000   |
| 137 | CuF      | 1        | 0.000000 |            | 3.342E-16  | 3.170E-16 | 0.9486    | 15.499   |
| 138 | CuOH     | 1        | 0.000000 |            | 4.425E-12  | 4.197E-12 | 0.9486    | 11.377   |
| 139 | Cu(OH)2  | 0        | 0.000087 |            | 8.968E-10  | 8.973E-10 | 1.0006    | 9.047    |
| 140 | Cu(OH)3  | -1       | 0.000000 |            | 5.833E-15  | 5.533E-15 | 0.9486    | 14.257   |
| 141 | Cu(OH)4  | -2       | 0.000000 |            | 1.395E-19  | 1.130E-19 | 0.8096    | 18.947   |
| 142 | Cu2(OH)2 | 2        | 0.000000 |            | 1.875E-18  | 1.518E-18 | 0.8096    | 17.819   |
| 143 | CuSO4 aq | 0        | 0.000000 |            | 4.554E-14  | 4.557E-14 | 1.0006    | 13.341   |
| 144 | Cu(HS)3  | -1       | 0.001119 |            | 6.875E-09  | 6.521E-09 | 0.9486    | 8.186    |
| 259 | Cu(S4)2  | -3       | 0.000000 |            | 8.418E-13  | 5.813E-13 | 0.6906    | 12.236   |
| 260 | CuS4S5   | -3       | 0.000000 |            | 1.565E-13  | 1.090E-13 | 0.6964    | 12.963   |
| 145 | Zn       | 2        | 0.000199 | 7.497E-09  | 3.051E-09  | 2.470E-09 | 0.8096    | 8.607    |
| 272 | ZnHCO3   | 1        | 0.000048 |            | 3.764E-10  | 3.571E-10 | 0.9486    | 9.447    |
| 273 | ZnCO3    | 0        | 0.000233 |            | 1.855E-09  | 1.856E-09 | 1.0006    | 8.731    |
| 274 | Zn(CO3)2 | -2       | 0.000034 |            | 1.847E-10  | 1.495E-10 | 0.8096    | 9.825    |
| 146 | ZnCl     | 1        | 0.000000 |            | 9.025E-13  | 8.561E-13 | 0.9486    | 12.067   |
| 147 | ZnCl2 aq | 0        | 0.000000 |            | 2.222E-16  | 2.223E-16 | 1.0006    | 15.653   |
| 148 | ZnCl3    | -1       | 0.000000 |            | 6.312E-20  | 5.987E-20 | 0.9486    | 19.223   |
| 149 | ZnCl4    | -2       | 0.000000 |            | 8.623E-24  | 6.981E-24 | 0.8096    | 23.156   |



| I   | Species     | Anal ppm | Calc ppm | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|-------------|----------|----------|------------|------------|-----------|-----------|----------|
| 150 | ZnF 1       |          | 0.000000 |            | 1.478E-13  | 1.402E-13 | 0.9486    | 12.853   |
| 151 | ZnOH 1      |          | 0.000007 |            | 8.453E-11  | 8.018E-11 | 0.9486    | 10.096   |
| 152 | Zn(OH)2 0   |          | 0.000032 |            | 3.254E-10  | 3.256E-10 | 1.0006    | 9.487    |
| 153 | Zn(OH)3 -1  |          | 0.000000 |            | 1.111E-13  | 1.053E-13 | 0.9486    | 12.977   |
| 154 | Zn(OH)4 -2  |          | 0.000000 |            | 2.110E-18  | 1.708E-18 | 0.8096    | 17.767   |
| 155 | ZnOHCl aq 0 |          | 0.000000 |            | 2.215E-12  | 2.216E-12 | 1.0006    | 11.654   |
| 156 | Zn(HS)2 0   |          | 0.000208 |            | 1.585E-09  | 1.586E-09 | 1.0006    | 8.800    |
| 157 | Zn(HS)3 -1  |          | 0.000000 |            | 6.561E-16  | 6.223E-16 | 0.9486    | 15.206   |
| 158 | ZnSO4 aq 0  |          | 0.000005 |            | 3.108E-11  | 3.110E-11 | 1.0006    | 10.507   |
| 159 | Zn(SO4)2 -2 |          | 0.000000 |            | 2.157E-14  | 1.746E-14 | 0.8096    | 13.758   |
| 229 | ZnBr 1      |          | 0.000000 |            | 4.879E-17  | 4.628E-17 | 0.9486    | 16.335   |
| 230 | ZnBr2 aq 0  |          | 0.000000 |            | 1.312E-24  | 1.312E-24 | 1.0006    | 23.882   |
| 231 | ZnI 1       |          | 0.000000 |            | 4.311E-20  | 4.089E-20 | 0.9486    | 19.388   |
| 232 | ZnI2 aq 0   |          | 0.000000 |            | 9.126E-27  | 9.131E-27 | 1.0006    | 26.039   |
| 160 | Cd 2        | 0.000100 | 0.000000 | 8.898E-10  | 2.439E-12  | 1.974E-12 | 0.8096    | 11.705   |
| 166 | Cd(CO3)3 -4 |          | 0.000000 |            | 4.077E-22  | 1.751E-22 | 0.4295    | 21.757   |
| 275 | CdHCO3 1    |          | 0.000000 |            | 3.009E-13  | 2.854E-13 | 0.9486    | 12.545   |
| 276 | CdCO3 0     |          | 0.000000 |            | 1.867E-12  | 1.868E-12 | 1.0006    | 11.729   |
| 161 | CdCl 1      |          | 0.000000 |            | 4.983E-14  | 4.727E-14 | 0.9486    | 13.325   |
| 162 | CdCl2 aq 0  |          | 0.000000 |            | 4.911E-17  | 4.914E-17 | 1.0006    | 16.309   |
| 163 | CdCl3 -1    |          | 0.000000 |            | 6.767E-21  | 6.418E-21 | 0.9486    | 20.193   |
| 164 | CdF 1       |          | 0.000000 |            | 1.293E-16  | 1.226E-16 | 0.9486    | 15.911   |
| 165 | CdF2 aq 0   |          | 0.000000 |            | 1.519E-21  | 1.520E-21 | 1.0006    | 20.818   |
| 167 | CdOH 1      |          | 0.000000 |            | 5.269E-15  | 4.998E-15 | 0.9486    | 14.301   |
| 168 | Cd(OH)2 0   |          | 0.000000 |            | 9.228E-17  | 9.233E-17 | 1.0006    | 16.035   |
| 169 | Cd(OH)3 -1  |          | 0.000000 |            | 1.117E-21  | 1.060E-21 | 0.9486    | 20.975   |
| 170 | Cd(OH)4 -2  |          | 0.000000 |            | 1.194E-27  | 9.667E-28 | 0.8096    | 27.015   |
| 171 | Cd2OH 3     |          | 0.000000 |            | 9.519E-26  | 5.917E-26 | 0.6217    | 25.228   |
| 172 | CdOHCl aq 0 |          | 0.000000 |            | 1.409E-15  | 1.410E-15 | 1.0006    | 14.851   |
| 173 | CdNO3 1     |          | 0.000000 |            | 1.162E-16  | 1.102E-16 | 0.9486    | 15.958   |
| 174 | CdSO4 aq 0  |          | 0.000000 |            | 3.136E-14  | 3.138E-14 | 1.0006    | 13.503   |
| 277 | Cd(SO4)2 -2 |          | 0.000000 |            | 2.861E-17  | 2.316E-17 | 0.8096    | 16.635   |
| 175 | CdHS 1      |          | 0.000122 |            | 8.356E-10  | 7.927E-10 | 0.9486    | 9.101    |
| 176 | Cd(HS)2 0   |          | 0.000009 |            | 4.928E-11  | 4.930E-11 | 1.0006    | 10.307   |
| 177 | Cd(HS)3 -1  |          | 0.000000 |            | 2.136E-16  | 2.026E-16 | 0.9486    | 15.693   |
| 178 | Cd(HS)4 -2  |          | 0.000000 |            | 1.053E-21  | 8.521E-22 | 0.8096    | 21.070   |
| 233 | CdBr 1      |          | 0.000000 |            | 2.364E-17  | 2.242E-17 | 0.9486    | 16.649   |
| 234 | CdBr2 aq 0  |          | 0.000000 |            | 7.953E-24  | 7.958E-24 | 1.0006    | 23.099   |
| 235 | CdI 1       |          | 0.000000 |            | 4.926E-18  | 4.673E-18 | 0.9486    | 17.330   |
| 236 | CdI2 aq 0   |          | 0.000000 |            | 1.390E-24  | 1.391E-24 | 1.0006    | 23.857   |
| 182 | Pb 2        | 0.000030 | 0.000001 | 1.448E-10  | 2.485E-12  | 2.012E-12 | 0.8096    | 11.696   |
| 278 | PbHCO3 1    |          | 0.000001 |            | 1.935E-12  | 1.835E-12 | 0.9486    | 11.736   |
| 241 | PbCO3 aq 0  |          | 0.000035 |            | 1.316E-10  | 1.317E-10 | 1.0006    | 9.880    |
| 187 | Pb(CO3)2 -2 |          | 0.000001 |            | 1.539E-12  | 1.246E-12 | 0.8096    | 11.904   |
| 183 | PbCl 1      |          | 0.000000 |            | 1.491E-14  | 1.414E-14 | 0.9486    | 13.850   |
| 184 | PbCl2 aq 0  |          | 0.000000 |            | 8.050E-18  | 8.055E-18 | 1.0006    | 17.094   |
| 185 | PbCl3 -1    |          | 0.000000 |            | 1.615E-21  | 1.532E-21 | 0.9486    | 20.815   |
| 186 | PbCl4 -2    |          | 0.000000 |            | 2.114E-25  | 1.712E-25 | 0.8096    | 24.767   |
| 188 | PbF 1       |          | 0.000000 |            | 1.861E-16  | 1.765E-16 | 0.9486    | 15.753   |
| 189 | PbF2 aq 0   |          | 0.000000 |            | 1.777E-20  | 1.778E-20 | 1.0006    | 19.750   |
| 190 | PbF3 -1     |          | 0.000000 |            | 6.700E-25  | 6.355E-25 | 0.9486    | 24.197   |
| 191 | PbF4 -2     |          | 0.000000 |            | 1.854E-30  | 1.501E-30 | 0.8096    | 29.824   |
| 192 | PbOH 1      |          | 0.000001 |            | 4.231E-12  | 4.014E-12 | 0.9486    | 11.396   |
| 193 | Pb(OH)2 0   |          | 0.000000 |            | 1.597E-13  | 1.598E-13 | 1.0006    | 12.796   |
| 194 | Pb(OH)3 -1  |          | 0.000000 |            | 1.979E-16  | 1.877E-16 | 0.9486    | 15.726   |
| 242 | Pb(OH)4 -2  |          | 0.000000 |            | 5.435E-20  | 4.400E-20 | 0.8096    | 19.357   |
| 195 | Pb2OH 3     |          | 0.000000 |            | 2.908E-22  | 1.808E-22 | 0.6217    | 21.743   |

## DK Nordstrom Test Data - Test Case #2 - Surface Water

B5

| I   | Species     | Anal ppm | Calc ppm | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|-------------|----------|----------|------------|------------|-----------|-----------|----------|
| 200 | Pb3(OH)4 2  |          | 0.000000 |            | 1.251E-28  | 1.013E-28 | 0.8096    | 27.995   |
| 196 | PbNO3 1     |          | 0.000000 |            | 4.310E-16  | 4.088E-16 | 0.9486    | 15.388   |
| 197 | PbSO4 aq 0  |          | 0.000000 |            | 6.887E-14  | 6.891E-14 | 1.0006    | 13.162   |
| 243 | Pb(SO4)2 -2 |          | 0.000000 |            | 2.721E-17  | 2.203E-17 | 0.8096    | 16.657   |
| 198 | Pb(HS)2 0   |          | 0.000001 |            | 2.760E-12  | 2.761E-12 | 1.0006    | 11.559   |
| 199 | Pb(HS)3 -1  |          | 0.000000 |            | 1.577E-18  | 1.496E-18 | 0.9486    | 17.825   |
| 237 | PbBr 1      |          | 0.000000 |            | 6.815E-18  | 6.464E-18 | 0.9486    | 17.189   |
| 238 | PbBr2 aq 0  |          | 0.000000 |            | 2.810E-25  | 2.812E-25 | 1.0006    | 24.551   |
| 239 | PbI 1       |          | 0.000000 |            | 2.486E-18  | 2.358E-18 | 0.9486    | 17.628   |
| 240 | PbI2 aq 0   |          | 0.000000 |            | 5.770E-25  | 5.773E-25 | 1.0006    | 24.239   |
| 204 | Ni 2        | 0.001800 | 0.000075 | 3.066E-08  | 1.282E-09  | 1.038E-09 | 0.8096    | 8.984    |
| 205 | NiBr 1      |          | 0.000000 |            | 2.464E-16  | 2.337E-16 | 0.9486    | 15.631   |
| 280 | NiHCO3 1    |          | 0.000021 |            | 1.734E-10  | 1.645E-10 | 0.9486    | 9.784    |
| 281 | NiCO3 0     |          | 0.003437 |            | 2.896E-08  | 2.897E-08 | 1.0006    | 7.538    |
| 282 | Ni(CO3)2 -2 |          | 0.000042 |            | 2.343E-10  | 1.897E-10 | 0.8096    | 9.722    |
| 206 | NiCl 1      |          | 0.000000 |            | 7.276E-13  | 6.901E-13 | 0.9486    | 12.161   |
| 279 | NiCl2 0     |          | 0.000000 |            | 6.632E-16  | 6.636E-16 | 1.0006    | 15.178   |
| 207 | NiF 1       |          | 0.000000 |            | 1.077E-13  | 1.021E-13 | 0.9486    | 12.991   |
| 208 | NiOH 1      |          | 0.000000 |            | 4.894E-12  | 4.643E-12 | 0.9486    | 11.333   |
| 209 | Ni(OH)2 0   |          | 0.000000 |            | 1.086E-12  | 1.086E-12 | 1.0006    | 11.964   |
| 210 | Ni(OH)3 -1  |          | 0.000000 |            | 1.172E-15  | 1.112E-15 | 0.9486    | 14.954   |
| 211 | NiSO4 aq 0  |          | 0.000002 |            | 1.070E-11  | 1.071E-11 | 1.0006    | 10.970   |
| 283 | Ni(SO4)2 -2 |          | 0.000000 |            | 4.980E-17  | 4.031E-17 | 0.8096    | 16.395   |
| 212 | Ag 1        | 0.000040 | 0.000000 | 3.709E-10  | 1.282E-16  | 1.216E-16 | 0.9486    | 15.915   |
| 213 | AgBr aq 0   |          | 0.000000 |            | 1.505E-19  | 1.506E-19 | 1.0006    | 18.822   |
| 214 | AgBr2 -1    |          | 0.000000 |            | 1.240E-23  | 1.176E-23 | 0.9486    | 22.930   |
| 244 | AgBr3 -2    |          | 0.000000 |            | 2.785E-29  | 2.255E-29 | 0.8096    | 28.647   |
| 215 | AgCl aq 0   |          | 0.000000 |            | 7.681E-17  | 7.685E-17 | 1.0006    | 16.114   |
| 216 | AgCl2 -1    |          | 0.000000 |            | 2.409E-18  | 2.285E-18 | 0.9486    | 17.641   |
| 217 | AgCl3 -2    |          | 0.000000 |            | 5.439E-22  | 4.403E-22 | 0.8096    | 21.356   |
| 218 | AgCl4 -3    |          | 0.000000 |            | 3.113E-25  | 1.935E-25 | 0.6217    | 24.713   |
| 219 | AgF aq 0    |          | 0.000000 |            | 1.785E-21  | 1.786E-21 | 1.0006    | 20.748   |
| 220 | AgHS aq 0   |          | 0.000052 |            | 3.702E-10  | 3.704E-10 | 1.0006    | 9.431    |
| 221 | Ag(HS)2 -1  |          | 0.000000 |            | 2.663E-13  | 2.526E-13 | 0.9486    | 12.598   |
| 222 | AgI aq 0    |          | 0.000000 |            | 6.511E-18  | 6.515E-18 | 1.0006    | 17.186   |
| 223 | AgI2 -1     |          | 0.000000 |            | 1.111E-21  | 1.054E-21 | 0.9486    | 20.977   |
| 245 | AgI3 -2     |          | 0.000000 |            | 1.047E-25  | 8.476E-26 | 0.8096    | 25.072   |
| 246 | AgI4 -3     |          | 0.000000 |            | 7.711E-34  | 4.794E-34 | 0.6217    | 33.319   |
| 224 | AgOH aq 0   |          | 0.000000 |            | 1.244E-20  | 1.244E-20 | 1.0006    | 19.905   |
| 225 | Ag(OH)2 -1  |          | 0.000000 |            | 1.342E-24  | 1.273E-24 | 0.9486    | 23.895   |
| 226 | AgSO4 -1    |          | 0.000000 |            | 1.327E-19  | 1.258E-19 | 0.9486    | 18.900   |
| 227 | AgNO3 aq 0  |          | 0.000000 |            | 8.565E-22  | 8.570E-22 | 1.0006    | 21.067   |
| 228 | Ag(NO2)2 -1 |          | 0.000000 |            | 3.266E-27  | 3.098E-27 | 0.9486    | 26.509   |
| 268 | Ag(S4)2 -3  |          | 0.000000 |            | 1.337E-14  | 9.194E-15 | 0.6875    | 14.037   |
| 269 | AgS4S5 -3   |          | 0.000000 |            | 6.478E-15  | 4.493E-15 | 0.6935    | 14.348   |
| 270 | Ag(HS)S4 -2 |          | 0.000000 |            | 2.967E-13  | 2.475E-13 | 0.8340    | 12.607   |
| 249 | As total 0  | 0.002000 |          | 2.670E-08  |            |           |           |          |
| 254 | H4AsO3 1    |          | 0.000000 |            | 8.038E-35  | 7.624E-35 | 0.9486    | 34.118   |
| 250 | H3AsO3aq 0  |          | 0.000000 |            | 1.574E-26  | 1.575E-26 | 1.0006    | 25.803   |
| 251 | H2AsO3 -1   |          | 0.000000 |            | 5.476E-28  | 5.194E-28 | 0.9486    | 27.284   |
| 252 | HAsO3 -2    |          | 0.000000 |            | 2.560E-32  | 2.072E-32 | 0.8096    | 31.684   |
| 253 | AsO3 -3     |          | 0.000000 |            | 7.511E-38  | 4.669E-38 | 0.6217    | 37.331   |
| 255 | H3AsO4aq 0  |          | 0.000000 |            | 1.806E-15  | 1.807E-15 | 1.0006    | 14.743   |
| 256 | H2AsO4 -1   |          | 0.000184 |            | 1.303E-09  | 1.236E-09 | 0.9486    | 8.908    |
| 257 | HAsO4 -2    |          | 0.003552 |            | 2.539E-08  | 2.055E-08 | 0.8096    | 7.687    |
| 258 | AsO4 -3     |          | 0.000001 |            | 5.735E-12  | 3.565E-12 | 0.6217    | 11.448   |

## Mole ratios from analytical molality - Log activity ratios

|         |   |            |                |     |   |         |
|---------|---|------------|----------------|-----|---|---------|
| Cl/Ca   | = | 9.1738E-01 | Log Ca         | /H2 | = | 12.4037 |
| Cl/Mg   | = | 9.0519E-01 | Log Mg         | /H2 | = | 12.4107 |
| Cl/Na   | = | 5.3498E-01 | Log Na         | /H1 | = | 4.7045  |
| Cl/K    | = | 7.7993E+00 | Log K          | /H1 | = | 3.5407  |
| Cl/Al   | = | 1.5069E+03 | Log Al         | /H3 | = | 9.1923  |
| Cl/Fe   | = | 1.0397E+03 | Log Fe         | /H2 | = | 9.3493  |
| Cl/SO4  | = | 3.4837E+00 | Log Ca/Mg      |     | = | -0.0070 |
| Cl/HCO3 | = | 2.2658E-01 | LOG NA/K       |     | = | 1.1638  |
| Ca/Mg   | = | 9.8671E-01 | Log Ca/K2      |     | = | 5.3222  |
| Na/K    | = | 1.4579E+01 | Log Diss Fe/H2 |     | = | 16.0200 |

| Phase             | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP   | Log KT   | Log MinKT | Log MaxKT |
|-------------------|-----------|----------|----------|--------------|--------------|----------|----------|-----------|-----------|
| 39 Adularia       | -0.786    | 0.000    | 0.000    | 0.000        | 0.000        | -22.598  | -21.812  | 0.000     | 0.000     |
| 40 Albite         | -2.391    | 0.000    | 0.000    | 0.000        | 0.000        | -21.434  | -19.043  | 0.000     | 0.000     |
| 140 AlOH3 (a)     | -2.275    | 0.000    | 0.000    | -1.586       | 0.000        | -34.408  | -32.133  | -32.822   | 0.000     |
| 471 AlOHSO4       | -7.813    | 0.000    | 0.000    | -7.653       | -7.973       | -11.043  | -3.230   | -3.390    | -3.070    |
| 472 Al4(OH)10SO4  | -6.166    | 0.000    | 0.000    | 0.000        | 0.000        | 16.534   | 22.700   | 0.000     | 0.000     |
| 157 Allophane(a)  | -0.581    | 0.000    | 0.000    | 0.000        | 0.000        | 7.176    | 7.757    | 0.000     | 0.000     |
| 158 Allophane(F)  | 0.400     | 0.000    | 0.000    | 0.000        | 0.000        | 7.176    | 6.775    | 0.000     | 0.000     |
| 338 Alum k        | -22.278   | 0.000    | 0.000    | 0.000        | 0.000        | -27.738  | -5.460   | 0.000     | 0.000     |
| 50 Alunite        | -10.021   | 0.000    | 0.000    | 0.000        | 0.000        | -96.553  | -86.533  | 0.000     | 0.000     |
| 42 Analcime       | -4.481    | 0.000    | 0.000    | 0.000        | 0.000        | -17.914  | -13.433  | 0.000     | 0.000     |
| 17 Anhydrite      | -3.346    | 0.000    | 0.000    | 0.000        | 0.000        | -7.832   | -4.486   | 0.000     | 0.000     |
| 113 Annite        | 45.546    | 0.000    | 0.000    | 0.000        | 0.000        | -42.610  | -88.156  | 0.000     | 0.000     |
| 41 Anorthite      | -5.614    | 0.000    | 0.000    | 0.000        | 0.000        | -25.794  | -20.179  | 0.000     | 0.000     |
| 21 Aragonite      | -0.787    | 0.000    | 0.020    | 0.000        | 0.000        | -9.040   | -8.253   | 0.000     | 0.000     |
| 150 Artinite      | -7.392    | 0.000    | 0.000    | 0.000        | 0.000        | 3.363    | 10.755   | 0.000     | 0.000     |
| 48 Beidellite     | 0.534     | 0.000    | 0.000    | 0.000        | 0.000        | -47.164  | -47.698  | 0.000     | 0.000     |
| 52 Boehmite       | -0.513    | 0.000    | 0.000    | 0.000        | 0.000        | -34.408  | -33.895  | -34.408   | 0.000     |
| 19 Brucite        | -5.418    | 0.000    | 0.000    | 0.000        | 0.000        | -16.656  | -11.238  | 0.000     | 0.000     |
| 12 Calcite        | -0.632    | 0.000    | 0.020    | -0.584       | 0.000        | -9.040   | -8.409   | -8.456    | 0.000     |
| 97 Chalcedony     | 0.189     | 0.000    | 0.000    | 0.000        | 0.000        | -3.520   | -3.708   | 0.000     | 0.000     |
| 49 Chlorite 14A   | -4.591    | 0.000    | 6.000    | 0.684        | -13.315      | 69.878   | 74.469   | 69.194    | 83.193    |
| 125 Chlorite 7A   | -8.115    | 0.000    | 6.000    | 0.000        | 0.000        | 69.878   | 77.993   | 0.000     | 0.000     |
| 20 Chrysotile     | -4.100    | 0.000    | 0.000    | 0.000        | 0.000        | -57.008  | -52.909  | 0.000     | 0.000     |
| 29 Clinoenstite   | -3.250    | 0.000    | 0.000    | -2.884       | -3.544       | -20.176  | -16.926  | -17.292   | -16.632   |
| 56 Clinoptilolite | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -26.807  | 0.000    | 0.000     | 0.000     |
| 99 Cristobalite   | 0.288     | 0.000    | 0.000    | 0.000        | 0.000        | -3.520   | -3.808   | 0.000     | 0.000     |
| 154 Diaspore      | 1.332     | 0.000    | 0.000    | 0.000        | 0.000        | -34.408  | -35.740  | 0.000     | 0.000     |
| 28 Diopside       | -3.405    | 0.000    | 0.000    | 0.000        | 0.000        | -40.359  | -36.954  | 0.000     | 0.000     |
| 11 Dolomite       | -1.407    | 0.000    | 0.000    | 0.000        | 0.000        | -18.074  | -16.667  | 0.000     | 0.000     |
| 340 Epsomite      | -5.571    | 0.000    | 0.000    | 0.000        | 0.000        | -7.825   | -2.253   | 0.000     | 0.000     |
| 55 Erionite       | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -23.194  | 0.000    | 0.000     | 0.000     |
| 112 Ferrihydrite  | 0.337     | 0.000    | 0.000    | 3.671        | 0.232        | 5.228    | 4.891    | 1.557     | 4.996     |
| 419 Fe3(OH)8      | -0.418    | 0.000    | 0.000    | 2.692        | -4.301       | 19.804   | 20.222   | 17.112    | 24.105    |
| 181 FeOH)2.7Cl.3  | 4.791     | 0.000    | 0.000    | 0.000        | 0.000        | 1.751    | -3.040   | 0.000     | 0.000     |
| 119 FeS ppt       | -2.312    | 0.000    | 0.000    | 0.000        | 0.000        | -6.227   | -3.915   | 0.000     | 0.000     |
| 401 Fe2(SO4)3     | -56.207   | 0.000    | 0.000    | -51.977      | 0.000        | -50.251  | 5.956    | 1.726     | 0.000     |
| 396 FCO3apatite   | 10.522    | 0.000    | 0.000    | 0.000        | 0.000        | -105.461 | -115.983 | 0.000     | 0.000     |
| 96 Fluorapatite   | -0.219    | 0.000    | 0.000    | 7.424        | 0.000        | -17.013  | -16.793  | -24.436   | 0.000     |
| 62 Fluorite       | -3.076    | 0.000    | 0.000    | 0.000        | 0.000        | -14.230  | -11.154  | 0.000     | 0.000     |
| 27 Forsterite     | -8.942    | 0.000    | 0.000    | 0.000        | 0.000        | -36.832  | -27.890  | 0.000     | 0.000     |
| 51 Gibbsite (c)   | -0.494    | 0.000    | 0.200    | -0.211       | -1.164       | 9.192    | 9.686    | 9.403     | 10.356    |
| 110 Goethite      | 4.146     | 0.000    | 0.800    | 0.000        | 0.000        | 5.228    | 1.082    | 0.000     | 0.000     |
| 111 Greenalite    | 0.198     | 0.000    | 0.000    | 0.000        | 0.000        | 21.008   | 20.810   | 0.000     | 0.000     |
| 118 Greigite      | 2.534     | 0.000    | 0.000    | 0.000        | 0.000        | -42.501  | -45.035  | 0.000     | 0.000     |
| 18 Gypsum         | -3.221    | 0.000    | 0.000    | 0.000        | 0.000        | -7.832   | -4.610   | 0.000     | 0.000     |
| 64 Halite         | -8.428    | 0.000    | 0.000    | 0.000        | 0.000        | -6.883   | 1.545    | 0.000     | 0.000     |
| 47 Halloysite     | -3.571    | 0.000    | 0.000    | 0.000        | 0.000        | -38.197  | -34.626  | 0.000     | 0.000     |
| 108 Hematite      | 13.223    | 0.000    | 0.000    | 0.000        | 0.000        | 10.455   | -2.768   | 0.000     | 0.000     |
| 117 Huntite       | -7.208    | 0.000    | 0.000    | 0.000        | 0.000        | -36.140  | -28.933  | 0.000     | 0.000     |
| 38 Hydrmagnesit   | -17.053   | 0.000    | 0.000    | 0.000        | 0.000        | -52.790  | -35.736  | 0.000     | 0.000     |
| 95 Hydroxyapati   | -1.728    | 0.000    | 0.000    | 0.801        | -8.389       | -3.696   | -1.968   | -4.497    | 4.693     |
| 45 Illite         | -0.459    | 0.000    | 0.000    | 0.000        | 0.000        | -42.924  | -42.465  | 0.000     | 0.000     |
| 204 Jarosite Na   | -10.337   | 0.000    | 1.000    | 0.000        | 0.000        | -20.083  | -9.746   | 0.000     | 0.000     |
| 205 Jarosite K    | -7.704    | 0.000    | 1.100    | 0.000        | -10.004      | -21.247  | -13.543  | 0.000     | -11.243   |
| 337 Jarosite H    | -14.904   | 0.000    | 0.000    | 0.000        | 0.000        | -24.788  | -9.883   | 0.000     | 0.000     |
| 46 Kaolinite      | 0.699     | 0.000    | 0.000    | 1.578        | -0.402       | -38.197  | -38.897  | -39.776   | -37.796   |
| 43 Kmica          | 5.468     | 0.000    | 1.300    | 6.866        | 3.789        | 20.558   | 15.090   | 13.692    | 16.769    |

| Phase            | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP   | Log KT   | Log MinKT | Log MaxKT |
|------------------|-----------|----------|----------|--------------|--------------|----------|----------|-----------|-----------|
| 128 Laumontite   | -0.281    | 0.000    | 0.000    | 0.000        | 0.000        | -32.834  | -32.552  | 0.000     | 0.000     |
| 147 Leonhardite  | 7.709     | 0.000    | 0.000    | 0.000        | 0.000        | -65.667  | -73.376  | 0.000     | 0.000     |
| 67 Mackinawite   | -1.579    | 0.000    | 0.000    | 0.000        | 0.000        | -6.227   | -4.648   | 0.000     | 0.000     |
| 98 Magadiite     | -6.799    | 0.000    | 0.000    | 0.000        | 0.000        | -21.099  | -14.300  | 0.000     | 0.000     |
| 109 Maghemite    | 4.069     | 0.000    | 0.000    | 0.000        | 0.000        | 10.455   | 6.386    | 0.000     | 0.000     |
| 10 Magnesite     | -1.252    | 0.000    | 0.000    | -1.002       | -1.502       | -9.033   | -7.781   | -8.031    | -7.531    |
| 107 Magnetite    | 14.039    | 0.000    | 0.000    | 14.409       | 11.181       | 19.804   | 5.765    | 5.395     | 8.623     |
| 339 Melanterite  | -8.301    | 0.000    | 0.000    | 0.000        | 0.000        | -10.886  | -2.585   | 0.000     | 0.000     |
| 63 Montmoril Ca  | 0.196     | 0.000    | 0.000    | 0.000        | 0.000        | -47.177  | -47.373  | 0.000     | 0.000     |
| 115 Montmoril BF | 1.030     | 0.000    | 0.000    | 0.000        | 0.000        | -33.883  | -34.913  | 0.000     | 0.000     |
| 116 Montmoril AB | 0.467     | 0.000    | 0.000    | 0.000        | 0.000        | -29.221  | -29.688  | 0.000     | 0.000     |
| 57 Mordenite     | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -25.047  | 0.000    | 0.000     | 0.000     |
| 66 Mirabilite    | -8.949    | 0.000    | 0.000    | 0.000        | 0.000        | -10.826  | -1.877   | 0.000     | 0.000     |
| 58 Nahcolite     | -5.548    | 0.000    | 0.000    | 0.000        | 0.000        | -6.245   | -0.698   | 0.000     | 0.000     |
| 60 Natron        | -10.091   | 0.000    | 0.000    | 0.000        | 0.000        | -12.035  | -1.944   | 0.000     | 0.000     |
| 149 Nesquehonite | -3.645    | 0.000    | 0.000    | -4.133       | -4.720       | -9.033   | -5.388   | -4.900    | -4.313    |
| 54 Phillipsite   | -2.142    | 0.000    | 0.000    | 0.000        | 0.000        | -22.016  | -19.874  | 0.000     | 0.000     |
| 44 Phlogopite    | -30.366   | 0.000    | 3.000    | 0.000        | 0.000        | 14.634   | 45.000   | 0.000     | 0.000     |
| 141 Prehnite     | -4.797    | 0.000    | 0.000    | 0.000        | 0.000        | -16.910  | -12.113  | 0.000     | 0.000     |
| 114 Pyrite       | 28.840    | 0.000    | 0.000    | 0.000        | 0.000        | 9.907    | -18.933  | 0.000     | 0.000     |
| 53 Pyrophyllite  | 3.077     | 0.000    | 0.000    | 6.373        | 1.243        | -45.237  | -48.314  | -51.610   | -46.480   |
| 101 Quartz       | 0.736     | 0.000    | 0.000    | 0.000        | 0.000        | -3.520   | -4.256   | 0.000     | 0.000     |
| 36 Sepiolite(c)  | -2.182    | 0.000    | 0.000    | 0.000        | 0.000        | 14.261   | 16.443   | 0.000     | 0.000     |
| 153 Sepiolite(a) | -4.399    | 0.000    | 0.000    | 0.000        | 0.000        | 14.261   | 18.660   | 0.000     | 0.000     |
| 9 Siderite       | -1.759    | 0.000    | 0.000    | -0.205       | 0.000        | -12.095  | -10.336  | -11.890   | 0.000     |
| 100 SiO2 (a,L)   | -0.323    | 0.000    | 0.000    | 0.000        | 0.000        | -3.520   | -3.196   | 0.000     | 0.000     |
| 395 SiO2 (a,M)   | -0.653    | 0.000    | 0.000    | 0.000        | 0.000        | -3.520   | -2.867   | 0.000     | 0.000     |
| 146 Strengite    | -2.847    | 0.000    | 0.000    | -0.124       | -3.012       | -29.165  | -26.318  | -29.041   | -26.153   |
| 37 Talc          | -0.110    | 0.000    | 2.000    | 2.058        | -1.858       | 23.152   | 23.262   | 21.094    | 25.010    |
| 402 Sulfur       | 18.073    | 0.000    | 0.000    | 19.147       | 0.000        | 2.730    | -15.344  | -16.418   | 0.000     |
| 65 Thenardite    | -10.670   | 0.000    | 0.000    | 0.000        | 0.000        | -10.826  | -0.156   | 0.000     | 0.000     |
| 61 Thermanatr    | -12.273   | 0.000    | 0.000    | 0.000        | 0.000        | -12.035  | 0.238    | 0.000     | 0.000     |
| 31 Tremolite     | -1.714    | 0.000    | 0.000    | 0.000        | 0.000        | -144.767 | -143.052 | 0.000     | 0.000     |
| 59 Trona         | -18.209   | 0.000    | 0.000    | 0.000        | 0.000        | -18.280  | -0.072   | 0.000     | 0.000     |
| 106 Vivianite    | -4.738    | 0.000    | 0.000    | 0.000        | 0.000        | -40.738  | -36.000  | 0.000     | 0.000     |
| 155 Wairkite     | -5.075    | 0.000    | 0.000    | 0.000        | 0.000        | -32.834  | -27.759  | 0.000     | 0.000     |
| 183 Pyrolusite   | -3.046    | 0.000    | 0.000    | 0.000        | -3.223       | 13.988   | 17.034   | 0.000     | 17.211    |
| 184 Birnessite   | -4.103    | 0.000    | 0.000    | 0.000        | 0.000        | 13.988   | 18.091   | 0.000     | 0.000     |
| 185 Nsutite      | -3.516    | 0.000    | 0.000    | 0.000        | 0.000        | 13.988   | 17.504   | 0.000     | 0.000     |
| 186 Bixbyite     | -3.736    | 0.000    | 0.000    | -2.121       | -3.917       | -3.734   | 0.002    | -1.613    | 0.183     |
| 187 Hausmannite  | -6.590    | 0.000    | 0.000    | 0.000        | 0.000        | 58.171   | 64.761   | 0.000     | 0.000     |
| 188 Pyrocroite   | -7.176    | 0.000    | 0.000    | 0.000        | -7.469       | 8.820    | 15.996   | 0.000     | 16.289    |
| 189 Manganite    | -1.629    | 0.000    | 0.000    | 0.000        | 0.000        | -1.867   | -0.238   | 0.000     | 0.000     |
| 190 Rhodochrosit | -2.297    | 0.000    | 0.000    | -1.688       | -2.714       | -12.624  | -10.326  | -10.935   | -9.909    |
| 191 MnCl2, 4H2O  | -16.365   | 0.000    | 0.000    | 0.000        | 0.000        | -14.354  | 2.011    | 0.000     | 0.000     |
| 192 Mns Green    | -10.789   | 0.000    | 0.000    | 0.000        | 0.000        | -6.756   | 4.033    | 0.000     | 0.000     |
| 182 MnSO4        | -14.706   | 0.000    | 0.000    | 0.000        | 0.000        | -11.415  | 3.291    | 0.000     | 0.000     |
| 134 Mn2(SO4)3    | -60.299   | 0.000    | 0.000    | 0.000        | 0.000        | -64.440  | -4.141   | 0.000     | 0.000     |
| 193 Mn3(PO4)2    | -18.412   | 0.000    | 0.000    | 0.000        | 0.000        | -42.325  | -23.912  | 0.000     | 0.000     |
| 194 MnHPO4       | -0.138    | 0.000    | 0.000    | 0.000        | 0.000        | -13.085  | -12.947  | 0.000     | 0.000     |
| 195 a-Cryptomeln | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -92.310  | 0.000    | 0.000     | 0.000     |
| 198 Todorokite   | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -42.025  | 0.000    | 0.000     | 0.000     |
| 200 Rancieite    | 0.000     | 0.000    | 0.000    | 0.000        | 0.000        | -39.821  | 0.000    | 0.000     | 0.000     |
| 223 Cu metal     | -14.975   | 0.000    | 0.000    | 0.000        | -14.935      | -24.424  | -9.449   | 0.000     | -9.489    |
| 224 Nantokite    | -12.994   | 0.000    | 0.000    | 0.000        | -13.124      | -20.155  | -7.161   | 0.000     | -7.031    |
| 225 CuF          | -29.462   | 0.000    | 0.000    | 0.000        | 0.000        | -21.885  | 7.577    | 0.000     | 0.000     |
| 226 Cuprite      | -15.336   | 0.000    | 0.000    | -15.016      | -16.186      | -17.137  | -1.801   | -2.121    | -0.951    |



| Phase              | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP  | Log KT  | Log MinKT | Log MaxKT |
|--------------------|-----------|----------|----------|--------------|--------------|---------|---------|-----------|-----------|
| 227 Chalcocite     | 3.889     | 0.000    | 0.160    | 4.190        | 0.170        | -32.713 | -36.603 | -36.904   | -32.884   |
| 536 Djurleite      | 4.568     | 0.000    | 0.150    | 0.000        | 0.000        | -31.276 | -35.845 | 0.000     | 0.000     |
| 535 Anilite        | 6.357     | 0.000    | 0.150    | 0.000        | 0.000        | -27.271 | -33.628 | 0.000     | 0.000     |
| 534 Blaublei II    | 7.628     | 0.000    | 0.150    | 0.000        | 0.000        | -19.651 | -27.279 | 0.000     | 0.000     |
| 533 Blaublei I     | 11.042    | 0.000    | 0.150    | 0.000        | 0.000        | -13.120 | -24.162 | 0.000     | 0.000     |
| 246 Covellite      | 13.060    | 0.000    | 0.110    | 0.000        | 12.192       | -10.943 | -24.003 | 0.000     | -23.135   |
| 228 Cu2SO4         | -35.605   | 0.000    | 0.000    | 0.000        | 0.000        | -37.372 | -1.767  | 0.000     | 0.000     |
| 229 Cuprousferit   | 5.426     | 0.000    | 0.000    | 0.000        | 3.386        | -3.341  | -8.767  | 0.000     | -6.727    |
| 230 Melanothalli   | -22.766   | 0.000    | 0.000    | 0.000        | -23.486      | -18.541 | 4.225   | 0.000     | 4.945     |
| 231 CuCO3          | -7.181    | 0.000    | 0.000    | -7.161       | -7.201       | -16.811 | -9.630  | -9.650    | -9.610    |
| 232 CuF2           | -21.916   | 0.000    | 0.000    | 0.000        | 0.000        | -22.001 | -0.085  | 0.000     | 0.000     |
| 233 CuF2, 2H2O     | -17.597   | 0.000    | 0.000    | 0.000        | 0.000        | -22.001 | -4.403  | 0.000     | 0.000     |
| 234 Cu(OH)2        | -4.620    | 0.000    | 0.000    | 0.000        | -5.180       | 4.633   | 9.253   | 0.000     | 9.813     |
| 235 Malachite      | -7.628    | 0.000    | 0.080    | -6.978       | -7.838       | -1.684  | 5.944   | 5.294     | 6.154     |
| 236 Azurite        | -12.992   | 0.000    | 0.090    | -10.422      | 0.000        | -8.001  | 4.991   | 2.421     | 0.000     |
| 237 Atacamite      | -10.412   | 0.000    | 0.000    | -10.312      | -10.562      | -2.321  | 8.091   | 7.991     | 8.241     |
| 238 Cu2(OH)3NO3    | -13.543   | 0.000    | 0.000    | 0.000        | -13.613      | -3.606  | 9.937   | 0.000     | 10.007    |
| 239 Antlerite      | -14.626   | 0.000    | 0.000    | 0.000        | -15.236      | -6.336  | 8.290   | 0.000     | 8.900     |
| 240 Brochantite    | -17.043   | 0.000    | 0.160    | -16.853      | -17.203      | -1.703  | 15.340  | 15.150    | 15.500    |
| 241 Langite        | -20.086   | 0.000    | 0.000    | 0.000        | -20.696      | -1.703  | 18.382  | 0.000     | 18.992    |
| 242 Tenorite       | -3.600    | 0.000    | 0.000    | -3.330       | -3.870       | 4.633   | 8.233   | 7.963     | 8.503     |
| 243 CuOCuSO4       | -39.949   | 0.000    | 0.000    | 0.000        | 0.000        | -26.989 | 12.960  | 0.000     | 0.000     |
| 244 Cu3(PO4)2      | -18.036   | 0.000    | 0.000    | 0.000        | -17.986      | -54.886 | -36.850 | 0.000     | -36.900   |
| 245 Cu3(PO4)2,3w   | -19.767   | 0.000    | 0.000    | 0.000        | 0.000        | -54.887 | -35.120 | 0.000     | 0.000     |
| 247 CuSO4          | -19.341   | 0.000    | 0.000    | -18.981      | -19.751      | -15.602 | 3.739   | 3.379     | 4.149     |
| 248 Chalcantite    | -12.905   | 0.000    | 0.000    | -12.585      | -13.410      | -15.602 | -2.698  | -3.018    | -2.193    |
| 420 Diopase        | -5.747    | 0.000    | 0.000    | 0.000        | 0.000        | 1.113   | 6.860   | 0.000     | 0.000     |
| 249 Cupricferrit   | 7.653     | 0.000    | 0.000    | 8.183        | 0.000        | 15.088  | 7.435   | 6.905     | 0.000     |
| 250 Chalcocopyrite | 19.526    | 0.000    | 0.000    | 0.000        | 15.046       | -17.170 | -36.696 | 0.000     | -32.216   |
| 459 CuBr           | -14.990   | 0.000    | 0.000    | 0.000        | 0.000        | -23.726 | -8.736  | 0.000     | 0.000     |
| 460 CuI            | -11.750   | 0.000    | 0.000    | 0.000        | 0.000        | -24.450 | -12.700 | 0.000     | 0.000     |
| 265 Zn metal       | -51.533   | 0.000    | 0.000    | 0.000        | -51.566      | -24.298 | 27.235  | 0.000     | 27.268    |
| 266 Zn(BO2)2       | -11.586   | 0.000    | 0.000    | 0.000        | 0.000        | -3.296  | 8.290   | 0.000     | 0.000     |
| 267 ZnCl2          | -23.494   | 0.000    | 0.000    | 0.000        | -23.524      | -15.761 | 7.733   | 0.000     | 7.763     |
| 268 Smithsonite    | -4.207    | 0.000    | 0.000    | -3.397       | -4.387       | -14.031 | -9.825  | -10.635   | -9.645    |
| 269 ZnCO3, 1H2O    | -3.771    | 0.000    | 0.000    | 0.000        | 0.000        | -14.031 | -10.260 | 0.000     | 0.000     |
| 270 ZnF2           | -18.227   | 0.000    | 0.000    | 0.000        | -18.667      | -19.221 | -0.994  | 0.000     | -0.554    |
| 271 Zn(OH)2 (a)    | -5.037    | 0.000    | 0.000    | -4.847       | -5.067       | 7.413   | 12.450  | 12.260    | 12.480    |
| 272 Zn(OH)2 (c)    | -4.787    | 0.000    | 0.000    | 0.000        | 0.000        | 7.413   | 12.200  | 0.000     | 0.000     |
| 273 Zn(OH)2 (b)    | -4.337    | 0.000    | 0.020    | -3.907       | -4.477       | 7.413   | 11.750  | 11.320    | 11.890    |
| 274 Zn(OH)2 (g)    | -4.297    | 0.000    | 0.000    | -3.777       | -4.427       | 7.413   | 11.710  | 11.190    | 11.840    |
| 275 Zn(OH)2 (e)    | -4.087    | 0.000    | 0.030    | -3.537       | -4.207       | 7.413   | 11.500  | 10.950    | 11.620    |
| 276 Zn2(OH)3Cl     | -11.962   | 0.000    | 0.000    | 0.000        | 0.000        | 3.238   | 15.200  | 0.000     | 0.000     |
| 277 Zn5(OH)8Cl     | -24.611   | 0.000    | 0.000    | 0.000        | 0.000        | 13.889  | 38.500  | 0.000     | 0.000     |
| 278 Zn2(OH)2SO4    | -12.910   | 0.000    | 0.000    | 0.000        | 0.000        | -5.410  | 7.500   | 0.000     | 0.000     |
| 279 Zn4(OH)6SO4    | -18.985   | 0.000    | 0.000    | 0.000        | 0.000        | 9.415   | 28.400  | 0.000     | 0.000     |
| 280 ZnNO3)2,6H2O   | -21.550   | 0.000    | 0.000    | 0.000        | 0.000        | -18.332 | 3.219   | 0.000     | 0.000     |
| 281 ZnO(active)    | -3.897    | 0.000    | 0.000    | -4.157       | -4.447       | 7.413   | 11.310  | 11.570    | 11.860    |
| 282 Zincite        | -4.606    | 0.000    | 0.000    | -4.456       | -5.006       | 7.413   | 12.019  | 11.869    | 12.419    |
| 283 Zn3O(SO4)2     | -39.745   | 0.000    | 0.000    | 0.000        | 0.000        | -18.233 | 21.512  | 0.000     | 0.000     |
| 284 Zn3(PO4)2,4w   | -14.507   | 0.000    | 0.000    | 0.000        | 0.000        | -46.547 | -32.040 | 0.000     | 0.000     |
| 285 Zns (a)        | 1.036     | 0.000    | 0.000    | 0.000        | 0.000        | -8.164  | -9.200  | 0.000     | 0.000     |
| 286 Sphalerite     | 3.786     | 0.000    | 0.000    | 5.380        | -1.880       | -8.164  | -11.950 | -13.544   | -6.284    |
| 287 Wurtzite       | 1.722     | 0.000    | 0.000    | 2.222        | 0.592        | -8.164  | -9.885  | -10.385   | -8.755    |
| 288 ZnSiO3         | 0.228     | 0.000    | 0.000    | 0.000        | 0.000        | 3.893   | 3.664   | 0.000     | 0.000     |
| 289 Willemite      | -5.366    | 0.000    | 0.000    | -3.386       | 0.000        | 11.305  | 16.671  | 14.691    | 0.000     |
| 290 Zincosite      | -16.604   | 0.000    | 0.000    | 0.000        | -17.524      | -12.823 | 3.782   | 0.000     | 4.702     |



| Phase                                       | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP  | Log KT  | Log MinKT | Log MaxKT |
|---------------------------------------------|-----------|----------|----------|--------------|--------------|---------|---------|-----------|-----------|
| 291 ZnSO <sub>4</sub> , 1H <sub>2</sub> O   | -12.680   | 0.000    | 0.000    | 0.000        | -12.750      | -12.823 | -0.142  | 0.000     | -0.072    |
| 292 Bianchite                               | -11.064   | 0.000    | 0.000    | 0.000        | -11.809      | -12.823 | -1.759  | 0.000     | -1.014    |
| 293 Goslarite                               | -10.730   | 0.000    | 0.000    | 0.000        | -10.820      | -12.823 | -2.093  | 0.000     | -2.003    |
| 461 ZnBr <sub>2</sub> , 2H <sub>2</sub> O   | -28.414   | 0.000    | 0.000    | 0.000        | 0.000        | -22.902 | 5.512   | 0.000     | 0.000     |
| 462 ZnI <sub>2</sub>                        | -32.120   | 0.000    | 0.000    | 0.000        | 0.000        | -24.349 | 7.770   | 0.000     | 0.000     |
| 312 Cd metal                                | -41.608   | 0.000    | 0.000    | 0.000        | -41.758      | -27.395 | 14.213  | 0.000     | 14.363    |
| 313 Gamma Cd                                | -41.714   | 0.000    | 0.000    | 0.000        | 0.000        | -27.395 | 14.319  | 0.000     | 0.000     |
| 314 Cd(BO <sub>2</sub> ) <sub>2</sub>       | -16.233   | 0.000    | 0.000    | 0.000        | 0.000        | -6.393  | 9.840   | 0.000     | 0.000     |
| 315 Otavite                                 | -3.412    | 0.000    | 0.000    | -3.342       | -5.942       | -17.129 | -13.717 | -13.787   | -11.187   |
| 316 CdCl <sub>2</sub>                       | -18.358   | 0.000    | 0.000    | 0.000        | -18.568      | -18.859 | -0.500  | 0.000     | -0.290    |
| 317 CdCl <sub>2</sub> , 1H <sub>2</sub> O   | -17.222   | 0.000    | 0.000    | 0.000        | 0.000        | -18.859 | -1.637  | 0.000     | 0.000     |
| 318 CdCl <sub>2</sub> , 2.5H <sub>2</sub> O | -16.850   | 0.000    | 0.000    | 0.000        | 0.000        | -18.859 | -2.009  | 0.000     | 0.000     |
| 319 CdF <sub>2</sub>                        | -19.729   | 0.000    | 0.000    | 0.000        | 0.000        | -22.318 | -2.589  | 0.000     | 0.000     |
| 320 Cd(OH) <sub>2</sub> (a)                 | -10.250   | 0.000    | 0.000    | -10.130      | -10.820      | 4.315   | 14.565  | 14.445    | 15.135    |
| 321 Cd(OH) <sub>2</sub> (c)                 | -9.335    | 0.000    | 0.040    | 0.000        | 0.000        | 4.315   | 13.650  | 0.000     | 0.000     |
| 322 CdOHC1                                  | -11.089   | 0.000    | 0.000    | -10.869      | 0.000        | -7.272  | 3.818   | 3.598     | 0.000     |
| 323 Cd3(OH)4SO <sub>4</sub>                 | -29.849   | 0.000    | 0.000    | 0.000        | 0.000        | -7.289  | 22.560  | 0.000     | 0.000     |
| 324 Cd3OH2(SO <sub>4</sub> ) <sub>2</sub>   | -34.234   | 0.000    | 0.000    | 0.000        | 0.000        | -27.524 | 6.710   | 0.000     | 0.000     |
| 325 Cd4(OH)6SO <sub>4</sub>                 | -31.374   | 0.000    | 0.000    | 0.000        | 0.000        | -2.974  | 28.400  | 0.000     | 0.000     |
| 326 Montepsonite                            | -11.800   | 0.000    | 0.000    | 0.000        | -12.420      | 4.315   | 16.115  | 0.000     | 16.735    |
| 327 Cd3(PO <sub>4</sub> ) <sub>2</sub>      | -23.239   | 0.000    | 0.000    | 0.000        | 0.000        | -55.839 | -32.600 | 0.000     | 0.000     |
| 328 CdSiO <sub>3</sub>                      | -8.933    | 0.000    | 0.000    | -7.833       | 0.000        | 0.795   | 9.728   | 8.628     | 0.000     |
| 329 CdSO <sub>4</sub>                       | -16.412   | 0.000    | 0.000    | -16.382      | -16.462      | -15.920 | 0.492   | 0.462     | 0.542     |
| 330 CdSO <sub>4</sub> , 1H <sub>2</sub> O   | -14.565   | 0.000    | 0.000    | -14.542      | -14.592      | -15.920 | -1.355  | -1.378    | -1.328    |
| 331 CdSO <sub>4</sub> , 2.7H <sub>2</sub> O | -14.220   | 0.000    | 0.000    | -14.203      | -14.233      | -15.920 | -1.700  | -1.717    | -1.687    |
| 332 Greenockite                             | 5.327     | 0.000    | 0.000    | 0.000        | 2.509        | -11.261 | -16.588 | 0.000     | -13.770   |
| 463 CdBr <sub>2</sub> , 4H <sub>2</sub> O   | -23.289   | 0.000    | 0.000    | 0.000        | 0.000        | -25.999 | -2.711  | 0.000     | 0.000     |
| 464 CdI <sub>2</sub>                        | -23.673   | 0.000    | 0.000    | 0.000        | 0.000        | -27.447 | -3.774  | 0.000     | 0.000     |
| 360 Pb metal                                | -31.641   | 0.000    | 0.000    | -31.441      | -31.681      | -27.387 | 4.254   | 4.054     | 4.294     |
| 361 Pb(BO <sub>2</sub> ) <sub>2</sub>       | -14.228   | 0.000    | 0.000    | 0.000        | 0.000        | -6.385  | 7.843   | 0.000     | 0.000     |
| 362 Cotunnite                               | -13.855   | 0.000    | 0.000    | -13.649      | -13.955      | -18.851 | -4.995  | -5.201    | -4.895    |
| 363 Matlockite                              | -10.831   | 0.000    | 0.000    | 0.000        | -11.661      | -20.580 | -9.750  | 0.000     | -8.920    |
| 364 Phosgenite                              | -16.161   | 0.000    | 0.000    | -16.031      | 0.000        | -35.971 | -19.810 | -19.940   | 0.000     |
| 365 Cerrusite                               | -3.795    | 0.000    | 0.000    | -3.485       | -4.095       | -17.120 | -13.325 | -13.635   | -13.025   |
| 366 PbF <sub>2</sub>                        | -14.898   | 0.000    | 0.000    | -14.768      | 0.000        | -22.310 | -7.412  | -7.542    | 0.000     |
| 367 Massicot                                | -9.261    | 0.000    | 0.000    | -9.141       | 0.000        | 4.324   | 13.584  | 13.464    | 0.000     |
| 368 Litharge                                | -9.055    | 0.000    | 0.000    | -8.975       | -9.405       | 4.324   | 13.378  | 13.298    | 13.728    |
| 369 PbO, .3H <sub>2</sub> O                 | -8.656    | 0.000    | 0.000    | 0.000        | 0.000        | 4.324   | 12.980  | 0.000     | 0.000     |
| 370 Pb2OCO <sub>3</sub>                     | -12.758   | 0.000    | 0.000    | -12.478      | 0.000        | -12.797 | -0.039  | -0.319    | 0.000     |
| 371 Larnakite                               | -11.567   | 0.000    | 0.000    | -5.547       | 0.000        | -11.588 | -0.021  | -6.041    | 0.000     |
| 372 Pb3O2SO <sub>4</sub>                    | -18.499   | 0.000    | 0.000    | 0.000        | 0.000        | -7.265  | 11.234  | 0.000     | 0.000     |
| 373 Pb4O3SO <sub>4</sub>                    | -26.451   | 0.000    | 0.000    | 0.000        | 0.000        | -2.941  | 23.510  | 0.000     | 0.000     |
| 374 PbHPO <sub>4</sub>                      | -5.838    | 0.000    | 0.000    | -1.668       | -7.398       | -17.581 | -11.743 | -15.913   | -10.183   |
| 375 Pb3(PO <sub>4</sub> ) <sub>2</sub>      | -11.236   | 0.000    | 0.000    | -0.876       | -13.526      | -30.839 | -19.603 | -29.963   | -17.313   |
| 376 Clpyromorph                             | -8.717    | 0.000    | 0.000    | 0.000        | -58.637      | -93.147 | -84.430 | 0.000     | -34.510   |
| 377 Hxypyromorph                            | -18.770   | 0.000    | 0.000    | 0.000        | 0.000        | -81.560 | -62.790 | 0.000     | 0.000     |
| 378 Pb3O2CO <sub>3</sub>                    | -20.556   | 0.000    | 0.000    | 0.000        | 0.000        | -8.473  | 12.082  | 0.000     | 0.000     |
| 379 Plumbgummit                             | -4.095    | 0.000    | 0.000    | 0.000        | 0.000        | -36.885 | -32.790 | 0.000     | 0.000     |
| 380 Hinsdalite                              | -20.228   | 0.000    | 0.000    | 0.000        | 0.000        | -22.728 | -2.500  | 0.000     | 0.000     |
| 381 Tsumebite                               | -11.323   | 0.000    | 0.000    | 0.000        | 0.000        | -21.113 | -9.790  | 0.000     | 0.000     |
| 382 PbSiO <sub>3</sub>                      | -6.889    | 0.000    | 0.000    | -5.689       | -7.209       | 0.804   | 7.692   | 6.492     | 8.012     |
| 383 Pb2SiO <sub>4</sub>                     | -15.678   | 0.000    | 0.000    | -15.138      | -16.418      | 5.127   | 20.805  | 20.265    | 21.545    |
| 384 Anglesite                               | -8.035    | 0.000    | 0.020    | -7.955       | 0.000        | -15.912 | -7.876  | -7.956    | 0.000     |
| 385 Galena                                  | 4.659     | 0.000    | 0.000    | 5.979        | 3.209        | -11.253 | -15.912 | -17.232   | -14.462   |
| 386 Plattnerite                             | -16.109   | 0.000    | 0.000    | -15.809      | 0.000        | 36.034  | 52.143  | 51.843    | 0.000     |
| 387 Pb2O <sub>3</sub>                       | -20.683   | 0.000    | 0.000    | 0.000        | 0.000        | 40.357  | 61.040  | 0.000     | 0.000     |
| 388 Minium                                  | -33.140   | 0.000    | 0.000    | -30.250      | 0.000        | 44.681  | 77.820  | 74.930    | 0.000     |

## DK Nordstrom Test Data - Test Case #2 - Surface Water

B5

| Phase             | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP   | Log KT  | Log MinKT | Log MaxKT |
|-------------------|-----------|----------|----------|--------------|--------------|----------|---------|-----------|-----------|
| 389 Pb(OH)2 (c)   | -4.389    | 0.000    | 0.000    | 0.000        | -9.869       | 4.324    | 8.712   | 0.000     | 14.192    |
| 390 Laurionite    | -7.887    | 0.000    | 0.000    | -7.439       | 0.000        | -7.264   | 0.623   | 0.175     | 0.000     |
| 391 Pb2(OH)3Cl    | -11.733   | 0.000    | 0.000    | 0.000        | 0.000        | -2.940   | 8.793   | 0.000     | 0.000     |
| 392 Hydcerussite  | -12.457   | 0.000    | 0.000    | 0.000        | 0.000        | -29.917  | -17.460 | 0.000     | 0.000     |
| 393 Pb2O(OH)2     | -17.553   | 0.000    | 0.000    | 0.000        | -18.453      | 8.647    | 26.200  | 0.000     | 27.100    |
| 465 PbBr2         | -20.485   | 0.000    | 0.000    | -20.325      | -21.255      | -25.991  | -5.506  | -5.666    | -4.736    |
| 466 PbBrF         | -15.661   | 0.000    | 0.000    | 0.000        | 0.000        | -24.151  | -8.490  | 0.000     | 0.000     |
| 467 PbI2          | -18.759   | 0.000    | 0.000    | 0.000        | 0.000        | -27.439  | -8.679  | 0.000     | 0.000     |
| 394 Pb4(OH)6SO4   | -24.041   | 0.000    | 0.000    | 0.000        | 0.000        | -2.941   | 21.100  | 0.000     | 0.000     |
| 410 NiCO3         | -7.968    | 0.000    | 0.000    | 0.000        | 0.000        | -14.408  | -6.440  | 0.000     | 0.000     |
| 411 Ni(OH)2       | -2.540    | 0.000    | 0.100    | -2.330       | -5.040       | 7.036    | 9.576   | 9.366     | 12.076    |
| 412 Ni4(OH)6SO4   | -24.091   | 0.000    | 0.000    | 0.000        | 0.000        | 7.909    | 32.000  | 0.000     | 0.000     |
| 413 Bunsenite     | -6.375    | 0.000    | 0.000    | 0.000        | -6.315       | 7.036    | 13.411  | 0.000     | 13.351    |
| 414 Ni3(PO4)2     | -16.377   | 0.000    | 0.000    | 0.000        | 0.000        | -47.677  | -31.300 | 0.000     | 0.000     |
| 415 Millerite     | -0.398    | 0.000    | 0.000    | -0.308       | 0.000        | -8.540   | -8.142  | -8.232    | 0.000     |
| 416 Retgersite    | -11.115   | 0.000    | 0.000    | 0.000        | 0.000        | -13.199  | -2.084  | 0.000     | 0.000     |
| 417 Morenosite    | -10.721   | 0.000    | 0.000    | 0.000        | 0.000        | -13.199  | -2.478  | 0.000     | 0.000     |
| 418 Ni2SiO4       | -5.329    | 0.000    | 0.000    | 0.000        | 0.000        | 10.552   | 15.881  | 0.000     | 0.000     |
| 437 Ag metal      | -9.236    | 0.000    | 0.000    | 0.000        | 0.000        | -23.760  | -14.524 | 0.000     | 0.000     |
| 438 Bromyrite     | -9.982    | 0.000    | 0.000    | 0.000        | 0.000        | -23.062  | -13.081 | 0.000     | 0.000     |
| 439 Cerargyrite   | -9.113    | 0.000    | 0.000    | 0.000        | 0.000        | -19.492  | -10.379 | 0.000     | 0.000     |
| 440 Ag2CO3        | -25.801   | 0.000    | 0.000    | 0.000        | 0.000        | -37.254  | -11.453 | 0.000     | 0.000     |
| 441 AgF, 4H2O     | -21.600   | 0.000    | 0.000    | 0.000        | 0.000        | -21.222  | 0.378   | 0.000     | 0.000     |
| 442 Iodyrite      | -6.638    | 0.000    | 0.000    | 0.000        | 0.000        | -23.786  | -17.148 | 0.000     | 0.000     |
| 443 Ag2O          | -28.809   | 0.000    | 0.100    | 0.000        | 0.000        | -15.810  | 12.999  | 0.000     | 0.000     |
| 444 Ag3PO4        | -40.558   | 0.000    | 0.000    | 0.000        | 0.000        | -58.108  | -17.550 | 0.000     | 0.000     |
| 445 Acanthite     | 6.806     | 0.000    | 0.000    | 0.000        | 0.000        | -31.386  | -38.192 | 0.000     | 0.000     |
| 446 Ag2SO4        | -30.954   | 0.000    | 0.000    | 0.000        | 0.000        | -36.045  | -5.091  | 0.000     | 0.000     |
| 488 As2O5         | -36.402   | 0.000    | 0.000    | 0.000        | -39.181      | -29.486  | 6.916   | 0.000     | 9.695     |
| 489 AlAsO4, 2H2O  | -10.449   | 0.000    | 0.000    | 0.000        | 0.000        | -26.286  | -15.837 | 0.000     | 0.000     |
| 490 Ca3AsO4)2, 4w | -14.840   | 0.000    | 0.000    | 0.000        | 0.000        | -33.745  | -18.905 | 0.000     | 0.000     |
| 491 Cu3AsO4)2, 6w | -21.934   | 0.000    | 0.000    | 0.000        | 0.000        | -57.057  | -35.123 | 0.000     | 0.000     |
| 492 FeAsO4, 2H2O  | -10.001   | 0.000    | 0.000    | 0.000        | 0.000        | -30.250  | -20.249 | 0.000     | 0.000     |
| 493 Mn3AsO4)2, 8w | -15.788   | 0.000    | 0.000    | 0.000        | 0.000        | -44.495  | -28.707 | 0.000     | 0.000     |
| 494 Ni3AsO4)2, 8w | -24.337   | 0.000    | 0.000    | 0.000        | 0.000        | -49.848  | -25.511 | 0.000     | 0.000     |
| 495 Pb3(AsO4)2    | -22.582   | 0.000    | 0.000    | 0.000        | 0.000        | -57.985  | -35.403 | 0.000     | 0.000     |
| 496 Zn3AsO4)2, 5w | -21.172   | 0.000    | 0.000    | 0.000        | 0.000        | -48.718  | -27.546 | 0.000     | 0.000     |
| 497 Arsenolite    | -99.834   | 0.000    | 0.000    | -99.776      | -99.907      | -103.211 | -3.377  | -3.435    | -3.304    |
| 498 Claudetite    | -99.612   | 0.000    | 0.000    | 0.000        | -99.656      | -103.211 | -3.599  | 0.000     | -3.555    |
| 499 AsI3          | -77.526   | 0.000    | 0.000    | 0.000        | 0.000        | -73.446  | 4.080   | 0.000     | 0.000     |
| 500 Orpiment      | -34.032   | 0.000    | 0.000    | 0.000        | -48.999      | -98.334  | -64.303 | 0.000     | -49.336   |
| 501 Realgar       | -36.259   | 0.000    | 0.000    | -29.432      | 0.000        | -57.234  | -20.975 | -27.802   | 0.000     |

|   |   |        |        |   |      |           |
|---|---|--------|--------|---|------|-----------|
| 0 | 0 | 001961 | 0      | 0 | 0    | 0         |
|   |   |        | TEMP   | = |      | 25.000000 |
|   |   |        | PH     | = |      | 0.300000  |
|   |   |        | EHM    | = |      | 9.900000  |
|   |   |        | DOC    | = |      | 0.000000  |
|   |   |        | DOX    | = |      | 0.000000  |
|   |   |        | CORALC | = |      | 0.000000  |
|   |   |        | FLG    | = | MG/L |           |
|   |   |        | DENS   | = |      | 1.000000  |
|   |   |        | PRNT   | = |      | 0         |
|   |   |        | PUNCH  | = |      | 1         |
|   |   |        | EHOPT  | = |      | 0         |
|   |   |        | EMPOX  | = |      | 0         |
|   |   |        | ITDS   | = |      | 0.000000  |
|   |   |        | COND   | = |      | 0.000000  |
|   |   |        | SIGMDO | = |      | 0.000000  |
|   |   |        | SIGMEH | = |      | 0.000000  |
|   |   |        | SIGMPH | = |      | 0.000000  |

| Species  |   | Index No |   | Input Concentration |
|----------|---|----------|---|---------------------|
| Ca       | : | 0        | : | 0.00000000          |
| Mg       | : | 1        | : | 0.00000000          |
| Na       | : | 2        | : | 24500.00000000      |
| K        | : | 3        | : | 8.20000000          |
| Cl       | : | 4        | : | 2770.00000000       |
| SO4      | : | 5        | : | 300.00000000        |
| HCO3     | : | 6        | : | 0.00000000          |
| Fe total | : | 16       | : | 0.00000000          |
| H2S aq   | : | 13       | : | 0.00000000          |
| CO3      | : | 17       | : | 0.00000000          |
| SiO2 tot | : | 34       | : | 10000.00000000      |
| NH4      | : | 38       | : | -1.00000000         |
| B tot    | : | 86       | : | 600.00000000        |
| PO4      | : | 44       | : | 0.00000000          |
| Al       | : | 50       | : | 0.00000000          |
| F        | : | 61       | : | 20000.00000000      |
| NO3      | : | 84       | : | 0.00000000          |

0 0 001961 0 0 0 0

| ITER | S1-AnalCO3   | S2-AnalSO4    | S3-AnalF     | S4-AnalPO4   | S5-AnalCL    | S6-AnalH2S   | S7-AnalFULV  | S8-AnalHUM   |
|------|--------------|---------------|--------------|--------------|--------------|--------------|--------------|--------------|
| 1    | 0.000000E-01 | 2.519282E-04  | 1.117197E+00 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 2    | 0.000000E-01 | 6.386244E-05  | 1.251975E+00 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 3    | 0.000000E-01 | -3.977902E-06 | 1.151618E+00 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 4    | 0.000000E-01 | -2.825563E-05 | 3.368368E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 5    | 0.000000E-01 | -1.981859E-06 | 2.889939E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 6    | 0.000000E-01 | -1.043526E-06 | 2.591614E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 7    | 0.000000E-01 | -6.773123E-07 | 2.396519E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 8    | 0.000000E-01 | -4.712498E-07 | 2.259319E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 9    | 0.000000E-01 | -3.445472E-07 | 2.156621E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 10   | 0.000000E-01 | -2.623583E-07 | 2.073750E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 11   | 0.000000E-01 | -2.080572E-07 | 1.998375E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 12   | 0.000000E-01 | -1.732962E-07 | 1.915414E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 13   | 0.000000E-01 | -1.541498E-07 | 1.800731E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 14   | 0.000000E-01 | -1.479215E-07 | 1.614252E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 15   | 0.000000E-01 | -1.496379E-07 | 1.305164E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 16   | 0.000000E-01 | -1.467603E-07 | 8.651874E-02 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 17   | 0.000000E-01 | -1.208841E-07 | 4.181143E-02 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 18   | 0.000000E-01 | -7.159288E-08 | 1.399602E-02 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 19   | 0.000000E-01 | -2.835299E-08 | 3.606945E-03 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |
| 20   | 0.000000E-01 | -8.119409E-09 | 8.384883E-04 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 | 0.000000E-01 |

Hawaii Kilauea Iki Volcanic Condensats,Drillholes & Vents unpub USGS 03 G5 Date = 9/12/86 9:57

0 0 001961 0 0 0 0  
 DOX = 0.0000 DOC = 0.0 INPUT TDS = 0.0  
 Anal Cond = 0.0 Calc Cond = 220479.3  
 Anal EPMCAT = 1632.9297 Anal EPMAN = 1207.3386 Percent difference in input cation/anion balance = 29.9684  
 ERROR IN CALCULATED CHARGE BALANCE GREATER THAN 30 PERCENT. CHECK INPUT DATA.

Calc EPMCAT = 1812.2583 Calc EPMAN = 441.1130 Percent difference in calc cation/anion balance = 121.6972  
 Total Ionic Strength (T.I.S.) from input data = 1.42345  
 Effective Ionic Strength (E.I.S.) from speciation = 1.28131

| Input | Sigma | Fe3/Fe2 | Sigma | Sato  | H2O2/O2 | Sigma | NO3/NO2 | Sigma | NO3/NH4 | Sigma | Calc  | H2O2/O2 | Sigma | SO4/S= | Sigma | As5/As3 | Sigma |
|-------|-------|---------|-------|-------|---------|-------|---------|-------|---------|-------|-------|---------|-------|--------|-------|---------|-------|
| 9.900 | 0.000 | 9.900   | 0.000 | 9.900 | 0.000   | 0.445 | 0.000   | 9.900 | 0.000   | 9.900 | 0.000 | 9.900   | 0.000 | 9.900  | 0.000 | 9.900   | 0.000 |

----- pE -----

|         |       |         |       |         |       |         |       |         |       |         |       |         |       |         |       |         |       |
|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|
| 100.000 | 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 | 100.000 | 0.000 | 100.000 | 0.000 |
|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|---------|-------|

| T     | pH    | TDS ppm | Effective | Ionic Str | pO2 Atm  | pCO2 Atm | pCH4 Atm | CO2 Tot  | Uncom CO2 | ppm Uncom CO2 | Ncrb Alk | aH2O   |
|-------|-------|---------|-----------|-----------|----------|----------|----------|----------|-----------|---------------|----------|--------|
| 25.00 | 0.300 | 58178.2 | 1.28131   | 0.00E-01  | 0.00E-01 | 0.00E-01 | 0.00000  | 0.00E-01 | 0.00E-01  | 0.00E-01      | 3.24E-11 | 0.9636 |

| I   | Species  | Anal ppm | Calc ppm  | Anal Molal | Calc Molal | Activity  | Act Coeff | -Log Act |
|-----|----------|----------|-----------|------------|------------|-----------|-----------|----------|
| 2   | Na       | 1        | 24500.000 | 24558.591  | 1.132E+00  | 1.131E+00 | 0.7306    | 0.083    |
| 43  | NaSO4    | -1       |           | 26.222     | 2.333E-04  | 1.963E-04 | 0.8417    | 3.707    |
| 297 | NaF aq   | 0        |           | 0.048      | 1.216E-06  | 1.633E-06 | 1.3432    | 5.787    |
| 3   | K        | 1        | 8.200     | 8.219      | 2.227E-04  | 1.305E-04 | 0.5862    | 3.884    |
| 45  | KSO4     | -1       |           | 0.006590   | 5.164E-08  | 4.346E-08 | 0.8417    | 7.362    |
| 63  | H        | 1        |           | 647.954    | 6.808E-01  | 5.012E-01 | 0.7362    | 0.300    |
| 26  | OH       | -1       |           | 0.000000   | 2.300E-14  | 1.936E-14 | 0.8417    | 13.713   |
| 5   | SO4      | -2       | 300.000   | 31.140     | 3.316E-03  | 3.433E-04 | 4.739E-05 | 0.1380   |
| 62  | HSO4     | -1       |           | 251.084    | 2.739E-03  | 2.306E-03 | 0.8417    | 2.637    |
| 61  | F        | -1       | 20000.000 | 0.360      | 1.118E+00  | 2.007E-05 | 1.689E-05 | 0.8417   |
| 125 | HF aq    | 0        |           | 175.733    | 9.302E-03  | 1.249E-02 | 1.3432    | 1.903    |
| 126 | HF2      | -1       |           | 0.035      | 9.542E-07  | 8.031E-07 | 0.8417    | 6.095    |
| 296 | H2F2 aq  | 0        |           | 11.828     | 3.131E-04  | 4.205E-04 | 1.3432    | 3.376    |
| 4   | Cl       | -1       | 2770.000  | 2777.200   | 8.296E-02  | 8.296E-02 | 0.5862    | 1.313    |
| 34  | SiO2 tot | 0        | 10000.000 |            | 1.767E-01  |           |           |          |
| 23  | H4SiO4aq | 0        |           | 2024.116   | 2.230E-02  | 2.996E-02 | 1.3432    | 1.524    |
| 24  | H3SiO4   | -1       |           | 0.000001   | 8.367E-12  | 7.042E-12 | 0.8417    | 11.152   |
| 25  | H2SiO4   | -2       |           | 0.000000   | 5.745E-23  | 2.883E-23 | 0.5018    | 22.540   |
| 124 | SiF6     | -2       |           | 20699.934  | 1.543E-01  | 7.743E-02 | 0.5018    | 1.111    |
| 86  | B tot    | 0        | 600.000   |            | 5.893E-02  |           |           |          |
| 35  | H3BO3 aq | 0        |           | 759.471    | 1.301E-02  | 1.747E-02 | 1.3432    | 1.758    |
| 36  | H2BO3    | -1       |           | 0.000001   | 2.396E-11  | 2.017E-11 | 0.8417    | 10.695   |
| 101 | BF(OH)3  | -1       |           | 0.011      | 1.396E-07  | 1.175E-07 | 0.8417    | 6.930    |
| 102 | BF2(OH)2 | -1       |           | 10.217     | 1.306E-04  | 1.100E-04 | 0.8417    | 3.959    |
| 103 | BF3OH    | -1       |           | 100.183    | 1.251E-03  | 1.053E-03 | 0.8417    | 2.978    |
| 104 | BF4      | -1       |           | 3647.838   | 4.450E-02  | 3.746E-02 | 0.8417    | 1.426    |
| 38  | NH4      | 1        | 0.000     |            |            |           |           |          |

## Mole ratios from analytical molality - Log activity ratios

|         |   |            |                |     |   |         |
|---------|---|------------|----------------|-----|---|---------|
| Cl/Ca   | = | 0.0000E-01 | Log Ca         | /H2 | = | 0.0000  |
| Cl/Mg   | = | 0.0000E-01 | Log Mg         | /H2 | = | 0.0000  |
| Cl/Na   | = | 7.3316E-02 | Log Na         | /H1 | = | 0.2173  |
| Cl/K    | = | 3.7257E+02 | Log K          | /H1 | = | -3.5844 |
| Cl/Al   | = | 0.0000E-01 | Log Al         | /H3 | = | 0.0000  |
| Cl/Fe   | = | 0.0000E-01 | Log Fe         | /H2 | = | 0.0000  |
| Cl/SO4  | = | 2.5018E+01 | Log Ca/Mg      |     | = | 0.0000  |
| Cl/HCO3 | = | 0.0000E-01 | LOG NA/K       |     | = | 3.8017  |
| Ca/Mg   | = | 0.0000E-01 | Log Ca/K2      |     | = | 0.0000  |
| Na/K    | = | 5.0818E+03 | Log Diss Fe/H2 |     | = | 0.6000  |



| Phase           | Log AP/KT | Sigma(A) | Sigma(T) | Log AP/MinKT | Log AP/MaxKT | Log AP  | Log KT  | Log MinKT | Log MaxKT |
|-----------------|-----------|----------|----------|--------------|--------------|---------|---------|-----------|-----------|
| 97 Chalcedony   | 2.032     | 0.000    | 0.000    | 0.000        | 0.000        | -1.491  | -3.523  | 0.000     | 0.000     |
| 99 Cristobalite | 2.096     | 0.000    | 0.000    | 0.000        | 0.000        | -1.491  | -3.587  | 0.000     | 0.000     |
| 64 Halite       | -2.978    | 0.000    | 0.000    | 0.000        | 0.000        | -1.396  | 1.582   | 0.000     | 0.000     |
| 98 Magadiite    | 0.196     | 0.000    | 0.000    | 0.000        | 0.000        | -14.104 | -14.300 | 0.000     | 0.000     |
| 66 Mirabilite   | -3.537    | 0.000    | 0.000    | 0.000        | 0.000        | -4.651  | -1.114  | 0.000     | 0.000     |
| 101 Quartz      | 2.515     | 0.000    | 0.000    | 0.000        | 0.000        | -1.491  | -4.006  | 0.000     | 0.000     |
| 100 SiO2 (a,L)  | 1.527     | 0.000    | 0.000    | 0.000        | 0.000        | -1.491  | -3.018  | 0.000     | 0.000     |
| 395 SiO2 (a,M)  | 1.219     | 0.000    | 0.000    | 0.000        | 0.000        | -1.491  | -2.710  | 0.000     | 0.000     |
| 65 Thenardite   | -4.311    | 0.000    | 0.000    | 0.000        | 0.000        | -4.490  | -0.179  | 0.000     | 0.000     |

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Attachment B. Program Listing of WATEQ4F

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|                                                                      |          |
|----------------------------------------------------------------------|----------|
| CWATEQ2 BEARBEITET VON D.W. ZACHMANN UND W. BAETHGE                  | WAT00020 |
| C                                                                    | WAT00030 |
| C       UEBERSETZT IN FORTRAN (W.BAETHGE)                            | WAT00040 |
| C                                                                    | WAT00050 |
| C       UNTERPROGRAMME :INTABL, PREP, SET, MAJEL, TREL,              | WAT00060 |
| C       SUMS, SOLUTS, RATIO, APCALC, ERRCLC, PHASES, OUTTBL          | WAT00070 |
| C       OUTPCH                                                       | WAT00080 |
| C                                                                    | WAT00090 |
| C       KANAL 1 -> EINLESEN DER DATENTABELLEN                        | WAT00100 |
| C       KANAL 2 -> EINLESEN DER MESSWERTE UND STEUERDATEN            | WAT00110 |
| C       KANAL 3 -> AUSGABE DER ERGEBNISSE                            | WAT00120 |
| C       KANAL 4 -> AUSGABE DER DATENTABELLEN MIT KOMMENTAR           | WAT00130 |
| C       KANAL 5 -> AUSGABE SUBROUTINE PUNCH (NOCH ANZUPASSEN)        | WAT00140 |
| C                                                                    | WAT00150 |
| C       UNIT NUMBERS CHANGED TO ACCOMMODATE IBM PC I/O REQUIREMENTS: |          |
| C                                                                    |          |
| C       UNIT 11 -> INPUT OF TABLE1 DATA                              |          |
| C       UNIT 13 -> INPUT OF TABLE2 DATA                              |          |
| C       UNIT 14 -> INPUT OF TABLE3 DATA                              |          |
| C       UNIT 15 -> INPUT OF TABLE4 DATA                              |          |
| C       UNIT 5 -> INPUT OF THE WATER ANALYSIS DATA                   |          |
| C       UNIT 6 -> OUTPUT OF THE RESULTS                              |          |
| C       UNIT 6 -> OUTPUT OF THE THERMODYNAMIC DATA                   |          |
| C       UNIT 7 -> OUTPUT OF SUBROUTINE OUTPUNCH (PLOT DATA)          |          |
| C                                                                    |          |
| REAL*8 ALFA(0:297),ANALMI(0:297),AP(0:543),CUNITS(0:297),DH(0:543)   | WAT00160 |
| *,DHA(0:297),ERR(0:543),ERRT(0:543),GAMMA(0:297),GFW(0:297),         | WAT00170 |
| *KT(0:543),LOGKT(0:543),LOGKTO(0:543),MAXKTO(0:543),                 | WAT00180 |
| *MI(0:297),MINKTO(0:543),SIGMA(0:297),V(0:297)                       | WAT00190 |
| C                                                                    | WAT00200 |
| INTEGER ANAL(0:297),INDEX(1:297),INDEX2(1:297),Z(0:297)              | WAT00210 |
| C                                                                    | WAT00220 |
| CHARACTER*12 PAGE2(0:543)                                            | WAT00230 |
| CHARACTER*8 PAGE1(0:297)                                             | WAT00240 |
| CHARACTER*80 CARD1,CARD2                                             | WAT00250 |
| CHARACTER*1 DEST                                                     |          |
| C                                                                    | WAT00260 |
| REAL*8 ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT            | WAT00270 |
| REAL*8 ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT,      | WAT00280 |
| *MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3        | WAT00290 |
| INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA,        | WAT00300 |
| *ITER,NMBR,PUNCH,RBIT,FLAG,ENDE                                      | WAT00310 |
| C                                                                    | WAT00320 |
| COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B,       | WAT00330 |
| *BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND,            | WAT00340 |
| *CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF,   | WAT00350 |
| *DISCHG,DOC,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT,      | WAT00360 |
| *EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,     | WAT00370 |
| *FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,      | WAT00380 |
| *ITDS,ITER,K,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL,     | WAT00390 |
| *NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE,      | WAT00400 |
| *PEAS,PEDO,PEDO2,PEFE,PEN,PENO2,PEPT,PES,PH,PRNT,PTOT,PUNCH,R,       | WAT00410 |
| *RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,                 | WAT00420 |
| *T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT               | WAT00430 |

```

COMMON/CHRDAT/CARD1,CARD2
C
C**** THE FOLLOWING SUPPRESSES UNDERFLOW ERRORS
C
C      IERRN = 208 WAT00440
C      CALL ERRSET(IERRN,256,-1,1,1,IERRN) WAT00460
C WAT00470
C      D = 297 WAT00480
C      E = 543 WAT00490
C      G = 297 WAT00500
C WAT00510
C      CALL INTABL(PAGE1,PAGE2,INDEX,Z,DHA,GFW,V,DH,LOGKTO,MAXKTO,MINKTO WAT00520
*,ERRT,INDEX2) WAT00530
DO 5 I = 1 , D WAT00540
SIGMA(I) = 0.0 WAT00550
5 CONTINUE WAT00560
NMBR=0 WAT00570
OPEN (UNIT=5,FILE='WATEQ4F.DAT',STATUS='OLD')
K=6
OPEN (UNIT=K,FILE='WATEQ4F.OUT')
OPEN (UNIT=7,FILE='CARDS.EQP')
1000 CONTINUE WAT00580
NMBR=NMBR+1 WAT00590
ENDE = 0 WAT00600
CALL PREP(PAGE1,ANAL,Z,ANALMI,CUNITS,DH,ERRT,GFW,LOGKTO,MI,SIGMA, WAT00610
*LOGKT,V,ENDE) WAT00620
IF (ENDE .NE. 0) GOTO 60 WAT00630
CALL SET(DH,GAMMA,KT,LOGKT,LOGKTO,MI) WAT00640
ITER = 0 WAT00650
RBIT = 1 WAT00660
DO 7 I = 0 , D WAT00670
ALFA(I) = 0.0 WAT00680
7 CONTINUE WAT00690
10 ITER = ITER + 1 WAT00700
CALL MAJEL(ALFA,CUNITS,DHA,GAMMA,KT,MI,Z) WAT00710
CALL TREL(ALFA,GAMMA,KT,LOGKT,MI) WAT00720
CALL SUMS(ALFA,GAMMA,KT,MI) WAT00730
IF (RBIT .NE. 0) GOTO 10 WAT00740
CALL SOLUTS(ANAL,Z,PAGE1,ALFA,ANALMI,CUNITS,GAMMA,GFW,KT,MI,LOGKT WAT00750
*,INDEX2,SIGMA,ERR) WAT00760
IF (PRNT .EQ. 1 .OR. PRNT .EQ. 3) GOTO 20 WAT00770
CALL RATIO(PAGE1,ALFA,CUNITS,Z,ANALMI) WAT00780
20 IF (PRNT .EQ. 2 .OR. PRNT .EQ. 3) GOTO 30 WAT00790
CALL APCALC(AP,ALFA,GAMMA,MI) WAT00800
30 DO 40 I = 0 , E WAT00810
ERR(I) = 2.0E7 WAT00820
40 CONTINUE WAT00830
CALL ERRCLC(CUNITS,SIGMA,ERR) WAT00840
IF (PUNCH .NE. 0) GOTO 50 WAT00850
CALL OUTPCH(ALFA,AP,CUNITS,LOGKT) WAT00860
50 IF (PRNT .EQ. 2 .OR. PRNT .EQ. 3) GOTO 1000 WAT00870
CALL PHASES(PAGE2,INDEX,AP,DH,LOGKT,MAXKTO,MINKTO,ERR,ERRT) WAT00880
GOTO 1000 WAT00900
60 CLOSE(5)

```

|   |                                                                                     |          |
|---|-------------------------------------------------------------------------------------|----------|
|   | CLOSE(K)                                                                            |          |
|   | CLOSE(7)                                                                            |          |
|   | STOP                                                                                | WAT00910 |
|   | END                                                                                 | WAT00920 |
|   | SUBROUTINE INTABL(PAGE1, PAGE2, INDEX, Z, DHA, GFW, V, DH, LOGKTO                   | WAT00950 |
|   | *, MAXKTO, MINKTO, ERRT, INDEX2)                                                    | WAT00960 |
| C |                                                                                     | WAT00970 |
|   | REAL*8 DH(0:543), DHA(0:297), ERRT(0:543), GFW(0:297), V(0:297),                    | WAT00980 |
|   | *LOGKTO(0:543), MAXKTO(0:543), MINKTO(0:543)                                        | WAT00990 |
|   | DIMENSION COEF(0:6, 23)                                                             |          |
|   | INTEGER INDEX(1:297), INDEX2(1:297),                                                | WAT01000 |
|   | *Z(0:297), LISTE2(39)                                                               | WAT01010 |
|   | CHARACTER*80 CARD1, CARD2                                                           | WAT01020 |
|   | CHARACTER*12 PAGE2(0:543)                                                           | WAT01030 |
|   | CHARACTER*8 PAGE1(0:297)                                                            | WAT01040 |
|   | CHARACTER*2 MARKE                                                                   | WAT01050 |
| C |                                                                                     | WAT01060 |
|   | REAL*8 ANLCO3, SO4TOT, FTOT, PTOT, CLTOT, H2STOT, FULVTT, HUMTOT                    | WAT01070 |
|   | REAL*8 ITDS, KTOT, KW, LAMBDA, LH2O, LITOT, MGTOT, MNTOT, EPMAN, EPMCAT,            | WAT01080 |
|   | *MO, NATOT, NEQU, NH4TOT, NI, NITOT, NONCRB, NORM, NO2TOT, PB, C1, C2, C3           | WAT01090 |
|   | INTEGER CORALK, D, E, G, H, PRNT, EHOPT, EMPOX, FULFLG, HUMFLG, ISDATA,             | WAT01100 |
|   | *ITER, NMBR, PUNCH, RBIT, FLAG                                                      | WAT01110 |
| C |                                                                                     | WAT01120 |
|   | COMMON A, AG, AGTOT, AH2O, ALTOT, ANLCO3, AS, ASTOTL, AS3TOT, AS5TOT, B,            | WAT01130 |
|   | *BATOT, BTOT, C, CARBON, CATOT, CD, CDTOT, CLTOT, CO, CONCLC, COND,                 | WAT01140 |
|   | *CORALK, CO2TIT, CO3ALC, CR, CSTOT, CU, CUTOT, C1, C2, C3, D, DATE, DENS, DIFF,     | WAT01150 |
|   | *DISCHG, DOC, DOX, E, EHAS, EHDO, EHDO2, EHFE, EHM, EHN, EHNO, EHOPT, EHPT,         | WAT01160 |
|   | *EHS, EMPOX, EPMAN, EPMCAT, F, FETOTL, FE2TOT, FE3TOT, FLAG, FTOT, FULFLG,          | WAT01170 |
|   | *FULVTT, G, H, HCO3TT, HG, HUMFLG, HUMTOT, H2STOT, ISDATA, NATOT, XMUSAV,           | WAT01180 |
|   | *ITDS, ITER, K, KTOT, KW, LAMBDA, LH2O, LITOT, MGTOT, MNTOT, MO, XMU, XMUHL,        | WAT01190 |
|   | *NEQU, NH4TOT, NI, NITOT, NMBR, NONCRB, NORM, NO2TOT, PB, PBTOT, PCO2, PE,          | WAT01200 |
|   | *PEAS, PEDO, PEDO2, PEFE, PEN, PENO2, PEPT, PES, PH, PRNT, PTOT, PUNCH, R,          | WAT01210 |
|   | *RBIT, RSDDO, SIGMDO, SIGMEH, SIGMPH, SITOT, SO4TOT, SRTOT,                         | WAT01220 |
|   | *T, TDS, TEMP, TENMPE, TENPH, XMI120, XMI121, XMI178, ZN, ZNTOT                     | WAT01230 |
|   | COMMON/CHRDAT/CARD1, CARD2                                                          |          |
| C |                                                                                     | WAT01240 |
|   | DATA COEF/12., -171.9065, -0.77993, 2839.319, 2*0., 71.595, 13., 6.368,             |          |
|   | *-0.016346, -3405.9, 3*0., 14., 39.478, -0.065927, -12355.1, 3*0., 21.,             |          |
|   | *-171.9773, -0.077993, 2903.293, 2*0., 71.595, 24., 0.684, 0.0051, 4*0.,            |          |
|   | * 25., 28.6059, 0.012078, 1573.21, 2*0., -13.2248, 26., 0.6322, -0.001225,          |          |
|   | *-2835.76, 3*0., 35., 356.3094, 0.06091964, -21834.37, 0., 1684915.,                |          |
|   | *-126.8339, 62., 109.25, 0.0024, -3120.98, -4.9D-7, -2088.47, -37.62424,            |          |
|   | * 68., 107.8871, 0.03252849, -5151.79, 0., 563713.9, -38.92561, 72.,                |          |
|   | *3.106, 0., -673.6, 3*0., 73., 0.991, 0.00667, 4*0., 74., 2.319, -0.011056,         |          |
|   | *0., 2.29812D-5, 2*0., 77., 1209.12, 0.31294, -34765.05, 2*0., -478.782,            |          |
|   | *78., -1228.732, -0.299444, 35512.75, 2*0., 485.818, 79., -3.248,                   |          |
|   | *0.014867, 4*0., 89., -5.3505, 0.0183412, 557.2467, 3*0., 91., 11.17,               |          |
|   | *-0.02386, -3279., 3*0., 135., -1.019, 0.012836, 4*0., 142., 155.0305, 0.,          |          |
|   | *-7239.594, 2*0., -56.58638, 157., 6*0., 158., 6*0., 220., 2.497, 0.,               |          |
|   | *-3833., 3*0./                                                                      |          |
| C | DATA LISTE1/12, 13, 14, 21, 24, 25, 26, 35, 62, 68, 72, 73, 74, 77, 78, 79, 89, 91, | WAT01360 |
| C | *135, 142, 157, 158, 220/                                                           |          |
|   | DATA LISTE2/0, 1, 2, 3, 4, 5, 6, 7, 8, 13, 16, 17, 34, 38, 44, 48, 50, 61, 80, 84,  | WAT01370 |
|   | *86, 87, 89, 94, 96, 97, 109, 130, 145, 160, 182, 202, 204, 212, 249, 261, 262,     | WAT01380 |

|      |                                                     |          |
|------|-----------------------------------------------------|----------|
|      | *284,285/                                           | WAT01390 |
| C    | NEQU = 23                                           | WAT01400 |
|      | DO 100 I = 0 , D                                    | WAT01410 |
|      | V(I) = 1.0                                          | WAT01420 |
|      | GFW(I) = 1.0                                        | WAT01430 |
|      | Z(I) = 1                                            | WAT01440 |
|      | DHA (I) = 1.0                                       | WAT01450 |
| 100  | CONTINUE                                            | WAT01460 |
|      | DO 110 I = 0 , E                                    | WAT01470 |
|      | LOGKTO(I) = 1.0                                     | WAT01480 |
|      | MINKTO(I) = 1.0                                     | WAT01490 |
|      | MAXKTO(I) = 1.0                                     | WAT01500 |
|      | DH (I) = 1.0                                        | WAT01510 |
|      | ERRT(I) = 0.1                                       | WAT01520 |
| 110  | CONTINUE                                            | WAT01530 |
|      | OPEN (UNIT=11,FILE='TABLE1',STATUS='OLD')           | WAT01540 |
|      | DO 120 N = 0 , D + 1                                | WAT01550 |
|      | READ (11,9000)I,PAGE1(I),Z(I),GFW(I),DHA(I)         | WAT01560 |
| 9000 | FORMAT(I4,1X,A8,I3,F9.4,F4.1)                       | WAT01570 |
| 120  | CONTINUE                                            | WAT01580 |
|      | CLOSE(11)                                           |          |
|      | OPEN (UNIT=13,FILE='TABLE2',STATUS='OLD')           |          |
|      | DO 130 N = 0 , E + 1                                | WAT01590 |
|      | READ (13,9010)I,PAGE2(I),DH(I),LOGKTO(I),MINKTO(I), | WAT01600 |
|      | *MAXKTO(I),ERRT(I)                                  | WAT01610 |
| 130  | CONTINUE                                            | WAT01620 |
| 9010 | FORMAT(I4,1X,A12,4(F9.3),F5.2)                      | WAT01630 |
|      | CLOSE(13)                                           |          |
| C    |                                                     | WAT01640 |
|      | OPEN (UNIT=14,FILE='TABLE3',STATUS='OLD')           |          |
|      | READ (14,*)(INDEX(I),I=1,D)                         | WAT01650 |
|      | CLOSE(14)                                           |          |
|      | OPEN (UNIT=15,FILE='TABLE4',STATUS='OLD')           |          |
|      | READ (15,*)(INDEX2(I),I=1,D)                        | WAT01660 |
|      | CLOSE(15)                                           |          |
| C    |                                                     | WAT01680 |
|      | DO 140 I = 0 , D                                    | WAT01690 |
|      | IF (INDEX(I) .LT. 900) G = I                        | WAT01700 |
|      | IF (INDEX2(I) .LT. 900) H = I                       | WAT01710 |
|      | V(I) = 1.0                                          | WAT01720 |
|      | IF (Z(I).EQ. 0) GOTO 140                            | WAT01730 |
|      | V(I) = ABS(Z(I))                                    | WAT01740 |
| 140  | CONTINUE                                            | WAT01750 |
|      | PRNT = 4                                            | WAT01760 |
|      | PUNCH = 0                                           | WAT01770 |
|      | EHOPT = 0                                           | WAT01780 |
|      | SIGMDO = 0.0                                        | WAT01790 |
|      | SIGMEH = 0.0                                        | WAT01800 |
|      | SIGMPH = 0.0                                        | WAT01810 |
| C    |                                                     | WAT01820 |
|      | C = 2.302585093                                     | WAT01830 |
|      | F = 23.0603                                         | WAT01840 |
|      | R = 1.98719E-3                                      | WAT01850 |



|      |                                                                    |          |
|------|--------------------------------------------------------------------|----------|
|      | IF (PRNT .NE. 4) GOTO 200                                          | WAT01860 |
|      | OPEN (UNIT=6,FILE='TABLES.OUT',STATUS='NEW')                       |          |
|      | WRITE(6,9025)                                                      |          |
| 9025 | FORMAT (1H1,' I Page2 dh MaxKto MinKto Lo                          |          |
|      | *gKto Error',9X,'I Page1 Z DHa GFW')                               |          |
|      | IN=0                                                               |          |
|      | DO 170 I = 0 , E                                                   | WAT01870 |
|      | MARKE = ' '                                                        | WAT01880 |
|      | DO 150 J = 1 , NEQU                                                | WAT01890 |
|      | IF(I.EQ.INT(COEF(0,J))) MARKE = ' *'                               | WAT01900 |
| 150  | CONTINUE                                                           | WAT01910 |
|      | IF (I.GT.D) GOTO 160                                               | WAT01920 |
|      | WRITE(6,9030)I,PAGE2(I),DH(I),MAXKTO(I),MINKTO(I),                 | WAT01930 |
|      | *LOGKTO(I),MARKE,ERRT(I),I,PAGE1(I),Z(I),DHA(I),GFW(I)             | WAT01940 |
|      | GOTO 165                                                           | WAT01950 |
| 160  | WRITE(6,9030)I,PAGE2(I),DH(I),MAXKTO(I),MINKTO(I),                 | WAT01960 |
|      | *LOGKTO(I),MARKE, ERRT(I)                                          | WAT01970 |
| 9030 | FORMAT(1H ,I3,2X,A12,4F10.3,A2,F8.3,I10,2X,A8,I4,F5.1,F10.4)       | WAT01980 |
| 165  | IN=IN+1                                                            |          |
|      | IF (IN.LT.59) GOTO 170                                             |          |
|      | IN=0                                                               |          |
|      | WRITE(6,9025)                                                      |          |
| 170  | CONTINUE                                                           | WAT01990 |
| C    |                                                                    | WAT02000 |
|      | WRITE(6,9040)                                                      | WAT02010 |
| 9040 | FORMAT(/,' "*" Denotes that an analytical expression for Kt has'   | WAT02020 |
|      | *' been used'/1H1,'Summary of analytical expressions of the form', | WAT02030 |
|      | *' Log K = A + B*T + C/T + D*T**2 + E/T**2 + F*LOG10(T)'           | WAT02040 |
|      | *' I React Product A B C                                           | WAT02050 |
|      | * D E F')                                                          | WAT02060 |
| C    |                                                                    | WAT02070 |
|      | DO 180 K = 1, NEQU                                                 | WAT02080 |
|      | I = INT(COEF(0,K))                                                 | WAT02090 |
|      | WRITE(6,9050) I,PAGE2(I),(COEF(J,K),J=1,6)                         | WAT02100 |
| 9050 | FORMAT(I4,2X,A12,3X,F12.4,F13.8,F13.4,3X,1PE12.5,E15.6,0PF12.5)    | WAT02110 |
| 180  | CONTINUE                                                           | WAT02120 |
|      | WRITE(6,9060)                                                      | WAT02130 |
| 9060 | FORMAT(1H1,'Reference numbers for all possible numbered input cons | WAT02140 |
|      | *tituents:')                                                       | WAT02150 |
|      | WRITE(6,9070)                                                      | WAT02160 |
| 9070 | FORMAT(/,' Number Constituent Z')                                  | WAT02170 |
| C    |                                                                    | WAT02180 |
|      | DO 190 J = 1 , 39                                                  | WAT02190 |
|      | I = LISTE2(J)                                                      | WAT02200 |
|      | WRITE(6,9080)I,PAGE1(I),Z(I)                                       | WAT02210 |
| 9080 | FORMAT(' ',I4,10X,A8,I3)                                           | WAT02220 |
| 190  | CONTINUE                                                           | WAT02230 |
|      | CLOSE(6)                                                           |          |
|      | PRNT=0                                                             |          |
| 200  | RETURN                                                             | WAT02240 |
|      | END                                                                | WAT02250 |
|      | SUBROUTINE PREP (PAGE1,ANAL,Z,ANALMI,CUNITS,DH,ERRT,GFW,           | WAT02280 |
|      | *LOGKTO,MI,SIGMA,LOGKT,V,ENDE)                                     | WAT02290 |
| C    |                                                                    | WAT02300 |

|     |                                                                    |          |
|-----|--------------------------------------------------------------------|----------|
|     | INTEGER ANAL(0:297),Z(0:297)                                       | WAT02310 |
|     | REAL*8 ANALMI(0:297),CUNITS(0:297),DH(0:543),ERRT(0:543),V(0:297), | WAT02320 |
|     | *GFW(0:297),LOGKTO(0:543),MI(0:297),SIGMA(0:297),LOGKT(0:543)      | WAT02330 |
|     | CHARACTER*80 CARD1,CARD2                                           | WAT02340 |
|     | CHARACTER*8 PAGE1(0:297)                                           | WAT02350 |
|     | CHARACTER*4 CHECK,START                                            | WAT02360 |
|     | CHARACTER*2 MARKE                                                  | WAT02370 |
|     | REAL*8 ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT          | WAT02380 |
|     | REAL*8 ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT,    | WAT02390 |
|     | *MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3      | WAT02400 |
|     | INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA,      | WAT02410 |
|     | *ITER,NMBR,PUNCH,RBIT,FLAG,ENDE                                    | WAT02420 |
| C   |                                                                    | WAT02430 |
|     | COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B,     | WAT02440 |
|     | *BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND,          | WAT02450 |
|     | *CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF, | WAT02460 |
|     | *DISCHG, DOX,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT,   | WAT02470 |
|     | *EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,   | WAT02480 |
|     | *FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,    | WAT02490 |
|     | *ITDS,ITER,K,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL,   | WAT02500 |
|     | *NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE,    | WAT02510 |
|     | *PEAS,PEDO,PEDO2,PEFE,PEN,PENO2,PEPT,PES,PH,PRNT,PTOT,PUNCH,R,     | WAT02520 |
|     | *RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,               | WAT02530 |
|     | *T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT             | WAT02540 |
|     | COMMON/CHRDAT/CARD1,CARD2                                          |          |
|     | DATA START/'****'/                                                 | WAT02550 |
| C   |                                                                    | WAT02560 |
| 330 | DO 140 I = 0 , D                                                   | WAT02570 |
|     | CUNITS(I) = 0.0                                                    | WAT02580 |
|     | MI(I) = 0.0                                                        | WAT02590 |
|     | ANALMI(I) = 1.0                                                    | WAT02600 |
|     | ANAL(I) = 0                                                        | WAT02610 |
| 140 | CONTINUE                                                           | WAT02620 |
|     | CORALK = 0                                                         | WAT02630 |
|     | EMPOX = 0.0                                                        | WAT02640 |
|     | FULFLG = 0                                                         | WAT02650 |
|     | HUMFLG = 0                                                         | WAT02660 |
|     | EHAS = 9.9                                                         | WAT02670 |
|     | EHFE = 9.9                                                         | WAT02680 |
|     | EHDO = 9.9                                                         | WAT02690 |
|     | EHDO2 = 9.9                                                        | WAT02700 |
|     | EHN = 9.9                                                          | WAT02710 |
|     | EHNO2 = 9.9                                                        | WAT02720 |
|     | EHS = 9.9                                                          | WAT02730 |
|     | PEAS = 100.                                                        | WAT02740 |
|     | PEPT = 100.                                                        | WAT02750 |
|     | PEFE = 100.                                                        | WAT02760 |
|     | PES = 100.                                                         | WAT02770 |
|     | PEN = 100.                                                         | WAT02780 |
|     | PENO2 = 100.                                                       | WAT02790 |
|     | PEDO = 100.                                                        | WAT02800 |
|     | PEDO2 = 100.                                                       | WAT02810 |
|     | DOX = -1.0                                                         | WAT02820 |
|     | DENS = 1.0                                                         | WAT02830 |

|       |                                                              |          |
|-------|--------------------------------------------------------------|----------|
| C     |                                                              | WAT02840 |
| C     | N ,AG ,AS ,CD ,CO ,CR ,CU ,HG ,MO ,NI ,PB ,ZN = 0.0          | WAT02850 |
| C     |                                                              | WAT02860 |
|       | READ(5,2222,END=150)CHECK                                    | WAT02870 |
| 2222  | FORMAT(A4)                                                   | WAT02880 |
|       | IF (CHECK .EQ. START) GOTO 155                               | WAT02890 |
| 150   | ENDE = 1                                                     | WAT02900 |
|       | RETURN                                                       | WAT02910 |
| C     |                                                              | WAT02920 |
| 155   | CALL INPUT(PAGE1,CUNITS,SIGMA,LOGKT,ENDE)                    | WAT02930 |
| C     |                                                              | WAT02940 |
|       | T = TEMP + 273.16E0                                          | WAT02950 |
| C     | IF( CUNITS(130) .EQ. 0.0) CUNITS(130)=CU                     | WAT02960 |
| C     | IF( CUNITS(145) .EQ. 0.0) CUNITS(145)=ZN                     | WAT02970 |
| C     | IF( CUNITS(160) .EQ. 0.0) CUNITS(160)=CD                     | WAT02980 |
| C     | IF( CUNITS(182) .EQ. 0.0) CUNITS(182)=PB                     | WAT02990 |
| C     | IF( CUNITS(204) .EQ. 0.0) CUNITS(204)=NI                     | WAT03000 |
| C     | IF( CUNITS(212) .EQ. 0.0) CUNITS(212)=AG                     | WAT03010 |
| C     | IF( CUNITS(249) .EQ. 0.0) CUNITS(249)=AS                     | WAT03020 |
|       | DO 160 I = 0, D                                              | WAT03030 |
|       | IF (CUNITS(I) .GE. 0.0) GOTO 160                             | WAT03040 |
|       | ANAL(I) = 1                                                  | WAT03050 |
|       | CUNITS(I) = 0.0                                              | WAT03060 |
| 160   | CONTINUE                                                     | WAT03070 |
|       | EHPT=EHM                                                     | WAT03080 |
|       | IF (EHM .GT. 9.0) PEPT = 100.                                | WAT03090 |
|       | IF (EHM .LE. 9.0) PEPT = EHM/(C*R*T/F)                       | WAT03100 |
|       | IF (CUNITS(284) .LE. 0.0) GOTO 200                           | WAT03110 |
|       | IF (GFW(284) .NE. 650.0) GOTO 200                            | WAT03120 |
|       | FULFLG = 1                                                   | WAT03130 |
|       | WRITE(K,970)                                                 | WAT03140 |
| 970   | FORMAT(/,' NO GFW INPUT WITH CONC VALUE FOR FULVIC ACID.',/, | WAT03150 |
|       | *' RESULTS WILL BE FLAGGED WITH ASTERISKS',                  | WAT03160 |
|       | *' TO SIGNIFY THAT THEY ARE PURELY QUALITATIVE.')            | WAT03170 |
| 200   | IF (CUNITS(285) .LE. 0.0 ) GOTO 210                          | WAT03180 |
|       | IF ( GFW(285) .NE. 2000.0) GOTO 210                          | WAT03190 |
|       | HUMFLG = 1                                                   | WAT03200 |
|       | WRITE(K,980)                                                 | WAT03210 |
| 980   | FORMAT (/,' NO GFW INPUT WITH CONC VALUE FOR HUMID ACID.',   | WAT03220 |
|       | *' RESULTS WILL BE FLAGGED WITH ASTERISKS TO SIGNIFY THAT',  | WAT03230 |
|       | *' THEY ARE PURELY QUALITATIVE.')                            | WAT03240 |
| 210   | WRITE(K,1020)CARD1                                           | WAT03250 |
| 1020  | FORMAT(1H1,A80)                                              | WAT03260 |
|       | WRITE(K,1030)CARD2                                           | WAT03270 |
| 1030  | FORMAT(1H ,A80,///)                                          | WAT03280 |
|       | WRITE(K,990)                                                 | WAT03290 |
| 990   | FORMAT(' ITER S1-AnalCO3 S2-AnalSO4',                        | WAT03300 |
|       | *' S3-AnalF S4-AnalPO4 S5-AnalCL ',                          | WAT03310 |
|       | *' S6-AnalH2S S7-AnalFULV S8-AnalHUM')                       | WAT03320 |
| C     |                                                              | WAT03330 |
| C**** | FE SPECIES INPUT ADJUSTMENT                                  |          |
| C     |                                                              |          |
|       | IF (CUNITS(16).GT.0.) THEN                                   |          |
|       | IF (CUNITS(8).LT.1D-78) THEN                                 |          |

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        IF (CUNITS(7).GT.0.) CUNITS(8)=DMAX1(OD0,CUNITS(16)-CUNITS(7))
        ELSE
        IF(CUNITS(7).LT.1D-78)CUNITS(7)=DMAX1(OD0,CUNITS(16)-CUNITS(8))
        END IF
    END IF
    IF (CUNITS(7).GT.0. .OR. CUNITS(8).GT.0.) CUNITS(16)=0.
C
C/* AS SPECIES INPUT ADJUSTMENT */
    IF (CUNITS(249).GT.0.) THEN
        IF (CUNITS(262).LT.1D-78) THEN
            IF (CUNITS(261).GT.0.)
                * CUNITS(262)=DMAX1(OD0,CUNITS(249)-CUNITS(261))
            ELSE
                IF (CUNITS(261).LT.1D-78)
                    * CUNITS(261)=DMAX1(OD0,CUNITS(249)-CUNITS(262))
                END IF
            END IF
        IF (CUNITS(261).GT.0. .OR. CUNITS(262).GT.0.) CUNITS(249)=0.
C
C****          CALCULATION OF ANALYZED MOLALITY
C
        IF (FLAG .NE.1) GOTO 220
C
C          1 -> 'MEQ/L'
        DO 215 I = 0, D
            CUNITS(I) = CUNITS(I) * GFW(I) / V(I)
215 CONTINUE
        FLAG = 2
C
C          FLAG='MG/L'
220 IF (FLAG .NE.2) GOTO 240
C
C          2 -> 'MG/L'
        DO 230 I = 0, D
            CUNITS(I) = CUNITS(I) /DENS
230 CONTINUE
        FLAG = 3
C
C          FLAG='PPM'
240 IF (FLAG .NE.3) GOTO 270
C
C          3 -> 'PPM'
        C1=0.0
        DO 250 I = 0 , D
            C1 = C1 + CUNITS(I)
250 CONTINUE
        DO 260 I = 0 , D
            MI(I) = CUNITS(I) * (1./ (1.-1E-6 * C1)) / (1000.* GFW(I))
260 CONTINUE
270 IF (FLAG .NE.4) GOTO 290
C
C          4 -> 'MOL'
        DO 280 I = 0 , D
            MI(I) = CUNITS(I)
            CUNITS(I) =MI(I) * 1E3 * GFW(I) * (1-1E-6*C1)
280 CONTINUE
290 DO 300 I = 0 , D
            ANALMI(I) = MI(I)
300 CONTINUE
        EPMCAT = 0.0

```

```

      EPMAN = 0.0
C
C***** CALCULATION OF CATION-ANION BALANCE *
C
      MI(63)=1D1*(-PH)
      DO 310 I = 0 , D
      IF (Z(I) .GT. 0) EPMCAT = EPMCAT + Z(I) * MI(I)
      IF (Z(I) .LT. 0) EPMAN = EPMAN - Z(I) * MI(I)
310 CONTINUE
      IF (MI(26) .LT. 1D-78) THEN
        KW=LOGKTO(152)-DH(152)*((298.16-T)/(298.16*T*C*R))
        EPMAN = EPMAN+1E1*(PH+KW)
      END IF
      DIFF = 0.0
      IF (ABS(EPMAN+EPMCAT) .GT. 0.0)
      *DIFF = ABS(2.*(EPMAN - EPMCAT) / (EPMAN+EPMCAT))
      IF (DIFF .LE. 0.3) GOTO 320
      WRITE(1,1000)
      WRITE(K,1000)
1000 FORMAT(/' ERROR IN INPUT CHARGE BALANCE GREATER THAN 30 PERCENT. '
      *,' CHECK INPUT DATA.')
```

```

      EPCAT1 = EPMCAT * 1000.
      EPMAN1 = EPMAN * 1000.
      WRITE(1,1010)EPCAT1,EPMAN1
      WRITE(K,1010)EPCAT1,EPMAN1
1010 FORMAT(' ANAL EPMCAT = ',F12.4,' ANAL EPMAN =',F10.4)
C
C***** Calculation of total ionic strength (from initial input data)
C
      320 XMUSAV=0E0
      DO 325 I=0,D
      IF (MI(I).GT.1D-78) XMUSAV=XMUSAV+0.5E0*MI(I)*Z(I)*Z(I)
      325 CONTINUE
C
C***** TEMP. AFFECTS ON DEBYE-HUCKEL SOLVENT CONSTANTS
C
      S1 = 374.11 - TEMP
      S2 = S1**.333333
      S3 = SQRT((1.0 +.1342489E0 * S2 - 3.946263E-3 * S1)/
      *(3.1975E0 -.3151548E0 *S2 -1.203374E-3 *S1+ 7.48908E-13 *S1**4))
      IF (T .LT. 373.16)
      *C1 = 87.74 -TEMP *(TEMP *(1.41E-6 *TEMP -9.398E -4)+.4008)
      IF (T .GE. 373.16)
      *C1 = 5321 / T+233.76 -T *(T* (8.292E-7 *T-1.417E-3) +.9297E0)
      C1 = SQRT ( C1 * T )
      A = 18246E2 * S3 / C1**3
      B = 50.29 * S3 / C1
      RETURN
      END
      SUBROUTINE SET (DH,GAMMA,KT,LOGKT,LOGKTO,MI)
C
      REAL*8 DH(0:543),GAMMA(0:297),KT(0:543),LOGKT(0:543),LOGKTO(0:543)
      *,MI(0:297)
      REAL*8 ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT,DT,D1
```

|       |                                                                    |          |
|-------|--------------------------------------------------------------------|----------|
|       | REAL*8 ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT,    | WAT04110 |
|       | *MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3      | WAT04120 |
|       | INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA,      | WAT04130 |
|       | *ITER,NMBR,PUNCH,RBIT,FLAG                                         | WAT04140 |
|       | CHARACTER*80 CARD1,CARD2                                           | WAT04150 |
| C     |                                                                    | WAT04160 |
|       | COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B,     | WAT04170 |
|       | *BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND,          | WAT04180 |
|       | *CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF, | WAT04190 |
|       | *DISCHG,DOC,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT,    | WAT04200 |
|       | *EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,   | WAT04210 |
|       | *FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,    | WAT04220 |
|       | *ITDS,ITER,K,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL,   | WAT04230 |
|       | *NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE,    | WAT04240 |
|       | *PEAS,PEDO,PEDO2,PEFE,PEN,PENO2,PEPT,PES,PH,PRNT,PTOT,PUNCH,R,     | WAT04250 |
|       | *RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,               | WAT04260 |
|       | *T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT             | WAT04270 |
|       | COMMON/CHRDAT/CARD1,CARD2                                          |          |
| C     |                                                                    | WAT04280 |
|       | INTEGER LISTE1(23)                                                 | WAT04290 |
|       | DATA LISTE1 /12,13,14,21,24,25,26,35,62,68,72,73,74,77,78,79,89,   | WAT04300 |
|       | * 91,135,142,157,158,220/                                          | WAT04310 |
| C     |                                                                    | WAT04320 |
|       | DO 10 I = 0 , E                                                    | WAT04330 |
|       | KT(I)= 1.0                                                         | WAT04340 |
|       | LOGKT(I) = 1.0                                                     | WAT04350 |
| 10    | CONTINUE                                                           | WAT04360 |
|       | DO 20 I = 0 , D                                                    | WAT04370 |
|       | GAMMA(I) = 1.0                                                     | WAT04380 |
| 20    | CONTINUE                                                           | WAT04390 |
| C     |                                                                    | WAT04400 |
| C**** | INITIALIZE STARTING VALUES FOR ITERATIVE LOOP AND CONSTANT GAMMAS  | WAT04410 |
| C     |                                                                    | WAT04420 |
|       | ANLCO3 = MI(6) + 2. * MI (17)                                      | WAT04430 |
|       | CO2TIT = MI(6) + 2. * MI(17)                                       | WAT04440 |
|       | SITOT = MI(34)                                                     | WAT04450 |
|       | IF (CORALK .EQ. 2) CO2TIT=MI(6) + MI(17) + MI(85)                  | WAT04460 |
|       | CATOT = MI(0)                                                      | WAT04470 |
|       | MGTOT = MI(1)                                                      | WAT04480 |
|       | NATOT = MI(2)                                                      | WAT04490 |
|       | KTOT = MI(3)                                                       | WAT04500 |
|       | SO4TOT = MI(5)                                                     | WAT04510 |
|       | FETOTL = MI(16)                                                    | WAT04520 |
|       | FE2TOT = MI(7)                                                     | WAT04530 |
|       | FE3TOT = MI(8)                                                     | WAT04540 |
|       | NO2TOT = MI(202)                                                   | WAT04550 |
|       | AGTOT = MI(212)                                                    | WAT04560 |
|       | PTOT = MI(44)                                                      | WAT04570 |
|       | MI(46) = MI(44)                                                    | WAT04580 |
|       | ALTOT = MI(50)                                                     | WAT04590 |
|       | FTOT = MI(61)                                                      | WAT04600 |
|       | BTOT = MI(86)                                                      | WAT04610 |
|       | LITOT = MI(80)                                                     | WAT04620 |
|       | NH4TOT = MI(38)                                                    | WAT04630 |



|         |                                                             |          |
|---------|-------------------------------------------------------------|----------|
| H2STOT  | = MI(13)                                                    | WAT04640 |
| SRTOT   | = MI(87)                                                    | WAT04650 |
| BATOT   | = MI(89)                                                    | WAT04660 |
| NITOT   | = MI(204)                                                   | WAT04670 |
| CSTOT   | = MI(48)                                                    | WAT04680 |
| CLTOT   | = MI(4)                                                     | WAT04690 |
| HCO3TT  | = MI(6)                                                     | WAT04700 |
| PBTOT   | = MI(182)                                                   | WAT04710 |
| MNTOT   | = MI(109)                                                   | WAT04720 |
| CUTOT   | = MI(130)                                                   | WAT04730 |
| ZNTOT   | = MI(145)                                                   | WAT04740 |
| CDTOT   | = MI(160)                                                   | WAT04750 |
| AS3TOT  | = MI(261)                                                   | WAT04760 |
| AS5TOT  | = MI(262)                                                   | WAT04770 |
| ASTOTL  | = MI(249)                                                   | WAT04780 |
| FULVTT  | = MI(284)                                                   | WAT04790 |
| HUMTOT  | = MI(285)                                                   | WAT04800 |
| MI(249) | = 0.0                                                       | WAT04810 |
| MI(261) | = 0.0                                                       | WAT04820 |
| MI(262) | = 0.0                                                       | WAT04830 |
| MI(34)  | = 0.0                                                       | WAT04840 |
| MI(16)  | = 0.0                                                       | WAT04850 |
| MI(86)  | = 0.0                                                       | WAT04860 |
| TENPH   | = 10**PH                                                    | WAT04870 |
| C       |                                                             | WAT04880 |
| C****   | VANT HOFF EQN. FOR EFFECT OF T ON K                         | WAT04890 |
| C       |                                                             | WAT04900 |
|         | C1 = (298.16 - T) / (298.16 * T * C * R)                    | WAT04910 |
|         | DO 340 I = 0 , E                                            | WAT04920 |
|         | LOGKT(I) = LOGKTO(I) - DH(I) * C1                           | WAT04930 |
|         | IF (ABS(LOGKT(I)).LT. 75.) KT(I) = 10**LOGKT(I)             | WAT04940 |
| 340     | CONTINUE                                                    | WAT04950 |
| C       |                                                             | WAT04960 |
| C****   | ANALYTICAL EXPRS. FOR EFFECT OF T ON K */                   | WAT04970 |
| C       |                                                             | WAT04980 |
|         | KW = KT(152)                                                | WAT04990 |
|         | C1 = ALOG10(T)                                              | WAT05000 |
|         | KT(12) = 1D1 ** (-171.9065-0.077993*T+2839.319/T+71.595*C1) |          |
|         | KT(13) = 1D1 ** (6.368E0-1.6346E-2*T-3405.9E0/T)            |          |
|         | KT(14) = 1D1 ** (39.478D0-6.5927D-2*T-12355.1D0/T)          |          |
|         | KT(21) = 1D1 ** (-171.9773-0.077993*T+2903.293/T+71.595*C1) |          |
|         | KT(24) = 1D1 ** (.684+.0051*T)                              |          |
|         | KT(25) = KW*1D1** (28.6059+0.012078*T+1573.21/T-13.2248*C1) |          |
|         | KT(26) = 1D1 ** (0.6322D0-1.225D-3*T-2835.76D0/T)           |          |
|         | KT(35) = 1D1** (356.3094+.06091964*T-21834.37/T-126.8339*C1 |          |
| *       | +1684915./T**2)                                             |          |
|         | KT(62) = 1D1 ** (109.25+.0024*T-3120.98/T-37.62424*C1       |          |
| *       | -2088.47/(T*T)-4.9D-7*T*T-(298.4/SQRT(T)))                  |          |
|         | KT(68) = 1D1 ** (107.8871+.03252849*T-5151.79/T-38.92561*C1 |          |
| *       | +563713.9/T**2)                                             |          |
|         | KT(72) = 1D1 ** (3.106D0-673.6D0/T)                         |          |
|         | KT(73) = 1D1 ** (.991+.00667*T)                             |          |
|         | KT(74) = 1D1 ** (2.319-.011056*T+2.29812D-5*T*T)            |          |
|         | KT(77) = 1D1 ** (1209.12+.31294*T-34765.05/T-478.782*C1)    |          |

|     |                                                                    |          |
|-----|--------------------------------------------------------------------|----------|
|     | KT(78) = 1D1 ** (-1228.732-.299444*T+35512.75/T+485.818*C1)        |          |
|     | KT(79) = 1D1 ** (-3.248+0.014867*T)                                |          |
|     | KT(89) = 10. ** (-5.3505+0.0183412*T+557.2467/T)                   | WAT05170 |
|     | KT(91) = 10. ** (11.17-0.02386*T-3279.0/T)                         | WAT05180 |
|     | KT(135) = 1D1 ** (-1.019+0.012826*T)                               |          |
|     | KT(142) = 1D1 ** (155.0305 -7239.594/T-56.58638*C1)                |          |
|     | KT(157) = 10. ** (-5.7 +1.68 *PH)                                  | WAT05190 |
|     | KT(158) = 10. ** (-5.4 +1.52 *PH)                                  | WAT05200 |
|     | KT(220) = 10. ** (2.497 -3833./T)                                  | WAT05210 |
| C   |                                                                    | WAT05220 |
| C   | LISTE1                                                             | WAT05230 |
| C   |                                                                    | WAT05240 |
|     | DO 350 J = 1 , 23                                                  | WAT05250 |
|     | I = LISTE1(J)                                                      | WAT05260 |
|     | LOGKT(I) = DLOG10 (KT(I))                                          | WAT05270 |
| 350 | CONTINUE                                                           | WAT05280 |
|     | RETURN                                                             | WAT05290 |
|     | END                                                                | WAT05300 |
|     | SUBROUTINE MAJEL(ALFA,CUNITS,DHA,GAMMA,KT,MI,Z)                    | WAT05350 |
| C   |                                                                    | WAT05360 |
|     | REAL*8 ALFA(0:297),CUNITS(0:297),DHA(0:297),GAMMA(0:297),          | WAT05370 |
|     | *KT(0:543),MI(0:297)                                               | WAT05380 |
|     | INTEGER Z(0:297)                                                   | WAT05390 |
|     | INTEGER LISTE(0:297),LISTE1(15),LISTE2(18),LISTE3(30),LISTE4(19)   | WAT05400 |
|     | CHARACTER*80 CARD1,CARD2                                           | WAT05410 |
| C   |                                                                    | WAT05420 |
|     | REAL*8 ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT          | WAT05430 |
|     | REAL*8 ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT,    | WAT05440 |
|     | *MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3      | WAT05450 |
|     | INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA,      | WAT05460 |
|     | *ITER,NMBR,PUNCH,RBIT,FLAG                                         | WAT05470 |
| C   |                                                                    | WAT05480 |
|     | COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B,     | WAT05490 |
|     | *BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND,          | WAT05500 |
|     | *CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF, | WAT05510 |
|     | *DISCHG,DOC,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT,    | WAT05520 |
|     | *EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,   | WAT05530 |
|     | *FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,    | WAT05540 |
|     | *ITDS,ITER,K,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL,   | WAT05550 |
|     | *NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE,    | WAT05560 |
|     | *PEAS,PEDO,PEDO2,PEFE,PEN,PENO2,PEPT,PES,PH,PRNT,PTOT,PUNCH,R,     | WAT05570 |
|     | *RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,               | WAT05580 |
|     | *T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT             | WAT05590 |
|     | COMMON/CHRDAT/CARD1,CARD2                                          |          |
| C   |                                                                    | WAT05600 |
|     | DATA LISTE1/6,17,63,68,88,259,260,263,264,265,266,267,268,269,270/ | WAT05610 |
|     | DATA LISTE2/8,9,12,14,15,27,32,76,77,78,98,105,106,107,108,123,    | WAT05620 |
|     | *288,289/                                                          | WAT05630 |
|     | DATA LISTE3/7,8,9,10,11,12,14,15,27,32,33,64,76,77,78,79,98,99,    | WAT05640 |
|     | *105,106,107,108,122,123,179,180,247,248,288,289/                  | WAT05650 |
|     | DATA LISTE4/9,12,14,15,27,32,76,77,78,98,105,106,107,108,123,179,  | WAT05660 |
|     | *180,288,289/                                                      | WAT05670 |
| C   |                                                                    | WAT05680 |
|     | DO 355 I = 0 , D                                                   | WAT05690 |

|                                                                               |          |
|-------------------------------------------------------------------------------|----------|
| LISTE(I) = 1                                                                  | WAT05700 |
| 355 CONTINUE                                                                  | WAT05710 |
| LISTE(16) = 0                                                                 | WAT05720 |
| LISTE(34) = 0                                                                 | WAT05730 |
| LISTE(65) = 0                                                                 | WAT05740 |
| LISTE(69) = 0                                                                 | WAT05750 |
| LISTE(70) = 0                                                                 | WAT05760 |
| LISTE(71) = 0                                                                 | WAT05770 |
| LISTE(83) = 0                                                                 | WAT05780 |
| LISTE(86) = 0                                                                 | WAT05790 |
| LISTE(249) = 0                                                                | WAT05800 |
| LISTE(261) = 0                                                                | WAT05810 |
| LISTE(262) = 0                                                                | WAT05820 |
| C                                                                             | WAT05830 |
| C**** CALC. OF TOTAL MOLALITY & AH2O */                                       | WAT05840 |
| C                                                                             | WAT05850 |
| C1=0.0                                                                        | WAT05860 |
| DO 360 I = 0 , D                                                              | WAT05870 |
| IF (LISTE(I).EQ.0) GOTO 360                                                   | WAT05880 |
| C1 = C1 + MI(I)                                                               | WAT05890 |
| 360 CONTINUE                                                                  | WAT05900 |
| AH2O = 1. - 1.7E-2 * C1                                                       | WAT05910 |
| IF (AH2O .LT. 0.0 ) GOTO 370                                                  | WAT05920 |
| LH2O = ALOG10(AH2O)                                                           | WAT05930 |
| GOTO 380                                                                      | WAT05940 |
| 370 LH2O = 0.0                                                                | WAT05950 |
| 380 CONTINUE                                                                  | WAT05960 |
| C                                                                             | WAT05970 |
| C**** CALC. OF ACTIVITY COEFFICIENTS                                          | WAT05980 |
| C                                                                             | WAT05990 |
| XMU = 0.0                                                                     | WAT06000 |
| DO 390 I = 0 , D                                                              | WAT06010 |
| IF (LISTE(I) .EQ. 0) GOTO 390                                                 | WAT06020 |
| XMU = XMU + 0.5 *MI(I) *Z(I) *Z(I)                                            | WAT06030 |
| 390 CONTINUE                                                                  | WAT06040 |
| XMUHL = SQRT(XMU)                                                             | WAT06050 |
| C1 = -A * 4. * XMUHL                                                          | WAT06060 |
| GAMMA(0) = 10. ** (C1 / (1. + B * 5. * XMUHL) + 0.165 * XMU)                  | WAT06080 |
| GAMMA(1) = 10. ** (C1 / (1. + B * 5.5 * XMUHL) + 0.2 * XMU)                   | WAT06090 |
| GAMMA(2) = 10. ** (-A * XMUHL / (1. + B * 4. * XMUHL) + 0.075 * XMU)          | WAT06100 |
| GAMMA(3) = 10. ** (-A * XMUHL / (1. + B * 3.5 * XMUHL) + 0.015 * XMU)         | WAT06110 |
| GAMMA(4) = GAMMA(3)                                                           | WAT06120 |
| GAMMA(5) = 10. ** (C1 / (1. + B * 5. * XMUHL) - 0.04 * XMU)                   | WAT06130 |
| C                                                                             | WAT06140 |
| C**** DAVIES EQUATION FOR MOST ACTIVITY COEFFS.                               | WAT06150 |
| C                                                                             | WAT06160 |
| DO 400 I = 6 , D                                                              | WAT06170 |
| IF (Z(I) .NE. 0) GOTO 410                                                     | WAT06180 |
| GAMMA(I) = 10. ** (.1 * XMU)                                                  | WAT06190 |
| GOTO 400                                                                      | WAT06200 |
| 410 GAMMA(I) = 10. ** (-A * Z(I) * Z(I) * (XMUHL / (1. + XMUHL) - 0.3 * XMU)) | WAT06210 |
| 400 CONTINUE                                                                  | WAT06220 |
|                                                                               | WAT06230 |
|                                                                               | WAT06240 |

|       |                                                                  |          |
|-------|------------------------------------------------------------------|----------|
| C     |                                                                  | WAT06250 |
| C**** | DEBYE-HUCKEL EQN FOR POLYSULFIDE SPECIES(DHA FROM CLOKE,1963),   | WAT06260 |
| C**** | CARBONATES, H+, AND Sr SPECIES                                   | WAT06270 |
| C     |                                                                  | WAT06280 |
|       | DO 420 J = 1 , 15                                                | WAT06290 |
|       | I = LISTE1(J)                                                    | WAT06300 |
|       | IF (DHA(I).GT. 0.0) GAMMA(I) = 10. ** (-A * Z(I) * Z(I) *        | WAT06310 |
|       | *XMUHL / (1.0 + DHA(I) * B * XMUHL))                             | WAT06320 |
| 420   | CONTINUE                                                         | WAT06330 |
|       | GAMMA(85) = 10.** (XMU* (170.01/T - .8798 + .0013935*T)+         | WAT06340 |
|       | * XMU * XMU* (28.81 / T - .2108 + .0003641 * T))                 | WAT06350 |
|       | GAMMA(87)= 10. ** (C1 / (1. + B * 5.26 * XMUHL) + 0.121 * XMU)   |          |
|       | GAMMA(95)= 10. ** (-0.5 * XMU)                                   |          |
| C     |                                                                  | WAT06360 |
| C**** | CALC OF MINOR ANION ACTIVITIES */                                | WAT06370 |
| C     |                                                                  | WAT06380 |
|       | ALFA(84) = MI(84) * GAMMA(84)                                    | WAT06390 |
|       | ALFA(96) = MI(96) * GAMMA(96)                                    | WAT06400 |
|       | ALFA(97) = MI(97) * GAMMA(97)                                    | WAT06410 |
|       | ALFA(202)= MI(202)* GAMMA(202)                                   | WAT06420 |
| C     |                                                                  | WAT06430 |
| C**** | CALC. OF PE & EHDO                                               | WAT06440 |
| C     |                                                                  | WAT06450 |
|       | IF (DOX .LE. 0.0) GOTO 430                                       | WAT06460 |
|       | PEDO= -(DLOG10(KT(136))+ PH+ 0.5 *LH2O -0.25 * ALOG10(DOX/32E3)) | WAT06470 |
|       | PEDO2=-(DLOG10(KT(151))+ PH+ 0.5 *LH2O -0.25 * ALOG10(DOX/32E3)) | WAT06480 |
|       | EHDO = PEDO * C * R * T / F                                      | WAT06490 |
|       | EHDO2 = PEDO2 * C * R * T / F                                    | WAT06500 |
| 430   | CONTINUE                                                         | WAT06510 |
|       | PE = PEPT                                                        | WAT06520 |
|       | IF (EHPT .LE. 9.0) GOTO 440                                      | WAT06530 |
|       | IF (DOX .LE. 0.0) GOTO 440                                       | WAT06540 |
|       | PE=PEDO                                                          | WAT06550 |
|       | IF (EMPOX .NE. 1) GOTO 440                                       | WAT06560 |
|       | PE=PEDO2                                                         | WAT06570 |
| 440   | CONTINUE                                                         | WAT06580 |
|       | TENMPE = 10.**(-PE)                                              | WAT06590 |
| C     |                                                                  | WAT06600 |
| C**** | ACTIVITIES OF OH & H+ SPECIES */                                 | WAT06610 |
| C     |                                                                  | WAT06620 |
|       | ALFA(26) = AH2O * KW * TENPH                                     | WAT06630 |
|       | MI(26) = ALFA(26) / GAMMA(26)                                    | WAT06640 |
|       | ALFA(63) = 10**(-PH)                                             | WAT06650 |
|       | MI(63) = 1. / (TENPH * GAMMA(63))                                | WAT06660 |
| C     |                                                                  | WAT06670 |
|       | IF (ITER .NE. 1) GOTO 560                                        | WAT06680 |
| C     |                                                                  | WAT06690 |
| C**** | INITIAL CO2 SPECIES */                                           | WAT06700 |
| C     |                                                                  | WAT06710 |
|       | IF (CORALK .EQ. 2) GOTO 460                                      | WAT06720 |
|       | C1 = 2.0 * TENPH / (KT(68) * GAMMA(17))                          | WAT06730 |
|       | MI(6) = CO2TIT / (1.0 + GAMMA(6) * C1)                           | WAT06740 |
|       | ALFA(6) = MI(6) * GAMMA(6)                                       | WAT06750 |
|       | C2 = KT(35) / (TENPH * GAMMA(85))                                | WAT06760 |

|                                                                     |          |
|---------------------------------------------------------------------|----------|
| MI(17) = C1 * ALFA(6) / 2.0                                         | WAT06770 |
| MI(85) = C2 * ALFA(6)                                               | WAT06780 |
| ALFA(17) = MI(17) * GAMMA(17)                                       | WAT06790 |
| ALFA(85) = MI(85) * GAMMA(85)                                       | WAT06800 |
| GOTO480                                                             | WAT06810 |
| 460 MI(6)=CO2TIT/(1EO + GAMMA(6)*((KT(35)/(TENPH*GAMMA(85)))+TENPH/ | WAT06820 |
| *(KT(68)*GAMMA(17))))                                               | WAT06830 |
| ALFA(6)=MI(6)*GAMMA(6)                                              | WAT06840 |
| MI(17)=ALFA(6)*TENPH/(GAMMA(17)*KT(68))                             | WAT06850 |
| MI(85)=ALFA(6)*KT(35)/(TENPH*GAMMA(85))                             | WAT06860 |
| ALFA(17) = MI(17) * GAMMA(17)                                       | WAT06870 |
| ALFA(85) = MI(85) * GAMMA(85)                                       | WAT06880 |
| C                                                                   | WAT06890 |
| C**** INITIAL SULFATE SPECIES */                                    | WAT06900 |
| C                                                                   | WAT06910 |
| 480 IF (SO4TOT .LE. 0.0) GOTO 490                                   | WAT06920 |
| MI(62)=KT(89)/(TENPH*GAMMA(62))                                     | WAT06930 |
| MI(5)=SO4TOT/(1EO + GAMMA(5)*MI(62))                                | WAT06940 |
| C1 = MI(5) * GAMMA(5)                                               | WAT06950 |
| ALFA(5) = C1                                                        | WAT06960 |
| MI(62)=C1 * MI(62)                                                  | WAT06970 |
| ALFA(62) = MI(62) * GAMMA(62)                                       | WAT06980 |
| C                                                                   | WAT06990 |
| C**** INITIAL FLUORIDE SPECIES */                                   | WAT07000 |
| C                                                                   | WAT07010 |
| 490 IF (FTOT .LE. 0.0) GOTO 500                                     | WAT07020 |
| MI(125) = KT(202) / (TENPH * GAMMA(125))                            | WAT07030 |
| MI(126) = KT(203) * MI(61) * GAMMA(61) / (TENPH * GAMMA(126))       | WAT07040 |
| MI(296) = KT(537) * MI(61) * GAMMA(61) / (TENPH**2 * GAMMA(296))    | WAT07050 |
| MI(61) = FTOT / (1 + GAMMA(61) * (MI(125) + MI(126) + MI(296)))     | WAT07060 |
| ALFA(61) = MI(61) * GAMMA(61)                                       | WAT07070 |
| C1 = MI(61) * GAMMA(61)                                             | WAT07080 |
| C                                                                   | WAT07090 |
| MI(125) = C1 * MI(125)                                              | WAT07100 |
| ALFA(125) = MI(125) * GAMMA(125)                                    | WAT07110 |
| MI(126) = C1 * MI(126)                                              | WAT07120 |
| ALFA(126) = MI(126)* GAMMA(126)                                     | WAT07130 |
| MI(296) = C1 * MI(296)                                              | WAT07140 |
| ALFA(296) = MI(296) * GAMMA(296)                                    | WAT07150 |
| C                                                                   | WAT07160 |
| C**** INITIAL PHOSPHATE SPECIES */                                  | WAT07170 |
| C                                                                   | WAT07180 |
| 500 IF (PTOT .LE. 0.0) GOTO 520                                     | WAT07190 |
| MI(46) = KT(15) / (TENPH * GAMMA(46))                               | WAT07200 |
| MI(47) = KT(16) / (TENPH**2 * GAMMA(47))                            | WAT07210 |
| MI(44) = PTOT/(1EO + GAMMA(44) * (MI(46) + MI(47)))                 | WAT07220 |
| ALFA(44) = MI(44) * GAMMA(44)                                       | WAT07230 |
| C1 = MI(44) * GAMMA(44)                                             | WAT07240 |
| DO 510 I = 46 , 47                                                  | WAT07250 |
| MI(I) = C1 * MI(I)                                                  | WAT07260 |
| ALFA(I) = MI(I) * GAMMA(I)                                          | WAT07270 |
| 510 CONTINUE                                                        | WAT07280 |
| C                                                                   | WAT07290 |
| C**** INITIAL CHLORIDE */                                           | WAT07300 |



|       |                                                                 |          |
|-------|-----------------------------------------------------------------|----------|
| C     |                                                                 | WAT07310 |
|       | 520 ALFA(4) = MI(4) * GAMMA(4)                                  | WAT07320 |
| C     |                                                                 | WAT07330 |
| C**** | INITIAL SULFIDE SPECIES */                                      | WAT07340 |
| C     |                                                                 | WAT07350 |
|       | IF (H2STOT .LE. 0.0) GOTO 540                                   | WAT07360 |
|       | MI(13) = 1 / (KT(91) * TENPH * GAMMA(13))                       | WAT07370 |
|       | MI(67) = KT(92) * TENPH / GAMMA(67)                             | WAT07380 |
|       | MI(263) = KT(502) * TENPH / GAMMA(263)                          | WAT07390 |
|       | MI(264) = KT(503) * TENPH / GAMMA(264)                          | WAT07400 |
|       | MI(265) = KT(504) * TENPH / GAMMA(265)                          | WAT07410 |
|       | MI(266) = KT(505) * TENPH / GAMMA(266)                          | WAT07420 |
|       | MI(267) = KT(506) * TENPH / GAMMA(267)                          | WAT07430 |
|       | MI(66) = H2STOT / (1.0 + GAMMA(66) * (MI(13) + MI(67) + MI(263) | WAT07440 |
|       | *+ MI(264) + MI(265) + MI(266) + MI(267)))                      | WAT07450 |
|       | C1 = MI(66) * GAMMA(66)                                         | WAT07460 |
|       | ALFA(66) = C1                                                   | WAT07470 |
|       | MI(13) = C1 * MI(13)                                            | WAT07480 |
|       | ALFA(13) = MI(13) * GAMMA(13)                                   | WAT07490 |
|       | MI(67) = C1 * MI(67)                                            | WAT07500 |
|       | ALFA(67) = MI(67) * GAMMA(67)                                   | WAT07510 |
|       | DO 530 I= 263 , 267                                             | WAT07520 |
|       | MI(I) = C1 * MI(I)                                              | WAT07530 |
|       | ALFA(I) = MI(I) * GAMMA(I)                                      | WAT07540 |
|       | 530 CONTINUE                                                    | WAT07550 |
| C     |                                                                 | WAT07560 |
| C**** | INITIAL ORGANIC LIGANDS */                                      | WAT07570 |
| C     |                                                                 | WAT07580 |
|       | 540 IF (FULVTT .LE. 0.0) GOTO 550                               | WAT07590 |
|       | MI(286) = KT(523) / (TENPH * GAMMA(286))                        | WAT07600 |
|       | MI(284) = FULVTT / (1 + GAMMA(284) * MI(286))                   | WAT07610 |
|       | C1=MI(284) * GAMMA(284)                                         | WAT07620 |
|       | ALFA(284) = C1                                                  | WAT07630 |
|       | MI(286) = C1 * MI(286)                                          | WAT07640 |
|       | ALFA(286) = MI(286) * GAMMA(286)                                | WAT07650 |
| C     |                                                                 | WAT07660 |
|       | 550 IF (HUMTOT .LE. 0.0) GOTO 580                               | WAT07670 |
|       | MI(287)=KT(524)/(TENPH*GAMMA(287))                              | WAT07680 |
|       | MI(285)=HUMTOT/(1 + GAMMA(285)*MI(287))                         | WAT07690 |
|       | C1 = MI(285) * GAMMA(285)                                       | WAT07700 |
|       | ALFA(285) = C1                                                  | WAT07710 |
|       | MI(287) = C1 * MI(287)                                          | WAT07720 |
|       | ALFA(287) = MI(287) * GAMMA(287)                                | WAT07730 |
|       | GOTO 580                                                        | WAT07740 |
|       | 560 ALFA(4) = MI(4) * GAMMA(4)                                  | WAT07750 |
|       | ALFA(5) = MI(5) * GAMMA(5)                                      | WAT07760 |
|       | ALFA(6) = MI(6) * GAMMA(6)                                      | WAT07770 |
|       | ALFA(17) = MI(17) * GAMMA(17)                                   | WAT07780 |
|       | ALFA(44) = MI(44) * GAMMA(44)                                   | WAT07790 |
|       | ALFA(46) = MI(46) * GAMMA(46)                                   | WAT07800 |
|       | ALFA(47) = MI(47) * GAMMA(47)                                   | WAT07810 |
|       | ALFA(61) = MI(61) * GAMMA(61)                                   | WAT07820 |
|       | ALFA(66) = MI(66) * GAMMA(66)                                   | WAT07830 |
|       | ALFA(284) = MI(284) * GAMMA(284)                                | WAT07840 |



|                                                                |          |
|----------------------------------------------------------------|----------|
| ALFA(285) = MI(285) * GAMMA(285)                               | WAT07850 |
| C                                                              | WAT07860 |
| C**** SILICA SPECIES */                                        | WAT07870 |
| C                                                              | WAT07880 |
| 580 C1 = KT(13) * TENPH / GAMMA(24)                            | WAT07890 |
| C2 = KT(14) * TENPH**2 / GAMMA(25)                             | WAT07900 |
| C3 = KT(201) * ALFA(61)**6 / (GAMMA(124) * TENPH**4 * AH2O**4) | WAT07910 |
| MI(23) = SITOT / (1EO + GAMMA(23) * (C1 + C2 + C3))            | WAT07920 |
| ALFA(23) = MI(23) * GAMMA(23)                                  | WAT07930 |
| MI(24) = ALFA(23) * C1                                         | WAT07940 |
| MI(25) = ALFA(23) * C2                                         | WAT07950 |
| MI(124) = ALFA(23) * C3                                        | WAT07960 |
| ALFA(24) = MI(24) * GAMMA(24)                                  | WAT07970 |
| ALFA(25) = MI(25) * GAMMA(25)                                  | WAT07980 |
| ALFA(124)=MI(124)*GAMMA(124)                                   | WAT07990 |
| C                                                              | WAT08000 |
| C**** BORON SPECIES */                                         | WAT08010 |
| C                                                              | WAT08020 |
| IF (BTOT .LE. 0.0) GOTO 600                                    | WAT08030 |
| MI(36) = KT(25) * TENPH / GAMMA(36)                            | WAT08040 |
| MI(101)= KT(161)* ALFA(61) / GAMMA(101)                        | WAT08050 |
| MI(102)= KT(162)* ALFA(61)**2 / (GAMMA(102) * ALFA(26))        | WAT08060 |
| MI(103)= KT(163)* ALFA(61)**3 / (GAMMA(103) * ALFA(26)**2)     | WAT08070 |
| MI(104)= KT(164)* ALFA(61)**4 / (GAMMA(104) * ALFA(26)**3)     | WAT08080 |
| MI(35) = BTOT / (1+GAMMA(35) * (MI(36) + MI(101) + MI(102)+    | WAT08090 |
| *MI(103) + MI(104)))                                           | WAT08100 |
| C1 = MI(35) * GAMMA(35)                                        | WAT08110 |
| ALFA(35) = C1                                                  | WAT08120 |
| MI(36) = C1 * MI(36)                                           | WAT08130 |
| ALFA(36) = MI(36) * GAMMA(36)                                  | WAT08140 |
| DO 590 I = 101 , 104                                           | WAT08150 |
| MI(I) = C1 * MI(I)                                             | WAT08160 |
| ALFA(I) = MI(I) * GAMMA(I)                                     | WAT08170 |
| 590 CONTINUE                                                   | WAT08180 |
| C                                                              | WAT08190 |
| C**** NITROGEN SPECIES */                                      | WAT08200 |
| C                                                              | WAT08210 |
| 600 C1 = TENPH * KT(26) / GAMMA(37)                            | WAT08220 |
| C2 = ALFA(5) * KT(131) / GAMMA(91)                             | WAT08230 |
| MI(38) = NH4TOT / (1.0 + GAMMA(38) * (C1 + C2))                | WAT08240 |
| ALFA(38) = MI(38) * GAMMA(38)                                  | WAT08250 |
| MI(37) = ALFA(38) * C1                                         | WAT08260 |
| ALFA(37) = MI(37) * GAMMA(37)                                  | WAT08270 |
| MI(91) = ALFA(38) * C2                                         | WAT08280 |
| ALFA(91) = MI(91) * GAMMA(91)                                  | WAT08290 |
| C                                                              | WAT08300 |
| C**** MG SPECIES */                                            | WAT08310 |
| C                                                              | WAT08320 |
| MI(18) = ALFA(26) * KT(24) / GAMMA(18)                         | WAT08330 |
| MI(19) = ALFA(61) * KT(22) / GAMMA(19)                         | WAT08340 |
| MI(20) = ALFA(17) * KT(73) / GAMMA(20)                         | WAT08350 |
| MI(21) = ALFA(6) * KT(74) / GAMMA(21)                          | WAT08360 |
| MI(22) = ALFA(5) * KT(75) / GAMMA(22)                          | WAT08370 |
| MI(39) = ALFA(44) * KT(123) / GAMMA(39)                        | WAT08380 |

|                                                               |          |
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| MI(40) = ALFA(47) * KT(124) / GAMMA(40)                       | WAT08390 |
| MI(72) = ALFA(46) * KT(33) / GAMMA(72)                        | WAT08400 |
| MI(1) = MGTOT / (1.0 + GAMMA(1) * (MI(18) + MI(19) + MI(20) + | WAT08410 |
| *MI(21) + MI(22) + MI(39) + MI(40) + MI(72)))                 | WAT08420 |
| C1 = MI(1) * GAMMA(1)                                         | WAT08430 |
| ALFA(1) = C1                                                  | WAT08440 |
| DO 610 I = 18 , 22                                            | WAT08450 |
| MI(I) = C1 * MI(I)                                            | WAT08460 |
| ALFA(I) = MI(I) * GAMMA(I)                                    | WAT08470 |
| 610 CONTINUE                                                  | WAT08480 |
| MI(39) = C1 * MI(39)                                          | WAT08490 |
| ALFA(39) = MI(39) * GAMMA(39)                                 | WAT08500 |
| MI(40) = C1 * MI(40)                                          | WAT08510 |
| ALFA(40) = MI(40) * GAMMA(40)                                 | WAT08520 |
| MI(72) = C1 * MI(72)                                          | WAT08530 |
| ALFA(72) = MI(72) * GAMMA(72)                                 | WAT08540 |
| C                                                             | WAT08550 |
| C***** CA SPECIES */                                          | WAT08560 |
| C                                                             | WAT08570 |
| MI(28) = ALFA(26) * KT(76) / GAMMA(28)                        | WAT08580 |
| MI(29) = ALFA(6) * KT(77) / GAMMA(29)                         | WAT08590 |
| MI(30) = ALFA(17) * KT(78) / GAMMA(30)                        | WAT08600 |
| MI(31) = ALFA(5) * KT(23) / GAMMA(31)                         | WAT08610 |
| MI(73) = ALFA(46) * KT(34) / GAMMA(73)                        | WAT08620 |
| MI(74) = ALFA(44) * KT(121) / GAMMA(74)                       | WAT08630 |
| MI(75) = ALFA(47) * KT(122) / GAMMA(75)                       | WAT08640 |
| MI(81) = ALFA(62) * KT(168) / GAMMA(81)                       |          |
| MI(100) = ALFA(61) * KT(160) / GAMMA(100)                     | WAT08650 |
| MI(0) = CATOT / (1.0 + GAMMA(0) * (MI(28) +MI(29) +MI(30) +   | WAT08660 |
| * MI(31) +MI(73) +MI(74) +MI(75) +MI(81) +MI(100)))           | WAT08670 |
| C1=MI(0)*GAMMA(0)                                             | WAT08680 |
| ALFA(0) = C1                                                  | WAT08690 |
| MI(28) = C1 * MI(28)                                          | WAT08700 |
| ALFA(28) = MI(28) * GAMMA(28)                                 | WAT08710 |
| MI(29) = C1 * MI(29)                                          | WAT08720 |
| ALFA(29) = MI(29) * GAMMA(29)                                 | WAT08730 |
| MI(30) = C1 * MI(30)                                          | WAT08740 |
| ALFA(30) = MI(30) * GAMMA(30)                                 | WAT08750 |
| MI(31) = C1 * MI(31)                                          | WAT08760 |
| ALFA(31) = MI(31) * GAMMA(31)                                 | WAT08770 |
| MI(73) = C1 * MI(73)                                          | WAT08780 |
| ALFA(73) = MI(73) * GAMMA(73)                                 | WAT08790 |
| MI(74) = C1 * MI(74)                                          | WAT08800 |
| ALFA(74) = MI(74) * GAMMA(74)                                 | WAT08810 |
| MI(75) = C1 * MI(75)                                          | WAT08820 |
| ALFA(75) = MI(75) * GAMMA(75)                                 | WAT08830 |
| MI(81) = C1 * MI(81)                                          |          |
| ALFA(81) = MI(81) * GAMMA(81)                                 |          |
| MI(100)= C1 * MI(100)                                         | WAT08840 |
| ALFA(100)= MI(100)* GAMMA(100)                                | WAT08850 |
| C                                                             | WAT08860 |
| C***** NA SPECIES */                                          | WAT08870 |
| C                                                             | WAT08880 |
| MI(41) = ALFA(17) * KT(69) / GAMMA(41)                        | WAT08890 |

|                                                                 |          |
|-----------------------------------------------------------------|----------|
| MI(42) = ALFA(6) * KT(70) / GAMMA(42)                           | WAT08900 |
| MI(43) = ALFA(5) * KT(71) / GAMMA(43)                           | WAT08910 |
| MI(49) = ALFA(46) * KT(30) / GAMMA(49)                          | WAT08920 |
| MI(297) = ALFA(61)* KT(540)/ GAMMA(297)                         |          |
| MI(2) = NATOT / (1.0 +GAMMA(2) * (MI(41)+MI(42)+MI(43)+MI(49)   | WAT08930 |
| * +MI(297)))                                                    |          |
| C1 = MI(2) * GAMMA(2)                                           | WAT08940 |
| ALFA(2) = C1                                                    | WAT08950 |
| MI(41) = C1 * MI(41)                                            | WAT08960 |
| ALFA(41) = MI(41) * GAMMA(41)                                   | WAT08970 |
| MI(42) = C1 * MI(42)                                            | WAT08980 |
| ALFA(42) = MI(42) * GAMMA(42)                                   | WAT08990 |
| MI(43) = C1 * MI(43)                                            | WAT09000 |
| ALFA(43) = MI(43) * GAMMA(43)                                   | WAT09010 |
| MI(49) = C1 * MI(49)                                            | WAT09020 |
| ALFA(49) = MI(49) * GAMMA(49)                                   | WAT09030 |
| MI(297)= C1 * MI(297)                                           |          |
| ALFA(297)= MI(297)* GAMMA(297)                                  |          |
| C                                                               | WAT09040 |
| C***** K SPECIES */                                             | WAT09050 |
| C                                                               | WAT09060 |
| MI(45) = ALFA(5) * KT(72) / GAMMA(45)                           | WAT09070 |
| MI(60) = ALFA(46) * KT(32) / GAMMA(60)                          | WAT09080 |
| MI(3) = KTOT / (1.0 +GAMMA(3) * (MI(45) + MI(60)))              | WAT09090 |
| C1 = MI(3) * GAMMA(3)                                           | WAT09100 |
| ALFA(3) = C1                                                    | WAT09110 |
| MI(45) = C1 * MI(45)                                            | WAT09120 |
| ALFA(45) = MI(45) * GAMMA(45)                                   | WAT09130 |
| MI(60) = C1 * MI(60)                                            | WAT09140 |
| ALFA(60) = MI(60) * GAMMA(60)                                   | WAT09150 |
| C                                                               | WAT09160 |
| C***** AL SPECIES */                                            | WAT09170 |
| C                                                               | WAT09180 |
| IF (ALTOT .LE. 0.0) GOTO 630                                    | WAT09190 |
| MI(51)=AH20*TENPH*KT(80)/GAMMA(51)                              | WAT09200 |
| MI(52)=(AH20*TENPH)**2*KT(81)/GAMMA(52)                         | WAT09210 |
| MI(53)=(AH20*TENPH)**4*KT(82)/GAMMA(53)                         | WAT09220 |
| MI(54)=ALFA(61)*KT(83)/GAMMA(54)                                | WAT09230 |
| MI(55)=ALFA(61)**2*KT(84)/GAMMA(55)                             | WAT09240 |
| MI(56)=ALFA(61)**3*KT(85)/GAMMA(56)                             | WAT09250 |
| MI(57)=ALFA(61)**4*KT(86)/GAMMA(57)                             | WAT09260 |
| MI(58)=ALFA(5)*KT(87)/GAMMA(58)                                 | WAT09270 |
| MI(59)=ALFA(5)**2*KT(88)/GAMMA(59)                              | WAT09280 |
| MI(181)=KT(336)*(AH20*TENPH)**3/GAMMA(181)                      | WAT09290 |
| MI(203)=ALFA(62)*KT(397)/GAMMA(203)                             |          |
| MI(50)=ALTOT/(1E0+GAMMA(50)*(MI(51)+MI(52)+MI(53)+MI(54)+MI(55) | WAT09300 |
| *+MI(56)+MI(57)+MI(58)+MI(59)+MI(181)+MI(203)))                 | WAT09310 |
| C1 = MI(50) * GAMMA(50)                                         | WAT09320 |
| ALFA(50) = C1                                                   | WAT09330 |
| DO 620 I = 51 , 59                                              | WAT09340 |
| MI(I) = C1 * MI(I)                                              | WAT09350 |
| ALFA(I) = MI(I) * GAMMA(I)                                      | WAT09360 |
| 620 CONTINUE                                                    | WAT09370 |
| MI(181) = C1 * MI(181)                                          | WAT09380 |

|                                                                    |          |
|--------------------------------------------------------------------|----------|
| ALFA(181) = MI(181) * GAMMA(181)                                   | WAT09390 |
| MI(203) = C1 * MI(203)                                             |          |
| ALFA(203) = MI(203) * GAMMA(203)                                   |          |
| GOTO 650                                                           | WAT09400 |
| 630 DO 640 I = 51 , 59                                             | WAT09410 |
| MI(I) = 0.0                                                        | WAT09420 |
| 640 CONTINUE                                                       | WAT09430 |
| MI(181) = 0.0                                                      | WAT09440 |
| MI(203) = 0.0                                                      |          |
| C                                                                  | WAT09450 |
| C***** FE SPECIES */                                               | WAT09460 |
| C                                                                  | WAT09470 |
| 650 IF( FE2TOT + FE3TOT .GT. 0.0) GOTO 660                         | WAT09480 |
| IF( EHM .LT. 9.9 .AND. FETOTL .GT. 0.0)GOTO 660                    | WAT09490 |
| GOTO 730                                                           | WAT09500 |
| C                                                                  | WAT09510 |
| C***** FE +2 SPECIES */                                            | WAT09520 |
| C                                                                  | WAT09530 |
| 660 MI(10) = KT(2) * AH2O*TENPH / GAMMA(10)                        | WAT09540 |
| MI(11) = KT(3) * AH2O**3 * TENPH**3 / GAMMA(11)                    | WAT09550 |
| MI(33) = KT(8) * ALFA(5) / GAMMA(33)                               | WAT09560 |
| MI(64) = KT(120) * ALFA(47) / GAMMA(64)                            | WAT09570 |
| MI(79) = KT(105) * (AH2O*TENPH)**2 / GAMMA(79)                     | WAT09580 |
| MI(99) = KT(138) * ALFA(46) / GAMMA(99)                            | WAT09590 |
| MI(122) = KT(148) * ALFA(62) / GAMMA(122)                          |          |
| MI(247) = KT(476) * ALFA(66)**2 / GAMMA(247)                       | WAT09600 |
| MI(248) = KT(477) * ALFA(66)**3 / GAMMA(248)                       | WAT09610 |
| C                                                                  | WAT09620 |
| C***** FE +3 SPECIES */                                            | WAT09630 |
| C                                                                  | WAT09640 |
| MI(9) = KT(1) * AH2O*TENPH / GAMMA(9)                              | WAT09650 |
| MI(12) = KT(139)* ALFA(46) / GAMMA(12)                             | WAT09660 |
| MI(14) = KT(4) * ALFA(5) / GAMMA(14)                               | WAT09670 |
| MI(15) = KT(5) * ALFA(4) / GAMMA(15)                               | WAT09680 |
| MI(27) = KT(6) * ALFA(4)**2 / GAMMA(27)                            | WAT09690 |
| MI(32) = KT(7) * ALFA(4)**3 / GAMMA(32)                            | WAT09700 |
| MI(76) = KT(102)*(AH2O*TENPH)**2/ GAMMA(76)                        | WAT09710 |
| MI(77) = KT(103)*(AH2O*TENPH)**3/ GAMMA(77)                        | WAT09720 |
| MI(78) = KT(104)*(AH2O*TENPH)**4/ GAMMA(78)                        | WAT09730 |
| MI(98) = KT(156) * ALFA(47) / GAMMA(98)                            | WAT09740 |
| MI(105) = ALFA(61) * KT(165) / GAMMA(105)                          | WAT09750 |
| MI(106) = ALFA(61)**2 * KT(166) / GAMMA(106)                       | WAT09760 |
| MI(107) = ALFA(61)**3 * KT(167) / GAMMA(107)                       | WAT09770 |
| MI(108) = KT(333)* ALFA(5)**2 / GAMMA(108)                         | WAT09780 |
| MI(123) = KT(159)* ALFA(62) / GAMMA(123)                           |          |
| MI(179) = KT(334)*(AH2O*TENPH)**2 *MI(8)*GAMMA(8) / GAMMA(179)     | WAT09790 |
| MI(180) = KT(335)*(AH2O*TENPH)**4 *(MI(8)*GAMMA(8))**2 /GAMMA(180) | WAT09800 |
| MI(288) = KT(525) * ALFA(284) / GAMMA(288)                         | WAT09810 |
| MI(289) = KT(526) * ALFA(285) / GAMMA(289)                         | WAT09820 |
| C                                                                  | WAT09830 |
| IF (FE2TOT + FE3TOT .LE. 0.0) GOTO 680                             | WAT09840 |
| C                                                                  | WAT09850 |
| C***** SPLIT IRON FE +2 SPECIES                                    | WAT09860 |
| C                                                                  | WAT09870 |

|       |                                                                   |          |
|-------|-------------------------------------------------------------------|----------|
|       | MI(7) = FE2TOT / (1.+ GAMMA(7) * (MI(10) + MI(11) + MI(33)+       | WAT09880 |
|       | *MI(64) + MI(79) + MI(99) + MI(122) + MI(247) + MI(248)))         | WAT09890 |
|       | C1 = MI(7) * GAMMA(7)                                             | WAT09900 |
|       | ALFA(7) = C1                                                      | WAT09910 |
| C     |                                                                   | WAT09920 |
|       | MI(10) = C1 * MI(10)                                              | WAT09930 |
|       | MI(11) = C1 * MI(11)                                              | WAT09940 |
|       | MI(33) = C1 * MI(33)                                              | WAT09950 |
|       | MI(64) = C1 * MI(64)                                              | WAT09960 |
|       | MI(79) = C1 * MI(79)                                              | WAT09970 |
|       | MI(99) = C1 * MI(99)                                              | WAT09980 |
|       | MI(122) = C1 * MI(122)                                            |          |
|       | MI(247)= C1 * MI(247)                                             | WAT09990 |
|       | MI(248)= C1 * MI(248)                                             | WAT10000 |
| C     |                                                                   | WAT10010 |
| C**** | SPLIT IRON            FE +3 SPECIES                               | WAT10020 |
| C     |                                                                   | WAT10030 |
|       | MI(8) = FE3TOT / (1.+ GAMMA(8) * (MI(9) +MI(12) +MI(14) +MI(15)   | WAT10040 |
|       | *+MI(27) + MI(32) + MI(76) + MI(77) + MI(78) + MI(98) + MI(105)+  | WAT10050 |
|       | *MI(106) + MI(107) + MI(108) + MI(123) + 2 *MI(179) + 3 *MI(180)+ | WAT10060 |
|       | *MI(288) + MI(289)))                                              | WAT10070 |
|       | C1 = MI(8) * GAMMA(8)                                             | WAT10080 |
|       | ALFA(8) = C1                                                      | WAT10090 |
| C     |                                                                   | WAT10100 |
|       | DO 670 J = 1 , 19                                                 | WAT10110 |
|       | I = LISTE4(J)                                                     | WAT10120 |
|       | MI(I) = C1 * MI(I)                                                | WAT10130 |
| 670   | CONTINUE                                                          | WAT10140 |
|       | GOTO 710                                                          | WAT10150 |
| C     |                                                                   | WAT10160 |
| 680   | MI(8) = 1.0 / GAMMA(8)                                            | WAT10170 |
|       | C1 = KT(0) / TENMPE                                               | WAT10180 |
| C     |                                                                   | WAT10190 |
|       | DO 690 J = 1 ,18                                                  | WAT10200 |
|       | I = LISTE2(J)                                                     | WAT10210 |
|       | MI(I) = C1 * MI(I)                                                | WAT10220 |
| 690   | CONTINUE                                                          | WAT10230 |
|       | MI(179)=KT(334)*C1**2*(AH2O*TENPH)**2*MI(7)*GAMMA(7)              | WAT10240 |
|       | */GAMMA(179)                                                      | WAT10250 |
|       | MI(180)=KT(335)*C1**3*(AH2O*TENPH)**4*(MI(7)*GAMMA(7))**2         | WAT10260 |
|       | */GAMMA(180)                                                      | WAT10270 |
|       | MI(7)=FETOTL/(1.0+GAMMA(7)*(MI(8)+MI(9)+MI(10)+MI(11)+MI(12)+     | WAT10280 |
|       | *MI(14)+MI(15)+MI(27)+MI(32)+MI(33)+MI(64)+MI(76)+MI(77)+         | WAT10290 |
|       | *MI(78)+MI(79)+MI(98)+MI(99)+MI(105)+MI(106)+MI(107)+             | WAT10300 |
|       | *MI(108)+MI(122)+MI(123)+2*MI(179)+3*MI(180)+MI(247)+MI(248)+     | WAT10310 |
|       | *MI(288)+MI(289)))                                                |          |
|       | C1 = MI(7) * GAMMA(7)                                             | WAT10320 |
|       | ALFA(7) = C1                                                      | WAT10330 |
| C     |                                                                   | WAT10340 |
|       | DO 700 J = 2 ,30                                                  | WAT10350 |
|       | I =LISTE3(J)                                                      | WAT10360 |
|       | MI(I)=C1*MI(I)                                                    | WAT10370 |
| 700   | CONTINUE                                                          | WAT10380 |
|       | ALFA(8)=MI(8)*GAMMA(8)                                            | WAT10390 |

|       |                                                                  |          |
|-------|------------------------------------------------------------------|----------|
| 710   | CONTINUE                                                         | WAT10400 |
| C     |                                                                  | WAT10410 |
|       | DO 720 J = 3 , 30                                                | WAT10420 |
|       | I = LISTE3(J)                                                    | WAT10430 |
|       | ALFA(I)=MI(I)*GAMMA(I)                                           | WAT10440 |
| 720   | CONTINUE                                                         | WAT10450 |
|       | GOTO 745                                                         | WAT10460 |
| C     |                                                                  | WAT10470 |
| 730   | DO 740 J = 1 , 30                                                | WAT10480 |
|       | I = LISTE3(J)                                                    | WAT10490 |
|       | MI(I) = 0.0                                                      | WAT10500 |
| 740   | CONTINUE                                                         | WAT10510 |
| 745   | IF (ALFA(7) * ALFA(8) .LE. 0.0) GOTO 750                         | WAT10520 |
|       | PEFE = -DLOG10(KT(0) * ALFA(7) / ALFA(8))                        | WAT10530 |
|       | EHFE = PEFE * C*R*T/F                                            | WAT10540 |
|       | IF (EHPT .LE. 9.0 .AND. EHPT .EQ. 0) GOTO 750                    | WAT10550 |
|       | EHM = EHFE                                                       | WAT10560 |
|       | PE = PEFE                                                        | WAT10570 |
|       | TENMPE = 10.0**(-PE)                                             | WAT10580 |
| 750   | CONTINUE                                                         | WAT10590 |
| C     |                                                                  | WAT10600 |
| C**** | LI, SR, BA, CS, RB SPECIES */                                    | WAT10610 |
| C     |                                                                  | WAT10620 |
|       | C2 = KT(126) * ALFA(5)/GAMMA(82)                                 | WAT10640 |
|       | MI(80) = LITOT/(1E0+GAMMA(80)*C2)                                | WAT10650 |
|       | ALFA(80) = MI(80)*GAMMA(80)                                      | WAT10660 |
|       | MI(82)=C2 * ALFA(80)                                             | WAT10680 |
|       | C1=KT(129) * ALFA(26)/GAMMA(88)                                  | WAT10690 |
|       | C2=KT(79) * ALFA(6)/GAMMA(68)                                    |          |
|       | C3=KT(135)* ALFA(17)/GAMMA(95)                                   |          |
|       | MI(87) = SRTOT/(1E0+GAMMA(87)*(C1+C2+C3))                        | WAT10700 |
|       | MI(88) = GAMMA(87)*MI(87)*C1                                     | WAT10710 |
|       | MI(68) = GAMMA(87)*MI(87)*C2                                     |          |
|       | MI(95) = GAMMA(87)*MI(87)*C3                                     |          |
|       | C1=KT(130)*AH20*TENPH/GAMMA(90)                                  | WAT10720 |
|       | C2=KT(543)*ALFA(5)/GAMMA(201)                                    |          |
|       | MI(89)=BATOT/(1E0+GAMMA(89)*(C1+C2))                             | WAT10730 |
|       | ALFA(89)=MI(89)*GAMMA(89)                                        |          |
|       | MI(90)=ALFA(89)*C1                                               | WAT10740 |
|       | MI(201)=ALFA(89)*C2                                              |          |
|       | ALFA(48) = MI(48) * GAMMA(48)                                    | WAT10750 |
|       | ALFA(68) = MI(68) * GAMMA(68)                                    |          |
|       | ALFA(82) = MI(82) * GAMMA(82)                                    | WAT10760 |
|       | ALFA(87) = MI(87) * GAMMA(87)                                    | WAT10770 |
|       | ALFA(88) = MI(88) * GAMMA(88)                                    | WAT10780 |
|       | ALFA(90) = MI(90) * GAMMA(90)                                    | WAT10800 |
|       | ALFA(94) = MI(94) * GAMMA(94)                                    | WAT10810 |
|       | ALFA(95) = MI(95) * GAMMA(95)                                    |          |
|       | ALFA(201)= MI(201)* GAMMA(201)                                   |          |
|       | RETURN                                                           | WAT10820 |
|       | END                                                              | WAT10830 |
|       | SUBROUTINE TREL(ALFA,GAMMA,KT,LOGKT,MI)                          | WAT10880 |
| C     |                                                                  | WAT10890 |
|       | REAL*8 ALFA(0:297),GAMMA(0:297),KT(0:543),LOGKT(0:543),MI(0:297) | WAT10900 |



|       |                                                                    |          |
|-------|--------------------------------------------------------------------|----------|
|       | INTEGER LISTE1(23),LISTE2(22),LISTE3(28),LISTE4(27),LISTE5(13),    | WAT10910 |
|       | *LISTE6(25)                                                        | WAT10920 |
|       | CHARACTER*80 CARD1,CARD2                                           | WAT10930 |
| C     |                                                                    | WAT10940 |
|       | REAL*8 ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT          | WAT10950 |
|       | REAL*8 ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT,    | WAT10960 |
|       | *MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3      | WAT10970 |
|       | INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA,      | WAT10980 |
|       | *ITER,NMBR,PUNCH,RBIT,FLAG                                         | WAT10990 |
| C     |                                                                    | WAT11000 |
|       | COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B,     | WAT11010 |
|       | *BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND,          | WAT11020 |
|       | *CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF, | WAT11030 |
|       | *DISCHG,DOC,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT,    | WAT11040 |
|       | *EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,   | WAT11050 |
|       | *FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,    | WAT11060 |
|       | *ITDS,ITER,K,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL,   | WAT11070 |
|       | *NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE,    | WAT11080 |
|       | *PEAS,PEDO,PEDO2,PEFE,PEN,PENO2,PEPT,PES,PH,PRNT,PTOT,PUNCH,R,     | WAT11090 |
|       | *RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,               | WAT11100 |
|       | *T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT             | WAT11110 |
|       | COMMON/CHRDAT/CARD1,CARD2                                          |          |
| C     |                                                                    | WAT11120 |
|       | DATA LISTE1/130,127,128,129,131,132,133,134,135,136,137,138,139    | WAT11130 |
|       | *,140,141,142,143,144,259,260,271,290,291/                         | WAT11140 |
|       | DATA LISTE2/145,146,147,148,149,150,151,152,153,154,155,156,157    | WAT11150 |
|       | *,158,159,229,230,231,232,272,273,274/                             | WAT11160 |
|       | DATA LISTE3/160,161,162,163,164,165,166,167,168,169,170,171,172    | WAT11170 |
|       | *,173,174,175,176,177,178,233,234,235,236,275,276,277,292,293/     | WAT11180 |
|       | DATA LISTE4/182,183,184,185,186,187,188,189,190,191,192,193,194    | WAT11190 |
|       | *,195,196,197,198,199,200,237,238,239,240,241,242,243,278/         | WAT11200 |
|       | DATA LISTE5/204,205,206,207,208,209,210,211,279,280,281,282,283/   | WAT11210 |
|       | DATA LISTE6/212,213,214,215,216,217,218,219,220,221,222,223,224    | WAT11220 |
|       | *,225,226,227,228,244,245,246,268,269,270,294,295/                 | WAT11230 |
| C     |                                                                    | WAT11240 |
| C**** | MN SPECIES */                                                      | WAT11250 |
| C     |                                                                    | WAT11260 |
|       | IF(MNTOT .LE. 0.0) GOTO 30                                         | WAT11270 |
| C     |                                                                    | WAT11280 |
| C**** | MN +2 SPECIES */                                                   | WAT11290 |
| C     |                                                                    | WAT11300 |
|       | MI(111)=KT(170)*ALFA(4)/GAMMA(111)                                 | WAT11310 |
|       | MI(112)=KT(171)*ALFA(4)**2/GAMMA(112)                              | WAT11320 |
|       | MI(113)=KT(172)*ALFA(4)**3/GAMMA(113)                              | WAT11330 |
|       | MI(114)=KT(173)*AH2O*TENPH/GAMMA(114)                              | WAT11340 |
|       | MI(115)=KT(174)*(AH2O*TENPH)**3/GAMMA(115)                         | WAT11350 |
|       | MI(116)=KT(175)*ALFA(61)/GAMMA(116)                                | WAT11360 |
|       | MI(117)=KT(176)*ALFA(5)/GAMMA(117)                                 | WAT11370 |
|       | MI(118)=KT(177)*ALFA(84)**2/GAMMA(118)                             | WAT11380 |
|       | MI(119)=KT(178)*ALFA(6)/GAMMA(119)                                 | WAT11390 |
| C     |                                                                    | WAT11400 |
|       | IF (EHM .GE. 9.9) GOTO 10                                          | WAT11410 |
| C     |                                                                    | WAT11420 |
| C**** | MN +3, +6, +7 SPECIES */                                           | WAT11430 |

|       |                                                                    |          |
|-------|--------------------------------------------------------------------|----------|
| C     |                                                                    | WAT11440 |
|       | MI(110) = KT(169)/(GAMMA(110)*TENMPE)                              | WAT11450 |
|       | XMI120 = LOGKT(179) +4. *LH20-(DLOG10(GAMMA(120)) -8.*PH -5.*PE)   | WAT11460 |
|       | IF (XMI120 .GT. -70.) MI(120)= 10**XMI120                          | WAT11470 |
|       | IF (XMI120 .LE. -70.) MI(120)= 0.0                                 | WAT11480 |
|       | XMI121 = LOGKT(180)+ 4. * LH20- (DLOG10(GAMMA(121)) -8.*PH -4.*PE) | WAT11490 |
|       | IF (XMI121 .GT. -70.) MI(121)=10**XMI121                           | WAT11500 |
|       | IF (XMI121 .LE. -70.) MI(121) = 0.0                                | WAT11510 |
| 10    | CONTINUE                                                           | WAT11520 |
|       | MI(109)=MNTOT/(1.+GAMMA(109)*(MI(110)+MI(111)+MI(112)+MI(113)+     | WAT11530 |
|       | *MI(114)+MI(115)+MI(116)+MI(117)+MI(118)+MI(119)+MI(120)           | WAT11540 |
|       | *+MI(121)))                                                        | WAT11550 |
|       | C1 = MI(109) * GAMMA(109)                                          | WAT11560 |
|       | ALFA(109) = C1                                                     | WAT11570 |
|       | DO 20 I = 110 , 121                                                | WAT11580 |
|       | MI(I) = C1 * MI(I)                                                 | WAT11590 |
|       | ALFA(I) = MI(I) * GAMMA(I)                                         | WAT11600 |
| 20    | CONTINUE                                                           | WAT11610 |
|       | GOTO 50                                                            | WAT11620 |
| 30    | DO 40 I = 109 , 121                                                | WAT11630 |
|       | MI(I) = 0.0                                                        | WAT11640 |
| 40    | CONTINUE                                                           | WAT11650 |
| C     |                                                                    | WAT11660 |
| C**** | CU SPECIES */                                                      | WAT11670 |
| C     |                                                                    | WAT11680 |
|       | 50 IF (CUTOT .LE. 0.0) GOTO 80                                     | WAT11690 |
|       | IF (EHM .GE. 9.9) GOTO 60                                          | WAT11700 |
| C     |                                                                    | WAT11710 |
| C**** | CU +1 SPECIES */                                                   | WAT11720 |
| C     |                                                                    | WAT11730 |
|       | MI(127) = KT(208) * TENMPE / GAMMA(127)                            | WAT11740 |
|       | MI(128) =KT(206) * ALFA(4)**2 * TENMPE / GAMMA(128)                | WAT11750 |
|       | MI(129) =KT(207) * ALFA(4)**3 * TENMPE / GAMMA(129)                | WAT11760 |
|       | MI(259) =KT(485) * (ALFA(66) * TENPH)**2 * TENMPE / GAMMA(259)     | WAT11770 |
|       | MI(260) =KT(486) * (ALFA(66) * TENPH)**2 * TENMPE / GAMMA(260)     | WAT11780 |
| 60    | CONTINUE                                                           | WAT11790 |
| C     |                                                                    | WAT11800 |
| C**** | CU +2 SPECIES */                                                   | WAT11810 |
| C     |                                                                    | WAT11820 |
|       | MI(131)=KT(209)*ALFA(17)/GAMMA(131)                                | WAT11830 |
|       | MI(132)=KT(210)*ALFA(17)**2/GAMMA(132)                             | WAT11840 |
|       | MI(133)=KT(211)*ALFA(4)/GAMMA(133)                                 | WAT11850 |
|       | MI(134)=KT(212)*ALFA(4)**2/GAMMA(134)                              | WAT11860 |
|       | MI(135)=KT(213)*ALFA(4)**3/GAMMA(135)                              | WAT11870 |
|       | MI(136)=KT(214)*ALFA(4)**4/GAMMA(136)                              | WAT11880 |
|       | MI(137)=KT(215)*ALFA(61)/GAMMA(137)                                | WAT11890 |
|       | MI(138)=KT(216)*AH20*TENPH/GAMMA(138)                              | WAT11900 |
|       | MI(139)=KT(217)*(AH20*TENPH)**2/GAMMA(139)                         | WAT11910 |
|       | MI(140)=KT(218)*(AH20*TENPH)**3/GAMMA(140)                         | WAT11920 |
|       | MI(141)=KT(219)*(AH20*TENPH)**4/GAMMA(141)                         | WAT11930 |
|       | MI(142)=KT(220)*MI(130)*GAMMA(130)*(AH20*TENPH)**2/GAMMA(142)      | WAT11940 |
|       | MI(143)=KT(221)*ALFA(5)/GAMMA(143)                                 | WAT11950 |
|       | MI(144)=KT(222)*ALFA(66)**3/GAMMA(144)                             | WAT11960 |
|       | MI(271)=KT(510)*ALFA(6)/GAMMA(271)                                 | WAT11970 |

|        |                                                               |          |
|--------|---------------------------------------------------------------|----------|
|        | MI(290)=KT(527)*ALFA(284)/GAMMA(290)                          | WAT11980 |
|        | MI(291)=KT(528)*ALFA(285)/GAMMA(291)                          | WAT11990 |
| C      |                                                               | WAT12000 |
|        | MI(130)=CUTOT/(1.+GAMMA(130)*(MI(127)+MI(128)+MI(129)+MI(131) | WAT12010 |
|        | *+MI(132)+MI(133)+MI(134)+MI(135)+MI(136)+MI(137)             | WAT12020 |
|        | *+MI(138)+MI(139)+MI(140)+MI(141)+2.*MI(142)+MI(143)          | WAT12030 |
|        | *+MI(144)+MI(259)+MI(260)+MI(271)+MI(290)+MI(291)))           | WAT12040 |
|        | C1 = MI(130) * GAMMA(130)                                     | WAT12050 |
|        | ALFA(130) = C1                                                | WAT12060 |
| C      |                                                               | WAT12070 |
|        | DO 70 J = 2 , 23                                              | WAT12080 |
|        | I = LISTE1(J)                                                 | WAT12090 |
|        | MI(I) = C1 * MI(I)                                            | WAT12100 |
|        | ALFA(I) = MI(I) * GAMMA(I)                                    | WAT12110 |
|        | 70 CONTINUE                                                   | WAT12120 |
|        | GOTO 100                                                      | WAT12130 |
| C      |                                                               | WAT12140 |
|        | 80 DO 90 J = 1 , 23                                           | WAT12150 |
|        | I = LISTE1(J)                                                 | WAT12160 |
|        | MI(I) = 0.0                                                   | WAT12170 |
|        | 90 CONTINUE                                                   | WAT12180 |
| C      |                                                               | WAT12190 |
| C***** | ZN SPECIES */                                                 | WAT12200 |
| C      |                                                               | WAT12210 |
|        | 100 IF (ZNTOT .LE. 0.0) GOTO 120                              | WAT12220 |
|        | MI(146)=KT(251)*ALFA(4)/GAMMA(146)                            | WAT12230 |
|        | MI(147)=KT(252)*ALFA(4)**2/GAMMA(147)                         | WAT12240 |
|        | MI(148)=KT(253)*ALFA(4)**3/GAMMA(148)                         | WAT12250 |
|        | MI(149)=KT(254)*ALFA(4)**4/GAMMA(149)                         | WAT12260 |
|        | MI(150)=KT(255)*ALFA(61)/GAMMA(150)                           | WAT12270 |
|        | MI(151)=KT(256)*AH2O*TENPH/GAMMA(151)                         | WAT12280 |
|        | MI(152)=KT(257)*(AH2O*TENPH)**2/GAMMA(152)                    | WAT12290 |
|        | MI(153)=KT(258)*(AH2O*TENPH)**3/GAMMA(153)                    | WAT12300 |
|        | MI(154)=KT(259)*(AH2O*TENPH)**4/GAMMA(154)                    | WAT12310 |
|        | MI(155)=KT(260)*AH2O*TENPH*ALFA(4)/GAMMA(155)                 | WAT12320 |
|        | MI(156)=KT(261)*ALFA(66)**2/GAMMA(156)                        | WAT12330 |
|        | MI(157)=KT(262)*ALFA(66)**3/GAMMA(157)                        | WAT12340 |
|        | MI(158)=KT(263)*ALFA(5)/GAMMA(158)                            | WAT12350 |
|        | MI(159)=KT(264)*ALFA(5)**2/GAMMA(159)                         | WAT12360 |
|        | MI(229)=KT(447)*ALFA(97)/GAMMA(229)                           | WAT12370 |
|        | MI(230)=KT(448)*ALFA(97)**2/GAMMA(230)                        | WAT12380 |
|        | MI(231)=KT(449)*ALFA(96)/GAMMA(231)                           | WAT12390 |
|        | MI(232)=KT(450)*ALFA(96)**2/GAMMA(232)                        | WAT12400 |
|        | MI(272)=KT(511)*ALFA(6)/GAMMA(272)                            | WAT12410 |
|        | MI(273)=KT(512)*ALFA(17)/GAMMA(273)                           | WAT12420 |
|        | MI(274)=KT(513)*ALFA(17)**2/GAMMA(274)                        | WAT12430 |
|        | MI(145)=ZNTOT/(1+GAMMA(145)*(MI(146)+MI(147)+MI(148)+MI(149)+ | WAT12440 |
| C      |                                                               | WAT12450 |
|        | *MI(150)+MI(151)+MI(152)+MI(153)+MI(154)+MI(155)+MI(156)      | WAT12460 |
|        | *+MI(157)+MI(158)+MI(159)+MI(229)+MI(230)+MI(231)             | WAT12470 |
|        | *+MI(232)+MI(272)+MI(273)+MI(274)))                           | WAT12480 |
|        | C1 = MI(145) * GAMMA(145)                                     | WAT12490 |
|        | ALFA(145)= C1                                                 | WAT12500 |
| C      |                                                               | WAT12510 |

|                                                                   |          |
|-------------------------------------------------------------------|----------|
| DO 110 J = 2 , 22                                                 | WAT12520 |
| I = LISTE2(J)                                                     | WAT12530 |
| MI(I) = C1 * MI(I)                                                | WAT12540 |
| ALFA(I) = MI(I) * GAMMA(I)                                        | WAT12550 |
| 110 CONTINUE                                                      | WAT12560 |
| GOTO 140                                                          | WAT12570 |
| C                                                                 | WAT12580 |
| 120 DO 130 J = 1 , 22                                             | WAT12590 |
| I = LISTE2(J)                                                     | WAT12600 |
| MI(I) = 0.0                                                       | WAT12610 |
| 130 CONTINUE                                                      | WAT12620 |
| C                                                                 | WAT12630 |
| C**** CD SPECIES */                                               | WAT12640 |
| C                                                                 | WAT12650 |
| 140 IF (CDTOT .LE. 0.0) GOTO 175                                  | WAT12660 |
| MI(161)=KT(294)*ALFA(4)/GAMMA(161)                                | WAT12670 |
| MI(162)=KT(295)*ALFA(4)**2/GAMMA(162)                             | WAT12680 |
| MI(163)=KT(296)*ALFA(4)**3/GAMMA(163)                             | WAT12690 |
| MI(164)=KT(297)*ALFA(61)/GAMMA(164)                               | WAT12700 |
| MI(165)=KT(298)*ALFA(61)**2/GAMMA(165)                            | WAT12710 |
| MI(166)=KT(299)*ALFA(17)**3/GAMMA(166)                            | WAT12720 |
| MI(167)=KT(300)*AH2O*TENPH/GAMMA(167)                             | WAT12730 |
| MI(168)=KT(301)*(AH2O*TENPH)**2/GAMMA(168)                        | WAT12740 |
| MI(169)=KT(302)*(AH2O*TENPH)**3/GAMMA(169)                        | WAT12750 |
| MI(170)=KT(303)*(AH2O*TENPH)**4/GAMMA(170)                        | WAT12760 |
| MI(171)=KT(304)*MI(160)*GAMMA(160)*AH2O*TENPH/GAMMA(171)          | WAT12770 |
| MI(172)=KT(305)*AH2O*TENPH*ALFA(4)/GAMMA(172)                     | WAT12780 |
| MI(173)=KT(306)*ALFA(84)/GAMMA(173)                               | WAT12790 |
| MI(174)=KT(307)*ALFA(5)/GAMMA(174)                                | WAT12800 |
| MI(175)=KT(308)*ALFA(66)/GAMMA(175)                               | WAT12810 |
| MI(176)=KT(309)*ALFA(66)**2/GAMMA(176)                            | WAT12820 |
| MI(177)=KT(310)*ALFA(66)**3/GAMMA(177)                            | WAT12830 |
| C                                                                 | WAT12840 |
| IF (ALFA(66) .LE. 0.0) GOTO 150                                   | WAT12850 |
| XMI178 = LOGKT(311) + 4E0 * DLOG10(ALFA(66)) - DLOG10(GAMMA(178)) | WAT12860 |
| IF (XMI178 .GT. -70) MI(178) = 10**XMI178                         | WAT12870 |
| GOTO 160                                                          | WAT12880 |
| 150 MI(178) = 0.0                                                 | WAT12890 |
| 160 MI(233)=KT(451)*ALFA(97)/GAMMA(233)                           | WAT12900 |
| MI(234)=KT(452)*ALFA(97)**2/GAMMA(234)                            | WAT12910 |
| MI(235)=KT(453)*ALFA(96)/GAMMA(235)                               | WAT12920 |
| MI(236)=KT(454)*ALFA(96)**2/GAMMA(236)                            | WAT12930 |
| MI(275)=KT(514)*ALFA(6)/GAMMA(275)                                | WAT12940 |
| MI(276)=KT(515)*ALFA(17)/GAMMA(276)                               | WAT12950 |
| MI(277)=KT(516)*ALFA(5)**2/GAMMA(277)                             | WAT12960 |
| MI(292)=KT(529)*ALFA(284)/GAMMA(292)                              | WAT12970 |
| MI(293)=KT(530)*ALFA(285)/GAMMA(293)                              | WAT12980 |
| C                                                                 | WAT12990 |
| MI(160)=CDTOT/(1+GAMMA(160)*(MI(161)+MI(162)+MI(163)+MI(164)+     | WAT13000 |
| *MI(165)+MI(166)+MI(167)+MI(168)+MI(169)+MI(170)+2*MI(171)        | WAT13010 |
| *+MI(172)+MI(173)+MI(174)+MI(175)+MI(176)+MI(177)+                | WAT13020 |
| *MI(178)+MI(233)+MI(234)+MI(235)+MI(236)+MI(275)+MI(276)+         | WAT13030 |
| *MI(277)+MI(292)+MI(293))                                         | WAT13040 |
| C1=MI(160)*GAMMA(160)                                             | WAT13050 |

|       |                                                                    |          |
|-------|--------------------------------------------------------------------|----------|
|       | ALFA(160) = C1                                                     | WAT13060 |
| C     |                                                                    | WAT13070 |
|       | DO 170J = 2 , 28                                                   | WAT13080 |
|       | I = LISTE3(J)                                                      | WAT13090 |
|       | MI(I) = C1 * MI(I)                                                 | WAT13100 |
|       | ALFA(I) = MI(I) * GAMMA(I)                                         | WAT13110 |
|       | 170 CONTINUE                                                       | WAT13120 |
|       | GOTO 190                                                           | WAT13130 |
| C     |                                                                    | WAT13140 |
|       | 175 DO 180 J = 1 , 28                                              | WAT13150 |
|       | I = LISTE3(J)                                                      | WAT13160 |
|       | MI(I) = 0.0                                                        | WAT13170 |
|       | 180 CONTINUE                                                       | WAT13180 |
| C     |                                                                    | WAT13190 |
| C**** | PB SPECIES */                                                      | WAT13200 |
| C     |                                                                    | WAT13210 |
|       | 190 IF (PBTOT .LE. 0.0) GOTO 210                                   | WAT13220 |
|       | MI(183)=KT(341)*ALFA(4)/GAMMA(183)                                 | WAT13230 |
|       | MI(184)=KT(342)*ALFA(4)**2/GAMMA(184)                              | WAT13240 |
|       | MI(185)=KT(343)*ALFA(4)**3/GAMMA(185)                              | WAT13250 |
|       | MI(186)=KT(344)*ALFA(4)**4/GAMMA(186)                              | WAT13260 |
|       | MI(187)=KT(345)*ALFA(17)**2/GAMMA(187)                             | WAT13270 |
|       | MI(188)=KT(346)*ALFA(61)/GAMMA(188)                                | WAT13280 |
|       | MI(189)=KT(347)*ALFA(61)**2/GAMMA(189)                             | WAT13290 |
|       | MI(190)=KT(348)*ALFA(61)**3/GAMMA(190)                             | WAT13300 |
|       | MI(191)=KT(349)*ALFA(61)**4/GAMMA(191)                             | WAT13310 |
|       | MI(192)=KT(350)*AH2O*TENPH/GAMMA(192)                              | WAT13320 |
|       | MI(193)=KT(351)*(AH2O*TENPH)**2/GAMMA(193)                         | WAT13330 |
|       | MI(194)=KT(352)*(AH2O*TENPH)**3/GAMMA(194)                         | WAT13340 |
|       | MI(195)=KT(353)*AH2O*TENPH*MI(182)*GAMMA(182)/GAMMA(195)           | WAT13350 |
|       | MI(196)=KT(354)*ALFA(84)/GAMMA(196)                                | WAT13360 |
|       | MI(197)=KT(355)*ALFA(5)/GAMMA(197)                                 | WAT13370 |
|       | MI(198)=KT(356)*ALFA(66)**2/GAMMA(198)                             | WAT13380 |
|       | MI(199)=KT(357)*ALFA(66)**3/GAMMA(199)                             | WAT13390 |
|       | MI(200)=KT(358)*(MI(182)*GAMMA(182))**2*(AH2O*TENPH)**4/GAMMA(200) | WAT13400 |
|       | MI(237)=KT(455)*ALFA(97)/GAMMA(237)                                | WAT13410 |
|       | MI(238)=KT(456)*ALFA(97)**2/GAMMA(238)                             | WAT13420 |
|       | MI(239)=KT(457)*ALFA(96)/GAMMA(239)                                | WAT13430 |
|       | MI(240)=KT(458)*ALFA(96)**2/GAMMA(240)                             | WAT13440 |
|       | MI(241)=KT(468)*ALFA(17)/GAMMA(241)                                | WAT13450 |
|       | MI(242)=KT(469)*(AH2O*TENPH)**4/GAMMA(242)                         | WAT13460 |
|       | MI(243)=KT(470)*ALFA(5)**2/GAMMA(243)                              | WAT13470 |
|       | MI(278)=KT(517)*ALFA(6)/GAMMA(278)                                 | WAT13480 |
| C     |                                                                    | WAT13490 |
|       | MI(182)=PBTOT/(1+GAMMA(182)*(MI(183)+MI(184)+MI(185)+MI(186)+      | WAT13500 |
|       | *MI(187)+MI(188)+MI(189)+MI(190)+MI(191)+MI(192)+MI(193)+          | WAT13510 |
|       | *MI(194)+2*MI(195)+MI(196)+MI(197)+MI(198)+MI(199)+3*MI(200)+      | WAT13520 |
|       | *MI(237)+MI(238)+MI(239)+MI(240)+MI(241)+MI(242)+                  | WAT13530 |
|       | *MI(243)+MI(278)))                                                 | WAT13540 |
|       | C1 = MI(182) * GAMMA(182)                                          | WAT13550 |
|       | ALFA(182) = C1                                                     | WAT13560 |
| C     |                                                                    | WAT13570 |
|       | DO 200 J = 2 , 27                                                  | WAT13580 |
|       | I = LISTE4(J)                                                      | WAT13590 |



|                                                               |          |
|---------------------------------------------------------------|----------|
| MI(I) = C1 * MI(I)                                            | WAT13600 |
| ALFA(I) = MI(I) * GAMMA(I)                                    | WAT13610 |
| 200 CONTINUE                                                  | WAT13620 |
| GOTO 230                                                      | WAT13630 |
| C                                                             | WAT13640 |
| 210 DO 220 J = 1 , 27                                         | WAT13650 |
| I = LISTE4(J)                                                 | WAT13660 |
| MI(I) = 0.0                                                   | WAT13670 |
| 220 CONTINUE                                                  | WAT13680 |
| C                                                             | WAT13690 |
| C***** NI SPECIES */                                          | WAT13700 |
| C                                                             | WAT13710 |
| 230 IF (NITOT .LE. 0.0) GOTO 250                              | WAT13720 |
| MI(205)=KT(403)*ALFA(97)/GAMMA(205)                           | WAT13730 |
| MI(206)=KT(404)*ALFA(4)/GAMMA(206)                            | WAT13740 |
| MI(207)=KT(405)*ALFA(61)/GAMMA(207)                           | WAT13750 |
| MI(208)=KT(406)*AH2O*TENPH/GAMMA(208)                         | WAT13760 |
| MI(209)=KT(407)*(AH2O*TENPH)**2/GAMMA(209)                    | WAT13770 |
| MI(210)=KT(408)*(AH2O*TENPH)**3/GAMMA(210)                    | WAT13780 |
| MI(211)=KT(409)*ALFA(5)/GAMMA(211)                            | WAT13790 |
| MI(279)=KT(518)*ALFA(4)**2/GAMMA(279)                         | WAT13800 |
| MI(280)=KT(519)*ALFA(6)/GAMMA(280)                            | WAT13810 |
| MI(281)=KT(520)*ALFA(17)/GAMMA(281)                           | WAT13820 |
| MI(282)=KT(521)*ALFA(17)**2/GAMMA(282)                        | WAT13830 |
| MI(283)=KT(522)*ALFA(5)**2/GAMMA(283)                         | WAT13840 |
| MI(204)=NITOT/(1+GAMMA(204)*(MI(205)+MI(206)+MI(207)+MI(208)+ | WAT13850 |
| *MI(209)+MI(210)+MI(211)+MI(279)+MI(280)+MI(281)+MI(282)+     | WAT13860 |
| *MI(283)))                                                    | WAT13870 |
| C1 = MI(204) * GAMMA(204)                                     | WAT13880 |
| ALFA(204)= C1                                                 | WAT13890 |
| C                                                             | WAT13900 |
| DO 240J = 2 , 13                                              | WAT13910 |
| I = LISTE5(J)                                                 | WAT13920 |
| MI(I) = C1 * MI(I)                                            | WAT13930 |
| ALFA(I) = MI(I) * GAMMA(I)                                    | WAT13940 |
| 240 CONTINUE                                                  | WAT13950 |
| GOTO 270                                                      | WAT13960 |
| C                                                             | WAT13970 |
| 250 DO 260 J = 1 , 13                                         | WAT13980 |
| I = LISTE5(J)                                                 | WAT13990 |
| MI(I) = 0.0                                                   | WAT14000 |
| 260 CONTINUE                                                  | WAT14010 |
| C                                                             | WAT14020 |
| C***** AG SPECIES */                                          | WAT14030 |
| C                                                             | WAT14040 |
| 270 IF (AGTOT .LE. 0.0) GOTO 290                              | WAT14050 |
| MI(213)=KT(421)*ALFA(97)/GAMMA(213)                           | WAT14060 |
| MI(214)=KT(422)*ALFA(97)**2/GAMMA(214)                        | WAT14070 |
| MI(215)=KT(423)*ALFA(4)/GAMMA(215)                            | WAT14080 |
| MI(216)=KT(424)*ALFA(4)**2/GAMMA(216)                         | WAT14090 |
| MI(217)=KT(425)*ALFA(4)**3/GAMMA(217)                         | WAT14100 |
| MI(218)=KT(426)*ALFA(4)**4/GAMMA(218)                         | WAT14110 |
| MI(219)=KT(427)*ALFA(61)/GAMMA(219)                           | WAT14120 |
| MI(220)=KT(428)*ALFA(66)/GAMMA(220)                           | WAT14130 |



|                                                               |          |
|---------------------------------------------------------------|----------|
| MI(221)=KT(429)*ALFA(66)**2/GAMMA(221)                        | WAT14140 |
| MI(222)=KT(430)*ALFA(96)/GAMMA(222)                           | WAT14150 |
| MI(223)=KT(431)*ALFA(96)**2/GAMMA(223)                        | WAT14160 |
| MI(224)=KT(432)*AH2O*TENPH/GAMMA(224)                         | WAT14170 |
| MI(225)=KT(433)*(AH2O*TENPH)**2/GAMMA(225)                    | WAT14180 |
| MI(226)=KT(434)*ALFA(5)/GAMMA(226)                            | WAT14190 |
| MI(227)=KT(435)*ALFA(84)/GAMMA(227)                           | WAT14200 |
| MI(228)=KT(436)*ALFA(202)**2/GAMMA(228)                       | WAT14210 |
| MI(244)=KT(473)*ALFA(97)**3/GAMMA(244)                        | WAT14220 |
| MI(245)=KT(474)*ALFA(96)**3/GAMMA(245)                        | WAT14230 |
| MI(246)=KT(475)*ALFA(96)**4/GAMMA(246)                        | WAT14240 |
| MI(268)=KT(507)*(ALFA(66)*TENPH)**2/GAMMA(268)                | WAT14250 |
| MI(269)=KT(508)*(ALFA(66)*TENPH)**2/GAMMA(269)                | WAT14260 |
| MI(270)=KT(509)*ALFA(66)**2*TENPH/GAMMA(270)                  | WAT14270 |
| MI(294)=KT(531)*ALFA(284)/GAMMA(294)                          | WAT14280 |
| MI(295)=KT(532)*ALFA(285)/GAMMA(295)                          | WAT14290 |
| C                                                             | WAT14300 |
| MI(212)=AGTOT/(1+GAMMA(212)*(MI(213)+MI(214)+MI(215)+MI(216)+ | WAT14310 |
| *MI(217)+MI(218)+MI(219)+MI(220)+MI(221)+MI(222)+MI(223)+     | WAT14320 |
| *MI(224)+MI(225)+MI(226)+MI(227)+MI(228)+MI(244)+MI(245)+     | WAT14330 |
| *MI(246)+MI(268)+MI(269)+MI(270)+MI(294)+MI(295)))            | WAT14340 |
| C1 = MI(212) * GAMMA(212)                                     | WAT14350 |
| ALFA(212) = C1                                                | WAT14360 |
| C                                                             | WAT14370 |
| DO 280 J = 2 , 25                                             | WAT14380 |
| I = LISTE6(J)                                                 | WAT14390 |
| MI(I) = C1 * MI(I)                                            | WAT14400 |
| ALFA(I) = MI(I) * GAMMA(I)                                    | WAT14410 |
| 280 CONTINUE                                                  | WAT14420 |
| GOTO 310                                                      | WAT14430 |
| C                                                             | WAT14440 |
| 290 DO 300 J = 1 , 25                                         | WAT14450 |
| I = LISTE6(J)                                                 | WAT14460 |
| MI(I) = 0.0                                                   | WAT14470 |
| 300 CONTINUE                                                  | WAT14480 |
| C                                                             | WAT14490 |
| C***** AS SPECIES */                                          | WAT14500 |
| C                                                             | WAT14510 |
| 310 IF (AS3TOT + AS5TOT .GT. 0.0) GOTO 420                    | WAT14520 |
| IF (EHM .LT. 9.9 .AND. ASTOTL .GT. 0.0) GOTO 420              | WAT14530 |
| GOTO 370                                                      | WAT14540 |
| 420 MI(251)=KT(478)*TENPH/GAMMA(251)                          | WAT14550 |
| MI(252)=KT(479)*TENPH**2/GAMMA(252)                           | WAT14560 |
| MI(253)=KT(480)*TENPH**3/GAMMA(253)                           | WAT14570 |
| MI(254)=KT(481)/(TENPH*GAMMA(254))                            | WAT14580 |
| MI(256)=KT(482)*TENPH/GAMMA(256)                              | WAT14590 |
| MI(257)=KT(483)*TENPH**2/GAMMA(257)                           | WAT14600 |
| MI(258)=KT(484)*TENPH**3/GAMMA(258)                           | WAT14610 |
| IF (AS3TOT + AS5TOT .LE. 0.0) GOTO320                         | WAT14620 |
| C                                                             | WAT14630 |
| C SPLIT-ARSENIC                                               | WAT14640 |
| C                                                             | WAT14650 |
| C***** AS +3 SPECIES */                                       | WAT14660 |
| C                                                             | WAT14670 |

|                                                                 |          |
|-----------------------------------------------------------------|----------|
| MI(250) = AS3TOT/(1E0 + GAMMA(250) * (MI(251) + MI(252) +       | WAT14680 |
| *MI(253) + MI(254)))                                            | WAT14690 |
| C1 = MI(250) * GAMMA(250)                                       | WAT14700 |
| ALFA(250) = C1                                                  | WAT14710 |
| DO 400 I = 251 , 254                                            | WAT14720 |
| MI(I) = C1 * MI(I)                                              | WAT14730 |
| 400 CONTINUE                                                    | WAT14740 |
| C                                                               | WAT14750 |
| C***** AS +5 SPECIES */                                         | WAT14760 |
| C                                                               | WAT14770 |
| MI(255) = AS5TOT/ (1E0 + GAMMA(255) * (MI(256) + MI(257) +      | WAT14780 |
| *MI(258)))                                                      | WAT14790 |
| C1 = MI(255) * GAMMA(255)                                       | WAT14800 |
| ALFA(255) = C1                                                  | WAT14810 |
| DO 410 I = 256 , 258                                            | WAT14820 |
| MI(I) = C1 * MI(I)                                              | WAT14830 |
| 410 CONTINUE                                                    | WAT14840 |
| GOTO 350                                                        | WAT14850 |
| C                                                               | WAT14860 |
| C                                                               | WAT14870 |
| C                                                               | WAT14880 |
| 320 MI(255) = 1.0 / GAMMA(255)                                  | WAT14890 |
| C1 = KT(487) * AH2O * TENPH**2 / TENMPE**2                      | WAT14900 |
| DO 330 I = 255 , 258                                            | WAT14910 |
| MI(I) = C1 * MI(I)                                              | WAT14920 |
| 330 CONTINUE                                                    | WAT14930 |
| MI(250)=ASTOTL/(1E0 + GAMMA(250)*(MI(251)+MI(252)+MI(253)+      | WAT14940 |
| *MI(254)+MI(255)+MI(256)+MI(257)+MI(258)))                      | WAT14950 |
| C1 = MI(250) * GAMMA(250)                                       | WAT14960 |
| ALFA(250) = C1                                                  | WAT14970 |
| DO 340 I = 251 , 258                                            | WAT14980 |
| MI(I) = C1 * MI(I)                                              | WAT14990 |
| 340 CONTINUE                                                    | WAT15000 |
| ALFA(255) = MI(255) * GAMMA(255)                                | WAT15010 |
| C                                                               | WAT15020 |
| 350 ALFA(251) = MI(251) * GAMMA(251)                            | WAT15030 |
| ALFA(252) = MI(252) * GAMMA(252)                                | WAT15040 |
| ALFA(253) = MI(253) * GAMMA(253)                                | WAT15050 |
| ALFA(254) = MI(254) * GAMMA(254)                                | WAT15060 |
| ALFA(256) = MI(256) * GAMMA(256)                                | WAT15070 |
| ALFA(257) = MI(257) * GAMMA(257)                                | WAT15080 |
| ALFA(258) = MI(258) * GAMMA(258)                                | WAT15090 |
| GOTO 390                                                        | WAT15100 |
| 370 DO 380 I = 250 , 258                                        | WAT15110 |
| MI(I) = 0.0                                                     | WAT15120 |
| 380 CONTINUE                                                    | WAT15130 |
| 390 RETURN                                                      | WAT15140 |
| END                                                             | WAT15150 |
| SUBROUTINE SUMS(ALFA,GAMMA,KT,MI)                               | WAT15200 |
| C                                                               | WAT15210 |
| REAL*8 ALFA(0:297),GAMMA(0:297),KT(0:543),MI(0:297)             | WAT15220 |
| REAL*8 ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT       | WAT15230 |
| REAL*8 S1,S2,S3,S4,S5,S6,S7,S8,M1,M2,M3,M4,M5,M6,M7,M8          | WAT15240 |
| INTEGER LISTE1(26),LISTE2(28),LISTE3(29),LISTE4(14),LISTE5(31), | WAT15250 |

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*LISTE6(25)
CHARACTER*80 CARD1,CARD2
C
REAL*8 ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT,
*MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3
INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA,
*ITER,NMBR,PUNCH,RBIT,FLAG
C
COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B,
*BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND,
*CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF,
*DISCHG,DOC,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT,
*EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,
*FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,
*ITDS,ITER,K,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL,
*NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE,
*PEAS,PEDO,PEDO2,PEFE,PEN,PENO2,PEPT,PES,PH,PRNT,PTOT,PUNCH,R,
*RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,
*T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT
COMMON/CHRDAT/CARD1,CARD2
C
DATA LISTE1/6,20,21,29,30,41,42,68,85,95,119,131,132,166,187,241,
* 271,272,273,274,275,276,278,280,281,282/
DATA LISTE2/14,22,31,33,43,45,58,59,62,81,82,91,108,117,122,123,
*143,158,159,174,197,201,203,211,226,243,277,283/
DATA LISTE3/19,54,55,56,57,100,101,102,103,104,105,106,107,116,
*124,125,126,137,150,164,165,188,189,190,191,207,219,296,297/
DATA LISTE4/12,39,40,46,47,49,60,64,72,73,74,75,98,99/
DATA LISTE5/15,27,32,111,112,113,128,129,133,134,135,136,146,147,
*148,149,155,161,162,163,172,183,184,185,186,206,215,216,217,
*218,279/
DATA LISTE6/13,67,247,248,144,156,157,175,176,177,178,198,199,
*220,221,259,260,263,264,265,266,267,268,269,270/
C
C***** SUMMATION OF ANION SPECIES */
C
C***** HCO3
C
M1 = MI(6)
IF (CORALK.NE.2) GOTO 10
S1 = MI(17) + MI(20) + MI(21) + MI(29)
*+ MI(30) + MI(41) + MI(42) + MI(85)
*+ MI(68) + MI(95)
*+ 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)
GOTO 20
10 S1 = 2. * MI(17) + 2. * MI(20) + MI(21) + MI(29)
*+ 2. * MI(30) + 2. * MI(41) + MI(42) + MI(119)
*+ MI(68) + 2. * MI(95)
*+ 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)

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|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <pre>           *+      MI(280) + 2. * MI(281) + 4. * MI(282) C C***** S04 C       20 M2 = MI(5)           S2 =      MI(14) +      MI(22) +      MI(31) +      MI(43)           *+      MI(45) +      MI(58) + 2. * MI(59) +      MI(62)           *+      MI(81) +      MI(82) +      MI(91) +      MI(33)           *+      MI(117) +      MI(122) +      MI(123) +      MI(143)           *+ 2. * MI(108) +      MI(158) + 2. * MI(159) +      MI(174)           *+      MI(197) +      MI(201) +      MI(203) +      MI(211)           *+      MI(226) + 2. * MI(243) + 2. * MI(277) + 2. * MI(283) C C***** F C           M3 = MI(61)           S3 =      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) C C***** PO4 C           M4 = MI(44)           S4 =      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) C C***** CL C           M5 = MI(4)           S5 =      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) +      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) C C***** H2S C           M6 = MI(13)           S6 =      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) </pre> | <pre> WAT15770 WAT15780 WAT15790 WAT15800 WAT15810 WAT15820 WAT15830 WAT15840 WAT15850 WAT15860 WAT15870 WAT15880 WAT15890 WAT15900 WAT15910 WAT15920 WAT15930 WAT15940 WAT15950 WAT15960 WAT15970 WAT15980 WAT15990 WAT16000 WAT16010 WAT16020 WAT16030 WAT16040 WAT16050 WAT16060 WAT16070 WAT16080 WAT16090 WAT16100 WAT16110 WAT16120 WAT16130 WAT16140 WAT16150 WAT16160 WAT16170 WAT16180 WAT16190 WAT16200 WAT16210 WAT16220 WAT16230 WAT16240 WAT16250 WAT16260 WAT16270 WAT16280 </pre> |
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      *+ 2. * MI(270)
C
C***** FULVATE
C
      M7 = MI(284)
      S7 = MI(286) + MI(288) + MI(290) + MI(292) + MI(294)
C
C***** HUMATE
C
      M8 = MI(285)
      S8 = MI(287) + MI(289) + MI(291) + MI(293) + MI(295)
C
C***** ANION MASS BALANCE CALCULATIONS */
C
C***** MASS BALANCE ON CARBON */
C
      IF (CO2TIT .LE. 0.0) GOTO 60
      MI(6) = KT(68) / (TENPH * GAMMA(6))
      MI(20) = KT(73) * ALFA(1) / GAMMA(20)
      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(68) = KT(79) * KT(68) * ALFA(87) / (TENPH * GAMMA(68))
      MI(85) = KT(35) * KT(68) / (TENPH**2 * GAMMA(85))
      MI(95) = KT(135) * ALFA(87) / GAMMA(95)
      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(160) / (TENPH * GAMMA(275))
      MI(276) = KT(515) * ALFA(160) / GAMMA(276)
      MI(278) = KT(517) * KT(68) * ALFA(182) / (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)
C
      IF (CORALK .NE. 2) GOTO 30
      MI(17) = ANLCO3 / (1.0 + GAMMA(17) * (MI(6) + MI(20)
      *+ MI(21) + MI(29) + MI(30) + MI(41) + MI(42) + MI(68) + MI(85)
      *+ MI(95) + 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)))
      GOTO 40
C
30 NONCRB = MI(24) + 2. * MI(25) + MI(26) + MI(36) + 2. * MI(44)

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WAT16290  
 WAT16300  
 WAT16310  
 WAT16320  
 WAT16330  
 WAT16340  
 WAT16350  
 WAT16360  
 WAT16370  
 WAT16380  
 WAT16390  
 WAT16400  
 WAT16410  
 WAT16420  
 WAT16430  
 WAT16440  
 WAT16450  
 WAT16460  
 WAT16470  
 WAT16480  
 WAT16490  
 WAT16500  
 WAT16510  
 WAT16520  
 WAT16530  
 WAT16540  
 WAT16550  
 WAT16560  
 WAT16570  
 WAT16580  
 WAT16590  
 WAT16600  
 WAT16610  
 WAT16620  
 WAT16630  
 WAT16640  
 WAT16650  
 WAT16660  
 WAT16670  
 WAT16680  
 WAT16690  
 WAT16700  
 WAT16710  
 WAT16720  
 WAT16730  
 WAT16740  
 WAT16750  
 WAT16760  
 WAT16770  
 WAT16780  
 WAT16790  
 WAT16800



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      *+ MI(46) + MI(53) + MI(66) + 2. * MI(67) + MI(81)
      IF (CORALK .EQ. 0) ANLCO3 = CO2TIT - NONCRB
C
      MI(17) = ANLCO3 / (2.0 + GAMMA(17) * (MI(6) + 2. * MI(20)
      *+MI(21) + MI(29) + 2. * MI(30) + 2. * MI(41) + MI(42) + MI(119)
      *+MI(68) + 2. * MI(95)
      *+ 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)))
C
40 C1 = MI(17) * GAMMA(17)
   ALFA(17) = C1
   DO 50J = 1 ,26
   I = LISTEL(J)
   MI(I) = C1 * MI(I)
   ALFA(I) = MI(I) * GAMMA(I)
50 CONTINUE
C
C***** MASS BALANCE ON SULFATE */
C
60 IF (SO4TOT .LE. 0.0) GOTO 80
   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)
   MI(59) = KT(88) * ALFA(50) * ALFA(5) / GAMMA(59)
   MI(62) = KT(89) / (TENPH * GAMMA(62))
   MI(81) = KT(168) * KT(89) * ALFA(0) / (TENPH * GAMMA(81))
   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(122) = KT(148) * KT(89) * ALFA(7) / (TENPH * GAMMA(122))
   MI(123) = KT(159) * KT(89) * ALFA(8) / (TENPH * GAMMA(123))
   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(201) = KT(543) * ALFA(89) / GAMMA(201)
   MI(203) = KT(397) * KT(89) * ALFA(50) / (TENPH * GAMMA(203))
   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)
   MI(5)=SO4TOT/(1EO + GAMMA(5)*(MI(14)+MI(22)+MI(31)+MI(33)+MI(43)+
   *MI(45)+MI(58)+2.*MI(59)+MI(62)+MI(81)+MI(82)+MI(91)+2.*MI(108)+
   *MI(117)+MI(122)+MI(123)+MI(143)+MI(158)+2.*MI(159)+MI(174)+
   *MI(197)+MI(201)+MI(203)+MI(211)+MI(226)+2*MI(243)+

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|       |                                                                   |          |
|-------|-------------------------------------------------------------------|----------|
|       | *2.*MI(277)+2.*MI(283)))                                          |          |
|       | ALFA(5)=MI(5)*GAMMA(5)                                            |          |
|       | C1=ALFA(5)                                                        |          |
| C     |                                                                   | WAT17310 |
|       | DO 70 J = 1 , 28                                                  | WAT17320 |
|       | I = LISTE2(J)                                                     | WAT17330 |
|       | MI(I) = C1 * MI(I)                                                | WAT17340 |
|       | ALFA(I) = MI(I) * GAMMA(I)                                        | WAT17350 |
|       | 70 CONTINUE                                                       | WAT17360 |
| C     |                                                                   | WAT17370 |
| C**** | MASS BALANCE ON FLUORIDE */                                       | WAT17380 |
| C     |                                                                   | WAT17390 |
|       | 80 IF (FTOT .LE. 0.0) GOTO 100                                    | WAT17400 |
|       | MI(19)=KT(22)*ALFA(1)/GAMMA(19)                                   | WAT17410 |
|       | MI(54)=KT(83)*ALFA(50)/GAMMA(54)                                  | WAT17420 |
|       | MI(55)=KT(84)*ALFA(50)*ALFA(61)/GAMMA(55)                         | WAT17430 |
|       | MI(56)=KT(85)*ALFA(50)*ALFA(61)**2/GAMMA(56)                      | WAT17440 |
|       | MI(57)=KT(86)*ALFA(50)*ALFA(61)**3/GAMMA(57)                      | WAT17450 |
|       | MI(100)=KT(160)*ALFA(0)/GAMMA(100)                                | WAT17460 |
|       | MI(101)=KT(161)*ALFA(35)/GAMMA(101)                               | WAT17470 |
|       | MI(102)=KT(162)*ALFA(35)*ALFA(61)/(ALFA(26)*GAMMA(102))           | WAT17480 |
|       | MI(103)=KT(163)*ALFA(35)*ALFA(61)**2/(ALFA(26)**2*GAMMA(103))     | WAT17490 |
|       | MI(104)=KT(164)*ALFA(35)*ALFA(61)**3/(ALFA(26)**3*GAMMA(104))     | WAT17500 |
|       | MI(105)=KT(165)*ALFA(8)/GAMMA(105)                                | WAT17510 |
|       | MI(106)=KT(166)*ALFA(8)*ALFA(61)/GAMMA(106)                       | WAT17520 |
|       | MI(107)=KT(167)*ALFA(8)*ALFA(61)**2/GAMMA(107)                    | WAT17530 |
|       | MI(116)=KT(175)*ALFA(109)/GAMMA(116)                              | WAT17540 |
|       | MI(124)=KT(201)*ALFA(23)*ALFA(61)**5/((TENPH*AH2O)**4*GAMMA(124)) | WAT17550 |
|       | MI(125)=KT(202)/(TENPH*GAMMA(125))                                | WAT17560 |
|       | MI(126)=KT(203)*ALFA(61)/(TENPH*GAMMA(126))                       | WAT17570 |
|       | MI(137)=KT(215)*ALFA(130)/GAMMA(137)                              | WAT17580 |
|       | MI(150)=KT(255)*ALFA(145)/GAMMA(150)                              | WAT17590 |
|       | MI(164)=KT(297)*ALFA(160)/GAMMA(164)                              | WAT17600 |
|       | MI(165)=KT(298)*ALFA(160)*ALFA(61)/GAMMA(165)                     | WAT17610 |
|       | MI(188)=KT(346)*ALFA(182)/GAMMA(188)                              | WAT17620 |
|       | MI(189)=KT(347)*ALFA(182)*ALFA(61)/GAMMA(189)                     | WAT17630 |
|       | MI(190)=KT(348)*ALFA(182)*ALFA(61)**2/GAMMA(190)                  | WAT17640 |
|       | MI(191)=KT(349)*ALFA(182)*ALFA(61)**3/GAMMA(191)                  | WAT17650 |
|       | MI(207)=KT(405)*ALFA(204)/GAMMA(207)                              | WAT17660 |
|       | MI(219)=KT(427)*ALFA(212)/GAMMA(219)                              | WAT17670 |
|       | MI(296)=KT(537)*ALFA(61)/(TENPH**2*GAMMA(296))                    | WAT17680 |
|       | MI(297)=KT(540)*ALFA(2)/GAMMA(297)                                |          |
|       | MI(61)=FTOT/(1.+GAMMA(61)*(MI(19)+MI(54)+2.*MI(55)+3.*MI(56)+     | WAT17690 |
|       | *4.*MI(57)+MI(100)+MI(101)+2.*MI(102)+3.*MI(103)+4.*MI(104)+      | WAT17700 |
|       | *MI(105)+2.*MI(106)+3.*MI(107)+MI(116)+6.*MI(124)+MI(125)+        | WAT17710 |
|       | *2.*MI(126)+MI(137)+MI(150)+MI(164)+2.*MI(165)+MI(188)+           | WAT17720 |
|       | *2.*MI(189)+3.*MI(190)+4.*MI(191)+MI(207)+MI(219)+2.*MI(296)+     | WAT17730 |
|       | *MI(297)))                                                        |          |
|       | C1 = MI(61) * GAMMA(61)                                           | WAT17740 |
|       | ALFA(61) = C1                                                     | WAT17750 |
| C     |                                                                   | WAT17760 |
|       | DO 90 J = 1 , 29                                                  | WAT17770 |
|       | I = LISTE3(J)                                                     | WAT17780 |
|       | MI(I) = C1 * MI(I)                                                | WAT17790 |

|                                                                  |          |
|------------------------------------------------------------------|----------|
| ALFA(I) = MI(I) * GAMMA(I)                                       | WAT17800 |
| 90 CONTINUE                                                      | WAT17810 |
| C                                                                | WAT17820 |
| C**** MASS BALANCE ON PHOSPHATE */                               | WAT17830 |
| C                                                                | WAT17840 |
| 100 IF (PTOT .LE. 0.0) GOTO 120                                  | WAT17850 |
| MI(12)=KT(139)*KT(15)*ALFA(8)/(TENPH*GAMMA(12))                  | WAT17860 |
| MI(39)=KT(123)*ALFA(1)/GAMMA(39)                                 | WAT17870 |
| MI(40)=KT(124)*KT(16)*ALFA(1)/(TENPH**2*GAMMA(40))               | WAT17880 |
| MI(46)=KT(15)/(TENPH*GAMMA(46))                                  | WAT17890 |
| MI(47)=KT(16)/(TENPH**2*GAMMA(47))                               | WAT17900 |
| MI(49)=KT(30)*KT(15)*ALFA(2)/(TENPH*GAMMA(49))                   | WAT17910 |
| MI(60)=KT(32)*KT(15)*ALFA(3)/(TENPH*GAMMA(60))                   | WAT17920 |
| MI(64)=KT(120)*KT(16)*ALFA(7)/(TENPH**2*GAMMA(64))               | WAT17930 |
| MI(72)=KT(33)*KT(15)*ALFA(1)/(TENPH*GAMMA(72))                   | WAT17940 |
| MI(73)=KT(34)*KT(15)*ALFA(0)/(TENPH*GAMMA(73))                   | WAT17950 |
| MI(74)=KT(121)*ALFA(0)/GAMMA(74)                                 | WAT17960 |
| MI(75)=KT(122)*KT(16)*ALFA(0)/(TENPH**2*GAMMA(75))               | WAT17970 |
| MI(98)=KT(156)*KT(16)*ALFA(8)/(TENPH**2*GAMMA(98))               | WAT17980 |
| MI(99)=KT(138)*KT(15)*ALFA(7)/(TENPH*GAMMA(99))                  | WAT17990 |
| MI(44)=PTOT/(1. + GAMMA(44)*(MI(12)+MI(39)+MI(40)+MI(46)+MI(47)+ | WAT18000 |
| *MI(49)+MI(60)+MI(64)+MI(72)+MI(73)+MI(74)+MI(75)+MI(98)+        | WAT18010 |
| *MI(99))                                                         | WAT18020 |
| C1 = MI(44) * GAMMA(44)                                          | WAT18030 |
| ALFA(44) = C1                                                    | WAT18040 |
| C                                                                | WAT18050 |
| DO 110J = 1 , 14                                                 | WAT18060 |
| I = LISTE4(J)                                                    | WAT18070 |
| MI(I) = C1 * MI(I)                                               | WAT18080 |
| ALFA(I) = MI(I) * GAMMA(I)                                       | WAT18090 |
| 110 CONTINUE                                                     | WAT18100 |
| C                                                                | WAT18110 |
| C**** MASS BALANCE ON CHLORIDE */                                | WAT18120 |
| C                                                                | WAT18130 |
| 120 IF (CLTOT .LE. 0.0) GOTO 140                                 | WAT18140 |
| MI(15) = KT(5) * ALFA(8) / GAMMA(15)                             | WAT18150 |
| MI(27) = KT(6) * ALFA(8) * ALFA(4) / GAMMA(27)                   | WAT18160 |
| MI(32) = KT(7) * ALFA(8) * ALFA(4)**2 / GAMMA(32)                | WAT18170 |
| MI(111) = KT(170) * ALFA(109) / GAMMA(111)                       | WAT18180 |
| MI(112) = KT(171) * ALFA(109) * ALFA(4) / GAMMA(112)             | WAT18190 |
| MI(113) = KT(172) * ALFA(109) * ALFA(4)**2 / GAMMA(113)          | WAT18200 |
| MI(128) = (KT(206) / KT(208)) * ALFA(127) * ALFA(4) / GAMMA(128) | WAT18210 |
| MI(129) = (KT(207) / KT(208)) * ALFA(127)*ALFA(4)**2 /GAMMA(129) | WAT18220 |
| MI(133) = KT(211) * ALFA(130) / GAMMA(133)                       | WAT18230 |
| MI(134) = KT(212) * ALFA(130) * ALFA(4) / GAMMA(134)             | WAT18240 |
| MI(135) = KT(213) * ALFA(130) * ALFA(4)**2 / GAMMA(135)          | WAT18250 |
| MI(136) = KT(214) * ALFA(130) * ALFA(4)**3 / GAMMA(136)          | WAT18260 |
| MI(146) = KT(251) * ALFA(145) / GAMMA(146)                       | WAT18270 |
| MI(147) = KT(252) * ALFA(145) * ALFA(4) / GAMMA(147)             | WAT18280 |
| MI(148) = KT(253) * ALFA(145) * ALFA(4)**2 / GAMMA(148)          | WAT18290 |
| MI(149) = KT(254) * ALFA(145) * ALFA(4)**3 / GAMMA(149)          | WAT18300 |
| MI(155) = KT(260) * ALFA(145) * AH2O*TENPH / GAMMA(155)          | WAT18310 |
| MI(161) = KT(294) * ALFA(160) / GAMMA(161)                       | WAT18320 |
| MI(162) = KT(295) * ALFA(160) * ALFA(4) / GAMMA(162)             | WAT18330 |

|                                                                    |          |
|--------------------------------------------------------------------|----------|
| MI(163) = KT(296) * ALFA(160) * ALFA(4)**2 / GAMMA(163)            | WAT18340 |
| MI(172) = KT(305) * ALFA(160) * AH2O*TENPH / GAMMA(172)            | WAT18350 |
| MI(183) = KT(341) * ALFA(182) / GAMMA(183)                         | WAT18360 |
| MI(184) = KT(342) * ALFA(182) * ALFA(4) / GAMMA(184)               | WAT18370 |
| MI(185) = KT(343) * ALFA(182) * ALFA(4)**2 / GAMMA(185)            | WAT18380 |
| MI(186) = KT(344) * ALFA(182) * ALFA(4)**3 / GAMMA(186)            | WAT18390 |
| MI(206) = KT(404) * ALFA(204) / GAMMA(206)                         | WAT18400 |
| MI(215) = KT(423) * ALFA(212) / GAMMA(215)                         | WAT18410 |
| MI(216) = KT(424) * ALFA(212) * ALFA(4) / GAMMA(216)               | WAT18420 |
| MI(217) = KT(425) * ALFA(212) * ALFA(4)**2 / GAMMA(217)            | WAT18430 |
| MI(218) = KT(426) * ALFA(212) * ALFA(4)**3 / GAMMA(218)            | WAT18440 |
| MI(279) = KT(518) * ALFA(204) * ALFA(4) / GAMMA(279)               | WAT18450 |
| C                                                                  | WAT18460 |
| MI(4) = CLTOT/(1.0 + GAMMA(4) * (MI(15) +2.*MI(27) +3.*MI(32)      | WAT18470 |
| *+MI(111) +2.*MI(112) +3.*MI(113) +2.*MI(128) +3.*MI(129)+         | WAT18480 |
| *MI(133) +2.*MI(134) +3.*MI(135) +4.*MI(136) +MI(146) +2.*MI(147)+ | WAT18490 |
| *3.*MI(148) +4.*MI(149) +MI(155) +MI(161) +2.*MI(162) +3.*MI(163)+ | WAT18500 |
| *MI(172) +MI(183) +2.*MI(184) +3.*MI(185) +4.*MI(186) +MI(206)+    | WAT18510 |
| *MI(215) +2.*MI(216) +3.*MI(217) +4.*MI(218) +2.*MI(279)))         | WAT18520 |
| C                                                                  | WAT18530 |
| CL = MI(4) * GAMMA(4)                                              | WAT18540 |
| ALFA(4) = CL                                                       | WAT18550 |
| DO 130 J = 1 , 31                                                  | WAT18560 |
| I = LISTE5(J)                                                      | WAT18570 |
| MI(I) = CL * MI(I)                                                 | WAT18580 |
| ALFA(I) = MI(I) * GAMMA(I)                                         | WAT18590 |
| 130 CONTINUE                                                       | WAT18600 |
| C                                                                  | WAT18610 |
| C**** MASS BALANCE ON SULFIDE */                                   | WAT18620 |
| C                                                                  | WAT18630 |
| 140 IF (H2STOT .LE. 0.0) GOTO 160                                  | WAT18640 |
| MI(13)=1/(KT(91)*TENPH*GAMMA(13))                                  | WAT18650 |
| MI(67)=KT(92)*TENPH/GAMMA(67)                                      | WAT18660 |
| MI(247)=KT(476)*ALFA(7)*ALFA(66)/GAMMA(247)                        | WAT18670 |
| MI(248)=KT(477)*ALFA(7)*ALFA(66)**2/GAMMA(248)                     | WAT18680 |
| MI(144)=KT(222)*ALFA(130)*ALFA(66)**2/GAMMA(144)                   | WAT18690 |
| MI(156)=KT(261)*ALFA(145)*ALFA(66)/GAMMA(156)                      | WAT18700 |
| MI(157)=KT(262)*ALFA(145)*ALFA(66)**2/GAMMA(157)                   | WAT18710 |
| MI(175)=KT(308)*ALFA(160)/GAMMA(175)                               | WAT18720 |
| MI(176)=KT(309)*ALFA(160)*ALFA(66)/GAMMA(176)                      | WAT18730 |
| MI(177)=KT(310)*ALFA(160)*ALFA(66)**2/GAMMA(177)                   | WAT18740 |
| MI(178)=KT(311)*ALFA(160)*ALFA(66)**3/GAMMA(178)                   | WAT18750 |
| MI(198)=KT(356)*ALFA(182)*ALFA(66)/GAMMA(198)                      | WAT18760 |
| MI(199)=KT(357)*ALFA(182)*ALFA(66)**2/GAMMA(199)                   | WAT18770 |
| MI(220)=KT(428)*ALFA(212)/GAMMA(220)                               | WAT18780 |
| MI(221)=KT(429)*ALFA(212)*ALFA(66)/GAMMA(221)                      | WAT18790 |
| MI(259)=KT(485)*ALFA(127)*ALFA(66)*TENPH**2/GAMMA(259)/KT(208)     | WAT18800 |
| MI(260)=KT(486)*ALFA(127)*ALFA(66)*TENPH**2/GAMMA(260)/KT(208)     | WAT18810 |
| MI(263)=KT(502)*TENPH/GAMMA(263)                                   | WAT18820 |
| MI(264)=KT(503)*TENPH/GAMMA(264)                                   | WAT18830 |
| MI(265)=KT(504)*TENPH/GAMMA(265)                                   | WAT18840 |
| MI(266)=KT(505)*TENPH/GAMMA(266)                                   | WAT18850 |
| MI(267)=KT(506)*TENPH/GAMMA(267)                                   | WAT18860 |
| MI(268)=KT(507)*ALFA(212)*ALFA(66)*TENPH**2/GAMMA(268)             | WAT18870 |

|                                                                   |          |
|-------------------------------------------------------------------|----------|
| MI(269)=KT(508)*ALFA(212)*ALFA(66)*TENPH**2/GAMMA(269)            | WAT18880 |
| MI(270)=KT(509)*ALFA(212)*ALFA(66)*TENPH/GAMMA(270)               | WAT18890 |
| MI(66)=H2STOT/(1.+GAMMA(66)*(MI(13)+MI(67)+2.*MI(247)+3.*MI(248)+ | WAT18900 |
| *3.*MI(144)+2.*MI(156)+3.*MI(157)+MI(175)+2.*MI(176)+3.*MI(177)+  | WAT18910 |
| *4.*MI(178)+2.*MI(198)+3.*MI(199)+MI(220)+2.*MI(221)+2.*MI(259)+  | WAT18920 |
| *2.*MI(260)+MI(263)+MI(264)+MI(265)+MI(266)+MI(267)+              | WAT18930 |
| *2.*MI(268)+2.*MI(269)+2*MI(270))                                 | WAT18940 |
| C1 = MI(66) * GAMMA(66)                                           | WAT18950 |
| ALFA(66) = C1                                                     | WAT18960 |
| DO 150 J = 1 , 25                                                 | WAT18970 |
| I = LISTE6(J)                                                     | WAT18980 |
| MI(I) = C1 * MI(I)                                                | WAT18990 |
| ALFA(I) = MI(I) * GAMMA(I)                                        | WAT19000 |
| 150 CONTINUE                                                      | WAT19010 |
| C                                                                 | WAT19020 |
| C**** MASS BALANCE ON FULVATE */                                  | WAT19030 |
| C                                                                 | WAT19040 |
| 160 IF (FULVTT .LE. 0.0) GOTO 180                                 | WAT19050 |
| MI(286)=KT(523)/(TENPH*GAMMA(286))                                | WAT19060 |
| MI(288)=KT(525)*ALFA(8)/GAMMA(288)                                | WAT19070 |
| MI(290)=KT(527)*ALFA(130)/GAMMA(290)                              | WAT19080 |
| MI(292)=KT(529)*ALFA(160)/GAMMA(292)                              | WAT19090 |
| MI(294)=KT(531)*ALFA(212)/GAMMA(294)                              | WAT19100 |
| MI(284)=FULVTT/(1.+ GAMMA(284)*(MI(286)+MI(288)+MI(290)+MI(292)+  | WAT19110 |
| *MI(294)))                                                        | WAT19120 |
| C1 = MI(284) * GAMMA(284)                                         | WAT19130 |
| ALFA(284) = C1                                                    | WAT19140 |
| DO 170 I=286 , 294 , 2                                            | WAT19150 |
| MI(I) = C1 * MI(I)                                                | WAT19160 |
| ALFA(I) = MI(I) * GAMMA(I)                                        | WAT19170 |
| 170 CONTINUE                                                      | WAT19180 |
| C                                                                 | WAT19190 |
| C**** MASS BALANCE ON HUMATE */                                   | WAT19200 |
| C                                                                 | WAT19210 |
| 180 IF (HUMTOT .LE. 0.0) GOTO 200                                 | WAT19220 |
| MI(287)=KT(524)/(TENPH*GAMMA(287))                                | WAT19230 |
| MI(289)=KT(526)*ALFA(8)/GAMMA(289)                                | WAT19240 |
| MI(291)=KT(528)*ALFA(130)/GAMMA(291)                              | WAT19250 |
| MI(293)=KT(530)*ALFA(160)/GAMMA(293)                              | WAT19260 |
| MI(295)=KT(532)*ALFA(212)/GAMMA(295)                              | WAT19270 |
| MI(285)=HUMTOT/(1.+ GAMMA(285)*(MI(287)+MI(289)+MI(291)+MI(293)+  | WAT19280 |
| *MI(295)))                                                        | WAT19290 |
| C1 = MI(285) * GAMMA(285)                                         | WAT19300 |
| ALFA(285) =C1                                                     | WAT19310 |
| DO 190 I = 287 , 295 , 2                                          | WAT19320 |
| MI(I) = C1 * MI(I)                                                | WAT19330 |
| ALFA(I) = MI(I) * GAMMA(I)                                        | WAT19340 |
| 190 CONTINUE                                                      | WAT19350 |
| C                                                                 | WAT19360 |
| C**** ITERATIVE TESTS */                                          | WAT19370 |
| C                                                                 | WAT19380 |
| 200 RBIT = 0                                                      | WAT19390 |
| IF (ABS(S1 + M1 - ANLCO3) .GT. 1E-3 * ANLCO3) RBIT = 1            | WAT19400 |
| IF (ABS(S2 + M2 - SO4TOT) .GT. 1E-3 * SO4TOT) RBIT = 1            | WAT19410 |



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IF (ABS(S3 + M3 - FTOT) .GT. 1E-3 * FTOT) RBIT = 1 WAT19420
IF (ABS(S4 + M4 - PTOT) .GT. 1E-3 * PTOT) RBIT = 1 WAT19430
IF (ABS(S5 + M5 - CLTOT) .GT. 1E-3 * CLTOT) RBIT = 1 WAT19440
IF (ABS(S6 + M6 - H2STOT) .GT. 1E-3 * H2STOT) RBIT = 1 WAT19450
IF (ABS(S7 + M7 - FULVTT) .GT. 1E-3 * FULVTT) RBIT = 1 WAT19460
IF (ABS(S8 + M8 - HUMTOT) .GT. 1E-3 * HUMTOT) RBIT = 1 WAT19470
C WAT19480
S1 = S1 + M1 - ANLCO3 WAT19490
S2 = S2 + M2 - SO4TOT WAT19500
S3 = S3 + M3 - FTOT WAT19510
S4 = S4 + M4 - PTOT WAT19520
S5 = S5 + M5 - CLTOT WAT19530
S6 = S6 + M6 - H2STOT WAT19540
S7 = S7 + M7 - FULVTT WAT19550
S8 = S8 + M8 - HUMTOT WAT19560
C WAT19570
WRITE(K,1000)ITER,S1,S2,S3,S4,S5,S6,S7,S8 WAT19580
1000 FORMAT(I4,1PE14.6,7E15.6) WAT19590
C WAT19600
C***** ITERATION MONITOR */ WAT19610
C WAT19620
IF (ITER .LT. 40) GOTO 210 WAT19630
RBIT = 0 WAT19640
WRITE(K,1010) WAT19650
1010 FORMAT(/,'*****' WAT19660
*****') WAT19670
WRITE(K,1020) WAT19680
1020 FORMAT(/,' CONVERGENCE NOT REACHED IN 40 ITERATIONS. CALCULATION WAT19690
*TERMINATED',/, ' PRINT OF CALCULATIONS FOLLOWS FOR CHECKING ONLY. ') WAT19700
WRITE(K,1010) WAT19710
WRITE(1,1030)
1030 FORMAT(/'CONVERGENCE NOT REACHED IN 40 ITERATIONS. CALCULATION TE
*RMINATED.'/RESULTS PRINTED OUT FOR CHECKING ONLY. ')
210 IF (ITER .LT. 2) RBIT = 1 WAT19720
RETURN WAT19730
END WAT19740
SUBROUTINE SOLUTS(ANAL,Z,PAGE1,ALFA,ANALMI,CUNITS,GAMMA,GFW,KT, WAT19760
*MI,LOGKT,INDEX2,SIGMA,ERR) WAT19770
C WAT19780
REAL*8 ALFA(0:297),ANALMI(0:297),CUNITS(0:297),ERR(0:543), WAT19790
*GAMMA(0:297),GFW(0:297),KT(0:543),MI(0:297),LOGKT(0:543), WAT19800
*SIGMA(0:297),RSD(0:297),LZERO(10),X(10),CONV(10) WAT19810
REAL*8 ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT WAT19820
REAL*8 S1,S2,S3,S4,S5,S6,S7,S8 WAT19830
INTEGER ANAL(0:297),INDEX2(1:297),Z(0:297),LISTE(9),LISTE1(63) WAT19840
CHARACTER*80 CARD1,CARD2 WAT19850
CHARACTER*8 PAGE1(0:297) WAT19860
CHARACTER*2 STARS WAT19870
C WAT19880
REAL*8 ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT, WAT19890
*MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3 WAT19900
INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA, WAT19910
*ITER,NMBR,PUNCH,RBIT,FLAG WAT19920
INTEGER*2 IDAY,IMONTH,IYEAR,IHOUR,IMIN,ISEC,IHSEC

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|    |                                                                    |          |
|----|--------------------------------------------------------------------|----------|
| C  | COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B,     | WAT19930 |
|    | *BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND,          | WAT19940 |
|    | *CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF, | WAT19950 |
|    | *DISCHG,DOC,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT,    | WAT19960 |
|    | *EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,   | WAT19970 |
|    | *FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,    | WAT19980 |
|    | *ITDS,ITER,K,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL,   | WAT19990 |
|    | *NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE,    | WAT20000 |
|    | *PEAS,PEDO,PEDO2,PEFE,PEN,PENO2,PEPT,PES,PH,PRNT,PTOT,PUNCH,R,     | WAT20010 |
|    | *RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,               | WAT20020 |
|    | *T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT             | WAT20030 |
|    | COMMON/CHRDAT/CARD1,CARD2                                          | WAT20040 |
| C  | DATA LISTE/5,7,8,13,38,84,202,261,262/                             | WAT20050 |
|    | DATA LISTE1/0,1,2,3,4,5,6,7,8,9,10,13,16,17,23,26,34,35,38,39,44,  | WAT20060 |
|    | *46,48,50,51,53,61,66,67,80,84,86,87,89,94,96,97,101,106,108,109,  | WAT20070 |
|    | *110,114,127,130,138,145,151,160,167,182,192,202,204,208,212,224,  | WAT20080 |
|    | *249,250,255,258,261,262/                                          | WAT20090 |
|    | DATA LZERO /59.5,53,50.1,73.5,76.35,80,44.5,71.46,349.8,198.3/     | WAT20100 |
|    | DATA X /115.1,109.2,41.8,47.1,47.8,133.9,40.5,46.7,110.42,75.73/   | WAT20110 |
|    | DATA CONV /4.99E-5,8.226E-5,4.35E-5,2.557E-5,2.821E-5,2.082E-5,    | WAT20120 |
|    | *1.639E-5,1.613E-5,99.209E-5,5.88E-5/                              | WAT20130 |
| C  | C2 = 0                                                             | WAT20140 |
|    | DO 10 N = 0 , D                                                    | WAT20150 |
|    | C2 = C2 + ANALMI(N) * GFW(N) * 1E3                                 | WAT20160 |
| 10 | CONTINUE                                                           | WAT20170 |
|    | C2 = C2 * 1E6 / (C2 + 1E6)                                         | WAT20180 |
| C  |                                                                    | WAT20190 |
| C  | CONDUCTANCE-TEST                                                   | WAT20200 |
| C  |                                                                    | WAT20210 |
|    | CUNITS(26) = MI(26) * 1E3 * GFW(26) * (1 - 1E-6 * C2)              | WAT20220 |
|    | CUNITS(63) = MI(63) * 1E3 * GFW(63) * (1 - 1E-6 * C2)              | WAT20230 |
|    | C1 = 0.0                                                           | WAT20240 |
|    | N = 0                                                              | WAT20250 |
|    | DO 15 I = 0 , 6                                                    | WAT20260 |
|    | N = N + 1                                                          | WAT20270 |
|    | LAMBDA = LZERO(N) - X(N) * XMUHL / (1E0 + XMUHL)                   | WAT20280 |
|    | NORM = CUNITS(I) * CONV(N)                                         | WAT20290 |
|    | C1 = C1 + LAMBDA * NORM                                            | WAT20300 |
| 15 | CONTINUE                                                           | WAT20310 |
|    | N = N + 1                                                          | WAT20320 |
|    | LAMBDA = LZERO(N) - X(N) * XMUHL / (1E0 + XMUHL)                   | WAT20330 |
|    | NORM = CUNITS(84) * CONV(N)                                        | WAT20340 |
|    | C1 = C1 + LAMBDA * NORM                                            | WAT20350 |
|    | N = N + 1                                                          | WAT20360 |
|    | LAMBDA = LZERO(N) - X(N) * XMUHL / (1E0 + XMUHL)                   | WAT20370 |
|    | NORM = CUNITS(63) * CONV(N)                                        | WAT20380 |
|    | C1 = C1 + LAMBDA * NORM                                            | WAT20390 |
|    | N = N + 1                                                          | WAT20400 |
|    | LAMBDA = LZERO(N) - X(N) * XMUHL / (1E0 + XMUHL)                   | WAT20410 |
|    | NORM = CUNITS(26) * CONV(N)                                        | WAT20420 |
|    | C1 = C1 + LAMBDA * NORM                                            | WAT20430 |
|    |                                                                    | WAT20440 |
|    |                                                                    | WAT20450 |



|                                                                   |          |
|-------------------------------------------------------------------|----------|
| CONCLC = 1E3 * C1                                                 | WAT20460 |
| CUNITS(26) = 0.0                                                  | WAT20470 |
| CUNITS(63) = 0.0                                                  | WAT20480 |
| C                                                                 | WAT20490 |
| C     END CONDUCTANCE-TEST                                        | WAT20500 |
| C                                                                 | WAT20510 |
| C**** AUXILIARY PE CALCULATIONS */                                | WAT20520 |
| C                                                                 | WAT20530 |
| SIGMPE = SIGMEH * F / (C*R*T)                                     | WAT20540 |
| IF (ALFA(5)*ALFA(13) .LE. 0.0) GOTO 20                            | WAT20550 |
| PES = 0.125 * DLOG10(KT(90))+0.125 * DLOG10(ALFA(5))-1.25*PH      | WAT20560 |
| *-0.125 * DLOG10(ALFA(13))-0.5*LH20                               | WAT20570 |
| EHS = PES* C*R*T / F                                              | WAT20580 |
| C     END                                                         | WAT20590 |
| 20 IF (ALFA(38)*ALFA(84) .LE. 0.0) GOTO 30                        | WAT20600 |
| PEN=(-LOGKT(127)+DLOG10(ALFA(84))- 10.0 * PH - DLOG10(ALFA(38))   | WAT20610 |
| *-3E0*LH20)/8E0                                                   | WAT20620 |
| EHN = PEN* C*R*T / F                                              | WAT20630 |
| C     END                                                         | WAT20640 |
| 30 IF (ALFA(202)*ALFA(84) .LE. 0.0) GOTO 40                       | WAT20650 |
| PEN02 = (LOGKT(400) + DLOG10(ALFA(84))-DLOG10(ALFA(202))          | WAT20660 |
| *-LH20-2*PH)/2                                                    | WAT20670 |
| EHNO2 = PEN02 * C*R*T/F                                           | WAT20680 |
| C     END                                                         | WAT20690 |
| 40 IF (ALFA(250)*ALFA(255) .LE. 0.0) GOTO 50                      | WAT20700 |
| PEAS = (DLOG10(ALFA(255)/ALFA(250)) - LOGKT(487)-LH20)/2E0-PH     | WAT20710 |
| EHAS = PEAS * C*R*T/F                                             | WAT20720 |
| C                                                                 | WAT20730 |
| C     EHERR                                                       | WAT20740 |
| C                                                                 | WAT20750 |
| 50 DO 45 I = 1, 296                                               | WAT20760 |
| RSD (I) = 2.0E7                                                   | WAT20770 |
| 45 CONTINUE                                                       | WAT20780 |
| C                                                                 | WAT20790 |
| DO 55 J = 1, 9                                                    | WAT20800 |
| I = LISTE(J)                                                      | WAT20810 |
| IF (CUNITS(I)*SIGMA(I) .GT. 0.0) RSD(I)=SIGMA(I)/CUNITS(I)/C      | WAT20820 |
| 55 CONTINUE                                                       | WAT20830 |
| IF (SIGMDO * DOX .GT. 0.0) RSDDO = SIGMDO / DOX / C               | WAT20840 |
| IF (SIGMDO * DOX .LE. 0.0) RSDDO = 2E7                            | WAT20850 |
| ERR(0)=SQRT(RSD(7)**2 + RSD(8)**2)                                | WAT20860 |
| ERR(1)=SQRT(SIGMPH**2 + RSDDO**2)                                 | WAT20870 |
| ERR(4)=ERR(1)                                                     | WAT20880 |
| ERR(2)=SQRT(SIGMPH**2+(.5*RSD(84))**2+(.5*RSD(202))**2)           | WAT20890 |
| ERR(3)=SQRT((1.125*SIGMPH)**2+(.125*RSD(84))**2+                  | WAT20900 |
| *(.125*RSD(38))**2)                                               | WAT20910 |
| ERR(5)=SQRT((1.125*SIGMPH)**2+(.125*RSD(5))**2+(.125*RSD(13))**2) | WAT20920 |
| ERR(6)=SQRT(RSD(261)**2+RSD(262)**2+(2*SIGMPH)**2)                | WAT20930 |
| DO 60 I = 0, 6                                                    | WAT20940 |
| IF (ERR(I).GT.1E2) ERR(I) = 0.0                                   | WAT20950 |
| ERR(I+7) = ERR(I) * C*R*T/F                                       | WAT20960 |
| 60 CONTINUE                                                       | WAT20970 |
| C                                                                 | WAT20980 |
| C**** PRINT OF INPUT */                                           | WAT20990 |

|       |                                                                    |          |
|-------|--------------------------------------------------------------------|----------|
| C     | CALL GETDAT(IYEAR,IMONTH,IDAY)                                     | WAT21000 |
|       | CALL GETTIM(IHOUR,IMIN,ISEC,IHSEC)                                 |          |
|       | WRITE(K,1003)CARD1,IMONTH,IDAY,IYEAR-1900,IHOUR,IMIN               |          |
| 1003  | FORMAT(1H1,1X,A80:,9X,'Date = ',I2,2('/',I2.2),2X,I2,':',I2.2)     |          |
| C     | WRITE(K,1003)CARD1                                                 | WAT21010 |
| C1003 | FORMAT(1H1,1X,A80)                                                 | WAT21020 |
|       | WRITE(K,1005) CARD2                                                | WAT21040 |
| 1005  | FORMAT(1H ,A80)                                                    | WAT21050 |
|       | WRITE(K,1010)DOX,DOC,ITDS                                          | WAT21060 |
| 1010  | FORMAT(' DOX = ',F11.4,' DOC = ',F8.1,                             | WAT21070 |
|       | *' INPUT TDS = ',F8.1)                                             | WAT21080 |
|       | WRITE(K,1040)COND,CONCLC                                           | WAT21090 |
| 1040  | FORMAT(' Anal Cond = ',F8.1,' Calc Cond = ',F8.1)                  | WAT21100 |
|       | INADD=0                                                            |          |
|       | IF (CUNITS(7) * CUNITS(8) .LE. 0.0) GOTO 70                        | WAT21110 |
|       | IF (EHPT .LE. 9E0 ) GOTO70                                         | WAT21120 |
|       | IF ( EHOPT .NE. 0 ) GOTO70                                         | WAT21130 |
|       | INADD=INADD+3                                                      |          |
|       | WRITE(K,1070)                                                      | WAT21140 |
| 1070  | FORMAT('/' ***** Eh and pE calculated from iron 2/3 activity ratio | WAT21150 |
|       | *have been substituted for input Eh data *****/')                  | WAT21160 |
| 70    | DIFF1 = 100. * (2.*(EPMCAT-EPMAN)/(EPMAN+EPMCAT))                  | WAT21170 |
|       | EPCAT1 = EPMCAT * 1000.                                            | WAT21180 |
|       | EPMAN1 = EPMAN * 1000.                                             | WAT21190 |
|       | WRITE(K,1080)EPCAT1,EPMAN1,DIFF1                                   | WAT21200 |
| 1080  | FORMAT(' Anal EPMCAT =',F10.4,' Anal EPMAN =',F10.4,               | WAT21210 |
|       | *' Percent difference in input cation/anion balance = ',F9.4)      | WAT21230 |
| C     |                                                                    | WAT21250 |
| C**** | RECALCULATION OF CATION-ANION BALANCE */                           | WAT21260 |
| C     |                                                                    | WAT21270 |
|       | EPMAN = 0.0                                                        | WAT21280 |
|       | EPMCAT = 0.0                                                       | WAT21290 |
|       | DO 100 I = 0 , D                                                   | WAT21300 |
|       | IF(I.EQ.16 .OR. I.EQ.34 .OR. I.EQ.69 .OR. I.EQ.70 .OR.I.EQ.71      | WAT21310 |
|       | *.OR. I.EQ.83 .OR. I.EQ.86) GOTO 100                               | WAT21320 |
|       | IF (Z(I) .GT. 0) EPMCAT = EPMCAT + Z(I) * MI(I)                    | WAT21330 |
|       | IF (Z(I) .LE. 0) EPMAN = EPMAN - Z(I) * MI(I)                      | WAT21340 |
| 100   | CONTINUE                                                           | WAT21350 |
|       | EPCAT1 = EPMCAT * 1000.                                            | WAT21360 |
|       | EPMAN1 = EPMAN * 1000.                                             | WAT21370 |
|       | DIFF1 = 100. * (2.*(EPMCAT-EPMAN)/(EPMAN+EPMCAT))                  | WAT21380 |
|       | IF (DIFF1.LE. 30.) GOTO 320                                        |          |
|       | INADD=INADD+2                                                      |          |
|       | WRITE(1,1000)                                                      |          |
|       | WRITE(K,1000)                                                      |          |
| 1000  | FORMAT( ' ERROR IN CALCULATED CHARGE BALANCE GREATER THAN 30 PERCE |          |
|       | *NT. CHECK INPUT DATA. '/')                                        |          |
|       | WRITE(1,1100)EPCAT1,EPMAN1,DIFF1                                   |          |
| C     |                                                                    |          |
| C**** | Calculation of total ionic strength (from speciation)              |          |
| C     |                                                                    |          |
| 320   | WRITE(K,1100)EPCAT1,EPMAN1,DIFF1                                   | WAT21390 |
| 1100  | FORMAT(' Calc EPMCAT =',F10.4,' Calc EPMAN =',F10.4,               | WAT21400 |



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WRITE(K,1130)PEPT,SIGMPE,PEFE,ERR(0),PEDO,ERR(1),PEN02,ERR(2),PEN,
*ERR(3),PEDO2,ERR(4),PES,ERR(5),PEAS,ERR(6)
WRITE(K,1178)
1178 FORMAT(/'                               Effective')
WRITE(K,1180)
S2 = 4.4E4*CARBON
1180 FORMAT( '      T      pH      TDS ppm  Ionic Str  pO2 Atm  pCO2 AtmWAT21880
*      pCH4 Atm   CO2 Tot   Uncom CO2  ppm Uncom CO2   Ncrb Alk   aHWAT21890
*20')
WRITE(K,1190)TEMP,PH,TDS,XMU,ALFA(69),PCO2,ALFA(70),S1,CARBON,
* S2,NONCRB,AH2O
1190 FORMAT(1X,F7.2,F8.3,F9.1,F10.5,3(1PE11.2),0PF10.5,1PE11.2,E13.2,
*E14.2,0PF11.4)
WRITE(K,1400)
1400 FORMAT (/ '      I Species          Anal ppm          Calc ppm      AnWAT21970
*al Molal   Calc Molal   Activity          Act Coeff    -Log Act')
C2=0
DO 140 N = 0 , D
C2 = C2 + MI(N) * GFW(N) * 1.E3
140 CONTINUE
C2 = C2 * 1E6 / (C2 + 1E6)
IN = 19 + INADD
DO 150 N = 1 , H
I=INDEX2(N)
IF (MI(I).LE.0.0.AND.ANALMI(I).LE.0.0.AND.ANAL(I).EQ.0) GOTO150
C1 = 0.0
STARS = ' '
IF (ALFA(I) .GT. 0.0) C1 = -DLOG10 (ALFA(I))
IF (FULFLG .NE. 1) GOTO 170
DO 160 J = 284 , 294 , 2
IF (I .EQ. J) STARS = '**'
160 CONTINUE
170 IF (HUMFLG .NE. 1) GOTO 185
DO 180 J = 285 , 295 , 2
IF (I .EQ. J) STARS= '**'
180 CONTINUE
185 S1 = CUNITS(I)
S2 = MI(I) * GFW(I) * 1E3 * (1. - 1E-6 * C2)
IF(S1.GT.0.0 .AND. MI(I).GT.0.0) THEN
  IF(S2.LT.1E-2) THEN
    WRITE(K,1300)I,STARS,PAGE1(I),Z(I),S1,S2,ANALMI(I),MI(I),
*   ALFA(I),GAMMA(I),C1
  ELSE
    WRITE(K,1301)I,STARS,PAGE1(I),Z(I),S1,S2,ANALMI(I),MI(I),
*   ALFA(I),GAMMA(I),C1
  END IF
ELSE
  IF(S1.LT.1D-78 .AND. MI(I).GT.0E0) THEN
    IF(S2.LT.1E-2) THEN
      WRITE(K,1302)I,STARS,PAGE1(I),Z(I),S2,MI(I),ALFA(I),
*   GAMMA(I),C1
    ELSE
      WRITE(K,1303)I,STARS,PAGE1(I),Z(I),S2,MI(I),ALFA(I),

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*      GAMMA(I),C1
      END IF
      ELSE
        IF(ANAL(I).EQ.0) THEN
          IF(S1.LT.1E-2) THEN
            WRITE(K,1304)I,STARS,PAGE1(I),Z(I),S1,ANALMI(I)
          ELSE
            WRITE(K,1305)I,STARS,PAGE1(I),Z(I),S1,ANALMI(I)
          END IF
        ELSE
          WRITE(K,1305)I,STARS,PAGE1(I),Z(I),S1
        END IF
      END IF
      END IF
      END IF
1300 FORMAT(' ',I3,A2,A8,I3,F16.6,F16.6,1X,3(1PE12.3),OPF12.4,F12.3)  WAT22240
1301 FORMAT(' ',I3,A2,A8,I3,F13.3,3X,F13.3,4X,3(1PE12.3),OPF12.4,F12.3)
1302 FORMAT(' ',I3,A2,A8,I3,16X,F16.6,13X,2(1PE12.3),OPF12.4,F12.3)
1303 FORMAT(' ',I3,A2,A8,I3,16X,F13.3,16X,2(1PE12.3),OPF12.4,F12.3)
1304 FORMAT(' ',I3,A2,A8,I3,F16.6,17X,1PE12.3)
1305 FORMAT(' ',I3,A2,A8,I3,F13.3,20X,1PE12.3)
      IN = IN + 1
      IF (IN .LT.57) GOTO 150
      IN = 0
      WRITE(K,1003) CARD1
      WRITE(K,1400)
150 CONTINUE
C
      IF (EHPT .GT. 9.0) PEPT = 999
      IF (CUNITS(7)*CUNITS(8) .LE. 0.0) PEF = 999
      IF (PE .GT. 9E1) PE = 2E1
C
C**** CONVERSION OF ALFA AND CUNITS TO LOG FORM FOR AP CALCS & PUNCHING
C
      DO 190 J = 1 ,63
        I = LISTE1(J)
        IF ( ALFA(I) .LE. 0.0) ALFA(I) = -2E4
        IF ( ALFA(I) .GT. 0.0) ALFA(I) = DLOG10(ALFA(I))
        IF (CUNITS(I) .LE. 0.0) CUNITS(I) = -2E4
        IF (CUNITS(I) .GT. 0.0) CUNITS(I) = DLOG10(CUNITS(I))
190 CONTINUE
      RETURN
      END
      SUBROUTINE RATIO(PAGE1,ALFA,CUNITS,Z,ANALMI)
C
      INTEGER Z(0:297),LISTE(7)
      REAL*8 ALFA(0:297),CUNITS(0:297),ANALMI(0:297)
      CHARACTER*80 CARD1,CARD2
      CHARACTER*8 PAGE1(0:297)
C
      REAL*8 ANLC03,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT
      REAL*8 ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT,
      *MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3
      INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA,
      *ITER,NMBR,PUNCH,RBIT,FLAG

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|       |                                                                    |          |
|-------|--------------------------------------------------------------------|----------|
| C     | COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B,     | WAT22590 |
|       | *BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND,          | WAT22600 |
|       | *CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF, | WAT22610 |
|       | *DISCHG, DOC,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT,   | WAT22620 |
|       | *EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,   | WAT22630 |
|       | *FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,    | WAT22640 |
|       | *ITDS,ITER,K,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL,   | WAT22650 |
|       | *NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE,    | WAT22660 |
|       | *PEAS,PEDO,PEDO2,PEFE,PEN,PENO2,PEPT,PES,PH,PRNT,PTOT,PUNCH,R,     | WAT22670 |
|       | *RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,               | WAT22680 |
|       | *T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT             | WAT22690 |
|       | COMMON/CHRDAT/CARD1,CARD2                                          | WAT22700 |
| C     | DATA LISTE/0,1,2,3,50,7,5/                                         | WAT22710 |
| C     |                                                                    | WAT22720 |
| C     |                                                                    | WAT22730 |
| C**** | CALCULATION OF MOLAR CONCENTRATION RATIOS AND LOG ACTIVITY RATIOS* | WAT22740 |
| C     | WRITE(K,980)CARD1                                                  | WAT22750 |
|       | 980 FORMAT(1H1//,1X,A80)                                           | WAT22760 |
|       | WRITE(K,1000)                                                      | WAT22770 |
| 1000  | FORMAT(/,18X,' Mole ratios from analytical molality - ',           | WAT22800 |
|       | *'Log activity ratios',/)                                          | WAT22810 |
|       | DO 20 J = 1,7                                                      | WAT22820 |
|       | I = LISTE(J)                                                       | WAT22830 |
|       | C1 = 0.0                                                           | WAT22840 |
|       | IF (ANALMI(I) .GT. 0.0) C1 = CLTOT/ANALMI(I)                       | WAT22850 |
|       | C2 = 0.0                                                           | WAT22860 |
|       | IF (ALFA(I) .GT. -1E3) C2 = Z(I) * PH + ALFA(I)                    | WAT22870 |
|       | IF (I .NE. 5) GOTO 10                                              | WAT22880 |
|       | C2 = ALFA(0) - ALFA(1)                                             | WAT22890 |
|       | WRITE(K,1010) PAGE1(I),C1,C2                                       | WAT22900 |
| 1010  | FORMAT(30X,'C1/',A8,' = ',1PE12.4,' Log Ca/Mg = '                  | WAT22910 |
|       | *,OPF11.4)                                                         | WAT22920 |
|       | GOTO 20                                                            | WAT22930 |
| 10    | WRITE(K,1020) PAGE1(I),C1,PAGE1(I),Z(I),C2                         | WAT22940 |
| 1020  | FORMAT(30X,'C1/',A8,' = ',1PE12.4,' Log ',A8,'/H',I1,' = '         | WAT22950 |
|       | *,OPF11.4)                                                         | WAT22960 |
| 20    | CONTINUE                                                           | WAT22970 |
|       | C1 = 0.0                                                           | WAT22980 |
|       | C2 = 0.0                                                           | WAT22990 |
|       | IF (CO2TIT .GT. 0.0) C1 = CLTOT/CO2TIT                             | WAT23000 |
|       | IF (ALFA(2)+ALFA(3) .GT. -1E4) C2 = ALFA(2)-ALFA(3)                | WAT23010 |
|       | WRITE(K,1040)C1,C2                                                 | WAT23020 |
| 1040  | FORMAT(30X,'CL/HCO3 = ',1PE12.4,' LOG NA/K = '                     | WAT23030 |
|       | *,OPF11.4)                                                         | WAT23040 |
|       | C1 = 0.0                                                           | WAT23050 |
|       | C2 = 0.0                                                           | WAT23060 |
|       | IF (ANALMI(1) .GT. 0.0) C1 = ANALMI(0)/ANALMI(1)                   | WAT23070 |
|       | IF (ALFA(0)+ALFA(3) .GT. -1E4) C2 = ALFA(0)-2*ALFA(3)              | WAT23080 |
|       | WRITE(K,1060)C1,C2                                                 | WAT23090 |
| 1060  | FORMAT(30X,'Ca/Mg = ',1PE12.4,' Log Ca/K2 = '                      | WAT23100 |
|       | *,OPF11.4)                                                         | WAT23110 |
|       | C1 = 0.0                                                           | WAT23120 |
|       |                                                                    | WAT23130 |



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C2 = 0.0 WAT23140
IF (ANALMI(3).GT.0.0)C1 = ANALMI(2)/ANALMI(3) WAT23150
IF (ANALMI(7).GT.-2E4) C2 = 2 * PH + ANALMI(7) WAT23160
WRITE(K,1080)C1,C2 WAT23170
1080 FORMAT(30X,'Na/K          = ',1PE12.4,'          Log Diss Fe/H2    = ' WAT23180
*,OPF11.4) WAT23190
RETURN WAT23200
END WAT23210
SUBROUTINE APCALC(AP,ALFA,GAMMA,MI) WAT23230
C WAT23240
REAL*8 AP(0:543),ALFA(0:297),GAMMA(0:297),MI(0:297) WAT23250
INTEGER LISTE(38) WAT23260
CHARACTER*80 CARD1,CARD2 WAT23270
C WAT23280
REAL*8 ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT WAT23290
REAL*8 ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT, WAT23300
*MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3 WAT23310
INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA, WAT23320
*ITER,NMBR,PUNCH,RBIT,FLAG WAT23330
C WAT23340
COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B, WAT23350
*BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND, WAT23360
*CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF, WAT23370
*DISCHG,DOC,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT, WAT23380
*EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG, WAT23390
*FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV, WAT23400
*ITDS,ITER,K,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL, WAT23410
*NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE, WAT23420
*PEAS,PEDO,PEDO2,PEFE,PEN,PENO2,PEPT,PES,PH,PRNT,PTOT,PUNCH,R, WAT23430
*RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT, WAT23440
*T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT WAT23450
COMMON/CHRDAT/CARD1,CARD2
C WAT23460
DATA LISTE/114,134,183,184,185,186,187,189,195,196,197,198,199, WAT23470
*200,223,224,225,226,227,228,229,265,312,313,360,386,387,388,402, WAT23480
*388,402,437,459,460,533,534,535,536/ WAT23490
C WAT23500
C**** CALC. OF ION ACTIVITY PRODUCTS (IN TERMS OF LOGS) */ WAT23510
C WAT23520
AP(9)=ALFA(7)+ALFA(17)
AP(10)=ALFA(1)+ALFA(17)
AP(11)=ALFA(0)+AP(10)+ALFA(17)
AP(12)=ALFA(0)+ALFA(17)
AP(21)=AP(12)
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)-6E0*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)=2*ALFA(1)+3*ALFA(23)+4*PH-0.5*LH2O

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AP(153)=AP(36)
AP(37)=3*ALFA(1)+4*ALFA(23)+6*PH-4*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)+3*(ALFA(50)+ALFA(23))+10*PH
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)=2E0*(ALFA(53)+ALFA(23)-PH          )-7E0*LH2O
AP(47)=AP(46)
IF ((MI(1)+MI(2)+MI(3)).LT.1D-78) THEN
  C1=2E4
ELSE
  C1=DLOG10(SQRT(MI(1)*GAMMA(1))+MI(2)*GAMMA(2)+MI(3)*GAMMA(3))
END IF
AP(48) = .33E0*C1+2.33E0*ALFA(53)+3.67E0*ALFA(23)-2E0*PH-12E0*LH2O
AP(49)=5*ALFA(1)+2*ALFA(50)+3*ALFA(23)+16*PH+6*LH2O
AP(125)=AP(49)
AP(50)=ALFA(3)+3E0*ALFA(50)+6E0*ALFA(26)+2E0*ALFA(5)
AP(51)=ALFA(50)+3E0*(LH2O+PH)
AP(52)=ALFA(50)+3E0*ALFA(26)-LH2O
AP(154)=AP(52)
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)).GT.1D-78) THEN
  AP(56)=.5E0*DLOG10(MI(2)*GAMMA(2)+MI(3)*GAMMA(3))+ALFA(53)
*      +5E0*ALFA(23)-8.5E0*LH2O
  AP(57)=.5E0*DLOG10(MI(2)*GAMMA(2)+MI(3)*GAMMA(3))+ALFA(53)
*      +4.5E0*ALFA(23)-8E0*LH2O
END IF
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)=ALFA(7)+ALFA(66)+PH
AP(119)=AP(67)
AP(95)=5E0*ALFA(0)+3E0*ALFA(46)+4E0*PH+LH2O
AP(96)=5E0*ALFA(0)+3E0*ALFA(46)+3E0*PH+ALFA(61)
AP(98)=ALFA(3)+7E0*ALFA(23)+PH          -9E0*LH2O
AP(97)=ALFA(23)-2E0*LH2O
AP(99)=AP(97)
AP(100)=AP(97)
AP(101)=AP(97)

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AP(395)=AP(97)
AP(106)=3E0*ALFA(7)+2E0*ALFA(44)+8E0*LH2O
AP(107)=2E0*ALFA(8)+ALFA(7)+4E0*LH2O+8E0*PH
AP(108)=2E0*ALFA(8)+3E0*LH2O+6E0*PH
AP(109)=AP(108)
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)=ALFA(3)+3*ALFA(7)+ALFA(53)+3*ALFA(23)-10*LH2O
AP(114)=ALFA(7)+2E0*(ALFA(66)+PE+PH)
C1=DLOG10(MI(2)*GAMMA(2)+MI(3)*GAMMA(3)+MI(63)*GAMMA(63))
AP(115)=0.83E0*C1+0.29E0*ALFA(1)+.23E0*ALFA(8)+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)-8E0*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)=(1E0-C1)*ALFA(50)+C1*ALFA(23)+(3E0-3E0*C1)*PH
AP(158)=AP(157)
AP(181)=ALFA(8)+0.3*ALFA(4)+2.7*(LH2O+PH)
AP(182)=ALFA(109)+ALFA(5)
AP(183)=ALFA(110)+2*LH2O+4*PH+PE
AP(184)=AP(183)
AP(185)=AP(183)
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)

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$AP(199) = 20 * ALFA(110) + 2 * ALFA(80) + 8 * ALFA(50) + 49 * LH2O + 70 * PH$   
 $*$   $- 8 * ALFA(109)$   
 $AP(200) = 8 * ALFA(110) + .44 * ALFA(0) + 12 * LH2O + 18 * PH - 3.44 * ALFA(109)$   
 $AP(204) = 3 * ALFA(8) + 2 * ALFA(5) + ALFA(2) + 6 * (LH2O + PH)$   
 $AP(205) = 3 * ALFA(8) + 2 * ALFA(5) + ALFA(3) + 6 * (LH2O + PH)$   
 $AP(223) = ALFA(127) - PE$   
 $AP(224) = ALFA(127) + ALFA(4)$   
 $AP(225) = ALFA(127) + ALFA(61)$   
 $AP(226) = 2 * ALFA(127) + LH2O + 2 * PH$   
 $AP(227) = 2 * ALFA(127) + ALFA(66) + PH$   
 $AP(228) = 2 * ALFA(127) + ALFA(5)$   
 $AP(229) = ALFA(127) + ALFA(8) + 2 * LH2O + 4 * PH$   
 $AP(230) = ALFA(130) + 2 * ALFA(4)$   
 $AP(231) = ALFA(130) + ALFA(17)$   
 $AP(232) = ALFA(130) + 2 * ALFA(61)$   
 $AP(233) = ALFA(130) + 2 * ALFA(61) + 2 * LH2O$   
 $AP(234) = ALFA(130) + 2 * LH2O + 2 * PH$   
 $AP(235) = 2 * ALFA(130) + 2 * LH2O + ALFA(6) + 3 * PH$   
 $AP(236) = 3 * ALFA(130) + 2 * LH2O + 2 * ALFA(6) + 4 * PH$   
 $AP(237) = 2 * ALFA(130) + 3 * LH2O + ALFA(4) + 3 * PH$   
 $AP(238) = 2 * ALFA(130) + 3 * LH2O + ALFA(84) + 3 * PH$   
 $AP(239) = 3 * ALFA(130) + 4 * LH2O + ALFA(5) + 4 * PH$   
 $AP(240) = 4 * ALFA(130) + 6 * LH2O + ALFA(5) + 6 * PH$   
 $AP(241) = 4 * ALFA(130) + 7 * LH2O + ALFA(5) + 6 * PH$   
 $AP(242) = ALFA(130) + LH2O + 2 * PH$   
 $AP(243) = 2 * ALFA(130) + LH2O + ALFA(5)$   
 $AP(244) = 3 * ALFA(130) + 2 * ALFA(44)$   
 $AP(245) = 3 * ALFA(130) + 2 * ALFA(44) + 3 * LH2O$   
 $AP(246) = ALFA(130) + ALFA(66) + PH$   
 $AP(247) = ALFA(130) + ALFA(5)$   
 $AP(248) = ALFA(130) + ALFA(5) + 5 * LH2O$   
 $AP(249) = ALFA(130) + 2 * ALFA(8) + 4 * LH2O + 8 * PH$   
 $AP(250) = ALFA(130) + ALFA(7) + 2 * (ALFA(66) + PH)$   
 $AP(265) = ALFA(145) - 2 * PE$   
 $AP(266) = ALFA(145) + 2 * ALFA(35) + 2 * PH - 2 * LH2O$   
 $AP(267) = ALFA(145) + 2 * ALFA(4)$   
 $AP(268) = ALFA(145) + ALFA(17)$   
 $AP(269) = ALFA(145) + ALFA(17) + LH2O$   
 $AP(270) = ALFA(145) + 2 * ALFA(61)$   
 $AP(271) = ALFA(145) + 2 * (LH2O + PH)$   
 $AP(272) = AP(271)$   
 $AP(273) = AP(271)$   
 $AP(274) = AP(271)$   
 $AP(275) = AP(271)$   
 $AP(276) = 2 * ALFA(145) + 3 * (LH2O + PH) + ALFA(4)$   
 $AP(277) = 5 * ALFA(145) + 8 * (LH2O + PH) + 2 * ALFA(4)$   
 $AP(278) = 2 * ALFA(145) + 2 * (LH2O + PH) + ALFA(5)$   
 $AP(279) = 4 * ALFA(145) + 6 * (LH2O + PH) + ALFA(5)$   
 $AP(280) = ALFA(145) + 2 * ALFA(84) + 6 * LH2O$   
 $AP(281) = ALFA(145) + LH2O + 2 * PH$   
 $AP(282) = AP(281)$   
 $AP(283) = 3 * ALFA(145) + 2 * ALFA(5) + LH2O + 2 * PH$   
 $AP(284) = 3 * ALFA(145) + 2 * ALFA(44) + 4 * LH2O$   
 $AP(285) = ALFA(145) + ALFA(66) + PH$

AP(286)=AP(285)  
 AP(287)=AP(285)  
 AP(288)=ALFA(145)+ALFA(23)+2\*PH-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\*LH2O  
 AP(293)=ALFA(145)+ALFA(5)+7\*LH2O  
 AP(312)=ALFA(160)-2\*PE  
 AP(313)=AP(312)  
 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)+LH2O  
 AP(318)=AP(316)+2.5\*LH2O  
 AP(319)=ALFA(160)+2\*ALFA(61)  
 AP(320)=ALFA(160)+2\*(LH2O+PH)  
 AP(321)=AP(320)  
 AP(322)=ALFA(160)+LH2O+PH+ALFA(4)  
 AP(323)=3\*ALFA(160)+4\*(LH2O+PH)+ALFA(5)  
 AP(324)=3\*ALFA(160)+2\*(LH2O+PH)+2\*ALFA(5)  
 AP(325)=4\*ALFA(160)+6\*(LH2O+PH)+ALFA(5)  
 AP(326)=ALFA(160)+LH2O+2\*PH  
 AP(327)=3\*ALFA(160)+2\*ALFA(44)  
 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)=ALFA(182)+LH2O+2\*PH  
 AP(368)=AP(367)  
 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

$AP(380) = ALFA(182) + 3 * ALFA(50) + ALFA(44) + 6 * (LH2O + PH) + ALFA(5)$   
 $AP(381) = ALFA(182) * 2 + ALFA(130) + ALFA(44) + 3 * PH + 6 * LH2O$   
 $AP(382) = ALFA(182) + ALFA(23) - LH2O + 2 * PH$   
 $AP(383) = ALFA(182) * 2 + ALFA(23) + 4 * PH$   
 $AP(384) = ALFA(182) + ALFA(5)$   
 $AP(385) = ALFA(182) + ALFA(66) + PH$   
 $AP(386) = ALFA(182) + 2 * LH2O + 4 * PH + 2 * PE$   
 $AP(387) = ALFA(182) * 2 + LH2O * 3 + 6 * PH + 2 * PE$   
 $AP(388) = ALFA(182) * 3 + LH2O * 4 + 8 * PH + 2 * PE$   
 $AP(389) = ALFA(182) + (LH2O + PH) * 2$   
 $AP(390) = ALFA(182) + LH2O + PH + ALFA(4)$   
 $AP(391) = ALFA(182) * 2 + (LH2O + PH) * 3 + ALFA(4)$   
 $AP(392) = ALFA(182) * 3 + (LH2O + PH) * 2 + ALFA(17) * 2$   
 $AP(393) = ALFA(182) * 2 + LH2O * 3 + 4 * PH$   
 $AP(394) = ALFA(182) * 4 + LH2O * 6 + 6 * PH + ALFA(5)$   
 $AP(396) = 9.496 * ALFA(0) + 0.36 * ALFA(2) + 0.144 * ALFA(1) + 4.8 * ALFA(44)$   
 $* + 1.2 * ALFA(17) + 2.48 * ALFA(61)$   
 $AP(398) = ALFA(89) + 2 * ALFA(61)$   
 $AP(399) = ALFA(87) + 2 * ALFA(61)$   
 $AP(401) = 2 * ALFA(8) + 3 * ALFA(5)$   
 $AP(402) = ALFA(67) + 2 * PE$   
 $AP(410) = ALFA(204) + ALFA(17)$   
 $AP(411) = ALFA(204) + 2 * (LH2O + PH)$   
 $AP(412) = 4 * ALFA(204) + 6 * (LH2O + PH) + ALFA(5)$   
 $AP(413) = ALFA(204) + LH2O + 2 * PH$   
 $AP(414) = 3 * ALFA(204) + 2 * ALFA(44)$   
 $AP(415) = ALFA(204) + ALFA(66) + PH$   
 $AP(416) = ALFA(204) + ALFA(5) + 6 * LH2O$   
 $AP(417) = AP(416) + LH2O$   
 $AP(418) = 2 * ALFA(204) + ALFA(23) + 4 * PH$   
 $AP(419) = 2 * ALFA(8) + ALFA(7) + 8 * (LH2O + PH)$   
 $AP(420) = ALFA(130) + ALFA(23) + 2 * PH$   
 $AP(437) = ALFA(212) - PE$   
 $AP(438) = ALFA(212) + ALFA(97)$   
 $AP(439) = ALFA(212) + ALFA(4)$   
 $AP(440) = 2 * ALFA(212) + ALFA(17)$   
 $AP(441) = ALFA(212) + ALFA(61) + 4 * LH2O$   
 $AP(442) = ALFA(212) + ALFA(96)$   
 $AP(443) = 2 * ALFA(212) + LH2O + 2 * PH$   
 $AP(444) = 3 * ALFA(212) + ALFA(44)$   
 $AP(445) = 2 * ALFA(212) + ALFA(66) + PH$   
 $AP(446) = 2 * ALFA(212) + ALFA(5)$   
 $AP(459) = ALFA(127) + ALFA(97)$   
 $AP(460) = ALFA(127) + ALFA(96)$   
 $AP(461) = ALFA(145) + 2 * ALFA(97) + 2 * LH2O$   
 $AP(462) = ALFA(145) + 2 * ALFA(96)$   
 $AP(463) = ALFA(160) + 2 * ALFA(97) + 4 * LH2O$   
 $AP(464) = ALFA(160) + 2 * ALFA(96)$   
 $AP(465) = ALFA(182) + 2 * ALFA(97)$   
 $AP(466) = ALFA(182) + ALFA(97) + ALFA(61)$   
 $AP(467) = ALFA(182) + 2 * ALFA(96)$   
 $AP(471) = ALFA(50) + ALFA(5) + LH2O + PH$   
 $AP(472) = 4 * ALFA(50) + ALFA(5) + 10 * (LH2O + PH)$   
 $AP(488) = 2 * ALFA(255) - 3 * LH2O$



|    |                                                                    |          |
|----|--------------------------------------------------------------------|----------|
|    | AP(489)=ALFA(50)+ALFA(258)+2*LH20                                  |          |
|    | AP(541)=3*ALFA(89)+2*ALFA(258)                                     |          |
|    | AP(490)=3*ALFA(0)+2*ALFA(258)+4*LH20                               |          |
|    | AP(491)=3*ALFA(130)+2*ALFA(258)+6*LH20                             |          |
|    | AP(492)=ALFA(8)+ALFA(258)+2*LH20                                   |          |
|    | AP(493)=3*ALFA(109)+2*ALFA(258)+8*LH20                             |          |
|    | AP(494)=3*ALFA(204)+2*ALFA(258)+8*LH20                             |          |
|    | AP(495)=3*ALFA(182)+2*ALFA(258)                                    |          |
|    | AP(496)=3*ALFA(145)+2*ALFA(258)+2.5*LH20                           |          |
|    | AP(497)=4*ALFA(250)-6*LH20                                         |          |
|    | AP(498)=AP(497)                                                    |          |
|    | AP(499)=ALFA(250)+3*ALFA(96)-3*(LH20+PH)                           |          |
|    | AP(500)=2*ALFA(250)+3*ALFA(66)-3*PH-6*LH20                         |          |
|    | AP(501)=ALFA(250)+ALFA(66)-3*LH20-2*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                 |          |
| C  |                                                                    | WAT26520 |
| C  | LISTE                                                              | WAT26530 |
| C  |                                                                    | WAT26540 |
|    | IF (ABS(PE) .LE. 19E0) GOTO 40                                     | WAT26550 |
|    | DO 30 J = 1,38                                                     | WAT26560 |
|    | I = LISTE(J)                                                       | WAT26570 |
|    | AP(I)=2E4                                                          | WAT26580 |
| 30 | CONTINUE                                                           | WAT26590 |
| 40 | CONTINUE                                                           | WAT26600 |
|    | RETURN                                                             | WAT26610 |
|    | END                                                                | WAT26620 |
|    | SUBROUTINE OUTPCH(ALFA,AP,CUNITS,LOGKT)                            | WAT26650 |
| C  |                                                                    | WAT26660 |
|    | REAL*8 ALFA(0:297),AP(0:543),CUNITS(0:297),LOGKT(0:543),LP(600)    | WAT26670 |
|    | CHARACTER*80 CARD1,CARD2                                           | WAT26680 |
|    | INTEGER LISTE(50),LISTE1(79),LISTE2(27)                            | WAT26690 |
| C  |                                                                    | WAT26700 |
|    | REAL*8 ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT          | WAT26710 |
|    | REAL*8 ITDS,KTOT,KW,LAMBDA,LH20,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT,    | WAT26720 |
|    | *MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3      | WAT26730 |
|    | INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA,      | WAT26740 |
|    | *ITER,NMBR,PUNCH,RBIT,FLAG                                         | WAT26750 |
| C  |                                                                    | WAT26760 |
|    | COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B,     | WAT26770 |
|    | *BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND,          | WAT26780 |
|    | *CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF, | WAT26790 |
|    | *DISCHG,DOC,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT,    | WAT26800 |
|    | *EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,   | WAT26810 |
|    | *FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,    | WAT26820 |
|    | *ITDS,ITER,K,KTOT,KW,LAMBDA,LH20,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL,   | WAT26830 |
|    | *NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE,    | WAT26840 |
|    | *PEAS,PEDO,PEDO2,PEFE,PEN,PENO2,PEPT,PES,PH,PRNT,PTOT,PUNCH,R,     | WAT26850 |
|    | *RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,               | WAT26860 |
|    | *T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT             | WAT26870 |
|    | COMMON/CHRDAT/CARD1,CARD2                                          |          |
| C  |                                                                    | WAT26880 |

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DATA LISTE/0,1,2,3,4,5,6,7,8,9,10,17,23,26,35,38,44,46,48,50,51, WAT26890
*61,67,80,84,87,89,94,96,97,101,106,108,109,114,130,138,145,151, WAT26900
*160,167,182,192,204,208,212,224,250,255,258/ WAT26910
DATA LISTE1/10,11,12,17,18,36,40,43,45,46,48,49,51,54,62,63,95,96, WAT26920
*97,99,100,106,110,111,112,114,119,128,140,155,157,158,159,47,50, WAT26930
*52,65,66,107,108,109,113,115,184,185,190,193,194,195,198,199,204, WAT26940
*205,239,240,242,248,288,289,292,293,330,331,337,338,339,340,365, WAT26950
*376,389,396,401,411,419,437,445,472,500,501/ WAT26960
DATA LISTE2/0,1,2,3,4,5,6,7,8,13,16,17,34,38,44,48,50,61,80,84,86, WAT26970
*87,89,94,96,97,202/ WAT26980
C WAT26990
C ** CONVERT VALUES OF ALPHA AND CUNITS TO LOG FORM FOR EQPLOT ** WAT27000
C ** PUNCHOUT BY INSERTING PAGE1 REFERENCE NUMBERS INTO CARDS ** WAT27010
C ** 5080 AND 5090 AT END OF PROCEDURE SOLUTS. ** WAT27020
C WAT27030
C**** DUPLICATE DESCRIPTOR CARDS */ WAT27040
C WAT27050
WRITE(7,1000) CARD1 WAT27060
WRITE(7,1000) CARD2 WAT27070
1000 FORMAT(A80) WAT27080
C WAT27090
C**** LOG ACTIVITY VALUES FOR SOLUTE CONSTITUENTS */ WAT27100
C WAT27110
N=0 WAT27120
C WAT27130
DO 10 J = 1, 50 WAT27140
I = LISTE(J) WAT27150
N=N+1 WAT27160
LP(N)=999. WAT27170
IF (ALFA(I).GT. -1D2 .AND. ALFA(I) .LT. 1D3) LP(N) = ALFA(I) WAT27180
10 CONTINUE WAT27190
C WAT27200
C**** LOG(AP) AND LOG(AP/K) FOR MINERAL PHASES */ WAT27210
C WAT27220
DO 20 J = 1, 79 WAT27230
I = LISTE1(J) WAT27240
N = N + 1 WAT27250
LP(N) = 999. WAT27260
IF (AP(I).GT. -1D3 .AND. AP(I) .LT. 1D3) LP(N) = AP(I) WAT27270
N=N+1 WAT27280
C3 = AP(I) - LOGKT(I) WAT27290
LP(N) = 999. WAT27300
IF (C3.GT. -1D2 .AND. C3.LT.1D3) LP(N) = C3 WAT27310
20 CONTINUE WAT27320
C WAT27330
C**** LOG CONCENTRATION OF MAJOR CONSTITUENTS */ WAT27340
C WAT27350
DO 25 J = 1, 27 WAT27360
I = LISTE2(J) WAT27370
N=N+1 WAT27380
LP(N) = 999. WAT27390
IF (CUNITS(I).GT. -1D2 .AND. CUNITS(I) .LT. 1D3) LP(N) = CUNITS(I) WAT27400
25 CONTINUE WAT27410
C WAT27420

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|                                                    |          |
|----------------------------------------------------|----------|
| C***** LOG CONCENTRATION(UG/L)OF TRACE ELEMENTS */ | WAT27430 |
| C                                                  | WAT27440 |
| N=N+1                                              | WAT27450 |
| LP(N) = 999.                                       | WAT27460 |
| IF (CUNITS(212).GT.-1D2 .AND. CUNITS(212).LT.1D3)  | WAT27470 |
| *LP(N)=CUNITS(212)+3.                              | WAT27480 |
| N=N+1                                              | WAT27490 |
| LP(N) = 999.                                       | WAT27500 |
| IF (CUNITS(249).GT.-1D2 .AND. CUNITS(249).LT.1D3)  | WAT27510 |
| *LP(N)=CUNITS(249)+3.                              | WAT27520 |
| N=N+1                                              | WAT27530 |
| LP(N) = 999.                                       | WAT27540 |
| IF (CUNITS(261).GT.-1D2 .AND. CUNITS(261).LT.1D3)  | WAT27550 |
| *LP(N)=CUNITS(261)+3.                              | WAT27560 |
| N=N+1                                              | WAT27570 |
| LP(N) = 999.                                       | WAT27580 |
| IF (CUNITS(262).GT.-1D2 .AND. CUNITS(262).LT.1D3)  | WAT27590 |
| *LP(N)=CUNITS(262)+3.                              | WAT27600 |
| N=N+1                                              | WAT27610 |
| LP(N) = 999.                                       | WAT27620 |
| IF (CUNITS(160).GT.-1D2 .AND. CUNITS(160).LT.1D3)  | WAT27630 |
| *LP(N)=CUNITS(160)+3.                              | WAT27640 |
| N=N+1                                              | WAT27650 |
| LP(N)=999.                                         | WAT27660 |
| IF (CO .GT. 0.0) LP(N)=DLOG10(CO*1D3)              | WAT27670 |
| N=N+1                                              | WAT27680 |
| LP(N) = 999.                                       | WAT27690 |
| IF (CR .GT. 0.0) LP(N) =DLOG10(CR*1D3)             | WAT27700 |
| N=N+1                                              | WAT27710 |
| LP(N) = 999.                                       | WAT27720 |
| IF (CUNITS(130).GT.-1D2 .AND. CUNITS(130).LT.1D3)  | WAT27730 |
| *LP(N)=CUNITS(130)+3                               | WAT27740 |
| N=N+1                                              | WAT27750 |
| LP(N) = 999.                                       | WAT27760 |
| IF (HG.GT.0.0) LP(N) = DLOG10(HG*1D3)              | WAT27770 |
| N=N+1                                              | WAT27780 |
| LP(N) = 999.                                       | WAT27790 |
| IF (CUNITS(109).GT.-1D2 .AND. CUNITS(109).LT.1D3)  | WAT27800 |
| *LP(N)=CUNITS(109)+3                               | WAT27810 |
| N=N+1                                              | WAT27820 |
| LP(N) = 999.                                       | WAT27830 |
| IF (MO.GT.0.0) LP(N) = DLOG10(MO*1D3)              | WAT27840 |
| N=N+1                                              | WAT27850 |
| LP(N) = 999.                                       | WAT27860 |
| IF (CUNITS(204).GT.-1D2 .AND. CUNITS(204).LT.1D3)  | WAT27870 |
| *LP(N)=CUNITS(204)+3.                              | WAT27880 |
| N=N+1                                              | WAT27890 |
| LP(N) = 999.                                       | WAT27900 |
| IF (CUNITS(182).GT.-1D2 .AND. CUNITS(182).LT.1D3)  | WAT27910 |
| *LP(N)=CUNITS(182)+3.                              | WAT27920 |
| N=N+1                                              | WAT27930 |
| LP(N) = 999.                                       | WAT27940 |
| IF (CUNITS(145).GT.-1D2 .AND. CUNITS(145).LT.1D3)  | WAT27950 |
| *LP(N)=CUNITS(145)+3.                              | WAT27960 |

|       |                                                                    |          |
|-------|--------------------------------------------------------------------|----------|
| C     | IF (PEPT.GT.19.) PEPT = 999.                                       | WAT27970 |
|       | IF (PEFE.GT.19.) PEFE = 999.                                       | WAT27980 |
|       | IF (PEN02.GT.19.) PEN02 = 999.                                     | WAT27990 |
| C     |                                                                    | WAT28000 |
| C**** | PUNCH OUT THE ARRAY LP WITH ALL SELECTED VALUES IN SEQUENCE */     | WAT28010 |
| C     |                                                                    | WAT28020 |
|       | WRITE(7,1010)TEMP,PH,PEPT,PEFE,PEN02,AH2O,(LP(I), I = 1, N)        | WAT28030 |
| 1010  | FORMAT(10F8.3)                                                     | WAT28040 |
| C     |                                                                    | WAT28050 |
| C**** | BLANK DATASET SEPARATOR CARD */                                    | WAT28060 |
| C     |                                                                    | WAT28070 |
|       | WRITE(7,1020)                                                      | WAT28080 |
| 1020  | FORMAT(1H ,1X)                                                     | WAT28090 |
|       | RETURN                                                             | WAT28100 |
|       | END                                                                | WAT28110 |
|       | SUBROUTINE ERRCLC(CUNITS,SIGMA,ERR)                                | WAT28120 |
| C     |                                                                    | WAT28150 |
|       | REAL*8 CUNITS(0:297),SIGMA(0:297),ERR(0:543),RSD(0:297)            | WAT28160 |
|       | INTEGER LISTE(40)                                                  | WAT28170 |
|       | CHARACTER*80 CARD1,CARD2                                           | WAT28180 |
| C     |                                                                    | WAT28190 |
|       | REAL*8 ANLCO3,SO4TOT,FTOT,PTOT,CLTOT,H2STOT,FULVTT,HUMTOT          | WAT28200 |
|       | REAL*8 ITDS,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,EPMAN,EPMCAT,    | WAT28210 |
|       | *MO,NATOT,NEQU,NH4TOT,NI,NITOT,NONCRB,NORM,NO2TOT,PB,C1,C2,C3      | WAT28220 |
|       | INTEGER CORALK,D,E,G,H,PRNT,EHOPT,EMPOX,FULFLG,HUMFLG,ISDATA,      | WAT28230 |
|       | *ITER,NMBR,PUNCH,RBIT,FLAG                                         | WAT28240 |
| C     |                                                                    | WAT28250 |
|       | COMMON A,AG,AGTOT,AH2O,ALTOT,ANLCO3,AS,ASTOTL,AS3TOT,AS5TOT,B,     | WAT28260 |
|       | *BATOT,BTOT,C,CARBON,CATOT,CD,CDTOT,CLTOT,CO,CONCLC,COND,          | WAT28270 |
|       | *CORALK,CO2TIT,CO3ALC,CR,CSTOT,CU,CUTOT,C1,C2,C3,D,DATE,DENS,DIFF, | WAT28280 |
|       | *DISCHG,DOC,DOX,E,EHAS,EHDO,EHDO2,EHFE,EHM,EHN,EHNO,EHOPT,EHPT,    | WAT28290 |
|       | *EHS,EMPOX,EPMAN,EPMCAT,F,FETOTL,FE2TOT,FE3TOT,FLAG,FTOT,FULFLG,   | WAT28300 |
|       | *FULVTT,G,H,HCO3TT,HG,HUMFLG,HUMTOT,H2STOT,ISDATA,NATOT,XMUSAV,    | WAT28310 |
|       | *ITDS,ITER,K,KTOT,KW,LAMBDA,LH2O,LITOT,MGTOT,MNTOT,MO,XMU,XMUHL,   | WAT28320 |
|       | *NEQU,NH4TOT,NI,NITOT,NMBR,NONCRB,NORM,NO2TOT,PB,PBTOT,PCO2,PE,    | WAT28330 |
|       | *PEAS,PEDO,PEDO2,PEFE,PEN,PEN02,PEPT,PES,PH,PRNT,PTOT,PUNCH,R,     | WAT28340 |
|       | *RBIT,RSDDO,SIGMDO,SIGMEH,SIGMPH,SITOT,SO4TOT,SRTOT,               | WAT28350 |
|       | *T,TDS,TEMP,TENMPE,TENPH,XMI120,XMI121,XMI178,ZN,ZNTOT             | WAT28360 |
|       | COMMON/CHRDAT/CARD1,CARD2                                          | WAT28370 |
| C     |                                                                    | WAT28380 |
|       | DATA LISTE/0,1,2,3,4,5,6,7,8,13,16,17,26,34,38,44,48,50,61,63,     | WAT28390 |
|       | *71,80,84,86,87,89,94,96,97,109,130,145,160,182,202,204,212,249,   | WAT28400 |
|       | *261,262/                                                          | WAT28410 |
|       | DO 10 I = 0, 296                                                   | WAT28420 |
|       | RSD(I) = 2E7                                                       | WAT28430 |
| 10    | CONTINUE                                                           | WAT28440 |
|       | DO 20 J = 1, 40                                                    | WAT28450 |
|       | I = LISTE(J)                                                       | WAT28460 |
|       | C1 = 10.**CUNITS(I)                                                | WAT28470 |
|       | IF (C1 * SIGMA(I) .GT. 0.0) RSD(I) = SIGMA(I)/C1/C                 | WAT28480 |
| 20    | CONTINUE                                                           | WAT28490 |
|       | IF (RSD(17).GT. 1E7) RSD(17) = RSD(6)                              | WAT28500 |
|       | IF (RSD(8) .GT. 1E7) RSD(8) = RSD(7) * 2                           | WAT28510 |

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ERR(9)=SQRT((RSD(7))**2+(RSD(17))**2) WAT28520
ERR(10)=SQRT((RSD(1))**2+(RSD(17))**2) WAT28530
ERR(11)=SQRT((RSD(0))**2+(RSD(1))**2+(2*RSD(17))**2) WAT28540
ERR(21) = SQRT((RSD(0))**2 + (RSD(17))**2) WAT28550
ERR(12) = ERR(21) WAT28560
ERR(18) = SQRT((RSD(0))**2 + (RSD(5))**2) WAT28570
ERR(17) = ERR(18) WAT28580
ERR(153)=SQRT((2*RSD(1))**2 + (3*RSD(34))**2 + (4*SIGMPH)**2) WAT28590
ERR(36) = ERR(153) WAT28600
ERR(40)=SQRT(RSD(2)**2+RSD(50)**2+(3*RSD(34))**2) WAT28610
ERR(41) = SQRT(RSD(0)**2 + (2*RSD(50))**2 + (2*RSD(34))**2) WAT28620
ERR(45) = SQRT((.6*RSD(3))**2 + (.25*RSD(1))**2 + (2.3*RSD(50))**2 WAT28630
*+(3.5*RSD(34))**2+(1.2*SIGMPH)**2) WAT28640
ERR(46) = SQRT((2*RSD(50))**2 + (2*RSD(34))**2 + (2*SIGMPH)**2) WAT28650
ERR(47) = ERR(46) WAT28660
ERR(168) = SQRT((RSD(50))**2+(3*SIGMPH)**2) WAT28670
ERR(51) = ERR(168) WAT28680
ERR(140)= ERR(168) WAT28690
ERR(54) =SQRT( (.5*(RSD(2)+RSD(3)))**2 + (RSD(50))**2+ WAT28700
*(3*RSD(34))**2) WAT28710
ERR(62) = SQRT((RSD(0))**2 + (2*RSD(61))**2) WAT28720
ERR(63) = SQRT((.167*RSD(0))**2 + (2.33*RSD(50))**2 WAT28730
*+(3.67*RSD(34))**2 + (2*SIGMPH)**2) WAT28740
ERR(67) = SQRT((RSD(7))**2+(RSD(13))**2) WAT28750
ERR(119) = ERR(67) WAT28760
ERR(95) = SQRT((5*RSD(0))**2 + (3*RSD(44))**2 + (4*SIGMPH)**2) WAT28770
C WAT28780
C**** SIO2 WAT28790
C WAT28800
ERR(97) = RSD(34) WAT28810
ERR(99) = RSD(34) WAT28820
ERR(100) = RSD(34) WAT28830
ERR(101) = RSD(34) WAT28840
ERR(395) = RSD(34) WAT28850
C WAT28860
ERR(106) = SQRT((3*RSD(7))**2 + (2*RSD(44))**2) WAT28870
ERR(112) = SQRT((RSD(8))**2 + (3*SIGMPH)**2) WAT28880
ERR(115) = SQRT((.277*RSD(2))**2 + (.277*RSD(3))**2 WAT28890
*+(.277*SIGMPH)**2 + (.29*RSD(1))**2 + (.23*RSD(8))**2 WAT28900
*+(1.58*RSD(50))**2 + (3.93*RSD(34))**2) WAT28910
ERR(116) = SQRT((.277*RSD(2))**2 + (.277*RSD(3))**2 WAT28920
*+(.277*SIGMPH)**2 + (.45*RSD(1))**2 + (.34*RSD(8))**2 WAT28930
*+(1.47*RSD(50))**2 + (3.82*RSD(34))**2 + (.76*SIGMPH)**2) WAT28940
ERR(117) = SQRT((3*RSD(1))**2 + (RSD(0))**2 + (4*RSD(17))**2) WAT28950
ERR(142) = SQRT(RSD(87)**2 + RSD(17)**2) WAT28960
ERR(143) = SQRT(RSD(87)**2 + RSD(5)**2) WAT28970
ERR(144) = SQRT(RSD(89)**2 + RSD(5)**2) WAT28980
ERR(145) = SQRT(RSD(89)**2 + RSD(17)**2) WAT28990
ERR(147) = SQRT((2*RSD(0))**2 + (4*RSD(50))**2 + (8*RSD(34))**2) WAT29000
C1 = 1.24 - .135*PH WAT29010
ERR(157) = SQRT(((1-C1)*RSD(50))**2 + (C1*RSD(34))**2 WAT29020
*+(3-3*C1)*SIGMPH)**2) WAT29030
ERR(158) = ERR(157) WAT29040
ERR(204) = SQRT((RSD(2))**2 + (2*RSD(5))**2 + (3*RSD(8))**2 WAT29050

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|      |                                                                                 |          |
|------|---------------------------------------------------------------------------------|----------|
|      | *+(6*SIGMPH)**2)                                                                | WAT29060 |
|      | ERR(205) = SQRT((RSD(3))**2 + (2*RSD(5))**2 + (3*RSD(8))**2                     | WAT29070 |
|      | *+(6*SIGMPH)**2)                                                                | WAT29080 |
|      | ERR(230) = SQRT((RSD(130))**2 + (2*RSD(4))**2)                                  | WAT29090 |
|      | ERR(235) = SQRT((2*RSD(130))**2 + (RSD(6))**2 + (3*SIGMPH)**2)                  | WAT29100 |
|      | ERR(236) = SQRT((3*RSD(130))**2 + (2*RSD(6))**2 + (4*SIGMPH)**2)                | WAT29110 |
|      | ERR(242) = SQRT((RSD(130))**2 + (2*SIGMPH)**2)                                  | WAT29120 |
|      | ERR(268) = SQRT((RSD(145))**2 + (RSD(17))**2)                                   | WAT29130 |
|      | ERR(269) = ERR(268)                                                             | WAT29140 |
|      | ERR(288) = SQRT((RSD(145))**2 + (RSD(34))**2 + (2*SIGMPH)**2)                   | WAT29150 |
|      | ERR(315) = SQRT((RSD(160))**2 + (RSD(17))**2)                                   | WAT29160 |
|      | ERR(339) = SQRT((RSD(7))**2 + (RSD(5))**2)                                      | WAT29170 |
|      | ERR(365) = SQRT((RSD(182))**2 + (RSD(17))**2)                                   | WAT29180 |
|      | ERR(374) = SQRT((RSD(182))**2 + (RSD(44))**2)                                   | WAT29190 |
|      | ERR(376) = SQRT((5*RSD(182))**2 + (3*RSD(44))**2 + RSD(4)**2)                   | WAT29200 |
|      | ERR(379) = SQRT((RSD(182))**2 + (3*RSD(50))**2 + (2*RSD(44))**2 +               | WAT29210 |
|      | *(5*SIGMPH)**2)                                                                 | WAT29220 |
|      | ERR(419) = SQRT((2*RSD(8))**2 + (RSD(7))**2 + 2*(2*RSD(8))*(RSD(7)              | WAT29230 |
|      | *)+(8*SIGMPH)**2)                                                               | WAT29240 |
|      | ERR(471) = SQRT((RSD(50))**2 + (RSD(5))**2 + SIGMPH**2)                         | WAT29250 |
|      | ERR(472) = SQRT((4*RSD(50))**2 + (RSD(5))**2 + (10*SIGMPH)**2)                  | WAT29260 |
|      | RETURN                                                                          | WAT29270 |
|      | END                                                                             | WAT29280 |
|      | SUBROUTINE PHASES(PAGE2, INDEX, AP, DH, LOGKT, MAXKTO, MINKTO, ERR, ERRT)       | WAT29300 |
| C    |                                                                                 | WAT29320 |
|      | REAL*8 AP(0:543), DH(0:543), LOGKT(0:543), MAXKTO(0:543),                       | WAT29330 |
|      | *MINKTO(0:543), ERR(0:543), ERRT(0:543)                                         | WAT29340 |
|      | INTEGER INDEX(1:297)                                                            | WAT29350 |
|      | CHARACTER*80 CARD1, CARD2                                                       | WAT29360 |
|      | CHARACTER*12 PAGE2(0:543)                                                       | WAT29370 |
| C    |                                                                                 | WAT29380 |
|      | REAL*8 ANLCO3, SO4TOT, FTOT, PTOT, CLTOT, H2STOT, FULVTT, HUMTOT                | WAT29390 |
|      | REAL*8 ITDS, KTOT, KW, LAMBDA, LH2O, LITOT, MGTOT, MNTOT, EPMAN, EPMCAT,        | WAT29400 |
|      | *MO, NATOT, NEQU, NH4TOT, NI, NITOT, NONCRB, NORM, NO2TOT, PB, C1, C2, C3       | WAT29410 |
|      | INTEGER CORALK, D, E, G, H, PRNT, EHOPT, EMPOX, FULFLG, HUMFLG, ISDATA,         | WAT29420 |
|      | *ITER, NMBR, PUNCH, RBIT, FLAG                                                  | WAT29430 |
| C    |                                                                                 | WAT29440 |
|      | COMMON A, AG, AGTOT, AH2O, ALTOT, ANLCO3, AS, ASTOTL, AS3TOT, AS5TOT, B,        | WAT29450 |
|      | *BATOT, BTOT, C, CARBON, CATOT, CD, CDTOT, CLTOT, CO, CONCLC, COND,             | WAT29460 |
|      | *CORALK, CO2TIT, CO3ALC, CR, CSTOT, CU, CUTOT, C1, C2, C3, D, DATE, DENS, DIFF, | WAT29470 |
|      | *DISCHG, DOC, DOX, E, EHAS, EHDO, EHDO2, EHFE, EHM, EHN, EHNO, EHOPT, EHPT,     | WAT29480 |
|      | *EHS, EMPOX, EPMAN, EPMCAT, F, FETOTL, FE2TOT, FE3TOT, FLAG, FTOT, FULFLG,      | WAT29490 |
|      | *FULVTT, G, H, HCO3TT, HG, HUMFLG, HUMTOT, H2STOT, ISDATA, NATOT, XMUSAV,       | WAT29500 |
|      | *ITDS, ITER, K, KTOT, KW, LAMBDA, LH2O, LITOT, MGTOT, MNTOT, MO, XMU, XMUHL,    | WAT29510 |
|      | *NEQU, NH4TOT, NI, NITOT, NMBR, NONCRB, NORM, NO2TOT, PB, PBTOT, PCO2, PE,      | WAT29520 |
|      | *PEAS, PEDO, PEDO2, PEFE, PEN, PENO2, PEPT, PES, PH, PRNT, PTOT, PUNCH, R,      | WAT29530 |
|      | *RBIT, RSDDO, SIGMDO, SIGMEH, SIGMPH, SITOT, SO4TOT, SRTOT,                     | WAT29540 |
|      | *T, TDS, TEMP, TENMPE, TENPH, XMI120, XMI121, XMI178, ZN, ZNTOT                 | WAT29550 |
|      | COMMON/CHRDAT/CARD1, CARD2                                                      |          |
| C    |                                                                                 | WAT29560 |
|      | WRITE(K, 1000) CARD1                                                            |          |
| 1000 | FORMAT(1H1, 1X, A80/)                                                           |          |
|      | WRITE(K, 1010)                                                                  | WAT29570 |
| 1010 | FORMAT (' Phase Log AP/KT Sigma(A) Sigma(T)                                     | WAT29580 |



|      |                                                                                 |          |
|------|---------------------------------------------------------------------------------|----------|
|      | *Log AP/MinKT    Log AP/MaxKT    Log AP    Log KT    Log MinKT    Log           | WAT29590 |
|      | *MaxKT')                                                                        | WAT29600 |
|      | IN = 0                                                                          | WAT29610 |
| C    |                                                                                 | WAT29620 |
|      | C1 = (298.16 - T) / (298.16 * T*C*R)                                            | WAT29630 |
|      | DO 10 N = 1, G                                                                  | WAT29640 |
|      | I = INDEX(N)                                                                    | WAT29650 |
|      | C2 = AP(I)                                                                      | WAT29660 |
|      | IF (ABS(C2) .GE. 5E2) GOTO 10                                                   | WAT29670 |
|      | S1 = 0.0                                                                        | WAT29680 |
|      | S2 = 0.0                                                                        | WAT29690 |
|      | IF (ABS(MINKTO(I)) .LT. 1D-78) GOTO 20                                          | WAT29700 |
|      | S1 = MINKTO(I) - DH(I) * C1                                                     | WAT29710 |
|      | S2 = C2 - S1                                                                    | WAT29720 |
| 20   | CONTINUE                                                                        | WAT29730 |
|      | S3 = 0.0                                                                        | WAT29740 |
|      | S4 = 0.0                                                                        | WAT29750 |
|      | S5 = LOGKT(I)                                                                   | WAT29760 |
|      | IF (ABS(MAXKTO(I)) .LT. 1D-78) GOTO 30                                          | WAT29770 |
|      | S3 = MAXKTO(I) - DH(I) * C1                                                     | WAT29780 |
|      | S4 = C2 - S3                                                                    | WAT29790 |
| 30   | S6 = 0.0                                                                        | WAT29800 |
|      | IF (ABS(LOGKT(I)) .GT. 1D-78) S6 = C2 - LOGKT(I)                                | WAT29810 |
|      | S7 = 0.0                                                                        | WAT29820 |
|      | S8 = 0.0                                                                        | WAT29830 |
|      | IF (ERR(I) .LT. 5E2) S7 = ERR(I)                                                | WAT29840 |
|      | IF (ERRT(I) .GT. 0.0) S8 = ERRT(I)                                              | WAT29850 |
|      | WRITE(K,1100) I, PAGE2(I), S6, S7, S8, S2, S4, C2, S5, S1, S3                   | WAT29860 |
| 1100 | FORMAT(' ', I3, 1X, A12, 3F11.3, 2F15.3, 4F11.3)                                | WAT29870 |
|      | IN = IN + 1                                                                     | WAT29880 |
|      | IF (IN .LT. 57) GOTO 10                                                         | WAT29890 |
|      | IN = 0                                                                          | WAT29900 |
|      | WRITE(K,1000) CARD1                                                             |          |
|      | WRITE(K,1010)                                                                   | WAT29910 |
| 10   | CONTINUE                                                                        | WAT29920 |
|      | RETURN                                                                          | WAT29930 |
|      | END                                                                             | WAT29940 |
|      | SUBROUTINE INPUT(PAGE1, CUNITS, SIGMA, LOGKT, ENDE)                             | WAT29970 |
| C    |                                                                                 | WAT29980 |
|      | REAL*8 XIN(17), CUNITS(0:297), SIGMA(0:297), LOGKTO(0:543)                      | WAT29990 |
|      | INTEGER LISTE(17), VAL(4)                                                       | WAT30000 |
|      | CHARACTER*80 CARD1, CARD2                                                       | WAT30010 |
|      | CHARACTER*8 PAGE1(0:297)                                                        | WAT30020 |
|      | CHARACTER*4 CARD(4), CONZ(4), WORD, FLG                                         | WAT30030 |
| C    |                                                                                 | WAT30040 |
|      | REAL*8 ANLCO3, SO4TOT, FTOT, PTOT, CLTOT, H2STOT, FULVTT, HUMTOT                | WAT30050 |
|      | REAL*8 ITDS, KTOT, KW, LAMBDA, LH2O, LITOT, MGTOT, MNTOT, EPMAN, EPMCAT,        | WAT30060 |
|      | *MO, NATOT, NEQU, NH4TOT, NI, NITOT, NONCRB, NORM, NO2TOT, PB, C1, C2, C3       | WAT30070 |
|      | INTEGER CORALK, D, E, G, H, PRNT, EHOPT, EMPOX, ENDE, FULFLG, HUMFLG, ISDATA,   | WAT30080 |
|      | *ITER, NMBR, PUNCH, RBIT, FLAG                                                  | WAT30090 |
| C    |                                                                                 | WAT30100 |
|      | COMMON A, AG, AGTOT, AH2O, ALTOT, ANLCO3, AS, ASTOTL, AS3TOT, AS5TOT, B,        | WAT30110 |
|      | *BATOT, BTOT, C, CARBON, CATOT, CD, CDTOT, CLTOT, CO, CONCLC, COND,             | WAT30120 |
|      | *CORALK, CO2TIT, CO3ALC, CR, CSTOT, CU, CUTOT, C1, C2, C3, D, DATE, DENS, DIFF, | WAT30130 |

|                                                                              |          |
|------------------------------------------------------------------------------|----------|
| *DISCHG, DOC, DOX, E, EHAS, EHDO, EHDO2, EHFE, EHM, EHN, EHNO, EHOPT, EHPT,  | WAT30140 |
| *EHS, EMPOX, EPMAN, EPMCAT, F, FETOTL, FE2TOT, FE3TOT, FLAG, FTOT, FULFLG,   | WAT30150 |
| *FULVTT, G, H, HCO3TT, HG, HUMFLG, HUMTOT, H2STOT, ISDATA, NATOT, XMUSAV,    | WAT30160 |
| *ITDS, ITER, K, KTOT, KW, LAMBDA, LH2O, LITOT, MGTOT, MNTOT, MO, XMU, XMUHL, | WAT30170 |
| *NEQU, NH4TOT, NI, NITOT, NMBR, NONCRB, NORM, NO2TOT, PB, PBTOT, PCO2, PE,   | WAT30180 |
| *PEAS, PEDO, PEDO2, PEFE, PEN, PENO2, PEPT, PES, PH, PRNT, PTOT, PUNCH, R,   | WAT30190 |
| *RBIT, RSDDO, SIGMDO, SIGMEH, SIGMPH, SITOT, SO4TOT, SRTOT,                  | WAT30200 |
| *T, TDS, TEMP, TENMPE, TENPH, XMI120, XMI121, XMI178, ZN, ZNTOT              | WAT30210 |
| COMMON/CHRDAT/CARD1, CARD2                                                   |          |
| C                                                                            | WAT30220 |
| DATA LISTE/0,1,2,3,4,5,6,16,13,17,34,38,86,44,50,61,84/                      | WAT30230 |
| DATA CARD/'CUN ', 'SIGM', 'LOKT', ' ' /                                      | WAT30240 |
| DATA CONZ/'MQ/L', 'MG/L', 'PPM ', 'MOL ' /                                   | WAT30250 |
| C                                                                            | WAT30260 |
| READ(5,560)CARD1                                                             | WAT30270 |
| READ(5,560)CARD2                                                             | WAT30280 |
| 560 FORMAT(A80)                                                              | WAT30290 |
| WRITE(1,560)CARD1                                                            | WAT30300 |
| 1011 FORMAT(1H1,1X,A80)                                                      | WAT30310 |
| 1111 FORMAT(1H ,A80)                                                         | WAT30330 |
| IF (K.NE.1) THEN                                                             |          |
| WRITE(K,1011)CARD1                                                           |          |
| WRITE(K,1111)CARD2                                                           |          |
| END IF                                                                       |          |
| READ(5,570)                                                                  | WAT30340 |
| READ(5,570) TEMP, PH, EHM, DOC, DOX, CORALC                                  | WAT30350 |
| 570 FORMAT (6(F8.2,1X))                                                      | WAT30360 |
| WRITE(K,1112)TEMP , PH ,EHM ,DOC ,DOX ,CORALC                                | WAT30370 |
| 1112 FORMAT (1X,' TEMP = ',F16.6,/,                                          | WAT30380 |
| *' PH = ',F16.6,/,                                                           | WAT30390 |
| *' EHM = ',F16.6,/,                                                          | WAT30400 |
| *' DOC = ',F16.6,/,                                                          | WAT30410 |
| *' DOX = ',F16.6,/,                                                          | WAT30420 |
| *' CORALC = ',F16.6)                                                         | WAT30430 |
| READ(5,575)                                                                  | WAT30440 |
| READ(5,575) FLG,DENS,PRNT,PUNCH,EHOPT                                        | WAT30450 |
| 575 FORMAT (A4,F11.5,3I6)                                                    | WAT30460 |
| IF (DENS .LT. 1D-78) DENS = 1.0                                              | WAT30470 |
| IF (FLG . EQ. CONZ(1)) FLAG = 1                                              | WAT30480 |
| IF (FLG . EQ. CONZ(2)) FLAG = 2                                              | WAT30490 |
| IF (FLG . EQ. CONZ(3)) FLAG = 3                                              | WAT30500 |
| IF (FLG . EQ. CONZ(4)) FLAG = 4                                              | WAT30510 |
| WRITE(K,1113)FLG, DENS,PRNT,PUNCH,EHOPT                                      | WAT30520 |
| 1113 FORMAT(' FLG = ',A4,/,                                                  | WAT30530 |
| *' DENS = ',F16.6,/,                                                         | WAT30540 |
| *' PRNT = ',I8,/,                                                            | WAT30550 |
| *' PUNCH = ',I8,/,                                                           | WAT30560 |
| *' EHOPT = ',I8)                                                             | WAT30570 |
| READ(5,570)                                                                  | WAT30580 |
| READ(5,585) EMPOX, ITDS, COND, SIGMDO, SIGMEH, SIGMPH                        | WAT30590 |
| 585 FORMAT(I8,1X,2(F8.2,1X),3F12.4)                                          |          |
| WRITE(K,1114)EMPOX,ITDS,COND,SIGMDO,SIGMEH,SIGMPH                            | WAT30630 |
| 1114 FORMAT(' EMPOX = ',I8,/,                                                | WAT30640 |
| *' ITDS = ',F16.6,/,                                                         | WAT30660 |

|      |                                        |          |                         |          |
|------|----------------------------------------|----------|-------------------------|----------|
| *'   | COND                                   | =        | ' ,F16.6,/,             | WAT30680 |
| *'   | SIGMDO                                 | =        | ' ,F16.6,/,             | WAT30690 |
| *'   | SIGMEH                                 | =        | ' ,F16.6,/,             | WAT30700 |
| *'   | SIGMPH                                 | =        | ' ,F16.6,/,             | WAT30710 |
| *'   | Species                                | Index No | Input Concentration'//, |          |
| *'   | -----')                                |          |                         |          |
|      | READ(5,620)                            |          |                         | WAT30720 |
|      | READ(5,620)(XIN(I),I=1,6)              |          |                         | WAT30730 |
|      | READ(5,620)                            |          |                         | WAT30740 |
|      | READ(5,620)(XIN(I),I=7,12)             |          |                         | WAT30750 |
|      | READ(5,620)                            |          |                         | WAT30760 |
|      | READ(5,620)(XIN(I),I=13,17)            |          |                         | WAT30770 |
| 620  | FORMAT(6F12.4)                         |          |                         | WAT30780 |
|      | DO 90 I=1,17                           |          |                         | WAT30790 |
|      | J = LISTE(I)                           |          |                         | WAT30800 |
|      | CUNITS(J) = XIN(I)                     |          |                         | WAT30810 |
|      | WRITE(K,1116)PAGE1(J),J,CUNITS(J)      |          |                         | WAT30820 |
| 1116 | FORMAT(' ,A8,' : ' ,I3,' : ' ,F16.8)   |          |                         | WAT30830 |
| 90   | CONTINUE                               |          |                         | WAT30840 |
|      | READ(5,620)                            |          |                         | WAT30850 |
| C    |                                        |          |                         | WAT30860 |
| 80   | READ(5,630) WORD,(VAL(I),XIN(I),I=1,4) |          |                         | WAT30870 |
| 630  | FORMAT(A4,4(1X,I3,1X,F12.5))           |          |                         | WAT30880 |
| C    |                                        |          |                         | WAT30890 |
|      | IF(WORD .NE. CARD(1)) GOTO 100         |          |                         | WAT30900 |
|      | DO 95 I = 1 ,4                         |          |                         | WAT30910 |
|      | IF (XIN(I) .LT. 1D-78) GOTO 95         |          |                         | WAT30920 |
|      | J = VAL(I)                             |          |                         | WAT30930 |
|      | CUNITS(J) = XIN(I)                     |          |                         | WAT30940 |
|      | WRITE(K,1116)PAGE1(J),J,CUNITS(J)      |          |                         | WAT30950 |
| 95   | CONTINUE                               |          |                         | WAT30960 |
|      | GOTO 80                                |          |                         | WAT30970 |
| C    |                                        |          |                         | WAT30980 |
| 100  | IF(WORD .NE. CARD(2)) GOTO 120         |          |                         | WAT30990 |
|      | DO 110 I = 1 ,4                        |          |                         | WAT31000 |
|      | IF (XIN(I) .LT. 1D-78) GOTO 110        |          |                         | WAT31010 |
|      | J = VAL(I)                             |          |                         | WAT31020 |
|      | SIGMA(J) = XIN(I)                      |          |                         | WAT31030 |
| 110  | CONTINUE                               |          |                         | WAT31040 |
|      | GOTO 80                                |          |                         | WAT31050 |
| C    |                                        |          |                         | WAT31060 |
| 120  | IF(WORD .NE. CARD(3)) GOTO 140         |          |                         | WAT31070 |
|      | DO 130 I = 1 ,4                        |          |                         | WAT31080 |
|      | IF (XIN(I) .LT. 1D-78) GOTO 130        |          |                         | WAT31090 |
|      | J = VAL(I)                             |          |                         | WAT31100 |
|      | LOGKTO(J) = XIN(I)                     |          |                         | WAT31110 |
| 130  | CONTINUE                               |          |                         | WAT31120 |
|      | GOTO 80                                |          |                         | WAT31130 |
| 140  | CONTINUE                               |          |                         |          |
| C    |                                        |          |                         | WAT31140 |
|      | IF ( WORD .EQ.CARD(4)) ENDE = 1        |          |                         | WAT31150 |
|      | RETURN                                 |          |                         | WAT31160 |
|      | END                                    |          |                         |          |



United States Department of the Interior

GEOLOGICAL SURVEY  
Pacific Northwest District, Oregon Office  
Water Resources Division  
847 NE 19th Avenue, Suite 300  
Portland, OR 97232  
June 20, 1988

## ERRATA AND REVISION SHEET FOR OPEN-FILE REPORT 87-50. WATEQ4F

On page 7, Line 19, which starts "CORALC", should read:

CORALK alkalinity correction flag I8 0, 1 or 2

On page 54 in Attachment B, Program Listing of WATEQ4F, the code in line 10, which starts with " 155 CALL INPUT . . ." has been changed to read:

```
155 CALL INPUT(PAGE1,CUNITS,SIGMA,LOGKTO,ENDE)                                WAT02930
```

On page 106, the code in line 38, which starts "SUBROUTINE INPUT . . ." has been changed to read:

SUBROUTINE INPUT(PAGE1,CUNITS,SIGMA,LOGKTO,ENDE) WAT29970

The purpose of these two changes is to pass the correct variable (LOGKTO, rather than LOGKT) to the input subroutine for the temporary replacement of  $\text{Log}_{10}K_r$  values in the optional input section of a data set.

On Page 107 of Attachment B, in the three lines in which the variable name CORALC appears, the computer code has been changed so that the variable name is CORALK. The line numbers are WAT30350, 30370, and 30430. The format code in line WAT30360 has been changed from (6(F8.2,1X)) to (5(F8.2,1X),I8), and the format in line WAT30430 has been changed from F16.6 to I9.

These changes have substituted the global integer variable CORALK for the local floating-point variable CORALC, and modified the format codes appropriately. The alkalinity input flag may now be used exactly as in the original WATEQ. WATEQ4F and WQ4FINPT versions mailed prior to 12/15/87 must be modified and replaced, respectively, if use of the CORALK parameter is desired. Note that the modified WATEQ4F will NOT read earlier data sets.

On page 81, line 2 (WAT16820) has been modified to read:

```
IF (CORALK .EQ. 0) ANLCO3 = DMAX1(0.0D0, (DBLE(CO2TIT)-NONCRB))
```

This is merely a safeguard to prevent program failure in the event that noncarbonate alkalinity becomes greater than input total (carbonate + noncarbonate) alkalinity. Users are cautioned, however, that the above condition is an indication that something is badly wrong with the input data, and modeling results may well be meaningless.



On page 89, line 42 (following WAT21380) has been modified to read:

```
IF (ABS(DIFF1) .LE. 30.) GOTO 320
```

This corrects a minor error in that a charge imbalance warning message was only printed if the charge imbalance was greater than +30%. The message is now printed if the charge imbalance is either greater than +30% or less than -30%.

On Page 51, following line 37 (WAT01680), a new DO loop has been constructed to correctly access members of the arrays INDEX and INDEX2, which have no zeroth member. The two records WAT01700 and WAT01710 have been moved into this loop.

### REVISIONS

A new version of subroutine PHASES has been written. The revised version places blank fields, rather than zero values, in the printed output of the mineral solubility calculations, in locations where no data are present.

In subroutine PREP, on page 56, near line 42 (WAT03960), a new expression for the dielectric constant of water from 0 to 100°C, from Uematsu and Franck (1980) has been added, per the recommendation of Nordstrom and others (1984), in WRI Report 84-4186.

In subroutine SET, on page 58, near line 36 (WAT04990), a new analytical expression for Kw has been added, from Olofsson and Olofsson (1981), per the recommendation of Nordstrom and others (1984), in WRI Report 84-4186.

J. W. Ball  
Chemist





BUREAU OF RECLAMATION  
DENVER OFFICE  
WATER QUALITY SECTION  
November 26, 1990

Memorandum

To: Judy Hamilton

From: Jim Yahnke

Subject: O'Neill Forebay Dam and Pumping Plant - Ground Water  
Quality Samples Collected October 30, 1990

I have taken the analytical results from the subject sampling and run them through the geochemical model WATEQ4F (Ball et al., 1987). There are a number of assumptions and conditions that I set in making the WATEQ runs that should be detailed. These include an assumed ambient temperature and dissolved oxygen (D.O.) for the samples, a computed Eh (reduction-oxidation potential), and an estimated H<sub>2</sub>S concentration. The temperature of all samples was set at 15° C, which was the temperature of most of the samples that I had to work with in my October memo. The D.O. was set at 0.0 mg/L in all samples; this is usually a reasonable assumption for ground water. The Eh was estimated from the pH using the following equation:

$$Eh = 0.70 - 0.06 \cdot pH$$

in accordance with the recommendation of Garrels (1960). Since there were oral reports of the presence of H<sub>2</sub>S in the samples at the time of collection, a small amount of H<sub>2</sub>S was added to each input data set for the WATEQ runs. The H<sub>2</sub>S was assumed to be greater than the threshold of detectable odor, which is estimated to be between 0.025 and 0.25 µg/L according to APHA (1989); H<sub>2</sub>S was arbitrarily set at 1 µg/L.

The WATEQ runs were made at both the field pH and the laboratory pH. This was done on the basis that the field pH was representative of *in situ* conditions, while the laboratory pH would represent a perturbed condition, although not necessarily that due to a dewatering well. One sample was also run with the H<sub>2</sub>S set to 0.0 mg/L.

The gypsum saturation indices of all samples at any pH or H<sub>2</sub>S concentration were well below saturation. This does not mean that there could be no precipitation of gypsum, but it does indicate that such precipitation is not to be expected.

Oversaturation with respect to calcite was shown in several of the samples at either the field or laboratory pH. All samples except that from DH-PTW-101-8 showed an increase in pH from the field to the laboratory. There was universal oversaturation with respect to calcite and aragonite at the laboratory pH. The saturation indices in all cases were fairly small, which would indicate that only small amounts of carbonates would be expected to precipitate from



```

PROGRAM WATEQF(INPUT,OUTPUT,TAPE9,TAPE5=INPUT)
C  **** PROGRAM WATEQF **** A FORTRAN IV VERSION OF WATEQ
C
C  REVISED FROM PL1 VERSION OF TRUESDELL AND JONES.
C  NIEL PLUMMER, SUMMER 1972.
C  LATEST REVISION DECEMBER, 1978.
C
C  **** DESCRIPTION OF INPUT - 5 CARDS ARE REQUIRED ****
C  CARD 1  TITLE, JOB DESCRIPTION. (20A4)
C  CARD 2  TEMP,PH,EHM,EHMC,EHMZ,DENS,DOX,FLAG,CORALK,PECALC,IGO,
C          (PRT(I),I=1,4),IDAVES,ISPEC,IMIN
C          (5(F6.0,1X),2F5.0,1X,9I1,2I3)
C  TEMP....TEMPERATURE IN DEGREES C
C  PH.....NEGATIVE LOG ACTIVITY H+
C  EHM.....PREFERRED EH ...SEE OPTIONS
C  EHMC....MEASURED EH ... SEE OPTIONS
C  EMFZ....MEASURED EH OF ZOBELL SOLUTION
C  DENS....DENSITY OF SOLUTION (G/CC)
C  DOX....DISSOLVED OXYGEN (MG/L)
C  FLAG....SIGNAL FOR UNITS OF INPUT CONCENTRATION.
C          0 (OR BLANK) = MMOL/L, 1=MEQ/L, 2=MG/L, 3=PPM, 4=MOLALITY.
C  CORALK..=0 IF ALKALINITY HAS NOT BEEN CORRECTED FOR BORON ETC.
C          AND THE ORIGINAL EXPRESSION OF WATEQ IS TO BE USED. =1 IF
C          CARBONATE ALKALINITY (CORRECTED FOR NON-CARBONATE ALKALINITY
C          SPECIES) HAS BEEN INPUT. =2 IF TOTAL INORGANIC CARBON IS
C          INPUT RATHER THAN ALKALINITY. =3 IF ALKALINITY HAS NOT BEEN
C          CORRECTED FRO BORON ETC. - SIMILAR TO CORALK=0, EXCEPT THAT
C          ALL POSSIBLE NON-CARBONATE ALKALINITY SPECIES ARE CONSIDERED.
C  PECALC..=0 WILL SET PE TO 100, =1 COMPUTES PE FROM EH,
C          =2 COMPUTES PE FROM DOX(THEORETICAL). = 3 COMPUTES PE FROM
C          THE SATO RELATION, = 4 COMPUTES PE FROM S-- - SO4--.
C  IGO..=0,OR BLANK, IF DESIRED TO HAVE DATA CHECKED FOR INPUT
C          ERROR. PH MUST BE GREATER THAN 3 AND LESS THAN 11, AND THE
C          ANALYSIS MUST HAVE LESS THAN 30% ERROR IN CHARGE BALANCE. =1
C          IF THIS CHECK IS NOT TO BE MADE.
C  (PRT(I),I=1,4), CAN BE SET TO 1 TO DELETE PRINT OF
C          THERMOCHEMICAL DATA,MASS BALANCE CONVERGENCE ITERATIONS,
C          RATIOS OF IONS, AND MINERAL SATURATION, RESPECTIVELY. PRT(I)
C          SHOULD BE SET TO ZERO OR BLANK TO OBTAIN THE RESPECTIVE PRINT.
C  IDAVES..=1, ACTIVITY COEFFICIENTS OF CHARGED ION PAIRS ARE
C          CALCULATED FROM THE DAVIES EQUATION. =0 (OR BLANK), ACTIVITY
C          COEFFICIENTS OF CHARGED ION PAIRS ARE CALCULATED FROM THE
C          DEBYE-HUCKEL EQUATION. IDAVES HAS NO EFFECT ON GAMMA(1)-
C          GAMMA(7), AND GAMMA(18).
C  ISPEC.. = NUMBER OF SPECIES DESIRED IN OUTPUT(IF LESS THAN TOTAL
C          POSSIBLE). TO OBTAIN OUTPUT OF MOLALITY, ACTIVITY, ETC. OF
C          ALL POSSIBLE SPECIES FOR THE DEFINED SYSTEM, LEAVE ISPEC
C          BLANK (OR ZERO). IF ISPEC GT. ZERO, ISPEC VALUES OF KSPEC
C          (SPECIES INDEX NUMBER) MUST BE READ (SEE BELOW). IF ISPEC =
C          BLANK (ZERO), OMIT KSPEC CARD(S).
C  IMIN.. = NUMBER OF MINERALS FOR WHICH SATURATION OUTPUT IS
C          DESIRED (IF LESS THAN TOTAL POSSIBLE). TO OBTAIN SATURATION
C          DATA ON ALL POSSIBLE MINERALS FOR THE DEFINED SYSTEM, LEAVE
C          IMIN BLANK (OR ZERO). IF IMIN GT. ZERO, IMIN VALUES OF KMIN
C          (MINERAL INDEX NUMBER) MUST BE READ (SEE BELOW). IF IMIN =
C          BLANK (OR ZERO), OMIT KMIN CARDS(S).
C  CARD 3  CA MG NA K CL SO4 (6(E12.5),8X)
C  CARD 4  HCO3 SIO2 FE PO4 SR F (6(E12.5),8X)
C          ... OPTIONAL CARDS OF TYPE 1 APPEAR HERE ...
C          ... OPTIONAL CARDS OF TYPE 2 APPEAR HERE ..
C  CARD 5  BLANK CARD (DENOTES END OF DATA FOR A PARTICULAR

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A  10
A  20
A  30
A  40
A  50
A  60
A  70
A  80
A  90
A 100
A 110
A 120
A 130
A 140
A 150
A 160
A 170
A 180
A 190
A 200
A 210
A 220
A 230
A 240
A 250
A 260
A 270
A 280
A 290
A 300
A 310
A 320
A 330
A 340
A 350
A 360
A 370
A 380
A 390
A 400
A 410
A 420
A 430
A 440
A 450
A 460
A 470
A 480
A 490
A 500
A 510
A 520
A 530
A 540
A 550
A 560
A 570
A 580
A 590
A 600
A 610

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C      WATER ANALYSIS.)
C
C      ....DESCRIPTION OF OPTIONAL INPUT....
C      ALL OPTIONAL INPUT MUST APPEAR BETWEEN CARDS 4 AND 5.
C      TYPE 1 CARDS MUST PRECEED TYPE 2 CARDS.
C
C      *****
C      TYPE 1 OPTIONAL INPUT CARDS
C      *****
C      (KSPEC(I),I=1,ISPEC) (1615) KSPEC(I) IS THE INDEX NUMBER OF THE
C      ITH SELECTED SPECIES FOR WHICH OUTPUT IS DESIRED. OMIT CARD
C      IF ISPEC = BLANK (OR ZERO).
C      (KMIN(I),I=1,IMIN) (1615) KMIN(I) IS THE INDEX NUMBER OF THE
C      ITH SELECTED MINERAL FOR WHICH SATURATION OUTPUT IS DESIRED.
C      OMIT CARD IF IMIN = BLANK (OR ZERO).
C      NOTE THAT IF BOTH KSPEC AND KMIN ARE READ, KSPEC(I) MUST BE READ
C      BEFORE KMIN(I).
C
C      *****
C      TYPE 2 OPTIONAL INPUT CARDS
C      *****
C      WORD,(INT(I),VAL(I),I=1,5) (A4,1X,5(I3,E12.5))
C      WORD = "CONC", "EROR", "DELH", "TABL", OR "LOGK".
C
C      "CONC"..ENTERS CONCENTRATION (UNITS OF FLAG) OF CONSTITUENTS
C      NOT ON CARDS 3 AND 4. INT(I) = 17(H2S),18(CO3),39(NH4),51(AL),
C      81(LI),85(NO3),86(H2CO3),87(B),90(BA),98(BR),AND 101(MN).
C      VAL(I) IS THE CONCENTRATION OF THE INT(I) CONSTITUENT.
C
C      "EROR"..OVERRIDES PRE-SET MASS BALANCE CONVERGENCE CONSTRAINTS
C      ON ANIONS. PER-SET VALUES OF EROR1-EROR5 ARE 0.001(0.1% ERROR
C      IN MASS BALANCE). EROR1-EROR5 ARE ENTERED ON THE "EROR" CARD
C      AS VAL(1)-VAL(5), IN THE ORDER 1=CARBON, 2=SULFATE, 3=FLUORIDE,
C      4=PHOSPHATE, 5=CHLORIDE. VALUES OF INT(I) ARE NOT USED.
C
C      "DELH"..OVERRIDES VALUES OF THE STANDARD DELTA ENTHALPY OF
C      REACTION (25 DEG. C) USED IN COMPUTING THE TEMPERATURE
C      DEPENDENCE OF EQUILIBRIUM CONSTANTS FROM THE VANT HOFF EQUATION.
C      INT(I) IS THE INDEX NUMBER OF THE ITH REACTION FOR WHICH DH(I)
C      IS TO BE CHANGED AND VAL(I) IS THE APPPRIATE NEW VALUE OF
C      DH(INT(I)).
C
C      "TABL"..OVERRIDES VALUES OF LOGKTO(INT(I)) (LOG K OF REACTION AT
C      25 DEG. C USED IN COMPUTING THE TEMPERATURE DEPENDENCE OF
C      EQUILIBRIUM CONSTANTS FROM THE VANT HOFF EQUATION). INT(I) IS
C      THE INDEX NUMBER OF THE ITH REACTION FOR WHICH LOGKTO IS TO BE
C      CHANGED AND VAL(I) IS THE APPROPRIATE NEW VALUE OF LOGKTO(I).
C
C      "LOGK"..OVERRIDES EXISTING ANALYTICAL EXPRESSIONS FOR LOG K AS A
C      FUNCTION OF T(DEG.K), OR ENTERS NEW, PREVIOUSLY UNDEFINED
C      ANALYTICAL EXPRESSIONS FOR LOG K(T DEG.K). THE FORM OF THE
C      ANALYTICAL EXPRESSION MUST BE
C      LOG KT(INT(I))=A+B*T+C/T+D*T**2+E/T**2
C      WHERE T IS TEMPERATURE IN DEG. K, AND A,B,C,D, AND E ARE FIT
C      PARAMETERS (MAY BE ZERO OR BLANK). INT(1) IS THE INDEX NUMBER
C      OF REACTION AND INT(2)-INT(5) ARE IGNORED. VAL(1)=A,VAL(2)=B,
C      VAL(3)=C,VAL(4)=D,VAL(5)=E.
C
C      IF ANY OF THE CARDS, "EROR","DELH","TABL","LOGK", ARE USED IN A
C      PARTICULAR WATER DATA SET, CALCULATIONS FOR THAT DATA SET AND ALL
C      SUBSEQUENT DATA SETS WILL USE THE NEW INPUT VALUES. DELH AND TABL

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A 620
A 630
A 640
A 650
A 660
A 670
A 680
A 690
A 700
A 710
A 720
A 730
A 740
A 750
A 760
A 770
A 780
A 790
A 800
A 810
A 820
A 830
A 840
A 850
A 860
A 870
A 880
A 890
A 900
A 910
A 920
A 930
A 940
A 950
A 960
A 970
A 980
A 990
A 1000
A 1010
A 1020
A 1030
A 1040
A 1050
A 1060
A 1070
A 1080
A 1090
A 1100
A 1110
A 1120
A 1130
A 1140
A 1150
A 1160
A 1170
A 1180
A 1190
A 1200
A 1210
A 1220
A 1230

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C CARDS CAN BE USED TO OVERRIDE PRE-EXISTING ANALYTICAL EXPRESSIONS. A 1240  
C THE ORDER OF TYPE 2 OPTIONAL INPUT CARDS IS "CONC","EROR","DELH", A 1250  
C "TABL",AND "LOGK", IF ALL 5 ARE USED. THE LAST CARD IN EACH WATER A 1260  
C ANALYSIS DATA SET MUST BE BLANK. A 1270  
C A 1280





