SOFTWARE NOTICE

PTA-SYSTEM: A Ge0-Calc software package for the calculation and display of activity-temperature-pressure phase diagrams*

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GENERAL SOFTWARE DESCRIPTION

Ge0-Calc is a microcomputer software package consisting of programs for calculation of phase diagrams, thermodynamic databases for minerals and aqueous species, and auxiliary programs for viewing and printing of computed phase diagrams. The two main ingredients of the Ge0-Calc package are the programs PTX-SYSTEM and PTA-SYSTEM. The former calculates complete pressure-temperature (P-T), temperature-composition (T-$X_{H_2O\text{-}CO_2}$), and pressure-composition (P-$X_{H_2O\text{-}CO_2}$) phase diagrams and has been previously described (Perkins et al., 1986; Berman et al., 1987; Brown et al., 1988). The latter program, described in this paper, calculates activity-activity (a-a), temperature-activity (T-a) and pressure activity (P-a) phase diagrams, where activity refers to the thermodynamic activity (or ratio and/or products of activities) of any mineral, gas species, or aqueous species. The minimum hardware requirements for using the software are an IBM or compatible personal computer with 640K memory, math coprocessor, and graphics card (CGA, EGA, or Hercules). the PTA version 2.0 release includes the programs described below.

PTA

The PTA-SYSTEM program has been adapted for microcomputer use from mainframe programs that are available from E. H. Perkins. The major differences between the mainframe version and this implementation are that the three mainframe programs have been combined into one program, user input is simplified, several run-time options have been modified or removed, and the program generates and calculates each reaction separately rather than generating coefficients for all reactions before calculating any individual reaction. This last modification was necessary because of the limited memory available on most microcomputers for calculating and storing a large number of reaction coefficients.

Execution times are dependent on hardware, the most important component being the math coprocessor speed. In general, AT compatibles run approximately 1.5–2 times faster than XT compatibles, and 386 machines run up to 10 times faster than XTs. Computation times is also affected by run-time options, increasing dramatically when calculations are carried out in the vicinity of the critical point of water. Activity-activity diagrams are calculated many times faster than temperature-activity and pressure-activity diagrams because the Gibbs free-energy functions need to be calculated only once in a given run. Total execution time should be on the order of seconds for systems with less than a hundred possible reactions, minutes for systems with several thousand possible reactions, and hours for systems with more than several hundred thousand possible reactions.

The output of PTA-SYSTEM can be plotted for visual representation of phase relations or inspected from a table. The program evaluates all possible reactions in the user-specified PTA space. At the user's option, each point of every reaction is tested for stability with respect to all other phases in the system, and metastable extensions are eliminated. If a curve is completely outside the P, T, and a limits of the diagram, any remaining reactions containing the metastable assemblage are removed from further consideration. Finally, all curves written to the plot file are labeled with stable assemblages. Run-time options include setting the P, T, and a limits of the diagram, the selection of ideal or nonideal H_2O-CO_2 (only for systems that do not involve aqueous species), and the specification of fixed phase activities. The user can also specify that only curves stable in the presence of a given phase or assemblage be computed so that the stability fields of particular phases or assemblages can be identified readily. Progress of the calculation can be followed in *graphics* or *text* mode. In *graphics* mode, each reaction curve is plotted on the screen as it is calculated, allowing the user to follow the search strategies and to see the phase diagram take shape. In *text* mode, calculations are summarized on a text screen that shows the current reaction being examined, the number of reactions already calculated, and an estimate of the percentage of reactions remaining to be calculated.

PTA-SYSTEM allows one to calculate any phase diagram using the variables P, T, or a (the activity of any phase or species), and faithfully calculates equilibrium curves defined by the equality of Gibbs free energy of reactants and products of each equilibrium. The user should be ever aware that the accuracy of calculated phase diagrams is a direct function of the quality of thermodynamic input data. The data distributed with this software are those presented by Helgeson et al. (1981) for aqueous species and those derived by Berman (1988) for minerals in the system Na_2O-K_2O-CaO-MgO-FeO-Fe_2O_3-Al_2O_3-SiO_2-TiO_2-H_2O-CO_2. Further details of the procedure used to derive this data set are given by Berman et al. (1986).

Also included on the distribution discs is an alternate database for minerals derived by Berman et al. (1985). Although the 1988 database represents an update and improvement of this data set, it is included in this package because several phases are present, notably zeolites, that are not present in the revised database. Note, however, that this database must be used in entirety; phases from this data set cannot be used meaningfully with phases from the revised data set.

PLOTS

The PLOTS program displays graphical output on video monitors using a Hercules card or an IBM or compatible color graph-
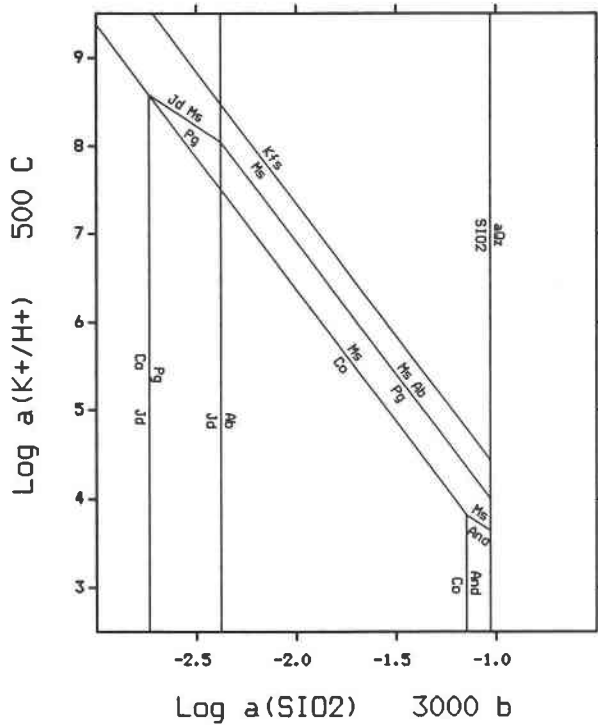
Fig. 1.   LASER plot of log a_{K_+}/a_{H_+} vs. log a_{SiO_2} diagram for the system K_2O-Na_2O-Al_2O_3-SiO_2-H_2O at 500 °C and 3000 bars.
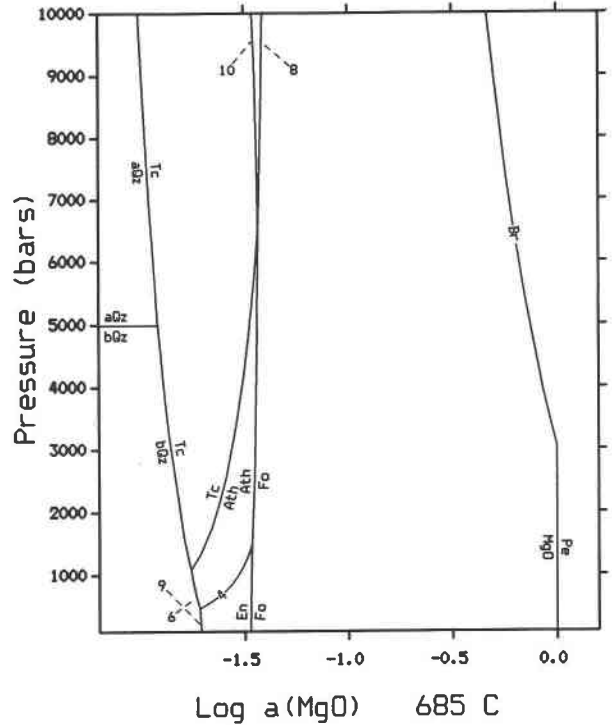

Fig. 3.   LASER plot of pressure vs. log a_{MgO} diagram for the system MgO-SiO_2-H_2O at 685 °C.
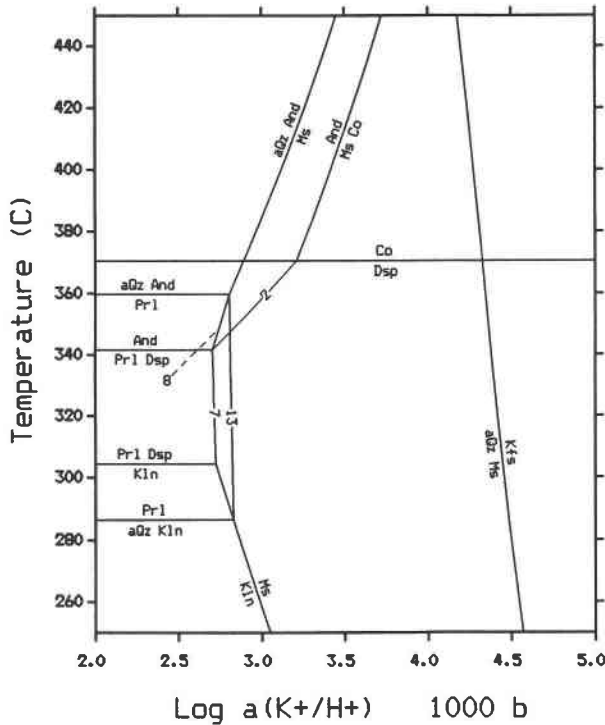

Fig. 2.   LASER plot of temperature vs. log a_{K_+}/a_{H_+} diagram for the system K_2O-Al_2O_3-SiO_2-H_2O at 1000 bars.

ics adapter (CGA) or enhanced graphics adapter (EGA). PLOTS offers a quick way to preview plots on the screen prior to making hard copies with the PRINTER or LASER programs (see below).

LASER

The LASER program makes high-resolution hard copies of the graphical output on HP-LASERJET-II printers with at least 1.5 MB of memory. Figures 1 to 3 show examples of phase diagrams printed on the laser printer. Provisions have been made to allow variable line types and widths.

PRINTER

The PRINTER program makes high-resolution hard copies of phase diagrams on EPSON or compatible dot matrix printers. The hard copies produced by PRINTER look similar to Figures 1 to 3 except the resolution is lower than that produced by LASER.

CLEAN

The graphical output of PTA-SYSTEM is often difficult to read because reaction labels overlap one another in any reasonably complex phase diagram. The program CLEAN improves the appearance of complicated phase diagrams on which the reaction labels overwrite one another. It either moves the labels to new positions or it replaces the conflicting reaction labels with numbers and writes a list of reactions that correspond to the numbers to a separate file. After executing CLEAN, the improved plot (i.e., Figs. 1 to 3) can be viewed on the screen with PLOTS or on hard copies made with PRINTER or LASER.

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