

THE "REETHERM" DATA BANK FOR MODELING OF GEOCHEMICAL PROCESSES WITH PARTICIPATION OF RARE-EARTH ELEMENTS

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The development of the data base (DB) of thermodynamic properties of minerals and aqueous species [1,2,etc.] gives a chance for physico-chemical modeling of the reasons and directions of REE and Y fractionation in the processes of hydrothermal ore-formation with the use of thermodynamic methods. The authors' experience suggests that the following well-known data base like the data bases included into the "Selector" program computing complex [3], the "UNITHERM" data base created for the "GIBBS" program of minimization of free energy [4], presently included into the Hch program complex [5], SUPCRT92 [6], SUPCRT96 [1], etc. are the suitable basis to solve this problem. The authors have created the "REETHERM" data bank, which uses the HKF equation as the main algorithm to provide possibilities for modeling hydrothermal equilibria with participation of REE. The use of the Delphi Client/Server program language and the presentation of information in the files of the dBase format make it possible to use the bank for work with information networks. The developed software is intended for use in the Windows operation system. The proposed bank of thermodynamic information consists of the following three connected data bases:

BASE1, BASE2 and BASE3. The structure of their files is shown in fig.1.

Fig.2 gives an arrangement of the program algorithm, the work of which consists of the following stages: 1) selection of the data of chemical formula of a required compound from the list in BASE1; 2) search of the required compound in the SPECIES field of the data base of HKF parameters with the help of SEARCH1 subprogram; 3) search of the reaction of the required compound in SPECIES field, connecting BASE1 and BASE2, with the help of SEARCH2 subprogram; 4) the execution of the operation to select from the equation of the reaction of complex formation of chemical formulae of all the particles, participating in the reaction and their corresponding stoichiometric coefficients by DISTINGUISH subprogram; 5) search of the components of the reaction on SPECIES field in the database of HKF parameters, using SEARCH3 subprogram; 6) creation the file of initial data and corresponding BASE3 bibliographic data of REFERENCE field; 7) computation and displaying the final result as the logarithms of stability constants of the given complex in the whole range of temperatures and pressures.

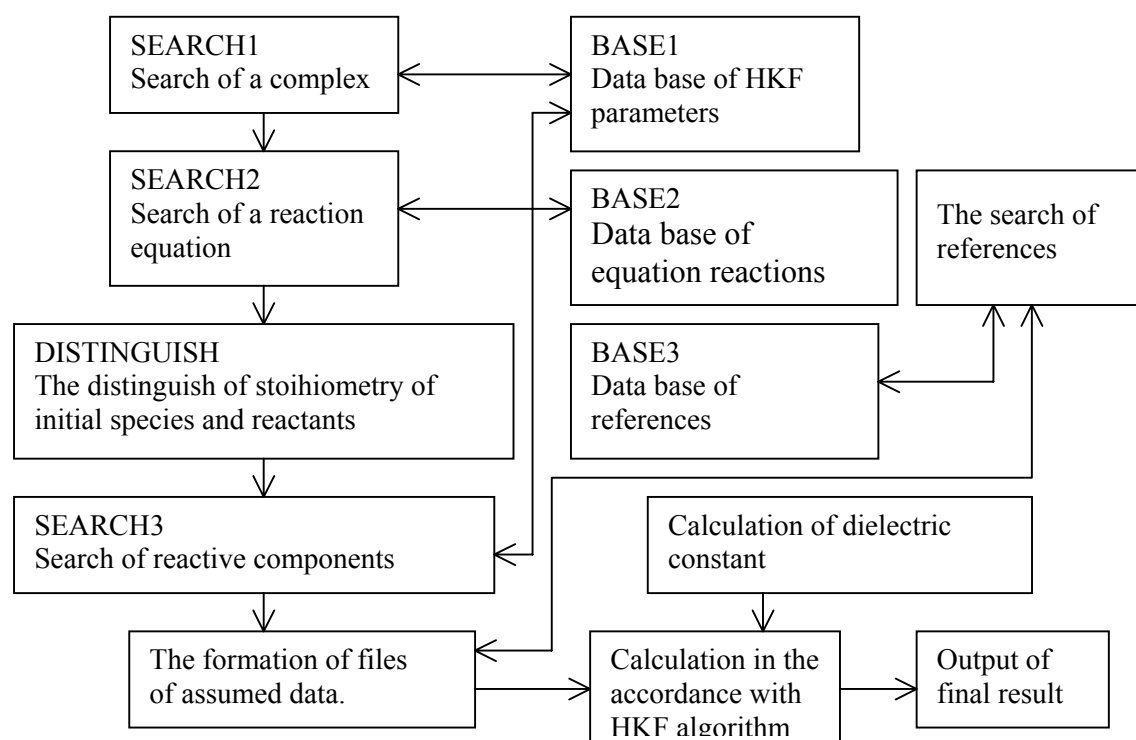


Fig 2. The general scheme of the used software

In the present stage of "REETHERM" data bank formation the main attention is paid to hydroxyl, fluoride, carbonate and bicarbonate complexes of REE, which play the main role in geochemical processes with participation of lanthanides. Moreover (In this case), the special program provides a means for the correction of the constants for two latter types of complexes in the context of change of dielectric permeability of the solvent with elevated contents of carbon dioxide as a nonpolar gas component [7].

The potential users can obtain (fuller) an extended information on "REETHERM" data bank and the possibility to use its data on the Web-page (<http://www.uiggm.nsc.ru:8082/uiggm/mineralogy/lab454/program.htm>) of the site of the United Institute of Geology, Geophysics and Mineralogy, SB RAS.

1. Haas J.R., Shock E.L., Sassani D.C. *Geochim. Cosmochim. Acta*, 1995, v.59, p.4329-4350.
2. Shock E.L., Sassani D.C., Willis M., Sverjensky D.A. *Geochim. Cosmochim. Acta*, 1997, v.61, №5, p.907-950.
3. Dorogokupetz P.I., Karpov I.K. *Thermodynamics of minerals and mineral equilibria*. Novosibirsk, Nauka (Russian), 1984, 184 p.
4. Borisov M.V., Shvarov Yu.V. *Thermodynamics of geochemical processes*. Moscow, Moscow State University publishing house (Russian), 1992, 256 p.
5. Shvarov Yu.V. *Geokhimiya* (Russian) 1999, №6, p.646-652.
6. Johnson J., Oelkers E., Helgeson H. *Computers and Geosciences*, 1992, v.18, p.899-947.
7. Kolonin G.R., Palyanova G.A., Shironosova G.P., Morgunov K.G. *Geokhimiya* (Russian), 1994, №12, p.1725-1733.

