A NEW EDITION OF THE "HANDBOOK OF THERMODYNAMIC DATA"

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The first edition of the "Handbook of Thermodynamic Data" by G.B.Naumov, B.N.Ryzhenko and I.L.Khodakovsky was published in 1971[1] in former USSR. It was translated into English in USA in 1974 [2]. The Handbook was intended for use by the Earth scientists. Thermodynamic values for minerals and many other crystal substances as well as Gibbs formation energies for ions and undissociated molecules of a number of acids and dissolved gasses in aqueous solutions at temperatures up to 350°C provided thermodynamic calculation of equilibrium constants for a great number of reactions in hydrothermal systems.

The new edition summarizes the systematic work on the thermodynamic data selection and critical assessment performed by a number of researchers at Vernadsky Institute in cooperation with scientific research workers at other Institutes of RAS, and (during the last years) – in cooperation with "Dubna" University. Simultaneously with that work, experimental determinations of thermodynamic properties of a number of minerals and aqueous species (ions, as well as complex ions and molecules) were performed , using predominantly calorimetry and solubility methods. The results of those determinations were published in the papers. A part of those results were incorporated, as accepted values, in fundamental Handbook of the USSR Academia of sciences ("Thermal constants of substances" [3]), and in other reference books [4, 5] as well.

It is expected that the Handbook will consist of three volumes. Each of these will involve several parts. The first volume of the Handbook will incorporate *main results of experimental investigations* on thermodynamics of chemical systems: (1) inorganic and simplest organic individual substances, as well as chemical reactions in which these substances participate; (2) aqueous species (ions and complex ions and molecules as well); (3) binary aqueous solutions; (4) gas mixtures; (5) solid solutions.

The main sources of the data: 1. Hand-written card indexes on thermodynamic properties (were regularly kept up to 1985. A total of about 12 thousands of cards); 2. VINITI summary card indexes (from 1985 to 1994. About 10 thousand of cards); 3. The reprints collection; 4. Computer bibliography and experimental databases contained in the DiaNIK-win" system.

The Handbook will be the first one to systematize experimentally studied chemical systems and chemical reactions. This enables to not only perform local and global consistency procedures, but to use the feed-back principle as well for the algorithms of correlation and calculation of the equilibrium composition of multicomponent systems of any phase constitution.

The second volume will incorporate *accepted values and substantiation of their selection* for a number of chemical systems. The selection of the systems was due to the problems which were solved by the authors since 1963. These problems were solved within the framework of application of the chemical thermodynamics methods to investigations of conditions of the mineral formation in different natural and technogenic systems. Thermodynamic properties of pure inorganic and simple organic substances, chemical reactions, aqueous species (ions, complex ions and molecules), and binary aqueous solutions will be considered as well. The first part of the second volume of the Handbook will incorporate the results of analysis of published experimental data for one- and two-component chemical systems.

All accepted values are consistent with the international recommendations of CODATA, IUPAC, IAEA, and UE, and they are related to the recommendations of the fundamental reference books.

The third volume will incorporate the *tables of thermodynamic properties* of minerals and principal mineral-forming substances, including aqueous species, in large temperature and pressure ranges. The tables will be prepared in the "DiaNIK-win" computer system.

In 2001 the first parts of the mentioned volumes (incorporated thermodynamic information on one- and twocomponent systems) will be published. The parts incorporated the data on three-, four-, five-component and more complicated systems are prepared in parallel.

1. *Наумов Г.Б., Рыженко Б.Н., Ходаковский И.Л.* Справочник термодинамических величин. М.: Атомиздат. 1971. 240 с.
2. *Naumov, G.B.; Ryzhenko, B.N.; Khodakovsky, I.L.* Handbook of Thermodynamic Data (PB-226 722/7GA) (NTIS: Springfield, Va.), 1974. 373 pp.
3. Термические константы веществ. Под ред. В.П.Глушко. Выпуски III-X, М.: АН СССР, 1968-1981 гг.
4. *Fuger J., Khodakovsky I.L., Sergeyeva E.I., Medvedev V.A., Navratil J.D.* The Chemical Thermodynamics of Actinide Elements and Compounds: Part 12. The Actinide Aqueous Inorganic Complexes; Vienna: International Atomic Energy Agency, 1992, 224 p.
5. CODATA International Geothermodynamic Tables. Editors: I.L.Khodakovsky, E. F. Westrum, Jr. and B.S. Hemingway. 1995. 276 p.