A Description of the *Handbook of Thermodynamic Values* Structure, the Software for the "DiaNIK-win" Database, and for the Website *Thermodynamics of Natural Processes*

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About 40 years ago a start has been made at Vernadsky Institute of RAS on the preparation of the card index on the results of experimental thermodynamic studies of inorganic substances (for about 10 thousand substances and several tens of thousands of references). The card index served as a basis for the preparation of «Handbook of thermodynamic values» («HTV») issued in former USSR in 1971 [1]. It was translated into English in USA in 1974 (PB-226 722/7GA, NTIS: Springfield, Va., 373 pp.) [2].

In 2001-2005 the first drafts of new edition of the «HTV» sums up systematic work of a number of researchers at Vernadsky Institute in cooperation with scientific research workers from other Institutes of Russian Academy of Sciences, and (during last years) – with Dubna University. It becomes apparent that a limited number of participants, together with limited time and budget, does not permit us to consider the all subsystems incorporated into the multicomponent system: O-H-F-Cl-S-N-P-C-Si-Th-U-Np-Pu-Se-As-Pb-Zn-Cd-Hg-Cu-Be). The experience of the last years is showing that publication of the «HTV» as a book is unsuitable (waste of time), because the content of this will be quickly out of date. Best way – to publish of the evolving «HTV» in the INTERNET.

«DiaNIK» computer database is an interactive research information system of chemical thermodynamic data for individual inorganic substances (including minerals) and aqueous systems [3, 4]. The development of the «DiaNIK» computer system under I.L. Khodakovsky's leadership was started in 1980 at Vernadsky Institute and at Dubna University (from 1999). The «DiaNIK» primary version was made using ES-1010 computer and finished in 1985. The software was written in FORTRAN-77 by A.I. Shapkin. During the next three years it was developed on computers of these series (ES-1035 and ES-1060). Then it was adapted to the IBM-PC platform without serious reprogramming by A.I.Shapkin and D.V. Nikolenko. Unfortunately, on some reasons, the «DiaNIK-2» version could not be finished and during 1992-1993 the Scientific Group "*DIANIK*" worked out the next «DiaNIK-3» version with new user interface (programming by V.S. Khudyaev). Programming languages FORTRAN and C were used for the «DiaNIK-3» programs. During 1994-1997 the described above studies have been suspended due to the essential restriction of funding from Russian Academy of Sciences.

The structure of thermodynamic database is based on the principles, developed by CODATA International Group on Geothermodynamic Data for working up thermodynamic information [5]. The principal unit of the database structure is a chemical system, because any pure substance corresponds in composition to a certain chemical system, as well as a chemical reaction takes place in a system which elemental composition corresponds to that both of the initial reagents and of the products of the reaction. According to the number of incorporated chemical elements all systems can be divided into one-, two-, three-, and *n*-component systems. The standard «Total Commander» program (version 5.51) was used for this deviation (and others) in the computer memory.

The accepted arrangement of chemical elements as a whole complies with the traditional «thermochemical» one, but differs from that only by sequence of the transition elements between Tl and Sc: Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Mn, Tc, Re, Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, Pt, Cu, Ag, Au, Zn, Cd, Hg). For the structure of «DiaNIK-win» database developing simple rules were used for defining the sequence of the chemical systems as well as pure substances, aqueous species, and chemical reactions [6]. The rules establish unique layout not only of the substances, but of the experimentally studies chemical reactions as well. They enable to use the feed-back principle as well for the algorithms of consistency procedures and calculation of the equilibrium composition of the multi-component system of phase composition [7].

To adequately present thermodynamic information in computer databases as well as to help users of different categories to conveniently access that, two information levels (main divisions in the «DiaNIK-win» and in the «HTV» published by INTERNET) are provided: a common user's one and an experts one. A common user needs only reference information presented by highly skilled experts in fundamental thermodynamic reference books. Hence, user interface helps common users to access internally consistent values recommended by basic thermodynamic reference books and to use those values in their practical thermodynamic calculations.

The main experimental results described in original publications are combined in the «Literature data» division of the «DiaNIK-win» database and of the «HTV». In the course of the consistency procedure the primary experimental data files for certain of the systems were developed by the experts of the «*DIANIK*» team. Those files are accessible to the experts of other scientific teams via CD. On the first stage we prepared the tables which incorporated the reference data and the *main results of experimental investigations* on thermodynamics

(brief summarizing information on available published experimental studies: property of interest, a method of the investigation, uncertainty of the data, for aqueous system temperature/concentrati on interval, ionic strength, supporting electrolyte, and a reference. The accepted structure allows performance of the following consistency procedure: (1) for the individual substance, binary aqueous solution and the individual chemical reaction as well (*"local consistency"*); (2) for the chemical systems, containing a set of substances (including aqueous species) and reactions (*"global consistency"*).

The use of the modern-day information technologies developed in Internet a start has been made on the development of the website «Thermodynamics of natural processes» (www.tnpdata.ru) in 2004 by the «*DIANIK*» team of Dubna University. The program «ChemNavi» (Chemical Navigator, © «*DIANIK*» team, 2002-2006) to perform out comfortable and quick search for different thermodynamic information on chemical system of expert interest. The Internet server «Apache», database «MySQL» and standard modern lengvidges «PHP», «SQL», «Javascript» is using in the site development. This give to possibility transfer of the calculated and information data in the standard modern programs: «EXCELL», «ACCESS» and others without additional formating.

We hope that the site could permit in future to join forces of highly skilled experts on chemical thermodynamics from different countries in order to perform successfully their work.

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1. Naumov, G.B, Ryzhenko, B.N., Khodakovsky I.L.: Handbook of Thermodynamic Values, Atomizdat, Moscow, 239 p. (1971), (in Russian).

2. Naumov, G.B., Ryzhenko, B.N., Khodakovsky, I.L.: Handbook of Thermodynamic Values, PB-226 722/7GA, NTIS: Springfield, Va., 373 p. (1974).

3. Khodakovsky I.L. Prospects for use of the computer for solving problems of chemical thermodynamics. Probl. Kalorimetrii i Khim. Termodinam. Dokl. na 10 Vses. Konf., 12-14 June, 1984, Chernogolovka, Vol. 1, Part 1, 116-121 (1984). (in Russian).

4. Khodakovsky I.L. «DiaNIK» - thermodynamic data bases of minerals and calculations of equilibrium compositions of natural systems. // Abstracts of the 12th IUPAC Conference on Chemical Thermodynamics and of the 47th Annual Calorimetry Conference in Snowbird, Utah, USA, (1992).

5. Khodakovsky I.L., Westrum E.F.,Ir., Hemingway B.S. // CODATA International Geothermodynamic Tables. Guidelines and set of prototype tables, 276 p. (beta version available from Edgar Westrum, University of Michigan, Department of Chemistry) (1995).

6 Semenov Yu.V., Shapkin, A.I., Khodakovsky I.L. The problems of classification and storage of thermodynamic data in computer systems. // In "Computer handling and dissemination of data" Glaeser, P.S., Ed., Elsevier Science Publishers B.V. (North- Holland), 262 (1987).

7. Khodakovsky, I.L. Feedback of algorithms of thermodynamic data consistency and computer simulation of geological systems; Proc. Int. CODATA Conf., Volume Date 1986, 10th (Comput. Handl. Dissemination Data), 270-274 (1987).