

**PACKAGE ID** - 000747IBMPC03 ZZ-HATCHES-14.0

**KWIC TITLE** - A Thermodynamic Database and Management System  
for Radio Chemical Modeling

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**LIMITATION CODE** -UNL                   **AUDIENCE CODE** - UNL

**COMPLETION DATE** - 02/20/2002   **PUBLICATION DATE** - 04/02/2002

**DESCRIPTION** - HATCHES is a collection of data for use in radiochemical modelling work. The data base includes thermodynamic data (the log formation constant and the enthalpy of formation for the chemical species) for the actinides U, Th, Pu, Np, Am and Cm and for fission products including Cs, Ru, Tc, and Sr. Compared to the previous version, this version contains the Technetium dataset taken from the 1999 NEA review "Chemical Thermodynamics of Technetium". A number of improvements have been made to clarify EQ3/6 mineral formula names. Ligrand and Reference fields have been checked and modified where necessary to improve consistency.

**PACKAGE CONTENTS** - Media Directory; Software Abstract; Information File; Media Includes User's Manual;

**SOURCE CODE INCLUDED?** - No

**MEDIA QUANTITY** - 1 CD ROM

**METHOD OF SOLUTION** - HATCHES has been created using the Microsoft Access software on a MS Windows computer. It consists of a database and a MS Access runtime version and is therefore independent of other software. The database is secured and can't be modified. Since it is an Access database the use of HATCHES is straightforward. Two applications for PHREEQE resp. EQ3/6 data conversion are included. The PICKER application, which extracts a part of the PHREEQE database, is also included. The thermodynamic constants (stability constants and solubility products) included in HATCHES have been selected as the best data available at the present time and the database is continuously being updated as improved data becomes available. In a number of cases, when there was evidence for the existence of a species by no good experimentally derived constants were found, estimated data has been included. Throughout the compilation of HATCHES every effort has been made to produce a self consistent database. Each entry includes a full description of the source of the data, together with details of any calculations that have been performed on the data, (e.g. correction to zero ionic strength). In addition, each entry includes all the associated input information required by the PHREEQE code (e.g. charge, stoichiometry, operational valency), together with comments concerning the validity of the data.

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**COMPUTER** - IBM PC

**OPERATING SYSTEMS** - Running under Microsoft Windows 95 or higher and NT. Microsoft Access executable is included.

**PROGRAMMING LANGUAGES** - Microsoft Access

**SOFTWARE LIMITATIONS** - At present the database has only been compiled for use at 25 C. In a limited number of cases the enthalpy data required for calculations at other temperatures is included, but it has not been used at Harwell. Complete validation of the HATCHES data would be an impossible task, however limited validation is achieved each time a database is used to successfully model experimental results. It is hoped that the wider use of HATCHES, to model a variety of different systems will result in an increased amount of validated data. The authors would therefore welcome any feedback from modellers using HATCHES concerning the validity of the data.

**SOURCE CODE AVAILABLE (Y/N)** - N

**RELATED SOFTWARE** - Two applications for PHREEQE resp. EQ3/6 data conversion are included. The PICKER application, which extracts a part of the PHREEQE database, is also included.

**HARDWARE REQS** - IBM-PC or compatible.

**REFERENCES** - Modeling, chemical reactions, database systems, data library, thermodynamic properties

**ABSTRACT STATUS** - Released AS-IS April 15, 2002.

**SUBJECT CLASS CODE** - MU

**SPONSOR** - NEA

**PACKAGE TYPE** - AS - IS