CODATA Thermodynamic Tables

SELECTIONS FOR SOME COMPOUNDS OF CALCIUM AND RELATED MIXTURES: A PROTOTYPE SET OF TABLES

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CODATA Series on Thermodynamic Properties

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Selections for Some Compounds of Calcium and Related Mixtures: A Prototype Set of Tables

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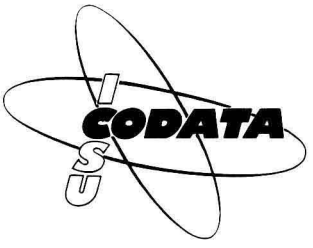
Report of the CODATA Task Group on Chemical Thermodynamic Tables.



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CODATA THERMODYNAMIC TABLES

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FOREWORD

CODATA* is particularly concerned with improvement of the quality and accessibility of data that span the interests of several scientific disciplines. Thermodynamics, with its broad importance in chemistry, physics, geology, and several branches of engineering, is clearly such a field. Thus CODATA has had an active interest in thermodynamic data since its inception.

The CODATA Task Group on Chemical Thermodynamic Tables has been charged with developing a comprehensive series of internationally accepted, thermodynamically consistent tables. This volume presents the first set of tables from the task group and is the prototype of what is intended to become a comprehensive series.

CODATA attaches great importance to this task and would welcome readers' comments on the format and content of these prototype tables.

David R. Lide
President, CODATA

* Committee on Data for Science and Technology of the International Council of Scientific Unions (ICSU)

PREFACE

Recommended values are presented for chemical thermodynamic properties of selected compounds of calcium and their mixtures. These have been prepared in accord with a previously developed plan and as a test of it. All values in the present table are mutually consistent and are consistent with the CODATA Key Values for Thermodynamics. The values are recommended for general use. This work has been an activity of the CODATA Task Group on Chemical Thermodynamic Tables.

This volume of chemical thermodynamic data is intended as the first of many to be prepared as a cooperative, ongoing international project by experts who are geographically separated, but in computer-to-computer communications, and share both data and calculational resources.

The evaluated data are for common compounds of calcium (element, oxide, hydroxide, peroxide, fluoride, chloride, sulfate, nitrate and carbonate, their hydrates and their ions in aqueous solution) and for three systems: Ca-Mg, $CaCl_2$-KCl and $CaCl_2$-H_2O.

Forty one tables of thermal functions (heat capacity, entropy, enthalpy, and Gibbs energy functions) are given for those compounds of magnesium, calcium and potassium for which the properties have been evaluated in this work. Twenty four tables of thermal functions are given for auxiliary substances. Each table spans the temperature range 0 to 4000 K, to the extent that data are available. Formation properties at 298.15 K (enthalpy and Gibbs energy of formation) are given for 68 compounds of calcium, magnesium and potassium plus the relevant values for 54 auxiliary substances. For each of the three systems the data given are mixing properties (enthalpies and Gibbs energies), partial molar or excess properties (activities, enthalpies, heat capacities) and phase transformation data. All selections of data are accompanied by uncertainties, and are documented. Detailed lists of the measurements used in the evaluations are given for the thermochemical, alloy, and aqueous solution sections.

The technical formalities needed for the project are described in an introduction (contents of tables, tabulation intervals, units, definitions of properties). Plans for the future are discussed.

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Chapter 1

INTRODUCTION

1.1 The CODATA Task Group on Chemical Thermodynamic Tables

The predecessor of this Task Group was the Task Group on Internationalization and Systematization of Thermodynamic Tables (ISTT). It was established at the 5th International CODATA Conference in Boulder, Colorado, in 1976, and reconstituted and given its present name in 1982. Most of the work reported on here was carried out during the period 1976-1985. The ISTT Task group was provided with the following terms of reference.

a. To reach international agreement on functions, conventions, standard states, intervals of tabulation, etc., for thermodynamic tables.

b. To develop a suitable system for international cooperation in compilation of papers, extraction of data, and storage of information and data, so that the same base of primary measurements will become available to all.

c. To develop suitable techniques for evaluation of data and the formation of tables such that the efforts of independent evaluators will lead to thermodynamically consistent tables, and new data and substances can be added in a consistent fashion to existing tables.

d. To promote international cooperation in the production of thermodynamic tables so that the needs of users can be met in a timely, efficient manner.

e. To provide a forum for discussion of the problems of preparing tables of critically evaluated chemical thermodynamic data and to develop an informative literature on the subject.

It is apparent that the principal thrust of the terms of reference is the development of a system of international cooperation leading to the preparation of thermodynamically consistent tables in a timely and efficient manner. In carrying out its responsibilities the Task Group focussed on chemical thermodynamics, that is the thermodynamics of chemical reactions and the thermodynamics of the change of state of a substance without chemical reaction.

The Task Group has accomplished four things:

a. It carried out an extensive systematic analysis of the preparation of large sets of tables of thermodynamic properties.

b. Using this analysis, it defined the structure of an international system and developed a plan for the preparation of tables as a joint international cooperative effort.

c. It specified the contents of several tables and data banks intended for general use.

d. It prepared a prototype set of tables using the plan and specifications mentioned above.

The purpose of this paper is to present this prototype set of Tables.

1.2 The Preparation of Thermodynamic Tables

The Task Group has already published the results of its analysis and planning under the title "Systematic Approach to the Preparation of Chemical Thermodynamic Tables" [82WHI]. This material will not be repeated in detail here. It does, however, underlie the tables and influences their structure and content.

Figure 1.2.1 is taken from the publication mentioned. It is a flow diagram through the proposed system. Raw data from the scientific literature enter at the top and comprehensive sets of evaluated data are produced at the bottom. The solid arrows indicate flow through the system as well as the intellectual input required in moving from one step to another. The small circles represent the intellectual synthesis of materials from several files. The bold broken arrows complete the major feedback loops. The rectangular boxes represent recognizable data files that are important states of the system. The tables and bibliography presented here give examples of files 1, 4A, 5A, 6, 7, 8, 9A, 9B and 10. Readers interested in the detailed explanation of Figure 1 are encouraged to read [82WHI].

1.3 The Prototype Tables

The tables focus on calcium, the element, and its compounds with hydrogen, oxygen and chlorine, as well as magnesium and potassium chloride. Additional compounds of calcium and other substances are also present. These are needed to solve the primary network of thermochemical reactions required to introduce thermodynamic consistency. The thermodynamic values chosen are consistent with the June 1984 draft of the final report on the CODATA Recommended Key Values for Thermodynamics [84COD], in which some values have been revised from the earlier publication [78COX] and take into account recent measurements. To the best of the Task Group's knowledge they provide as reliable a set of values as exists for the substances concerned.