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NBS Technical Note 1243

Thermodynamic Properties of the Alkaline Earth Metal Hydroxides (MOH) I. Literature Citations

Malcolm W. Chase

National Bureau of Standards

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- Neutron Measurements and Research
- Neutron Dosimetry
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- X-Ray Physics
- Dosimetry

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Engages in forefront research in nuclear and elementary particle physics; performs highly accurate measurements and theoretical analyses which probe the structure of nuclear matter; and improves the quantitative understanding of physical processes that underlie measurement science.

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Malcolm W. Chase

Chemical Thermodynamics Division
Center for Chemical Physics
National Measurement Laboratory
National Bureau of Standards
Gaithersburg, MD 20899

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THERMODYNAMIC PROPERTIES OF THE ALKALINE EARTH METAL HYDROXIDES (MOH)
I. Literature Citations

Table of Contents

ABSTRACT

A bibliographic collection is provided on data which are necessary for the calculation of the thermochemical properties of the gaseous alkaline earth metal (mono)hydroxides (MOH) and their positive ions (MOH^+), where M = Be, Mg, Ca, Sr, and Ba. This is the first in a series of articles that will document the information used in the critical evaluation of the thermodynamic properties for the JANAF Thermochemical Tables.

The collection contains references which have been published through the end of 1985, with a limited number of 1986 references. Five bibliographies are given, one for each of the alkaline earth metals. In each bibliography, the references are listed chronologically; alphabetically by first author within each year. The names of the ten species are given according to the Chemical Abstracts system of nomenclature (as of the Tenth Collective Index). The Chemical Abstracts Registry Numbers are also given for each of the species. A brief summary of the type of available information is given.

Keywords: alkaline earth hydroxides, bibliography, electron affinity, electronic energy levels, equilibrium data, formation properties, ionization potential, molecular structure, review articles, thermochemistry, thermodynamic properties, vibrational frequencies

INTRODUCTION

This is the first in a series of articles that will document the information used in the critical evaluation of the thermodynamic properties of chemical species for the JANAF Thermochemical Tables. In this particular article, thermochemical tables for the gaseous alkaline earth metal hydroxides (MOH) and their positive ions (MOH^+) are being prepared. For the current project, the alkaline earth metals (M) include Be, Mg, Ca, Sr, and Ba. There are no data available for the Ra species. The preparation of these thermochemical tables has been divided into a series of sequential sections, each section containing documentation. This permits the technical community not only to have access to all the available pertinent references early in the investigation but also to view the progress in the critical evaluation of the thermodynamic properties for the JANAF Thermochemical Tables. It is hoped that this will stimulate interested scientists to comment on the documentation so that we can make this documentation as complete as possible. The goal is to construct a complete bibliographic resource, upon which future studies can be built, and to eliminate the need for another search of the past literature on these species. In the future, one only should have to be concerned with current updates to this survey. A possible limitation is in the appearance of pertinent data in journals not accessed by the abstracting services. For example, much of the work on the beryllium species was done under DOD contracts and was often reported only in progress reports and military reports; these were often not made available to the abstracting services.

Since the final recommended thermochemical values for these hydroxides are tied in with the results of other species (e.g. the five (di)hydroxides and five oxides), there are other stepwise documentation projects in progress.

In general, the first two steps involve the construction of the bibliographies, followed by a set of data summaries (i.e., summaries of the reported data in a tabular and graphical format). Subsequently, there will be published preliminary thermal functions, preliminary formation properties, and then the final thermochemical tables. The latter normally would be a fine-adjustment of the preliminary values. This fine-adjustment would result from the examination of data consistency as viewed from a larger group of species, i.e. a mathematical solution of a thermochemical network or consideration of trends in the periodic table. From a network solution, there is obtained a statistical assessment of the overall uncertainties in the formation properties and a better understanding of the interconsistency of all data used in the network.

NOMENCLATURE

The species of interest in this bibliographic section are given below with their names and registry numbers as obtained from Chemical Abstracts On-Line (Registry File) in December 1986. Historically, these species have often been called monohydroxides, but this naming convention currently is not used by Chemical Abstracts.

formula	name	registry number
BeOH	beryllium hydroxide	20768-68-7
MgOH	magnesium hydroxide	12141-11-6
CaOH	calcium hydroxide	12177-67-2
SrOH	strontium hydroxide	12131-14-9
BaOH	barium hydroxide	12009-08-4
$BeOH^+$	hydroxyberyllium(1+)	12280-09-0
$MgOH^+$	hydroxymagnesium(1+)	60172-61-4
$CaOH^+$	hydroxycalcium(1+)	36812-31-4
$SrOH^+$	hydroxystrontium(1+)	36812-32-5
$BaOH^+$	hydroxybarium(1+)	68193-67-9

LITERATURE COVERAGE

All pertinent references have been collected into five bibliographies, one for each of the five alkaline earth metals [there are no data available for the radium species]. These references were taken primarily from a search of Chemical Abstracts up to and including the 1986 volumes (i.e. Volumes 104 and 105). However, a scanning of the retrieved articles, manual scanning of selected journals, and use of personal contacts has yielded additional publications. Since the number of references for these hydroxides is not excessive, all published sources could have been listed. Instead, only those articles are included which have some data pertinent to the thermochemical calculations. The literature collection maintained by the National Bureau of Standards Ion Energetics and Kinetics Data Center was searched to include articles pertaining to the ionization potential and appearance potential of the five alkaline earth (mono-) hydroxides. The collection should be complete through 1986 with the following constraints:

1. All articles referring to aqueous solutions involving MOH+ are not included. We are interested only in the gaseous MOH and MOH+ species. Occasionally, this type of article discusses solution spectra of the OH group; in this case, the article is included.

2. Many articles published in astrophysical journals are not included because they are not presenting new spectral information. More often, existing spectral data is used to identify species in stars.

3. Early studies in flame spectroscopy, in which alkaline earth metal-containing species were added to flames, may not be extensively covered in this bibliography. In the early investigation of these flames, the assignment of spectral lines to a given species was not always definitive.

4. Analytical chemistry articles which deal with the interferences of MOH(g) electronic bands with other bands usually are not included. These articles normally do not give definitive values for the electronic bands nor do they present data relevant to this particular thermodynamic study.

5. Articles using existing thermochemical values for the hydroxides in calculations are not included, unless the article includes a discussion of problems in the calculated results.

6. During the 1960's there was a large effort directed towards the measurement of properties of beryllium and its species by government agencies and their contractors. Much of this work was documented in technical progress reports. A critically reviewed publication did not necessarily follow. There is a high probability that not all of these reports have been accessed.

7. At this time, only those critical reviews which deal exclusively with hydroxides are included.

The inclusion of an article in this collection does not imply that it will be of high importance in the final selection of data. Since there is not much data, we have probably been rather unselective in our choice of entries in these bibliographies, and have extracted some articles which will not be useful. With the possible shortage of information, the hope was that some useful information may be hidden in these articles. The initial examination of the literature suggests that sufficient reliable information is available to generate sound thermochemical tables for the alkaline earth metal hydroxides (MOH), except for BeOH(g). In fact, there are no experimental studies on BeOH since 1969, except for the ESR study in 1976. The five positive ions lack experimental structural and vibrational frequency information.

In generating these bibliographic files, the intent is to add information progressively as the evaluation procedure progresses. Thus, at the start, the prime effort is to list authors and the journal citation. As the literature searching progresses and as articles are obtained, additional information is added (e.g., article title, Chemical Abstracts reference). Thus, some citations may be incomplete at this time. In general, the majority of the bibliographic citations will (should) eventually contain:

authors
title of the article
journal citation
abstract citation (Chemical Abstracts, Physics Abstacts, etc.)
short annotation as to information in the article

At this point for the alkaline earth metal hydroxides (MOH), we have collected the majority of the available data, with no statement as to its value. During the data evaluation process, some citations may well be deleted, as well as additional citations discussed.

DATA SUMMARIES

The next publication in this series will be a set of tabular information which will summarize the relevant data, as it was presented in the original publication. These summaries will help direct attention to the data actually available for use in generating thermochemical tables. In the case of these hydroxides, data summaries will be given for the following information:

molecular structure (bond angles and bond distances)
vibrational frequencies
electronic energy levels
dissociation energy, in terms of $MOH = M + OH$
ionization potential, in terms of $MOH = MOH^{+} + e^{-}$

The same information will be summarized for the positive ions, except for the ionization potential. In all cases, experimental and theoretical data are included.

At this time, it is interesting to summarize briefly the nature and quantity of data available. The following table is intended to give a rough sense of the distribution of data for the hydroxides. A more exact summary of the data will be available after a thorough examination of all references.

SUBJECT COVERAGE IN REFERENCES ON ALKALINE EARTH HYDROXIDES (MOH)

	Be	Mg	Ca	Sr	Ba
total references	34	32	71	64	48
structure					
estimated/calculated	6	11	11	14	11
experimental	1	2	3	2	1
vibrational frequencies					
estimated/calculated	2	11	11	14	11
experimental	-	1	3	2	1
electronic energy levels					
bands	-	10	15	18	12
precise values	-	1	3	2	1
enthalpy of formation					
indirect (flame studies)	-	2	12	11	12
direct (mass spec)	17	3	3	2	3
ionization potential	7	5	10	10	9

Since some articles may contain information pertaining to more than one category listed above, the sum does not equal the total. In addition, some articles do not report any data, but, instead, discuss the interpretation of previously reported data. As a side note, the large number (17) of references for the enthalpy of formation of beryllium hydroxide is misleading since many are progress reports in which the same data are reported repeatedly.

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The support of the U. S. Air Office of Scientific Research, Directorate of Aerospace Sciences, with program directors Dr. L. H. Caveny and Dr. R. Vondra, is gratefully acknowledged. This activity began while the JANAF Thermochemical Tables project (AFOSR Contract No. F49620-85-C-0076) was at The Dow Chemical Company. Numerous people helped in the initial collecting and typing of these references. Special thanks go to Ms.' Betty Clark, Rhoda Toth, Barbara Meier, and Ann Schmidt. When this project was transferred to the U. S. National Bureau of Standards (AFOSR-ISSA-86-0063), the conversion of the files from word processor floppy disks to the local Chemical Thermodynamic Data Centers computer system was expedited by Mr. Ronen Lamden and Dr. David Neumann. The NBS BIB computer system, written by Dr. David Neumann, Ms. Dorothy Bickham, and Mr. Robert Conyne, was used for the conversion of numerous literature formats into the form used in this publication. The final processing of the literature citations was aided by Ms. Cynthia Jackson and Dr. David Neumann. The assistance of Ms. Rhoda Levin in the preparation of this article for publication, both in terms of cross-checking the references for inclusion in the bibliographies and improving the clarity of the work, is greatly appreciated.

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60MAD Mader, C. L., "Thermodynamic properties of detonation products", U.S. At. Energy Comm., AECU-4508(Suppl), 57 pp (1960), CA 57 15891j, thermochemical table

62HIL/THE Hildenbrand, D. L., Theard, L. P., "Thermodynamic properties of rocket combustion products", Ford Motor Company, Aeronutronic Division, Second Quarterly Technical Progress Report, U-1546 (February 1, 1962), enthalpy of formation

62HIL/THE2 Hildenbrand, D. L., Theard, L. P., "Thermodynamic properties of rocket combustion products", Ford Motor Company, Aeronutronic Division, Final Technical Report, U-1784 (31 July 1962), enthalpy of formation

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A bibliographic collection is provided on data which are necessary for the calculation of the thermochemical properties of the gaseous alkaline earth metal (mono)hydroxides (MOH) and their positive ions (MOH^+), where M = Be, Mg, Ca, Sr, and Ba. This is the first in a series of articles that will document the information used in the critical evaluation of the thermodynamic properties for the JANAF Thermochemcial Tables. The collection contains references which have been published through the end of 1985, with a limited number of 1986 references. Five bibliographies are given, one for each of the alkaline earth metals. In each bibliography, the references are listed chronologically; alphabetically by first author within each year. The names of the ten species are given according to the Chemical Abstracts system of nomenclature (as of the Tenth Collective Index). The Chemical Abstracts Registry Numbers are also given for each of the species. A brief summary of the type of available information is given.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

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U.S. Department of Commerce
National Bureau of Standards
Gaithersburg, MD 20899