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## **NBS Technical Note 1244**

# *Thermodynamic Properties of Halides, Hydrides, and Deuterides of Cobalt, Iron, and Nickel*

## *I. Literature Citations*

*Cynthia R. Jackson and Malcolm W. Chase*

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## NBS Technical Note 1244

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Cynthia R. Jackson and Malcolm W. Chase

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

December 1987



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THERMODYNAMIC PROPERTIES OF HALIDES, HYDRIDES, AND DEUTERIDES OF COBALT, IRON, AND NICKEL  
I. Literature Citations

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## ABSTRACT

A bibliographic collection is provided on data which are necessary for the calculation of the thermochemical properties of the gaseous metal halides, hydrides (deuterides) and their positive and negative ions ( $\text{MX}$ ,  $\text{MX}^+$  and  $\text{MX}^-$ ), where  $\text{M} = \text{Co}$ ,  $\text{Fe}$ , and  $\text{Ni}$  and  $\text{X} = \text{Br}$ ,  $\text{Cl}$ ,  $\text{F}$ ,  $\text{H(D)}$ , and  $\text{I}$ . This is the first in a series of articles that will document the information used in the critical evaluation of the thermodynamic properties of these substances for the JANAF Thermochemical Tables.

The collection contains references which have been published through the end of 1986 with some 1987 references. Fifteen bibliographies are given, one for each species. In all bibliographies, the references are listed chronologically; alphabetically by first author within each year. The names of the species are given according to the Chemical Abstracts system of nomenclature (as of the Tenth Collective Index) when possible. The Chemical Abstracts Registry Numbers, if assigned, are also given for each of the species. A brief summary of the type of available information is given.

**Keywords:** bibliography, electron affinity, electronic energy levels, equilibrium data, formation properties, ionization potential, molecular structure, review articles, thermochemistry, thermodynamic properties, transition metal halides and hydrides, 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 iron, cobalt and nickel halides, hydrides (deuterides) and their positive and negative ions ( $\text{MX}$ ,  $\text{MX}^+$ ,  $\text{MX}^-$ ) are being prepared. The iron species are also being studied for use in the CODATA Task Group on Chemical Thermodynamics Tables. 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 it 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 in this coverage is in the appearance of pertinent data in journals not accessed by the abstracting services.

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 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. In the species studied here, however, the data are not strongly linked via chemical reactions to other species. Thus, a network solution may not be necessary. However, a comparison of the results of this study with the results for other transition metal species would be beneficial in confirming possible trends and identifying possible discrepancies.

## NOMENCLATURE

The species of interest in this bibliographic collection are given below with their names and registry numbers, as obtained from Chemical Abstracts On-Line (Registry File) in October 1987. Only 31 of the potentially relevant 54 species have been assigned registry numbers. The remaining 23 species, which are not listed in the following table, are named in analogy with those given. Historically, these species have often been called monohalides, monohydrides, and monodeuterides, but these designations are not used. In addition, names such as "chloronickel ion" have been used in the past but are no longer used by Chemical Abstracts. Although our intent was to cover the positive and negative ions of the above mentioned eighteen neutral species, not all of these species have been listed in the Chemical Abstracts Registry Number system, and thus are not listed here. Interestingly, there is no data reported in Chemical Abstracts for NiI(g), but there is information for the positive ion. On the other hand, data are given in the literature for FeI<sup>+</sup>, but no access to this species is given in Chemical Abstracts through the Formula Index.

formula	name	registry number
CoBr	Cobalt Bromide	22584-72-1
CoCl	Cobalt Chloride	34240-80-7
CoCl+	Chlorocobalt(1+)	52082-14-1
CoD+	Hydro-d-cobalt(1+)	87136-05-8
CoD	Cobalt Hydride (CoD)	76622-37-2**
CoD	Cobalt Hydride (CoD)	40418-24-4**
CoD	Cobalt Deuteride	37362-92-8**
CoF	Cobalt Fluoride	67321-83-9
CoF+	Fluorocobalt(1+)	21773-33-1
CoH	Cobalt Hydride	14994-20-8
CoH+	Hydrocobalt(1+)	12378-09-5
CoH-	Hydrocobaltate(1-)	65899-90-7
CoI	Cobalt Iodide	101015-09-2
FeBr	Iron Bromide	12514-32-8
FeBr+	Bromoiron(1+)	90143-36-5
FeCl	Iron Chloride	27846-09-9
FeD	Iron Deuteride	40418-23-3
FeF	Iron Fluoride	41428-55-1
FeH	Iron Hydride	15600-68-7
FeH+	Hydroiron(1+)	71899-96-2
FeH-	Hydroferrate(1-)	64899-88-3
FeI	Iron Iodide	33019-21-5
NiBr	Nickel Bromide	71939-11-2
NiCl	Nickel Chloride	13931-83-4
NiCl+	Chloronickel(1+)	52082-15-2
NiD	Nickel Deuteride	14989-21-0
NiD+	Hydro-d-nickel(1+)	75181-24-7

NiF	Nickel Fluoride	13783-64-7
NiF+	Fluoronickel(1+)	26024-87-3
NiH	Nickel Hydride	14332-32-2
NiH+	Hydronickel(1+)	75181-25-8
NiH-	Hydronickelate(1-)	64899-92-9
NiI+	Iodonickel(1+)	53290-74-7

\*\* NOTE: There are three registry numbers assigned to CoD.

#### LITERATURE COVERAGE

All references, which appear to have some data pertinent to the thermochemical calculations, have been collected into fifteen bibliographies, one for each of the halides and hydrides (deuterides) of cobalt, iron and nickel. The references for the deuterides are contained in the hydride bibliographies. These references were taken primarily from a search of Chemical Abstracts, from the First Collective Index, which includes 1907-1916, to the 11th Collective Index, which includes 1982-1986. However, we have included some 1987 publications in the bibliographies. In addition, scanning of the retrieved articles, manual scanning of selected resources, using personal contacts, searching the Chemical Thermodynamics Data Centers abstract files, and searching the Ion Kinetics and Energetics Data Center data base have yielded additional publications. It is hoped that the collection is complete through 1986 within the following constraints:

1. Articles referring to aqueous solutions involving  $MX^+$  and  $MX^-$  usually are not included. We are interested only in the gaseous  $MX$ ,  $MX^+$  and  $MX^-$  species.
2. Articles referring to estimated thermochemical values for  $MX(cr)$  are not included.
3. Articles published in astrophysical journals often are not included since they usually are not presenting new spectral information. More often, existing spectral data are given.

4. Analytical chemistry articles which deal with the interferences of MX(g) electronic bands with other bands typically 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 hydrides (deuterides) and halides in calculations are not included, unless the article includes a discussion of problems in the calculated results.
6. At this time, only those critical reviews which deal exclusively with halides and hydrides (deuterides) are included. The more general critical reviews (i.e. JANAF Thermochemical Tables) will be included in the next publication of this series.

The inclusion of an article in this collection does not necessarily imply that it will be of high importance in the final selection of data. Since there is not an overabundance of data, we have been unselective in our choice of entries in these bibliographies, and have extracted some articles which are tangential to our work with the hope that some useful information may be hidden in them. The initial examination of the literature suggests that sufficient reliable information is not available to generate sound thermochemical tables for some halides and hydrides (deuterides). Many will be estimated tables.

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

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

At this time for these metal halides and hydrides (deuterides), we have collected the majority of the available data, with no statement as to its reliability or usefulness.

## DATA SUMMARIES

The next publication in this series will contain sets of tabular information which will summarize the relevant data, as 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 halides and hydrides (deuterides), data summaries will be presented for the following information:

- dissociation energy
- electronic energy levels and configurations
- vibration-rotation constants
- ionization potential
- electron affinity

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

The following table summarizes briefly the nature and quantity of data available for the halides and hydrides (deuterides).

SUBJECT COVERAGE IN REFERENCES ON COBALT, IRON, AND NICKEL SPECIES

	CoBr	CoCl	CoD	CoF	CoH	CoI
total references	7	13	8	4	29	1
electronic energy information						
electronic energy levels	6	9	4	-	11	-
vibrational analysis	4	7	2	-	9	-
rotational analysis	-	-	3	-	-	-
dissociation energy	-	1	-	1	12	1
ionization potential	-	-	1	1	2	-
electron affinity	-	-	1	-	-	-
	FeBr	FeCl	FeD	FeF	FeH	FeI
total references	6	21	7	17	44	3
electronic energy information						
electronic energy levels	4	11	3	3	15	-
vibrational analysis	4	8	1	-	7	-
rotational analysis	-	1	1	1	-	-
dissociation energy	-	6	1	5	20	1
ionization potential	-	-	1	-	3	3
electron affinity	-	-	1	-	1	-
	NiBr	NiCl	NiD	NiF	NiH	NiI
total references	15	27	10	15	48	1
electronic energy information						
electronic energy levels	10	14	3	7	19	-
vibrational analysis	9	14	2	3	14	-
rotational analysis	-	1	2	2	3	-
dissociation energy	1	7	1	3	17	3
ionization potential	-	1	1	-	3	-
electron affinity	1	1	1	-	-	-

Since any one article may contain information pertaining to more than one category listed on the previous page, the sum within any column will not necessarily equal the total. In addition, some articles do not report any data, but instead discuss the interpretation of previously reported data.

#### ACKNOWLEDGEMENT

This activity is partially supported by the U. S. Air Force Office of Scientific Research (AFOSR-ISSA-86-0063) and by the Office of Standard Reference Data of the National Bureau of Standards. The work was undertaken not only as a contribution to the JANAF Thermochemical Tables but also as a contribution to the CODATA Task Group on Chemical Thermodynamic Tables. The more recent Russian references for the iron compounds were obtained from the reaction catalog provided by the Institute for High Temperatures (Moscow, USSR) to NBS for the CODATA Task Group. The help of the personnel of the Chemical Thermodynamics Data Centers is greatly appreciated. Special thanks go to Ms. Rhoda Levin of the Ion Kinetics and Energetics Data Center for assistance in the preparation of this article, both in terms of cross-checking the references for inclusion in the bibliographies, improving the clarity of the work, and proof-reading the text. Thanks are also extended to Dr. Vivian B. Parker and Dr. David Garvin for their comments on this article.

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- 37MES Mesnage, P., "Molecular emission spectra of some metallic salts", Compt. Rend., 204, 1929-1931 (1937), CA31:6108(8), emission spectra, electronic energy levels
- 39MES Mesnage, P., "Researches on high-frequency discharges and their application to molecular spectroscopy", Ann. Phys., (11), 12, 5-87 (1939), CA33:8112(4), vibrational analysis, emission spectra, electronic energy levels
- 52KRI Krishnamurty, V.G., "Structure of the band spectra of the halides of Co and Ni", Dissertation, Univ. Andhra, Doctoral Thesis (1952), emission spectra, electronic energy levels
- 62RAO/RAO Rao, S.V.K., Rao, P.T., "The spectrum of CoBr in the visible (4300-4700 A.)", Indian J. Phys., 36, 609-612 (1962), CA59:3442b, emission spectra, electronic energy levels, vibrational analysis
- 68RAO/RAO Rao, N. V. K., Rao, P. T., "New band systems of CoBr in the photographic infrared", Curr. Sci., 37(21), 608-609 (1968), CA70(12):52722b, emission spectra, vibrational analysis, electronic energy levels
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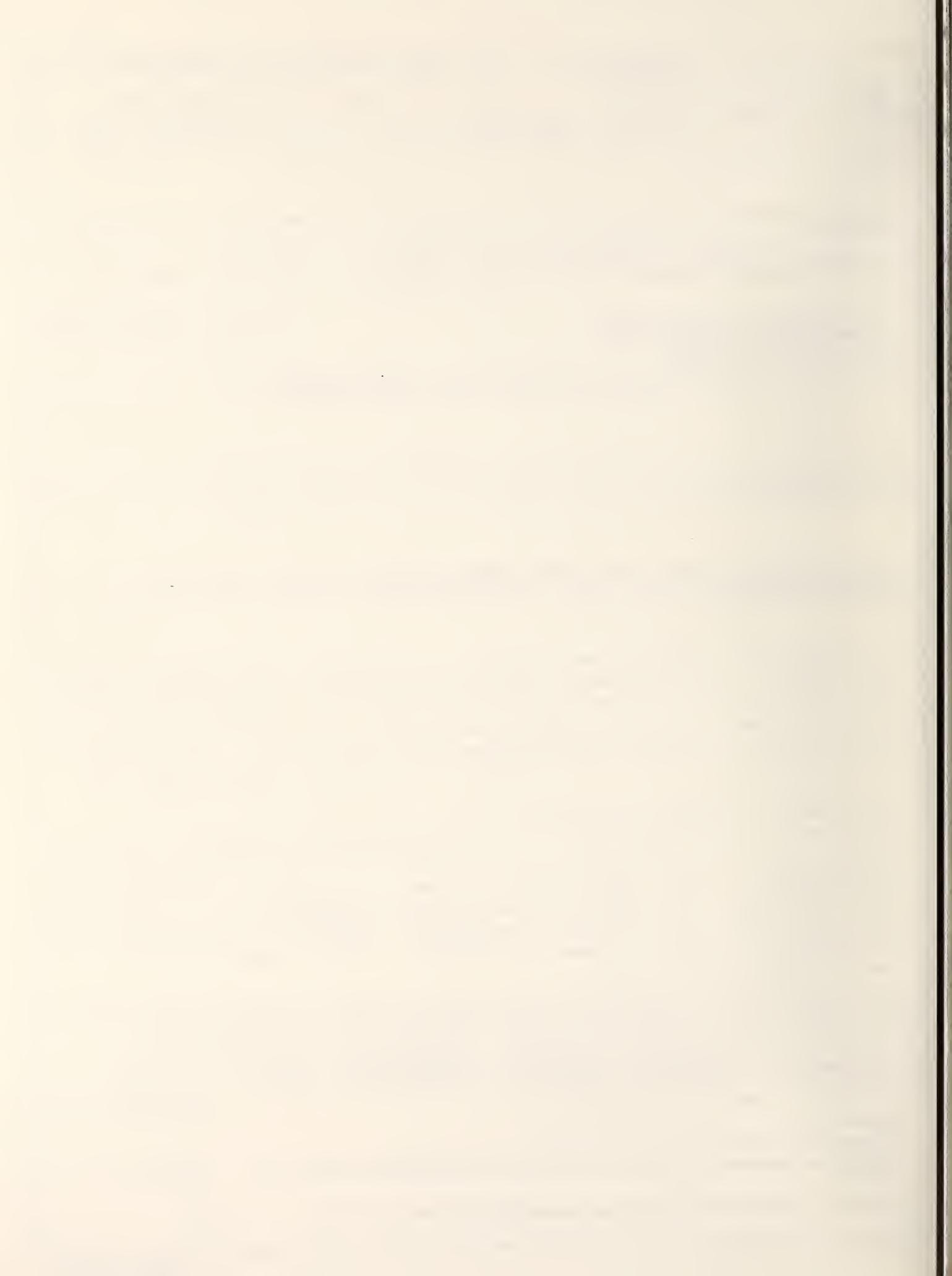
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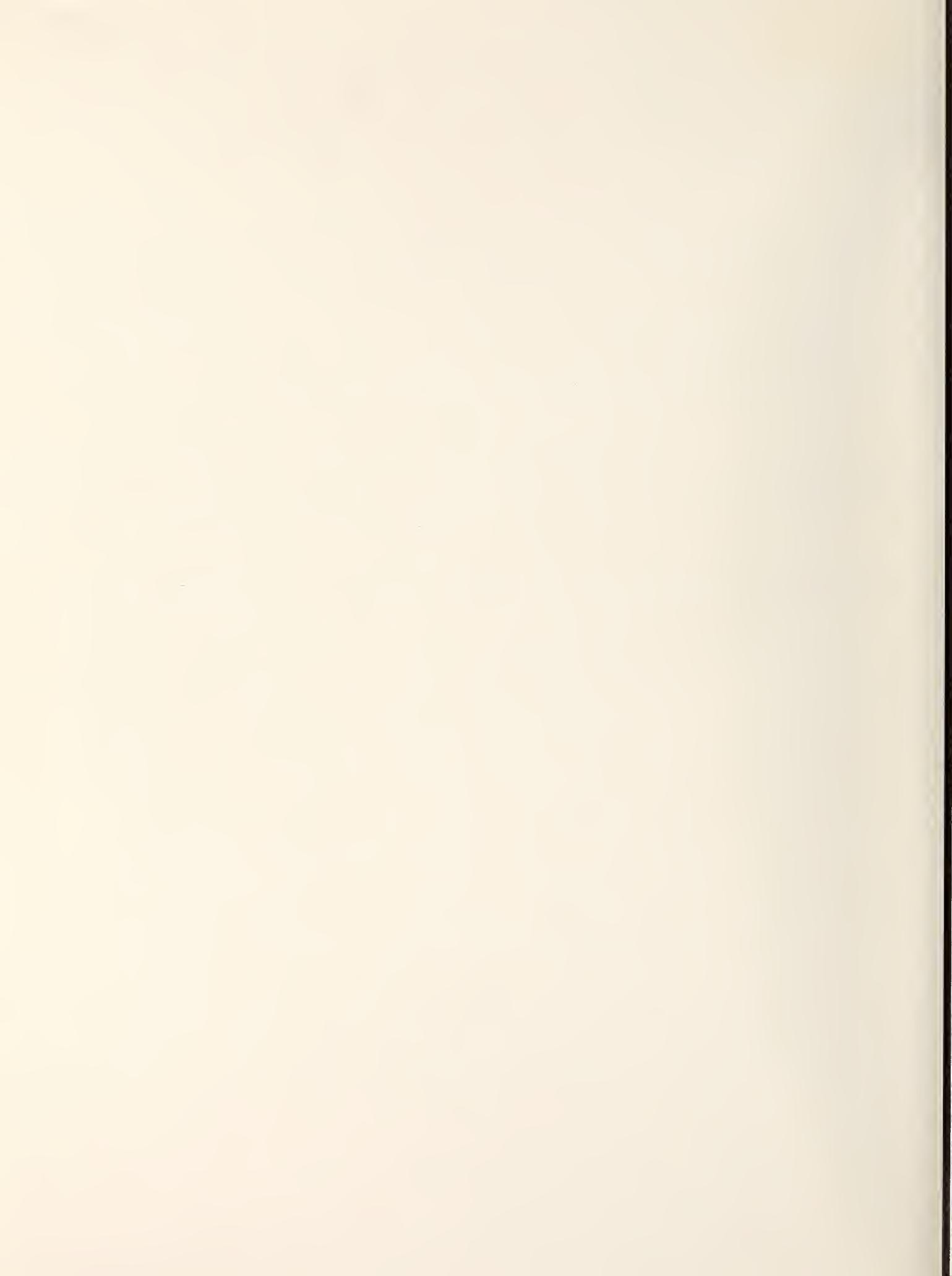
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