NIST–JANAF Thermochemical Tables for the Iodine Oxides

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NIST–JANAF Thermochemical Tables for the Iodine Oxides

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The thermodynamic and spectroscopic properties of the iodine oxide species have been reviewed. Recommended NIST–JANAF Thermochemical Tables are given for six gaseous iodine oxides: IO, OIO, IOO, IOI, IIO, and IOI. Sufficient information is not available to generate thermochemical tables for any condensed phase species. Annotated bibliographies (over 400 references) are provided for all neutral iodine oxides which have been reported in the literature. There is a lack of experimental thermodynamic and spectroscopic information for all iodine oxide species, except IO(g) and OIO(g). The recommended thermochemical tables are based on estimates for the structure, vibrational frequencies, and enthalpy of formation based in part on the spectroscopic and thermodynamic data for the other halogen oxides [J. Phys. Chem. Ref. Data 25, 551 (1996); 25, 1061 (1996)]. Although there is a definite lack of information in comparison with the other halides, this information is provided for the iodine oxides for the following reasons: (1) to complete the study of the halogen oxide family and (2) to stress the need for additional experimental measurements. Of all the species mentioned in the literature, many have not been isolated or characterized. In fact, some do not exist. Throughout this paper, uncertainties attached to recommended values correspond to the uncertainty interval, equal to twice the standard deviation of the mean. © 1996 American Institute of Physics and American Chemical Society.

Key words: evaluated/recommended data; iodine oxides; literature survey; spectroscopic properties; thermodynamic properties.

Contents

1. Introduction .................................. 1298
   1.1 References for Introduction ............ 1299
2. Chemical Species Coverage .................. 1300
3. Historical Perspective of Iodine Oxide Studies 1300
4. Summary of the Data for the Iodine Oxide Species .................. 1301
   4.1 Spectroscopic Information .............. 1301
   4.2. Thermodynamic Information .......... 1301
5. Discussion of the Literature Data .......... 1302
   5.1 IO .................................. 1302
   5.2 IO 2 .................................. 1304
   5.3 Iodyl–IO 2 ................................ 1304
   5.4 IOO .................................. 1305
   5.5 IO 2+ .................................. 1305
   5.6 IOI .................................. 1305
   5.7 IO .................................. 1305
   5.8 I 2O .................................. 1306
   5.9 I 2O 2 .................................. 1306
   5.10 I 2O 3 .................................. 1306
   5.11 I 3O .................................. 1306
   5.12 I 3O 2 .................................. 1307
   5.13 I 3O 3 .................................. 1308
   5.14 I 3O 4 .................................. 1308
   5.15 I 3O 5 .................................. 1309
   5.16 I 3O 6 .................................. 1309
   5.17 I 3O 7 .................................. 1309
   5.18 I 3O 8 .................................. 1309
6. NIST–JANAF Thermochemical Tables ........ 1320
   6.1 IO(g) .................................. 1321
   6.2 OIO(g) .................................. 1322
   6.3 IOO(g) .................................. 1323
   6.4 IOI(g) .................................. 1324
   6.5 IIO(g) .................................. 1325
   6.6 IIOI(g) .................................. 1326
7. Conclusions .................................. 1327
8. Acknowledgments ............................. 1327
9. References—Annotated Bibliography .......... 1327

List of Tables

1a. Solid iodine oxide species: Preparation and related reactions 1310
1b. Solid iodine oxide species: Decomposition and related reactions 1311
2. Iodine oxide species: Neutrals, radicals, and ions in solution 1314
3. Iodine oxide species: Electronic energy levels ... 1315
4. Iodine oxide species (IO): Dissociation energy (D0) 1317
5. Iodine oxide species: Structures and vibrational frequencies 1318
6. Thermodynamic properties of the iodine oxides 1327

0047-2689/96/25(5)/1297/44/$14.00

1. Introduction

As a continuation of previous studies which dealt with the thermodynamic properties of the chlorine oxides,\(^1\) oxygen fluorides,\(^2\) and bromine oxides,\(^3\) this study deals with the iodine oxides. We will not discuss the astatine oxides, as there appears to be only an estimated \(D_T\) value reported in the literature for AtO(g). Specifically, this study examines the thermodynamic properties of the neutral oxides, not the gaseous ionic and aqueous ionic species. The main purpose of this article is to generate thermochemical tables for iodine oxide species. In general, there are scant data available for the description of the spectroscopic and thermodynamic data for any of the iodine oxides, except for IO(g) and OIO(g). Although the prime emphasis was on the diatomic and triatomic species, a thorough search of all iodine oxygen species was conducted to decide which species had sufficient data. Of the iodine oxides mentioned in the literature, only five have been isolated and (at least, partially) characterized: IO(g), OIO(g), \(\text{I}_2\text{O}_5\)(cr), \(\text{I}_2\text{O}_7\)(cr), \(\text{I}_2\text{O}_9\)(cr).

For the time period 1907–1994, there are only 354 citations in Chemical Abstract Services (CAS) dealing with the iodine oxides; of these, 196 are for \(\text{I}_2\text{O}_3\) (with the majority of these dealing with commercial applications, as opposed to providing property data) and 73 references deal with IO. Of the approximately 20 oxides mentioned in the literature, however, some do not exist.

Iodine oxides are also of interest due to their involvement in the transport of iodine in a post-accident nuclear environment, while IO is of interest both because of its similarity to CIO (ozone depletion) and as a tropospheric ozone sink. Spectroscopic studies have shown that the ground and first excited electronic states of the halogen monoxides play an intermediate role in the photochemistry of upper atmosphere (e.g., CIO in stratosphere and IO in ionosphere limit the atmospheric abundance of ozone). \(\text{I}_2\text{O}_3\) is discussed in many articles dealing with the compound’s preparation or reaction. Specifically, \(\text{I}_2\text{O}_3\) has key applications in detecting CO(g). Despite this relevance of the halogen oxides, basic physical properties, in particular the vibrational frequencies and molecular geometries, are poorly characterized.

The current study is aimed at providing a complete and thorough coverage of the literature for spectroscopic and thermodynamic information. Although it is not the purpose of this article to summarize and critique the chemistry of the iodine oxides, all such references are provided here. The references were obtained primarily by use of commercial abstracting services and all NIST Data Centers.\(^8\) Since the literature survey revealed so few references in total for all iodine oxides, all citations are listed in Sec. 9 (References—Annotated Bibliography), except the approximately fifty patents which are not listed or discussed. It should be noted that the reading of the individual articles yielded many additional references, most of which are included in the attached bibliography. Not included are those articles or books (textbooks and handbooks) which are simply presenting a summary of properties, with no critical evaluation. Note that the earliest reference for any iodine oxide species was in the 1800s. However, these bibliographies are not complete in their coverage for the 1800s. Even though many of these citations are not relevant to this study, future investigators will not have to search the past literature, but simply concentrate on the publications since 1994.

The current edition (i.e., 1985) of the JANAF Thermochmical Tables\(^4\) does not include any iodine oxygen species, whereas the Thermodynamic Properties of Individual Substances\(^5\) only includes IO(g). This latter critical review referred to data from four spectroscopic studies, three ESR studies, one microwave study, and four dissociation energy studies, the latest of all these citations being dated 1975. The NBS tables\(^6\) gave information for IO(g) at 298.15 K, for \(C, S, H,\) and the formation properties, but only an enthalpy of formation for \(\text{I}_2\text{O}_5\)(cr). (Information for four iodine oxide aqueous ions is also included.) Similar information was given in Thermal Constants of Substances,\(^7\) although these authors additionally include an enthalpy of formation of a pentoxide hydrate. (Information for one iodine oxide aqueous ion is included.) These latter two evaluations were performed in 1964 and 1965, respectively, and were based on the same references.

There are many NASA-JPL publications on chemical kinetics in which enthalpy of formation tables are given. Of all the iodine oxides, only IO(g) is listed by NASA-JPL.\(^8\) These data are presented without citation or reference to the original source. Most of the recommendations are based upon data in the IUPAC Evaluation (Atkinson et al., 1989,\(^9\) 1992\(^10\)). Some of the values are different from the current IUPAC recommendations, reflecting recent studies that have not yet been accepted and incorporated into that publication. IUPAC cites the origin of their values. All citations given by IUPAC are included in this article.

Iodine and its oxides were reviewed by Roman\(^11\) for the Gmelin series. This review covered the literature through 1933 and is an excellent source of information on the oxides for the period of the 1800s. All these references are not included in this article. The Roman review discussed (see pages 432 to 442) the following compounds: I, I\(_2\), \(\text{I}_2\text{O}_3\), \(\text{I}_2\text{O}_4\) (or IO\(_2\)), \(\text{I}_2\text{O}_5\), \(\text{I}_2\text{O}_7\), IO\(_4\), \(\text{I}_2\text{O}_9\), \(\text{I}_2\text{O}_{10}\), and \(\text{I}_2\text{O}_{13}\). The latter two compounds were stated not to exist. The text discussed the formation and stability of the condensed phase oxides. In general, there were property data presented only for the pentoxide. There was a short mention of the thermodynamic information on the formation of \(\text{I}_2\text{O}_5\)(cr) at the time of this review. There were no experimental studies for the gaseous iodine oxides mentioned.

In a 1963 review article, Schmied and Brandle\(^12\) summarized the data pertaining to the properties and chemistry of the halogen–oxygen compounds. Although these authors did not specifically discuss IO, they highlighted the fact that
only \( \text{IO}_2 \) was well defined with only two other oxides having been isolated, but not unequivocally characterized—\( \text{I}_2 \text{O}_2 \) and \( \text{I}_2 \text{O}_4 \). A 1968 article by Selte and Kjekshus\(^1\) stated that two oxides \( \text{I}_2 \text{O}_3 \) and \( \text{I}_2 \text{O}_4 \) were properly established whereas the rest have a high degree of uncertainty associated with them. In a 1972 review of the halogen oxides, Brison\(^2\) discussed seven iodine oxide species: \( \text{I}_2 \text{O}_2 \), \( \text{IO}_2 \), \( \text{IO}_3 \), \( \text{IO}_4 \), \( \text{I}_2 \text{O}_3 \), and \( \text{I}_2 \text{O}_4 \). Whereas there was a spectroscopic characterization given for \( \text{IO}_2 \), there was only structural information in the condensed phase given for \( \text{I}_2 \text{O}_2 \) and \( \text{I}_2 \text{O}_3 \). \( \text{IO}_2 \) and \( \text{IO}_3 \) were mentioned only in terms of their presumed formation in iodate solutions. A later review (1980) by Wikjord et al.\(^3\) suggested that \( \text{I}_2 \text{O}_4 \), \( \text{I}_2 \text{O}_5 \), and \( \text{I}_2 \text{O}_6 \) have been isolated and fully characterized, crystallographically.

In 1977, Clyne and Curran\(^4\) surveyed the kinetics of halogen atoms, excited molecular halogens, and halogen oxide radicals. The authors covered the literature through early 1976. Their discussion provided a summary of the bimolecular reactions of \( \text{Cl}_2 \), \( \text{HBr} \), and \( \text{Br}_2 \). The authors stated that so far no systematic kinetic studies of \( \text{IO}_2 \) had been performed.

After this article was written and reviewed, we became aware of the existence of another review article by Wayne et al.\(^5\). This article provides discussion on the thermodynamic and spectroscopic data on many bromine oxides. Although not of importance for our purposes, the article also discusses many other topics, including photochemistry and kinetics.

In reading Sec. 5, the reader will soon learn that the existence of the iodine oxide compounds is questionable. The thermal instability of the iodine oxides has led to numerous difficulties in characterizing specific iodine oxides. The syntheses are not always reproducible. The following summarizes our interpretations of the probable existence of the compounds mentioned:

**Exist and have been observed:** \( \text{IO}_2 \); \( \text{IO}_3 \);

**Postulated:** \( \text{IO}_2 \text{O}_2 \); \( \text{IO}_3 \); \( \text{I}_2 \text{O}_3 \); \( \text{I}_2 \text{O}_4 \); \( \text{I}_2 \text{O}_5 \);

**Hypothetical molecule to describe ternary systems:** \( \text{I}_2 \text{O}_3 \); \( \text{I}_2 \text{O}_2 \); \( \text{IO}_3 \); \( \text{I}_2 \text{O}_4 \);

**No conclusive confirmation as to existence:** \( \text{I}_2 \text{O}_3 \); \( \text{I}_2 \text{O}_5 \); \( \text{I}_2 \text{O}_6 \);

In the following discussions, analyses and calculations, the 1993 atomic weights of the elements are used:\(^1\) \( A(\text{I}) = 126.904 \pm 0.004 \); \( A(\text{O}) = 15.9994 \pm 0.0003 \). Since the mid-1950s, the relative atomic weight of oxygen has changed by 0.0006 to 15.9994. Similarly for iodine, the relative atomic weight has changed by 0.005 53 to 126.904 47. However, since 1961 the change has been 0.0003. Relatively speaking, these changes are sufficiently small that we will not consider any conversions due to relative atomic weights.

In addition, the 1986 fundamental constants are used:\(^2\) \( R = 8.314 \cdot 510 \cdot 0.000 070 \, \text{J K}^{-1} \cdot \text{mol}^{-1} \). In comparison to the 1973 fundamental constants (16), \( R \) has changed by +0.0001 \( \text{J K}^{-1} \cdot \text{mol}^{-1} \).

SI units are used for the final recommendations. Since we are dealing only with spectroscopic information, the resulting calculated thermodynamic tables will refer to thermodynamic temperatures. Thus, no temperature scale conversions are necessary.

In the following discussions, the numeric values (and their uncertainties if given) presented are those reported in the original publication in addition to the SI value. This is to ensure quick confirmation of the extracted results and their uncertainties. These uncertainties (not always based on experimental and mathematical analyses) are the values quoted by the original authors and are often not fully described as to their origins. Our reported uncertainties for \( S^0 \) and \( \Delta H^\circ \) are calculated using a propagation of errors approach.

The recommended data presented in the NIST–JANAF Thermochemical Tables are a result of a combined appraisal of results from experimental studies, calculations (e.g., quantum-mechanical treatments) and estimations. All tables are calculated using the full significance of all numeric values. Rounding occurs at the end of the calculations. The uncertainty given represents our best attempt for twice the standard deviation.

The NIST–JANAF Thermodynamic Tables (Sec. 6) are calculated using the current atomic weights and fundamental constants, as well as the thermochemical tables for monatomic and diatomic iodine and oxygen. These latter reference state thermochemical tables, as originally calculated, were based on the 1973 fundamental constants\(^6\) and the 1981 relative atomic weights.\(^7\) This will cause a slight offset in the formation properties of the order 0.01 kJ mol\(^{-1}\) at most; such an offset is still outside the uncertainty range of the enthalpy of formation of the iodine oxides. Neumann\(^8\) has presented an identical thermodynamic table for \( \text{IO}_2 \); this table was prepared jointly with this author.

### 1.1 References for Introduction

7. V. P. Glushko and V. A. Medvedev, Thermal Constants of Substances (Academy of Sciences, Moscow, 1965).
2. Chemical Species Coverage

The following is a list of all iodine oxide species cited in the Chemical Abstracts Services (CAS) Indices (formula and substance). Aqueous ions and positive/negative gaseous ions are not included in this study. The chemical name, formula, and CAS Registry Number (when available) are given. This list is complete through Volume 121 of Chemical Abstracts Services (December, 1994). Numerous citations, covering 1995–1996 are included, but the coverage may not be complete. It is important to note that this listing includes species which now are known not to exist, but they were cited in the early literature. Deleted CAS Registry Numbers are given to assure the reader that all past citations were retrieved. There are difficulties in discussing “a” oxide such as IO₂ in which references are made to IO₂ and I₂O₃ as the same compound. Similar problems exist with IO₃/I₂O₅ and IO₂/I₂O₃. There is not sufficient experimental information to confirm the existence of six of the listed oxides (I₂O, I₂O₂, I₂O₅, I₂O₇, I₃O₁₃, and I₄O₁₀). In addition, there are no experimental data on the gaseous radicals IO₂ and IO₃. Many of the reported species have been proposed in reaction schemes, but not characterized. Also, it is important to note that there is no information available to suggest the existence of asymmetric isomers of the triatomic species IOO and IIO, although the former has been proposed in a kinetic scheme. Such asymmetric isomers exist for the chlorine, fluorine, and bromine oxides.

### Iodine oxide species

<table>
<thead>
<tr>
<th>Formula</th>
<th>Name</th>
<th>CAS Collective Registry Numbers</th>
</tr>
</thead>
<tbody>
<tr>
<td>IO (IO)</td>
<td>Iodine oxide</td>
<td>50400-00-5</td>
</tr>
<tr>
<td>IO₂ (IO₂)</td>
<td>Iodyl</td>
<td>71132-73-5</td>
</tr>
<tr>
<td>I₂O₃ (IO₃)</td>
<td>Iodine oxide</td>
<td>13494-92-3</td>
</tr>
<tr>
<td>I₂O₅ (IO₅)</td>
<td>Iodyl</td>
<td>116854-14-9</td>
</tr>
<tr>
<td>I₂O₇ (IO₇)</td>
<td>Iodyl</td>
<td>...</td>
</tr>
<tr>
<td>I₂O₉ (IO₉)</td>
<td>Iodyl</td>
<td>...</td>
</tr>
<tr>
<td>I₃O₁₀ (IO₁₀)</td>
<td>Iodine oxide</td>
<td>108216-85-9</td>
</tr>
<tr>
<td>I₃O₁₂ (IO₁₂)</td>
<td>Iodine oxide</td>
<td>13870-16-1</td>
</tr>
<tr>
<td>I₃O₁₄ (IO₁₄)</td>
<td>Iodine oxide</td>
<td>11074-36-5</td>
</tr>
<tr>
<td>I₃O₁₆ (IO₁₆)</td>
<td>Iodine oxide</td>
<td>39319-71-6</td>
</tr>
<tr>
<td>I₃O₁₈ (IO₁₈)</td>
<td>Iodine oxide</td>
<td>...</td>
</tr>
<tr>
<td>I₃O₂₀ (IO₂₀)</td>
<td>Iodine oxide</td>
<td>11085-17-9</td>
</tr>
<tr>
<td>I₃O₂₂ (IO₂₂)</td>
<td>Iodine oxide</td>
<td>12399-08-5</td>
</tr>
<tr>
<td>I₃O₂₄ (IO₂₄)</td>
<td>Iodine oxide</td>
<td>7790-35-4</td>
</tr>
<tr>
<td>I₃O₂₆ (IO₂₆)</td>
<td>Iodine oxide</td>
<td>64052-04-6</td>
</tr>
<tr>
<td>I₃O₂₈ (IO₂₈)</td>
<td>Iodidexygen</td>
<td>65355-99-9</td>
</tr>
<tr>
<td>I₄O₃₆ (IO₃₆)</td>
<td>Iodide</td>
<td>63912-61-8</td>
</tr>
<tr>
<td>I₅O₄₆ (IO₄₆)</td>
<td>Iodine oxide</td>
<td>20270-38-6</td>
</tr>
<tr>
<td>I₄O₅₄ (IO₅₄)</td>
<td>Iodine oxide</td>
<td>81756-07-2</td>
</tr>
<tr>
<td>I₅O₆₄ (IO₆₄)</td>
<td>Iodine oxide</td>
<td>73560-00-6</td>
</tr>
<tr>
<td>I₆O₇₄ (IO₇₄)</td>
<td>Iodine oxide</td>
<td>66523-94-2</td>
</tr>
<tr>
<td>I₇O₈₄ (IO₈₄)</td>
<td>Iodine oxide</td>
<td>...</td>
</tr>
<tr>
<td>I₈O₉₄ (IO₉₄)</td>
<td>Iodine oxide</td>
<td>...</td>
</tr>
</tbody>
</table>

The second formula is intended to suggest the assigned structure. If there is no secondary formula given, this means that no structure has been determined for this species, but the atomic ratio is known.

Articles exist which refer to this species, but there are no definitive data to prove its existence.

In those cases where a deleted CAS Registry Number exists, but no current CAS Registry Number exists, the species has been reassigned to another CAS Registry Number. This is discussed in a later section.

If no CAS Registry Number appears in this column, then the species is assumed NOT to exist or no characterization has been made.

3. Historical Perspective of the Iodine Oxide Studies

It is informative to briefly summarize the types of studies which have been conducted through the years on the iodine oxides. Specific references are given in Sec. 9. This section is intended to simply highlight developments through the years.

Using the CAS Collective Indices as a backdrop for these introductory comments, the period of 1907 to 1926 (the First and Second Collective Indices) reveals no information as to the thermodynamic and spectroscopic properties of any iodine oxides. For this time period, there are twelve citations (of which nine are for I₂O₅); some of these articles refer to additional work in this time period (although not noted by CAS) as well as earlier work. The retrieved information suggests that the preparation and identification of the various condensed phase oxides were still in their infancy. For example, there are articles which suggest that the earlier identification (pre-1907) of the oxides I₂O₃ and I₆O₉ was incorrect and that the oxide was in fact I₂O₅ which was (at that time) called, iodine isodate (IO·IO₃). Another article suggested that it was not as clear as whether the molecular spe-
cies was I$_2$O$_3$ or I$_2$O$_4$. In any event, there is information on the preparation, existence (or lack thereof), and reactivity of four iodine oxides (all in the condensed or aqueous phase)—I$_2$O$_4$, I$_2$O$_5$, I$_2$O$_7$, and I$_2$O$_9$—but not any spectroscopic and thermodynamic data. Of the nine pentoxide articles, four deal with preparative techniques and two with thermal stability.

From 1927 to 1946 (the Third and Fourth Collective Indices), there is continued activity in the preparation of various iodine oxides (only in the condensed or aqueous phase). Three articles involve the preparation of lower oxides (I$_2$O$_3$ and I$_2$O$_5$) and their relationship to I$_2$O$_5$. The remaining 25 citations deal with the pentoxide. There is considerable effort in reaction schemes involving the preparation and identification of the pentoxide and its hydrates. Articles on density and diamagnetism (structure) are the first citations on the properties of the pentoxide. Thermal decomposition (to the elements) studies suggest that decomposition “point” is 275°C.

For the time period 1947 to 1961 (the Fifth and Sixth Collective Indices), I$_2$O(g) has now been detected in flames and preliminary spectroscopic data were recorded yielding dissociation energy and rotation–vibration information. Of the 41 citations in this period, 23 deal with the pentoxide, with most of these involving commercial applications. However, some articles report the IR spectrum and structure of the condensed phase of the tetroxide and pentoxide.

In the time period 1962 to 1971 (the Seventh and Eighth Collective Indices), there are 87 references of which 44 refer to the pentoxide. Additional information on the spectroscopic properties of I$_2$O(g) was published. The first calculational information on the vibrational behavior of I$_2$O$_3$(g) appeared, as well as three articles dealing with the structure and spectra of I$_2$O$_5$ in the condensed phase. Although the majority of the pentoxide references deal with reactions and commercial applications, there are four articles which deal with the structure and spectra. No experimental information on the enthalpy of formation has appeared for any of the oxides except I$_2$O(g) and some pre-1900 studies of I$_2$O$_3$.

Of the 95 articles which are reported in the literature for the time period 1972 to 1981 (the Ninth and Tenth Collective Indices), the majority of the articles deal with I$_2$O(g) and I$_2$O$_5$(cr). There are numerous spectroscopic and dissociation energy studies on the monoxide. The pentoxide work was heavy on applications, including many patents, although there was continued examination of the relative stability among condensed phase oxides. There were also calculations and estimations involving I$_2$O(g), but no experimental studies.

In the time period 1982 to 1991 (the Eleventh and Twelfth Collective Indices), the literature deals primarily (again) with I$_2$O(g) and I$_2$O$_5$(cr). The pentoxide studies deal mostly with reactions and applications, with no definitive property characterization. Even the work involving I$_2$O(g) was related more to reactions, rather than spectroscopic and thermodynamic determinations.

In summary, there are no heat capacity, enthalpy, or vapor pressure studies for any of the iodine oxides, with the exception of one sublimation study for I$_2$O$_3$. There are many articles which detail the preparation and decomposition temperature of various crystalline oxides. There are some early (pre-1900) enthalpy of formation data for I$_2$O$_5$(cr). The spectroscopic properties and dissociation energy for I$_2$O(g) have been studied adequately, but the complete spectroscopic determination and enthalpy of formation values for any of the other iodine oxides are lacking. For the iodine oxides, many vibrational frequencies have been determined for the crystalline phase but none for the gas phase except I$_2$O$_3$. In addition, only I$_2$O and I$_2$O$_3$ have been studied in the gas phase. There are some experimental studies in a solution or a matrix.

4. Summary of the Data for the Iodine Oxide Species

4.1 Spectroscopic Information

The construction of thermodynamic tables for polyatomic gas phase species requires a knowledge of the spectroscopic constants of the molecule including electronic energy levels and degeneracies, vibrational frequencies and molecular structure (including bond angles and bond lengths). This information is necessary for any low-lying excited electronic states, as well as the ground state. These data are obtained from direct spectroscopic measurements, from theory, or by analogy with other similar chemical compounds. In some cases, theoretical quantum mechanical calculations are used. There is some spectral information available on a limited number of iodine oxides in the condensed phase. However, depending on information from the fluorine, chlorine, and bromine oxides, estimates can be made for the structure and spectroscopic properties of I$_2$O$_2$(g) and I$_2$O$_4$(g), as well as for the asymmetric isomer.

For the diatomic molecules, spectroscopic information on the electronic energy levels and vibrational–rotational structure is necessary. Experimental data of this type are available for I$_2$O(g). Similar information on ClO and BrO is available for comparison.

4.2 Thermodynamic Information

The literature survey revealed little or no information on the thermodynamic properties of any of the iodine oxides, except for I$_2$O(g), which was derived from spectroscopic data. Although not explicitly cited in Chemical Abstracts, there is a reference for the enthalpy of formation for I$_2$O$_3$(g) and I$_2$O$_5$(cr). There are, however, numerous citations as to the thermal stability of the various condensed phase oxides.

There are insufficient data available to permit the calculation of thermodynamic functions for the condensed phase of any of the iodine oxides. No heat capacity or enthalpy data are reported in the literature for any of these oxides. There are also no data for the melting of the various condensed phase. Limited stability information is available which refers to the decomposition of I$_2$O$_4$, I$_2$O$_5$, and I$_2$O$_9$. Melting, if observed, is in combination with decomposition.

For the gas phase species, only IO(g) has dissociation energy information available so that an enthalpy of formation may be calculated. No experimental formation information has been reported in the literature for any of the other iodine oxides.

5. Discussion of Literature Data

The information is discussed in terms of the individual iodine oxide species. All species cited in the Chemical Abstracts formula and substance index are discussed as well as those additional species which are mentioned in the individual articles. This is not to imply that all those species exist or have been isolated and characterized. For example, I$_2$O$_3$ and I$_2$O$_6$ do not exist, whereas I$_2$O$_5$ and I$_2$O$_7$, although discussed in many articles, have never been isolated. The references for each of the following subsections are found in the corresponding subsection of References—Annotated Bibliography (Sec. 9).

5.1 IO

There is a discontinued CA Registry Number 50400-00-5 that presumably referred to an unspecified iodine oxide compound, in which the iodine to oxygen ratio was one to one.

The reported references for IO(g) may be arbitrarily categorized as follows:

1. Spectra (see Table 3)
   - [37VAI], [46BLA/IRE], [48COL/GAY], [50HER], [58DUR/RAM], [60DAS/WAD], [60DUR/LEG], [72YAN], [73KAP], [73SAI], [79HUB/HER], [80LOE/MIL], [83BEK/MEE], [83ENG/TAL], [84BUR/LAW], [91GIL/POL], [92GIL/POL]

2. Preparation/formation/reaction (see Tables 1a, 1b, 2)
   - [60DAS/WAD], [62GUR/KHA], [69HAT/HUS], [73PAR/HER], [82ANT], [82FUR/NUO], [80BAR/BEC], [85BUX/KIL], [90BRA/HER], [90DAY/WYN], [90DAY/WIN], [90VOH/BAD], [92BUL/LAR], [92DUB/SKU], [92HEL/FOG]

3. Dissociation energy (see Table 4)
   - [30HER], [33GAY], [54COT], [58Bre], [58DUR/RAM], [61LIP/STE], [61PHI/SUG], [62GUR/KHA], [63SCH], [65SIN/RAI], [66VED/GUR], [68WAG/EVA], [69BRE/ROS], [69HER/HUI], [70CLY/CRU], [70DAR], [72RAI/SHA], [72TRI/GOH], [74RAO/RAO], [75RAD/WHI], [77GIL], [79ADD/DOJ], [79HUB/HER], [80KER/TRO], [82BAU/COX], [83BUS/SIB], [88TYK], [89GUR/VEY], [89RED/RAO], [92MAG/LAV], [94RUS/BER], [95HUI/LAS], [95ZHA/MON], [96GIL/TUR]

4. EPR (see Table 3)
   - [67CAR/DYE], [67CAR/CUR], [69CAR], [70CAR/DYE], [71BYF/CAR], [71MIL], [72BRO/BYF]

5. Radiolysis/photoysis


[61MCK/NOR], [63BUR/NOR], [70AMI/TRE], [70AMI/TRE2], [73STU/TEZ], [76CAL/MET], [77ANT/BUR], [77CAL/MET], [83COX/CKO], [83NIO/SUZ], [85BUX/SEL], [92KAR/END]

6. Kinetics
   - [67MCE/PHI], [69HER/HUI], [70COL/CRU], [75CLY/WAT], [75RAD/WHI], [75RAD/WHI2], [77CLY/CUR], [79ADD/DOJ], [79BRU/FIE], [79GOR/NOV], [79GOR/NOV2], [80KER/TRO], [81GAR/WAT], [81RAY/WAT], [82BAU/COX], [83BUS/SIB], [83THO/ZA6], [85JEN/COX], [86SAN], [87BAR/BEC], [87ELO/RYN], [87MAR/JOH], [87MAR/JOH2], [88CONS/TEN], [88STE/HYN], [90BAR/BAS], [91BAR/BAS], [91JEN/COX], [91MAG/MEL], [92MAG/LAV], [92WHI/SMI], [95TUR/GIL]

7. Other
   - [67STU/HUS], [69BRE/ROS], [71KAU/KOL], [74DHA/CL], [74DHA/CL2], [74SCH], [76REF/FRA], [76REF/FRA2], [77VOG/DRE], [77VOG/MIS], [81GRO/LAV], [81SEH/SUT], [82GAR], [84SAU/TAT], [87KAR], [92GIL/POL], [94SOL/GAR]

Fortunately, there is sufficient information on the spectroscopic properties (including a rotational–vibrational analysis) of IO(g) to characterize the thermodynamic properties of this chemical species. The results are in reasonable agreement with the results of the other halogen monoxides. It is not the intent of this article to discuss the articles dealing with formation, reaction and kinetics.

Durie et al. [60DUR/LEG] photographed the methyl iodide flame bands lying in the region 4100–6300 Å. These bands are attributed to the A$^1$I–X$^2$I transition of the IO molecule. A rotational and vibrational analysis was carried out to provide the molecular constants for the X$^2$I$^2$ and A$^1$I$^2$ states. This paper builds on and extends the earlier observations and analyses of [37VAI], [48COL/GAY], and [58DUR/RAM]. Blake and Iredale [46BLA/IRE] published a revised analysis of portions of the [37VAI] data. Coleman et al. [48COL/GAY] stated that this led to an unsatisfactory intensity distribution. Thus, [48COL/GAY] remeasured the bands and extended the system to larger wavelengths. Durie and Ramsay [58DUR/RAM] measured the absorption spectra of IO and derived a vibrational analysis consistent with Coleman et al. [48COL/GAY]. Engleman et al. [83ENG/PAL] observed an absorption spectrum of 1$_2$O which was in agreement with that predicted by [60DUR/LEG]. This spectrum was recorded as part of a high temperature spectra of a quartz cell containing an I$_2$–O$_2$ mixture. The recommended spectroscopic information for the X and A states is very similar to that recommended by Huber and Herzberg [79HUB/HER]. These authors relied on the experimental data of [48COL/GAY], [58DUR/RAM], and [60DUR/LEG]. The earlier review by Herzberg [50HER] was based on the data of [46BLA/IRE], [48COL/GAY], and [37VAI] and is superseded by [79HUB/HER]. Information published since these reviews provided more definitive vibration and rotation constants [83BEK/MEE].
Using a high resolution laser-rf spectroscopy on the $A^2\Pi_{3/2} \rightarrow X^2\Pi_{3/2}$ system of iodine oxide, the vibrational and rotational constants for the ground state have been refined from those previously recommended by Durie et al. [60DUR/LEG].

The ground state configuration, $X^2\Pi_{3/2}$ (inverted doublet), was confirmed by the EPR measurements of [70CAR/DYE] and [72BRO/BYF]. [70CAR/DYE] determined the fine structure splitting to be $A = -446 \pm 70$ cm$^{-1}$, although they questioned the validity of this value and felt that independent determinations should be made. Brown et al. [72BRO/BYF] also used ESR techniques to determine the spin–orbit coupling constant $A$ and the ground electronic state. The authors derived $A = -2330 \pm 230$ cm$^{-1}$. Both studies indicated that the value of $A$ was suspect and should be of the order of 1000 cm$^{-1}$.

Gilles et al. [91GIL/POL] used photoelectron spectroscopy to obtain the spectra for $IO^3_2\Pi_{3/2}$, $^2\Pi_{1/2}$; $v^+$+$\epsilon^- \rightarrow IO^{-}\left(\Sigma^{+}; v\right)$ This measurement provided direct structure information on $IO^{-}\left(g\right)$ and reported the first observation of the ground state $^2\Pi_{3/2} \rightarrow ^2\Pi_{3/2}$ spin–orbit splitting for IO. The authors observed two vibrational progressions separated by 2091(40) cm$^{-1}$ which they attributed to the spin–orbit components of the IO ground state. In their analysis of the data, the authors adopted the $r_e$, $\omega_s$, $\omega_\sigma r_e$ values from [83BEK/MEE] and derived the values for these three parameters in the $^2\Pi_{3/2}$ component. This work was continued and further discussed in [92GIL/POL]. We recommend an excited state at 22469.8 cm$^{-1}$ based on the values from [83BEK/MEE].

The dissociation energy has been calculated by many different techniques. The various studies have not improved the reliability of the dissociation energy. These values are summarized in Table 4. The derived values range from 176 to 249 kJ/mol, as referenced in Table 4. The values may be grouped into two types: (1) derived from a treatment of the observed vibrational energy levels and (2) extracted from kinetic studies. The largest value is derived from the curve fitting approach of [89RED/RAO], using a three-parameter modified Lippencott potential function (based on the spectroscopic data of [83BEK/MEE]).

Coleman et al. [48COL/GAY], from their study of the IO spectrum in flames, used a graphical Birge–Spencer technique to give $1.9 \pm 0.2$ eV (44 kcal/mol). Durie and Ramsay [85DUR/BYF] stated that since only six bands were observed in their study of the absorption spectrum of IO, it was not possible to obtain an accurate value for the dissociation energy of the ground state. They derived an upper limit from the observed predissociation. Thus, they calculated a value $<21.976$ cm$^{-1}$ (62.8 kcal/mol or 2.72 ev). However, Durie and Ramsay felt that a better estimate could be obtained from a Birge–Spencer extrapolation of the first four vibrational levels in the upper state. This led to 10.200 cm$^{-1}$. However, since the accepted values (at that time, 1958) for ClO and BrO were approximately 10% less than the values calculated by the same procedure, they applied the same correction to IO and calculated 14800$\pm$1800 cm$^{-1}$ (42$\pm$5 kcal/mol or 1.8$\pm$0.2 eV). Subsequent work by Durie, which led to vibrational constants with greater precision, would not lead to any improvement in the calculation of the dissociation energy due to considerable extrapolation.

Using flame photometry, Phillips and Sugden [61PHI/SUG] measured the intensity of the (0,4) band of IO at 5307 Å to determine the temperature dependent (1900–2700 K) equilibrium constant for the dissociation energy of IO. They determined a value of $57 \pm 6$ kcal/mol at 0 K. This value was calculated from the assumed enthalpy of formation value of 63 kcal/mol at 2000 K. This value is considerably higher than the earlier determined values. Herron and Huie [69HER/HUI], in their study of the rate constants of atomic oxygen with chloroalkanes and bromoalkanes, stated that the bond dissociation of IO (238$\pm$24 kJ mol$^{-1}$), as derived from [61PHI/SUG], is the value which is compatible with their iodine atom abstraction mechanism. The value from the [85DUR/BYF] study was too small.

Singh and Rai [65SIN/RAI] calculated RRK potential energy curves for the $X^2\Pi$ and $A^2\Pi$ states of IO. The spectroscopic data used as the basis for this calculation were those of Durie et al. [60DUR/LEG] and Durie and Ramsay [85DUR/BYF]. Using the three-parameter Lippencott function to calculate the dissociation energy from the potential energy curve, the authors arrived at 20,000 cm$^{-1}$. This is compared with an earlier reported value of 1.9$\pm$0.2 eV, which undoubtedly is the value of Coleman et al.

A least-squares fitting of the RRK curve with the Hulburt–Hirshfelder formation gave a dissociation energy value of 1.94 eV [72TRI/GOH]. The authors stated that the three-parameter Lippencott potential function fails to reproduce the experimental potential energy curve in the case of IO.

Rao, Rao, and Rao [74RAO/RAO] estimated the dissociation energy of the upper state of IO, the $A$ state, by fitting an empirical potential energy curve from Lippencott’s three-parameter function and the Hulburt–Hirshfelder function with the true potential energy curve. They determined the value 1.425 eV for the upper state and confirmed the value of Trivedi and Gohel, that is, 1.94 eV for the ground state. This value was also supported by fitting an electronegativity function suggested by Szoke and Baitz. As mentioned earlier, [89RED/RAO], using a three-parameter modified Lippencott potential function, based on the spectroscopic data of [83BEK/MEE], calculated a dissociation energy of 59.6 kcal/mol. However, recall [72TRI/GOH] claimed this technique was not acceptable as stated earlier.

Baulch et al. [82BAUL/COX] listed a dissociation value of 184$\pm$21 kJ/mol as given by [80KER/TRA].

Maguin et al. [92MAG/LEV], in studying the kinetics of the reactions of IO radicals with NO$_2$ and HO$_2$, reported three enthalpy of formation values for IO. They referred to $\Delta H_{296K} = 172$ kJ/mol from [90DEM/MOL], 132 kJ/mol from [89GUR/VEY], and 107 kJ/mol from [89RED/RAO]. Although these authors did not recommend a specific value for $\Delta H$, they implied that the latter value from [89RED/RAO] was not consistent with their kinetic observations.
Herron and Huie [69HER/HUI] and Huie and Laszlo [95HUI/LAS], in their kinetic studies, have questioned the validity of the spectroscopically derived dissociation energy values. Whereas [69HER/HUI] preferred the results of [61PHI/SUG], Huie and Laszlo [95HUI/LAS] have adopted an enthalpy of formation value of 130 kJ/mol based on the molecular beam studies of [75RAD/WHI] and [83BUS/SIB] (refer to Table 4).

The recommended thermodynamic properties of IO(g) by Wagman et al. [82WAG/EVA] were based on the spectroscopic measurements of Durie and Ramsay [58DUR/RAM] and Durie, Legay, and Ramsay [60DUR/LEG]. The corresponding publication by Glushko and Medvedev [65GLU/MED] based their recommended thermal function values on the earlier interpretation by Gurvich et al. [1962] and the dissociation energy value on the results of Coleman, Gaydon, and Vaidya [1948], Durie and Ramsay [1958], and Phillips and Sugden [1961]. The most recent analysis of Gurvich et al. [62GUR/KHA] relied on the results of Vaidya [1937], Blake and Iredale [1946], Coleman, Gaydon, and Vaidya [1948], Durie and Ramsay [1958], and Durie, Legay, and Ramsay [1960]. The recommended spectroscopic information given by Huber and Herzberg [79HUB/HER] was based on the data of Coleman et al. [1948], Durie and Ramsay [1958], and Durie et al. [1960]. The thermochemical table of Brewer and Rosenblatt [69BRE/ROS] is based on the earlier vibrational and rotational constants data of Durie et al. [1960] and the energy level values of Durie et al. [1960], Moore [1958], and Herzberg [1950]. The recommended dissociation value of 46±7 kcal was based on the results of Coleman et al. [1948], Durie and Ramsay [1958], and Phillips and Sugden [1961].

5.2 IO₂

The articles dealing with IO₂ can be classified as follows. Of prime importance to this article are the spectroscopic and properties studies.
1. Radiolysis/photolysis
   - [69BAR/GIL], [70AMI/TRE], [70AMI/TRE2], [72BAR/GIL], [73TEN/FAR], [86BYB], [89SAG], [92KAR/END]
2. Reactions
   - [69MUI], [64GIL/SEN]
3. Intermediates
   - [61PAV/RAF], [80COO], [82FUR/NOY], [82FUR/NOY2]
4. Spectroscopy/structure
   - [60DAS/WAD], [60DUV/LEC], [81ELL/WOL], [92GIL/POL]
5. Preparation/formation
   - [1844.IL], [60DAS/WAD], [80WIK/TAY]
6. Properties
   - [67STU/HUS], [80WIK/TAY], [81ATH/MOR], [86BYB], [88BYB], [92GIL/POL], [94FJE/KJE]

There is only one reported study involving this oxide in the gas phase [92GIL/POL], but there is no experimental structural or enthalpy of formation information. Most citations deal with the assumed existence in an aqueous or matrix media.

CA Registry Number 116854-14-9 corresponds to the isotope I²O₂ (one reference which deals with ESR spectrum [88BYB]). The author measured the ESR spectra of this dioxide in KClO₄. From the complicated I²O₂ hyperfine structure, he determined the hyperfine and quadrupole tensors of I²O. Byberg [88BYB] stated that the ground state of the free IO₂ molecule belonged to the representation B₁ of the point group C₂ᵥ. The author assumed the bond angle of OIO to be 118°. The analysis of the I²O₂ hyperfine patterns of I²O₂ supported the earlier conclusion that the electronic properties closely resemble those of ClO₂ and BrO₂.

An EPR study [81ATH/MOR] suggests that IO₂ in a γ-irradiated KIO₃F₂ crystal is a bent symmetric radical, OIO, as are the chlorine and bromine counterparts in comparable studies.

An ESR spectrum of IO₂ was obtained from the selective photolysis at room temperature of IO₂⁻ in KCIO₄ crystals and the subsequent x irradiation at low temperatures [86BYB]. The authors’ conclusion was that the C₂ᵥ nuclear geometry of IO₂ in KClO₄ resembles that of ClO₂ in the gas phase. Thus, the bond length of IO₂, 1.815 Å, was taken as that of ClO₂ (1.475 Å), corrected for the difference between the covalent radii of chlorine and iodine (0.34 Å). However, the bond angle of IO₂ in this lattice could be significantly smaller than that of ClO₂, 117.6°.

Gilles et al. [92GIL/POL] measured the photoelectron spectra of OIO⁻(g). In addition to deriving the electron affinity of OIO, the authors determined two vibrational frequencies [the symmetric stretch (765 cm⁻¹) and bend (192 cm⁻¹)]. The structure of the molecule was not determined, but was assumed to be of C₂ᵥ symmetry.

Numerous other studies involve the kinetic description of the formation and decay of this transient species in aqueous medium, as well as reactions involving IO₂ as an intermediate.

A confusing aspect for this chemical species involves the condensed phase characterization: is the "molecule" IO₂ or IO? The Chemical Abstracts literature references for IO₂ include I₂O₃ references. The early references for the dioxide are in fact for the tetroxide. There are two citations for IO, which deal with the crystal structure of I₂O₃. Indications are that the structure of the species in the condensed phase is perhaps IO - IO₂. The most recent reference to this species is a crystal structure study of I₂O₃ in which it was concluded that a chain structure exists: (⋯-I-O-I0₂-O-⋯).
on the oxidation of Fe(II) to Fe(III) by IO$_3^-$ in strongly acidic aqueous media. IO and IO$_2$ are among the seven proposed reactive intermediates.

5.4 IOO

There are three references which propose this species as an intermediate in aqueous reaction schemes [70UCY/CURU, 77CLY/CURU, 77WY/CURU]. This species has not been isolated or characterized.

The thermodynamic properties of IOO(g) could be estimated in comparison with the properties of FOO and CIOO, both of which were well characterized. Unfortunately, BrOO is not well characterized.

5.5 IO$_2$$_{24}$

There is only one reference to this species in which its formation in the reaction of iodine with ozone is discussed [80VIK/TOR].

5.6 IO$_3$

The articles dealing with IO$_3$ can be classified as follows. Of prime importance to this article are the spectroscopic and enthalpy of formation studies.

1. Enthalpy of formation
   - [48FAR/KLE]

2. Vibrational frequencies/structure
   - [56VEN/SUN], [63VEN/RAJ], [64RAO/SAN], [72RAO], [78THI/CH]

3. Formation/preparation
   - [186IKAE], [58ODE], [59HAU], [63PAC/HAU], [68SEL/KJE], [77SEL/WEI], [80VIK/TOR]

4. Related spectra
   - [60DAS/WAD], [77SEL/WEI]

5. Intermediate
   - [61PAV/RAF], [82NOS/NOS]

6. Photolysis/radiolysis
   - [69BAR/GIL], [70AMTI/RE], [70AMTI/RE2], [72BAR/GIL], [73TEN/FAR], [81KLA/SEH], [82WAG/STR], [85BUK/SEL]

There is no reported information as to the experimental determination of the enthalpy of formation of this radical. There is a calculated value reported by [48FAR/KLE] of -28 kcal/mol. Although the authors, Farkas and Klein, stated that they calculated the enthalpy of formation of IO$_3$, the formula given is IO$_3^-$.

There are five references of a theoretical nature which deal specifically with the structure and spectroscopic properties of the gaseous trioxide. Unfortunately, there are no experimental studies involving the radical in the gas phase.

The spectroscopic articles for the gas phase radical involve force field calculations of pyramidal X$\equiv$Y$_3$ type molecules [56VEN/SUN, 63VEN/RAJ, 64RAO/SAN, 72RAO, 78THI/CH]. Contrary to the implications of these five articles, there is no observed structural information or is there any observed vibrational information. Upon examination of the earlier literature cited by these authors, vibrational frequency information was found for IO$_3^-$ in a crystalline environment. Two of the four vibrational frequencies matched exactly with those reported for IO$_3^-$.

These articles have assumed a pyramidal structure with a O-I-O angle of 89° (same angle was used for the chlorine, bromine, and iodine trioxides); a bond distance I-0 of 1.79 Å (from Badger's rule), and vibrational frequencies (in cm$^{-1}$) of $\nu_1=780$ [A$_3$], $\nu_2=357$ [A$_2$], $\nu_3=809$ [E], and $\nu_4=326$ [E]. Unfortunately, $\nu_4$ is reported as 326 cm$^{-1}$ by Venkateswarlu and Sundaram [56VEN/SUN] and as 362 cm$^{-1}$ by Thirugnanasambandam and Mohan [78THI/CH]. From an examination of the calculations and the trends in the series of the three halogen trioxides, it is apparent that the frequency should be 326 cm$^{-1}$.

Many other references deal with (1) the thermal decomposition of orthoperiodic acid [59HAU, 63PAC/HAU], and NH$_4$IO$_3$ [61PAV/RAF], (2) the existence of solid IO$_6$ (not IO$_5$) and its Raman spectra [77SEL/WEI], (3) infrared and visible spectra of IO$_3^-$ [60DAS/WAD], and (4) numerous articles on the production of the transient radical in an aqueous medium through flash photolysis and pulse radiolysis of aqueous iodate solutions. The emphasis in these latter type articles is the explanation of the chemistry through a kinetic interpretation.

Farkas and Klein [48FAR/KLE] studied the decomposition of bromate ion in aqueous solution. IO$_3$ was proposed as an intermediate to describe the kinetics of the decomposition process.

There are three flash photolysis studies of periodate solutions by Barat and Gillies [72BAR/CH], Klaning and Sehested [81KLA/SEH], and Wagner and Strehlow [82WAG/STR]. Barat assumes the radical IO$_4$ is an intermediate whereas Klaning assumes IO$_3$ and an unspecified I(VIII) species are intermediates. In Wagner and Strehlow, the increase in the resistance of the solution during the flash was attributed to the reaction

$$\text{IO}_4^-+\text{H}^+\rightarrow\text{IO}_3^-+\text{OH}^-$$

Two methods proposed for the elimination of the radical were the dimerization to IO$_5$ and the reaction with ozone to yield IO$_4$.

5.7 IO$_4$

There are no reported studies involving this oxide in the gas phase: i.e., there is no experimental structural, vibrational frequency or enthalpy of formation information. A CA Registry Number exists for IO$_4$, but the structure is not determined. The existence of the IO$_4$ radical had been "established" as a short lived species by Gomberg as early as 1923 [23GOM]. Selte and Kjekshus [68SEL/KJE], in their study of the H$_2$O-I$_2$O$_5$ system, questioned the existence of IO$_4$.

There are four recent references which discuss the existence of the IO$_4$ radical. They all involve the existence of this radical in an aqueous medium, not in the gas phase. The studies involve the pulsed radiolysis [71LES/CH], flash
photolysis [82WAG/STR], laser flash photolysis and pulsed radiolysis [81KLA/SEH], and radiation induced redox [85BUX/SEL] of aqueous periodate solutions. Neither study reports any information as to the structure of the radical, its vibrational frequencies, or its enthalpy of formation. Thermal functions for this radical cannot be reliably estimated since there are no related substantial data for the other halogen oxides $\text{XO}_4(g)$.

Lesigne et al. [71LES/BAR] studied the $\text{IO}_4^{-2}$ aqueous ions and $\text{IO}_3^{-}$ radicals formed by the pulse radiolysis of periodate ion in aqueous medium. The authors state that they also observed this transient species by flash photolysis of deaerated periodate solution.

Ten years later, Wagner and Strehlow [82WAG/STR] studied the flash photolysis of periodate in the pH range 2.44 to 4.99 in which three reactions were observed. In this experiment, the authors discuss the formation of the $\text{IO}_4^{-}$ radical and its dimerization to $\text{IO}_6^{3-}$ and the related kinetics.

Klingner et al. [81KLA/SEH] also used flash photolysis to study periodate solutions. They assumed the formation of $\text{IO}_3^{-}$ and an unspecified $\text{I}^{(VIII)}$ species.

Buxton and Sellers [85BUX/SEL] proposed the formation of $\text{IO}_3^{-}$ as an intermediate species in the pulsed radiolysis of aqueous periodate solutions.

### 5.8 $\text{I}_2\text{O}$

There is no thermodynamic or spectroscopic information available for this chemical species. Most of the reported information deals with the reactivity of this oxide as an intermediate in various reactions: [38MAS], [72FOR/GOO], [76CAM/HAY], [82NOS/NOS]. There are two articles from which spectroscopic information might be extracted: [60DUV/LEC], [83BUS/SIB], [60DUV/LEC] have studied the vibrational frequencies of $\text{I}_2\text{O}_3(\text{cr})$, including the $\text{IO}_3$ bridging frequencies. Buss et al. [83BUS/SIB], in their discussion of the triatomic molecules $\text{XO}_3$, mentioned that the ground state is a singlet. However, there is no additional information as to the precise structure or vibrational frequencies. There are two additional articles: a patent [84DRA/TRI] and a dissertation [31CHI]. The species has not been isolated as a pure compound. No structure is associated with this CAS Registry Number.

### 5.9 $\text{I}_2\text{O}_2$

There is no information to confirm the existence of this compound, which has been reported in the literature four times: in a 1930 review [30BRA], in 1970 [70AM/TRE], in 1985 [85BUX/SEL], and in 1992 [92MAG/LAV]; in two cases it is suggested as an intermediate compound in an aqueous reaction scheme; whereas in the latter two cases it is presented as an intermediate in the gas phase self-reaction of IO. [70AM/TRE] suggested dimerization of IO to describe the decay of IO. Similarly, Cox and Coker [83COX/COK], in studying the rate of IO decay, proposed that the initial stages of the reaction involved the formation of $\text{I}_2\text{O}_2$.

### 5.10 $\text{I}_2\text{O}_4$

There is no thermodynamic or spectroscopic information reported for this compound. In fact, this compound has not been isolated or characterized as a separate entity. Although citations are given for this oxide, the discussions only deal with adducts with $\text{SO}_2$ or the like. The CAS Registry Number corresponds to composition $\text{I}_2\text{O}_4$ but no structure is associated with this formula.

The references include: [1896CHR], [1898CHR], [12KAP], [35BAH/PAR], [36FIC/DIN], [37MAS], [38MAS/ARG], [54WOO], [57SEM], [57SYM], [59LEH/HES], [60DAS/WAD], [62FIA/TAR], [63PAC/HAU], [64DAE/KJE], [68SEL/KJE], [71SEL/KJE], and [89SAG].

### 5.11 $\text{I}_2\text{O}_4$

The CAS Registry Number corresponding to $\text{I}_2\text{O}_4$ has been discontinued. This compound is now referred to as $\text{IO}_2$. The $\text{IO}_4$ unit is normally used in reference to the condensed phase, whereas in solution or gas phases, $\text{IO}_3$ is the entity discussed. For this reason, the literature is somewhat confusing for this compound, since in the early studies, the dioxide was mentioned where, in fact, the $\text{IO}_3$ species was really being discussed. There is no thermodynamic information reported for this oxide, although there is some data for the thermal stability (refer to Tables 1a and 1b). There are numerous studies which report structural and vibrational frequency information for the crystalline phase (refer to Table 5).

A CAS Registry Number 99690-81-0 corresponds to iodosyl iodate with the inferred structure $\text{IO}_2^{-}$ $\text{IO}_4^{-}$ $\text{IO}_3$. There is one reference to this compound [60DAS/WAD]. Dassent and Waddington [60DAS/WAD, 63DAS/WAD] have provided tentative information concerning the crystalline structure on the basis of infrared spectra, whereas [68SEL/KJE] used a combination of x-ray diffraction, density, ir spectra, proton magnetic resonance, DTA and TGA to examine the formation and stability of $\text{I}_2\text{O}_4(\text{cr})$. [60DAS/WAD] prepared iodine dioxide by Muir's method [09MUI] and gave frequency assignments for iodine dioxide in terms of $\text{I}_2\text{O}_4$. They state that the formation of $\text{I}_2\text{O}_4$ as iodosyl iodate was satisfactory if it was remembered that IO was not present as a discrete cation.

The numerous citations on $\text{I}_2\text{O}_4$ may be arbitrarily classified as follows.

1. Preparation/formation
   - [1884MIL], [1898CHR], [09MUI], [12KAP], [15FIC/KAP], [35BAH/PAR], [39BAH/SIN], [60DAS/WAD], [80WIK/TAY]
2. Reaction
   - [57SEM], [59LEH/HES], [61VLA/ATI], [62FIA/TAR], [64GIL/SENI], [70KUZ/KOT]
3. Properties
   - [50WIL/DHA], [57SYM], [62ARO/MIS], [68SEL/KJE]
4. Spectroscopy/structure

5.12 I₂O₅

There are numerous studies on the pentoxide. However, the only direct thermodynamically related information is early references to formation data. (See Table 1.) There are no heat capacity or enthalpy data, or melting information. There are numerous references to the fact that this oxide sublimes.

The discontinued CAS Registry Number 7790-35-4 probably referred to I₂O₅ before its structure was known. The current CAS Registry Number 12029-98-0 refers to I₂O₅ with a structure O₃I–O₂I. The numerous citations on I₂O₅ may be arbitrarily classified as follows. Note that the distinction between the categories of reaction, detection, and commercial applications is often not clear.

1. Enthalpy of formation

2. Preparation/formation

3. Reaction

4. Detection

5. Decomposition

6. Commercial applications

7. Properties
1308 MALCOLM W. CHASE

[23LAM/PHI], [30GRA/FAR], [32HUL/BLI], [32MOL/PER], [36MOL/DIL], [36VIL/MOL], [38WEB], [40BAK/KEL], [54SHI/KOS], [55KWI/TSU], [60DUX/LAC], [62ARO/MIS], [66SOL/VAI], [68SEL/KJE], [68VEP/HAI], [70SEL/KJE], [70SHE/TUR], [73SEM/MOS], [75BAR/BUL], [76DAL/CAR], [76SHE], [78KET/GOF], [78CHR/WI], [78CER/KO], [78PEN/BOC], [79PET/LO], [80RUB/SA], [81ELL/WOL], [84GOR/AND], [85SUN/WRE]

8. Hydrate

[33GAR], [33MOL/PAR]

9. Review

[51ADA/SIM], [54COU], [60GEO], [63SCH/BRA], [71SEL/KJE], [76SEL]

10. Ternary systems

[51RIC/AMR], [52RIC/FRE], [56NIK/BUS]

There has been extensive work on the preparation, crystal structure, Raman spectra, and decomposition. The crystal structure studies suggest that the molecule is of the form $\text{IO}_2\cdot\text{O}^{-}\text{IO}_2$. TGA and DTA results consistently show that $\text{I}_2\text{O}_3$ decomposes in the range 570–730 K to the elements [68SEL/KJE, 85VII/MAC].

Farkas and Klein [48PAR/KLE] reported an enthalpy of formation for $\text{I}_2\text{O}_3$ as $-42.0$ kcal/mol, but do not give any source for this number. The enthalpy of formation value ($-37.78$ kcal mol$^{-1}$) recommended by Brewer and Rosenb­

The 1982 republication of Wagman et al. recommended an enthalpy of formation for $\text{I}_2\text{O}_3$ based on a study by Spencer and Hepler [1960]. The evaluation was performed in 1964. The study involved the reaction of $\text{I}_2\text{O}_3$ (cr) with aqueous KOH. There are no recent calorimetric determinations of $\Delta H^0$ either through formation from or decomposition to the elements. At the time of the Wagman evaluation, four other solution processes led to formation values within 1.3 kcal mol$^{-1}$ range.

5.13 $\text{I}_2\text{O}_5$

The study of $\text{I}_2\text{O}_5$ is confusing since we must examine four different species: (1) iodyl periodate [77SIE/WEI], (2) iododioxygen periodate [77SIE/WEI], (3) iodine oxide, and (4) iodine trioxide (IO$_5$). Early references were to IO$_2$ and an unspecified IO$_3$. It is not clear as to which species truly exists in the condensed phase.

The references for the discontinued CAS Registry Number for $\text{I}_2\text{O}_5$ (64052-04-6) are not included under IO$_2$ references. Via a Chemical Abstract literature search, there is one IO$_3$ reference [77SIE/WEI] referring to iododioxygen periodate with a presumed structure $\text{IO}_2\cdot\text{IO}_2\cdot$. However, [77SIE/WEI] referred to $\text{I}_2\text{O}_5$ in its study as iodyl periodate which was given a Registry Number of 63912-61-8 in CAS. No references are listed under this registry number.

The early references for IO$_2$ in fact discussed IO$_6$. This compound was presumably formed by the decomposition of periodic acid [186KAE], [58ODE], [63PAC/HAU] and orthoperiodic acid, $\text{H}_3\text{IO}_6$ [59HAI]. Only one paper presents evidence in which this species was isolated; Siebert et al. [77SIE/WEI] confirmed its existence. The compound was prepared by two techniques and was confirmed as a distinct species by its individual Raman spectra. Diamagnetism studies proved that it is a mixed valence entity; perceived as iodyl periodate, $\text{IO}_2\cdot\text{IO}_2\cdot$, as discussed in Table 5. There are no thermodynamically related data.

A recent study [95KRA/JAN] determined the crystal structure of $\text{IO}_3$ as a mixed valent oxide, I(VII).

Alternatively, Wagner and Strelo­[82WAG/STR] suggest that this species supposedly formed from the dimerization of the IO$_5$ radical in aqueous periodate solutions as a result of flash photolysis.

5.14 $\text{I}_2\text{O}_7$

This condensed phase compound has not been isolated or characterized. It is often cited in terms of being the end member in ternary systems, but the $\text{I}_2\text{O}_7$ portion of the triangular diagram has not been studied. There are fourteen references for this compound: six preparations and eight ternary systems (X-$\text{I}_2\text{O}_7\cdot\text{H}_2\text{O}$). $\text{I}_2\text{O}_7$ is considered the hypothetical anhydride of periodic acid $\text{H}_3\text{IO}_6$.

The current CA Registry Number refers to an iodine–oxygen compound in which the atomic ratio is 2:7 but no structure is given. (There is a discontinued CA Registry Number 20270-38-6.)

The ternary systems are as follows:

[51GAY] Ag$_2$O–$\text{I}_2\text{O}_7$–H$_2$O
[53HES/SOU] I$_2$O$_7$–Li$_2$O–H$_2$O
[64DRA/TER] $\text{I}_2$O$_7$–CaO–H$_2$O and BaO–$\text{I}_2$O$_7$–H$_2$O
[66DRA/KOS] $\text{I}_2$O$_7$–MgO–H$_2$O
[68PAC/BOH] $\text{I}_2$O$_7$–Cd$_2$(IO$_3$)$_2$–H$_2$O
[74DEI/HEJ] $\text{I}_2$O$_7$–NaO$_2$–H$_2$O and $\text{I}_2$O$_7$–SO$_2$–H$_2$O
[67BIA/SAB] $\text{I}_2$O$_7$–K$_2$O–H$_2$O
[67SAB/BIA] $\text{I}_2$O$_7$–Na$_2$O–H$_2$O.

The following citations deal with the preparation and subsequent decomposition of $\text{I}_2\text{O}_7$:

• [58ODE] studied the dehydration of $\text{H}_3\text{IO}_6$;
• [62MIS/SYM] dealt with the formation from the reaction of $\text{H}_3\text{IO}_6$ with concentrated sulfuric acid (deduced that the compound was unstable; isolation often resulted in decomposition with explosive violence);
• [63PAC/HAU] dealt with the thermal decomposition of $\text{H}_3\text{IO}_6$ and the possible formation of a product of the form $\text{I}_2\text{O}_7$–$\text{I}_2\text{O}_5$ [68SEL/KJE], whose data was consistent with the results of [63PAC/HAU].
• Wagner and Strelo­[82WAG/STR] suggested a reaction scheme in which ozone oxidized $\text{I}_2\text{O}_5$ to $\text{I}_2\text{O}_7$. 

Chladek and Troenel [93CHL/TRO] established a relationship between the bond length and the bond strength for numerous oxides.

5.15 \( \text{I}_2\text{O}_8 \)

This condensed phase compound has not been isolated or characterized. It is postulated to exist in aqueous reaction schemes. The CAS Registry Number corresponds to the structure \( \text{O}_2\text{I}--\text{O}--\text{I}_3 \).

Wagner and Strehlow [82WAG/STR], in the flash photolysis of periodate in the pH range 2.44 to 4.90 using conductometric detection, observed three reactions, one of which was attributed to the hydrolysis of \( \text{I}_2\text{O}_8 \). The authors stated that ozone oxidized \( \text{IO}_3^- \) to form \( \text{IO}_4^- \), which in turn dimerized to \( \text{I}_2\text{O}_8 \). This citation provided no indication of the structure.

There are sufficient reliable studies to indicate that this compound does exist in the crystalline phase. The current CAS Registry Number corresponds to a structure \( \text{I}(\text{IO}_3)\) and a name, iodine iodate. (A discontinued CAS Registry Number 73560-00-6 also exists, which most likely refers to an \( \text{I}_2\text{O}_9 \) species with an unknown structure.) There are no studies which provide numeric thermodynamic information. That is, there are no studies on the heat capacity, enthalpy, melting, or enthalpy of formation.

The information on \( \text{I}_2\text{O}_9 \) may be arbitrarily classified as follows:
1. Preparation/formation
   [09BER], [99FIC/ROH], [15FIC/KAP], [35BAH/PAR], [35BAH/PERA], [68SEL/KJE], [80WIK/TAY], [83COX/COK], [85SUNI/WRE], [85VIK/MAC]
2. Decomposition
   [35BAH/PAR], [55KIK], [80WIK/TAY]
3. Reactions/intermediates
   [61VLA/ATI], [62ARO/MIS], [80WIK/TAY]
4. Review
   [63SCH/BRA]
5. Iodine transport
   [81VIK/FUR], [84VIK], [89SAG]
6. Characterization (crystal)
   [85SUNI/WRE]

There are many articles which deal with the formation of \( \text{I}_2\text{O}_9 \) and the subsequent decomposition to \( \text{I}_2\text{O}_5 \). There are three preferred methods of preparation: (1) the reaction of \( \text{I}_2 \) with ozone, (2) thermal treatment of iodine with anhydrous \( \text{HPO}_3 \), and (3) heating iodine acid with orthophosphoric acid. This oxide decomposes above 350 K to yield the pentoxide \( \text{I}_2\text{O}_5 \). See Table 1b for details. Additional studies include irradiation [61VLA/ATE], a magnetic susceptibility measurement [62ARO/MIS], and Raman spectra [85SUNI/WRE].

The experimental studies by Selte and Kjekshus [68SEL/KJE] did not support the results of [15FIC/KAP] and [35BAH/PAR]. By following the procedures of the latter two studies, Selte and Kjekshus could not produce \( \text{I}_2\text{O}_9 \). In addition these results also suggested that the reactions between iodine and ozone took place in \( \text{CCl}_4 \) solutions rather than in the gas phase, in contrast to [09BER] and [55KIK]. Selte and Kjekshus did not comment on the formation of \( \text{I}_4\text{O}_8 \) as described in [99FIC/ROH].

Sunder et al. [85SUNI/WRE] isolated amorphous and crystalline \( \text{I}_2\text{O}_9 \) and determined the Raman spectra. They established conclusively that it was a distinct molecular species and not a mixture of \( \text{I}_2\text{O}_5 \) and \( \text{I}_2\text{O}_4 \). This study provided tentative vibrational assignments for five types of vibrations \( (\text{I}=\text{O} \text{ stretch}, \text{O}--\text{I}=\text{O} \text{ symmetric stretch}, \text{I}=\text{O} \text{ stretch}, \text{O}1\text{O} \text{ deformation}, \text{IO}1 \text{ deformation).} \) The vibrational frequency assignments were made by analogy with \( \text{I}_2\text{O}_5 \) and \( \text{I}_2\text{O}_4 \).

5.16 \( \text{I}_4\text{O}_9 \)

The earliest reference dealing with the preparation of this solid compound is by Kaemmerer (1861).

The study by Kappeler [12KAP] questioned the existence of this oxide and indicated that it was most probably \( \text{I}_2\text{O}_4 \). This conclusion was further supported by [64DAE/KJE]. There are no studies since 1912 which have been able to prepare this species. This compound is assumed not to exist.

5.17 \( \text{I}_4\text{O}_{13} \)

The earliest reference dealing with the preparation of this solid compound is by Millon (1844/45).

The study by Kappeler [12KAP] questioned the existence of this oxide and indicated that it was most probably \( \text{I}_2\text{O}_4 \). This conclusion was further supported by [64DAE/KJE]. There are no studies since 1912 which have been able to prepare this species. This compound is assumed not to exist.

5.18 \( \text{I}_2\text{O}_{19} \)

The earliest reference dealing with the preparation of this solid compound is by Millon (1844/45).

The study by Kappeler [12KAP] questioned the existence of this oxide and indicated that it was most probably \( \text{I}_2\text{O}_4 \). This conclusion was further supported by [64DAE/KJE]. There are no studies since 1912 which have been able to prepare this species. This compound is assumed not to exist.
**Table 1a. Solid iodine oxide species: Preparation and related reactions**

<table>
<thead>
<tr>
<th>Source</th>
<th>Reaction</th>
<th>Temperature</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>IO</td>
<td>Quadrupole coupling constants for $^{127}$I</td>
<td></td>
<td>Comparison of calculated and experimental values; reference to earlier experimental study?</td>
</tr>
<tr>
<td>IO$_2$ (I$_3$O$_4$)</td>
<td>Formation of IO$_2$ from the photolysis and x-irradiation of I$_2$ embedded in KCIO$_4$</td>
<td>26 K</td>
<td>Observation and calculation of ESR spectra to determine structure</td>
</tr>
<tr>
<td>86BYB</td>
<td>I$_2$ + HNO$_3$ $\rightarrow$ I$_3$O$_3$</td>
<td></td>
<td>Reference to earlier preparative procedures by 1844 Millon</td>
</tr>
<tr>
<td>1844MIL</td>
<td>H$_2$SO$_4$($\text{hot, conc.}$)+HI$O_3$ $\rightarrow$ I$_2$O$_4$</td>
<td>[85 °C]</td>
<td>Reaction gives yellow granular nonhygroscopic I$_2$O$_4$ which, when heated above 85 °C forms I$_2$O$_3$. I$_2$O$_3$, formed by 1$_2$-I$_2$O$_2$ radioactive exchange system reacts with excess I$_2$O$_2$ to yield I$_2$O$_4$.</td>
</tr>
<tr>
<td>35BAHIPAR</td>
<td>H$_2$SO$_4$($\text{hot, conc.}$)+HI$O_3$ $\rightarrow$ I$_2$O$_4$</td>
<td>[85 °C]</td>
<td>Cryoscopy used to determine $T_fus$ for information, see Table 1, pp. 973-4) of I$_2$O$_4$ in sulfuric acid solutions; interpolation; used method of 35BAHIPAR</td>
</tr>
<tr>
<td>62FIA/TAR</td>
<td>I$_2$O$_3$+[IO]$_2$ $\rightarrow$ $2$(IO)(IO)$_3$</td>
<td>138 210 °C</td>
<td>I$_2$O$_3$, used to form the complex with sulfuric acid.</td>
</tr>
<tr>
<td>64GIL/SEN</td>
<td>HIO$_3$+H$_2$SO$_4$ $\rightarrow$(IO)$_3$</td>
<td></td>
<td>In concentrated sulfuric acid, I$_2$O$_3$, SO$_3$ takes up elementary iodine to form a brown solute; I$_2$O$_3$ was not isolated, only the complex with sulfuric acid</td>
</tr>
<tr>
<td>35BAHIPAR</td>
<td>I$_2$O$_3$+[IO]$_2$ $\rightarrow$ $2$(IO)(IO)$_3$</td>
<td>138 210 °C</td>
<td>The exchange of iodine in the I$_2$-I$_2$O$_3$ systems has been studied by use of radioactive isotope $^{131}$I</td>
</tr>
<tr>
<td>35BAHIPAR</td>
<td>Preparation apparently involves I$_2$O$_3$ and H$_2$SO$_4$ complex</td>
<td></td>
<td>Preparation of I$_2$O$_3$ and I$_2$O$_5$ in sulfate compounds: I$_2$O$_4$,H$_2$SO$_4$ and I$_2$O$_5$,H$_2$SO$_4$, respectively</td>
</tr>
<tr>
<td>38MAS</td>
<td>2I$_2$+3I$_2$O$_3$ $\rightarrow$ I$_3$O$_5$; shaken yellow solution $\rightarrow$I$_2$O$_3$.SO$_3$(c)</td>
<td></td>
<td>In concentrated sulfuric acid, I$_2$O$_3$, SO$_3$ takes up elementary iodine to form a brown solute; I$_2$O$_3$ was not isolated, only the complex with sulfuric acid</td>
</tr>
<tr>
<td>12GUIL2</td>
<td>Examined the exothermic reaction: I$_2$(g) + 2O$_3$(g) $\rightarrow$I$_2$O$_5$(c)</td>
<td>173 °C</td>
<td>Equilibrium pressure of system was calculated to 173° based on the earlier Berthelot data; concluded that direct oxidation of iodine is not a create practical preparation of anhydride; refers to two earlier studies of Berthelot and Thomsen in which enthalpy of formation is given I$_2$O$_3$, produced by dehydration of HIO$_3$ contains less I (and more O) than corresponds to the theoretical formula</td>
</tr>
<tr>
<td>31BAX/BUT</td>
<td>Formation from dehydration of HIO$_3$</td>
<td></td>
<td>Action of HNO$_3$ on I$_2$ gives hygroscopic I$_2$O$_5$; I$_2$O$_5$ reaction occurs in vapor phase; yellow hygroscopic crystals obtained; decomposition between 85 and 120° gives I$_2$O$_3$.</td>
</tr>
<tr>
<td>35BAHIPAR</td>
<td>H$_2$SO$_4$($\text{hot, conc.}$)+HI$O_3$ $\rightarrow$ I$_2$O$_4$</td>
<td>[85 °C]</td>
<td>Formation of I$_2$O$_5$ by dehydration of hydrate in vapor over KOH</td>
</tr>
<tr>
<td>36VIL/MOL</td>
<td>Formation of I$_2$O$_5$ · H$_2$O from reaction of hot I$_2$ with HNO$_3$</td>
<td></td>
<td>In concentrated sulfuric acid, I$_2$O$_3$ · SO$_3$ takes up elementary iodine to form a brown solute</td>
</tr>
<tr>
<td>38MAS</td>
<td>2I$_2$+3I$_2$O$_3$ $\rightarrow$ I$_3$O$_5$; shaken yellow solution $\rightarrow$I$_2$O$_3$.SO$_3$(c)</td>
<td></td>
<td>Directions for production of HIO$_3$ and subsequent preparation of I$_2$O$<em>5$: $\Delta</em>{f}H^\circ = -42.0$ kcal mol$^{-1}$ enthalpy of formation is stated; no reference given to the source of this value</td>
</tr>
<tr>
<td>40KONI</td>
<td>Formation by heating HIO$_3$</td>
<td></td>
<td>Infrared absorption spectra observed and compared with earlier studies; rapid dissociation and sublimation above 410 °C; no enthalpy values given</td>
</tr>
<tr>
<td>48FAR/KLE</td>
<td>No experimental procedure for formation of I$_2$O$_5$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>57DUV</td>
<td>Step-wise dissociation: sublimation of HIO$_3$ $\rightarrow$I$_2$O$_5$</td>
<td>248-410 °C</td>
<td></td>
</tr>
</tbody>
</table>

Table 1a. (Continued.)

<table>
<thead>
<tr>
<th>Source</th>
<th>Reaction</th>
<th>Temperature</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>57DUV2</td>
<td>Preparation of mixture: 2KIO₃ + I₂O₅; dissociation; sublimation</td>
<td>180–370 °C</td>
<td>Infrared absorption spectra studies; iodic anhydride disappears at 500 °C with the start of dissociation and sublimation</td>
</tr>
<tr>
<td>62FIA/TAR</td>
<td>Reversible redox reaction: I₂ + I₂O₅ → I₂O₆ + I₄; energy of activation = 10 kcal mol⁻¹</td>
<td>138–210 °C</td>
<td>The exchange of iodine in the I₂–I₂O₅ systems has been studied by use of radioactive isotope ¹²³I</td>
</tr>
<tr>
<td>84VIK</td>
<td>Preparation</td>
<td></td>
<td>Uses uv light; I₄ then reacted with O₃ to form solid I₂O₆ or I₂O₇</td>
</tr>
<tr>
<td>62MIS/SYM</td>
<td>H₂IO₆ + 65% oleum → I₂O₅</td>
<td></td>
<td>Spectrophotometry; assumed of new solid formation to be I₂O₆ in vacuo</td>
</tr>
<tr>
<td>15FCI/KAP</td>
<td>Formation of I(1O₂)₁₃</td>
<td></td>
<td>Two references to earlier preparation procedures: 1909 Fichter and Rohner; 1906 Beger</td>
</tr>
<tr>
<td>35BAH/PAR</td>
<td>Ozone reaction with iodine vapor to form I₂O₆ containing some unoxidized iodine</td>
<td></td>
<td>Reaction in vapor phase; yellow hygroscopic crystals obtained; decomposes at 75 °C</td>
</tr>
<tr>
<td>55KIK</td>
<td>Preparation</td>
<td></td>
<td>Uses uv light; I₄ then reacted with O₃ to form solid I₂O₆ or I₂O₇</td>
</tr>
<tr>
<td>84VIK/MAC</td>
<td>Formation: 4I₂(g) + 6O₃ → 2I₂O₅(c)</td>
<td>293–370 K</td>
<td>Stoichiometric composition of I₂O₆ in flow system; kinetic data given</td>
</tr>
<tr>
<td>I₂O₆/I₃O₈/12KAP</td>
<td>Preparation</td>
<td></td>
<td>Using earlier preparation method, the author suggests that the two oxides were misidentified and should be I₂O₆</td>
</tr>
</tbody>
</table>

Table 1b. Solid iodine oxide species: Decomposition and related reactions

<table>
<thead>
<tr>
<th>Source</th>
<th>Reaction</th>
<th>Temperature</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>Decomposition</td>
<td></td>
<td>Mass spectra; no values given; IO⁺ and IO₂⁺ undergo marked fluctuations in intensity; independent existence for I₂O₆ in gases produced by vaporization of I₂O₅</td>
</tr>
<tr>
<td>09MUI</td>
<td>Decomposition: I₂O₅ → I₂O₆ + I₂O₃</td>
<td>130 °C</td>
<td>Aqueous compositions/mixtures mostly; molecular weight not determined (I₂O₅ or I₂O₆); density values given; I₂O₅ is not hygroscopic</td>
</tr>
<tr>
<td>35BAH/PAR</td>
<td>Decomposition: 5I₂O₅ = 4I₂O₆ + I₂</td>
<td>130 °C</td>
<td>I₂O₅ decomposes slowly at 85 °C but more rapidly at 130 °C; decomposition does not proceed as stated by 09MUI; it is not hygroscopic</td>
</tr>
<tr>
<td>64DAE/KJE</td>
<td>Decomposition: 5I₂O₅ = 4I₂O₆ + H₂O</td>
<td>100–230 °C</td>
<td>Decomposition in moist air; enthalpy: x-ray diffraction analysis; density values given</td>
</tr>
<tr>
<td>68SEL/KJE</td>
<td>Decomposition: 5I₂O₅ = 4I₂O₆ + 2H₂O</td>
<td>20–240 °C</td>
<td>Differential thermogravimetric (DTG) analysis data (215–260 °C; 300–415 °C); x-ray diffraction data; proton magnetic resonance studies; density measurements included</td>
</tr>
<tr>
<td>71SEL/KJE</td>
<td>Decomposition: 3I₂O₅ = 2I₂O₆ + I₂O₃</td>
<td>125–250 °C</td>
<td>Statement of previous observations</td>
</tr>
<tr>
<td>80VIK/TAY</td>
<td>Decomposition: 9I₂O₅ = 8I₂O₆ + 2H₂O</td>
<td>460 K</td>
<td>Thermogravimetry; x-ray diffraction measurements; differential thermal analysis (DTA)</td>
</tr>
<tr>
<td>I₂O₅</td>
<td>Decomposition</td>
<td></td>
<td>Reaction with excess I₂O₅</td>
</tr>
<tr>
<td>63PAC/HAL</td>
<td>Decomposition of orthoperiodic acid (H₂IO₆) → I₂O₅ + I₂O₃</td>
<td>138–210 °C</td>
<td>Thermogravimetry; possible classification of product as I₂O₅</td>
</tr>
<tr>
<td>1. Decomposition</td>
<td></td>
<td></td>
<td>Decomposition in contact with humid air, water, or alcohol; preparation of crystallized substance</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Source</th>
<th>Reaction</th>
<th>Temperature</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>31MOL/PER</td>
<td>Decomposition</td>
<td>275 °C</td>
<td>Decomposition of pure dry I$_2$O$_3$ in dry air</td>
</tr>
<tr>
<td>32MOL/VIT</td>
<td>Decomposition</td>
<td>275 °C</td>
<td>Initial temperature of decomposition; $\Delta H^\circ$ reactions are</td>
</tr>
<tr>
<td></td>
<td>$\Delta H^\circ$ dissociation = -9.2</td>
<td></td>
<td>deduced</td>
</tr>
<tr>
<td></td>
<td>kcal mol$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\Delta H^\circ$ hydration = 2.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>kcal mol$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>32MOL/VIT2</td>
<td>Initial decomposition:</td>
<td>275 °C</td>
<td>Decomposition of I$_2$O$_3$ at 275 °C determined by the</td>
</tr>
<tr>
<td></td>
<td>I$_2$O$_3$ - I$_2$ + O$_2$</td>
<td></td>
<td>modified method of Tzentnershver and Andrusov; $\Delta H$ solution</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>of I$_2$O$_3$ given presumably in water</td>
</tr>
<tr>
<td>38MAS/ARG</td>
<td>Decomposition</td>
<td>215–220 K</td>
<td>Chretien's iodous sulfate; reaction occurring in</td>
</tr>
<tr>
<td></td>
<td>I$_2$O$_3$ - I$_2$O$_2$ + O$_2$</td>
<td></td>
<td>fuming sulfuric acid; product stabilized as an</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>iodous sulfate</td>
</tr>
<tr>
<td>64DAE/KJE</td>
<td>Decomposition</td>
<td>330–460 °C</td>
<td>Decomposition; thermogravimetric analysis; x-ray</td>
</tr>
<tr>
<td></td>
<td>I$_2$O$_3$ - O$_2$ + I$_2$</td>
<td></td>
<td>diffraction investigation</td>
</tr>
<tr>
<td>67STU/HUS</td>
<td>Decomposition</td>
<td>25°C</td>
<td>Mass spectra; no numeric information provided; six ions detected;</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>HIO$_3$ dehydrated to I$_2$O$_3$; sufficient</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>volatization occurred so that mass spectrum could</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>be obtained</td>
</tr>
<tr>
<td>68SEL/KJE</td>
<td>Decomposition:</td>
<td>&gt;[280 °C]</td>
<td>Differential thermogravimetric analysis (355–240 °C); x-ray</td>
</tr>
<tr>
<td></td>
<td>2I$_2$O$_3$ - 2I$_2$ + 5O$_2$</td>
<td>[250 °C]</td>
<td>diffraction data; crystallization from aqueous solutions with</td>
</tr>
<tr>
<td></td>
<td>sublimation</td>
<td></td>
<td>degrees of acidity; density measurements included</td>
</tr>
<tr>
<td>78CER/KO</td>
<td>Reaction:</td>
<td>25 °C</td>
<td>Proton magnetic resonance studies; it studies</td>
</tr>
<tr>
<td></td>
<td>$\frac{1}{2}$I$_2$O$_6$(c) + $\frac{3}{2}$H$_2$O(l) = H$^+$ (aq) + IO$_3^-$ (aq)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\frac{1}{2}$I$_2$O$_6$(c) + OH$^-$ (aq) = IO$_3^-$ (aq) + $\frac{1}{2}$H$_2$O(l)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>80WIK/TAY</td>
<td>Decomposition:</td>
<td>600–710 K</td>
<td>Thermogravimetry; x-ray diffraction measurements; differential</td>
</tr>
<tr>
<td></td>
<td>2I$_2$O$_3$ - 2I$_2$ + 5O$_2$</td>
<td></td>
<td>thermal analysis</td>
</tr>
<tr>
<td>85WIK/MAN</td>
<td>Decomposition:</td>
<td>570–730 K</td>
<td>TGA and DTA study of I$_2$O$_3$</td>
</tr>
</tbody>
</table>

### 2. Decomposition Reactions Leading to I$_2$O$_3$

<table>
<thead>
<tr>
<th>Source</th>
<th>Decomposition</th>
<th>Temperature</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>09GUI</td>
<td>I$_2$O$_3$ - I$_2$ + O$_2$</td>
<td>350–270 K</td>
<td>Reaction of iodine anhydride when exposed to heat; reaction starts at</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>350 K but gradually reaches 270 K by the end; preparation of substances</td>
</tr>
<tr>
<td>09MUI</td>
<td>I$_2$O$_3$ + SO$_3$</td>
<td>100 °C</td>
<td>Similar to earlier studies by Kammerer and Weber; presumed product is</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>I$_2$O$_3$; 25O$_3$ which differs from results of other two studies</td>
</tr>
<tr>
<td>11GUI</td>
<td>Decomposition of anhydride</td>
<td>250 °C</td>
<td>Preparative technique of anhydride; study of decomposition in vacuum</td>
</tr>
<tr>
<td>12GUI</td>
<td>Decomposition of I$_2$O$_3$ into iodic acid and oxygen</td>
<td>250 °C</td>
<td>Decomposition in vacuum, during 100 hours</td>
</tr>
<tr>
<td>32MOL/VIT2</td>
<td>Stepwise dehydration:</td>
<td>70 °C</td>
<td>The systematic thermal dehydration of HIO$_3$ yielded 3I$_2$O$_3$H$_2$O</td>
</tr>
<tr>
<td></td>
<td>HIO$_3$ - I$_2$O$_3$ - H$_2$O - I$_2$O$_3$</td>
<td></td>
<td>at 70 °C; at higher temperature, loss of H$_2$O is very small up to</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>200 °C where total dehydration gives I$_2$O$_3$</td>
</tr>
<tr>
<td>59HAU</td>
<td>Stepwise decomposition:</td>
<td>115–151 °C</td>
<td>Thermal decomposition</td>
</tr>
<tr>
<td></td>
<td>H$_2$IO$_3$ - I$_2$O$_3$</td>
<td></td>
<td>Decomposition of NH$_4$I$_3$O$_5$ in vacuum to form I$_2$O$_3$</td>
</tr>
<tr>
<td>61PAV/RAF</td>
<td>Decomposition of NH$_4$I$_3$O$_5$ in vacuum to form I$_2$O$_3$</td>
<td>100–170 °C</td>
<td>as an intermediate; I$_3$(g) was also a product</td>
</tr>
<tr>
<td>68SEL/KJE</td>
<td>Decomposition of 2HI$_2$O$_4$</td>
<td>190–250 °C</td>
<td>Discussion on I$_2$O$_3$ sublimation; DTG data (355–420 °C); x-ray</td>
</tr>
<tr>
<td></td>
<td>3I$_2$O$_3$ - H$_2$O</td>
<td></td>
<td>diffraction data; recrystallization from aqueous solutions with degrees</td>
</tr>
<tr>
<td></td>
<td>Stepwise dehydration:</td>
<td></td>
<td>of acidity; density measurements included</td>
</tr>
<tr>
<td>71SEL/KJE</td>
<td>I$_2$O$_3$ - 4I$_2$O$_3$ + I$_2$</td>
<td>125–250 °C</td>
<td>Statement of previous observations</td>
</tr>
</tbody>
</table>

### NIST–JANAF THERMOCHEMICAL TABLES FOR THE IODINE OXIDES

**Table 1b. (Continued.)**

<table>
<thead>
<tr>
<th>Source</th>
<th>Reaction</th>
<th>Temperature</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>3SBASH/PAR</td>
<td>Decomposition: 4I₂O₉ → 6I₂O₅ + 2I₂ + 3O₂</td>
<td>*85–120 °C</td>
<td>*I₂O₉ begins to decompose at 75 °C but reaches its peak at 85–120 °C; it is very hygroscopic; comments on many reactions of I₂O₉ are also given</td>
</tr>
<tr>
<td>80WIK/TAY</td>
<td>Decomposition: 5I₂O₉ → 9I₂O₅ + I₂</td>
<td>415–460 K</td>
<td>Thermogravimetry; x-ray diffraction measurements; differential thermal analysis.</td>
</tr>
<tr>
<td>83COX/COK</td>
<td>Decomposition: 5I₂O₉ → 9I₂O₅ + I₂</td>
<td>460 K</td>
<td>Authors state that these data from [80WIK/TAY] are consistent with observations in their system</td>
</tr>
<tr>
<td>85SUN/WRE</td>
<td>Decomposition: 5I₂O₉ → 9I₂O₅ + I₂</td>
<td></td>
<td>Crystalline compound thermal decomposition—see 85VIKMAK</td>
</tr>
<tr>
<td>85VIKMAK</td>
<td>I₂O₉ → I₂O₅ + I₂</td>
<td></td>
<td>Thermogravimetry and differential thermal analysis of I₂O₉ indicates two transitions, the last one of which appears to be the decomposition of I₂O₉</td>
</tr>
</tbody>
</table>

### Table 2. Iodine oxide species: Neutrals, radicals, and ions in solution

<table>
<thead>
<tr>
<th>Source</th>
<th>Compound</th>
<th>Reaction</th>
<th>Temperature</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1896CHR</td>
<td>I₂O₂</td>
<td>Decomposition: 3I₂O₂ + H₂O = 2I₂O₃ + H₂O</td>
<td>250-260 °C</td>
<td>Immediate decomposition in contact with H₂O; HI cannot exist in the presence of iodic acid, hence the second reaction</td>
</tr>
<tr>
<td>1898CHR2</td>
<td>I₂O₃</td>
<td>Decomposition: I₂O₃ + H₂O = 2I₂O₂ + H₂</td>
<td>250-260 °C</td>
<td>Immediate decomposition in contact with water; HI cannot exist in presence of iodic acid, hence the second reaction</td>
</tr>
<tr>
<td>23GOM</td>
<td>I₂O₄</td>
<td>(ClO₃)⁻ + I₃⁻ = I₂O₄ + Cl⁻</td>
<td></td>
<td>Probable formation of I₂O₄ in ether; I₂O₄ presumably unstable to I₂ and O₂.</td>
</tr>
<tr>
<td>30BRA</td>
<td>I₂O₃</td>
<td>*Preparation of I₂O₃ from photodecomposition of iodate ion in solution</td>
<td></td>
<td>*Preparation of I₂O₃ · SO₃H₂O but no data of I₂O₃ itself.</td>
</tr>
<tr>
<td>36FIC/DIN</td>
<td>I₂O₅</td>
<td>Formation of I₂O₅ from decomposition of iodate ion in solution</td>
<td></td>
<td>It appears that the ΔG°* calculated value is for the radical not the ion, as indicated in the article</td>
</tr>
<tr>
<td>72FOR/GOO</td>
<td>I₂O₅</td>
<td>Hypoiodate reaction: HgO + 2I₂O₅ = I₂O₃ + 2H₂O</td>
<td>18 °C</td>
<td>Stability and reactivity of mercuric oxide with iodine reagent in solution; these reactions (among others) are proposed to describe the hypoiodate reaction</td>
</tr>
<tr>
<td>740DE/DEJ</td>
<td>I₂O₃</td>
<td>Solubility of I₂O₃ in ternary systems</td>
<td>0, 25 °C</td>
<td>Solubility in the I₂O₃ · Na₂SO₄·H₂O and I₂O₃ · SO₃·H₂O systems studied; I₂O₃ was never isolated</td>
</tr>
<tr>
<td>80COO</td>
<td>I₂O₇</td>
<td>Chloride ion; I₂O₇ catalyzed oxidation reaction scheme</td>
<td>50 °C</td>
<td>Kinetic data; chloride ions may influence the production of the free radical iodine dioxide; I₂O₇ and I₂O₇ are intermediates in the reaction scheme; no thermochemical data present</td>
</tr>
<tr>
<td>81KLA/SEN</td>
<td>I₂O₇⁻</td>
<td>2I₂O₇⁻ + O⁻ = I₂O₇²⁻</td>
<td>± 7 °C</td>
<td>Radiolysis and flash photolysis of aqueous iodate and periodate solutions; ΔG°(I₂O₇) = 190 kJ/mol, presumably in aqueous solution; spectrum and decay kinetics of the assumed I₂O₇ are determined</td>
</tr>
<tr>
<td>82PUR/NOY</td>
<td>I₂O₇</td>
<td>Oscillatory Briggs-Rauscher reaction (acidic aqueous solution)</td>
<td>25 °C</td>
<td>Postulates that I₂O₇ and I₂O₃ exist as intermediates in acidic aqueous reactions in the kinetic description of this reaction</td>
</tr>
<tr>
<td>82NOS/NOS</td>
<td>I₂O₇</td>
<td>Oscillatory reactions for ion selective electrodes</td>
<td>24±1 °C</td>
<td>Preparation of iodide-free HOI; I₂O₇ in an intermediate</td>
</tr>
<tr>
<td>83WAG/STR</td>
<td>I₂O₅</td>
<td>Hydrolysis: 2I₂O₅ + H₂O + I₂O₅⁻ + 2I₂O₃⁻ + 2H²⁻</td>
<td>278-298 K</td>
<td>Flash photolysis of periodate in pH range 2.44-4.90; I₂O₃ formed in the photolysis can be further reacted with O₃ to form I₂O₅; both I₂O₃ and I₂O₇ can further dimerize; all species used to describe kinetics</td>
</tr>
<tr>
<td>85BUX/SEL</td>
<td>I₂O₇</td>
<td>*I₂O₅ + I₂O₇⁻ = I₂O₇⁺</td>
<td>25 °C</td>
<td>Pulse radiolysis of iodate and iodate solutions; spectrophotometry of I₂O₇ equilibria in periodate solutions; *in analogy with Cl and Br systems authors suggest formation of I₂O₅⁻; dimerization of I₂O₅ to I₂O₇ proposed to explain kinetics in alkaline solution</td>
</tr>
<tr>
<td>86VIK/TOR</td>
<td>I₂O₇</td>
<td>Gas phase reaction to form oxides followed by reaction/solution with H₂O</td>
<td></td>
<td>I₂O₇ reacts with O₃ to form iodine oxides that, on contact with H₂O, would be washed into the aqueous phase as I₂O₅;</td>
</tr>
</tbody>
</table>

### Table 3. Iodine oxide species: Electronic energy levels

<table>
<thead>
<tr>
<th>Source</th>
<th>Transition</th>
<th>Energy level (cm⁻¹)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>IO(g)</td>
<td>B–X system</td>
<td>21 557</td>
<td>( T_v ) value; gas phase study</td>
</tr>
<tr>
<td>37VAI</td>
<td></td>
<td>21 565</td>
<td>Flame spectra data; estimated vibrational constants for both states; provides comments on earlier studies by Vaidya and by Blake and Iredale</td>
</tr>
<tr>
<td>48COL/GAY</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>58DUR/RAM</td>
<td>( ^2\Pi_{1/2} - ^2\Pi_{3/2} )-X</td>
<td>23 420.3, 22 958.9, 22 478.0, 21 981.9, 21 804.5, 21 481.4</td>
<td>Absorption spectra of IO during flash photolysis of I₂O₃ mixtures; vibrational analysis consistent with scheme developed by Coleman, Gaydon, and Vaidya</td>
</tr>
<tr>
<td>60DAS/WAD</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>60DUR/LEG</td>
<td>( \Delta \Pi - X^\Pi )</td>
<td>24 390–15 873</td>
<td></td>
</tr>
<tr>
<td>61PH/SUG</td>
<td></td>
<td>18 843</td>
<td></td>
</tr>
<tr>
<td>65SIR/RAI</td>
<td>( ^3\Pi - X^\Pi )</td>
<td>21 565</td>
<td></td>
</tr>
<tr>
<td>70AMI/TRE</td>
<td></td>
<td>22 222.2</td>
<td></td>
</tr>
<tr>
<td>70AMI/TRE2</td>
<td></td>
<td>21 739.1</td>
<td></td>
</tr>
<tr>
<td>70CL/YCRU</td>
<td>( ^1\Pi - X^\Pi )</td>
<td>21 277–23 923</td>
<td></td>
</tr>
<tr>
<td>72BRO/BYP</td>
<td>( \Sigma^+ ) ( ^3\Pi - X^\Pi )</td>
<td>[30 000]</td>
<td></td>
</tr>
<tr>
<td>73SAI</td>
<td>( \Delta \Pi - X^\Pi )</td>
<td>[49 615.5–50 403.2, 49 959.6]</td>
<td>Estimated value of excited state in comparison with IO radical; energy separation of ( ^3\Pi_{1/2} ) and ( ^3\Pi_{3/2} ) is 2330 cm⁻¹; ( B_0(\Pi_{3/2})=10 157.08±0.18 ) MHz; microwave spectra; ( r_0=1.8677±0.0028 ) A; value is calculated from effective rotational constant ( R(\Pi_{3/2}) ) combined with ( \alpha_s ) from ( \Delta \Pi - X^\Pi ) transition of 60DUR/LEG; comparison of molecular constants given</td>
</tr>
<tr>
<td>77CAL/MET</td>
<td>( \beta \Pi - X^\Pi )</td>
<td>50 000–55 555.5</td>
<td>Fluorescence absorption spectra; ( ^3\Pi ) transition of IO₂ solutions leads to dissociation of IO by light absorption and optical filters; (?) new system with 3 bandheads observed in ultraviolet</td>
</tr>
<tr>
<td>83BEK/MEE</td>
<td>( \Delta \Pi_{3/2} - X^\Pi_{3/2} )</td>
<td>22 469.8</td>
<td>High resolution molecular-beam laser excitation spectroscopy; microwave optical double resonance; equilibrium rotational constant ( B_0=10 083 ) MHz derived using estimated ( A_0=233 ) cm⁻¹; calculated vibrational frequency ( \omega_u ) of 669.7 and corresponding equilibrium internuclear distance ( \xi_0=0.187 84 ) Å; spin–orbit coupling constrained to be ( A=2330 ) cm⁻¹</td>
</tr>
<tr>
<td>83COX/COX</td>
<td>( \Delta \Pi - X^\Pi )</td>
<td>21 277–24 096</td>
<td>No direct analysis of the vibrational and rotational structure; absorption by molecular modulation technique</td>
</tr>
<tr>
<td>85BUX/SEI</td>
<td></td>
<td>20 408</td>
<td>Radiolysis spectrophotometry of aqueous HIO; spectra of IO obtained by oxidation of IO with O²⁻ in aqueous solution at pH ≥ 13; band maximum reported</td>
</tr>
<tr>
<td>89RED/RAO</td>
<td></td>
<td></td>
<td>Potential energy curves for the ground state constructed by Rydberg–Klein–Rees method as modified by Vanderslice et al.; no values given; dissociation energy provided</td>
</tr>
<tr>
<td>IO(matrix)</td>
<td>( \Delta \Pi - X )</td>
<td>21 043±34</td>
<td>Absorption and emission spectra of IO in solid argon matrix at 20 K; ( T_v ) values; prepared by microwave discharge</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Source</th>
<th>Transition</th>
<th>Energy level (cm(^{-1}))</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>I(_2)(cr)</td>
<td>69BAR/GIL</td>
<td>20 833.3</td>
<td>Absorption spectra; flash photolysis of aqueous solutions of iodate ions; maximum absorption band at 480 nm attributed to I(_2) radical</td>
</tr>
<tr>
<td>70AMI/TRE</td>
<td>[29411.8]</td>
<td></td>
<td>Flash photolysis of IO(_3^-) and IO(_5^-) in aqueous solution; absorption spectra in decay kinetics studied by pulse radiolysis; estimated value, maximum intensity of band structure at approximately 715 nm</td>
</tr>
<tr>
<td>70AMI/1KE2</td>
<td>27 261.2</td>
<td></td>
<td>Flash photolysis of IO(_3^-) in boric acid glass; maximum intensity absorption band at 655 nm</td>
</tr>
<tr>
<td>72BAR/GIL</td>
<td>20 833.3</td>
<td></td>
<td>Pulse radiolysis and flash photolysis of aqueous solutions in iodate ions; absorption band maximum at 480–490 nm attributed to IO(_3^-)</td>
</tr>
<tr>
<td>7JEN/FAR</td>
<td>20 408.2</td>
<td></td>
<td>Transient absorption spectra; maintains that the 490 nm band is related to IO(_3^-) rather than IO(_3) (as suggested by 70AMI/TRE); pulse radiolysis technique</td>
</tr>
<tr>
<td>81ATH/MOR</td>
<td>0 (B(_2)); A(_1)B(_1)</td>
<td></td>
<td>EPR spectra; in (\gamma)-irradiated KIO(_3) crystals, reassigns spectra originally thought to be IO(_2)F to IO(_3^-)</td>
</tr>
<tr>
<td>86BYB</td>
<td>1(^3)O(_2)</td>
<td></td>
<td>EPR spectra, electronic properties closely resemble those of ClO(_2^-) and BrO(_2^-)</td>
</tr>
<tr>
<td>IO(_2)</td>
<td>69BAR/GIL</td>
<td>38 461.5–52 631.6</td>
<td>IO(_2) radical not observed under these experimental conditions; absorption spectra; flash photolysis of aqueous solutions of iodate ions</td>
</tr>
<tr>
<td>70AMI/TRE</td>
<td>26 315.8</td>
<td></td>
<td>Flash photolysis of IO(_3^-) and IO(_5^-) in aqueous solution; absorption spectra in decay kinetics studied by pulse radiolysis; maximum intensity of band structure at 380 nm</td>
</tr>
<tr>
<td>70AMI/TRE2</td>
<td>25 316.5</td>
<td></td>
<td>Flash photolysis of IO(_3^-) in boric acid glass; maximum intensity of absorption band at 395 nm</td>
</tr>
<tr>
<td>72BAR/GIL</td>
<td>27 777.8</td>
<td></td>
<td>Pulse radiolysis and flash photolysis of aqueous solutions of iodate ions; absorption band maximum at 360 nm attributed to IO(_3^-)</td>
</tr>
<tr>
<td>7JEN/FAR</td>
<td>27 777.8</td>
<td></td>
<td>Transient absorption spectra; though spectra are observed for IO(_3^-), the author attributes them to (IO(_3)(_2); pulse radiolysis technique</td>
</tr>
<tr>
<td>IO(_3)</td>
<td>7ILES/8BAR</td>
<td></td>
<td>Absorption spectra; pulse radiolysis periodate aqueous solutions; IO(_3) proposed as reaction intermediate</td>
</tr>
<tr>
<td>I(_2)O(_5)</td>
<td>57SYM</td>
<td></td>
<td>Absorption of IO(_3^-) spectra observed from solutions of iodine in concentrated H(_2)SO(_4); spectra used as evidence that I(_2)O(_5) is ionic having the structure IO(_3^-)IO(_2)(_5^-)</td>
</tr>
<tr>
<td>60DAS/WAD</td>
<td>45 000–85 000</td>
<td></td>
<td>Infrared absorption spectra</td>
</tr>
<tr>
<td>61WIS/HAN</td>
<td>11 049.7; 75 188.0 (9.05 (\mu)m) (13.30 (\mu)m)</td>
<td></td>
<td>Infrared absorption spectra studies of I(_2)O(_5) in pressed KBr pellets; of the two strong bands, 13.30 (\mu)m is attributed to IO(_3^-) and 9.05 (\mu)m, obtained from stoichiometry, was identified with IO(_5^-)</td>
</tr>
<tr>
<td>69GRU/MUR</td>
<td>132 000</td>
<td></td>
<td>Mössbauer spectrum measured at 80 K treating I(_2)O(_5) as absorber; scheme is put forward for the structure of I(_2)O(_5) built of IO groups bound covalently to IO(_3^-) groups through the O atom</td>
</tr>
<tr>
<td>I(_2)O(_5)</td>
<td>61DUR/LEC</td>
<td></td>
<td>*Study of structure by infrared spectroscopy from 2–33 (\mu)m shows existence of 1–O–1 bridge analogues to that of I(_2)O(_5)</td>
</tr>
<tr>
<td>70SHE/TUR</td>
<td></td>
<td></td>
<td>Mass spectra studies of I(_2)O(_5); author believes earlier studies' peaks assigned to I(_2)O(_5) to be incorrect; evaporation of I(_2)O(_5) only above [280]°C</td>
</tr>
</tbody>
</table>

### Table 3. (Continued.)

<table>
<thead>
<tr>
<th>Source</th>
<th>Transition</th>
<th>Energy level (cm(^{-1}))</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>I(_2)O(_6)</td>
<td>62MIS/SYM</td>
<td></td>
<td></td>
</tr>
<tr>
<td>I(_2)O(_4)(cr)</td>
<td>85SUN/WRE</td>
<td>15 453.6</td>
<td></td>
</tr>
</tbody>
</table>

Ultraviolet spectra at 77 K; no values given; uv spectra at room temperature are irreproducible.

Raman spectrometry of crystalline and amorphous solids; formed by gas phase reaction of I\(_2\) with O\(_3\); I\(_2\)O\(_4\) is a distinct molecular species (not a mixture of I\(_2\)O\(_3\) and I\(_2\)O\(_5\)).

---

### Table 4. Iodine oxide species (I\(_2\O\)): Dissociation energy (\(D_0\))

<table>
<thead>
<tr>
<th>Source</th>
<th>(D_0) (kJ mol(^{-1}))</th>
<th>Temperature</th>
<th>Comments (as reported values)</th>
</tr>
</thead>
<tbody>
<tr>
<td>48COL/GAY</td>
<td>184±21</td>
<td></td>
<td>From graphical Birge–Sponer extrapolation for ground state ([X^2\Pi (v, 0–12)] D_0); flame spectral data (twelve ground state vibrational levels); 44±5 kcal mol(^{-1})</td>
</tr>
<tr>
<td>50HER</td>
<td>183.3</td>
<td></td>
<td>No specific source cited; 1.9 eV</td>
</tr>
<tr>
<td>53GAY</td>
<td>183.3±19</td>
<td></td>
<td>Value based on 37VAY, 48COL/GAY; LBX(v, 0–12); this is supported by extrapolation of upper state and predissociation giving a value of ≲ 1.95 eV; 1.9±0.2 eV</td>
</tr>
<tr>
<td>54COT</td>
<td>183.3±19</td>
<td></td>
<td>Value based on 53GAY; Cottrell stated that this value seemed fairly well established; 1.9±0.2 eV</td>
</tr>
<tr>
<td>58BRE</td>
<td>184</td>
<td></td>
<td>Value given by Brewer with a &quot;?&quot;; no explanation as to source; 44 kcal mol(^{-1})</td>
</tr>
<tr>
<td>58DUR/RAM</td>
<td>176±21</td>
<td></td>
<td>Dissociation energy for ground state is calculated from absorption spectra; a linear Birge–Sponer extrapolation of four upper state vibrational levels yielded 45 kcal mol(^{-1}); Birge–Sponer extrapolation was decreased by 10% in analogy with ClO and BrO; 42±5 kcal mol(^{-1})</td>
</tr>
<tr>
<td>60DUR/LEG</td>
<td>192±21</td>
<td></td>
<td>Graphical Birge–Sponer extrapolation for A(^2\Pi (\mu, 0–5, perturbed) state; predissociation &lt; 2.72 eV; 46±5 kcal mol(^{-1})</td>
</tr>
<tr>
<td>61LIP/STE</td>
<td>249.9 or 248.0</td>
<td></td>
<td>Calculated from three- and five-parameter potential functions; 2.59 eV or 2.57 eV</td>
</tr>
<tr>
<td>61PHI/SUG</td>
<td>238±25</td>
<td>0 K</td>
<td>(D_0) deduced from the temperature variation of the equilibrium constant; flame photometry; 57±6 kcal mol(^{-1})</td>
</tr>
<tr>
<td>62GUR/KHA</td>
<td>184±21</td>
<td></td>
<td>Corresponds to an enthalpy of formation of 40.574±5 kcal mol(^{-1}) value based on data from 48COL/GAY; mentions work of 58DUR/RAM; 44±5 kcal mol(^{-1})</td>
</tr>
<tr>
<td>63SCH</td>
<td>183.3±19</td>
<td></td>
<td>(D_0) deduced from 53GAY; 1.9±0.2 eV</td>
</tr>
<tr>
<td>65SIN/RAJ</td>
<td>239.3</td>
<td></td>
<td>(D_0) calculated from RKRV potential energy curves 120 000 cm(^{-1}); no uncertainty given; 57.2 kcal mol(^{-1})</td>
</tr>
<tr>
<td>66VED/GUR</td>
<td>184±21</td>
<td>238±25</td>
<td>L.B.S. for the (X^2\Pi) and (A^2\Pi) states, assuming that the dissociation limit corresponds to (I(\Sigma_d^+))+O((^1)D); dissociation equilibria in flames; 44±5 and 57±6 kcal mol(^{-1})</td>
</tr>
<tr>
<td>67CAR/DYE</td>
<td>176±21</td>
<td></td>
<td>Based on the spectroscopic measurements of 58DUR/RAM and 60DUR/LEG; 42.3 kcal mol(^{-1})</td>
</tr>
<tr>
<td>68WAG/EVA</td>
<td>177.0</td>
<td>0 K</td>
<td>Value based on analysis of 48COL/GAY, 58DUR/RAM, and 61PHI/SUG; 46±7 kcal mol(^{-1})</td>
</tr>
<tr>
<td>69BRE/ROS</td>
<td>192±29</td>
<td></td>
<td>Suggests that (D_0) = 238±24 kcal mol(^{-1}); [61PHI/SUG] is compatible with iodine abstraction mechanism but not (D_0 = 174 ± 19 \text{ kcal mol}^{-1}) [58DUR/RAM]</td>
</tr>
<tr>
<td>69HER/HUI</td>
<td>167±21</td>
<td></td>
<td>(D_0) calculated from linear extrapolation of the upper state (A (^2\Pi)) vibrational levels; *rapid bimolecular disproportionation at 293 K occurring through transition state [I–O–O–I]; bond angles are 120°; r distances are O–O=0.15 nm, I–O=0.22 nm, I–O=0.188 nm; the latter value is from 60DUR/LEG</td>
</tr>
</tbody>
</table>

TABLE 4. (Continued.)

<table>
<thead>
<tr>
<th>Source</th>
<th>$D_o^e$ (kJ mol$^{-1}$)</th>
<th>Temperature</th>
<th>Comments (as reported values)</th>
</tr>
</thead>
<tbody>
<tr>
<td>70DAR</td>
<td>180±21</td>
<td></td>
<td>Based on 58DUR/RAM, 61PHI/SUG, 62VED/GUR, and 68WAG/EVA; 43±5 kcal mol$^{-1}$</td>
</tr>
<tr>
<td>72TRI/GOH</td>
<td>183.3±19</td>
<td></td>
<td>Experimental value in agreement with the least-squares fitting of the RKR curve and Hulburt–Hirschfelder value of 44.7; 43.3±6.6 kcal mol$^{-1}$</td>
</tr>
<tr>
<td>74RAO/RAO</td>
<td>dissociation ($A^3Π_{3/2}$): 137.5</td>
<td></td>
<td>Dissociation of upper state calculated by fitting an empirical potential energy curve using Lippencott's three-parameter function and Hulburt–Hirschfelder function with Franck–Condon factors; r centroids of $A^3Π_{3/2}$–$X^3Π_{1/2}$ system; 32.86 kcal mol$^{-1}$</td>
</tr>
<tr>
<td>75RAD/WHI</td>
<td>222±13</td>
<td>0 K</td>
<td>Reaction in crossed molecular beams of O+ICl led to a measured bond energy value; result based on dissociation energy of ICl; 53±3 kcal mol$^{-1}$</td>
</tr>
<tr>
<td>79ADD/DON</td>
<td>≥210</td>
<td></td>
<td>Kinetic dissociation energy value is consistent with 75RAD/WHI</td>
</tr>
<tr>
<td>79HUB/HER</td>
<td>173.7</td>
<td></td>
<td>Based on extrapolations of the vibrational levels of $A^3Π_{3/2}$ and the assumption that $A^1Π_{3/2}$Br$^+$+D$^0$(0) flame photometry [61PHI/SUG] gives 2.4 eV (less likely as it is as high as BrO); observed predissociation in A gives $D_o^e$&lt;2.72 eV; extrapolation of ground state gives 1.94 eV [72TRI/GOH]; 1.8 eV</td>
</tr>
<tr>
<td>82BAU/COX</td>
<td>182±21</td>
<td></td>
<td>Derived heat of formation at 298 K to be 172 kcal mol$^{-1}$; authors refer to the work of [80KER/TRO] whose results have been taken from other sources</td>
</tr>
<tr>
<td>83BUS/SIL</td>
<td>230±8</td>
<td></td>
<td>O+Cl reaction in crossed molecular beams; authors preferred a slightly higher IO bond energy value than that proposed by 75RAD/WHI; 55±2 kcal mol$^{-1}$</td>
</tr>
<tr>
<td>88TYK</td>
<td>atomization: $\Delta_H^o = 181$</td>
<td>25°C</td>
<td>Calculated from reaction trends in log $\Delta_H^o$; trends based on data from JANAF Thermochemical Tables (1985 Supplement) and NBS Tables of Chemical Thermodynamic Properties (1982)</td>
</tr>
<tr>
<td>89RED/RAO</td>
<td>249.4±1.7</td>
<td></td>
<td>Estimated from the Lippencott three-parameter potential function; author referred to three other values for the $D_o^e$: 2.4 eV from flame photometry, &lt;2.74 eV from absorbed predissociation A state, and 1.94 eV from extrapolation of ground state; 59.6±0.4 kcal mol$^{-1}$</td>
</tr>
<tr>
<td>92MAG/LAV</td>
<td>$\Delta_H^o = 172$</td>
<td></td>
<td>Used value reported by 90DEM/MOL, JPL report mentioned in Introduction; $\Delta_H^o = 41.1$ kcal mol$^{-1}$; two values given by 89GUR/VEY and 89RED/RAO are mentioned but not used</td>
</tr>
<tr>
<td>94RUS/BER</td>
<td>201.2±21</td>
<td></td>
<td>Roughly the mean of the preferred values of 75RAD/WHI and 68GAY; 50±5 kcal mol$^{-1}$</td>
</tr>
<tr>
<td>95MON/STI</td>
<td>226</td>
<td></td>
<td>Use of photoionization efficiency spectra</td>
</tr>
<tr>
<td>96GIL/TUR</td>
<td>$\Delta_H^o &lt; 120.5$</td>
<td></td>
<td>Determined rate constants for the reaction O(\textit{P}) with alkyl iodides; suggested $\Delta_H^o$ (IO, 298 K) &lt;28.8 kcal mol$^{-1}$</td>
</tr>
</tbody>
</table>

TABLE 5. Iodine oxide species: Structures and vibrational frequencies

<table>
<thead>
<tr>
<th>Source</th>
<th>Structure</th>
<th>Bond distance X–Y (Å)</th>
<th>Vibrational frequencies (cm$^{-1}$)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>IO I</td>
<td>37VAI</td>
<td>2.1</td>
<td>600, 1100, 1300</td>
<td>Vibrational analysis; $\omega_3$ and $\omega_3\gamma_4$ values given</td>
</tr>
<tr>
<td></td>
<td>80LOE/MIL</td>
<td></td>
<td></td>
<td>Vibrational analysis; $\omega_3$ and $\omega_3\gamma_4$ values given</td>
</tr>
<tr>
<td></td>
<td>90DAS/WAD</td>
<td>$\text{IO}_2$ (complex iodates)</td>
<td>$\text{IO}_2$ (iodoxy benzenes)</td>
<td>Spectrum interpreted in terms of a network of IO$_2$ groups and polymerized ion chains; IO symmetric and antisymmetric stretching frequencies are estimated by trends in many iodine compounds</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Source</th>
<th>Structure</th>
<th>Bond distance X–Y (Å)</th>
<th>Vibrational frequencies (cm⁻¹)</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>IO₂</td>
<td>60DUV/LEC</td>
<td></td>
<td>ν₁(sym.) 420 ν₂ (asym.) ν₃</td>
<td>Absorption spectra of IO₂; the three vibrational frequencies given are assumed to represent the IO₂ fragment of IO₂₃</td>
</tr>
<tr>
<td>86BYB</td>
<td>C₂v point group</td>
<td></td>
<td>ν₁ ν₂ 765±25 192±35 ν₃</td>
<td>Observation and calculation of EPR spectrum of structure in KCIO₄ crystal</td>
</tr>
<tr>
<td>88BYB IO₂</td>
<td>C₂v point group</td>
<td></td>
<td></td>
<td>EPR spectra interpreted in terms of bond angle of 118°; no bond distances given</td>
</tr>
<tr>
<td>92GIL/POL</td>
<td>Pyramidal C₃v point group</td>
<td>1.79 A₁(sym) 357 780</td>
<td>E(asym.) 326 809</td>
<td>Photoelectron spectroscopy</td>
</tr>
<tr>
<td>56VEN/SUN</td>
<td>Pyramidal C₃v point group</td>
<td>1.79 ν₁ ν₂ 765±25 192±35</td>
<td>E(asym.) 326 809</td>
<td>Raman effect data; type E frequencies are doubly degenerate; observed interbond angles and observed frequencies are presumably taken from Landolt–Bornstein Tables 1951 (data could not be found in this publication); X–Y distances calculated by Badger’s rule; force constants given; I–O–I bond angle is 89°</td>
</tr>
<tr>
<td>6-4RAO/SAN</td>
<td>Pyramidal C₃v point group</td>
<td>1.79 ν₁ ν₂ 765±25 192±35</td>
<td>E(asym.) 326 809</td>
<td>Identiﬁes vibrational frequencies, two symmetrical (A₁) and two doubly degenerate E modes but no values given; uses 56VEN/SUN values to calculate mean square amplitudes</td>
</tr>
<tr>
<td>72RAO</td>
<td>Pyramidal C₃v point group</td>
<td>1.79 ν₁ ν₂ 765±25 192±35</td>
<td>E(asym.) 326 809</td>
<td>Identifies XY₃ pyramidal type molecule with six vibrations (two symmetric A₁ and two doubly degenerate E modes) but no values given; calculations based on 56VEN/SUN; calculation of centriﬁetal distortion constants</td>
</tr>
<tr>
<td>78THI/MOH</td>
<td>Pyramidal C₃v point group</td>
<td>1.79 ν₁ ν₂ 765±25 192±35</td>
<td>E(asym.) 326 809</td>
<td>Frequency analysis from Landolt–Bornstein tables; authors cite origin of data in three references which do not deal with IO₃</td>
</tr>
<tr>
<td>I₂O</td>
<td>60DUV/LEC</td>
<td>IOI</td>
<td>ν₁ ν₂ ν₃ 597 170 688</td>
<td>Absorption spectra of IO₂; frequencies given for I₂O but no indication as to origin of these values</td>
</tr>
<tr>
<td>I₂O₂</td>
<td>30BRA</td>
<td>IOI or OIO</td>
<td></td>
<td>Established existence as an intermediate in the equilibrium involving IO₂⁻ and H₃IO₃</td>
</tr>
<tr>
<td>I₂O₃</td>
<td>50WIL/DHA</td>
<td>Diamagnetic; IO₂⁻; IO₂⁻;</td>
<td>ν₁ ν₂ 622 s 408 825 w 578 s</td>
<td>Monomeric IO₃ unit does not occur in solid state; stable compound at room temperature; assumed structure</td>
</tr>
<tr>
<td>57SYM</td>
<td>Diamagnetic; IO⁻</td>
<td>ν₁ ν₂ 622 s 408 825 w</td>
<td>ν₃ 578 s 783 s ν₄ 745 s</td>
<td>Absorption spectra; structure and diamagnetic attribute based on 50WIL/DHA observations; ultraviolet absorption spectrum interpreted in terms of a network of IO₂ groups and polymerized IO chains; spectrum estimated in analogy to TeO frequency of 796 cm⁻¹</td>
</tr>
<tr>
<td>60DAS/WAD</td>
<td>IO⁻ IO₂⁻</td>
<td>ν₁ ν₂ 622 s 408 825 w</td>
<td>ν₃ 578 s 783 s ν₄ 745 s</td>
<td>Structure determination from infrared spectra; infra-red spectrum in Nujol mulls and structure: critique of earlier work by Wise and Hannan, Dassent and Waddington (1960); IO₂⁻ spectrum explained in terms of polymerized I–OI chains and IO₂ groups; Mössbauer study of the oxide; conclusions: there are two sterically and chemically inequivalent states of iodine; there is no undeformed IO⁻⁻ ion</td>
</tr>
<tr>
<td>61WIS/HAN</td>
<td>IO⁻ IO₂⁻</td>
<td>ν₁ ν₂ 622 s 408 825 w</td>
<td>ν₃ 578 s 783 s ν₄ 745 s</td>
<td>Structure determination from infrared spectra; infra-red spectrum in Nujol mulls and structure: critique of earlier work by Wise and Hannan, Dassent and Waddington (1960); IO₂⁻ spectrum explained in terms of polymerized I–OI chains and IO₂ groups; Mössbauer study of the oxide; conclusions: there are two sterically and chemically inequivalent states of iodine; there is no undeformed IO⁻⁻ ion</td>
</tr>
<tr>
<td>63DAS/WAD</td>
<td>Diamagnetic</td>
<td>ν₁ ν₂ 622 s 408 825 w</td>
<td>ν₃ 578 s 783 s ν₄ 745 s</td>
<td>Infrared spectra, partial Raman spectra; &quot;vibrational frequency stretching of solid state from 900–550 cm⁻¹ but no assignment made; structure of I₂O₂ is similar to I₂O₃</td>
</tr>
<tr>
<td>69GRU/MUR</td>
<td>Nonionic</td>
<td>ν₁ ν₂ 622 s 408 825 w</td>
<td>ν₃ 578 s 783 s ν₄ 745 s</td>
<td>Infrared spectra, partial Raman spectra; &quot;vibrational frequency stretching of solid state from 900–550 cm⁻¹ but no assignment made; structure of I₂O₂ is similar to I₂O₃</td>
</tr>
<tr>
<td>70GRU/LUR</td>
<td>Nonionic</td>
<td>ν₁ ν₂ 622 s 408 825 w</td>
<td>ν₃ 578 s 783 s ν₄ 745 s</td>
<td>Infrared spectra, partial Raman spectra; &quot;vibrational frequency stretching of solid state from 900–550 cm⁻¹ but no assignment made; structure of I₂O₂ is similar to I₂O₃</td>
</tr>
<tr>
<td>75ION</td>
<td>OIO₂ (IO⁻ IO₂⁻)</td>
<td>ν₁ ν₂ 622 s 408 825 w</td>
<td>ν₃ 578 s 783 s ν₄ 745 s</td>
<td>Infrared spectra, partial Raman spectra; &quot;vibrational frequency stretching of solid state from 900–550 cm⁻¹ but no assignment made; structure of I₂O₂ is similar to I₂O₃</td>
</tr>
<tr>
<td>76DAL/CAR</td>
<td>OIO₂ (IO⁻ IO₂⁻)</td>
<td>ν₁ ν₂ 622 s 408 825 w</td>
<td>ν₃ 578 s 783 s ν₄ 745 s</td>
<td>Infrared spectra, partial Raman spectra; &quot;vibrational frequency stretching of solid state from 900–550 cm⁻¹ but no assignment made; structure of I₂O₂ is similar to I₂O₃</td>
</tr>
</tbody>
</table>
## Table 5. (Continued.)

<table>
<thead>
<tr>
<th>Source</th>
<th>Structure</th>
<th>Bond distance X-Y (Å)</th>
<th>Vibrational frequencies</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>81ELWOL</td>
<td>Centrosymmetric O=I-O=IO₂</td>
<td>*</td>
<td></td>
<td>Infrared and Raman spectroscopy of crystal; 5 infrared and 3 Raman bands were observed between 830 and 735 cm⁻¹ for I=O stretch, and 9 infrared and 6 Raman bands between 670 and 400 cm⁻¹ are possible for I-O stretch but no assignments are made; discussion of structural models; partial force constants given</td>
</tr>
<tr>
<td>87LEH/CHR</td>
<td>(P2₁/c) space group</td>
<td>v₁, v₂</td>
<td>804, 835</td>
<td>Nuclear quadrupole data</td>
</tr>
<tr>
<td>55KOJ/TSU</td>
<td></td>
<td>v₁, v₃</td>
<td>804, 355</td>
<td>Infrared absorption spectra with rapid dissociation and sublimation at 410°; vibrational frequencies are based on earlier interpretations</td>
</tr>
<tr>
<td>57DULV</td>
<td></td>
<td>v₁, v₂</td>
<td>804, 355</td>
<td>Absorption spectra; redefinition of structure is symmetrical</td>
</tr>
<tr>
<td>60DULV/LEC</td>
<td></td>
<td>v₁ sym., v₂ asym.</td>
<td>804, 355</td>
<td>*712; *supplementary bands are due to the existence of the acid function</td>
</tr>
<tr>
<td>61SEL/KJE</td>
<td>Two IO₃ pyramids</td>
<td>Intramolecular</td>
<td></td>
<td>Monoclinic crystal structure studies of crystalline compound; authors disagree with 60DULV/LEC C₂ᵥ symmetry attributed to I₂O₅</td>
</tr>
<tr>
<td>73SEM/MOS</td>
<td>Crystal symmetry</td>
<td>v₃</td>
<td>355</td>
<td>X-ray spectrum of solid I₂O₅</td>
</tr>
<tr>
<td>76DUL/CE</td>
<td>I-O-I</td>
<td></td>
<td></td>
<td>Infrared spectra, partial Raman spectra; *bond length—see 70SEL/KJE</td>
</tr>
<tr>
<td>81ELWOL</td>
<td>(quasi-)monomeric IO₂</td>
<td>v₁</td>
<td>804</td>
<td>Infrared and Raman spectroscopy of crystal; *I=O-I stretch vibrations of bands 610–400 cm⁻¹, 12 infrared bands observed between 850 and 670 cm⁻¹ attributed to I=O stretch, four I=O-I bending modes attributed to bands around 100 cm⁻¹ but no assignment made; discussion of structural models; partial force constants given</td>
</tr>
<tr>
<td>I₂O₅</td>
<td></td>
<td>v₁</td>
<td></td>
<td>Existence of I₂O₅ is confirmed, according to Raman spectra and vibrational frequencies; diamagnetism proves mixed valence iodine; the compound is described as an iodyl periodate</td>
</tr>
<tr>
<td>78MSE/WIE</td>
<td>IO₂=IO₅</td>
<td>v₁</td>
<td></td>
<td>*Raman spectra of amorphous solid at room temperature observed and tentative assignments made: strong Raman bands at 800 cm⁻¹ attributed to I=O stretch, bands in frequency range 400–500 cm⁻¹ attributed to I-O-I stretch, and the band at 692 cm⁻¹ is assigned to O–I=O symmetric stretch; confirms I₂O₅ existence</td>
</tr>
</tbody>
</table>

**6. NIST-JANAF Thermochemical Tables**

NIST–JANAF Thermochemical Tables for IO(g) (Sec. 6.1), OIO(g) (Sec. 6.2), IOO(g) (Sec. 6.3), IO3(g) (Sec. 6.4), IOI(g) (Sec. 6.5), and IIO(g) (Sec. 6.6) are presented on the following pages.
Enthalpy of Formation
The dissociation energy has been determined in the flame photometry, Phillips and Ramsay measured the intensity of the (0,0) band of IO at 2900 cm
-1 to give a new value for the enthalpy of formation $\Delta H^\circ (-1)$ = 21557.81 cm
-1.

Additional data needed for the calculations presented here, e.g. thermal functions for I(g), I2 (g), Au(g) and O(g), are taken from JANAF Thermochemical Tables. A recent photoionization study of Phillips and Durie and Huie and Hersch all adopted an enthalpy of formation based on the kinetic studies of Rudolph et al., $\Delta H^\circ (-1)$ = 226 ± 13 kJ·mol
-1 and Bassi et al., $\Delta H^\circ (-1)$ = 210 ± 81 kJ·mol
-1.

Recent determinations of the dissociation energy for IO in the IO, I2 and I2 systems are in agreement with the arguments of Huie, Herron and Laszlo we adopt the 21557.81 cm
-1 value for the enthalpy of formation of IO and use the enthalpy of formation of I and I2 to give an estimate for the enthalpy of formation of I2. The dissociation energy for IO, $\Delta H^\circ (-1)$ = 145 kJ·mol
-1 is used to calculate the temperature dependence of the equilibrium constant for the dissociation of IO and I2.

The dissociation energy for IO is calculated from the observed values of $\Delta H^\circ (-1)$ = 21557.81 cm
-1 used. We use the enthalpies of formation for I(g), I2 and I2 to give an estimate of the heat of formation for IO and use this to calculate the heat of formation for IO at 298 K.

The heat of formation of IO is calculated from the observed values of $\Delta H^\circ (-1)$ = 21557.81 cm
-1 used. We use the enthalpies of formation for I(g), I2 and I2 to give an estimate of the heat of formation for IO and use this to calculate the heat of formation for IO at 298 K.

The heat of formation of IO is calculated from the observed values of $\Delta H^\circ (-1)$ = 21557.81 cm
-1 used. We use the enthalpies of formation for I(g), I2 and I2 to give an estimate of the heat of formation for IO and use this to calculate the heat of formation for IO at 298 K.

The heat of formation of IO is calculated from the observed values of $\Delta H^\circ (-1)$ = 21557.81 cm
-1 used. We use the enthalpies of formation for I(g), I2 and I2 to give an estimate of the heat of formation for IO and use this to calculate the heat of formation for IO at 298 K.
Iodine oxide (OIO)

Ideal Gas

\[ M = 158.90327 \]

**Electronic Level and Quantum Weight state**

- \[ \text{Electronic state } n \text{, cm}^{-1} \]
- \[ X^3B_2 \]
- \[ 0.0 \]
- \[ 2 \]

**Vibrational Frequencies and Degeneracies**

- \[ \text{v, cm}^{-1} \]
- \[ \text{g} \]

- \[ 765(1) \]
- \[ 1921(1) \]
- \[ 800(1) \]

- \[ \sigma = 2 \]

**Product of the Moments of Inertia**

- \[ \text{IP} = 0.25 	imes 10^{-11} \text{g} \cdot \text{cm}^2 \]

**Enthalpy of Formation**

For the system O\(\text{IO}(g)\) where X = F, Cl, Br, I, there are only reliable experimental data for O\(\text{IO}(g)\). Assuming that the values O\(\text{IO}(g)\) and \(\Delta_\text{H}^\circ(\text{IO},g)\) are reasonable, we adopt the ratio of the numbers (1.94) to apply for a similar relationship between IO\(\text{(g)}\) and O\(\text{IO}(g)\). Thus, \(\Delta_\text{H}^\circ(\text{IO},g) = 1.94 \Delta_\text{H}^\circ(\text{IO},g) = 438 \text{kJ} \cdot \text{mol}^{-1} \)

**Heat Capacity and Entropy**

Based on the ESR study by Blyberg, the ground state of the free IO molecule belongs to the representation \(B_2\) of the point group \(C_\infty\). This symmetry, best molecule is estimated to have an 0-0-0 angle of 112°8 and a bond length of 1.8 A in analogy with the corresponding fluorine, chlorine, and bromine oxide molecules. The principal moments of inertia in g cm\(^2\) are: \(I_1 = 3.43 \times 10^{-20}, I_2 = 1.26 \times 10^{-17}, I_3 = 16.59 \times 10^{-17}\).

- Two of the three vibrational frequencies have been derived by Giles et al. Using photodetachment spectroscopic techniques. \(\nu\) is estimated based on anticipated trends with the \(\text{OIO}(g)\) family and assuming \(\nu = \beta\).

**References**

Iodine oxide (IO) Ideal Gas

$$S'(298.15K) = [296.4 \pm 4] \text{J K}^{-1} \text{mol}^{-1}$$

$$\Delta_f^{\text{r}}(0K) = [119 \pm 40] \text{kJ mol}^{-1}$$

$$\Delta_f^{\text{r}}(298.15K) = [116.5 \pm 40] \text{kJ mol}^{-1}$$

Electronic Level and Quantum Weight


Vibrational Frequencies and Degeneracies $v (\text{cm}^{-1})$

| Product of the Moments of Inertia: $I_{dO} = [1134.2931 \times 10^{-18}] \text{g cm}^2$ |

Enthalpy of Formation

Following trends is the reaction $\text{XOO}(g) \rightarrow \text{X}(g) + \text{O}(g)$, a reasonable estimate for the iodine reaction would be 470 $\text{kJ mol}^{-1}$ which yields $\Delta_f^{\text{r}}(0K) = -91.25 \text{kJ mol}^{-1}$. However, looking at the trends in the reaction $\text{XO}(g) \rightarrow \text{X}(g) + \text{O}(g)$, a reasonable estimate for the iodine reaction would be 260 $\text{kJ mol}^{-1}$ which leads to a $\Delta_f^{\text{r}}(0K) = -119 \text{kJ mol}^{-1}$. This large discrepancy in estimates is a result of the estimates and uncertainties in all X-O enthalpies of formation. We adopt the value based on the trend involving an X-O bond breakage. 

Heat Capacity and Entropy

The vibrational frequencies and strengths are estimated based on the existing data for $\text{FOO}(g)$, $\text{CIOO}(g)$, and $\text{BrOO}(g)$. The principal moments of inertia in g cm$^2$ are: $\lambda_1 = 1331.9 \times 10^{-24}$, $\lambda_2 = 3.4021 \times 10^{-24}$, and $\lambda_3 = 5.4512 \times 10^{-24}$. 

References

1NIST-JANAF Thermochemical Tables: FOO(g), 1995; CIOO(g), 1996; BrOO(g), 1996.
Iodine oxide (IO₂)

**Ideal Gas**

\[ M_r = 174.90267 \]

\[ \Delta H_f(0 K) = (248 \pm 50) \text{kJ/mol} \cdot 1 \]

\[ \Delta H_f(298.15 K) = (241.9 \pm 55) \text{kJ/mol} \cdot 1 \]

<table>
<thead>
<tr>
<th>Electronic Level and Quantum Weight state</th>
<th>( g )</th>
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<tbody>
<tr>
<td>( \Delta \epsilon )</td>
<td>0</td>
</tr>
</tbody>
</table>

Vibrational Frequencies and Degeneracies \( \nu, \text{ cm}^{-1} \):

\[
\begin{align*}
\nu(\text{cm}^{-1}) & \quad \text{MHz} \\
780.1(1) & \quad 0 \#
\end{align*}
\]

Point Group: \( C_2 \)

Bond Distance: \( r_{\text{IO}} = 1.79 \AA \)

Bond Angle: \( \theta_{\text{I-O}} = 89 \degree \)

Product of the Moments of Inertia: \( I_{\text{IO}}/M_r = 5642.359 \times 10^{-44} \text{g} \cdot \text{cm}^2 \)

**Enthalpy of Formation**

The enthalpy of formation value which is based on an assumed relationship of \( \Delta H_f(0 K) = 3.05 D(\text{IO}_2) \).

As an entropy of formation value has been reported by Farkas and Klein. This value, \( -98 \text{ kcal mol}^{-1} \) \((-127 \text{ kJ mol}^{-1}) \), is derived from absorption spectra measurements of iodate ions in solutions. There is considerable uncertainty in this value, both in terms of the experimental measurements and the fact that the authors have interchanged \( \text{IO}_3^- \) and \( \text{IO}_4^- \). This corresponds to an average bond energy of 241.9 kJ/mol. Since this value is greater than 250 kJ/mol, it is suspect.

**Heat Capacity and Entropy**

The structure of this molecule is estimated to be pyramidal with \( \theta_{\text{I-O}} = 89 \degree \) and a bond length of 1.79 \AA\ in analogy with the corresponding chlorine and bromine oxide molecules. Venkateswara and Sundaram, Venkateswara and Rajalakshmi, Rao and Sastham, Rao, and Dhoopnanaa and Mohan assumed the same structure and bond angle for \( \text{IO}_3^- \), \( \text{IO}_4^- \), and \( \text{IO}_5^- \). Using Badger's rule, the authors examined the relationship between the vibrational frequencies and force constants for the three pyramidal molecules \( \text{ClO}_3^- \), \( \text{BrO}_3^- \), and \( \text{IO}_3^- \). Although these authors refer to early measurements of the vibrational frequencies, the values appear to be in part of those of the iodates. Their reported values are adopted here although we treat them as estimated values. The vibrational frequencies are derived from the force constants which describe the other halogen oxide molecules. The principal moments of inertia in g.cm² are: \( \alpha = 14.765 \times 10^{-44} \), \( \beta = 14.760 \times 10^{-44} \), and \( \gamma = 16.720 \times 10^{-44} \).

**References**


**David M. Chase**
Iodine oxide (IO)  
\[ \Delta H^\circ(10 \text{ K}) = 348 \pm 2 \text{ kJ mol}^{-1} \]
\[ S^{\circ}(298.15 \text{ K}) = 330.1 \pm 4 \text{ J K}^{-1} \text{ mol}^{-1} \]

### Ideal Gas

Electronic Level and Quantum Weight

- \[ \ell \ellA \]
- \[ \ell \ell \ellA \]
- \[ \ell \ell \ell \ellA \]

### Vibrational Frequencies and Degeneracies

- \[ \nu \text{ cm}^{-1} \]
- \[ \nu \text{ cm}^{-1} \]
- \[ \nu \text{ cm}^{-1} \]

\[ \text{Point Group: } \text{C}_2h \]
\[ \text{Bond Distance: } \text{I-O} = [2.0] \AA \]
\[ \text{Bond Angle: } \text{I-O-I} = [115] \]

Product of the Moments of Inertia: \[ I_{\text{tot}} = 4.2498.6720 \times 10^{-11} \text{ kg m}^2 \]

### Enthalpy of Formation

For the series XOX(g) (where X = F, Cl, Br, I), there are only reliable experimental data for ClOCl(g). Assuming that the values \( E(X) \) and \( \Delta H^\circ(X\text{Cl}) \) are reasonable, we adopt the ratio of the numbers (1.52) to apply for a similar relationship between IO(g) and ICl(g). The ratio for the corresponding bromine oxides is approximately 1.6.

### Heat Capacity and Entropy

The structure of this molecule is estimated to be bent with a 1-O-I angle of [115] and a bond length of [2.0] \AA in analogy with the corresponding fluoro, chloro, and bromine oxide molecules. The principal moments of inertia in g cm\(^2\) are \( I_x = 2.8860 \times 10^{-42} \text{ kg m}^2 \), \( I_y = 1.9913 \times 10^{-43} \text{ kg m}^2 \), and \( I_z = 1.7803 \times 10^{-43} \text{ kg m}^2 \). The vibrational frequencies are estimated from known frequencies of FOF(g), ClOCl(g), and BrOBr(g) and expected trends in this halogen oxide family.

### References

### Enthalpy of Formation

For the four halogen oxide species, XXO(g) where X = F, Cl, Br, I, there are no experimental data related to the enthalpy of formation. Thus the enthalpy of formation is estimated based on assumption that the X−XX bond in XXO(g) is 0.6 kcal mol⁻¹. This leads to a ΔH°(0 K) = −110.5 kcal mol⁻¹, which is closer to the enthalpy of formation of CICIO, which is −133.1 kcal mol⁻¹.

### Heat Capacity and Entropy

The structure of this molecule is estimated to be bent with a θ−XX angle of 125° and bond distances r(XX) = 1.29 Å and r(XX) = 1.30 Å. This structure is estimated in analogy with the corresponding chlorine and bromine molecules. The vibrational frequencies are estimated from the known frequencies of ClXX and BrXX. The principal moments of inertia in g cm⁻² are: Iₐ = 3.51 × 10⁻¹⁰, Iₐ = 115.54 × 10⁻¹⁰, and Iₐ = 174.48 × 10⁻¹⁰.

### References

1. NIST-JANAF Thermochemical Tables, CRC10(g), March 1996; BrBrO(g): March 1996.
7. Conclusions

Of the iodine oxides mentioned in the literature, only five have been isolated and (at least, partially) characterized: \( \text{IO(g)}, \text{OIO(g)}, \text{I}_2\text{O}_4(\text{cr}), \text{I}_2\text{O}_5(\text{cr}) \). Only early studies mention \( \text{I}_2\text{O}_3 \) and \( \text{I}_2\text{O}_6 \); it would appear that these species do not exist. \( \text{IO}_2 \) and \( \text{OIO}_2 \) are proposed as intermediates in solutions or crystalline environments, with only an absorption maximum as a characterization. The other species are proposed to exist but there are no definitive studies as to their isolation and characterization.

In Table 6, a summary of the recommended thermodynamic properties at ambient conditions for six gaseous iodine oxides (\( \text{IO}, \text{OIO}, \text{IOO}, \text{IO}_1, \text{IO}_2 \)) are given. Even though there is a severe lack of experimental or calculational data for these six iodine oxides, tables are being generated for these species to match the corresponding fluorine, chlorine, and bromine oxides. The brackets indicate estimated values. The recommended values contain significant uncertainties. In all cases, experimental enthalpy of formation data are needed. However, the prime effort should be directed at confirming the dissociation energy of \( \text{IO(g)} \) and determining the enthalpy of formation of \( \text{IOO(g)} \). Further efforts should be directed towards establishing the enthalpy of formation for the remaining four gaseous species. For any of the polyatomic gaseous species (except \( \text{IO} \)), spectroscopic measurements for the geometry and vibrational frequencies would greatly reduce the uncertainties in the resulting thermal functions. For \( \text{OIO(g)} \), two of the three vibrational frequencies have been observed experimentally.

<table>
<thead>
<tr>
<th>Table 6. Thermodynamic properties of the iodine oxides</th>
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<tbody>
<tr>
<td>Compound</td>
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<tr>
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</tr>
<tr>
<td>IO(g)</td>
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<tr>
<td>OIO(g)</td>
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<td>IOO(g)</td>
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<td>IO(g)</td>
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<td>IO(g)</td>
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<tr>
<td>IO(g)</td>
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</table>

The main thrust in this study of the iodine oxygen system is to verify the existence of the various iodine oxygen species and to obtain spectroscopic data for them. Additional confirmation is needed as to the existence of the condensed phases, although this is a much lower priority. There seems to be little demand for heat capacity and enthalpy measurements at this time.

Note added. After this article was accepted for publication, two additional references on the dissociation energy of \( \text{IO(g)} \) were brought to our attention:

\[ \Delta H(\text{IO}) = 234±5 \text{ kJ mol}^{-1}; \Delta R(\text{IO}) = 120±5 \text{ kJ mol}^{-1} \]


\[ \Delta H^\circ(\text{IO}) = 219±4 \text{ kJ mol}^{-1}; \Delta R^\circ(\text{IO}) = 135±4 \text{ kJ mol}^{-1} \]


8. Acknowledgments

This work was undertaken as part of a larger study to provide JANAF Thermochemical Tables for as many halogen oxide species as possible. This particular study for the iodine oxides was supported by the Standard Reference Data Program at the U.S. National Institute of Standards and Technology.

The author is particularly grateful for the help of Sabina Crisen, who confirmed the completeness of the annotated bibliographies, created the numerous tables which summarize the reported experimental studies, and obtained copies of the pertinent articles. The contribution of Stanley Abramowitz in discussions on the spectroscopic properties of the triatomic molecules is greatly appreciated; appreciation is also extended to R. B. Klemm (Brookhaven National Laboratory) and A. R. Ravishankara (NOAA) for information pertaining to the enthalpy of formation of IO. Appreciation is also extended to Karl Irikura (NIST) for providing us with a calculated value for the dissociation energy of IO and providing comments on the text. The IO thermal function calculations were performed by David Neumann.

9. References—Annotated Bibliography

The following articles are a combination of all references dealing with the iodine oxides. Where possible, we have tried to include all authors, title, journal, a citation to Chemical Abstracts, and an annotation indicating the type of study. In general, dissertations (especially non-U.S.) have not been obtained and read.

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1882THO J. Thomsen, Thermochromische Untersuchungen Barth, Leipzig (1882–1886); heat of formation.


07BER M. Berthelot, “On the chemical action of radium,” Ann. 351, 504 (1907); CA 1 2214(6): decomposition by radium.

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NIST–JANAF THERMOCHEMICAL TABLES FOR THE IODINE OXIDES

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**NIST-JANAF THERMOCHEMICAL TABLES FOR THE IODINE OXIDES**

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