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# NATIONAL BUREAU OF STANDARDS REPORT

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## THERMODYNAMIC DATA FOR INDUSTRIAL INCINERATORS

Thermochemistry Section  
Physical Chemistry Division  
Institute for Materials Research  
for  
Office of Standard Reference Data



U.S. DEPARTMENT OF COMMERCE  
NATIONAL BUREAU OF STANDARDS

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# NATIONAL BUREAU OF STANDARDS REPORT

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### THERMODYNAMIC DATA FOR INDUSTRIAL INCINERATORS with Guides to the Use of the Tables

By  
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and  
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Final Technical Report  
to  
American Society of Mechanical Engineers  
Research Committee on Industrial Wastes

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## Part II. The Scientific Approach

### Thermodynamic Data for Industrial Incinerators with Guides for the Use of the Tables

#### 20.0 Preface

##### 20.1 Introduction

Maintenance of a high-quality clean environment in our current technological civilization has many facets; however, there is no question that effective disposal of waste materials is a primary factor in achieving this desirable goal. The neglect of this perennial, necessary, housekeeping chore would lead to accumulation of discarded materials in a way that could not be ignored for reasons of health, safety, efficient performance of activities, and aesthetic impact. The means of accomplishing the disposal of waste have varied with the state of development of our civilization and technology and in the most primitive procedures consisted of dumping or dispersal on land, into oceans and lakes, into rivers, or into the atmosphere.

More sophisticated techniques consist of chemical or physical processing to modify the form of the wastes and then dumping as before. Still more sophisticated techniques include chemical or physical processing as before, but modified or selected to achieve a goal of partial or complete re-use of the waste materials.

The initial cost and effort of devising ways to carry out methods of disposal increased rapidly with their increasing degree of sophistication. As a result, mostly for economic reasons, the least sophisticated

and most direct means are usually used. Satisfactory and optimum technological procedures for the more sophisticated means of disposal have not been developed yet for many forms of waste.

Among the chemical processing techniques of moderate sophistication incineration ranks as an important and widely used device for converting wastes to less undesirable forms before dumping or dispersal. Incineration is applicable to gaseous, liquid, or solid wastes. It reduces the residual bulk of many solid or liquid wastes, converts most organic materials into gases which are already part of the natural atmosphere and can be released directly into it, generates heat which can be used in some instances, uses readily available oxygen or air as its principal chemical agent, causes chemical processes that are comparatively well understood, and is readily carried out rapidly on large quantities of materials in apparatus of comparatively simple design.

Disadvantages of incineration are its generation of some noxious or toxic gases, smoke, and other atmospheric pollutants unless specially designed equipment is used, and the low economic value of the products of combustion. The generation of atmospheric pollutants can be largely controlled by proper design of the incineration apparatus or by further processing of the effluent gases before emitting them to the atmosphere. The ultimate limitation on the usefulness of incineration as a waste disposal technique (with respect to combustible substances) is probably going to be the implicit extravagance of its use.

Nevertheless, because of several advantages listed above, incineration as a waste disposal technique is going to be in use for a long time into the foreseeable future. As indicated above, the proper design

of incinerators is, therefore, environmentally and economically desirable, and, because of legal specifications on emission, may also be required.

The American Society of Mechanical Engineers (ASME) recognized this problem as of growing importance in the light of increasing professional and public awareness of the whole waste-disposal problem and its environmental implications. The ASME Research Committee on Industrial Wastes undertook to provide a guide to the design of industrial incinerators as an ASME publication. In collaboration with a task group of his committee, the National Bureau of Standards through the Office of Standard Reference Data (OSRD) has prepared this compilation of thermodynamic data on potential ingredients and products of combustion of industrial wastes. Some guides to the use of the data for computation of thermodynamic parameters associated with the incineration process are also given. The use of this type of data is essential in the calculation of incinerator design parameters for particular disposal problems.

Incineration will undoubtedly assume a well-defined place in the spectrum of methods available for waste disposal. The field at present is in a state of considerable innovation and flux; but also includes non-combustion chemical treatments, pyrolysis, and atomization. The data and the accompanying guides to their use will probably find application in these areas too because parameters of many of the processes involved can be calculated using the same input thermodynamic data.

## 20.2 Anticipated Needs for Thermodynamic Data

In the design of industrial waste disposal units, in particular--incinerators, the engineer has two major problems which must be solved

in an internally consistent way in order to obtain satisfactory performance. (a) The composition of the mix of input materials, which may consist in general terms of waste, added fuel, and combustion air or oxygen, must be understood and adjusted in such a way as to allow the requisite combustion processes to be carried out leading to known products. (b) The heat balance of the process based on energies of combustion (or other reaction) must be known at various stages of the process, in order to allow proper temperature control to be maintained. To meet these requirements there is need for a substantial body of thermochemical data for ingredients of waste, either as enthalpy of combustion or enthalpy of formation at room temperature, and need for some information on products of combustion at high temperatures such as their enthalpies of formation, heat capacities and Gibbs energies. These needs resemble in many ways those which have been met in the past few years for quantities of thermodynamic data on rather large numbers of substances as for example in the rocket propulsion program.

Looking at the waste disposal problem from another point of view one sees that the use of incinerators has two quite different aspects. In the first instance, mechanical engineers involved in incinerator design are faced with the problem of obtaining effective combustion and therefore must know the combustion performance of the materials they put into the incinerator in an approximate way. Under many existing circumstances a high degree of precision in the calculations is not required. However a secondary problem now is known and is likely to be of considerably more importance in the future. This is the control of noxious substances

emitted by the incinerator which tend to pollute the atmosphere. Because of the human factors involved in the exposure of the public to the emission products and because of federal, state, or municipal control mechanisms which are likely to be specified to limit pollution of the atmosphere, it will be very important ultimately to know the kind of substances that will be present in the products of combustion and to guarantee the upper limits of specified substances. In order to be able to estimate the combustion product concentrations with assurance we anticipate that considerably more accurate knowledge of the enthalpies of formation of the ingredients, and the enthalpies of formation and other thermodynamic properties of a much wider range of products will be required than are needed in the first instance.\*

To meet the requirements for thermodynamic data by engineers and designers, a handbook is needed which will provide (a) tables of thermodynamic data applicable to common problems of waste disposal by incineration and (b) guidance in the use of the tables and in obtaining supplementary information. The handbook may appropriately contain a discussion of the application of thermodynamic data to calculation of heat balances, and the effects of the composition of the input materials on the output composition; also, a discussion of the limitations of accuracy of the calculations, and the possible need for more elaborate analysis and more accurate data on input materials if output products must be closely controlled (as for pollution control).

The required tables are enthalpies of formation and Gibbs energies of as large as practical a number of potential input materials at 25°C,

and of potential incineration products at 25°C and elevated temperatures ranging to 2000°C or higher.

An important feature of the presentation of technical data should be a format suitable for engineering use, and rather detailed guidance as to use of the data. In addition, as it is not practicable to include available thermodynamic data on all substances, nor do data exist on all substances that are potentially of interest, it is important to provide two specific supplements to the thermodynamic data: (a) bibliographic references to reliable and extensive collections of data on additional materials, (b) selected lists of methods of estimation of the properties. A discussion of the merits of these referenced collections and methods of estimation will be helpful to the engineer.

### 20.3 Scope and Preparation of Tables

Following general lines of the discussion presented above, preparation of material for a handbook of thermodynamic data for industrial incinerator design and operation was undertaken.

As an initial step in limiting the coverage of substances to be included, a survey was made by Mr. Wayman L. Calhoun (Union Carbide Corp.) of the ASME Research Committee on Industrial Wastes. The persons queried were primarily members of the Subcommittee on Coordination with Associations and Government. The results of this survey in general indicated the following points:

- (a) A large fraction of the industrial waste to be disposed of consists of organic materials which fall generally into three categories:

- (1) pure substances, well defined
  - (2) organic materials of variable composition but resolvable into known components
  - (3) poorly defined mixtures
- (b) A smaller amount consists of inorganic materials. Among these, ingredients include essentially all the elements in small amounts and some, such as ferrous and non-ferrous metals, in relatively large amounts.

On the basis of this survey, the time and effort available, and the desire to have the tables available in a reasonably short time to enhance their early usefulness, the final plan for the tables was as follows:

Enthalpies of formation at 25°C (298.15K) were agreed to be of primary importance. Tables of thermodynamic functions of temperature are of less immediate importance as many of these are available in the extensive JANAF Thermochemical Tables and the computer tapes associated with them (See source 20, Section 22.0).

The scope of the substance coverage was established as follows:

- (a) Organic compounds. All organic substances for which experimental data are available, within the limits of time and effort available.
- (b) Organic materials (not well characterized). Limited to polymeric substances to which a reasonably good formula can be attributed.
- (c) Inorganic compounds. Inorganic oxides, only.

The decision not to list poorly defined materials was made deliberately because of the open-ended nature of the list, the lack of carefully screened sources of data, and the possibility of approximating combustion values from data on related pure substances. The alternative decision was made to include all polymers for which data could be found, as polymeric substances were prominent among the large volume waste products.

For the above three classes of substances enthalpies of formation at 298.15K are provided in tables obtained as described below.

To prepare Table I, "Enthalpies of Formation of Organic Compounds at 298.15 K", advantage was taken of the fact that in the Chemical Thermodynamics Data Center a comprehensive monograph is in preparation for the OSRD. Files of compounds for which enthalpies of combustion have been determined now comprise about 4000 compounds. The data on these have not all been evaluated. The tabulated list, therefore, comprises the 1000 compounds for which work had been completed. The selection of these compounds was made on the basis of (a) important functional groups and, (b) importance of the compound. The selection of appropriate substances was aided by the fact that a recent previous review had been made for NASA in which compounds of primary interest in biology and biochemistry had been selected for early evaluation.

In the selection of values for enthalpies of formation, the data were derived from measured values of enthalpies of combustion, usually performed by bomb calorimetry. The measurements had been made, in some cases, over a period of a hundred years, and hence were of very non-

uniform quality. The data for each substance were evaluated and updated according to uniform criteria, which are described by Domalski (source 4, Section 22.0). They represent the best values that can be derived from existing data.

Because of the prospective repetition of needs to tabulate organic compounds with their enthalpies of formation and other data, a permanent, machine-readable file was organized during the course of this work. The final listing of compounds which forms Table I was prepared from this file.

To prepare Table II, "Enthalpies of Formation of Organic Polymers at 298.15 K", the Chemical Thermodynamics Data Center file of enthalpies of combustion of organic compounds was combed for relevant substances. Recent reviews of enthalpies of formation of organic polymers were also searched. All polymers were included for which reliable enthalpies of formation could be determined from their enthalpies of combustion. The final table comprises 39 polymers.

The values listed in Table II were arrived at in the same way as those in Table I; hence, they represent the best values available on the basis of existing experimental data.

To prepare Table III, "Enthalpies of Formation of Inorganic Oxides at 298.15 K", the recent set of NBS compilations of critically evaluated data on the thermodynamic properties of inorganic substances was the principal source. These tables (NBS Technical Note 270, D. D. Wagman, et al., 1965-1971 and continuing) are the most recent comprehensive critical evaluation on inorganic compounds, and have the title "Selected

Values of Chemical Thermodynamic Properties". Oxides for which enthalpies of formation were known to have been determined, but not yet found in completed sections of TN 270 were obtained principally from the JANAF tables. References to the sources of data are given appended to Table III.

Each of the sources listed above is a tabulation of values by competent reviewers who have devoted years of systematic study to the selection and evaluation of chemical thermodynamic data. The tabulations quoted in each case are authoritative and may be said to represent the best values available on the basis of existing experimental data. Only one or two estimated values have been included.

The prepared descriptive material consists of:

(a) general background of thermodynamic definitions and formulas necessary to an understanding of the discussion; (b) detailed discussion of the calculation of thermodynamic quantities at 298.15 K, using the material from the tables; (c) a brief general discussion of calculations involving elevated temperatures; (d) supplementary sources of thermodynamic data, and methods of estimation, and (e) an appendix giving auxiliary constants, symbols, and units of measurement.

#### 20.4 Status of Thermodynamic Data and Auxiliary Aids: Recommendations for Further Action

Listed below are the stronger impressions obtained concerning needs for information as compared with its availability and completeness. A few recommendations are made for action to alleviate some deficiencies or fill certain needs.

1. A large category of ingredients for incinerator processes was found to be "poorly characterized materials": materials which by dint of some effort could be resolved into well defined substances, and materials for which this might not even be possible. These materials are not included in the tables for the handbook. However, the practical incinerator process manager is going to need information to allow him to make ad-hoc decisions. This information can take the form of (a) tables of classes of ingredients of typical poorly characterized materials, together with appropriate elemental composition and enthalpies of combustion or a pseudo-enthalpies of formation; (b) tables of enthalpies of combustion or pseudo-enthalpies of formation of well known classes of materials for which only average values can be cited. Such materials as coal, hard-woods, soft-woods, petroleum oils, fall in this category. The accuracy of the enthalpy values may not be high, but the elemental composition and a pseudo-enthalpy of formation would allow such materials to be fed into computer programs for calculating high temperature equilibria as well as any well-defined substance. Only the products of combustion enter the final equilibria, and their proportions will be fixed by the proportions of the elements and parameters independent of the nature of the combustible material.

2. In reviewing the reactions for possible combustion reactions involving water and various volatile acids, it became apparent that conditions of operation of an incinerator (for example: using scrubbing water on effluent gases) can be readily envisioned which will require vapor-liquid equilibria of a few volatile acid-water solutions. The

relevant data include such parameters as partial pressures of HCl and H<sub>2</sub>O as functions of temperature and mole ratios for solutions of HCl in water. Other acid gases such as HF, SO<sub>2</sub>, SO<sub>3</sub>, P<sub>4</sub>O<sub>10</sub>, N<sub>2</sub>O<sub>5</sub> also enter such equilibria. Satisfactory data for these equilibria probably exist, but could not be organized within the scope of this project.

The number of organic substances for which enthalpies of combustion are known is much larger than those tabulated. The critical review of the data is proceeding rapidly, and a much longer list will be available in perhaps two years. The list given as Table I could then be augmented.

A serious deficiency exists in the availability of experimental enthalpies of combustion (and formation) of organic polymers. This is made quite obvious by the availability of reliable combustion data for only 39 out of the multitude of polymers in large scale industrial use. More experimental values are needed on these large-volume chemicals, to provide additional data for an augmented Table II. There are also other important uses for such data.

#### 20.5 Collaborative Arrangements

As the administrators of the National Standard Reference Data System (NSRDS), the Office of Standard Reference Data (OSRD) at NBS (Dr. D. R. Lide, Director) agreed to provide the handbook materials to ASME for its Research Committee on Industrial Wastes (E. S. Monroe, Chairman). The working organization within NBS which was assigned by OSRD to carry out the project was the Thermochemistry Section of the Physical Chemistry Division, Institute for Materials Research. Dr. George T. Armstrong and Dr. Eugene S. Domalski carried out the work,

using the resources of the Chemical Thermodynamics Data Center (Mr. D. D. Wagman, Manager), which is organizationally located in the Thermochemistry Section.

The organization of the work was planned by Mr. E. S. Monroe (E. I. du Pont de Nemours and Company, Inc.), Mr. R. A. Conway (Union Carbide Corp.), Mr. W. L. Calhoun (Union Carbide Corp.) and Dr. S. R. Beitler (Director of Research, A.S.M.E.) all representing the A.S.M.E., and by Dr. H. J. White, (OSRD), Dr. George T. Armstrong, Chief, Thermochemistry Section, Dr. C. W. Beckett, Physical Chemistry Division Office, and Dr. David Garvin, Coordinator of Data Programs for the Physical Chemistry Division Office. During the early part of 1971, after the project was started, Mr. F. H. Small (Union Carbide Corp.) replaced Mr. Conway.

During the course of the work, continuing guidance was received from the ASME Research Committee on Industrial Wastes. Assistance from the staff of the Chemical Thermodynamics Data Center, in particular Mrs. J. J. Grimes and Miss B. Beckwith is acknowledged, in setting up a mechanism for information storage and retrieval of enthalpies of formation of organic compounds, and from Mr. J. I. Minor of the Thermochemistry Section in processing the data files.

## 21.0 Discussion and Aids for the Use of the Tables

### 21.1 Processes Occurring in Incinerator Combustion

Thermochemical and thermodynamic data have well defined applications in the analysis of incinerator processes and in the design of incinerators. The energy released during the combustion process appears as heat. This heat causes the gases formed in the reaction to be hot, and the non-volatile materials to form hot ash, cinders, or molten refractory materials. It may be carried away in hot effluent gases or by conduction through the walls. The heat must be under control in that the incinerator must be designed to withstand it, and possibly, by heat exchangers, to make use of it in an auxiliary operation. This heat may be used to volatilize non-combustible substances in the ingredients, such as water, which needs only to be volatilized in order to make it an acceptable effluent into the atmosphere. Under any circumstances the heat will be carried away from the reaction zone; and the mechanism by which this is to be done is an important part of the incinerator design. The reaction processes may require supplementary heat or possibly damping in order to make the combustion complete or to provide gaseous or solid products as appropriate at the end of the process. Information required for the calculation of these processes are the nature of the ingredients and products, and the values of their enthalpies of formation, heat capacities or enthalpies of the products as functions of temperature.

The heat of the reaction may cause some of the products formed to be partially or completely dissociated. The temperature to which the effluent gases and the residues are heated, and the nature of the products found in them are determined to a large extent by the dissociation equilibria and other equilibria that can occur as a result of interactions between the products of combustion. The proportions of materials present in the products are strongly dependent upon the equilibrium constants of the various possible reactions. The important thermodynamic data here are the Gibbs (free) energies of formation and the equilibrium constants of formation of the products of reaction at the possible temperatures. The occurrence of spontaneous reactions in a constant pressure system is governed by a decrease in Gibbs energy; and the equilibrium proportions of substances present are determined (as the equilibrium constant) from sums of the Gibbs energies of formation from the elements. Available data may be the Gibbs energy or it may be enthalpy and entropy data from which the Gibbs energy may be calculated. The equilibria are strongly temperature dependent; hence there are strong connections among the enthalpy of reaction, the heat capacities of the substances, heat retention in the incinerator, and the proportions of products that will be present following the reaction.

A third area of importance of the thermodynamic data is in the possible interaction of ingredients or products of combustion with the materials of construction of the incinerator. Here much more flexibility occurs. The materials to be burned may be relatively fixed before incinerator design is attempted, or on the other hand the variety of materials may be very great. The selection of materials of construction may depend upon knowledge of volatility or refractoriness of substances possibly to be formed by interaction of the hot incinerator gases with the walls.

Thermodynamic data applicable to the solution of some of these problems are discussed in the following parts of Section 21. This presentation and some general principles of their use is not an attempt to recommend methods for calculation of specific incinerator design parameters, but rather to provide a ready reference to the meaning and typical applications of thermodynamic data of special value in such applications.

## 21.2 Definitions of Thermodynamic Terms

21.2.1 Temperature. Temperature is a measure of the hotness of a system. Note: A system may be a given quantity of a single substance, or it may be a complex mixture or aggregate of material.

When analyzed in terms of the motions of the atoms or molecules constituting a material, the temperature is a measure of the

average kinetic energies of their random movement. Substances in a system and all parts of a system tend to approach the same temperature, and will attain the same temperature if disturbing processes are absent.

The temperature occurs as a parameter of importance in all heat transfer processes, in chemical reaction processes, and in the properties of materials and chemical substances.

All thermodynamic formulas and laws involving temperature with a basis in theory require temperature to be expressed in terms of the thermodynamic or absolute temperature scale. The internationally agreed version of the thermodynamic temperature scale is the International Practical Temperature Scale. The kelvin (symbol K) is the unit of temperature and the size of the kelvin is determined by defining the temperature of the triple point of water as 273.16 K. The freezing point of water (melting point under 1 atm pressure of air) is defined as 0.01 K below the triple point, hence the normal ice point is 273.15 K.

The ice point temperature is 0°C on the frequently used Celsius (centigrade) temperature scale. The size of the temperature units is the same on the Celsius and the thermodynamic scales. The relationship between the scales is expressed by the equation

$$t = T - 273.15$$

where  $t$  is the temperature ( $^{\circ}\text{C}$ ) on the Celsius scale, and  $T$  is the temperature (K) on the thermodynamic scale.

### 21.2.2 Energy of a System

Every physical system has associated with it a certain amount of energy which is variously described in terms of several state functions--internal energy, enthalpy, Gibbs energy, or Helmholtz energy--depending upon the use to which the information is to be put.

The energy of a system is an extensive parameter; that is, the amount of energy is proportional to the mass (kilograms) or the amount (moles) of each substance present.

Note: The unit of energy is the joule (symbol J), though values are commonly given also in calories (symbol cal) and, in engineering practice are sometimes given in British thermal units (symbol Btu). The amount of substance referred to in an equation is in terms of moles (symbol mol). In this handbook, unless otherwise specified, a tabulated enthalpy, or other thermodynamic quantity attributed to a particular substance is for a mole of that substance as described by its formula. The mass corresponding to a mole is found by taking the molecular weight in grams. The engineering unit pound mole (symbol lb-mol) is not used in this handbook. See Appendix section 25 for definitions of the units of measure and for relationships between the units.

### 21.2.3 State Function

State functions are any of several extensive thermodynamic functions, relating to the energy of a system, of which the values are uniquely defined for a given system when its state is defined. These include internal energy, enthalpy, Gibbs energy, Helmholz energy, entropy, and some functions derived from them. The state of a system is defined when

it is at equilibrium in a given physical state at a given temperature, and under a given set of external stresses, such as a given pressure. The important feature of a state function is that the value does not depend upon the path by which the specified state of the system is reached. Put in another way, the difference in value of a state function in two states of a system is independent of the path by which the system is changed from one state to the other.

It should be noted that all the state functions defined below are not required for direct use in incineration design. However, they need to be defined here, because of their uses in tabulation of thermal data (see Sec.21.3) in some of the auxiliary reference sources to be cited later.

#### 21.2.4 Internal Energy

A system is said to have internal energy (symbol  $U$ ) which changes as heat is added or removed, and work is done on or by the system. While the absolute value of the internal energy of a system is arbitrary, and unimportant for the purposes of thermodynamics, changes in internal energy can be measured. The equivalence of heat and work in their influence on the internal energy of a system is expressed by the equation

$$\Delta U = q + w$$

In the above equation,  $\Delta U$  represents a change in internal energy. An increase  $\Delta U$  in the internal energy of a system

may be caused by supplying an amount of heat,  $q$ , to the system and doing an amount of work,  $w$ , on the system. The two quantities,  $w$  and  $q$ , are not state functions, but depend on the path followed. They have the same energy units, may be applied simultaneously or sequentially, and may have any values relative to one another. The direction of heat and work transfer as denoted by their signs must be chosen in a consistent manner. There is no universally accepted convention as to the signs of heat and work energy supplied to a system, so care should be taken to note the convention used in any particular presentation.

The internal energy is a function of temperature, pressure, and other parameters, which has a characteristic value for a fixed amount of a particular substance in a defined state. Another common symbol for internal energy is  $E$ .

In a reaction carried out at constant volume the heat effect of the process measures a change  $\Delta U$  (or  $\Delta E$ ) in the substances. If heat is produced by the reaction (exothermic reaction) the change  $\Delta U$  is negative. An engineer examining combustion measurements made in a bomb calorimeter may find the data expressed as  $\Delta U$  or  $\Delta E$  as this is a constant volume process.

#### 21.2.5 Enthalpy

The enthalpy, sometimes called heat content, (symbol  $H$ ), of a system is a measure of its energy which differs from the

internal energy by the amount of work done by the system against the pressure of the surrounding medium. The enthalpy is defined by the following relationship

$$H = U + pV$$

in which  $U$  is the internal energy,  $p$  is the pressure of the surrounding medium, and  $V$  is the volume of the system. The enthalpy and the internal energy of a system are the same when the  $pV$  term is zero. This occurs only when (1) the system is a condensed phase and the external pressure is zero, or (2) when the system is an ideal gas at the absolute zero of temperature.

In a constant pressure process, (i.e. a process in which initial and final pressure are the same) the change in enthalpy is given by the following equation

$$\Delta H = \Delta U + p\Delta V$$

The change in enthalpy associated with a process is equal to the change in internal energy only when (1) the  $pV$  terms are all zero as above, or (2) when the volume of the products is the same as the volume of the reactants.

As in the case of internal energy, the absolute value of the enthalpy is arbitrary and only changes in enthalpy can be measured.

For processes occurring at constant pressure, such as combustion at normal atmospheric pressure, if the products are cooled to the starting temperature, the heat effect observed

is the enthalpy change  $\Delta H$ . For an exothermic reaction  $\Delta H$  is negative. See Section 21.5 for illustrations of calculations of  $\Delta U$  and  $\Delta H$ .

When two molecular species in a system react to form another molecular species, such as



and the reaction is exothermic ( $\Delta H$  is negative) we can say that the molecular arrangement of the products is more stable, or gives stronger bonds than those of the reactants. This excess energy released by forming the stronger bonds becomes available and may be released as heat. A decrease in internal energy, or enthalpy is a driving force which tends to cause a process to occur spontaneously (in order to arrive at a more stable state), but though it is a dominant effect, it is not sufficient in itself.

#### 21.2.6 Entropy

The entropy (symbol S) is a measure of the disorder or randomness in a system. Another way of putting it is that the entropy of a system is directly related to the number of states of existence available to it. If the number of states of existence for a collection of atoms is greater in one molecular configuration than in another configuration the entropy will also be greater. The difference in the entropy of liquid water and gaseous water may be used as an example. When water is condensed to liquid its

molecules have much less freedom of movement than when the water is a gas. The gas molecules have many more configurations available to them, and so at a given temperature the entropy of a given amount of water vapor is much greater than that of the same amount of water liquid.

Heating a body reversibly increases its entropy by an amount equal to the quantity of heat divided by the absolute temperature. Thus an infinitesimal amount of heat,  $\delta q$ , supplied reversibly increases the entropy of a body by  $d\delta$  where

$$d\delta = \frac{\delta q}{T}$$

For a given substance the kinetic, rotational, and vibrational movement of the molecules increases with temperature. The amount of disorder therefore increases with temperature and the entropy of a substance is greater at a high temperature than at a low temperature.

The tendency for entropy to increase is a driving force which causes processes to occur spontaneously, but is not sufficient in itself. It is usually not sufficient to overcome an opposing energy change and where it is sufficient we will have a spontaneous endothermic process. The entropy in any closed system tends to increase with time, with an ultimate maximum when equilibrium has been reached.

When reactions are carried out rapidly and under non-equilibrium conditions, hence irreversibly, as is the common practice in rapid combustion, the increase in entropy of the

whole system is always greater than that calculated for the reversible reaction.

### 21.2.7 Free Energy

See Gibbs Energy; see also Helmholtz Energy.

### 21.2.8 Free Energy Function

See Planck Function; see also Massieu Function

### 21.2.9 Helmholtz energy

The Helmholtz energy (symbol A) is a measure of the maximum work that can be done by a system. It is defined by the equation

$$A = U - TS$$

The change in Helmholtz energy that occurs in a process at constant temperature is given by the equation

$$\Delta A = \Delta U - T\Delta S$$

In an isothermal process, the maximum amount of work that can be done by a system is  $-\Delta A$ , the decrease in Helmholtz energy.

The Helmholtz energy is a valid measure of the tendency for a process to occur spontaneously. For a process occurring at constant temperature and constant volume, the necessary condition for the process to occur spontaneously is a decrease in the Helmholtz energy.

$$\Delta A < 0$$

For an isothermal process occurring at constant volume the necessary condition for equilibrium is that

$$dA = 0$$

The Helmholtz energy may be found referred to as Helmholtz free energy or Helmholtz function. It should not be confused with the Gibbs energy discussed below.

#### 21.2.10 Massieu Function

The Massieu function (symbol J) is the negative of Helmholtz energy divided by temperature ( $J = -A/T$ ). The Massieu function does not contain any new information not found in the Helmholtz energy; but it is a useful form for calculation of equilibrium processes at constant volume. The Massieu function is found less commonly tabulated than its Gibbs energy analog, the Planck function.

#### 21.2.11 Gibbs Energy

The Gibbs energy (symbol G) is a measure of the maximum work that can be done by a system. It is defined by the equations:

$$G = U + pV - TS = H - TS$$

The change in Gibbs energy that occurs in an isothermal process at constant pressure is:

$$\Delta G = \Delta U + p\Delta V - T\Delta S = \Delta H - T\Delta S$$

For the isothermal process, the maximum work other than expansion work that can be performed by a system is  $-\Delta G$ , the decrease in Gibbs energy.

The Gibbs energy is also a valid measure of the tendency for a reaction to occur spontaneously. For an isothermal

process subject to a constant pressure, the necessary condition for the process to occur spontaneously is a decrease in the Gibbs energy

$$\Delta G < 0$$

For an isothermal process subject to a constant pressure, the necessary condition for equilibrium is that

$$dG = 0$$

An important consequence of this condition is that the Gibbs energy provides one criterion for the maximum temperature reached in a combustion zone. At the temperature of the combustion zone the proportions of substances present will be governed by the fact that this isothermal Gibbs energy change will be zero for each possible reaction. That is each reaction will establish an equilibrium at that temperature. See Section 21.7 for discussion and an example.

The Gibbs energy is frequently found referred to as merely free energy, and any references to free energy without qualifying adjectives should be taken to mean Gibbs energy. It is also called Gibbs free energy or Gibbs function by some users.

#### 21.2.12 Planck Function

The Planck function (symbol Y) is the negative of Gibbs energy divided by temperature (-G/T). The Planck function does not contain any new information not found in the Gibbs energy; but it is a very useful form for calculation of

equilibrium processes at constant pressure. (See Section 23.3.2). The Planck function is more commonly referred to as free energy function. The terms fef or Gibbs energy function are also sometimes found referring to this function.

### 21.2.13 Heat Capacity

The heat capacity is the ratio of the energy supplied to the temperature change of a body. It may be an average heat capacity over a temperature range or the limiting ratio over an infinitesimal temperature change. If the system is maintained at constant pressure, the heat capacity,  $C_p$ , is the rate of change of enthalpy with temperature.

$$\left(\frac{\delta q}{\delta T}\right)_p = C_p = \left(\frac{\delta H}{\delta T}\right)_p$$

If the system is maintained at constant volume, the heat capacity,  $C_v$ , is the rate of change of internal energy with temperature

$$\left(\frac{\delta q}{\delta T}\right)_v = C_v = \left(\frac{\delta U}{\delta T}\right)_v$$

The heat capacity allows one to calculate temperature changes to be expected from liberation of specified amounts of heat, or the amount of heat needed to create a given temperature change.

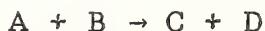
### 21.2.14 Enthalpy of Reaction (Heat of Reaction)

For a reaction that goes to completion, the enthalpy of reaction at constant temperature is the negative of the observed calorimetric heat when carried out at constant

pressure and with the products brought to the same temperature as the reactants. It could be logically considered to be the sum of the enthalpies of the products of reaction minus the sum of the enthalpies of the reactants.

This concept, however, leads to a practical difficulty. The enthalpies of individual substances are based on arbitrary scales and cannot be added or subtracted without adjustment. This adjustment is made by relating the enthalpy scales of various substances through their enthalpies of formation (heats of formation) (See Section 21.2.15). On this basis the enthalpy of reaction is the sum of the enthalpies of formation of the products minus the sum of the enthalpies of formation of the reactants. If the sum of the enthalpies of formation at the temperature of interest is less after the reaction than before, then the enthalpy of the system has been reduced and the excess enthalpy will have appeared as heat.

For reaction (1)



$$\Delta H_r = \Delta H_f[C] + \Delta H_f[D] - \Delta H_f[A] - \Delta H_f[B] \quad (1)$$

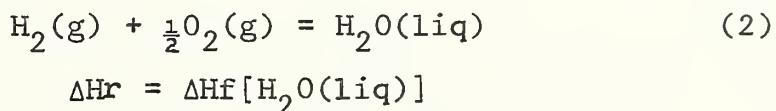
In the example,  $\Delta H_r$  is the enthalpy of reaction, and the other enthalpy terms are the enthalpies of formation of the substances contained in the brackets. A negative enthalpy of reaction means that the reaction is exothermic while a

positive enthalpy of reaction means that the reaction is endothermic.

#### 21.2.15 Enthalpy of Formation (Heat of Formation)

For the special case in which a single product is formed and the reactants are the elements in a standard reference state defined for each element, the enthalpy of reaction is called the enthalpy of formation, and has the symbol  $\Delta H_f$ .

For reaction (2)



$\Delta H_f$ , which has a characteristic set of values for any substance is a very important thermodynamic function. The enthalpy change occurring in any reaction can be calculated if the enthalpies of formation are known for all the substances participating as reactants or products. By convention the enthalpies of formation of the elements in their standard reference states are zero, at any temperature (see Section 21.2.16). An element not in its standard reference will, in general, have a non-zero enthalpy of formation. The standard reference state for hydrogen is the gas composed of molecules,  $\text{H}_2(\text{g})$ . On the other hand the gas consisting of hydrogen atoms  $\text{H}(\text{g})$  is not the standard reference state for hydrogen. Thus  $\Delta H_f^\circ[\text{H}(\text{g})]$  at 298K =  $52.04 \text{ kcal mol}^{-1}$  while  $\Delta H_f^\circ[\text{H}_2(\text{g})] = 0$ , at all temperatures.

### 21.2.16 Thermodynamic Standard States and Standard Reference States

The molal values of the internal energy, enthalpy, Gibbs energy, Helmholtz energy, entropy, heat capacity and enthalpy of formation are functions of the temperature. For simplicity and convenience the values that these thermodynamic properties have for particular substances are usually tabulated for the substances in their standard states (indicated by a superscript zero on the thermodynamic symbol as in  $\Delta H_f^\circ$ ,  $C_p^\circ$ , etc. The standard states are defined as follows: For a pure solid or liquid the standard state is the substance in the condensed phase under a pressure of one atmosphere. For a gas the standard state is the ideal gas at a pressure of one atmosphere. For the functions  $\Delta H_f$ ,  $\Delta G_f$ , and  $\log K_f$  the values tabulated usually represent the quantities appropriate for the reaction by which the substance is formed in its standard state from the elements in their standard reference states. The conventional notations in this case are  $\Delta H_f^\circ$ ,  $\Delta G_f^\circ$ ,  $\log K_f^\circ$ . For this purpose, in the usual case, the standard reference states of the elements are taken to be the molecular form and phase that are stable at one atm pressure at  $25^\circ\text{C}$  ( $298.15\text{ K}$ ). A few of the elements, oxygen, nitrogen, hydrogen, fluorine, and chlorine, are diatomic gases under these conditions. The inert gases (He, Ne, etc.) are monatomic gases. Bromine and mercury are liquids. For the solid elements the stable crystal phase at  $298.15\text{ K}$  is the

standard reference state. The single exception to this is phosphorus, for which white crystal phosphorus is used because the more stable forms have not been well characterized thermochemically. In the use of any tables other than those in this handbook, care should be taken to understand the standard states used for the elements, as there is some non-uniformity in this, particularly at temperatures different from 25°C.

### 21.3 Tabulated Thermal Functions

Tabulated values for the thermodynamic functions are given in terms of carefully defined observables that can be evaluated by experimental means or derived easily by unambiguous calculation from experimental and theoretical relationships. The functions discussed up to this point such as internal energy, enthalpy, Gibbs energy, Helmholtz energy, and entropy suffer from vagueness, particularly with respect to the energy base to which they are referred, but also in other ways. The tabulated thermal functions found in this handbook and in the references given in Section 22.0 are designed to avoid such vagueness. The same criteria are not used in every tabulation, however. It is important to note certain descriptive features of the terminology in order to distinguish the basis of the values in a particular set of tables. When differences in the function descriptions are

noted, in some cases they are unimportant for many calculations, but in other cases are very important. The principal distinctions that may be observed are given below, with some notes as to their importance in particular applications.

Because changes to achieve international uniformity have been made just recently, many tables which had been published present the thermal functions in terms of an older and still widely used system of notation. The principal identities are

$$E = U ; F = G$$

The symbols E and F represent the Lewis and Randall (Reference 14, Section 22.0) notations. U and G represent the IUPAC or IUPAP notation. Practically all earlier tables for Gibbs energy and various derivative functions of it published in the United States use the symbol F and the term free energy for Gibbs energy. The same tables usually use E for internal energy.

#### 21.3.1 Non-Standard-State vs. Standard-State Functions

The superscript zero is placed by a function to indicate that the substance is in the standard state. The presence of a superscript zero by a standard-state function and its absence by a non-standard-state function should be deliberate distinctions, though this is not always made clear in the presentation of a table. U as compared to  $U^\circ$ , H vs  $H^\circ$ , G vs  $G^\circ$ ,  $C_p$  vs  $C_p^\circ$  differ by amounts that are usually small for

liquids and solids near 1 atm pressure, because of their low compressibility. They become important at high pressures and in the region of the critical temperature. For gases the differences should not be ignored. In this case, the distinction is between the real gas and the ideal gas. For detailed energy balances the real gas state is preferable. Unfortunately real gas functions are unavailable for large numbers of substances. However, the steam tables (Section 22.0, References 2, 7, 8, 13), and the NBS Tables (Section 22.0, Reference 5) apply to real gases.

### 21.3.2 Different Temperatures for the Energy Base

Internal energy, enthalpy, Gibbs energy, Helmholtz energy, entropy, and certain derived functions are cumulative functions of temperature; and the numerical value given to them, therefore, represents an increment as the temperature of the substance is changed from some reference temperature. The commonly used reference temperatures are 0 K and 298.15 K (The subscript 298 is often used in referring to 298.15 K).

(a) The quantity tabulated for internal energy may be

$$U^\circ - U_0^\circ \text{ or } U^\circ - U_{298}^\circ$$

depending on the base of temperature used. These two quantities differ by a constant term:

$$(U^\circ - U_0^\circ) - (U^\circ - U_{298}^\circ) = (U_{298}^\circ - U_0^\circ)$$

The quantity  $(U_{298}^\circ - U_0^\circ)$  may be found tabulated occasionally.

(b) The quantity tabulated for the enthalpy may be

$$H^\circ - H_0^\circ \text{ or } H^\circ - H_{298}^\circ$$

depending on the base of the temperature used. These two quantities differ by a constant term:

$$(H^\circ - H_0^\circ) - (H^\circ - H_{298}^\circ) = H_{298}^\circ - H_0^\circ$$

The quantity  $(H_{298}^\circ - H_0^\circ)$  may be found in many tables.

(c) The quantity tabulated for entropy is usually

$$S^\circ \text{ or } S^\circ - S_{298}^\circ$$

The quantity  $S^\circ$ , rather than  $S^\circ - S_0^\circ$  is usually tabulated on the assumption that  $S_0^\circ$  can be exactly determined. It is usually zero, but may be a constant non-zero quantity. The difference between the above terms is  $S_{298}^\circ$ ; and this is found in many tables.

(d) The quantity tabulated for Gibbs energy is usually

$$G^\circ - H_0^\circ \text{ or } G^\circ - H_{298}^\circ$$

The base  $H_0^\circ$  instead of  $G_0^\circ$  is chosen because the relationship

$$G_T^\circ = H_T^\circ - TS_T^\circ \text{ gives us } G_0^\circ = H_0^\circ \text{ when } T = 0.$$

The terms differ by the constant term  $(H_{298}^\circ - H_0^\circ)$ , which as mentioned above, may be found in some tables.

(e) The quantities usually tabulated for the Planck function  $(-G/T)$  are

$$-(G^\circ - H_0^\circ)/T \text{ or } -(G^\circ - H_{298}^\circ)/T$$

These quantities differ by the amount

$$-(H_{298}^\circ - H_0^\circ)/T$$

which is not a constant, since  $T$  is in the denominator.

Despite its anomalous character the function  $-(G^\circ - H_{298}^\circ)/T$  is very useful, because it allows calculations to be made involving processes for which  $\Delta H_{298}^\circ$  is known. These include enthalpies of reaction, enthalpies of phase transition, and so on. Such calculations are quite practical with this function even if the quantity  $H_{298}^\circ - H_0^\circ$  may never have been measured, as would be necessary to obtain  $-(G^\circ - H_0^\circ)/T$ . The negative function is used for the Planck function because most table entries then become positive.

(f) The quantities tabulated for enthalpy of formation ( $\Delta H_f$ ) are

$$\Delta H_f^\circ(\text{at } 0 \text{ K}) \text{ and } \Delta H_f^\circ(\text{at } 298.15 \text{ K})$$

These quantities differ by the amount

$$\Delta H_f^\circ(\text{at } 298.15 \text{ K}) - \Delta H_f^\circ(\text{at } 0 \text{ K}) = \sum_i v_i (H_{298}^\circ - H_0^\circ)_i$$

where the sum of enthalpy increments  $(H_{298}^\circ - H_0^\circ)_i$  is taken over all the  $i$  products and reactants, with the number of moles of each given by  $v_i$ , where  $v_i$  is positive for the products and negative for the reactants. The quantity  $\Delta H_f^\circ(\text{at } T)$  is also frequently given at a series of temperatures.

## 21.4 Calculation of Thermochemical Quantities

### 21.4.1 Additivity of Chemical Processes

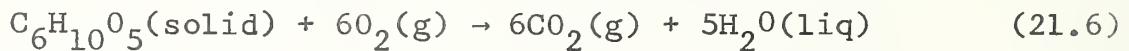
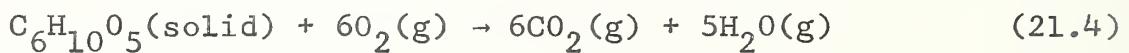
Any chemical process can be conceived as occurring in stages, for each of which a chemical reaction can be written. These processes are additive in effect, and the overall reaction is the sum of the reactions into which it has been

resolved. As an example, we give the combustion of carbon to form carbon monoxide (equation 21.1) followed by the combustion of carbon monoxide to form carbon dioxide (equation 21.2). Energies are in kcal mol<sup>-1</sup>.



The sum of the reactions is the appropriate reaction for the complete combustion of carbon directly to form carbon dioxide (equation 21.3). In summing such a sequence of reactions the same substance is not ordinarily shown on both sides of the final reaction, but only the excess on one side or the other.

As another illustration we give the combustion of an organic substance (for example, cellulose for which the repeating unit is C<sub>6</sub>H<sub>10</sub>O<sub>5</sub>) to form carbon dioxide and gaseous water (equation 21.4), followed by condensation of the water to liquid (equation 21.5). The overall reaction may be written as the combustion of the organic substance to form gaseous carbon dioxide and liquid water (equation 21.6).



#### 21.4.2 Additivity of Thermodynamic Quantities (Law of Hess)

When a sequence of chemical processes is carried out, as illustrated in Section 21.4.1, the thermodynamic quantities associated with the reaction are additive in the same way as the chemical reactions. The overall thermodynamic change of the final process is the sum of the thermodynamic changes of the intermediate or postulated processes into which it has been resolved.

Changes of enthalpy, internal energy, Gibbs energy, Helmholtz energy, and entropy are additive in this way. The enthalpy changes associated with reactions (21.1), (21.2), and (21.3) are given beside the equations for illustration. A sequence of processes of any desired length can be added this way.

## 21.5 Enthalpy and Internal Energy of Combustion

### 21.5.1 Calculation of Observed Heat Effects from Enthalpies of Formation

Combustion processes can be carried out practically in a variety of ways. Commercially, for example, combustion is often carried out as a flowing, nearly adiabatic process operated at constant pressure. The heat of reaction is dissipated through insulated walls, to heat exchange surfaces, and in heating quench water, or is carried up the stack in the products of combustion. Adiabatic constant-volume calculations are also useful in a practical way to determine pressure and temperature build-up from explosive combustions which might occur in incinerators.

In order to calculate the enthalpy of combustion ( $\Delta H_c$ ) or internal energy of combustion ( $\Delta U_c$ ) of a substance, it is essential to know the products of combustion and their proportions. The products and their proportions depend, first of all, on the composition of the substances burned and the oxidizer used. In addition, however, they depend upon the conditions of the combustion process. Factors involved include the pressure of the oxidizing air, the temperature and pressure reached by the reacting system, the relative proportions of elements present, and the rates at which substances pass through various reaction zones.

In this space it is impossible to give a complete analysis of the factors involved and methods for making calculations. However, the processes involved can be resolved into idealized simpler processes; the

isothermal process and the adiabatic process. A brief discussion of some of the factors involved in adiabatic processes and other processes, in which the reaction products are hot, is given in Sections 21.6 and 21.7. In the following two sections (21.5.2 and 21.5.3) we limit ourselves to enthalpy and internal energy changes and the related heat effects for some isothermal processes representing the combustion of substances as determined under idealized conditions. In Section 21.5.4 we extend the discussion to the combustion of several types of organic compounds, and in Section 21.5.5 discuss some other formalized fuel combustion reactions. We shall restrict our discussion to combustion in which oxygen (or air) is the oxidizer.

The isothermal process is a convenient form for presenting carefully defined thermodynamic information in a standard way, in which the heat observed can be expressed in terms of enthalpies of formation listed in tables of this handbook. Isothermal combustion can be carried out at constant pressure or at constant volume. These two processes are discussed below.

#### 21.5.2 Isothermal Constant-Pressure Combustion

Combustion can be carried out in an open burner as a constant-pressure process with all reactants and products at the same initial and final temperature and pressure. The heat effect observed,  $Q_p(\text{obs})$ , in which the subscript p represents the constant-pressure process is a measure of the enthalpy change.

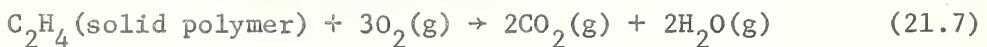
In a constant-pressure process, typically though not necessarily, water and any other appreciably volatile substance among the products

remain in the gas phase, and oxygen is present in excess. In this case the observed heat effect which we shall calculate is closely related but not identical to the quantity, net heat of combustion, used in fuel technology (See Section 21.5.6).

For the purpose of this illustration we shall presume that  $\Delta H$  and  $\Delta H^\circ$  do not differ significantly. Hence we may write:

$$Q_p(\text{obs}) = -\Delta H_c(\text{at T K}) \approx -\Delta H_c^\circ(\text{at T K})$$

For a typical reaction, the combustion of polyethylene, equation (21.7) represents the process per mole of monomer unit.



The enthalpy change for reaction (21.7) can be calculated from data in Tables I, II, and III.

$$\begin{aligned}\Delta H_c^\circ(\text{at } 298 \text{ K}) &= 2\Delta H_f^\circ[\text{CO}_2(\text{g})] + 2\Delta H_f^\circ[\text{H}_2\text{O}(\text{g})] - \Delta H_f^\circ[\text{C}_2\text{H}_4(\text{solid polymer})] \\ &= 2(-393.509) + 2(-241.818) - (-56.48) \text{ kJ mol}^{-1} \\ &= -1214.17 \text{ kJ mol}^{-1}\end{aligned}$$

$$Q_p(\text{obs}) \approx \Delta H_c^\circ(\text{at } 298 \text{ K}) = -1214.17 \text{ kJ mol}^{-1}$$

As the molecular weight of polyethylene (monomer unit) is 28.0542 g (0.0280542 kg) the specific net heat of combustion of polyethylene is  $\frac{-1214.17}{28.0542} = -43.28 \text{ MJ/kg}$ .

During the reaction an increase in volume occurs, representing principally the increase in number of moles of gas,  $\Delta n$ . The increase in the amount of gas is 1 mole of gas per mole of reactant (4 moles of gas formed minus 3 moles of gas reacted). On the basis that the volume of

solid reactant is small compared to the increase in volume of the gases, and that the gases follow the ideal gas law, the work term  $p \Delta V$  is expressible as

$$p \Delta V \approx \Delta n RT$$

At 298.15 K,  $RT$  has the value  $2.479 \text{ kJ mol}^{-1}$ . As  $\Delta n = 1$ ,  $p \Delta V = 2.48 \text{ kJ mol}^{-1}$ .

If for any reason one wishes to calculate the internal energy change,  $\Delta U^\circ$  (at 298 K) for reaction (21.7) it may now be done

$$\begin{aligned}\Delta U_c^\circ (\text{at } 298 \text{ K}) &= \Delta H_c^\circ (\text{at } 298 \text{ K}) - p \Delta V \\ &= -1214.17 - 2.48 \text{ kJ mol}^{-1} \\ &= -1216.65 \text{ kJ mol}^{-1} \\ &= -43.37 \text{ MJ kg}^{-1}\end{aligned}$$

### 21.5.3 Isothermal Constant-Volume Combustion

Combustion can be carried out in a closed burner as a constant-volume process with all reactants and products contained in the same volume and at the same temperature at beginning and end of the reaction. In a constant-volume process, it is customary to achieve complete combustion by using oxygen in excess and under a pressure of 20 to 30 atmospheres. In this case the heat effect,  $Q_v$ , to which the subscript  $v$  has been added to represent the constant-volume process, is a measure of the internal energy change.

$$Q_v(\text{obs}) = -\Delta U_c \approx \Delta U_c^\circ$$

If it is possible to devise a system in which all the products of reaction (21.7) remain in the gaseous state, then  $-\Delta U_c^\circ$  (at 298 K) would be as we have calculated it before and  $Q_v(\text{obs})$  would be  $1216.65 \text{ kJ mol}^{-1}$  ( $43.37 \text{ MJ kg}^{-1}$ ).

A more usual circumstance for a constant-volume process is for the condensable products of combustion to be condensed to the liquid state. In this case, the observed heat effect which we shall calculate is closely related, though not identical, to the gross heat of combustion (see Section 21.5.6) used in fuel technology. In this case, the observed reaction would be given by equation (21.8).



The enthalpy change again can be computed using data from Tables I, II, and III

$$\begin{aligned}\Delta H^\circ \text{ (at 298 K)} &= 2\Delta H_f^\circ [\text{CO}_2(\text{g})] + 2\Delta H_f^\circ [\text{H}_2\text{O}(\text{liq})] - \Delta H_f^\circ [\text{C}_2\text{H}_4 \text{ (solid polymer)}] \\ &= 2(-393.509) + 2(-285.830) - (-56.99) \text{ kJ mol}^{-1} \\ &= -1302.20 \text{ kJ mol}^{-1} \\ &= -46.42 \text{ MJ kg}^{-1}\end{aligned}$$

As before, we can now calculate the internal energy change. In this case, because the water was condensed, the number of moles of gas is reduced;  $\Delta n = -1$  mole per mole of reactant.

$$\begin{aligned}p\Delta V &\approx \Delta n RT = -2.48 \text{ kJ mol}^{-1} \\ \Delta U_c^\circ \text{ (at 298 K)} &= \Delta H_c^\circ \text{ (at 298 K)} - p\Delta V \\ &= -1302.20 - (-2.48) \text{ kJ mol}^{-1} \\ &= -1299.72 \text{ kJ mol}^{-1} \\ &= -46.33 \text{ MJ kg}^{-1}\end{aligned}$$

Thus for this constant volume process

$$\begin{aligned}Q_v(\text{obs}) &\approx -\Delta U^\circ \text{ (at 298 K)} = 1299.72 \text{ kJ mol}^{-1} \\ &= 46.33 \text{ MJ kg}^{-1}\end{aligned}$$

Note that both  $\Delta U_c^\circ$  (at 298 K) and  $\Delta H_c^\circ$  (at 298 K) are more negative for reaction (21.8) than the corresponding values for reaction (21.7), and the reaction is, therefore, more exothermic. The extra heat comes from the condensation of the water.

#### 21.5.4 Type Reactions for Combustion of Organic Compounds- Calculation of Enthalpy of Combustion for the Isothermal Process

The substances present in the combustion products depend first upon the elements present. The phases of the products (gas, liquid, or solid) depend upon the temperatures and partial pressures of the substances at the conclusion of the process.

Calculations of  $\Delta U_c$  or  $\Delta H_c$  (at 298 K) such as are shown in the preceding section can be made for any given process, provided the equation can be written for the process, and provided the enthalpies of formation of reactants and products are known.

To assist in the calculation of the energy changes, equations are given in Table 21.1 and Table 21.3 for a standard type reaction for each of several classes of organic compounds.

The classes of compounds are based on the elements present in an empirical formula, and are not functional classes. Compound classes containing various typical combinations of the elements C, H, N, O, P, S, F, Cl, Br, and I are given. Not all possible combinations are given. However, the pattern of the reactions should be clear from the table, and it should be possible for the user to extend the table to include all the information required for other combinations of the same elements.

The products of combustion that will be encountered are different, depending upon whether the process is carried out at constant volume or at constant pressure, and the product in which a given element is found depends to some extent upon other elements present.

For the combustion processes, we make the following somewhat arbitrary presumptions. Some water will have been supplied in the constant-volume process to dissolve the soluble acids formed.

The product of combustion of carbon is  $\text{CO}_2(\text{g})$ .

The product of combustion of hydrogen is  $\text{H}_2\text{O}(\text{g})$  in the constant-pressure process, and  $\text{H}_2\text{O}(\text{liq})$  in the constant-volume process. If the halogens F or Cl are present, some of the hydrogen may be present as  $\text{HF}(\text{g})$  or  $\text{HCl}(\text{g})$  in the constant-pressure process in which water is formed as a gas, or as  $\text{HF}(\text{aq})$  or  $\text{HCl}(\text{aq})$  in the constant-volume process in which condensables are condensed. If sulfur or phosphorus is present, some of the hydrogen may be present as  $\text{H}_2\text{SO}_4(\text{aq})$  or  $\text{H}_3\text{PO}_4(\text{aq})$  in the constant-volume process, in which water and other condensables have condensed.

The product of combustion of organic nitrogen is taken to be the gaseous element,  $\text{N}_2(\text{g})$ . Some oxides of nitrogen may be formed in the constant-pressure process, and some  $\text{HNO}_3(\text{aq})$  may be formed in the constant-volume process. A correction to the enthalpy change of the type process may be required, to obtain the observed heat, if appreciable quantities of either are formed. Some oxides of nitrogen or nitric acid may also be formed, even if the element is absent in the combustible substance, because nitrogen from the combustion air may combine with

oxygen at the temperature and pressure of the combustion reaction. The occurrence of nitrogen-oxygen compounds may be expected to be much more pronounced in the constant-volume process than in the constant-pressure process, because of the higher temperatures usually reached in the constant-volume process, and possibly also because of the reduction in number of moles of gas caused by formation of the compounds.

The product of combustion of organic phosphorus is taken here to be  $P_4O_{10}(g)$  in the constant-pressure process and  $H_3PO_4(aq)$  in the constant-volume process. The presumed concentration of  $H_3PO_4$  is one mole in 40 moles of  $H_2O$ . If the resulting concentration in an actual combustion differs appreciably from this, a dilution correction may be required in order to calculate  $Qv(obs)$ . Note that some compilations of enthalpies of combustion of phosphorus compounds presume the final form of the phosphorus to be  $H_3PO_4(c)$ , and hence care must be taken when comparing enthalpies of combustion from various sources.

The product of combustion of organic sulfur is taken to be  $SO_2(g)$  in the constant-pressure process and  $H_2SO_4(aq)$  in the constant-volume process. The conversion to the higher oxidation state is catalyzed by oxides of nitrogen, and the conversion may be expected to be nearly complete if appreciably high pressures and temperatures are developed. The presumed concentration of  $H_2SO_4$  is one mole in 115 moles of  $H_2O$ . If the resulting concentration in an actual combustion differs appreciably from this, a dilution correction may be required in order to calculate  $Qv(obs)$ .

The product of combustion of organic fluorine is taken to be HF(g) in the constant-pressure process, and HF(aq) in the constant-volume process. The presumed concentration of HF is one mole in 20 moles of H<sub>2</sub>O. If the resulting concentration in an actual combustion differs from this by an appreciable amount, a dilution correction may be required in order to calculate Qv(obs). The formation of HF by burning an organic compound in oxygen depends upon the presence of hydrogen in the combustion material. If hydrogen is not present in sufficient quantity to combine with all the fluorine, the balance of the fluorine will appear as CF<sub>4</sub>, or possibly COF<sub>2</sub>, unless other elements (such as metals) are present. If not wanted, this contingency can be avoided by adding an auxiliary combustible which contains enough hydrogen to combine with the fluorine. The equation for this alternate process is given (Equation 9, Table 21.3). If CF<sub>4</sub> or COF<sub>2</sub> are formed and their avoidance is not deemed necessary, the calculation of Qv(obs) will be affected by the proportions present, which may be determined by analysis or by calculation from equilibria.

The product of combustion of organic chlorine is taken to be HCl(g) in the constant-pressure process, and HCl(aq) in the constant-volume process. The presumed concentration of HCl is one mole of HCl in 600 moles of H<sub>2</sub>O. If the resulting concentration differs appreciably from this, a dilution correction may be required in order to calculate Qv(obs) accurately. Because oxygen and chlorine are of comparable electronegativity, the possibility of forming elemental chlorine, Cl<sub>2</sub>(g), exists. If its presence is objectionable, it may be possible to remove it by use of a reducing agent, such as As<sub>2</sub>O<sub>3</sub>(aq), outside the combustion

zone. A correction must be applied to  $Q_v(\text{obs})$  for the reduction process. If the presence of  $\text{Cl}_2(g)$  must be allowed, the calculation of  $Q_v(\text{obs})$  is affected, and the proportions of  $\text{Cl}_2$  and  $\text{HCl}$  may have to be determined by analysis or from equilibrium calculations in order to determine  $Q_v(\text{obs})$ . Experience indicates that 15 to 20% of the chlorine is formed as  $\text{Cl}_2$  and 80 to 85% as  $\text{HCl}$  in the constant-volume process.

The product of combustion of organic bromine is taken to be elemental bromine, as the gas in the constant-pressure process and as the liquid in the constant-volume process. The form of the bromine in a given reaction system should be determined by analysis. In calculating  $Q_v(\text{obs})$  or  $Q_p(\text{obs})$ , a correction can be applied to  $\Delta U$  or  $\Delta H$  for any deviation from the equation given. Experience indicates that 90 to 97% of the bromine is formed as  $\text{Br}_2(\text{liq})$  in the constant-volume process.

The product of combustion of organic iodine is taken to be elemental iodine, as the gas in the constant-pressure process. For a given reaction system, the form of the iodine should be determined by actual analysis. In calculating  $Q_v(\text{obs})$  or  $Q_p(\text{obs})$  a correction can be applied to  $\Delta U$  or  $\Delta H$  for any deviation from the equation.

Table 21.1 presents type equations for combustion reactions of organic compounds burning at constant pressure in an atmosphere of oxygen. The equations are balanced with generalized letter coefficients derived from the letter subscripts of the elements in the formula. The stoichiometric amount of oxygen and the amounts of the type reaction products are given. Table 21.1 is supplemented by Table 21.2 which gives for the reactions the elements present, the increase in quantity of gas,  $\Delta n$ , calculated from the amounts of gaseous products and reactants

Table 21.1

Type Combustion Reactions of Organic Compounds Burning at Constant Pressure in an Atmosphere of Oxygen  
All Products Emitted as Gases

| Substance (*)                                  | Stoichiometric oxygen   | Products   |
|--|---|--|
| (1) $C_aH_b$ (c,liq)                           | + $(a + \frac{b}{4}) O_2$ (g)   | $\rightarrow a CO_2$ (g) + $\frac{b}{2} H_2O$ (g)  |
| (2) $C_aH_bN_c$ (c,liq)                        | + $(a + \frac{b}{4}) O_2$ (g)   | $\rightarrow a CO_2$ (g) + $\frac{b}{2} H_2O$ (g) + $\frac{c}{2} N_2$ (g)  |
| (3) $C_aH_bO_d$ (c,liq)                        | + $(a + \frac{b}{4} - \frac{d}{2}) O_2$ (g)                                   | $\rightarrow a CO_2$ (g) + $\frac{b}{2} H_2O$ (g)  |
| (4) $C_aH_bN_cO_d$ (c,liq)                     | + $(a + \frac{b}{4} - \frac{d}{2}) O_2$ (g)                                   | $\rightarrow a CO_2$ (g) + $\frac{b}{2} H_2O$ (g) + $\frac{c}{2} N_2$ (g)  |
| (5) $C_aH_bO_dP_e$ (c,liq)                     | + $(a + \frac{b}{4} - \frac{d}{2} + \frac{5}{4}e) O_2$ (g)                    | $\rightarrow a CO_2$ (g) + $\frac{b}{2} H_2O$ (g) + $\frac{e}{4} P_4O_{10}$ (g)                                      |
| (6) $C_aH_bO_dS_f$ (c,liq)                     | + $(a + \frac{b}{4} - \frac{d}{2} + f) O_2$ (g)                               | $\rightarrow a CO_2$ (g) + $\frac{b}{2} H_2O$ (g) + $f SO_2$ (g)   |
| (7) $C_aH_bN_cO_dS_f$ (c,liq)                  | + $(a + \frac{b}{4} - \frac{d}{2} + f) O_2$ (g)                               | $\rightarrow a CO_2$ (g) + $\frac{b}{2} H_2O$ (g) + $\frac{c}{2} N_2$ (g) + $f SO_2$ (g)                             |
| (8) $C_aH_bF_g$ (c,liq)                        | + $(a + \frac{b}{4} - \frac{g}{4}) O_2$ (g)                                   | $\rightarrow a CO_2$ (g) + $(\frac{b}{2} - \frac{g}{2}) H_2O$ (g) + $g HF$ (g)                                       |
| (9) $C_aH_bF_g$ (c,liq) + $x C_aH_b$ (c,liq) + | $(a + x\acute{a} + \frac{b}{4} + \frac{x\acute{b}}{4} - \frac{g}{4}) O_2$ (g) | $\rightarrow (a + x\acute{a}) CO_2$ (g) + $(\frac{b}{2} + \frac{x\acute{b}}{2} - \frac{g}{2}) H_2O$ (g) + $g HF$ (g) |
| (10) $C_aH_bCl_h$ (c,liq)                      | + $(a + \frac{b}{4} - \frac{h}{4}) O_2$ (g)                                   | $\rightarrow a CO_2$ (g) + $(\frac{b}{2} - \frac{h}{2}) H_2O$ (g) + $h HCl$ (g)                                      |
| (11) $C_aH_bBr_i$ (c,liq)                      | + $(a + \frac{b}{4}) O_2$ (g)   | $\rightarrow a CO_2$ (g) + $\frac{b}{2} H_2O$ (g) + $\frac{i}{2} Br_2$ (g)   |
| (12) $C_aH_bI_j$ (c,liq)                       | + $(a + \frac{b}{4}) O_2$ (g)   | $\rightarrow a CO_2$ (g) + $\frac{b}{2} H_2O$ (g) + $\frac{j}{2} I_2$ (g)  |

(\*) (c,liq) indicates that the equations are valid for either solid or liquid substance  
(g) indicates that the equations are valid for gaseous substance.

Table 21.2, Enthalpy Changes for Table 21.1

| Reaction | Elements      | $\Delta n^*$                                   | $p\Delta V = \Delta n RT = 0.592 \Delta n$   | $\Delta H^\circ (\text{at } 298 \text{ K}), \text{kcal mol}^{-1}$   | $\Delta H^\circ (\text{at } 298 \text{ K}), \text{kJ mol}^{-1}$ |
|----------|---------------|--|--|---|---|
| (1)      | C, H          | $(\frac{b}{4})$                                | -94.051a -57.796 $\frac{b}{2}$ - $\Delta Hf$ [substance]   | -393.51a -241.82 $\frac{b}{2}$ - $\Delta Hf$ [substance]  |   |
| (2)      | C, H, N       | $(\frac{b}{4} + \frac{c}{2})$                  | -94.051a -57.796 $\frac{b}{2}$ - $\Delta Hf$ [substance]   | -393.51a -241.82 $\frac{b}{2}$ - $\Delta Hf$ [substance]  |   |
| (3)      | C, H, O       | $(\frac{b}{4} + \frac{d}{2})$                  | -94.051a -57.796 $\frac{b}{2}$ - $\Delta Hf$ [substance]   | -393.51a -241.82 $\frac{b}{2}$ - $\Delta Hf$ [substance]  |   |
| (4)      | C, H, N, O    | $(\frac{b}{4} + \frac{c}{2} + \frac{d}{2})$    | -94.051a -57.796 $\frac{b}{2}$ - $\Delta Hf$ [substance]   | -393.51a -241.82 $\frac{b}{2}$ - $\Delta Hf$ [substance]  |   |
| (5)      | C, H, O, P    | $(\frac{b}{4} + \frac{d}{2} - e)$              | -94.051a -57.796 $\frac{b}{2}$ -677.4 $\frac{e}{4}$ - $\Delta Hf$ [substance]                          | -393.51a -241.82 $\frac{b}{2}$ -2834.2 $\frac{e}{4}$ - $\Delta Hf$ [substance]  |   |
| (6)      | C, H, O, S    | $(\frac{b}{4} + \frac{d}{2})$                  | -94.051a -57.796 $\frac{b}{2}$ -70.94f - $\Delta Hf$ [substance]                                       | -393.51a -241.82 $\frac{b}{2}$ -296.83f - $\Delta Hf$ [substance]   |   |
| (7)      | C, H, N, O, S | $(\frac{b}{4} + \frac{c}{2} + \frac{d}{2})$    | -94.051a -57.796 $\frac{b}{2}$ -70.94f - $\Delta Hf$ [substance]                                       | -393.51a -241.82 $\frac{b}{2}$ -296.83f - $\Delta Hf$ [substance]   |   |
| (8)      | C, H, F       | $(\frac{b}{4} + \frac{3g}{4})$                 | -94.051a -57.796 $(\frac{b}{2} - \frac{g}{2})$ -65.15g<br>- $\Delta Hf$ [substance]                    | -393.51a -241.82 $(\frac{b}{2} - \frac{g}{2})$ -272.55g<br>- $\Delta Hf$ [substance]                                    |   |
| (9)      | C, H, F,      | $(\frac{b}{4} + \frac{x^b}{4} + \frac{3g}{4})$ | -94.051(a + $x^a$ ) -57.796 $(\frac{b}{2} + \frac{x^b}{2} - \frac{g}{2})$<br>- $\Delta Hf$ [substance] | -393.51(a + $x^a$ ) -241.82 $(\frac{b}{2} + \frac{x^b}{2} - \frac{g}{2})$<br>- $\Delta Hf$ [substance] -xHf [auxiliary] |   |
| (10)     | C, H, Cl      | $(\frac{b}{4} + \frac{3h}{4})$                 | -94.051a -57.796 $(\frac{b}{2} - \frac{h}{2})$ -22.06h<br>- $\Delta Hf$ [substance]                    | -393.51a -241.82 $(\frac{b}{2} - \frac{h}{2})$ -92.31h<br>- $\Delta Hf$ [substance]                                     |   |
| (11)     | C, H, Br      | $(\frac{b}{4} - \frac{i}{2})$                  | -94.051a -57.796 $\frac{b}{2}$ + 7.39 $\frac{i}{2}$ - $\Delta Hf$ [substance]                          | -393.51a -241.82 $\frac{b}{2}$ + 30.91 $\frac{i}{2}$ - $\Delta Hf$ [substance]  |   |
| (12)     | C, H, I       | $(\frac{b}{4} + \frac{j}{2})$                  | -94.051a -57.796 $\frac{b}{2}$ + 14.92 $\frac{j}{2}$ - $\Delta Hf$ [substance]                         | -393.51a -241.82 $\frac{b}{2}$ + 62.44 $\frac{j}{2}$ - $\Delta Hf$ [substance]  |   |

\*  $\Delta n$  is the increase in number of moles of gas when the combustible material is not a gas. Under some circumstances  $\Delta n$  may be negative.

$p\Delta V = \Delta n RT$  on the basis that (a) the gases are ideal, and (b) the volume of the condensed phase can be neglected in comparison with change in volume of gas.

Table 21.3 Type Combustion Reactions of Organic Compounds Burning at Constant Volume in an Atmosphere of Oxygen (Excess Water Present)

Products are Formed as Gases and Aqueous Solutions

| Substance                                      | Stoichiometric Oxygen  | Products   |
|--|--|--|
| (1) $C_aH_bN_d(c, liq)$                        | + $(a + \frac{b}{2}) O_2(g)$   | $\rightarrow a CO_2(g) + \frac{b}{2} H_2O(1iq)$  |
| (2) $C_aH_bN_c(c, liq)$                        | + $(a + \frac{b}{4}) O_2(g)$   | $\rightarrow a CO_2(g) + \frac{b}{2} H_2O(1iq) + \frac{c}{2} N_2(g)$   |
| (3) $C_aH_bO_d(c, liq)$                        | + $(a + \frac{b}{4} - \frac{d}{2}) O_2(g)$                                 | $\rightarrow a CO_2(g) + \frac{b}{2} H_2O(1iq)$  |
| (4) $C_aH_bN_cO_d(c, liq)$                     | + $(a + \frac{b}{4} - \frac{d}{2}) O_2(g)$                                 | $\rightarrow a CO_2(g) + \frac{b}{2} H_2O(1iq) + \frac{c}{2} N_2(g)$   |
| (5) $C_aH_bO_dP_e(c, liq)$                     | + $(a + \frac{b}{4} - \frac{d}{2} + \frac{5}{4}e) O_2(g)$                  | $\rightarrow a CO_2(g) + (\frac{b}{2} - \frac{3e}{2}) H_2O(1iq) + e H_3PO_4$<br>(aq in 40 H <sub>2</sub> O)                  |
| (6) $C_aH_bO_dS_f(c, liq)$                     | + $(a + \frac{b}{4} - \frac{d}{2} + \frac{3f}{2}) O_2(g)$                  | $\rightarrow a CO_2(g) + (\frac{b}{2} - f) H_2O(1iq) + f H_2SO_4$<br>(aq in 115 H <sub>2</sub> O)                            |
| (7) $C_aH_bN_eO_dS_f(c, liq)$                  | + $(a + \frac{b}{4} - \frac{d}{2} + \frac{3f}{2}) O_2(g)$                  | $\rightarrow a CO_2(g) + (\frac{b}{2} - f) H_2O(1iq) + \frac{c}{2} N_2(g) + f H_2SO_4$<br>(aq in 115 H <sub>2</sub> O)       |
| (8) $C_aH_bF_g(c, liq)$                        | + $(a + \frac{b}{4} - \frac{g}{4}) O_2(g)$                                 | $\rightarrow a CO_2(g) + (\frac{b}{2} - \frac{g}{2}) H_2O(1iq) + g HF(aq in 20 H_2O)$  |
| (9) $C_aH_bF(c, liq)$<br>+ $xC'_aH'_b(c, liq)$ | + $(a + x\bar{a} + \frac{b}{4} + \frac{x\bar{b}}{4} - \frac{g}{4}) O_2(g)$ | $\rightarrow (a + x\bar{a}) CO_2(g) + (\frac{b}{2} + \frac{x\bar{b}}{2} - \frac{g}{2}) H_2O(1iq)$<br>+ $g HF(aq in 20 H_2O)$ |
| (10) $C_aH_bCl_h(c, liq)$                      | + $(a + \frac{b}{4} - \frac{h}{4}) O_2(g)$                                 | $\rightarrow a CO_2(g) + (\frac{b}{2} - \frac{h}{2}) H_2O(1iq) + h HCl$ (aq in 600 H <sub>2</sub> O)                         |
| (11) $C_aH_bBr_i(c, liq)$                      | + $(a + \frac{b}{4}) O_2(g)$   | $\rightarrow a CO_2(g) + \frac{b}{2} H_2O(1iq) + \frac{i}{2} Br_2(1iq)$  |
| (12) $C_aH_bI_j(c, liq)$                       | + $(a + \frac{b}{4}) O_2(g)$   | $\rightarrow a CO_2(g) + \frac{b}{2} H_2O(1iq) + \frac{j}{2} I_2(c)$   |

Table 21.4 Enthalpy Changes for Table 21.3

| Reaction | Elements      | $\Delta n^*$   | $p \Delta V \approx \Delta n RT = 0.592 \Delta n$                                      | $\Delta H^\circ \text{ (at 298 K), kcal mol}^{-1}$ | $\Delta n$ | $p \Delta V \approx \Delta n RT = 2.477 \Delta n$                                      | $\Delta H^\circ \text{ (at 298 K), kJ mol}^{-1}$ |
|----------|---------------|--|--|--|------------|--|--|
| (1)      | C, H          | (- $\frac{b}{4}$ )   | -94.051a - $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                              |  |            | -393.51a -285.83 $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                        |  |
| (2)      | C, H, N       | ( $\frac{c}{2}$ - $\frac{b}{4}$ )                                  | -94.051a - $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                              |  |            | -393.51a -285.83 $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                        |  |
| (3)      | C, H, O       | ( $\frac{d}{2}$ - $\frac{b}{4}$ )                                  | -94.051a -68.315 $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                        |  |            | -393.51a -285.83 $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                        |  |
| (4)      | C, H, N, O    | ( $\frac{c}{2}$ - $\frac{d}{2}$ - $\frac{b}{4}$ )                  | -94.051a -68.315 $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                        |  |            | -393.51a -285.83 $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                        |  |
| (5)      | C, H, O, P    | ( $\frac{d}{2}$ - $\frac{b}{4}$ )                                  | -94.051a -68.315 ( $\frac{b}{2}$ - $\frac{3e}{2}$ ) -308.032e                          |  |            | -393.51a -285.83 ( $\frac{b}{2}$ - $\frac{3e}{2}$ ) -1288.81e                          |  |
| (6)      | C, H, O, S    | ( $\frac{d}{2}$ - $\frac{b}{4}$ - $\frac{3f}{2}$ )                 | -94.051a -68.315 ( $\frac{b}{2}$ - $\frac{f}{2}$ ) -212.192f                           |  |            | -393.51a -285.83 ( $\frac{b}{2}$ - $\frac{f}{2}$ ) -887.81f                            |  |
| (7)      | C, H, N, O, S | ( $\frac{c}{2}$ + $\frac{d}{2}$ - $\frac{b}{4}$ - $\frac{3f}{2}$ ) | -94.051a -68.315 ( $\frac{b}{2}$ - $\frac{f}{2}$ ) -212.192f                           |  |            | -393.51a -285.83 ( $\frac{b}{2}$ - $\frac{f}{2}$ ) -887.81f                            |  |
| (8)      | C, H, F       | ( $\frac{g}{4}$ - $\frac{b}{4}$ )                                  | -94.051a -68.315 ( $\frac{b}{2}$ - $\frac{g}{2}$ ) -76.71g                             |  |            | -393.51a -285.83 ( $\frac{b}{2}$ - $\frac{g}{2}$ ) -320.95g                            |  |
| (9)      | C, H, Cl      | ( $\frac{g}{4}$ - $\frac{b}{4}$ - $\frac{x\bar{b}}{4}$ )           | -94.051(a + x\bar{a}) -68.315 ( $\frac{b}{2}$ + $\frac{x\bar{b}}{2}$ - $\frac{g}{2}$ ) |  |            | -393.51(a + x\bar{a}) -285.83 ( $\frac{b}{2}$ + $\frac{x\bar{b}}{2}$ - $\frac{g}{2}$ ) |  |
| (10)     | C, H, Cl      | ( $\frac{h}{4}$ - $\frac{b}{4}$ )                                  | -76.71g - $\Delta H_f[\text{substance}]$   |  |            | -320.95g - $\Delta H_f[\text{substance}]$  |  |
| (11)     | C, H, Br      | (- $\frac{b}{4}$ )   | -94.051a -68.315 ( $\frac{b}{2}$ - $\frac{h}{2}$ ) -39.823h                            |  |            | -393.51a -285.83 ( $\frac{b}{2}$ - $\frac{h}{2}$ ) -166.62h                            |  |
| (12)     | C, H, I       | (- $\frac{b}{4}$ )   | -94.051a -68.315 $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                        |  |            | -393.51a -285.83 $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                        |  |
|          |               |  | -94.051a -68.315 $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                        |  |            | -393.51a -285.83 $\frac{b}{2}$ - $\Delta H_f[\text{substance}]$                        |  |

\* See footnote Table 21.2

Table 21.5 Auxiliary Data for Determining Enthalpies  
of Combustion of Organic Compounds

| Substance<br>(state)                                  | $\Delta H_f^\circ$<br>kcal mol <sup>-1</sup> | $\Delta H_f^\circ$<br>kJ mol <sup>-1</sup> | Reference |
|---|--|--|-----------|
| CO <sub>2</sub> (g)                                   | -94.051                                      | -393.51                                    | [1]       |
| H <sub>2</sub> O(g)                                   | -57.796                                      | -241.82                                    | [1]       |
| H <sub>2</sub> O(liq)                                 | -68.315                                      | -285.83                                    | [1]       |
| HF(g)   | -65.14                                       | -272.55                                    | [2]       |
| HF(aq) (20 H <sub>2</sub> O)                          | -76.71                                       | -320.95                                    | [3]       |
| HCl(g)  | -22.062                                      | -92.31                                     | [1]       |
| HCl(aq) (600 H <sub>2</sub> O)                        | -39.823                                      | -166.62                                    | [1]       |
| HBr(g)  | -8.70  | -36.40                                     | [1]       |
| HBr(aq) (600 H <sub>2</sub> O)                        | -28.935                                      | -121.06                                    | [1]       |
| HI(g)   | +6.33  | +26.48                                     | [1]       |
| HI(aq) (600 H <sub>2</sub> O)                         | -13.088                                      | -54.76                                     | [1]       |
| H <sub>3</sub> PO <sub>4</sub> (40 H <sub>2</sub> O)  | -308.032                                     | -1288.81                                   | [1]       |
| P <sub>4</sub> O <sub>10</sub> (g)                    | -677.4                                       | -2834.2                                    | [2]       |
| SO <sub>2</sub> (g)                                   | -70.944                                      | -296.83                                    | [1]       |
| H <sub>2</sub> SO <sub>4</sub> (115 H <sub>2</sub> O) | -212.192                                     | -887.81                                    | [1]       |
| Br <sub>2</sub> (g)                                   | +7.387                                       | +30.91                                     | [1]       |
| I <sub>2</sub> (g)                                    | +14.923                                      | +62.44                                     | [1]       |
| I <sub>2</sub> (c)                                    | 0.0  | 0.0  | [1]       |
| Br <sub>2</sub> (liq)                                 | 0.0  | 0.0  | [1]       |

- [1] Wagman, D. D., Evans, W.H., Parker, V. B., Harlow, I., Bailey, S. M., and Schumm, R. H., Nat. Bur. Standards Technical Note 270-3, January 1968.
- [2] Stull, D. R., and Prophet, H., JANAF Thermochemical Tables, 2nd Edition, National Standard Reference Data System, NSRDS-NBS-37, 1141 pp. (June 1971) (U.S. Government Printing Office, Washington, D. C. 20402).
- [3] Domalski, E. S. and Armstrong, G. T., J. Research NBS 71A, 105-118 (1967).

determined from the stoichiometry, and expressions for calculating  $\Delta H^\circ$  (at 298 K) in kcal mol<sup>-1</sup> and kJ mol<sup>-1</sup> from the enthalpies of formation of products and reactants given in Tables I, II, and III and Table 21.5.

Table 21.3 presents type reactions for combustion reactions of organic compounds burning at constant volume in an atmosphere of oxygen, with water added to dissolve product acids, and all water formed condensed to the liquid state. In other respects Tables 21.3 and 21.4 are similar to Tables 21.1 and 21.2, respectively.

Table 21.5 gives the values of  $\Delta H_f^\circ$  (at 298 K) in kcal mol<sup>-1</sup> and in kJ mol<sup>-1</sup> for products found in Tables 21.1 and 21.3. These data were used in deriving the equations of Tables 21.2 and 21.4. They can be used to calculate the enthalpy and internal energy changes for combustion of particular substances, and for other reactions, following the procedures described in this and the preceding sections.

#### 21.5.5 Enthalpies of Formation by Estimation

Supplementary sources of enthalpies of formation, many of which are not found in Tables I, II, or III may be found in monographs listed in Section 22.0.

If the value of the enthalpy of formation (or enthalpy of combustion) is not found in any available reference source, it is possible to estimate a value which is reasonably accurate. Monographs, chapters of books, and review articles giving methods for estimating various thermodynamic quantities are given in Section 23.0. Values of enthalpies of formation estimated using these methods may be in error by one to five kcal mol<sup>-1</sup> (4 to 20 kJ mol<sup>-1</sup>).

### 21.5.6 Calorific Values or Heating Values of Fuels

The terminology of heating values used in the fuel industries and applied to coal, coke, petroleum products, and natural or manufactured gas, refers to quantities closely related to the enthalpy and internal energy of combustion as discussed in this book. The terms given below may be found in use. The following definitions are quoted from ASTM methods referenced.

Standard Definition of the Terms Gross Calorific Value and Net Calorific Value of Solid and Liquid Fuels (Definitions (1) and (2) are found in Reference (1) below).

(1) gross calorific value (gross heat of combustion),  $Q_g$  in the case of solid fuels and liquid fuels of low volatility, the heat produced by combustion of unit quantity, at constant volume, in an oxygen bomb calorimeter, under specified conditions.

Note - The conditions are initial oxygen pressure of 20 to 40 atm, final temperature of 68 to 95 F (20 to 35 C), products in form of ash, liquid water, and gaseous  $\text{CO}_2$ ,  $\text{SO}_2$ , and nitrogen. This definition is not applied to gaseous or highly volatile liquid fuels.

(2) net calorific value, (net heat of combustion),  $Q_n$  in the case of solid fuels and liquid fuels of low volatility, a lower value calculated from the gross calorific value as the heat produced by combustion of unit quantity, at constant atmospheric pressure, under conditions such that all water in the products remains in the form of vapor.

Note - The net calorific value (net heat of combustion) is calculated from the gross calorific value (gross heat of combustion) at 68°F (20°C) by making a deduction of 1030 Btu/lb. (572 cal/g) of water derived from unit

quantity of fuel, including both the water originally present as moisture and that formed by combustion. The deduction is not equal to the latent heat of vaporization of water (1055 Btu/lb. at 68 F (20 C) because the calculation is made to reduce from gross value at constant volume to net value at constant pressure, for which the appropriate factor under these conditions is 1030 Btu/lb.

Definitions (1) and (2) are found in Reference (1) below. The quantities  $H_i$  and  $H_s$  found in Reference (1) are respectively  $Q_g$  and  $Q_n$  above. Slightly variant definitions can be found in other places. Also, in different ASTM methods different base temperatures are found. The quantities gross and net heat of combustion are therefore not very explicitly defined.

For the conversion from gross to net heat of combustion, several nearly equivalent formulas are found in the standard test literature. These take into account the per cent hydrogen in the sample.

|   | <u>Relation (at 25°C)</u> | <u>Units</u> | <u>ASTM Method</u> | <u>Fuel Type</u>   |
|---|---------------------------|--------------|--------------------|--------------------|
| (1) $Q_n$   | $= Q_g - 10.30(Hx9)$      | Btu/lb       | D271-70;D2015-66   | Coal, coke         |
| (2) $Q_n$   | $= Q_g - 5.72(Hx9)$       | cal/g        | D271-70            | Coal, coke         |
| (3) $Q_p(\text{net}) = Q_v(\text{gross}) - 91.23(H)$    |                           | Btu/lb       | D240-64;D2382-65   | Petroleum Products |
| (4) $Q_p(\text{net}) = 0.7195 Q_v(\text{gross}) + 4310$ | Btu/lb                    |              | D240-64;D2382-65   | Petroleum Products |

In the above equations  $H$  is per cent hydrogen by weight.

$Q_g$  is found referred to in the methods as  $H_s$ ,  $H_g$ ,  $Q_g$  (gross at 25 C, or the letters B and C).

$Q_n$  is found referred to in the methods as  $H_i$ ,  $H_n$  or  $Q_n$  (net at 25 C) or the letters N and N'.

The terminology  $Q_p$  (net, at 25°C) and  $Q_v$  (gross, at 25°C) is due to Jessup (Reference (3)). It uses  $Q$  for heat in a positive sense, uses subscript  $p$  to indicate the constant pressure process and  $v$  to indicate the constant volume process, and in parentheses states whether the net or gross heating value is referred to and the temperature to which the heat effect refers. It is a more explicit statement of the conditions for which the heat effect is valid than are the other samples in use.

The slight discrepancy between formula (1) and formula (3) should not be of concern. While formula (3) is probably based on a more accurate analysis of the thermal effects involved, the inaccuracy with which  $H$  is known and the variations from sample to sample in measuring the heating value probably introduce larger uncertainties than the differences.

To convert  $Q_g$  to  $Q_n$  the hydrogen content of the fuel must be known. This is preferably determined by analysis. In the absence of a measured value an estimate of the difference ( $Q_g - Q_n$ ) for petroleum fuels can be made. Equation (4) is a relationship based on an experimental correlation between  $Q_g$  and per cent hydrogen for liquid hydrocarbons and hydrocarbon mixtures. It is not as accurate as equations (1) or (3).

Equation (2) differs from equation (1) only in the factor  
1.8 Btu/lb = 1.0 cal/g.

Definitions of Terms for Gaseous Fuels (Reference (1c), (1d) below).

(3) total calorific value, the total calorific value of a gas is the number of British thermal units evolved by the complete combustion, at constant pressure, of one standard cubic foot of gas with air, the

temperature of the gas, air, and products of combustion being 60°F, and all the water formed by the combustion reaction being condensed to the liquid state.

(4) net calorific value, the net calorific value of a gas is the number of British thermal units evolved by the complete combustion, at constant pressure, of one standard cubic foot of gas with air, the temperature of the gas, air, and products of combustion being 60°F and all of the water formed by the combustion reaction remaining in the vapor state.

Note 1 - The net calorific value of a gas is its total calorific value minus the latent heat of evaporation at standard temperature of the water formed by the combustion reaction.

Note 2 - The definitions given [Terms (3) and (4)] are for total and net calorific values per standard cubic foot of gas. The definitions corresponding to any other unit quantity of gas are obtained by substituting the name of the desired unit in place of the term "standard cubic foot" in the definitions. Methods of calculating calorific values per cubic foot of gas under any desired conditions of pressure, temperature, and water vapor content are specified [in the ASTM method].

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Definitions (3) and (4) are found in

ASTM Designation D900-55

Standard Method of Test for Calorific Value of Gaseous Fuels  
by the Water Flow Calorimeter. See Reference (1) below.

Definition (3) is also found in:

ASTM Designation D1826-64

Standard Method of Test for Calorific Value of Gases in Natural Gas Range by Continuous Recording Calorimeter. See Reference (1) below.

The British thermal unit used in the gas industry and the standard cubic foot of gas are also defined in these methods.

The gross heat of combustion at constant volume,  $Q_v(\text{gross})$  approximates  $-\Delta U$ , the change in internal energy of the combustion process with water formed in the liquid state. The negative sign appears because  $Q_v(\text{gross})$  is positive for an exothermic reaction, while  $\Delta U$  is negative.

The net heat of combustion at constant pressure,  $Q_p(\text{net})$ , approximates  $-\Delta H$ , the change in enthalpy of the combustion process with water formed in the gaseous state. The negative sign appears as above.

In ASTM Method D-2382 (See reference (2) below), the following caution is noted: Users of this method desiring to calculate  $\Delta H_c^\circ$  at 298 K for a pure compound should note that corrections must be applied to the value of  $Q_v(\text{gross})$  for buoyancy of air, heat capacities of reaction components, reduction to a constant-pressure process, and deviation of the reaction from the thermodynamic standard state.

The total calorific value and the net calorific value of a gas differ only in that the water formed is condensed to determine the former and not the latter. Thus the value of the net heating value of a gas approximates the net heat of combustion at constant pressure but on a volumetric basis rather than a mass basis. The total calorific

value of a gas could be given the name gross heat of combustion at constant pressure, a term which is rarely if ever used.

#### References to Section 21.5

- (1) 1971 Annual Book of ASTM Standards, Part 19. Gaseous Fuels; Coal and Coke. (American Society for Testing and Materials, Philadelphia, Pa., 19103).
  - (a) D 271-70 Standard Method of Test for Analysis of Coal and Coke.
  - (b) D 407-44 Standard Definitions of the Term Gross Calorific Value and Net Calorific Value of Solid and Liquid Fuels.
  - (c) D 900-35 Standard Method of Test for Calorific Value of Gases by the Water Flow Calorimeter.
  - (d) D 1826-64 Standard Method of Test for Calorific Value of Gases in Natural Gas Range by Continuous Recording Calorimeter.
  - (e) D 2015-66 Standard Method of Test for Calorific Value by Adiabatic Bomb Calorimeter.
- (2) 1971 Annual Book of ASTM Standards, Part 17, Petroleum Products-Fuels-Solvents; Burner Fuel Oils; Lubricating Oils; Cutting Oils; Lubricating Greases; Hydraulic Fluids. (American Society for Testing and Materials, Philadelphia, Pa. 19103).
  - (a) D 240-64 Heat of Combustion of Liquid Hydrocarbon Fuels by Bomb Calorimeter;
  - (b) D 2382-65 Heat of Combustion of Hydrocarbon Fuels by Bomb Calorimeter (High-Precision Method).
- (3) R. S. Jessup, Precise Determination of Heat of Combustion by Bomb Calorimeter, Nat'l Bur. Standards Monograph 7, 1960. (U. S. Government Printing Office, Washington, D. C.).

## 21.6 Reaction Energy and Temperature

### 21.6.1 Effect of Temperature on Enthalpy of Reaction

The enthalpy change in a reaction (for instance, the enthalpy of combustion) is a function of the temperature at which the reaction occurs, and of the nature of the reacting substances. We may illustrate the relationships involved by reference to Figure 21.1. Figure 21.1 is a schematic diagram of enthalpy states of a system in which a reaction can occur and the temperature can change.

At  $T_1$  the sum of the enthalpies of formation of the reactants may be represented as point A; the sum of the enthalpies of formation of the products by point B. The enthalpy change of the isothermal reaction, reactants  $\rightarrow$  products, at  $T_1$  is

$$\begin{aligned}\Delta H(B - A) &= \Delta H(\text{reaction, at } T_1) \\ &= \Sigma \Delta H_f(\text{products, at } T_1) - \Sigma \Delta H_f(\text{reactants, at } T_1)\end{aligned}\quad (1)$$

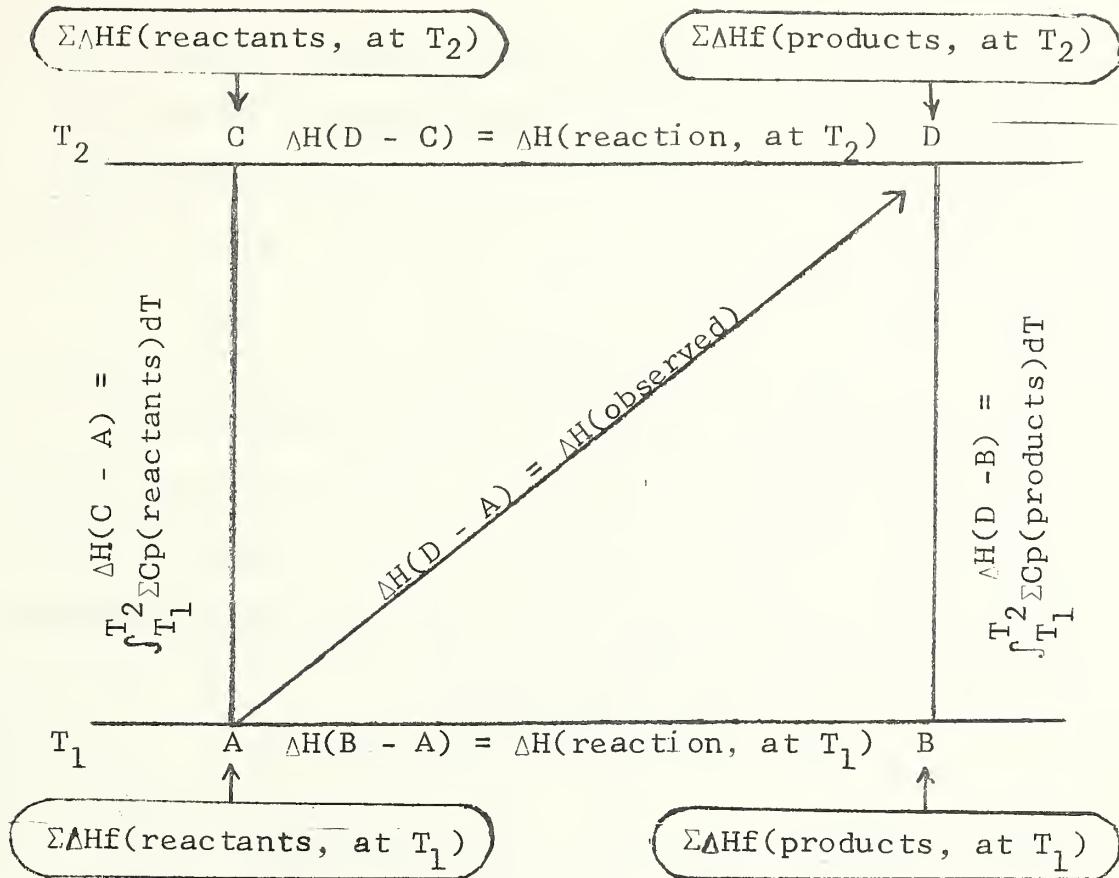


Figure 21.1 Effect of Temperature on Enthalpy of Reaction

A, B, C, D, are points on the state diagram for enthalpy of a system in which a reaction can occur and the temperature can change. An observed process, the transition from state A to state D can be resolved into two components as shown. In one component the enthalpy changes with composition, and in the other component the enthalpy changes with temperature.

At  $T_2$  the sum of the total enthalpies of formation of the reactants may be represented by point C; the sum of the enthalpies of formation of the products, by point D. The enthalpy change of the isothermal reaction, Reactants  $\rightarrow$  Products, at  $T_2$  is

$$\Delta H(D - C) = \Delta H(\text{reaction, at } T_2)$$

$$= \Sigma \Delta H_f(\text{products, at } T_2) - \Sigma \Delta H_f(\text{reactants, at } T_2) \quad (2)$$

To heat the reactants from  $T_1$  (point A) to  $T_2$  (point C) requires that an enthalpy equal to the difference between C and A be added to the reactants. This enthalpy is mathematically given by the relationship:

$$\Delta H(C - A) = \int_{T_1}^{T_2} \Sigma C_p(\text{reactants}) dT \quad (3)$$

or equally well

$$= \Sigma(H - H_0)(\text{reactants, at } T_2) - \Sigma(H - H_0)(\text{reactants, at } T_1)$$

$$= \Sigma(H - H_{298})(\text{reactants, at } T_2) - \Sigma(H - H_{298})(\text{reactants, at } T_1) \quad (3')$$

$$= \Sigma(H - H_{298})(\text{reactants, at } T_1) \quad (3'')$$

Depending upon the availability of data,  $\Delta H(C - A)$  may be evaluated by summing the enthalpy terms  $H - H_0$  or  $H - H_{298}$  or by summing and integrating the heat capacity terms. The term  $\int_{T_1}^{T_2} \Sigma C_p(\text{reactants}) dT$  may be approximated over small temperature ranges by  $\Sigma C_p(\text{reactants})(T_2 - T_1)$ ; that is, by assuming the  $C_p$ 's are constant. (The abbreviation  $\Sigma C_p(\text{reactants})$  should be understood to mean the total heat capacity of all the reactants, and so the individual heat capacities must be weighed according to the amounts of substance involved.)

To heat the products from  $T_1$  (point B) to  $T_2$  (point D) requires that an enthalpy equal to the difference between D and B be added to the products. This enthalpy is mathematically exactly given by the relationship:

$$\Delta H(D - B) = \int_{T_1}^{T_2} \Sigma C_p(\text{products}) dT \quad (4)$$

or equally well  $= \Sigma(H - H_0)(\text{products, at } T_2) - \Sigma(H - H_0)(\text{products, at } T_1) \quad (4')$

or  $= \Sigma(H - H_{298})(\text{products, at } T_2) - \Sigma(H - H_{298})(\text{products, at } T_1) \quad (4'')$

The term  $\int_{T_1}^{T_2} \Sigma C_p(\text{products}) dT$  may be approximated over small temperature ranges by  $\Sigma C_p(\text{products})(T_2 - T_1)$  that is, by assuming the  $C_p$ 's are constant.

#### 21.6.2 Relationships between Enthalpies of Isothermal Reactions at Different Temperatures

The difference in enthalpy between points D and A (Figure 21.1) is constant for a given reaction. Advantage may be taken of this fact to demonstrate a method of calculating the relationship between  $\Delta H(\text{reaction, at } T_1)$  and  $\Delta H(\text{reaction, at } T_2)$ . The energy difference is independent of the path followed. Thus a path  $A \rightarrow C \rightarrow D$  may be followed or a path  $A \rightarrow B \rightarrow D$  may equally well be followed. An arbitrary path  $A \rightarrow D$ , represented by the diagonal may also be followed.

Mathematically:  $\Delta H(D - A) = \Delta H(D - C) + \Delta H(C - A) \quad (5)$

$$= \Delta H(D - B) + \Delta H(B - A) \quad (6)$$

Substituting quantities from the above discussion we have

$$\begin{aligned}\Delta H(D - A) &= \Delta H(\text{reaction, at } T_2) + \int_{T_1}^{T_2} \sum C_p(\text{reactants}) dT \\ &= \int_{T_1}^{T_2} \sum C_p(\text{products}) dT + \Delta H(\text{reaction, at } T_1)\end{aligned}\quad (7)$$

In the simple case where  $C_p$ 's are independent of  $T$ , the above relationship is sometimes simplified to the following:

$$\Delta H(\text{reaction at } T_2) = \Delta H(\text{reaction at } T_1) + \Delta C_p(T_2 - T_1) \quad (8)$$

in which  $\Delta C_p$  is the difference: heat capacity of products minus heat capacity of reactants.

### 21.6.3 Enthalpy Relations When the Temperature of the System is Allowed to Change (at Constant Pressure)

The enthalpy difference between point D and point A,  $\Delta H(D - A)$  is a function only of the ingredients of the system and the temperatures  $T_2$  and  $T_1$ . Pressure effects are negligible except in unusual cases. We shall consider only the isobaric process.\* For a given system, the difference,  $\Delta H(D - A)$ , is dependent on  $T_2$  and  $T_1$ . For a given system, if  $T_2$  and  $T_1$  are fixed, then  $\Delta H(D - A)$  is also fixed. The relevant relationships are given by equation (7). If a reaction occurs in which the reactants are at  $T_1$  (point A) and the products are at temperature  $T_2$  (point D), the enthalpy change is  $\Delta H(\text{observed})$ .

This appears or is evident as heat,  $Q = -\Delta H(\text{observed})$ .

Two extreme cases can be recognized.

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\* The only work done is presumed to be pressure-volume work.

(a) The adiabatic process. No heat transfer between the system and the external world occurs in the adiabatic process. Mathematically this is equivalent to saying

$$Q = -\Delta H(\text{observed}) = 0$$

Since  $\Delta H(\text{observed}) = \Delta H(\text{reaction, at } T_1) + \int_{T_1}^{T_2} \sum C_p(\text{products}) dT$  this means that for the adiabatic process,  $-\Delta H(\text{reaction, at } T_1) = \int_{T_1}^{T_2} \sum C_p(\text{products}) dT$ . This is a mathematical way of saying the enthalpy of reaction, being retained in the system, if exothermic causes the temperature of the products to rise an amount determined by their specific heat.

The temperature rise that will occur is often determined by a method of successive approximation. An estimate is made of the temperature rise. The specific heats are used to calculate the necessary  $-\Delta H(\text{reaction at } T_1)$ . If the value for  $-\Delta H(\text{reaction, at } T_1)$  calculated in this way is less than the true value obtained from the Tables, the estimated temperature is increased, and the process repeated. If the value calculated for  $-\Delta H(\text{reaction, at } T_1)$  is larger than the true value, the estimated temperature is decreased. The iteration is repeated until the calculated and tabular values of  $-\Delta H(\text{reaction, at } T_1)$  are as close to one another as desired.

(b) The isothermal process. Heat transfer between the system and the external world is complete in the isothermal process, so that the temperature of the system always remains at  $T_1$ . No practical system is completely adiabatic, and more

or less heat transfer will be encountered in any real reaction process. At the other extreme, the amount of heat transferred equals the negative of the enthalpy of the isothermal process,

$$-Q = \Delta H(\text{observed}) = \Delta H(\text{reaction at } T_1) + \int_{T_1}^{T_2} \sum C_p (\text{products}) dT$$

Since  $T_1 = T_2$  the second term of the right hand side is zero, and

$$Q = -\Delta H(\text{reaction, at } T_1)$$

The temperature rise of the products of reaction can be regulated by allowing the transfer of varying amounts of heat. The maximum possible temperature rise is, of course, the adiabatic temperature rise. This maximum temperature can be regulated to some extent by varying the composition of the system.

### 21.7 Reaction Equilibrium and Temperature

Data in the tables of this monograph and in additional tables of thermal functions referred to in Section 22.0 are suitable for calculations of thermodynamic equilibria at the final temperature in reactions involving a few or many species. We limit ourselves here to a very brief outline of the procedures and refer the reader to other sources for detailed procedures. Several references to more detailed presentations of the general problems of handling high temperature equilibria of multicomponent systems are found in Section 24.0. Because several parameters must be adjusted simultaneously or at least in a mutually consistent way and because many variables are present in a multicomponent system, the solution of such problems may be very time consuming and arduous unless assisted by rapid machine calculation. The techniques for using such aids change rather rapidly and the user may find being developed from time to time procedures that are more efficient in the use of machine time. All discussion presented here is based on an assumption of equilibrium in the gaseous state. Equilibrium may be quite closely reached in hot reacting systems; but even in the absence of equilibrium the results of equilibrium calculations may provide a useful approximation to the real situation. There is currently much work being done on the application of thermodynamics and kinetics to estimate dynamic non-equilibrium performance. Some such work is described in references in Section 24.0 (see, for example, references [5, 8, 29]).

When a complex mixture is allowed to react until it comes to equilibrium, two general limiting cases can be readily identified and described. (1) The resulting temperature is determined by the energy

of reaction--no energy losses being allowed. (2) Energy exchange is allowed, and the combustion products are brought to the same final temperature as the initial temperature. These two situations represent the adiabatic and isothermal process, respectively. The real situation lies somewhere in between. There are always some heat losses to the surroundings.

The equilibrium thermodynamic state of the system comprising the products of combustion can be completely described by specifying the composition and enthalpies of the initial materials that have been burned and the final pressure at which the products will be present. The final temperature and product composition will then be given in terms of four sets of simultaneous equations giving: (a) mass balance; (b) enthalpy balance; (c) pressure balance; and (d) chemical equilibria.

(a) The equations for the conservation of mass are summarized as equations (1A) and (1B).

$$\sigma_i = \sum_{k=1}^{\alpha} a_{ik} n_k \text{ for the reactants} \quad (1A)$$

As an initial step the number of gram-atoms,  $\sigma_i$ , of the  $i$ 'th element, which we shall identify as  $A_i$ , introduced into the reaction zone is calculated from equation (1A);  $\sigma_i$  is the sum of the number of gram-atoms of  $A_i$  in the substances introduced. There are  $\alpha$  different substances introduced, which we shall identify as  $B_k$ , and these are enumerated from  $k = 1$  to  $k = \alpha$ . The number of moles  $B_k$  is  $n_k$  and the subscript of  $A_i$  in the chemical formula of  $B_k$  is  $a_{ik}$ . If there are  $N$  elements present,  $i$  will range from 1 to  $N$  and there will be  $N$  such equations.

As an example let us consider a combustion mix introduced into the furnace and consisting of one kilogram of cellulose (monomer formula,

$C_6H_{10}O_5$ ; molecular weight, 242), one kilogram of benzene (formula,  $C_6H_6$ ; molecular weight, 80), and thirty kilograms of combustion air (approximate formula, 78%  $N_2$ ; 20%  $O_2$ ; 2%  $H_2O$ ; molecular weights,  $N_2$ , 28;  $O_2$ , 32;  $H_2O$ , 18).

The numbers of moles  $n_k$  of the various substances are calculated as follows [for simplicity approximate atomic weights are used]:

$$n_1 \text{ (cellulose)} = 1000/242 = 4.13 \text{ moles}$$

$$n_2 \text{ (benzene)} = 1000/80 = 12.50 \text{ moles}$$

$$n_3 \text{ ( $O_2$ )} = (0.20) (30000/32) = 187.50 \text{ moles}$$

$$n_4 \text{ ( $N_2$ )} = (0.78) (30000/28) = 835.71 \text{ moles}$$

$$n_5 \text{ ( $H_2O$ )} = (0.02) (30000/18) = 33.33 \text{ moles}$$

The numbers of gram atoms,  $\sigma_i$ , of the various elements are calculated as follows:

$$\sigma_1 \text{ (carbon)} = 6(4.13) + 6(12.50) = 99.78 \text{ gram atoms}$$

$$\sigma_2 \text{ (hydrogen)} = 10(4.13) + 6(12.50) + 2(33.33) = 182.96 \text{ gram atoms}$$

$$\sigma_3 \text{ (oxygen)} = 5(4.13) + 2(187.50) + 33.33 = 428.98 \text{ gram atoms}$$

$$\sigma_4 \text{ (nitrogen)} = 2(835.71) = 1671.42 \text{ gram atoms}$$

For this example  $N$  is 4 and  $\alpha$  is 5.

Having established the composition of the combustion mix a necessary step in the calculation of the mass balance is to list the presumed reaction products to be considered. This is a critical step, depending upon the judgement of the individual; there being no way a priori to establish definitively what products will be formed.

Referring to the above example we shall expect to find  $CO_2$ ,  $H_2O$ ,  $O_2$ , and  $N_2$  as major components of the combustion products. However, if care is to be used in controlling effluent gases we must also take into account

the possibility of formation of CO, NO, NO<sub>2</sub>, and HNO<sub>3</sub>. As a matter of procedure we shall also consider the gaseous monatomic elements, C, O, N, H, as being present. If the amount of oxygen is limited, one must also consider such possibilities as unburned or partially burned ingredients such as gaseous H<sub>2</sub>, CH<sub>4</sub>, CH, C<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, and HCO. There are a very large number of potential components resulting from incomplete combustion. The variety of potential products of combustion will increase rapidly as additional elements are included in the combustion mixture.

When this has been done, the number of gram-atoms of the elements can be expressed as the sum of their presence in the products of combustion by equation (1B).

$$\sigma_i = \sum_{j=1}^{\beta} a_{ij} n_j \text{ for the combustion products} \quad (1B)$$

In equation (1B),  $\sigma_i$  is the same series of quantities calculated by equation (1A). There are  $\beta$  presumed products of combustion, and there are  $n_j$  moles of product  $B_j$  in the formula in which the subscript of the element A<sub>i</sub> is  $a_{ij}$ .

Equations (1B) become:

$$\sigma_1 \text{ (carbon)} = n_C + n_{CO} = n_{CO_2} + n_{CH_4} + n_{CH} + 2n_{C_2} + 2n_{C_2H_2} + n_{HCO}$$

$$\sigma_2 \text{ (hydrogen)} = n_H + 2n_{H_2} + 2n_{H_2O} + 4n_{CH_4} + n_{CH} + 2n_{C_2H_2} + n_{HCO} + n_{HNO_3}$$

$$\sigma_3 \text{ (oxygen)} = n_O + 2n_{O_2} + n_{NO} + 2n_{NO_2} + n_{H_2O} + 3n_{HNO_3} + n_{CO} + 2n_{CO_2} + n_{HCO}$$

$$\sigma_4 \text{ (nitrogen)} = n_N + 2n_{N_2} + n_{NO} + n_{NO_2} + n_{HNO_3}$$

The values assigned to the n's cannot be made final without solving the equilibrium equations.

(b) Equation (2) is the equation for the conservation of energy in the case where all energy of reaction goes to heating the products of combustion.

$$\begin{aligned} \sum_{k=1}^{\alpha} n_k [\Delta H_f^{\circ} \text{ of } B_k + (H_{T_1} - H_{298}) \text{ of } B_k] \\ = \sum_{j=1}^{\beta} n_j [\Delta H_f^{\circ} \text{ of } B_j + (H_{T_2} - H_{298}) \text{ of } B_j] \end{aligned} \quad (2)$$

As before there are  $\alpha$  ingredient substances (or reactants)  $B_k$  in the combustion mix, and these are enumerated from  $k = 1$  to  $k = \alpha$ . The enthalpy contribution of each ingredient is given by a term on the left hand side of the equation and consists of the number of moles  $n_k$  times its enthalpy of formation at 298 K plus an enthalpy increment if the initial temperature  $T_1$  of the ingredients differs from 298 K.

The enthalpy requirements to form the products of combustion and bring them to the final temperature  $T_2$  are given by the right hand side of the equation. There are  $\beta$  combustion products  $B_j$  and these are enumerated from  $j = 1$  to  $j = \beta$ . The enthalpy requirement for each combustion product is given by a term which consists of the number of moles  $n_j$  times its enthalpy of formation at 298 K plus an enthalpy increment to bring its final temperature to  $T_2$ .

Note that the number of moles of each substance formed in the products will depend upon the temperature of the products, and this dependence will be particularly pronounced if some comparatively unstable combustion products can be formed. Therefore the quantities  $n_j$  must be made consistent with the requirements of the possible equilibria at the final temperature. The quantities  $n_k$ , on the other hand, depend only on the mixture burned.

Note also that if energy losses occur, such as losses through the furnace walls, the final temperature  $T_2$  will not be as high as if there were no such losses.

(c) Equation (3) is the pressure balance equation.

$$P_t = \sum_{j=1}^{\beta} P_j \quad (3)$$

In equation (3)  $P_t$  is the total pressure in the chamber where the combustion products are present, and  $P_j$  is the partial pressure of the  $j$ 'th product,  $B_j$ . The partial pressures are given in terms of the number of moles and the total pressure by equation (3'), assuming the fugacities

$$\frac{P_j}{P_t} = \frac{n_j}{\sum_{j=1}^{\beta} n_j} \quad (3')$$

are all proportional to the pressures. Note that the partial pressures can be calculated only after the mole ratios are known.

(d) Equations (4) and (4') are the equations for the reaction equilibria involved. There are various ways in which the equilibria may be specified. An unambiguous way which assures that all possible equilibria are implicitly included is to give the equilibrium constant of formation of each substance from the atoms of the elements present.

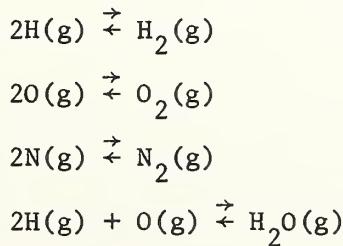
$$RT \ln K_j = RT \ln f_j - \sum_{i=1}^N a_{ij} \ln f_i \quad (4)$$

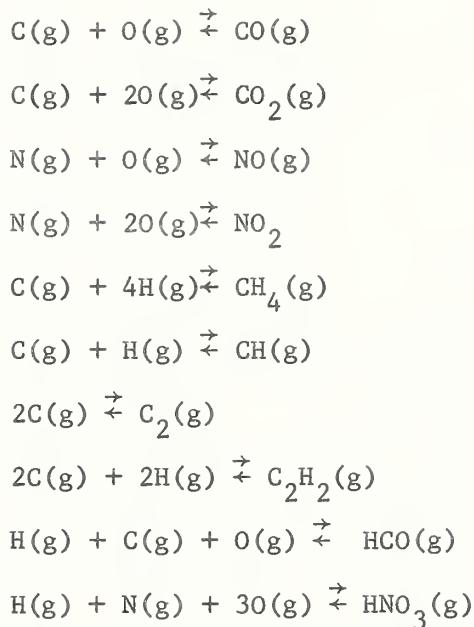
$$RT \ln K_j = (-\Delta H_f^\circ)_j - (G_T^\circ - H_o^\circ)_j + \sum_{i=1}^N a_{ij} [(\Delta H_f^\circ)_i + (G_T^\circ - H_o^\circ)_i] \quad (4')$$

The constant  $K_j$  is the equilibrium constant of formation of  $B_j$ , the  $j$ 'th constituent of the products, from the atoms of the elements. There are

N elements present, and so for each substance present the elements in it are enumerated from  $i = 1$  to  $i = N$ . The coefficient  $a_{ij}$  represents the subscript of element  $i$  in the formula for the substance  $B_j$ . The equilibrium constant can be expressed in two ways represented by equations (4) and (4') respectively. Equation (4) represents the definition of the equilibrium constant of formation from the gaseous monatomic elements in terms of the fugacities of the elements and of the combustion products,  $f_i$  and  $f_j$ , respectively. Equation (4') represents the equilibrium constant in terms of the Gibbs energies of the substance and of the elements respectively, and the enthalpy of reaction, which can be derived from the enthalpies of formation of the substance and the elements respectively. The reader should note that the elements as used in the equations (4) and (4') are not in their standard reference states, but are in the form of the gaseous monatomic species. The elimination of  $RT \ln K_j$  from equations (4) and (4') allows a single equation to represent the equilibrium for each reaction. For gases at not too high pressures the fugacity equals the pressure (i.e.,  $f_j = P_j$ ). For gases to which this equality does not apply, a correction term may have to be applied. For condensed phase products formed  $f_j$  is considered to be unity.

We may illustrate the equilibria involved in the previous example in the following way:





This sequence of reaction is sufficient to specify the equilibria involving the formation of the substances specifically listed above. It will be apparent from the above sequence of reactions that a number of the proposed species will be found only in extremely small quantities and a way can probably be found to reduce the number of equations by eliminating these species. In addition, it can easily become apparent that one or more additional species are important enough for inclusion. The criteria for inclusion will differ for different species depending upon contribution to the mass or pressure balance, toxicity, corrosiveness or other factors. The equilibria shown were chosen as a systematic way of identifying unambiguously a sufficient number of non-redundant equations including all the substances under consideration. An attempt to write down directly the equilibria that are of real importance may lead to problems because of redundancies or because they form an insufficient set. Provided that all substances of importance have been listed a set involving formation of a substance from the gaseous atoms such as those given above, includes implicitly or explicitly all equilibria of importance.

The mass balance equations for the combustion products can now be listed.

$$\sigma_1 \text{ (carbon)} = n(C) + n(CO) + n(CO_2) + n(CH_4) + n(CH) + 2n(C_2) \\ + 2n(C_2H_2) + n(HCO)$$

$$\sigma_2 \text{ (hydrogen)} = n(H) + 2n(H_2) + 2n(H_2O) + n(HNO_3) + 4n(CH_4) + n(CH) \\ + 2n(C_2H_2) + n(HCO)$$

$$\sigma_3 \text{ (oxygen)} = n(O) + 2n(O_2) + n(H_2O) + n(CO) + 2n(CO_2) + n(NO) \\ + 2n(NO_2) + n(HCO)$$

$$\sigma_4 \text{ (nitrogen)} = n(N) + 2n(N_2) + n(NO) + n(NO_2) = n(HNO_3)$$

The pressure balance equation can be written:

$$P_t = P(C) + P(CO) + P(CO_2) + P(CH_4) + P(CH) + P(C_2) + P(C_2H_2) \\ + P(HCO) + P(H) + P(H_2) + P(H_2O) + P(O) + P(O_2) + P(NO) \\ + P(NO_2) + P(HNO_3) + P(N) + P(N_2).$$

An iterative procedure for calculating equilibrium compositions and energies is as follows:

(1) Prepare equations for reactions that may participate in equilibria at the resulting temperature.

(2) Write mass balance equations for each element in terms of molecular species present based on combustion ingredients introduced.

(3) Write expressions for equilibrium constants.

(4) Assume a temperature  $T_2$  and a number of moles for each product and try the consistency of the equations. Calculate the number of moles of gas and test the material balance. If material imbalances result adjust  $n$ . When  $n$  has been adjusted to balance, the temperature,  $T_2$  and

moles of products  $n_j$  are consistent. This gives a product profile for a given  $T_2$ . However,  $T_2$  may be incorrect for the enthalpy. Calculate the enthalpies of the products at  $T_2$  (including enthalpies of formation and enthalpy increments to  $T_2$ ).

(5) Then repeat determinations of product profiles until enthalpies of products and of reactants are equal. This gives the correct  $T_2$ , and the remaining quantities, moles of each product, partial pressures, etc., are then correct.

A different approach is to find the composition of the combustion which minimizes Gibbs energy of the system. This approach is discussed in References [33] and [34] of Section 24.0. Only the principle of this method will be mentioned here. The procedures for carrying out a calculation may be found in reference [33].

The condition for a minimum (or a maximum) in a mathematical function is that the derivative or differential be zero. The condition for thermochemical equilibrium is that the Gibbs energy,  $dG$ , be a minimum for the system. This is expressed by the statement which sets the differential equal to zero (equation (5))

$$dG = 0 \quad (5)$$

At a fixed temperature and pressure and for a specified set of combustion products  $B_j$  the differential  $dG$  is given by equation (6).

$$dG = \sum_{j=1}^{\beta} \mu_j dn_j \quad (6)$$

Here  $dn_j$  is a differential change in the number of moles  $n_j$  of component  $B_j$ , and  $\mu_j$  is the chemical potential of the species  $B_j$ . The chemical

potential of  $B_j$  is the differential rate of change of the Gibbs energy of the system per mole of  $B_j$  added to the system (equation (7)).

$$\mu_j = \frac{\partial G}{\partial n_j} \quad (7)$$

For an ideal gas :

$$\mu_j = G_j^\circ + RT \ln P_j$$

This system is subject to the same constraints as before, that the mass balance must be maintained and that the energy balance must be maintained.

By consideration of all of the possible chemical products and maintaining the mass balance of the elements present, a set of mole numbers for the combustion products can be calculated which leads to a minimum Gibbs energy and equilibrium temperatures for the whole system by an iterative process.

## 22.0 Supplementary Sources of Thermodynamic Data on Chemical Substances and Materials

The following monographs are collections of thermodynamic data compiled from the original literature by competent thermochemists and presented in a well organized way. These sources have been selected to provide reasonably comprehensive coverage but are by no means a complete list of compilations of thermodynamic data. Except for the Landolt-Börnstein tables, foreign language compilations have not been included because of their limited accessibility. The extensive Russian compilations of thermodynamic tables are essentially very similar to some of the more comprehensive compilations listed here. Two general texts on thermodynamics and thermochemistry are also included.

1. Ashcroft, S. J., and Mortimer, C. T.

Thermochemistry of Transition Metal Complexes  
(Academic Press, London, New York, 1970).

This book surveys the literature to 1968 on energy processes involving transition metal complexes including both organic and inorganic ligands. A critical review of the thermochemical data for over 1500 systems of complexes is given. Comparable data from various sources are shown in juxtaposition. Values of  $\Delta H$ ,  $\Delta G$ , and  $\Delta S$  for various stages of complex formation are usually listed for processes in aqueous solution.  $\Delta H_f^\circ$ ,  $\Delta G_f^\circ$ ,  $\Delta S_f^\circ$  for crystalline complex substances are given where available. In many instances correlations of the data for various metals with a single ligand, and for various related complexes of a given metal, are given graphically or by means of bond-energy estimates based on the data.

2. Bain, R. W.

National Engineering Laboratory (NEL) Steam Tables, 1964

Physical Properties of Water and Steam 0-800°C, 0-1000 Bars

(Her Majesty's Stationary Office, Edinburgh)

These are typical steam tables, with data tabulated in SI units, except that pressure is in bars and temperature in °C. The tables were ratified by the Sixth International Conference on the Properties of Steam. An introduction to the tables is given. See also sources (8, 13).

3. Cox, J. D., and Pilcher, G.

Thermochemistry of Organic and Organometallic Compounds

(Academic Press, London, New York, 1970)

This monograph is a critical compilation of thermochemical data published since 1930. The heats of formation of some 3000 substances are listed, with estimates of error. Where enthalpies of vaporization are known or can be reliably estimated these are listed and in these cases the enthalpies of formation of both gaseous and condensed phases are given. Extensive introductory material presents experimental procedures and procedures for reduction of experimental data of the type found in the book. Applications of thermochemical data are given, and there is a section on methods of estimating enthalpies of formation of organic compounds.

## 4. Domalski, E. S.

Selected Values of Heats of Combustion and Heats of Formation  
of Organic Compounds Containing the Elements C, H, N, O, P, and S.  
(Journal of Physical and Chemical Reference Data 1, 221-277 (1972))

Selected values of the enthalpies of combustion and enthalpies of formation of 719 organic compounds are reported. These are essentially the same as in the present compilation, but the selected values are augmented by commentary and original source references. The Wiswesser Line Notation is also given for each compound. The methods used in updating older work are described.

5. Hilsenrath, J., Beckett, C. W., Benedict, W. S., Fano, L.,  
Hoge, H. S., Masi, J. F., Nuttall, R. L., Touloukian, Y. S.,  
and Woolley, H. W.

Tables of Thermal Properties of Gases

National Bureau of Standards Circular 564, (1955)

(U. S. Government Printing Office, Washington, D. C. 20402)

This monograph gives tables of compressibility factor, density, entropy, enthalpy, specific heat, specific-heat ratio, and sound velocity for the real gases: air, argon,  $\text{CO}_2$ , CO,  $\text{H}_2$ ,  $\text{N}_2$ ,  $\text{O}_2$ , and steam over the range 0.01 to 100 atm and to 3000 K (in most cases). It also gives ideal-gas thermodynamic functions to 5000 K. Vapor pressures, thermal conductivity, viscosity and Prandtl number are given over the range of available experimental data. Critical commentaries and descriptions of the analyses of the data are provided.

6. Hultgren, R., Orr, R. L., Anderson, P. D., and Kelley, K. K.  
Selected Values of Thermodynamic Properties of Metals and Alloys  
(John Wiley and Sons, Inc., New York, London, 1963).

This volume gives the results of critical evaluations of the thermodynamic properties of the 63 metallic elements and 168 alloy systems. Self-consistency of the data, consistency with known thermodynamic relationships, consistency with known phase diagrams, and agreement between similar measurements, formed the bases for selection of the values. Heat capacities ( $C_p$ ) at low and high temperatures and vapor pressure data are reviewed and references are given. Values are tabulated for  $C_p$ ,  $H_T - H_{298}$ , and  $-(G_T - H_{298})/T$ , for condensed and gas phases, with T as the principal variable; and values of P,  $\Delta G$ , and  $\Delta H$  of the vaporization process are given. Values for  $H_{298} - H_0$ ,  $S_{298}$ ,  $T_m$ ,  $\Delta H_m$  and  $\Delta S_m$ , and analytical expressions for  $H_T - H_{298}$  as functions of T are given.

A supplement containing information on three additional elements and 4 alloy systems was issued in 1966.

7. Joshi, R. M., and Zwolinski, B. J.

Vinyl Polymerization, Volume 1, Part I, edited by G. E. Ham  
(Marcel Dekker, Inc., New York, 1967)

Chapter 8: Heats of Polymerization and their Structural and Mechanistic Implications

The authors discuss experimental methods used to measure and derive heats of polymerization. A listing of experimental data on heats of

polymerization is provided for 81 organic polymerization reactions. Other tables give heats of formation, heats of vaporization, entropies, Gibbs' energies, equilibrium constants, rate constants and activation energies at 25°C for a variety of polymerization processes. A discussion of the structural influence upon the heat of polymerization is also given. At the end of the chapter, 164 references are cited.

8(a). Keenan, H. J., Keyes, F. G., Hill, P. G., and Moore, J. G.

#### Steam Tables

Thermodynamic Properties of Water, including Vapor, Liquid, and Solid Phases (International Edition, Metric Units)

(John Wiley and Sons, Inc., New York, London, Sydney, Toronto, 1969)

This book presents the results of a new and independent correlation of all the new thermodynamic data and all previously existing data. It constitutes a complete revision of the Keenan and Keyes Tables of 1936 and an extension of range to 1000 bars and about 1300°C.

Values of the thermodynamic properties specific volume, internal energy, enthalpy, and entropy are tabulated with pressure and temperature as parameters, for vapor-liquid equilibrium, vapor-solid equilibrium, superheated vapors, and compressed liquid. Mollier and temperature-entropy charts are included along with charts of heat capacity of liquid and vapor, Prandtl number, and isentropic expansion coefficient. A detailed table for the critical region shows volume and temperatures as parameters.

The present tables are in no sense a formulation of the International Skeleton Tables (1963). In general they are in good accord with, and their values fall within the tolerance of the International Skeleton Tables.

Exceptions are discussed. Extensive tables of viscosity and thermal conductivity are reproduced from the documents of the Sixth International Conference on the Properties of Steam.

Energy units are joules, temperatures are K or °C, pressures are in bars, volumes in  $\text{cm}^3$  and masses in grams. The data and tables are discussed in an appendix of 25 pages; and a list of 37 references is given. The introduction is in English, French, German, Italian, Japanese, Russian, and Spanish. See also sources (2, 13).

8(b). Keenan, J. H., Keyes, F. G., Hill, P.G., and Moore, J. G.

#### Steam Tables

Thermodynamic Properties of Water, including Vapor, Liquid,  
and Solid Phases (English Units)

(John Wiley and Sons, Inc., New York, London, Sydney, Toronto,  
1969).

This edition of the Steam Tables supplies the same basic information as source (8a) except that English units are used.

A review of the sources of data and comparison of derived tabulated values with experiment, and a summary of the equations used in deriving the tabulated data are given in an appendix of 29 pages. Tables for the vapor give specific volume, specific internal energy, specific enthalpy, and specific entropy at temperatures from 32° to 2400°F, and at pressure intervals from 0.2 to 15,000  $\text{lb/in}^2$ ; as well as several properties of the very low pressure gas. Similar tables are given for the liquid, covering somewhat different ranges. See also sources (2, 13).

## 9. Kelley, K. K.

Contributions to the Data on Theoretical Metallurgy

XV. A Reprint of Bulletins 383, 384, 393, and 406

Bureau of Mines Bulletin 601 (1962)

(U. S. Government Printing Office, Washington, D. C.)

This monograph is a reprint collection of previous monographs having the same principal title. The subtitles of these are listed below.

III. The Free Energies of Vaporization and Vapor Pressures of Inorganic Substances. Bureau of Mines Bulletin 383 (1935).

IV. Metal Carbonates--Correlations and Applications of Thermodynamic Properties. Bureau of Mines Bulletin 384 (1935).

V. Heats of Fusion of Inorganic Substances. Bureau of Mines Bulletin 393 (1936).

VII. The Thermodynamic Properties of Sulfur and Its Inorganic Compounds. Bureau of Mines Bulletin 406 (1937).

This volume together with Bureau of Mines Bulletins 542, 584, and 592 constitute a complete set of the thermodynamic data series.

A typical presentation of the selected data for vaporization gives  $C_p(g)$ ,  $C_p(liq)$ ,  $C_p(c)$ ,  $\Delta C_p$ ,  $\Delta H_{vap}$ ,  $\Delta G_{vap}$  as analytical equations in temperature, and values of  $\Delta H_{298}$ ,  $S_{298}$ , and  $T_b$ . The monograph on metal carbonates gives selected values and equations for  $C_p$ ,  $S$ ,  $\Delta G_f^\circ$ ,  $\Delta H_f^\circ$  for  $CO$ ,  $CO_2$ ,  $H_2O$ , carbonate(aq) and bicarbonate(aq) ions, and 25 metal carbonates or bicarbonates. A table of dissociation pressures is given. The monograph on enthalpies of fusion gives selected values of  $\Delta H_m$  for

63 elements and many of their compounds. The monograph on sulfur compounds gives similar information for elemental sulfur, a few gaseous non-metallic compounds, and for the sulfides and sulfates. Illustrations of the uses of thermochemical data, critical discussions of the source data, and bibliographies are given in each monograph.

10. Kelley, K. K.

Contributions to the Data on Theoretical Metallurgy  
XIII. High-Temperature Heat-Content, Heat-Capacity, and Entropy  
Data for the Elements and Inorganic Compounds.  
Bureau of Mines Bulletin 584, (1960).  
(U. S. Government Printing Office, Washington, D. C.)

This comprehensive monograph gives procedures used in the correlations, and gives selected values, tables, and analytical functions in temperature for the subject thermodynamic data of several hundred substances. A bibliography of sources is provided. The breadth of coverage is very great. Substances for which data are provided include the first 92 elements and many of their acids, oxides, carbides, nitrides, hydrides, hydroxides, halides, carbonates, nitrates, phosphates, sulfates, borates, cyanides, mixed oxides and intermetallic compounds.

11. Kubaschewski, O., Evans, E. Ll., and Alcock, C. B.

Metallurgical Thermochemistry, 4th Edition

(Pergamon Press, Oxford, New York, and other cities, 1967)

This monograph is a standard reference work for metallurgists, and deals with the thermochemistry in a rather broad way with special emphasis on inorganic compounds and alloys. About 140 pages of tables of thermochemical data are given in which are presented  $\Delta H_f^\circ$ ,  $S^\circ$ ,  $T_{trans}$ ,  $T_m$ ,  $T_b$ , structural information,  $\Delta H_m$ ,  $\Delta H_{vap}$ , and  $\Delta H_{subl}$ , for elements and compounds.

Constants of analytical expressions for  $C_p$ , the vapor pressure, and  $\Delta G_f^\circ$  or  $\Delta G$  for a reaction, with temperature as the variable, together with the temperature range of applicability, are given for many substances. A separate table gives the thermodynamic properties of mixing for alloys. The tabulated data are derived from other compilations and the original literature.

The accompanying text, comprising some 300 pages, gives the theoretical basis of the deviation and application of thermochemical data, a discussion of the estimation of thermochemical data, and examples of thermochemical treatment of metallurgical problems.

12. Merrill, A. L., and Watt, B. K.

(a) Energy Value of Foods; Basis and Derivation  
Agriculture Handbook No. 74, 1955.

(b) Watt, B. K., and Merrill, A. L.  
Composition of Foods; Raw, Processed, Prepared  
Agriculture Handbook No. 8, revised, 1963

(U. S. Government Printing Office, Washington, D. C. 20402)

This pair of monographs provides numerous composition and energy values for food and foodstuff ingredients. It should be noted, of course, that the Calorie used in food energy values is 1 kcal as used in this handbook. In Agriculture Handbook No. 74, Part I gives a discussion of the sources of food energy in terms of organic compound class, and of the experimental determination of heats of combustion. Parts II, III, and IV apply the data to physiological processes. An appendix gives composition and heat of combustion of foods. Tables 1-5 and table 24 give heats of combustion of specific food items or component substances. Care should be used in taking values from the numerous tables, as correction factors have sometimes been applied to adjust for physiological processes. These adjustments are indicated by footnotes. In Agriculture Handbook No. 8, Appendix A is of particular interest as it gives notes on energy values and nutrients, including (adjusted) heats of combustion of many foods and food ingredients.

13. Meyer, C. S., McClintock, R. B., Silvestri, G. J., and Spencer, R. C., Jr.

ASME Steam Tables 1967

Thermodynamic and Transport Properties of Steam; comprising Tables and Charts for Steam and Water

(American Society of Mechanical Engineers, New York, N.Y., 10017)

These tables give an introductory discussion of their source. Nine tables and thirteen charts of thermodynamic properties are given. The data were computed from equations adopted in the IFC\*, Formulation for

\*International Formulation Committee of the Sixth International Conference on the Properties of Steam.

Industrial Use, which is reproduced. Reference is made to computer procedures for handling the source equations. Three tables of transport properties are given, based on the skeleton tables and empirical equations developed by the Sixth International Conference. The principal tables are in U. S. Customary units. See also sources (2, 8).

14. Pitzer, K. S., and Brewer, L.

Thermodynamics: Gilbert N. Lewis and Merle Randall (Second edition)  
(McGraw Hill Book Company, Inc., New York, Toronto, London, 1961)

This monograph on thermodynamics and its application to physics and chemistry is a revision and updating of the classical work by Lewis and Randall, that did much to shape the development of thermodynamics in the 20th century. It provides a reasonably complete presentation of the principal subjects of thermodynamics. In addition it provides in the appendices (among other subjects) tables and discussions of (1) properties of normal solutions, (2) properties of gaseous solutions, (3) a tabular summary of thermodynamic formulas, (4) tables of thermodynamic properties. The latter tables include  $\Delta H_f^\circ_{298}$  and  $-(G^\circ - H^\circ_{298})/T$  for halides, oxides, sulfides and related compounds, carbides, and nitrides, at 298, 500, 1000, 1500, and 2000 K. Values of  $-(G - H_0^\circ)/T$  at the same temperatures,  $H_0^\circ - H_0^\circ$ , and  $\Delta H_f^\circ_0$  are given for some of the elements. Also,  $-(G - H_0^\circ)/T$  at the same temperatures,  $\Delta H_f^\circ_{298}$ ,  $\Delta H_f^\circ_0$ , and  $H_0^\circ - H_0^\circ$  are given for some gaseous carbon compounds, halides, oxides, hydrides, and related compounds. Sources of data are given.

15. Rossini, F. D., Pitzer, K. S., Taylor, W. J., Ebert, J. P., Kilpatrick, J. E., Beckett, C. W., Williams, M. D., and Werner, H. G.

Selected Values of Properties of Hydrocarbons

National Bureau of Standards Circular C461, (1947).

(U. S. Government Printing Office, Washington, D. C.)

This monograph was prepared as part of the work of the American Petroleum Institute (API) Research Project 44. Values are given for some 36 physical and thermodynamic properties of several hundred hydrocarbons in metric and in U. S. Customary units. The data in most instances represent values found from careful studies, many of which were done in connection with the same API Research Project. Experimental data are supplemented by theoretical calculations or empirical correlations. References to the source data and a bibliography are given. The data in many instances are identical to those in the Carnegie Press publication by the same name listed below. See also source (16).

16. Rossini, F. D., Pitzer, K. S., Arnett, R. L., Brown, R. M., and Primentel, G. C.

Selected Values of Physical and Thermodynamic Properties of

. Hydrocarbons and Related Compounds

(Carnegie Press, Pittsburgh, Pennsylvania, 1953)

This monograph resulted from the work of American Petroleum Institute (API) Research Project 44. Values are given for 40-odd physical and thermodynamic properties of several hundred hydrocarbons in metric and U. S. Customary units. The data in most instances represent selected values from

careful studies, many of which were done in connection with the same API Research Project. Experimental data are supplemented by theoretical calculations or empirical correlations. References to the source data and a bibliography are given. The data in many instances are identical to those in NBS Circular C461, listed above. See also source (15).

17. Rossini, F. D., Wagman, D. D., Evans, W. H., Levine, S., and Jaffe, I.  
Selected Values of Chemical Thermodynamic Properties .  
National Bureau of Standards Circular 500 (1952)  
(U. S. Government Printing Office, Washington, D. C. 20402)

This was for many years the most comprehensive authoritative compilation of thermochemical data at 298.15 K for inorganic substances. All inorganic substances and organic substances containing two carbon atoms or fewer per molecule are included if thermodynamic data exist for calculating one of the properties tabulated. Properties tabulated in Part I are  $\Delta H_f^\circ$ ,  $\Delta H_f^\circ_{298}$ ,  $\Delta G_f^\circ_{298}$ ,  $\log K_f$ ,  $S^\circ_{298}$ , and  $C_p^\circ_{298}$ . Properties tabulated in Part II are temperature, pressure, enthalpy change, entropy change and heat capacity change for the phase changes: transition, fusion, and vaporization. The data from original sources were critically evaluated by competent thermochemists and best values selected for the functions tabulated, maintaining internal consistency by the relationship:  $\Delta G_f^\circ_{298} = \Delta H_f^\circ_{298} - T\Delta S^\circ_{298}$ . The sources of data for each data item are listed and a bibliography is included. Some information in this book can still not be found readily elsewhere as the revision is not yet complete. See Wagman, et al, (source [24]) below.

## 18. Schäfer, D., and Lax, E. (editors)

Landolt-Börnstein

Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie,  
Geophysik, und Technik, Sechste Auflage

Eigenschaften der Materie in Ihren Aggregatzuständen

4 Teil, Kalorische Zustandgrößen

(Springer-Verlag, Berlin, Göttingen, Heidelberg, 1961)

This most recent issue of thermodynamic information of the famous Landolt-Börnstein series gives thermal properties: molar heat capacity, entropy, enthalpy, enthalpy of formation, Gibbs energy of formation, in the standard state, and enthalpies of phase changes for many organic and inorganic substances in SI units. The dependence of thermal functions and heat capacity upon temperature is given for many substances. Some other thermodynamic quantities are given. Extensive tables are given of group contributions to enthalpy of formation and the Gibbs energy of formation of organic substances (gases) in  $\text{kcal mol}^{-1}$  and  $\text{kJ mol}^{-1}$ . Many of the heat capacity data are presented in diagrams.

## 19. Stern, K. H., and Weise, E. L.

High Temperature Properties and Decomposition of Inorganic Salts

Part 1. Sulfates - NSRDS-NBS-7 (1966)

Part 2. Carbonates - NSRDS-NBS-30 (1969)

(U. S. Government Printing Office, Washington, D. C.)

These two monographs treat the thermodynamics and kinetics of decomposition of sulfates of over 60 metals, and carbonates of over 21 metals in a systematic way. The general features of the decomposition chemistry, phase transition temperatures, densities, and decomposition equilibria as functions of temperature are discussed. Also the mechanism of endothermic solid state decomposition, kinetic equations, and surface area changes during decomposition, and several parameters affecting rate of decomposition are discussed. These parameters include pressure, activation energy, method of preparation, heat transfer and crystal imperfections. Data given for each of the substances involved include density, thermal expansion coefficient, transition temperatures, entropy at 298 K, enthalpy of formation at 298 K, as well as the following functions of temperature: Gibbs energy of decomposition, equilibrium constant K and Log K of decomposition, and the Gibbs energy functions  $-(G^\circ - H_{298}^\circ)/T$ . The coverage is not uniform as all the data have not been measured for all the compounds. The substances involved are  $SO_3$ ,  $SO_2$ ,  $O_2$ ,  $CO_2$ , CO, the carbonates, the sulfates, and the oxides. The values obtained are the results of a critical review of the original literature sources.

20. Stull, D. R., and Prophet, H., editors

JANAF Thermochemical Tables, 2nd Edition, 1971

National Standard Reference Data Series NSRDS-NBS 37, (1971)

(U. S. Government Printing Office, Washington, D. C. 20402)

This work appeared first as a series of loose-leaf data sheets, revised at intervals as new information became available. Each sheet

was dated. The first bound edition of the work (1965-1966) was issued by the Clearinghouse for Federal Scientific and Technical Information (since changed to: National Technical Information Service) as Document PB-168370 and supplements. This has been somewhat revised for the second edition. Approximately 1000 compounds, elemental molecules, and atomic species, including a few gaseous ions, are included in this work. The elements included were selected for relevance in rocket propellant ingredients or products of combustion, and hence the elements of lower atomic weight and substances formed from them predominate. However a few heavier elements such as Pb, Hg, and W are included. Thermal functions  $C_p^\circ$ ,  $S^\circ$ ,  $-(G^\circ - H_{298}^\circ)/T$ ,  $H^\circ - H_{298}^\circ$ ,  $\Delta H_f^\circ$ ,  $\Delta G_f^\circ$ , and Log  $K_p$  are tabulated from 0 to 6000 K or to a lower temperature limit of meaningful data.  $\Delta H_f^\circ$  at 0 K and 298 K,  $S_{298}^\circ$ ,  $\Delta H_m$  and  $T_m$  as well as spectroscopic information needed for statistical mechanical computation of thermodynamic properties are listed. The sources of data are listed and briefly discussed. A lengthy introduction discusses sources, methods of treatment, and methods of application of the tables.

21. Stull, D. R., and Sinke, G. H.

Thermodynamic Properties of the Elements

Advances in Chemistry Series, Number 18

(American Chemical Society, Washington, D. C., 1956)

Tabulated values of  $C_p^\circ$ ,  $H^\circ - H_{298}^\circ$ ,  $S^\circ$ ,  $-(G^\circ - H_{298}^\circ)/T$ ,  $\Delta H_f^\circ$ ,  $\Delta G_f^\circ$ , and log  $K_f$  are given for the solid, liquid, and gas states of the first 92 elements over the temperature range 298 to 3000 K. Also given, where

available, are  $H_{298}^\circ - H_0^\circ$ , temperatures of phase changes and the associated enthalpy changes, and critical constants. The source data for each element are cited and briefly discussed. While now 15 years old, this book is still the most convenient reference for high temperature properties of some of the heavier elements.

22. Stull, D. R., Westrum, E. F., and Sinke, G. H.

The Chemical Thermodynamics of Organic Compounds

(John Wiley and Sons, Inc., New York, London, Sydney, Toronto, 1969)

This monograph is divided into three parts. The first part gives theoretical basis and principles of thermodynamics and thermochemistry, some experimental and computational methods used, and some applications to industrial problems. The second part gives thermal and thermochemical properties in the ideal gas state from 298 to 1000 K. In this section, the sources of data are listed and discussed and standardized tables are presented for 918 organic compounds. Values of  $C_p^\circ$ ,  $S^\circ$ ,  $-(G - H_{298}^\circ)/T$ ,  $H^\circ - H_{298}^\circ$ ,  $\Delta H_f^\circ$ ,  $\Delta H_f^\circ$ , and  $\log K_p$  are given at 100 K intervals. In the third section are listed selected values of enthalpy of formation, entropy, and consistent values of  $\Delta G_f^\circ$  and  $\log K_p$  of organic compounds at 298 K. In excess of 4000 compounds are listed. A very few inorganic compounds are also found in this book. A chapter very briefly discusses methods of estimating thermodynamic quantities.

23. Touloukian, Y. S.

Retrieval Guide to Thermophysical Properties Research Literature  
(McGraw Hill Book Co., New York, 1960- )

These volumes, which are a continuing series, contain thoroughly cross-indexed references to the source literature for bulk transport and thermodynamic properties. The properties first covered are: thermal conductivity, specific heat, viscosity, thermal radiative properties, thermal diffusivity, diffusivity, diffusion coefficient, and Prandtl number. A limited but continually increasing number of data sheets are available on materials and pure substances, giving charts and tabulated values based on a critical evaluation, analysis, and correlation of existing data. These are separately supplied by the Thermophysical Properties Research Center (Purdue University) on a subscription basis. These comprise the Data Book: Volume I, Metallic Elements and Their Alloys; Vol. II, Non-metallic Elements, Compounds, and Mixtures (in Liquid and Gaseous States at Normal Temperature and Pressure); and Vol. III. Non-metallic Elements, Compounds, and Mixtures (in the Solid State at Normal Temperature and Pressure).

24. Wagman, D. D., Evans, W. H., Parker, V. B., and (in various individual parts) Halow, I., Bailey, S. M., Schumm, R. H., Churney, K. L.

Selected Values of Chemical Thermodynamic Properties  
National Bureau of Standards Technical Note 270, October 1965  
(and continuing)

(U. S. Government Printing Office, Washington, D. C. 20402)

This technical note is a revision of NBS Circular 500 Part I (see above) and is issued in parts as segments of the work relating to selected sequences of elements are completed. The following parts had been issued as of 1971.

270-1 Tables for the first twenty-three elements in the standard order of arrangement

270-2 Tables for elements 24-32 -- elements in the standard order of arrangement

270-3 Tables for the first thirty-four elements in the standard order of arrangement

270-4 Tables for elements 35-53 in the standard order of arrangement

270-5 Tables for elements 54-61 in the standard order of arrangement

270-6 Tables for the alkaline earth elements, elements 92-97 in the standard order of arrangement.

The remaining elements will be covered in two or three additional parts to appear over a period of about two years. Documentation and references have not yet been issued.

This is the most comprehensive recent compilation in English of critically evaluated thermochemical data at 298.15 K for inorganic substances. All inorganic substances and organic substances containing two carbon atoms or fewer per molecule are included if thermodynamic data exist for calculating any of the properties tabulated. The coverage when complete will be approximately 12,000 substances. Properties tabulated are  $\Delta H_f^\circ$ ,  $\Delta H_f^\circ_{298}$ ,  $\Delta G_f^\circ$ ,  $H^\circ_{298.15} - H^\circ_0$ ,  $S^\circ_{298}$ ,  $C_p^\circ_{298.15}$ . The data from original sources have been critically evaluated by competent thermochemists and best values selected for the functions tabulated, maintaining internal consistency by the relationships  $\Delta G_f^\circ_{298} = \Delta H_f^\circ_{298} - T\Delta S^\circ_{298}$ , and  $\Delta H_f^\circ_{298} = \Delta H_f^\circ_0 + \sum (H^\circ_{298} - H^\circ_0)$ .

25. Watt, B. K. and Merrill, A. L. (see Merrill, A. L. and Watt, B. K., source 12).

26. Wicks, C. E., and Block, F. E.

Thermodynamic Properties of 65 Elements - Their Oxides, Halides, Carbides, and Nitrides

Bureau of Mines Bulletin 605, (1963).

(U. S. Government Printing Office, Washington, D. C.)

Part I of this monograph is a seven page introduction to the application of thermodynamic functions, with particular reference to metallurgical process. Part II gives tabular data and graphs of enthalpy, enthalpy of formation, and Gibbs energy, for the substances listed in the title. Also listed are  $S_{298}$ ,  $T_m$ ,  $\Delta H_m$ ,  $T_b$ ,  $\Delta H_v$ , and analytic expressions for  $C_p$ ,  $H_T - H_{298}$ , and  $G_T - H_{298}$ . The units are the calorie, the mole, and the kelvin. References to sources of information are given. The sources included original sources, reviews by other groups, and estimates. The data are, therefore, of very non-uniform reliability.

27. Wilhoit, R. C., and Zwolinski, B. J.

Handbook on Vapor Pressures and Heats of Vaporization

of Hydrocarbons and Related Compounds (API 44 - TRC)

(Thermodynamics Research Center, Texas A and M Research Foundation, College Station, Texas, 1971)

This handbook gives subject data on 680 hydrocarbons, 95 sulfur compounds, and water from 0 to 150°C. It is indexed by compound name, and by boiling point.

28. Zemansky, M. W.

Heat and Thermodynamics, 5th edition

(McGraw Hill Book Company, New York, Etc., 1968)

This well known textbook provides a clear pedagogical presentation of the principal subjects of thermodynamics.

### 23.0 Methods of Estimation of Thermodynamic Data

Because of the essentially unlimited number of possible organic compounds, and the very large number of inorganic compounds, the probability of encountering a substance or material for which the thermodynamic properties have not been measured is quite large. Methods of estimation are, therefore, essential to supplement tabulated values of thermodynamic properties based on experimental studies. Some guides to the more commonly used methods are listed below. This is by no means a complete list, as there have been some hundreds of studies of methods of correlation or estimation.

#### 1. American Society for Testing and Materials

Estimation of Net Heat of Combustion of Aviation Fuels

ASTM Method of Test D-1405

ASTM Standards, Part 17, Petroleum Products

(American Society for Testing and Materials, Philadelphia, Penn;  
annual)

This method of test allows an estimate accurate to about 0.5 percent to be made of net heat of combustion of petroleum fuels having well defined characteristics. Fuels included are certain classes of aviation gasoline, jet engine fuels and kerosines. The required measurements are aniline point and API gravity, which are routine laboratory tests applied to most batches of petroleum products. The estimates have reduced validity if applied to fuels not meeting the specifications for which the method was developed. The experimental studies and the correlations were performed at the National Bureau of Standards.

2. American Society for Testing and Materials

(1) Proposed Method for Estimation of Net and Gross Heat of

Combustion of Burner and Diesel Fuels

ASTM Standards, Part 17, Petroleum Products, January 1969,

Appendix XI, D-2-1968

(2) Proposed Method of Test for Estimation of Net Heat of

Combustion of Distillate and Residual Fuels

ASTM Standards on Petroleum Products, December 1962, Vol. I,

Appendix XII, D-2-1962, pp. 1247-1259.

(American Society for Testing and Materials, Philadelphia, Penna)

These tables, relating net and gross heat of combustion to API gravity of diesel and burner fuels and distilled and residual fuels were published for information by ASTM Committee D-2 on Petroleum Products and Lubricants, but failed of acceptance as a standard method of test. The deviations of individual actual fuels from the correlation and the disagreement between these two sets of tables occurs principally in the very low API-gravity range. The estimate of net heat of combustion may still be expected to be valid to within a few percent. It is necessary to measure API gravity in order to use this method for a particular batch of fuel.

3. Benson, S. W.

Thermochemical Kinetics

Methods for the Estimation of Thermochemical Data and Rate Parameters

(John Wiley and Sons, Inc., New York, London, Sydney, 1968)

This monograph gives tables of necessary data and descriptions of methods of their use for calculating  $\Delta H_f$ ,  $C_p$ , and  $S$ , at  $25^\circ C$  for gas phase mole-

cules and radicals and for extrapolating them to higher temperatures. The procedures can be applied to hydrocarbons, oxygen-containing compounds, nitrogen-containing compounds, haloalkanes, organo-sulfur compounds, and organo-metallic compounds; and deal principally with organic compounds.

4. Benson, S. W., Cruickshank, F. R., Golden, D. M., Haugen, G. R., O'Neal, H. E., Rogers, A. S., Shaw, R., and Walsh, R.  
Additivity rules for the estimation of thermochemical properties.  
*Chem. Rev.* 69, 279-324 (1969)

This lengthy technical article gives procedures for calculating the properties  $\Delta H_f^\circ$ ,  $S^\circ$ ,  $C_p^\circ$ , for organic compounds in the gas phase. Parameters for calculating  $C_p$  are given for temperatures from 300 to 1500 K at intervals. The availability of  $C_p$  at T allows calculation of  $\Delta H_f^\circ$  and  $S^\circ$  at the same temperatures. The necessary constants for making the calculations are given for individual chemical groupings in some 38 tables. Many classes of functional groups and molecular conformations are included. Examples are given comparing calculated and observed values. Agreements of 1 kcal mol<sup>-1</sup> or less in  $\Delta H_f^\circ$  and 1 cal mol<sup>-1</sup> K<sup>-1</sup> or less in  $C_p^\circ$  and  $S^\circ$  are generally found.

5. Bondi, A.

*Physical Properties of Molecular Crystals, Liquids, and Glasses*  
(John Wiley and Sons, Inc., New York, London, Sydney, 1968)

This monograph is designed for the use of chemical engineers to estimate physical properties needed in design calculations, as well as of physical chemists and synthetic chemists who need to understand the relationship between structure and physical properties. Correlations of several kinds

are described in the text. These are then restated as methods for estimation of the properties.

Substances considered include non-polar and polar gases, non-polar and polar liquids, associated liquids, crystalline solids, glasses, polymers, and polymer melts, as well as others. Procedures given include many variants, depending upon the properties given as initial information. Among the properties for which procedures are given are: density, heat capacity, enthalpy, entropy, enthalpy and entropy of fusion, enthalpy of sublimation and vapor pressure, cubical thermal expansion coefficient, bulk modulus, Young's modulus, compressibility, thermal conductivity, rotational diffusion constant, relaxation times, mass diffusion, viscosity, and others.

#### 6. Cox, J. D., and Pilcher, G.

Thermochemistry of Organic and Organometallic Compounds  
(Academic Press, London, New York, 1970)

In this monograph, Chapter 7, "Some Theoretical Applications of Thermochemical Data", gives a discussion of the application of schemes for calculating  $\Delta H_f$  (or equally well,  $\Delta H_c$ ).

The group-contribution method of Benson and Buss is discussed and tables of group contributions are given. The bond-energy schemes (by which  $\Delta H$  (atomization) and hence  $\Delta H_f$  or  $\Delta H_c$  can be calculated) developed by Laidler, and by Allen, are discussed and tables of contributing terms are given. Other schemes developed by Tatevskii, Platt, Greenshields-Rossini, and Somayajulu-Zwolinski, are briefly described. Special factors affecting these methods are discussed and illustrated including

steric effects, ring strain, and resonance. The accuracy of the estimates is discussed and examples of the use of the methods are given.

7. Janz, G. J.

Thermodynamic Properties of Organic Compounds

Estimation methods, principles and practice (revised edition)

(Academic Press, Inc., New York, London, 1967)

This well established monograph discusses computation of thermodynamic properties such as heat capacities, entropies, enthalpies and Gibbs energies by statistical mechanical methods, by methods of structural similarity, by methods of group contributions, by methods of group equations, and by methods of generalized vibrational assignments. The chemical properties: enthalpy of formation, and enthalpy of combustion are treated in terms of bond energies and group increments. Some 78 tables are given of increments, group contributions, and bond contributions as specifically needed for estimation of particular properties.

8. Joshi, R. M., and Zwolinski, B. J.

Vinyl Polymerization, Volume 1, Part I, edited by G. E. Ham

(Marcel Dekker, Inc., New York, 1967)

Chapter 8: Heats of Polymerization and their Structural and Mechanistic Implications

The application of various semi-empirical bond-energy schemes to the calculation of heats of polymerization are discussed.

9. Kubaschewski, O., Evans, E. Ll., and Alcock, C. B.

Metallurgical Thermochemistry, 4th edition

(Pergamon Press, Oxford, New York, and other cities, 1967)

This book contains a chapter of 35 pages on estimation of thermochemical data. Methods are given for calculation of heat capacities ( $C_p$ ) of gases, solids, and liquids, and constants are given for estimating  $\Delta C_p$  for some reactions involving gases. Estimation of entropies and enthalpies of evaporation and fusion is briefly treated. Tables and charts are given for estimating entropies of solids and gases. Charts are given illustrating regularities in enthalpies of formation of compounds, and special attention is given to estimating enthalpies of formation of inter-metallic compounds and sulfides, selenides, and tellurides.

10. Mason, D. M., and Eakin, B. E.

Calculation of Heating Value and Specific Gravity of Fuel Gases  
Institute of Gas Technology Research Bulletin 32, (1961), 18 pp.  
(Institute of Gas Technology, Chicago, Illinois )

This pamphlet gives procedures for calculating heating value and specific gravity of a gaseous fuel from an analysis of its component substances. It is applicable to commercial fuel gases. Compressibility factors are taken into account. The heating value calculation has errors less than 1%.

11. Pauling, L.

The Nature of the Chemical Bond, 3rd edition  
(Cornell University Press, Ithaca, New York, 1960 )

This well established monograph provides general information about the nature of chemical binding in (principally) inorganic compounds which is fundamentally very important for the estimation of enthalpies of formation, but not always easily applied.

## 12. Pitzer, K. S., and Brewer, L.

Thermodynamics: Gilbert N. Lewis and Merle Randall, 2nd edition  
(McGraw Hill Book Co., New York, etc., 1961)

Chapter 32 of this book describes methods for estimating entropies and other thermodynamic properties. The emphasis is on entropy, but energies of inorganic substances are also briefly treated showing the use of a Born-Haber cycle. Ad hoc procedures are suggested for estimating enthalpies of formation of inorganic compounds for which data are not available.

## 13. Reid, Robert C., and Sherwood, T. K.

The Properties of Gases and Liquids, their Estimation and Correlation, 2nd edition.  
(McGraw Hill Book Co., New York, etc., 1966)

This lengthy monograph follows the procedure of discussing various methods available for calculating or estimating particular properties of particular materials, and then provides recommendations for action with respect to each kind of property. Included in the book are procedures for making estimates of critical constants, normal boiling temperatures, Lennard-Jones-potential parameters, compressibility factors and equations of state, liquid molal volumes and densities, and vapor pressures. Estimates of enthalpies of vaporization, and of ideal-gas heat capacities, enthalpies and Gibbs energies of formation are treated. For real fluids variations of enthalpy, entropy, internal energy, and heat capacity with pressure are treated. Some methods are given for estimating the properties of fluid mixtures. Surface tension and the transport properties

--viscosity, diffusion coefficient and thermal conductivity--are discussed. Numerous tables present comparisons of observed and calculated properties.

14. Schafer, K., and Lax, E. (editors)

Landolt-Börnstein

Eigenschaften der Materie in Ihren Aggregatzuständen

4 Teil. Kalorische Zustandsgrossen, pp. 18-32

(Springer-Verlag, Berlin, Gottingen, Heidelberg, 1961)

Extensive tables are given of group contributions to enthalpy of formation and Gibbs energy of formation of organic substances (gases) in  $\text{kcal mol}^{-1}$  and  $\text{kJ mol}^{-1}$ . They form a suitable basis for estimating properties of gases.

15. Tatevskii, V. M., Benderskii, V. A., and Yarovoī, S. S.

Rules and Methods for Calculating the Physico-chemical Properties  
of Paraffinic Hydrocarbons

(Translated from the Russian by M. F. Mullins and edited by B. P.  
Mullins)

(Pergamon Press, New York, Oxford, London, Paris, 1961)

This monograph is a summary and a consolidation of the results of some years of work by Tatevskii and others, extending and elaborating some procedures introduced by Rossini and others. It suffers from ambiguity of statement which is somewhat distracting, but the methods presented in it have been attracting increasing attention recently. Properties calculated include: molar volume, molar refraction, vapor pressure, enthalpy of formation from atoms or elements, Gibbs energy of formation, and

enthalpy of combustion. Three different methods are used. Tables of constants and illustrations of the accuracy of the methods are given.

24.0 Selected References on Combustion and High Temperature Reaction Equilibria

1. Bahn, Gilbert S., and Zukoski, Edward S., editors  
Kinetics, Equilibria, and Performance of High Temperature Systems.  
(Proceedings of the First Conference, 2-5 Nov., 1959)  
(Butterworths, Washington, D. C., 1960)

This conference proceedings is directed primarily to rocket propulsion systems and to chemical and phsycial processes occurring in propulsion systems. There are several papers describing procedures for calculating equilibria and temperatures of complex reacting systems. Several of these use digital computer programs which are described. See also proceedings of the second conference by the same title.

2. Berenblut, I. I., and Downes, A. B.  
Tables for Petroleum Gas - Oxygen Flames: Combustion Products and Thermodynamic Properties.  
(Oxford Press, New York and Oxford, 1960).
3. Bradley, J. N.  
Flame and Combustion Phenomena  
(Menthuen, Barnes & Noble, New York, 1969).
4. Combustion (Serial)  
(Combustion Publishing Co., Inc. New York, N. Y.)

5. Combustion and Flame (The Journal of the Combustion Institute)  
(Butterworths, London, 1957- )

This journal publishes experimental and theoretical investigations dealing with combustion, detonation, and explosion, including such topics as: combustion in practical systems, fires, fluid dynamics, heat transfer and radiation; heterogeneous combustion; ignition; instability; mechanisms and kinetics; phase changes; thermal decomposition; thermochemistry and thermodynamics; and other topics.

6. Combustion Science and Technology (Serial)  
(Gordon and Breach, London, 1959- ).

7. Corey, Richard C.

Principles and Practice of Incineration  
(John Wiley and Sons, New York, N. Y., 1969).

8. Ducarme, J., Gerstein, M., and LeFebre, A. H., editors (Serial)  
Progress in Combustion Science and Technology  
(Pergamon Press, New York, 1961- ).

9. Fleming, Donald K.

Aerothermochemistry  
(First Biennial Gas Dynamics Symposium, 1956)  
(Northwestern University Press, Evanston, Ill.).

10. Fristrom, R. M. and Westenberg, A. A.

Flame Structure  
(McGraw-Hill Book Co., Inc., New York, N.Y., 1965).

11. Gaydon, A. G., and Wolfhard, H. G.

Flames, Their Structure, Radiation and Temperature  
(Chapman and Hall, Ltd., London, 1970).
12. Hougen, Olaf A., Watson, Kenneth M., and Ragatz, Roland R.

Chemical Process Principles, Part II Thermodynamics  
(John Wiley and Sons, Inc., New York, N.Y.; Chapman & Hall,  
Ltd, London, 2nd ed. 1959).

Chapter 25, "Chemical Equilibrium Constants, Chapter 26, "Equilibria in Chemical Reactions," and Chapter 27, "Equilibria in Complex Reactions", are of particular relevance to the determination of temperatures and products of combustion resulting from combustion processes. Charts and illustrative problems are given.
13. Jost, Wilhelm (H. O. Croft, translator)

Explosion and Combustion Processes in Gases  
(McGraw-Hill Book Co., Inc., New York, N.Y., 1946).
14. Lewis, B., Pease, R. N., and Taylor, H. S. (editors)

Combustion Processes  
(High Speed Aerodynamics and Jet Propulsion, Volume 2)  
(Princeton University Press, Princeton, N. J., 1956)

In this large volume there are numerous chapters on the combustion of solids, liquids, and gases, the kinetics of combustion reactions and on detonation process by various authors. Chapter A by Carter and Altman discusses reaction equilibrium and the temperatures obtained by the combustion energy. Chapter C by S. R. Brinkley, Jr., discusses computational methods for complex reacting systems.

15. Lewis, Bernard, and Von Elbe, G.  
Combustion, Flames and Explosions of Gases, 2nd ed.  
(Academic Press, New York, N. Y., 1961)
16. Minkoff, G. J. and Tippen, C.F.H.  
Chemistry of Combustion Reactions  
(Butterworths, London, 1962).
17. Mullins, B. P.  
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25.0 Tables of Thermodynamic Data25.1 Description of the Tables

Table I-A Enthalpies of Formation of Some Organic Compounds  
and Inorganic Carbon Compounds at 298.15 K.

Content. Table I-A is a list of about 1000 carbon compounds (989 compounds, some differing in physical state or stereochemical configuration gave a total of 1093 entries) in which the information given in columns, left to right, is: molecular formula, formula weight, name (physical state), enthalpy (heat) of formation in kcal mol<sup>-1</sup>, enthalpy (heat) of formation in kJ mol<sup>-1</sup>, references for enthalpy data.

Formula format. A molecular formula (for substances consisting of discrete molecules) is given in which the elements are listed in a partially alphabetical order with the numbers of atoms as subscripts. Carbon is always the first element. Hydrogen, if present, is always the second element. The remaining elements follow in the alphabetical order of their chemical symbols. Empirical formulas are given for ionic solids.

Arrangement of compounds. The formulas are listed in alphabetical order following the arrangement of the Chemical Abstracts Formula Index (Hill arrangement, E. A. Hill, J. Am. Chem. Soc. 22, 478-494 (1900)). The compounds are also in numerical order of the number of atoms per molecule. Beginning with the element on the left, the lowest subscripts are listed first and increase to higher numbers only when all elements

to the right have been listed from the lowest to the highest number. Thus, all compounds with  $C_1$  are listed before any with  $C_2$ ; all compounds with  $C_1A_1$  before any with  $C_1A_2$ , and so on. The arrangement is illustrated in figure 25.1.

$C_1A_1$   
 $C_1A_1B_1$   
 $C_1A_2$   
 $C_1A_2B_1$   
-----

Figure 25.1

alphabetic-numeric

$C_1H_1$   
 $C_1H_1A_1$   
 $C_1H_2$   
 $C_1H_2A_1$   
-----

arrangement of compounds

$C_1Z_1$   
 $C_1Z_2$   
 $C_2A_1$   
-----

Compound name (and physical state). A well known name for each compound is given to make a positive identification of the substance and remove any ambiguity resulting from the possibility of several isomeric forms having the same composition and molecular weight. The physical state of the compound is listed: gas (g), Liquid (liq), or crystal (c).

Enthalpy of formation. (Sometimes called heat of formation). The enthalpy of formation of the compound from the elements is given in two columns, respectively in kilocalories per mole and in kilojoules per mole. In the table of data the uncertainties are not given explicitly. The values in general are accurate to between one and 10 parts in the last figure given. A negative enthalpy of formation means the reaction of formation from the elements is exothermic.

Reference. The values of enthalpies of formation were taken from a few collections of carefully evaluated data and represent the best current appraisal of the available experimental data. The source references are listed at the end of the table.

Table I-B Compound Name-Formula Index (of Carbon Compounds)

Content. Table I-B is a name-formula index of all the compounds in Table I-A arranged alphabetically in order of the name. For some compounds, an alternative name is listed with a cross reference to the name found in Table I-A.

Use of Table I - To find the enthalpy (heat) of formation of a compound. Write the molecular formula of the compound in the format given in paragraph 2 above, and then look for the formula in Table I-A following the arrangement listed in paragraph 3 above. Some formulas represent more than one substance. Distinguish between them by the name and physical state.

If the formula is not known, look up the name in the alphabetical listing in Table I-B to find the formula, and then proceed as before. Failure to find the name in the alphabetical listing does not mean for

sure that the compound is not listed, as it has been impossible to list all the names that may be used for the compounds. In event the compound is not found in the alphabetical name index, look for alternate names, or determine the formula and proceed as above.

Table II - Enthalpies of Formation of Organic Polymers at 298.15 K.

Content. Table II is a list of 39 organic polymers, in which the information given in columns, left to right is: chemical formula of the repeating unit, formula weight of the repeating unit, name (and physical state), enthalpy (heat) of formation in  $\text{kcal mol}^{-1}$ , enthalpy (heat) of formation in  $\text{kJ mol}^{-1}$ , references for enthalpy data.

Formula format. Same as Table I-A.

Arrangement of Compounds. Same as Table I-A.

Compound name, (and physical state). A name based on the monomer is frequently given. A few common names and trade names are used.

Enthalpy (heat) of formation. The value cited represents the enthalpy of formation of the repeating unit from the elements. Uncertainties are not explicitly given. The values, in general, are accurate to between one and ten parts in the last figure given.

Reference. The original source of the heat of combustion data is given. A list of references is found at the end of the table.

Table III - Enthalpies of Formation of Inorganic Oxides at 298.15 K.

Content. Table III is a list of 285 inorganic oxides, in which the information given in columns, left to right is: empirical or molecular formula (and physical state), formula weight, name, enthalpy

(heat) of formation in  $\text{kcal mol}^{-1}$ , enthalpy (heat) of formation in  $\text{kJ mol}^{-1}$ , reference for enthalpy data.

Formula format. Solids forming continuous covalent or ionic lattices have the empirical formula given. Gases, liquids, or solids having molecules (as for instance  $\text{As}_4\text{O}_6(\text{c})$ ) are represented as the molecular formula. Oxygen is listed last in the formula. The state: gas (g), liquid (liq), or solid (c) is listed in parenthesis following the formula. When more than one crystal form is known, the crystal form is listed. Non-crystalline solids are listed as amorphous (amorph).

Arrangement of compounds. The formulas are listed in alphabetical order of the symbol of the first element and in order of increasing numbers of atoms of each element in the formula. Phases of the same compound are listed in the order (g), (liq), (c).

Compound name. A descriptive chemical name is given. In a few cases a common synonym or a mineral name is given.

Enthalpy of formation. (Sometimes called heat of formation). The enthalpy of formation from the elements is given in two columns, respectively in kilocalories per mole, and kilojoules per mole. In the table the uncertainties are not given explicitly. The values in general are accurate to between one and ten parts in the last figure given. A negative enthalpy of formation means the reaction of formation from the elements is exothermic.

Reference. Numerical references refer to the source of the data in the list of references at the end of the table. All data were taken from reliable collections of carefully evaluated data and represent the best current appraisal of the available experimental data.

25.2 TABLE I-A

## ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula                                      | Formula<br>Weight | Name (state)                 | Enthalpy of Formation<br>kcal mol <sup>-1</sup><br>kJ mol <sup>-1</sup> | Ref |
|--|-------------------|------------------------------|---|-----|
| C <sub>2</sub> H <sub>2</sub> O <sub>3</sub> | 275.7494          | Silver carbonate (c)         | -120.9  | (3) |
| CBrF <sub>3</sub>                            | 148.9154          | Bromotrifluoromethane (g)    | -153.6  | (2) |
| CBr <sub>2</sub> O                           | 187.8286          | Carbonyl dibromide (g)       | -23.0   | (2) |
| CBr <sub>2</sub> F                           | 187.8286          | Carbonyl dibromide (liq)     | -30.4   | (2) |
| CBr <sub>2</sub>                             | 251.7382          | Carbon tribromide (g)        | *42.  | (2) |
| CBr <sub>3</sub>                             | 331.6472          | Carbon tetrabromide (g)      | *19.  | (2) |
| CBr <sub>4</sub>                             | 331.6472          | Carbon tetrabromide (c)      | *4.5  | (2) |
| CBr <sub>4</sub>                             | 104.4594          | Chlorotrifluoromethane (g)   | -166.   | (2) |
| CCl <sub>3</sub> F                           | 120.9140          | Dichlorodifluoromethane (g)  | -114.   | (2) |
| CCl <sub>2</sub> F <sub>2</sub>              | 98.9166           | Carbonyl dichloride (g)      | -52.3   | (2) |
| CCl <sub>2</sub> O                           | 118.3702          | Carbon trichloride (g)       | *14.  | (2) |
| CCl <sub>3</sub> P                           | 137.3686          | Fluorotrifluoromethane (g)   | -66.  | (2) |
| CCl <sub>3</sub> P                           | 137.3686          | Fluorotrichloromethane (liq) | -72.02  | (2) |
| CCl <sub>4</sub>                             | 153.8232          | Carbon tetrachloride (g)     | -24.6   | (2) |
| CCl <sub>4</sub>                             | 153.8232          | Carbon tetrachloride (liq)   | -32.37  | (2) |
| CCo <sub>2</sub> O <sub>3</sub>              | 118.9426          | Cobalt carbonate (c)         | -170.4  | (3) |
| CP <sub>2</sub> O                            | 66.0074           | Carbonyl difluoride (g)      | -151.7  | (2) |
| CF <sub>3</sub>                              | 69.0064           | Carbon trifluoride (g)       | -114.   | (2) |
| CF <sub>4</sub>                              | 88.0048           | Carbon tetrafluoride (g)     | -223.0  | (2) |
| CF <sub>4</sub>                              | 115.8564          | Iron (III) carbonato (c)     | -177.00   | (3) |
| CHBr <sub>3</sub>                            | 252.7461          | Bromoform (g)                | *4.   | (2) |
| CHBr <sub>3</sub>                            | 252.7461          | Bromoform (liq)              | -6.8  | (2) |
| CHCl <sub>3</sub>                            | 119.3781          | Chloroform (g)               | -24.65  | (2) |
| CHCl <sub>3</sub>                            | 119.3781          | Chloroform (liq)             | 32.14   | (2) |
| CHF <sub>3</sub>                             | 70.0143           | Fluoroform (g)               | -164.5  | (2) |
| CHI <sub>3</sub>                             | 393.7323          | Iodoform (c)                 | *33.7   | (2) |
| CH <sub>2</sub> Cl <sub>2</sub>              | 84.9331           | Methylene dichloride (g)     | -22.10  | (2) |
| CH <sub>2</sub> Cl <sub>2</sub>              | 84.9331           | Methylene dichloride (liq)   | -29.03  | (2) |
| CH <sub>2</sub> F <sub>2</sub>               | 52.0239           | Methylene difluoride (g)     | -106.8  | (2) |
| CH <sub>2</sub> I <sub>2</sub>               | 267.8359          | Methylene diiodide (g)       | *27.0   | (2) |
| CH <sub>2</sub> I <sub>2</sub>               | 267.8359          | Methylene diiodide (liq)     | *16.0   | (2) |
| CH <sub>2</sub> N <sub>4</sub>               | 70.0539           | Tetrazole (c)                | *56.7   | (1) |
| CH <sub>2</sub> N <sub>4</sub> O             | 86.0533           | 5-Hydroxytetrazole (c)       | *1.5  | (1) |
| CH <sub>2</sub> O                            | 30.0265           | Formaldehyde (g)             | -25.95  | (1) |
| CH <sub>2</sub> O <sub>2</sub>               | 46.0259           | Formic acid (liq)            | -101.51   | (1) |
| CH <sub>3</sub> BO <sub>3</sub>              | 41.8455           | Carbonyl borane (g)          | -26.58  | (2) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 299.15 K

| Formula                                       | Formula Weight | Name (state)                                | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Enthalpy of Formation<br>kJ mol <sup>-1</sup> | Ref |
|---|----------------|---|---|---|-----|
| CH <sub>3</sub> Br                            | 94.9441        | Methyl bromide (g)                          | -94.4   | -35.1   | (2) |
| CH <sub>3</sub> Cl                            | 50.4881        | Methyl chloride (g)                         | -19.32  | -80.33  | (2) |
| CH <sub>3</sub> Hg                            | 215.6251       | Methyl mercury (g)                          | +40.  | +167.   | (3) |
| CH <sub>3</sub> I                             | 141.9395       | Methyl iodide (g)                           | +3.1  | +13.0   | (2) |
| CH <sub>3</sub> I                             | 141.9395       | Methyl iodide (liq)                         | -3.7  | -15.5   | (2) |
| CH <sub>3</sub> NH                            | 45.0412        | Formamide (liq)                             | -60.7   | -254.0  | (1) |
| CH <sub>3</sub> N <sub>2</sub>                | 85.0686        | 5-Aminotetrazole (c)                        | +49.7   | +207.9  | (1) |
| CH <sub>3</sub> N <sub>5</sub>                | 235.4045       | Thallium methoxide (c)                      | -27.5   | -115.1  | (2) |
| CH <sub>3</sub> OTl                           | 16.0430        | Methane (g)                                 | -17.89  | -74.85  | (1) |
| CH <sub>4</sub>                               | 60.0558        | Urea (c)                                    | -79.71  | -333.51                                       | (1) |
| CH <sub>4</sub> N <sub>2</sub> S              | 76.1204        | Thiourea (c)                                | -21.13  | -83.41  | (1) |
| CH <sub>4</sub> N <sub>6</sub> O <sub>3</sub> | 148.0814       | 5-Aminotetrazole nitrate (c)                | -6.6  | -27.6   | (1) |
| CH <sub>4</sub> O                             | 32.0424        | Methanol (g)                                | -47.96  | -200.66                                       | (1) |
| CH <sub>4</sub> O                             | 32.0424        | Methanol (liq)                              | -57.04  | -238.66                                       | (1) |
| CH <sub>4</sub> S                             | 48.1070        | Methanethiol (liq)                          | -11.08  | -46.36  | (1) |
| CH <sub>5</sub> N                             | 31.0577        | Methylamine (liq)                           | -11.3   | -47.3   | (1) |
| CH <sub>5</sub> N <sub>3</sub>                | 59.0711        | Guanidine (c)                               | -13.39  | -56.02  | (1) |
| CH <sub>5</sub> N <sub>3</sub> O <sub>4</sub> | 123.0687       | Urea nitrate (c)                            | -134.8  | -564.0  | (1) |
| CH <sub>5</sub> N <sub>5</sub> O <sub>2</sub> | 119.0833       | Nitroamino guanidine (c)                    | +5.29   | +22.13  | (1) |
| CH <sub>6</sub> N <sub>2</sub> O <sub>3</sub> | 94.0706        | Methylamine nitrate (c)                     | -84.7   | -354.4  | (1) |
| CH <sub>6</sub> N <sub>4</sub> O <sub>3</sub> | 122.0840       | Guanidine nitrate (c)                       | -92.5   | -387.0  | (1) |
| CH <sub>6</sub> N <sub>6</sub> O <sub>3</sub> | 152.1133       | Sym-Diamino guanidine nitrate (c)           | -37.57  | -157.19                                       | (1) |
| Cm <sup>3+</sup>                              | 114.9474       | Manganese carbonate, natural (c)            | -213.7  | -894.1  | (3) |
| CmO <sub>3</sub>                              | 114.9474       | Manganese carbonate, precipitated (c)       | -211.1  | -883.2  | (3) |
| C <sub>0</sub> 3Tl <sub>2</sub>               | 468.7494       | Thallium carbonate (c)                      | -167.3  | -700.0  | (2) |
| C <sub>0</sub> Zn                             | 125.3794       | Zinc carbонate (c)                          | -194.26   | -812.78                                       | (2) |
| C <sub>2</sub> Ag <sub>2</sub> O <sub>4</sub> | 303.7599       | Silver oxalate (c)                          | -160.9  | -673.2  | (3) |
| C <sub>2</sub> Br <sub>2</sub> F <sub>4</sub> | 259.0339       | 1,2-Dibromo-1,1,2,2-tetrafluoroethane (g)   | -186.5  | -780.3  | (2) |
| C <sub>2</sub> CdO <sub>4</sub>               | 200.4199       | Cadmium oxalate (c)                         | -218.1  | -912.5  | (2) |
| C <sub>2</sub> ClF <sub>3</sub>               | 116.4705       | Chlorotrifluoroethylene (g)                 | -132.7  | -555.2  | (2) |
| C <sub>2</sub> Cl <sub>2</sub> F <sub>2</sub> | 132.9251       | 1,2-Dichloro-1,2-difluoroethylene (g)       | -76.3   | -319.2  | (2) |
| C <sub>2</sub> Cl <sub>2</sub> F <sub>4</sub> | 170.9219       | 1,1,2,2-Tetrafluoro-1,2-dichloroethane (g)  | -212.0  | -890.4  | (2) |
| C <sub>2</sub> Cl <sub>3</sub> F <sub>3</sub> | 187.3765       | 1,1,2-Trichloro-2,2,1-trifluoroethane (g)   | -161.5  | -759.4  | (2) |
| C <sub>2</sub> Cl <sub>3</sub> F <sub>3</sub> | 187.3765       | 1,1,2-Trichloro-2,2,1-trifluoroethane (liq) | -138.37   | -739.16                                       | (2) |
| C <sub>2</sub> Cl <sub>4</sub>                | 165.8343       | Tetrachloroethylene (g)                     | -12.9   | -12.1   | (2) |

TABLE II-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 293.15 K

| Formula   | Formula Weight | Name (state)                               | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Enthalpy of Formation<br>kJ mol <sup>-1</sup> | Ref  |
|---|----------------|--|---|---|------|
| C <sub>2</sub> Cl <sub>4</sub>                                | 165.8343       | Tetrachloroethylene (liq)                  | -12.5   | -52.3   | (2)  |
| C <sub>2</sub> Cl <sub>4</sub> F <sub>2</sub>                 | 203.8311       | 1,1,1,2-Tetrachloro-2,2-difluoroethane (g) | -117.1  | -489.9  | (2)  |
| C <sub>2</sub> Cl <sub>4</sub> O                              | 181.8337       | Trichloroacetyl chloride (liq)             | -66.65  | -278.95                                       | (2)  |
| C <sub>2</sub> Cl <sub>6</sub>                                | 236.7403       | Hexachloroethane (c, I)                    | -46.0   | -192.5  | (2)  |
| C <sub>2</sub> Cl <sub>6</sub>                                | 236.7403       | Hexachloroethane (c, II)                   | -47.9   | -200.4  | (2)  |
| C <sub>2</sub> Cl <sub>6</sub>                                | 236.7403       | Hexachloroethane (c, III)                  | -48.5   | -202.9  | (2)  |
| C <sub>2</sub> Cl <sub>6</sub>                                | 236.7403       | Hexachloroethane (c, IV)                   | -33.9   | -141.9  | (2)  |
| C <sub>2</sub> Cl <sub>6</sub>                                | 146.9531       | Hexachloroethane (f)                       | -20.3.5   | -851.4  | (3)  |
| C <sub>2</sub> CoO <sub>4</sub>                               | 100.0159       | Cobalt oxalate (c)                         | -155.5  | -650.6  | (2)  |
| C <sub>2</sub> F <sub>4</sub>                                 | 138.0127       | Tetrafluoroethylene (g)                    | -310.   | -1297.  | (2)  |
| C <sub>2</sub> F <sub>6</sub>                                 | 213.8421       | Hexafluoroethane (f)                       | -107.9  | -451.5  | (2)  |
| C <sub>2</sub> HBrCl <sub>2</sub> F <sub>2</sub>              | 180.9329       | 1,1,2,2-Tetrafluorobromoethane (g)         | -197.0  | -824.2  | (2)  |
| C <sub>2</sub> HBrF <sub>3</sub>                              | 280.7567       | Bromal (liq)                               | -31.13  | -130.25                                       | (2)  |
| C <sub>2</sub> HClF <sub>2</sub>                              | 98.4801        | 1,1-Difluoro-2-chloroethylene (g)          | -75.4   | -315.5  | (2)  |
| C <sub>2</sub> HCl <sub>3</sub>                               | 131.3893       | Trichloroethylene (g)                      | -1.86   | -7.78   | (2)  |
| C <sub>2</sub> HCl <sub>3</sub>                               | 131.3893       | Trichloroethylene (liq)                    | -10.1   | -42.3   | (2)  |
| C <sub>2</sub> HCl <sub>3</sub> O                             | 147.3837       | Chloral (g)                                | -47.0   | -196.6  | (2)  |
| C <sub>2</sub> HCl <sub>3</sub> O                             | 147.3887       | Dichloroacetyl chloride (liq)              | -56.45  | -236.19                                       | (2)  |
| C <sub>2</sub> HCl <sub>3</sub> O                             | 147.3887       | Dichloroacetic acid (c)                    | -67.27  | -281.46                                       | (2)  |
| C <sub>2</sub> HCl <sub>3</sub> O <sub>2</sub>                | 163.3881       | Trichloroacetic acid (c)                   | -120.7  | -505.0  | (2)  |
| C <sub>2</sub> HCl <sub>5</sub>                               | 202.2953       | Pentachloroethane (liq)                    | -44.9   | -187.9  | (2)  |
| C <sub>2</sub> HNS  | 95.0638        | 5-Cyanotetrazole (c)                       | +96.1   | +402.1  | (11) |
| C <sub>2</sub> H <sub>2</sub>                                 | 26.0382        | Acetylene (g)                              | +54.19  | +225.73                                       | (11) |
| C <sub>2</sub> H <sub>2</sub> Br <sub>2</sub> Cl <sub>2</sub> | 256.7622       | 1,2-Dibromo-1,2-dichloroethane (g)         | +8.8  | -36.8   | (2)  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>                 | 96.9442        | 1,1-Dichloroethylene (g)                   | +0.58   | +2.43   | (2)  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>                 | 96.9442        | 1,1-Dichloroethylene (liq)                 | -5.8  | -24.3   | (2)  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>                 | 96.9442        | cis-1,2-Dichloroethylene (g)               | +0.9  | +3.9  | (2)  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>                 | 96.9442        | cis-1,2-Dichloroethylene (liq)             | -6.6  | -27.6   | (2)  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>                 | 96.9442        | trans-1,2-Dichloroethylene (g)             | +1.47   | +6.15   | (2)  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>                 | 96.9442        | trans-1,2-Dichloroethylene (liq)           | -5.53   | -23.14  | (2)  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> O               | 112.9436       | Chloroacetyl chloride (liq)                | -67.85  | -283.68                                       | (2)  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> O <sub>2</sub>  | 128.9430       | Dichloroacetic acid (liq)                  | -119.0  | -497.9  | (2)  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub>                 | 167.8502       | 1,1,2,2-Tetrachloroethane (g)              | -35.7   | -149.4  | (2)  |
| C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub>                 | 167.8502       | 1,1,2,2-Tetrachloroethane (liq)            | -47.0   | -196.6  | (2)  |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula<br>Weight  | Name (state) | Enthalpy of Formation<br>kcal mol <sup>-1</sup><br>kJ mol <sup>-1</sup> | Ref          |
|--|--------------|---|--------------|
| C <sub>2</sub> H <sub>2</sub> COθ <sub>4</sub>               | 148.9690     | Cobaltous formate (c)   | -208.7 (-3)  |
| C <sub>2</sub> H <sub>2</sub> Cuθ <sub>4</sub>               | 153.5758     | Copper (II) formate (c)   | -186.7 (-3)  |
| C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>                 | 64.0350      | 1,1-Difluoroethylene (g)  | -78.6 (-2)   |
| C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> θ <sub>2</sub>  | 96.0338      | Difluoroacetic acid (liq)   | -207.8 (-2)  |
| C <sub>2</sub> H <sub>2</sub> Mnθ <sub>4</sub>               | 144.9738     | Manganese formate (c)   | -249.7 (-3)  |
| C <sub>2</sub> H <sub>2</sub> N <sub>6</sub>                 | 110.0784     | 3-Azido-S-triazole (c)  | -1044.7 (-3) |
| C <sub>2</sub> H <sub>2</sub> Niθ <sub>4</sub>               | 148.7458     | Nickel formate (c)  | -105.5 (-1)  |
| C <sub>2</sub> H <sub>2</sub> O <sub>2</sub>                 | 58.0370      | Glyoxal (g)   | -208.4 (-3)  |
| C <sub>2</sub> H <sub>2</sub> O <sub>2</sub>                 | 90.0358      | oxalic acid (c,α)   | -50.66 (-1)  |
| C <sub>2</sub> H <sub>2</sub> O <sub>4</sub>                 | 90.0358      | oxalic acid (c,β)   | -197.7 (-1)  |
| C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> Pb              | 297.2253     | Lead formate (c)  | -197.4 (-1)  |
| C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> Zn              | 155.4058     | Zinc formate (c)  | -210.0 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Agθ <sub>2</sub>               | 166.9150     | Silver acetate (c)  | -235.8 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Br                             | 106.9552     | Vinyl bromide (g)   | -95.3 (-3)   |
| C <sub>2</sub> H <sub>3</sub> Brd                            | 122.9546     | Acetyl bromide (liq)  | +18.7 (-2)   |
| C <sub>2</sub> H <sub>3</sub> Br <sub>3</sub> θ <sub>2</sub> | 298.7720     | Bromal hydrate (c)  | +53.39 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Cl                             | 62.4992      | Vinyl chloride (g)  | -112.2 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Cl                             | 62.4992      | Vinyl chloride (liq)  | +8.5 (-2)    |
| C <sub>2</sub> H <sub>3</sub> Clθ                            | 78.4986      | Acetyl chloride (g*)  | +3.5 (-2)    |
| C <sub>2</sub> H <sub>3</sub> Clθ                            | 78.4986      | Acetyl chloride (liq)   | -58.20 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Clθ                            | 78.4986      | Monochloroacetaldehyde (liq)  | -65.44 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Clθ                            | 78.4986      | Monochloroacetic acid (c, I)  | -61.5 (-2)   |
| C <sub>2</sub> H <sub>3</sub> Clθ <sub>2</sub>               | 94.4980      | Monochloroacetic acid (c, II)   | -122.3 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Clθ <sub>2</sub>               | 94.4980      | Monochloroacetic acid (c, III)  | -122.12 (-2) |
| C <sub>2</sub> H <sub>3</sub> Clθ <sub>2</sub>               | 94.4980      | Monochloroacetic acid (c, III)  | -121.46 (-2) |
| C <sub>2</sub> H <sub>3</sub> Cl <sub>2</sub>                | 133.4052     | 1,1,2-Trichloroethane (g)   | -33.94 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Cl <sub>2</sub>                | 133.4052     | 1,1,2-Trichloroethane (liq)   | -43.5 (-2)   |
| C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> θ <sub>2</sub> | 165.4040     | Chloral hydrate (c)   | -137.7 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> θ <sub>2</sub> | 165.4040     | Chloral hydrate (g)   | -107.2 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Fθ <sub>2</sub>                | 62.0440      | Acetyl fluoride (g)   | -104.9 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Fθ                             | 62.0440      | Acetyl fluoride (liq)   | -110.83 (-2) |
| C <sub>2</sub> H <sub>3</sub> Fθ <sub>2</sub>                | 78.0434      | Fluoroacetic acid (c)   | -164.5 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Fθ <sub>2</sub>                | 84.0414      | 1,1,1-Trifluoroethane (g)   | -176.0 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Fθ <sub>2</sub>                | 84.0414      | 1,1,2-Trifluoroethane (g)   | -174.7 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Fθ <sub>3</sub>                | 100.0408     | 2,2,2-Trifluoroethanol (liq)  | -205.4 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Iθ <sub>2</sub>                | 169.9500     | Acetyl iodide (liq)   | -38.84 (-2)  |
| C <sub>2</sub> H <sub>3</sub> Nθ <sub>3</sub>                | 89.0511      | Uranic acid (c)   | -671.1 (-1)  |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula   | Formula Weight | Name (state)                   | Enthalpy of Formation<br>kcal mol <sup>-1</sup><br>kJ mol <sup>-1</sup> | Ref |
|---|----------------|--------------------------------|---|-----|
| C <sub>2</sub> H <sub>3</sub> N <sub>7</sub>                | 125.0931       | 4-Amino-3-azido-s-triazole (c) | *136.5  | (1) |
| C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> Tl             | 263.4150       | Thallium acetate (c)           | -126.1  | (2) |
| C <sub>2</sub> H <sub>4</sub>                               | 28.0542        | Ethylene (g)                   | *12.50  | (1) |
| C <sub>2</sub> H <sub>4</sub> BrI                           | 234.8676       | 1-Bromo-2-iodoethane (c)       | -11.3   | (2) |
| C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub>               | 187.9722       | 1,2-Dibromoethane (g)          | -9.16   | (2) |
| C <sub>2</sub> H <sub>4</sub> Br <sup>2</sup>               | 187.8722       | 1,2-Dibromoethane (liq)        | -19.4   | (2) |
| C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>               | 98.9602        | 1,1-Dichloroethane (g)         | -30.93  | (2) |
| C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>               | 98.9602        | 1,1-Dichloroethane (liq)       | -38.3   | (2) |
| C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>               | 98.9602        | 1,2-Dichloroethane (g)         | -31.02  | (2) |
| C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>               | 98.9602        | 1,2-Dichloroethane (liq)       | -39.49  | (2) |
| C <sub>2</sub> H <sub>4</sub> F <sub>2</sub>                | 66.0510        | 1,1-Difluoroethane (g)         | -114.3  | (2) |
| C <sub>2</sub> H <sub>4</sub> F <sub>2</sub> Ø              | 82.0504        | 2,2-Difluoroethanol (liq)      | -164.8  | (2) |
| C <sub>2</sub> H <sub>4</sub> I <sub>2</sub>                | 281.8630       | 1,2-Diiodoethane (c)           | +0.1  | (2) |
| C <sub>2</sub> H <sub>4</sub> I <sub>2</sub>                | 281.8630       | 1,2-Diiodoethane (g)           | *15.9   | (2) |
| C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> Ø <sub>2</sub> | 88.0664        | Formylurea (c)                 | -118.   | (1) |
| C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> Ø <sub>2</sub> | 88.0664        | Formamide (c)                  | -123.0  | (1) |
| C <sub>2</sub> H <sub>4</sub> N <sub>4</sub>                | 84.0810        | 3-Amino-1,2,4-triazole (c)     | *18.4   | (1) |
| C <sub>2</sub> H <sub>4</sub> N <sub>4</sub> Ø              | 100.0804       | 5-Methoxytetrazole (c)         | +16.6   | (1) |
| C <sub>2</sub> H <sub>4</sub> N <sub>4</sub> Ø <sub>2</sub> | 116.0798       | Azodicarbamide (c)             | -69.90  | (1) |
| C <sub>2</sub> H <sub>4</sub> N <sub>10</sub>               | 168.1212       | 5,5'-Hydrazotetrazole (c)      | *135.1  | (1) |
| C <sub>2</sub> H <sub>4</sub> Ø <sub>2</sub>                | 44.0536        | Acetaldehyde (g)               | -39.72  | (1) |
| C <sub>2</sub> H <sub>4</sub> Ø <sub>2</sub>                | 44.0536        | Acetaldehyde (liq)             | -45.96  | (1) |
| C <sub>2</sub> H <sub>4</sub> Ø <sub>2</sub>                | 76.1176        | Thioacetic acid (liq)          | -52.39  | (1) |
| C <sub>2</sub> H <sub>4</sub> Ø <sub>2</sub>                | 60.0530        | Acetic acid (liq)              | -115.71   | (1) |
| C <sub>2</sub> H <sub>4</sub> Ø <sub>2</sub>                | 60.0530        | Methyl formate (g)             | -83.7   | (1) |
| C <sub>2</sub> H <sub>4</sub> Ø <sub>2</sub>                | 60.0530        | Methyl formate (liq)           | -90.6   | (1) |
| C <sub>2</sub> H <sub>5</sub> Br                            | 76.0524        | Glycolic acid (c)              | -158.6  | (1) |
| C <sub>2</sub> H <sub>5</sub> Br                            | 92.0518        | Glyoxylic acid (c)             | -199.7  | (1) |
| C <sub>2</sub> H <sub>5</sub> S                             | 60.1182        | Thiacyclopropane (liq)         | *12.41  | (1) |
| C <sub>2</sub> H <sub>5</sub> Br                            | 108.9712       | Ethyl bromide (g)              | -15.42  | (2) |
| C <sub>2</sub> H <sub>5</sub> Br                            | 108.9712       | Ethyl bromide (liq)            | -21.99  | (2) |
| C <sub>2</sub> H <sub>5</sub> Cl                            | 64.5152        | Ethyl chloride (g)             | -26.81  | (2) |
| C <sub>2</sub> H <sub>5</sub> Cl                            | 64.5152        | Ethyl chloride (liq)           | -32.63  | (2) |
| C <sub>2</sub> H <sub>5</sub> ClØ                           | 80.5146        | Ethylen chlorohydrin (liq)     | -70.6   | (2) |
| C <sub>2</sub> H <sub>5</sub> PF <sub>3</sub>               | 64.0600        | 2-Fluoroethanol (liq)          | -111.3  | (2) |
| C <sub>2</sub> H <sub>5</sub> Fr                            | 155.9666       | Ethyl iodide (g)               | -1.84   | (2) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 293.15 K

| Formula   | Weight   | Name (state)                       | Enthalpy of Formation<br>kcal mol <sup>-1</sup> kJ mol <sup>-1</sup> | Perf |
|---|----------|------------------------------------|--|------|
| C <sub>2</sub> H <sub>5</sub> I                             | 155.9666 | Ethyl iodide (liq)                 | -9.6<br>-40.2  | (2)  |
| C <sub>2</sub> H <sub>5</sub> N                             | 43.0689  | Ethylenimine (liq)                 | +21.97<br>+91.92   | (1)  |
| C <sub>2</sub> H <sub>5</sub> Nθ                            | 59.0683  | Acetamide (c)                      | -76.0<br>-318.0  | (1)  |
| C <sub>2</sub> H <sub>5</sub> Nθ <sub>2</sub>               | 75.0677  | Glycine (c)                        | -126.22<br>-528.10   | (1)  |
| C <sub>2</sub> H <sub>5</sub> N <sub>5</sub>                | 99.0957  | 1-Methyl-5-amino tetrazole (c)     | +46.25<br>+193.51  | (1)  |
| C <sub>2</sub> H <sub>5</sub> N <sub>5</sub>                | 99.0957  | 2-Methyl-5-amino tetrazole (c)     | +50.4<br>+210.9  | (1)  |
| C <sub>2</sub> H <sub>5</sub> N <sub>5</sub>                | 99.0957  | 5-Methylamino tetrazole (c)        | +48.4<br>+202.5  | (1)  |
| C <sub>2</sub> H <sub>5</sub> N <sub>5</sub> θ <sub>3</sub> | 147.0939 | 3-Amino-1,2,4-triazole nitrate (c) | -40.9<br>-171.1  | (1)  |
| C <sub>2</sub> H <sub>5</sub> N <sub>5</sub> θ <sub>3</sub> | 147.0939 | 1-Formamido-2-nitroguanidine (c)   | -35.1<br>-146.9  | (1)  |
| C <sub>2</sub> H <sub>5</sub> N <sub>7</sub>                | 127.1091 | 5-Guanylaminotetrazole (c)         | +40.5<br>+169.5  | (1)  |
| C <sub>2</sub> H <sub>5</sub> O <sub>2</sub> Tl             | 249.4316 | Thallium ethoxide (liq)            | -56.5<br>-236.4  | (2)  |
| C <sub>2</sub> H <sub>6</sub>                               | 30.0701  | Ethane (g)                         | -20.24<br>-84.68   | (1)  |
| C <sub>2</sub> H <sub>6</sub> Cd                            | 142.7401 | Dimethyl cadmium (g)               | +24.27<br>+101.55  | (2)  |
| C <sub>2</sub> H <sub>6</sub> Cd                            | 142.4701 | Dimethyl cadmium (liq)             | +15.2<br>+63.6   | (2)  |
| C <sub>2</sub> H <sub>6</sub> Hg                            | 230.6601 | Dimethyl mercury (g)               | +22.56<br>+94.39   | (3)  |
| C <sub>2</sub> H <sub>6</sub> Hg                            | 230.6601 | Dimethyl mercury (liq)             | +14.3<br>+59.3   | (3)  |
| C <sub>2</sub> H <sub>6</sub> Nθ <sub>5</sub>               | 138.0805 | Glycine nitrate (c)                | -174.1<br>-728.4   | (1)  |
| C <sub>2</sub> H <sub>6</sub> N <sub>4</sub> θ <sub>2</sub> | 118.0957 | Hydrazodicarbamide (c)             | -119.19<br>-498.69   | (1)  |
| C <sub>2</sub> H <sub>6</sub> O                             | 46.0695  | Dimethyl ether (g)                 | -43.99<br>-184.05  | (1)  |
| C <sub>2</sub> H <sub>6</sub> O                             | 45.0695  | Ethanol (g)                        | +56.19<br>-235.10  | (1)  |
| C <sub>2</sub> H <sub>6</sub> O                             | 46.0695  | Ethanol (liq)                      | -66.37<br>-277.69  | (1)  |
| C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>                | 62.0689  | 1,2-Ethanediol (liq)               | -108.70<br>-454.80   | (1)  |
| C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>                | 126.0665 | oxalic acid dihydrate (c)          | -341.0<br>-1420.7  | (1)  |
| C <sub>2</sub> H <sub>6</sub> S                             | 62.1341  | Ethanethiol (liq)                  | -17.53<br>-73.35   | (1)  |
| C <sub>2</sub> H <sub>6</sub> S                             | 62.1341  | 2-Thiapropane (liq)                | -15.55<br>-65.06   | (1)  |
| C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>                | 94.1981  | 2,3-Dithiabutane (liq)             | -14.82<br>-62.01   | (1)  |
| C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>                | 94.1981  | 1,2-Ethanedithiol (liq)            | -12.83<br>-53.63   | (1)  |
| C <sub>2</sub> H <sub>6</sub> Si                            | 58.1561  | Vinylsilane (g)                    | -2.<br>-8.   | (2)  |
| C <sub>2</sub> H <sub>6</sub> Zn                            | 95.4401  | Dimethyl zinc (g)                  | +12.67<br>+53.01   | (2)  |
| C <sub>2</sub> H <sub>6</sub> Zn                            | 95.4401  | Dimethyl zinc (liq)                | +5.6<br>+23.4  | (2)  |
| C <sub>2</sub> H <sub>7</sub> Bθ <sub>2</sub>               | 73.8379  | Dimethoxyborane (g)                | -138.5<br>-579.5   | (2)  |
| C <sub>2</sub> H <sub>7</sub> Bθ <sub>2</sub>               | 73.8379  | Dimethoxyborane (liq)              | -144.7<br>-605.4   | (2)  |
| C <sub>2</sub> H <sub>7</sub> N                             | 45.0848  | Dimethylamine (liq)                | -10.5<br>-43.9   | (1)  |
| C <sub>2</sub> H <sub>7</sub> N                             | 45.0848  | Ethylamine (liq)                   | -17.7<br>-74.1   | (1)  |
| C <sub>2</sub> H <sub>7</sub> Nθ <sub>3</sub> S             | 125.1470 | 2-Aminooctane-1-sulfonic acid (c)  | -187.7<br>-785.3   | (1)  |
| C <sub>2</sub> H <sub>7</sub> Nθ <sub>4</sub>               | 165.1092 | Guanylurea nitrate (c)             | -102.1<br>-427.2   | (1)  |

TABLE I-A

| Formula  | Formula Weight | Name (state)   | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Enthalpy of Formation<br>kJ mol <sup>-1</sup> | Ref |
|--|----------------|--|---|---|-----|
| C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> <sup>0</sup>    | 60.0995        | Ethylenediamine (liq)                                | -15.06  | -63.01  | (1) |
| C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> <sup>0</sup> 3  | 108.0977       | Dimethylamine nitrate (c)                            | -79.6   | -333.0  | (1) |
| C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> <sup>0</sup> 3  | 108.0977       | Ethylamine nitrate (c)                               | -87.7   | -366.9  | (1) |
| C <sub>2</sub> H <sub>8</sub> Sn                             | 150.7761       | Dimethyl tin (g)                                     | +21.  | +98.  | (2) |
| C <sub>2</sub> H <sub>8</sub> Sn                             | 150.7761       | Dimethyl tin (liq)                                   | +14.5   | +60.7   | (2) |
| C <sub>2</sub> H <sub>8</sub> N <sub>10</sub> <sup>0</sup>   | 188.1525       | 1-(5-Tetrazoyl)-4-quaternyltetrazene monohydrate (c) | +45.2   | +189.1  | (1) |
| C <sub>2</sub> H <sub>10</sub> N <sub>4</sub> <sup>0</sup> 6 | 186.1252       | Ethylenediamine dinitrate (c)                        | -156.2  | -653.5  | (1) |
| C <sub>2</sub> I <sub>4</sub>                                | 531.6399       | Tetraiodoethylene (c)                                | +73.  | +305.   | (2) |
| C <sub>2</sub> NI <sub>6</sub> <sup>4</sup>                  | 146.7299       | Nickel oxalate (c)                                   | -204.8  | -856.9  | (3) |
| C <sub>3</sub> H <sub>2</sub> N <sub>2</sub> <sup>0</sup> 3  | 114.0610       | Parabanic acid (c)                                   | -138.0  | -577.4  | (1) |
| C <sub>3</sub> H <sub>4</sub>                                | 40.0653        | Propadiene (g)                                       | +45.93  | +192.17                                       | (4) |
| C <sub>3</sub> H <sub>4</sub>                                | 40.0653        | Propyne (g)  | +44.33  | +185.48                                       | (4) |
| C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>                 | 68.0787        | Imidazole (c)  | +14.5   | +60.7   | (1) |
| C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>                 | 68.0787        | Pyrazole (c)   | +28.3   | +118.4  | (1) |
| C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> <sup>0</sup> S  | 116.1421       | Thiohydantoin (c)                                    | -59.5   | -248.9  | (1) |
| C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> <sup>0</sup> 2  | 100.0775       | Hydantoin (c)  | -107.2  | -448.5  | (1) |
| C <sub>3</sub> H <sub>4</sub> N <sub>6</sub>                 | 124.1055       | 3-Azido-5-methyl-s-triazole (c)                      | +93.8   | +392.5  | (1) |
| C <sub>3</sub> H <sub>4</sub> <sup>0</sup> 2                 | 72.0641        | Acrylic acid (liq)                                   | -91.8   | -384.1  | (1) |
| C <sub>3</sub> H <sub>4</sub> <sup>0</sup> 2                 | 72.0641        | $\beta$ -Propiolactone (g)                           | -67.61  | -282.68                                       | (1) |
| C <sub>3</sub> H <sub>4</sub> <sup>0</sup> 2                 | 72.0641        | $\beta$ -Propiolactone (liq)                         | -78.85  | -329.91                                       | (1) |
| C <sub>3</sub> H <sub>4</sub> <sup>0</sup> 3                 | 88.0635        | Ethylene carbonate (c)                               | -138.9  | -581.2  | (1) |
| C <sub>3</sub> H <sub>4</sub> <sup>0</sup> 3                 | 88.0635        | Pyruvic acid (c)                                     | -140.3  | -587.0  | (1) |
| C <sub>3</sub> H <sub>4</sub> <sup>0</sup> 4                 | 104.0629       | Malonic acid (c)                                     | -212.96   | -891.02                                       | (1) |
| C <sub>3</sub> H <sub>4</sub> <sup>0</sup> 6                 | 136.0617       | Mesoxalic acid (c)                                   | -290.7  | -1216.3                                       | (1) |
| C <sub>3</sub> H <sub>5</sub> N <sub>5</sub> <sup>0</sup>    | 127.1062       | 5-Acetamidotetrazole (c)                             | -1.2  | -5.0  | (1) |
| C <sub>3</sub> H <sub>5</sub> N <sub>7</sub>                 | 139.1202       | 4-Amino-3-azido-5-methyl-s-triazole (c)              | +115.6  | +483.7  | (1) |
| C <sub>3</sub> H <sub>6</sub>                                | 42.0813        | Cyclopropane (g)                                     | +12.75  | +53.35  | (1) |
| C <sub>3</sub> H <sub>6</sub>                                | 42.0813        | Propene (g)  | +4.89   | +20.46  | (4) |
| C <sub>3</sub> H <sub>6</sub> <sup>0</sup> 2                 | 102.0935       | Malonamide (c)                                       | -130.5  | -546.0  | (1) |
| C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> <sup>0</sup> 2S | 134.1575       | Thiobutyric acid (c)                                 | -132.6  | -554.8  | (1) |
| C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> <sup>0</sup> 3  | 118.0929       | Hydantoinic acid (c)                                 | -179.   | -749.   | (1) |
| C <sub>3</sub> H <sub>6</sub> N <sub>4</sub>                 | 98.1081        | 1,5-Dimethyltetrazole (c)                            | +45.1   | +188.7  | (1) |
| C <sub>3</sub> H <sub>6</sub> N <sub>4</sub>                 | 114.1075       | 1,4-Dimethyl-5-tetrazolone (c)                       | -6.6  | -27.6   | (1) |
| C <sub>3</sub> H <sub>6</sub> N <sub>6</sub>                 | 126.1215       | Melanine (c)   | -17.3   | -72.4   | (1) |
| C <sub>3</sub> H <sub>6</sub> <sup>0</sup>                   | 58.0807        | Oxacyclobutane (g)                                   | -19.25  | -80.54  | (1) |

TABLE I-A

## ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula   | Weight   | Name (state)                                | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Ref |
|---|----------|---|---|-----|
| C <sub>3</sub> H <sub>6</sub> O                             | 58.0807  | Propanone (g)                               | -51.78  | (1) |
| C <sub>3</sub> H <sub>6</sub> O                             | 58.0807  | Propanone (liq)                             | -59.18  | (1) |
| C <sub>3</sub> H <sub>6</sub> O                             | 58.0807  | n-Propionaldehyde (liq)                     | -53.0   | (1) |
| C <sub>3</sub> H <sub>6</sub> O                             | 74.0801  | Methyl acetate (liq)                        | -106.4  | (1) |
| C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>                | 74.0801  | Propionic acid (liq)                        | -122.07   | (1) |
| C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> S              | 106.1441 | $\beta$ -Thiolactic acid (liq)              | -111.6  | (1) |
| C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> S              | 90.0795  | Glyceraldehyde (liq)                        | -143.   | (1) |
| C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>                | 90.0795  | D-Lactic acid (c)                           | -165.88   | (1) |
| C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>                | 90.0795  | DL-Lactic acid (liq)                        | -160.3  | (1) |
| C <sub>3</sub> H <sub>6</sub> S                             | 74.1453  | Thiacyclobutane (liq)                       | +5.93   | (1) |
| C <sub>3</sub> H <sub>7</sub> NO                            | 73.0953  | N,N-Diethylformamide (liq)                  | -57.2   | (1) |
| C <sub>3</sub> H <sub>7</sub> NO                            | 73.0953  | Propionamide (c)                            | -81.7   | (1) |
| C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>               | 89.0947  | DL-Alanine (c)                              | -134.55   | (1) |
| C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>               | 89.0947  | L-Alanine (c)                               | -133.96   | (1) |
| C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>               | 89.0947  | Ethyl carbamate (c)                         | -124.4  | (1) |
| C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>               | 89.0947  | Sarcosine (c)                               | -121.2  | (1) |
| C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S             | 121.1587 | L-Cysteine (c)                              | -124.6  | (1) |
| C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>               | 105.0941 | L-Tyrosine (c)                              | -177.8  | (1) |
| C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>               | 105.0941 | L-Serine (c)                                | -173.6  | (1) |
| C <sub>3</sub> H <sub>7</sub> N <sub>5</sub>                | 113.1227 | 5-Vinylaminotetrazole (c)                   | +43.6   | (1) |
| C <sub>3</sub> H <sub>7</sub> N <sub>5</sub> O <sub>3</sub> | 161.1209 | 1-Acetamido-2-nitroguanidine (c)            | -46.3   | (1) |
| C <sub>3</sub> H <sub>7</sub> N <sub>5</sub> O <sub>3</sub> | 161.1209 | 3-Amino-5-methyl-1,2,4-triazole nitrate (c) | -54.6   | (1) |
| C <sub>3</sub> H <sub>8</sub>                               | 44.0972  | Propane (g)                                 | -24.81  | (1) |
| C <sub>3</sub> H <sub>8</sub> Hg                            | 244.6872 | Methyl ethyl mercury (liq)                  | +11.1   | (3) |
| C <sub>3</sub> H <sub>8</sub> N <sub>6</sub> O <sub>3</sub> | 176.1356 | 1,3-Dimethyl-5-iminotetrazole nitrate (c)   | +46.4   | (1) |
| C <sub>3</sub> H <sub>8</sub> O                             | 60.0966  | Methyl ethyl ether (g)                      | -1.3  | (1) |
| C <sub>3</sub> H <sub>8</sub> O                             | 60.0966  | 1-Propanol (liq)                            | -51.72  | (1) |
| C <sub>3</sub> H <sub>8</sub> O                             | 60.0966  | 2-Propanol (liq)                            | -72.66  | (1) |
| C <sub>3</sub> H <sub>8</sub> O                             | 76.0960  | 1,2-Propanediol (liq)                       | -75.97  | (1) |
| C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>                | 76.0960  | 1,3-Propanediol (liq)                       | -119.6  | (1) |
| C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>                | 76.0960  | 1,2,3-Propanetriol (liq)                    | -124.4  | (1) |
| C <sub>3</sub> H <sub>8</sub> O <sub>3</sub>                | 92.0954  | 1,2,3-Propanetriol (liq)                    | -159.76   | (1) |
| C <sub>3</sub> H <sub>8</sub> S                             | 76.1612  | 1-Propane thiol (liq)                       | -23.78  | (1) |
| C <sub>3</sub> H <sub>8</sub> S <sub>2</sub>                | 108.2252 | 1,3-Propanedithiol (liq)                    | -18.83  | (1) |
| C <sub>3</sub> H <sub>9</sub> Al                            | 72.0867  | Trimethyl aluminum (g)                      | -17.7   | (2) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Formula Weight | Name (state)                      | Ref | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | kJ mol <sup>-1</sup> |
|--|----------------|-----------------------------------|-----|---|----------------------|
| C <sub>3</sub> H <sub>9</sub> Al                             | 72.0867        | Trimethyl aluminum (liq)          | (2) | -32.6   | -136.4               |
| C <sub>3</sub> H <sub>9</sub> B                              | 55.9162        | Trimethyl boron (g)               | (2) | -29.7   | -124.3               |
| C <sub>3</sub> H <sub>9</sub> B                              | 55.9162        | Trimethyl boron (liq)             | (2) | -34.2   | -143.1               |
| C <sub>3</sub> H <sub>9</sub> B <sup>0</sup> 3               | 103.9144       | Trimethoxyborane (g)              | (2) | -215.0  | -899.6               |
| C <sub>3</sub> H <sub>9</sub> B <sup>0</sup> 3               | 103.9144       | Trimethoxyborane (liq)            | (2) | -223.2  | -933.9               |
| C <sub>3</sub> H <sub>9</sub> Ga                             | 114.8252       | Trimethyl gallium (g)             | (2) | -10.8   | -45.2                |
| C <sub>3</sub> H <sub>9</sub> Ga                             | 114.8252       | Trimethyl gallium (liq)           | (2) | -18.7   | -78.2                |
| C <sub>3</sub> H <sub>9</sub> N                              | 59.1119        | Isopropylamine (liq)              | (1) | -26.83  | -112.26              |
| C <sub>3</sub> H <sub>9</sub> N                              | 59.1119        | n-Propylamine (liq)               | (1) | -24.26  | -101.50              |
| C <sub>3</sub> H <sub>9</sub> N                              | 59.1119        | Trimethylamine (liq)              | (1) | -11.0   | -46.0                |
| C <sub>3</sub> H <sub>9</sub> N <sup>0</sup> 4               | 179.1363       | Acetanilidoguanidine nitrate (c)  | (1) | -118.1  | -494.1               |
| C <sub>3</sub> H <sub>9</sub> P                              | 76.0790        | Trimethylphosphine (liq)          | (1) | -30.  | -126.                |
| C <sub>3</sub> H <sub>10</sub> N <sup>2</sup>                | 74.1266        | 1,2-Propanediamine (liq)          | (1) | -23.38  | -97.82               |
| C <sub>3</sub> H <sub>10</sub> N <sup>2</sup> <sup>0</sup> 3 | 122.1248       | Trimethylamine nitrate (c)        | (1) | -74.1   | -310.0               |
| C <sub>3</sub> H <sub>10</sub> N <sup>2</sup> Si             | 122.1974       | Trimethoxysilane (liq)            | (2) | -199.   | -833.                |
| C <sub>3</sub> H <sub>10</sub> Sn                            | 164.8032       | Trimethyl tin (g)                 | (2) | *5.   | *21.                 |
| C <sub>3</sub> H <sub>10</sub> Sn                            | 164.8032       | Trimethyl tin (liq)               | (2) | -2.1  | -8.3                 |
| C <sub>3</sub> H <sub>12</sub> N <sup>2</sup> <sup>0</sup> 3 | 180.1675       | Guanidine carbonate (c)           | (1) | -232.10   | -971.11              |
| C <sub>4</sub> H <sub>2</sub> N <sub>2</sub> S               | 110.1379       | 4-Cyanothiazole (c)               | (1) | *52.63  | *220.20              |
| C <sub>4</sub> H <sub>2</sub> <sup>0</sup> 3                 | 98.0587        | Maleic anhydride (c)              | (1) | -112.42   | -470.37              |
| C <sub>4</sub> H <sub>4</sub> N                              | 80.0899        | Pyrazine (c)                      | (1) | *33.41  | *139.79              |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>                 | 80.0899        | Pyrazine (g)                      | (1) | *46.86  | *196.06              |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>                 | 80.0899        | Pyridazine (g)                    | (1) | *66.52  | *278.32              |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>                 | 80.0899        | Pyridazine (liq)                  | (1) | *53.74  | *224.85              |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>                 | 80.0899        | Pyrimidine (g)                    | (1) | *46.99  | *196.51              |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>                 | 80.0899        | Pyrimidine (liq)                  | (1) | *35.04  | *146.61              |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> <sup>0</sup> 3  | 128.0881       | Barbituric acid (c)               | (1) | -152.2  | -636.8               |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> <sup>0</sup> 3  | 144.0875       | Dialuric acid (c)                 | (1) | -314.4  | -1315.4              |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> <sup>0</sup> 4  | 160.0869       | Alloxan monohydrate (c)           | (1) | -239.08   | -1000.31             |
| C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> <sup>0</sup> 5  | 68.0759        | Furan (g)                         | (1) | -8.23   | -34.43               |
| C <sub>4</sub> H <sub>4</sub> O                              | 68.0759        | Furan (liq)                       | (1) | -14.84  | -62.09               |
| C <sub>4</sub> H <sub>4</sub> O <sup>0</sup> 3               | 84.0753        | β-Methylene-β-propiolactone (liq) | (1) | -55.72  | -233.13              |
| C <sub>4</sub> H <sub>4</sub> O <sup>0</sup> 2               | 100.0747       | Succinic anhydride (c)            | (1) | -143.8  | -601.7               |
| C <sub>4</sub> H <sub>4</sub> O <sup>0</sup> 3               | 116.0741       | Fumaric acid (c)                  | (1) | -193.84   | -811.03              |
| C <sub>4</sub> H <sub>4</sub> O <sup>0</sup> 4               | 116.0741       | Maleic acid (c)                   | (1) | -188.94   | -790.52              |
| C <sub>4</sub> H <sub>4</sub> S                              | 84.1405        | Thiophene (liq)                   | (1) | *19.24  | *80.50               |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula   | Formula<br>Weight | Name (state)                                 | Enthalpy of Formation<br>kcal. mol. <sup>-1</sup> | Ref |
|---|-------------------|--|---|-----|
| C <sub>4</sub> H <sub>5</sub> N                             | 67.0912           | Pyrrole (g)                                  | +25.88  | (1) |
| C <sub>4</sub> H <sub>5</sub> N                             | 67.0912           | Pyrrole (liq)                                | +108.28<br>+63.09                                 | (1) |
| C <sub>4</sub> H <sub>5</sub> NH <sub>3</sub>               | 115.0894          | Sarcosine-N-carboxylic acid anhydride<br>(c) | -144.1<br>-602.9                                  | (1) |
| C <sub>4</sub> H <sub>5</sub> NS                            | 99.1552           | 4-Methylthiazole (liq)                       | +16.31<br>+58.24                                  | (1) |
| C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O <sub>3</sub> | 143.1028          | Uramil (c)                                   | -16.2<br>-703.7                                   | (1) |
| C <sub>4</sub> H <sub>6</sub>                               | 54.0924           | 1,2-Butadiene (g)                            | +38.77<br>+162.21                                 | (4) |
| C <sub>4</sub> H <sub>6</sub>                               | 54.0924           | 1,3-Butadiene (g)                            | +26.33<br>+110.16                                 | (4) |
| C <sub>4</sub> H <sub>6</sub>                               | 54.0924           | 1-Butyne (g)                                 | +39.49<br>+155.23                                 | (4) |
| C <sub>4</sub> H <sub>6</sub>                               | 54.0924           | 2-Butyne (g)                                 | +34.98<br>+146.36                                 | (4) |
| C <sub>4</sub> H <sub>6</sub> CO <sub>6</sub>               | 213.6288          | Copper (II) glycollate (c)                   | -299.1<br>-1251.4                                 | (3) |
| C <sub>4</sub> H <sub>6</sub> CO <sub>6</sub>               | 181.6300          | Copper (II) acetate (c)                      | -213.5<br>-893.3                                  | (3) |
| C <sub>4</sub> H <sub>6</sub> MnO <sub>4</sub>              | 173.0280          | Manganese acetate (c)                        | -274.4<br>-1148.1                                 | (3) |
| C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> | 114.1046          | Glycine anhydride (c)                        | -106.0<br>-443.5                                  | (1) |
| C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> | 114.1046          | 5-Methyl hydantoin (c)                       | -116.3<br>-436.6                                  | (1) |
| C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>3</sub> | 158.1174          | Allantoin (c)                                | -171.51<br>-717.60                                | (1) |
| C <sub>4</sub> H <sub>6</sub> N <sub>6</sub>                | 138.1326          | 3-Azido-5-ethyl-s-triazole (c)               | +87.4<br>+365.7                                   | (1) |
| C <sub>4</sub> H <sub>6</sub> N <sub>8</sub>                | 166.1460          | 1,2-Di-(5-tetrazolyl)ethane (c)              | +106.2<br>+444.3                                  | (1) |
| C <sub>4</sub> H <sub>6</sub> N <sub>10</sub>               | 194.1594          | cis-1,1'-Dimethyl-5,5'-azotetrazole (c)      | +188.6<br>+789.1                                  | (1) |
| C <sub>4</sub> H <sub>6</sub> N <sub>10</sub>               | 194.1594          | trans-1,1'-Dimethyl-5,5'-azotetrazole<br>(c) | +189.3<br>+792.0                                  | (1) |
| C <sub>4</sub> H <sub>6</sub> N <sub>10</sub>               | 194.1594          | 2,2'-Dimethyl-5,5'-azotetrazole (c)          | +180.3<br>+754.4                                  | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>                | 86.0912           | 2,3-Butanedione (liq)                        | -87.44<br>-365.35                                 | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>                | 86.0912           | cis-Crotonic acid (liq)                      | -83.  | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>                | 86.0912           | trans-Crotonic acid (c)                      | -102.9  | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>                | 102.0906          | Acetic anhydride (liq)                       | -149.45<br>-625.30                                | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>                | 118.0900          | Dimethyl oxalate (liq)                       | -181.0<br>-757.3                                  | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>                | 118.0900          | Succinic acid (c)                            | -224.79<br>-940.52                                | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> Pb             | 325.2800          | Lead acetate (c)                             | -230.36<br>-963.83                                | (2) |
| C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> Zn             | 183.4600          | Zinc acetate (c)                             | -257.8<br>-1073.5                                 | (2) |
| C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>                | 134.0894          | DL-Malic acid (c)                            | -264.27<br>-1105.71                               | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>                | 134.0894          | L-Malic acid (c)                             | -263.78<br>-1103.66                               | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>6</sub>                | 150.0898          | DL-Tartaric acid (c)                         | -308.5<br>-1290.8                                 | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>6</sub>                | 150.0888          | L-Tartaric acid (c)                          | -306.5<br>-1282.4                                 | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>6</sub>                | 150.0888          | meso-Tartaric acid (c)                       | -305.9<br>-1279.9                                 | (1) |
| C <sub>4</sub> H <sub>6</sub> O <sub>6</sub> Zn             | 215.4588          | Zinc glycollate (c)                          | -350.6<br>-1466.9                                 | (2) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula   | Formula Weight | Name (state)                            | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Ref |
|---|----------------|---|---|-----|
| C <sub>4</sub> H <sub>7</sub> NO                            | 85.1065        | $\alpha$ -Pyrrolidone (c)               | -68.3   | (1) |
| C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub>               | 101.1059       | Diacetamide (c)                         | -117.   | (1) |
| C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub>               | 133.1047       | L-Aspartic acid (c)                     | -232.47   | (1) |
| C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub>               | 133.1047       | D,L-Glycolamidic acid (c)               | -219.5  | (1) |
| C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> O              | 113.1199       | Creatinine (c)                          | -56.77  | (1) |
| C <sub>4</sub> H <sub>7</sub> N <sub>5</sub>                | 125.1339       | 1-Allyl-5-amino-tetrazole (c)           | -63.4   | (1) |
| C <sub>4</sub> H <sub>7</sub> N <sub>5</sub>                | 125.1339       | 2-Allyl-5-amino-tetrazole (c)           | -67.6   | (1) |
| C <sub>4</sub> H <sub>7</sub> N <sub>5</sub> O <sub>2</sub> | 157.1327       | 5-Tetraazoylurethan (c)                 | -52.6   | (1) |
| C <sub>4</sub> H <sub>7</sub> N <sub>7</sub>                | 153.1473       | 4-Amino-3-azido-5-e-thyl-8-triazole (c) | -118.5  | (1) |
| C <sub>4</sub> H <sub>8</sub>                               | 56.1084        | Cyclobutane (liq)                       | -0.76   | (1) |
| C <sub>4</sub> H <sub>8</sub>                               | 56.1084        | 1-Butene (g)                            | -0.03   | (4) |
| C <sub>4</sub> H <sub>8</sub>                               | 56.1084        | cis-2-Butene (g)                        | -1.67   | (4) |
| C <sub>4</sub> H <sub>8</sub>                               | 56.1084        | trans-2-Butene (g)                      | -2.67   | (4) |
| C <sub>4</sub> H <sub>8</sub>                               | 56.1084        | 2-Methyl 1-propene (g)                  | -4.04   | (4) |
| C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> | 116.1206       | Succinamide (c)                         | -138.9  | (1) |
| C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> | 132.1200       | L-Asparagine (c)                        | -188.50   | (1) |
| C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> | 132.1200       | Glycylglycine (c)                       | -178.51   | (1) |
| C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> | 148.1194       | L-Tartramide (c)                        | -222.9  | (1) |
| C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> | 148.1194       | meso-Tartramide (c)                     | -223.5  | (1) |
| C <sub>4</sub> H <sub>8</sub> O                             | 72.1078        | Butanone (g)                            | -50.26  | (1) |
| C <sub>4</sub> H <sub>8</sub> O                             | 72.1078        | Butanone (liq)                          | -65.29  | (1) |
| C <sub>4</sub> H <sub>8</sub> O                             | 72.1078        | n-Butyraldehyde (liq)                   | -57.3   | (1) |
| C <sub>4</sub> H <sub>8</sub> O                             | 72.1078        | Tetrahydrofuran (g)                     | -44.03  | (1) |
| C <sub>4</sub> H <sub>8</sub> O                             | 72.1078        | Tetrahydrofuran (liq)                   | -51.1   | (1) |
| C <sub>4</sub> H <sub>8</sub> O <sup>2</sup>                | 88.1072        | Butyric acid (liq)                      | -127.59   | (1) |
| C <sub>4</sub> H <sub>8</sub> O <sup>2</sup>                | 88.1072        | 1,3-Dioxane (liq)                       | -89.99  | (1) |
| C <sub>4</sub> H <sub>8</sub> O <sup>2</sup>                | 88.1072        | 1,4-Dioxane (liq)                       | -84.47  | (1) |
| C <sub>4</sub> H <sub>8</sub> O <sup>2</sup>                | 88.1072        | Gycol acetal (liq)                      | -91.1   | (1) |
| C <sub>4</sub> H <sub>8</sub> O <sup>2</sup>                | 104.1066       | DL- $\beta$ -Hydroxybutyric acid (liq)  | -162.3  | (1) |
| C <sub>4</sub> H <sub>8</sub> O <sup>2</sup>                | 104.1066       | Hydroxyisobutyric acid (c)              | -177.9  | (1) |
| C <sub>4</sub> H <sub>8</sub> O <sup>2</sup>                | 168.1042       | DL-Tartaric acid monohydrate (c)        | -371.   | (1) |
| C <sub>4</sub> H <sub>8</sub> O <sup>2</sup>                | 88.10724       | Thiacyclopentane (liq)                  | -17.39  | (1) |
| C <sub>4</sub> H <sub>8</sub> S                             | 88.1072        | Pyrrotidine (g)                         | -0.89   | (1) |
| C <sub>4</sub> H <sub>9</sub> N                             | 71.1230        | Pyrrolidine (liq)                       | -9.87   | (1) |
| C <sub>4</sub> H <sub>9</sub> N                             | 71.1230        | n-Butyramide (c)                        | -87.5   | (1) |
| C <sub>4</sub> H <sub>9</sub> NO                            | 87.1224        | $\gamma$ -Aminobutyric acid (c)         | -138.1  | (1) |
| C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>               | 103.1218       |   | -577.9  | (1) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Formula weight | Name (state)                      | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Enthalpy of Formation<br>kJ mol <sup>-1</sup> | Ref <sup>f</sup> |
|--|----------------|-----------------------------------|---|---|------------------|
| C <sub>4</sub> H <sub>9</sub> N <sup>0</sup> 3               | 119.1212       | DL-Threonine (c)                  | -181.4  | -759.0  | (1)              |
| C <sub>4</sub> H <sub>9</sub> N <sup>0</sup> 3               | 119.1212       | L-Threonine (c)                   | -191.4  | -759.0  | (1)              |
| C <sub>4</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>  | 131.1352       | Creatine (c)                      | -128.16   | -536.22                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub>                               | 58.1243        | n-Butane (g)                      | -30.10  | -125.94                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub> Hg                            | 258.7143       | Diethyl mercury (g)               | +18.0   | +75.3   | (3)              |
| C <sub>4</sub> H <sub>10</sub> Hg                            | 258.7143       | Diethyl mercury (liq)             | +7.2  | +30.1   | (3)              |
| C <sub>4</sub> H <sub>10</sub> N <sub>2</sub>                | 86.1377        | Piperazine (c)                    | -10.90  | -45.61  | (1)              |
| C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> | 150.1353       | L-Asparagine monohydrate (c)      | -259.52   | -1085.83                                      | (1)              |
| C <sub>4</sub> H <sub>11</sub> N <sub>3</sub> S              | 149.1506       | Creatine hydrate (c)              | -199.1  | -833.0  | (1)              |
| C <sub>4</sub> H <sub>10</sub> O                             | 74.1237        | 1-Butanol (liq)                   | -78.25  | -327.40                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub> O                             | 74.1237        | 2-Butanol (liq)                   | -81.88  | -342.59                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub> O                             | 74.1237        | Diethyl ether (g)                 | -60.26  | -252.13                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub> O                             | 74.1237        | 2-Methyl-1-propanol (liq)         | -79.85  | -334.09                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub> O                             | 74.1237        | 2-Methyl-2-propanol (liq)         | -85.86  | -359.24                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>                | 90.1231        | 1,2-Dimethoxyethane (liq)         | -90.02  | -376.64                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub> O <sub>4</sub>                | 122.1219       | meso-1,2,3,4-Butanetetrol (c)     | -217.56   | -910.27                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub> S                             | 90.1863        | 1-Butanethiol (liq)               | -29.69  | -124.22                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub> S <sub>2</sub>                | 122.2523       | 1,4-Butanedithiol (liq)           | -25.11  | -105.06                                       | (1)              |
| C <sub>4</sub> H <sub>10</sub> Zn                            | 123.4943       | Diethyl zinc (g)                  | +12.1   | +50.6   | (2)              |
| C <sub>4</sub> H <sub>10</sub> Zn                            | 123.4943       | Diethyl zinc (liq)                | +2.5  | +10.5   | (2)              |
| C <sub>4</sub> H <sub>11</sub> N                             | 73.1390        | n-Butylamine (liq)                | -30.52  | -127.70                                       | (1)              |
| C <sub>4</sub> H <sub>11</sub> N                             | 73.1390        | sec.-Butylamine (liq)             | -32.87  | -137.53                                       | (1)              |
| C <sub>4</sub> H <sub>11</sub> N                             | 73.1390        | tert.-Butylamine (liq)            | -35.97  | -150.50                                       | (1)              |
| C <sub>4</sub> H <sub>11</sub> N                             | 73.1390        | Diethylamine (liq)                | -24.7   | -103.3  | (1)              |
| C <sub>4</sub> H <sub>11</sub> N                             | 73.1390        | Isobutylamine (liq)               | -31.68  | -132.55                                       | (1)              |
| C <sub>4</sub> H <sub>12</sub> N <sub>2</sub>                | 88.1536        | 1,2-Butanediamine (liq)           | -28.74  | -120.25                                       | (1)              |
| C <sub>4</sub> H <sub>12</sub> N <sub>2</sub>                | 88.1536        | 2-Methyl-1,2-propanediamine (liq) | -32.00  | -133.89                                       | (1)              |
| C <sub>4</sub> H <sub>12</sub> N <sup>0</sup> 3              | 136.1518       | Diethylamine nitrate (c)          | -100.1  | -418.8  | (2)              |
| C <sub>4</sub> H <sub>12</sub> O <sub>4</sub> Si             | 152.2238       | Tetramethoxysilane (liq)          | -302.   | -1264.  | (2)              |
| C <sub>4</sub> H <sub>12</sub> Pb                            | 267.3302       | Tetramethyl lead (g)              | +32.48  | +135.90                                       | (2)              |
| C <sub>4</sub> H <sub>12</sub> Pb                            | 267.3302       | Tetramethyl lead (liq)            | +23.4   | +97.9   | (2)              |
| C <sub>4</sub> H <sub>12</sub> Si                            | 88.2262        | Tetramethylsilane (g)             | -57.1   | -238.9  | (2)              |
| C <sub>4</sub> H <sub>12</sub> Si                            | 88.2262        | Tetramethylsilane (liq)           | -63.  | -254.   | (2)              |
| C <sub>4</sub> H <sub>12</sub> Sn                            | 178.8302       | Diethyl tin (g)                   | +11.0   | +46.0   | (2)              |
| C <sub>4</sub> H <sub>12</sub> Sn                            | 178.8302       | Diethyl tin (liq)                 | +2.1  | +8.8  | (2)              |
| C <sub>4</sub> H <sub>12</sub> Sn                            | 178.8302       | Tetraethyl tin (g)                | -4.5  | -18.8   | (2)              |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Formula Weight | Name (state)                     | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Ref   |
|--|----------------|----------------------------------|---|-------|
| C <sub>4</sub> H <sub>12</sub> Sn                            | 178.8302       | Tetramethyl tin (liq)            | -112.5  | (2)   |
| C <sub>4</sub> H <sub>22</sub> N <sub>2</sub> O <sub>6</sub> | 194.2297       | Piperazine hexahydrate (c)       | -436.8  | (1)   |
| C <sub>4</sub> NiO <sub>4</sub>                              | 170.7522       | Nickel carbonyl (g)              | -144.10   | (3)   |
| C <sub>4</sub> NiO <sub>4</sub>                              | 170.7522       | Nickel carbonyl (liq)            | -151.3  | (3)   |
| C <sub>5</sub> FeO <sub>5</sub>                              | 195.8998       | Iron pentacarbonyl (g)           | -175.4  | (3)   |
| C <sub>5</sub> FeO <sub>5</sub>                              | 195.8998       | Iron pentacarbonyl (liq)         | -185.0  | (3)   |
| C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>  | 136.1138       | Hypoxanthine (c)                 | -26.24  | (1)   |
| C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>  | 136.1138       | 8-Oxypurine (c)                  | -15.4   | (1)   |
| C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>  | 152.1132       | Xanthine (c)                     | -90.49  | (1)   |
| C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>  | 168.1126       | Isouric' acid (c)                | -147.9  | (1)   |
| C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>  | 168.1126       | Uric acid (c)                    | -147.73   | (1)   |
| C <sub>5</sub> H <sub>4</sub> O <sub>2</sub>                 | 96.0864        | Furfural (liq)                   | -47.8   | (1)   |
| C <sub>5</sub> H <sub>4</sub> O <sub>3</sub>                 | 112.0858       | 2-Furoic acid (c)                | -119.1  | (1)   |
| C <sub>5</sub> S <sub>5</sub> N                              | 79.1023        | Pyridine (g)                     | +33.61  | (1)   |
| C <sub>5</sub> S <sub>5</sub> N                              | 79.1023        | Pyridine (liq)                   | +23.96  | (1)   |
| C <sub>5</sub> S <sub>5</sub> NO                             | 95.1017        | Pyrrolaldehyde (c)               | -24.8   | (1)   |
| C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>                 | 135.1291       | Adenine (c)                      | +23.21  | (1)   |
| C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O               | 151.1285       | Guanine (c)                      | -43.72  | (1)   |
| C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>  | 110.1164       | Pyrrolidoxime                    | +3.7  | (1)   |
| C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>  | 126.1158       | 4-Methyl uracil (c)              | -109.2  | (1)   |
| C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>  | 126.1158       | Thymine (c)                      | -111.9  | (1)   |
| C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>  | 142.1152       | Dimethyl parabanic acid (c)      | -137.0  | (1)   |
| C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>  | 186.1280       | Pseudouric acid (c)              | -221.7  | (1)   |
| C <sub>5</sub> H <sub>6</sub> O <sub>4</sub>                 | 98.1024        | Furfuryl alcohol (liq)           | -66.0   | (1)   |
| C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>                 | 98.1024        | Levulinic lactone (liq)          | -76.2   | (1)   |
| C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>                 | 130.1012       | Citraconic acid (c)              | -197.04   | (1)   |
| C <sub>5</sub> H <sub>6</sub> O <sub>4</sub>                 | 130.1012       | Iaconic acid (c)                 | -201.06   | (1)   |
| C <sub>5</sub> H <sub>6</sub> O <sub>4</sub>                 | 130.1012       | Mesaconic acid (c)               | -197.   | (1)   |
| C <sub>5</sub> H <sub>6</sub> O <sub>4</sub>                 | 146.1006       | $\alpha$ -Keto glutaric acid (c) | -245.35   | (1)   |
| C <sub>5</sub> H <sub>6</sub> S                              | 98.1676        | 2-Methyl thiophene (liq)         | +10.75  | (1)   |
| C <sub>5</sub> H <sub>6</sub> S                              | 98.1676        | 3-Methyl thiophene (liq)         | +10.38  | (1)   |
| C <sub>5</sub> H <sub>7</sub> N <sub>3</sub>                 | 109.1316       | 2,6-Diaminopyridine (c)          | -1.5  | (1)   |
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195        | 2-Methyl-1,3-butadiene (g)       | +18.10  | (4,5) |
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195        | 2-Methyl-1,3-butadiene (liq)     | +11.80  | (4)   |
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195        | 1,2-Pentadiene (g)               | +33.63  | (5)   |
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195        | 1-cis-3-Pentadiene (g)           | +19.79  | (5)   |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Formula<br>Weight | Name (state)                        | Enthalpy of<br>Formation<br>kcal mol <sup>-1</sup> | Ref     |
|--|-------------------|-------------------------------------|--|---------|
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195           | 1-trans-3-Pentadiene (g)            | +18.13   | +75.86  |
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195           | 1,4-Pentadiene (g)                  | +25.43   | +106.40 |
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195           | 2,3-Pentadiene (g)                  | +31.81   | +133.09 |
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195           | 3-Methyl 1,1-butyne (g)             | +32.62   | +136.48 |
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195           | 1-Pentyne (g)                       | +34.52   | +144.43 |
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195           | 2-Pentyne (g)                       | +30.81   | +128.91 |
| C <sub>5</sub> H <sub>8</sub>                                | 68.1195           | Spiropentane (g)                    | +44.26   | +185.18 |
| C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>  | 128.1317          | 5,5-Dimethyl hydantoin (c)          | +126.4   | +528.9  |
| C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>  | 128.1317          | 4-Methyl hydouracil (c)             | +125.5   | +525.1  |
| C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>5</sub>  | 176.1299          | Glycylglycine-N-carboxylic acid (c) | +273.0   | +1142.2 |
| C <sub>5</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub>  | 172.1445          | Methyl allantoin (c)                | +177.0   | +740.6  |
| C <sub>5</sub> H <sub>8</sub> O                              | 84.1189           | Dihydropyran, 4H (liq)              | -37.5  | -156.9  |
| C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>                 | 100.1183          | Aniglic acid (c)                    | -108.9   | -455.6  |
| C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>                 | 100.1183          | Tiglic acid (c)                     | -117.3   | -490.8  |
| C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>                 | 116.1177          | Levulinic acid (c)                  | -166.6   | -697.1  |
| C <sub>5</sub> H <sub>8</sub> O <sub>4</sub>                 | 132.1171          | Dimethyl malonate (liq)             | -190.2   | -795.8  |
| C <sub>5</sub> H <sub>8</sub> O <sub>4</sub>                 | 132.1171          | Glutaric acid (c)                   | -229.44  | -959.98 |
| C <sub>5</sub> H <sub>8</sub> O <sub>5</sub>                 | 148.1165          | D-Arabonic acid-γ-lactone (c)       | -238.2   | -996.6  |
| C <sub>5</sub> H <sub>8</sub> O <sub>7</sub>                 | 180.1153          | DL-Trihydroxybutyric acid (c)       | -356.  | -1490.  |
| C <sub>5</sub> H <sub>9</sub> N                              | 83.1342           | 1,2,5,6-Tetrahydropyridine (liq)    | +8.0   | +33.5   |
| C <sub>5</sub> H <sub>9</sub> NO                             | 99.1336           | N-Methyl pyrrolidone (liq)          | -62.64   | -262.09 |
| C <sub>5</sub> H <sub>9</sub> NO                             | 99.1336           | α-Piperidone (c)                    | -73.3  | -306.7  |
| C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>                | 115.1330          | DL-Proline (c)                      | -125.7   | -525.9  |
| C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>                | 131.1324          | L-Hydroxyproline (c)                | -158.1   | -661.5  |
| C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>                | 147.1318          | L-Glutamic acid (c)                 | -241.5   | -1010.4 |
| C <sub>5</sub> H <sub>10</sub>                               | 70.1355           | Cyclopentane (liq)                  | -25.28   | -105.77 |
| C <sub>5</sub> H <sub>10</sub>                               | 70.1354           | 2-Methyl 1-butene (g)               | -8.66  | -36.23  |
| C <sub>5</sub> H <sub>10</sub>                               | 70.1354           | 2-Methyl 1,2-butene (g)             | -10.15   | -42.47  |
| C <sub>5</sub> H <sub>10</sub>                               | 70.1354           | 3-Methyl 1,1-butene (g)             | -6.90  | -28.87  |
| C <sub>5</sub> H <sub>10</sub>                               | 70.1354           | 1-Pentene (g)                       | -4.98  | -20.44  |
| C <sub>5</sub> H <sub>10</sub>                               | 70.1354           | cis-2-Pentene (g)                   | -6.49  | -27.15  |
| C <sub>5</sub> H <sub>10</sub>                               | 70.1354           | trans-2-Pentene (g)                 | -7.57  | -31.67  |
| C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> | 146.1471          | DL-Alanyl glycine (c)               | +185.64  | +776.72 |
| C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> | 146.1471          | L-Glutawine (c)                     | +197.3   | +925.5  |
| C <sub>5</sub> H <sub>10</sub> O                             | 86.1349           | 2-Pentanone (liq)                   | -71.05   | -297.27 |
| C <sub>5</sub> H <sub>10</sub> O                             | 86.1349           | 3-Pentanone (liq)                   | -70.87   | -296.52 |

TABLE I-a

| Formula  | Formula Weight | Name (state)                     | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Enthalpy of Formation<br>kJ mol <sup>-1</sup> | Ref |
|--|----------------|----------------------------------|---|---|-----|
| C <sub>5</sub> H <sub>10</sub> O <sup>6</sup>                | 86.1349        | Tetrahydropyran (g)              | -53.39  | -223.38                                       | (1) |
| C <sub>5</sub> H <sub>10</sub> O                             | 86.1349        | Tetrahydropyran (liq)            | -61.1   | -255.6  | (1) |
| C <sub>5</sub> H <sub>10</sub> O                             | 86.1349        | n-Valealdehyde (liq)             | -70.  | -293.   | (1) |
| C <sub>5</sub> H <sub>10</sub> O <sup>2</sup>                | 102.1343       | 5-Hydroxy-1-pentanal (liq)       | -114.7  | -479.9  | (1) |
| C <sub>5</sub> H <sub>10</sub> O <sup>2</sup>                | 102.1343       | Tetrahydrofurfuryl alcohol (liq) | -104.1  | -435.6  | (1) |
| C <sub>5</sub> H <sub>10</sub> O <sup>2</sup>                | 102.1343       | Valeric acid (liq)               | -133.71   | -559.44                                       | (1) |
| C <sub>5</sub> H <sub>10</sub> O <sup>2</sup>                | 134.1331       | Glyceryl-1-acetate (liq)         | -217.5  | -910.0  | (1) |
| C <sub>5</sub> H <sub>10</sub> O <sup>4</sup>                | 150.1325       | $\beta$ -D-Arabinose (c)         | -252.84   | -1057.98                                      | (1) |
| C <sub>5</sub> H <sub>10</sub> O <sup>5</sup>                | 150.1325       | $\beta$ -L-Arabinose (c)         | -252.84   | -1057.98                                      | (1) |
| C <sub>5</sub> H <sub>10</sub> O <sup>5</sup>                | 150.1325       | $\beta$ -D-Ribose (c)            | -251.16   | -1050.85                                      | (1) |
| C <sub>5</sub> H <sub>10</sub> O <sup>5</sup>                | 150.1325       | $\alpha$ -D-Xylose (c)           | -252.8  | -1057.7                                       | (1) |
| C <sub>5</sub> H <sub>10</sub> S                             | 102.1995       | Thiacyclohexane (liq)            | -25.33  | -105.98                                       | (1) |
| C <sub>5</sub> H <sub>11</sub> N                             | 85.1501        | Piperidine (liq)                 | -21.05  | -88.07  | (1) |
| C <sub>5</sub> H <sub>11</sub> NO <sup>2</sup>               | 117.1489       | 6-Aminovaleric acid (c)          | -144.5  | -604.6  | (1) |
| C <sub>5</sub> H <sub>11</sub> NO <sup>2</sup>               | 117.1489       | DL-Valine (c)                    | -148.2  | -620.1  | (1) |
| C <sub>5</sub> H <sub>11</sub> NO <sup>2</sup>               | 117.1489       | L-Valine (c)                     | -148.2  | -620.1  | (1) |
| C <sub>5</sub> H <sub>11</sub> NO <sup>2</sup> S             | 149.2129       | L-Methionine (c)                 | -180.4  | -754.8  | (1) |
| C <sub>5</sub> H <sub>12</sub>                               | 72.1514        | 2,2-Dimethylpropane (g)          | -39.76  | -166.36                                       | (4) |
| C <sub>5</sub> H <sub>12</sub>                               | 72.1514        | 2-Methylbutane (g)               | -36.91  | -154.43                                       | (4) |
| C <sub>5</sub> H <sub>12</sub>                               | 72.1514        | n-Pentane (g)                    | -35.08  | -146.77                                       | (1) |
| C <sub>5</sub> H <sub>12</sub>                               | 72.1514        | n-Pentane (liq)                  | -41.47  | -173.51                                       | (1) |
| C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sup>6</sup> | 132.1636       | DL-Glutathione (c)               | -156.0  | -652.7  | (1) |
| C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sup>2</sup> | 88.1508        | 1-Pentanol (liq)                 | -84.27  | -352.59                                       | (1) |
| C <sub>5</sub> H <sub>12</sub> O <sup>4</sup>                | 136.1490       | Pentaerythritol (c)              | -220.0  | -920.5  | (1) |
| C <sub>5</sub> H <sub>12</sub> O <sup>5</sup>                | 152.1484       | L-Arabinitol (c)                 | -268.7  | -1124.2                                       | (1) |
| C <sub>5</sub> H <sub>12</sub> O <sup>5</sup>                | 152.1484       | Xylitol (c)                      | -267.32   | -1118.47                                      | (1) |
| C <sub>5</sub> H <sub>12</sub> S                             | 104.2154       | 1-Pentanethiol (liq)             | -35.72  | -149.45                                       | (1) |
| C <sub>6</sub> CrO <sub>6</sub>                              | 220.0593       | Chromium hexacarbonyl (g)        | -240.4  | -1005.8                                       | (3) |
| C <sub>6</sub> CrO <sub>6</sub>                              | 220.0593       | Chromium hexacarbonyl (c)        | -257.4  | -1077.0                                       | (3) |
| C <sub>6</sub> H <sub>4</sub> N <sub>2</sub>                 | 104.1122       | 3-Cyanopyridine (c)              | +4.6.23   | +193.43                                       | (1) |
| C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>                | 123.1123       | Picolinic acid (c)               | -83.7   | -350.2  | (1) |
| C <sub>6</sub> H <sub>5</sub> N <sub>3</sub>                 | 119.1269       | Benzotriazole (c)                | +59.74  | +249.95                                       | (1) |
| C <sub>6</sub> H <sub>6</sub>                                | 78.1147        | Benzene (g)                      | +19.81  | +32.39  | (1) |
| C <sub>6</sub> H <sub>6</sub>                                | 78.1147        | Benzene (liq)                    | +11.71  | +48.99  | (1) |
| C <sub>6</sub> H <sub>6</sub> N <sub>4</sub>                 | 134.1415       | 7-Methyl purine (c)              | +51.3   | +214.6  | (1) |
| C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O               | 150.1409       | 7-Methylhypoxanthine (c)         | -9.9  | -41.4   | (1) |

TABLE I-A

## ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Name (state)                       | Weight                             | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Ref<br>kJ mol <sup>-1</sup> |
|--|------------------------------------|------------------------------------|---|-----------------------------|
| C <sub>6</sub> H <sub>6</sub> O                              | Phenol (c)                         | 94.1141                            | -39.45  | -165.06                     |
| C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>                 | Hydroquinone (c)                   | 110.1135                           | -87.47  | -365.97                     |
| C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>                 | Pyrocatechol (c)                   | 110.1135                           | -86.3   | -361.1                      |
| C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>                 | Resorcinol (c)                     | 110.1135                           | -87.95  | -367.98                     |
| C <sub>6</sub> H <sub>6</sub> O <sub>6</sub>                 | cis-Aconitic acid (c)              | 174.1111                           | -292.7  | -1124.7                     |
| C <sub>6</sub> H <sub>6</sub> O <sub>6</sub>                 | trans-Aconitic acid (c)            | 174.1111                           | -294.7  | -1233.0                     |
| C <sub>6</sub> H <sub>6</sub> O <sub>6</sub>                 | D-Mannonic-1,4-3,6-dilactone (c)   | 174.1111                           | -254.6  | -1065.2                     |
| C <sub>6</sub> H <sub>6</sub> S                              | Benzene thiol (liq)                | 110.1787                           | +15.32  | +64.10                      |
| C <sub>6</sub> H <sub>7</sub> N                              | Aniline (liq)                      | 93.1294                            | +7.55   | +31.59                      |
| C <sub>6</sub> H <sub>7</sub> N                              | 2-Methyl pyridine (g)              | 93.1294                            | +24.05  | +100.63                     |
| C <sub>6</sub> H <sub>7</sub> N                              | 2-Methyl pyridine (liq)            | 93.1294                            | +13.83  | +57.36                      |
| C <sub>6</sub> H <sub>7</sub> N                              | 3-Methyl pyridine (g)              | 93.1294                            | +26.30  | +110.34                     |
| C <sub>6</sub> H <sub>7</sub> N                              | 3-Methyl pyridine (liq)            | 93.1294                            | +15.57  | +67.14                      |
| C <sub>6</sub> H <sub>7</sub> N                              | 4-Methyl pyridine (g)              | 93.1294                            | +24.44  | +102.26                     |
| C <sub>6</sub> H <sub>7</sub> N                              | 4-Methyl pyridine (liq)            | 93.1294                            | +13.58  | +55.32                      |
| C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>  | Aniline nitrate (c)                | 156.1423                           | -43.7   | -182.8                      |
| C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>                 | Sorbic acid (c)                    | 112.1295                           | -93.4   | -390.8                      |
| C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>                 | Dimethyl fumarate (liq)            | 144.1283                           | -174.3  | -729.3                      |
| C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>                 | Dimethyl maleate (liq)             | 144.1283                           | -168.2  | -703.7                      |
| C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>                 | Hexa-2-ene-1,6-dioic acid (c)      | 144.1283                           | -279.   | -874.                       |
| C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>                 | Hexa-3-ene-1,6-dioic acid (c)      | 144.1283                           | -209.   | -874.                       |
| C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>                 | Lactide (c)                        | 144.1283                           | -184.2  | -770.7                      |
| C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>                 | L-Ascorbic acid (c)                | 176.1271                           | -278.34   | -1164.57                    |
| C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>                 | Citric acid, anhydrous (c)         | 192.1265                           | -369.0  | -1543.9                     |
| C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>                 | D-Glucaric acid id-1,4-lactone (c) | 192.1265                           | -343.2  | -1435.9                     |
| C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>                 | D-Glucaric acid id-3,6-lactone (c) | 192.1265                           | -343.6  | -1437.6                     |
| C <sub>6</sub> H <sub>9</sub> AlO <sub>6</sub>               | Aluminum trilactate (c)            | 204.1165                           | -462.3  | -1892.4                     |
| C <sub>6</sub> H <sub>9</sub> NO <sub>6</sub>                | 191.1417                           | Nitrilotriacetic acid (c)          | -312.5  | -1307.5                     |
| C <sub>6</sub> H <sub>10</sub>                               | 82.1466                            | 1-Hexyne (g)                       | +29.57  | +123.72                     |
| C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> | 142.1588                           | Alanine anhydride (c)              | -128.0  | -535.6                      |
| C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> | 142.1588                           | 5-Methyl-5-ethyl hydantoin (c)     | -135.0  | -554.8                      |
| C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> | 174.1576                           | Serine anhydride (c)               | -209.5  | -876.5                      |
| C <sub>6</sub> H <sub>10</sub> N <sub>10</sub>               | 222.2136                           | 2,2'-Diethyl-5,5'-azotetrazole (c) | +156.6  | +655.2                      |
| C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>                | 114.1454                           | Hydrosorbic acid (liq)             | -110.2  | -461.1                      |
| C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>                | 130.1448                           | Acetone glyceraldehyde (liq)       | -180.   | -753.                       |
| C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>                | 146.1442                           | Adipic acid (c)                    | -237.60   | -994.12                     |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula   | Weight   | Name (state)                                  | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Enthalpy of Formation<br>kJ mol <sup>-1</sup> | Ref |
|---|----------|---|---|---|-----|
| C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>                               | 146.1442 | Dimethyl succinate (liq)                      | -199.6  | -835.1  | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>                               | 146.1442 | Erythritol diformal (c)                       | -161.8  | -677.0  | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>4</sub> S <sub>2</sub>                | 210.2722 | $\beta$ , $\beta'$ -Dithiodilactic acid (liq) | -230.9  | -966.1  | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>5</sub>                               | 162.1436 | Levoglucosan (c)                              | -229.3  | -959.4  | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>5</sub>                               | 162.1436 | Saccharinic acid lactone (c)                  | -249.6  | -1044.3                                       | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>                               | 178.1430 | D-Galactonic acid- $\gamma$ -lactone (c)      | -298.3  | -1248.1                                       | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>                               | 178.1430 | D-Gluconic acid- $\delta$ -lactone (c)        | -300.3  | -1256.5                                       | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>                               | 178.1430 | L-Gulonic acid- $\gamma$ -lactone (c)         | -291.5  | -1219.6                                       | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>                               | 178.1430 | D-Mannonic acid- $\gamma$ -lactone (c)        | -296.2  | -1239.3                                       | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>                               | 210.1418 | Allomuic acid (c)                             | -412.   | -1724.  | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>8</sub>                               | 210.1418 | Citric acid monohydrate (c)                   | -439.40   | -1838.45                                      | (1) |
| C <sub>6</sub> H <sub>10</sub> O <sub>8</sub>                               | 210.1418 | Malic acid (c)                                | -423.   | -1770.  | (1) |
| C <sub>6</sub> H <sub>11</sub> N <sub>6</sub>                               | 113.1607 | $\epsilon$ -Caprolactam (c)                   | -78.6   | -328.9  | (1) |
| C <sub>6</sub> H <sub>11</sub> N <sub>6</sub>                               | 113.1607 | N-Methyl piperidone (liq)                     | -70.00  | -292.86                                       | (1) |
| C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub>                | 189.1723 | Diglycylglycine (c)                           | -230.8  | -965.7  | (1) |
| C <sub>6</sub> H <sub>12</sub>  | 84.1625  | Cyclohexane (liq)                             | -37.33  | -156.19                                       | (1) |
| C <sub>6</sub> H <sub>12</sub>  | 84.1625  | 1-Hexene (g)                                  | -9.94   | -41.59  | (4) |
| C <sub>6</sub> H <sub>12</sub>  | 84.1625  | Methylcyclopentane (liq)                      | -33.06  | -138.32                                       | (4) |
| C <sub>6</sub> H <sub>12</sub> N <sub>2</sub>                               | 112.1759 | Triethylendiamine (c)                         | -3.4  | -14.2   | (1) |
| C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>                | 160.1741 | Ethyl glycylglycinate (c)                     | -170.5  | -713.4  | (1) |
| C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub> | 240.3015 | L-Cystine (c)                                 | -245.7  | -1028.0                                       | (1) |
| C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>5</sub>                | 192.1729 | Serylserine (c)                               | -281.8  | -1179.1                                       | (1) |
| C <sub>6</sub> H <sub>12</sub> N <sub>4</sub>                               | 140.1893 | Hexamethylene tetraamine (c)                  | +28.7   | +120.1  | (1) |
| C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> S <sub>4</sub>                | 240.4319 | Tetramethylthiuram disulfide (c)              | +9.94   | +41.59  | (1) |
| C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> S <sub>3</sub>                | 208.3679 | Tetramethylthiuram monosulfide (c)            | +11.60  | +48.53  | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>                               | 116.1613 | Caproic acid (liq)                            | -139.71   | -584.55                                       | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>                               | 116.1613 | Methyl valerate (liq)                         | -122.89   | -514.17                                       | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>                               | 132.1607 | Acetone glycerol (liq)                        | -163.   | -682.   | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>3</sub>                               | 132.1607 | Paraldehyde (liq)                             | -164.2  | -687.0  | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>                               | 164.1595 | D-Fucose (c)                                  | -262.7  | -1099.1                                       | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>                               | 164.1595 | $\beta$ -L-Khamnose (c)                       | -256.5  | -1073.2                                       | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                               | 180.1589 | $\beta$ -D-Fructose (c)                       | -302.2  | -1264.4                                       | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                               | 180.1589 | $\alpha$ -D-Galactose (c)                     | -304.1  | -1272.4                                       | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                               | 180.1589 | $\alpha$ -D-Glucose (c)                       | -304.26   | -1273.02                                      | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                               | 180.1589 | $\beta$ -D-Glucose (c)                        | -302.76   | -1266.75                                      | (1) |
| C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                               | 180.1589 | D-Mannose (c)                                 | -301.9  | -1263.1                                       | (1) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Formula<br>Weight | Name (state)                         | Enthalpy of<br>Formation<br>kcal mol <sup>-1</sup> | Formation<br>kJ mol <sup>-1</sup> | Ref  |
|--|-------------------|--------------------------------------|--|-----------------------------------|------|
| C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                | 180.1589          | L-Sorbose (c)                        | -303.6   | -1270.3                           | {11} |
| C <sub>6</sub> H <sub>12</sub> O <sub>7</sub>                | 196.1583          | D-Galactonic acid (c)                | -384.8   | -1610.0                           | {11} |
| C <sub>6</sub> H <sub>12</sub> O <sub>7</sub>                | 196.1583          | D-Gluconic acid (c)                  | -379.3   | -1587.0                           | {11} |
| C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>               | 131.1760          | $\alpha$ -Aminocaproic acid (c)      | -152.7   | -638.9                            | {11} |
| C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>               | 131.1760          | $\gamma$ -Aminocaproic acid (c)      | -154.5   | -646.4                            | {11} |
| C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>               | 131.1760          | $\delta$ -Aminocaproic acid (c)      | -153.7   | -643.1                            | {11} |
| C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>               | 131.1760          | $\epsilon$ -Aminocaproic acid (c)    | -152.7   | -638.9                            | {11} |
| C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>               | 131.1760          | DL-Isoleucine (c)                    | -151.8   | -635.1                            | {11} |
| C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>               | 131.1760          | L-Isoleucine (c)                     | -151.8   | -635.1                            | {11} |
| C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>               | 131.1760          | D-Leucine (c)                        | -151.97  | -635.84                           | {11} |
| C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>               | 131.1760          | DL-Leucine (c)                       | -152.74  | -639.06                           | {11} |
| C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>               | 131.1760          | L-Leucine (c)                        | -151.97  | -635.84                           | {11} |
| C <sub>6</sub> H <sub>14</sub>                               | 86.1785           | 2,2-Dimethylbutane (liq)             | -50.99   | -213.34                           | {4}  |
| C <sub>6</sub> H <sub>14</sub>                               | 86.1785           | 2,3-Dimethylbutane (liq)             | -49.46   | -206.94                           | {4}  |
| C <sub>6</sub> H <sub>14</sub>                               | 86.1785           | n-Hexane (liq)                       | -47.50   | -198.74                           | {4}  |
| C <sub>6</sub> H <sub>14</sub>                               | 86.1785           | 2-Methylpentane (liq)                | -48.80   | -204.18                           | {4}  |
| C <sub>6</sub> H <sub>14</sub>                               | 86.1785           | 3-Methylpentane (liq)                | -48.26   | -201.92                           | {4}  |
| C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> | 146.1907          | DL-Lysine (c)                        | -162.2   | -678.6                            | {11} |
| C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> | 174.2041          | L-Arginine (c)                       | -148.66  | -621.99                           | {11} |
| C <sub>6</sub> H <sub>14</sub> N <sub>6</sub> O <sub>2</sub> | 266.2151          | Hexamethylenetetramine dinitrate (c) | -68.6  | -370.7                            | {11} |
| C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>                | 102.1779          | 1-Hexanol (liq)                      | -90.65   | -379.28                           | {11} |
| C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>                | 182.1749          | Dulcitol (c)                         | -321.83  | -1346.54                          | {11} |
| C <sub>6</sub> H <sub>14</sub> O <sub>6</sub>                | 192.1749          | D-Mannitol (c)                       | -319.54  | -1336.96                          | {11} |
| C <sub>6</sub> H <sub>14</sub> O <sub>6</sub>                | 182.1749          | $\alpha$ -L-Rhamnose monohydrate (c) | -331.3   | -1386.2                           | {11} |
| C <sub>6</sub> H <sub>14</sub> O <sub>6</sub>                | 198.1743          | $\alpha$ -D-Glucose hydrate (c)      | -374.97  | -1568.87                          | {11} |
| C <sub>6</sub> H <sub>14</sub> S                             | 118.2425          | 1-Hexanethiol (liq)                  | -41.84   | -175.06                           | {11} |
| C <sub>6</sub> H <sub>15</sub> B                             | 97.9974           | Triethyl boron (g)                   | -37.69   | -157.69                           | {2}  |
| C <sub>6</sub> H <sub>15</sub> B                             | 97.9974           | Triethyl boron (liq)                 | -46.5  | -194.6                            | {2}  |
| C <sub>6</sub> H <sub>15</sub> BO <sub>3</sub>               | 145.9956          | Triethoxyborane (g)                  | -240.4   | -1005.9                           | {2}  |
| C <sub>6</sub> H <sub>15</sub> BO <sub>3</sub>               | 145.9956          | Triethoxyborane (liq)                | -250.8   | -1049.3                           | {2}  |
| C <sub>6</sub> H <sub>15</sub> N                             | 101.1932          | Triethylamine (liq)                  | -32.1  | -134.3                            | {11} |
| C <sub>6</sub> H <sub>15</sub> OP                            | 182.1578          | Triethyl phosphate (liq)             | -297.  | -1243.                            | {11} |
| C <sub>6</sub> H <sub>15</sub> NO <sub>2</sub>               | 164.2060          | Triethylamine nitrate (c)            | -98.9  | -413.3                            | {11} |
| C <sub>6</sub> H <sub>16</sub> Si <sub>3</sub>               | 165.2786          | Triethoxysilane (liq)                | -226.  | -946.                             | {2}  |
| C <sub>6</sub> H <sub>16</sub> Si <sub>1</sub>               | 116.2804          | Triethylsilane (liq)                 | -54.   | -226.                             | {2}  |
| C <sub>6</sub> H <sub>18</sub> Al <sub>2</sub>               | 144.1734          | Hexamethyl dialuminum (g)            | -55.19   | -230.91                           | {2}  |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 293.15 K

| Formula   | Formula Weight | Name (state)                    | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Enthalpy of Formation<br>kJ mol <sup>-1</sup> | Ref |
|---|----------------|---------------------------------|---|---|-----|
| C <sub>6</sub> H <sub>18</sub> OSi <sub>2</sub>             | 162.3818       | Hexamethyldisiloxane (g)        | -185.88   | -777.72                                       | (2) |
| C <sub>6</sub> H <sub>18</sub> OSi <sub>2</sub>             | 162.3818       | Hexamethylidisiloxane (liq)     | -194.8  | -815.0  | (2) |
| C <sub>6</sub> H <sub>18</sub> Sn <sub>2</sub>              | 327.5904       | Hexamethyl ditin (liq)          | -21.6   | -90.4   | (2) |
| C <sub>5</sub> MoO <sub>6</sub>                             | 264.0033       | Molybdenum hexacarbonyl (g)     | -218.0  | -912.1  | (3) |
| C <sub>5</sub> MoO <sub>6</sub>                             | 264.0033       | Molybdenum hexacarbonyl (c)     | -234.9  | -982.8  | (3) |
| C <sub>7</sub> H <sub>6</sub> N <sub>4</sub>                | 146.1527       | 1-Phenyltetrazole (c)           | +86.5   | +361.9  | (1) |
| C <sub>7</sub> H <sub>6</sub> N <sub>4</sub>                | 146.1527       | 5-Phenyltetrazole (c)           | +70.0   | +292.9  | (1) |
| C <sub>7</sub> H <sub>6</sub> N <sub>4</sub> O              | 162.1521       | 1-Phenyl-5-hydroxytetrazole (c) | +26.7   | +111.7  | (1) |
| C <sub>7</sub> H <sub>6</sub> O                             | 106.1253       | Benzaldehyde (liq)              | -20.1   | -84.1   | (1) |
| C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>                | 122.1247       | Benzoic acid (c)                | -92.03  | -385.05                                       | (1) |
| C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>                | 122.1247       | Salicylaldehyde (liq)           | -66.9   | -279.9  | (1) |
| C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>                | 138.1241       | Salicylic acid                  | -140.9  | -589.5  | (1) |
| C <sub>7</sub> H <sub>7</sub> N                             | 105.1405       | 2-Vinylpyridine (liq)           | +37.2   | +155.6  | (1) |
| C <sub>7</sub> H <sub>7</sub> N <sub>2</sub> O              | 121.1399       | Benzamide (c)                   | -48.42  | -202.59                                       | (1) |
| C <sub>7</sub> H <sub>7</sub> N <sub>2</sub> O              | 121.1399       | Formanilide (c)                 | -36.2   | -151.5  | (1) |
| C <sub>7</sub> H <sub>7</sub> N <sub>2</sub> O <sub>2</sub> | 137.1393       | m-Aminobenzoic acid (c)         | -98.2   | -410.9  | (1) |
| C <sub>7</sub> H <sub>7</sub> N <sub>2</sub> O <sub>2</sub> | 137.1393       | o-Aminobenzoic acid (c)         | -95.8   | -400.8  | (1) |
| C <sub>7</sub> H <sub>7</sub> N <sub>2</sub> O <sub>2</sub> | 137.1393       | p-Aminobenzoic acid (c)         | -98.8   | -413.4  | (1) |
| C <sub>7</sub> H <sub>7</sub> N <sub>5</sub>                | 161.1673       | 1-Phenyl-5-aminotetrazole (c)   | +74.3   | +310.9  | (1) |
| C <sub>7</sub> H <sub>7</sub> N <sub>5</sub>                | 161.1673       | 5-Phenylaminotetrazole (c)      | +72.9   | +305.0  | (1) |
| C <sub>7</sub> H <sub>8</sub>                               | 92.1418        | Toluene (liq)                   | +2.88   | +12.05  | (4) |
| C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub> | 180.1674       | Theobromine (c)                 | -86.4   | -361.5  | (1) |
| C <sub>7</sub> H <sub>8</sub> O                             | 108.1412       | m-Cresol (c)                    | -46.37  | -194.01                                       | (1) |
| C <sub>7</sub> H <sub>8</sub> O                             | 108.1412       | o-Cresol (c)                    | -48.90  | -204.60                                       | (1) |
| C <sub>7</sub> H <sub>8</sub> O                             | 108.1412       | p-Cresol (c)                    | -47.63  | -199.28                                       | (1) |
| C <sub>7</sub> H <sub>8</sub> S                             | 124.2058       | Benzyl mercaptan (liq)          | +10.5   | +43.9   | (1) |
| C <sub>7</sub> H <sub>8</sub> S                             | 124.2058       | Phenylmethylsulfide (liq)       | +11.5   | +48.1   | (1) |
| C <sub>7</sub> H <sub>9</sub> N                             | 107.1565       | 2,3-Dimethylpyridine (liq)      | +4.62   | +19.33  | (1) |
| C <sub>7</sub> H <sub>9</sub> N                             | 107.1565       | 2,4-Dimethylpyridine (liq)      | +3.85   | +16.11  | (1) |
| C <sub>7</sub> H <sub>9</sub> N                             | 107.1565       | 2,5-Dimethylpyridine (liq)      | +4.45   | +18.62  | (1) |
| C <sub>7</sub> H <sub>9</sub> N                             | 107.1565       | 2,6-Dimethylpyridine (liq)      | +3.02   | +12.64  | (1) |
| C <sub>7</sub> H <sub>9</sub> N                             | 107.1565       | 3,4-Dimethylpyridine (liq)      | +4.36   | +18.24  | (1) |
| C <sub>7</sub> H <sub>9</sub> N                             | 107.1565       | 3,5-Dimethylpyridine (liq)      | +5.36   | +22.43  | (1) |
| C <sub>7</sub> H <sub>9</sub> N                             | 107.1565       | 2-Ethylpyridine (liq)           | -1.2  | -5.0  | (1) |
| C <sub>7</sub> H <sub>9</sub> N                             | 107.1565       | N-Methyllaniline (liq)          | +7.7  | +32.2   | (1) |
| C <sub>7</sub> H <sub>10</sub> O <sub>4</sub>               | 158.1554       | Terebic acid (c)                | -929.   | (1)   |     |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Name (state)                                      | Weight   | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Ref     |     |
|--|---|----------|---|---------|-----|
| C <sub>7</sub> H <sub>10</sub> O <sub>4</sub>                | Tetraconic acid (c)                               | 158.1554 | -204.   | (1)     |     |
| C <sub>7</sub> H <sub>11</sub> N <sub>5</sub>                | 1-Allyl-5-allylaminotetrazole (c)                 | 165.1992 | +83.7   | (1)     |     |
| C <sub>7</sub> H <sub>11</sub> N <sub>5</sub>                | 5-Diallylaminotetrazole (c)                       | 165.1992 | +83.9   | (1)     |     |
| C <sub>7</sub> H <sub>12</sub>                               | 1-Heptyne (g)                                     | 96.1737  | +24.64  | (4)     |     |
| C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> | Glycylvalyl anhydride (c)                         | 156.1859 | -120.5  | (1)     |     |
| C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>                | Dimethyl glutarate (liq)                          | 160.1713 | -205.9  | (1)     |     |
| C <sub>7</sub> H <sub>12</sub> O <sub>4</sub>                | Glycerol-1,3-diacetate (liq)                      | 176.1707 | -268.2  | (1)     |     |
| C <sub>7</sub> H <sub>12</sub> O <sub>5</sub>                | D-Gluco-D-sulohexonic acid- $\gamma$ -lactone (c) | 208.1695 | -1122.1   | (1)     |     |
| C <sub>7</sub> H <sub>12</sub> O <sub>7</sub>                | $\zeta$ -Enantholactam (c)                        | 127.1878 | -355.6  | (1)     |     |
| C <sub>7</sub> H <sub>13</sub> N <sub>9</sub>                | N-Methylcapro lactam (liq)                        | 127.1878 | -83.2   | (1)     |     |
| C <sub>7</sub> H <sub>13</sub> N <sub>9</sub>                | 5-Methylcapro lactam (c)                          | 127.1878 | -73.3   | (1)     |     |
| C <sub>7</sub> H <sub>13</sub> N <sub>9</sub>                | 7-Methylcapro lactam (c)                          | 127.1878 | -86.9   | (1)     |     |
| C <sub>7</sub> H <sub>13</sub> N <sub>9</sub>                | N-Formyl-DL-leucine (c)                           | 159.1866 | -86.5   | (1)     |     |
| C <sub>7</sub> H <sub>13</sub> N <sub>9</sub>                | 98.1896 Cycloheptane (liq)                        | -222.1   | -929.3  | (1)     |     |
| C <sub>7</sub> H <sub>14</sub>                               | 98.1896 1-Heptene (g)                             | -37.47   | -156.77   | (1)     |     |
| C <sub>7</sub> H <sub>14</sub>                               | 98.1896 1,1-Dimethylcyclopentane (liq)            | -14.87   | -62.22  | (4)     |     |
| C <sub>7</sub> H <sub>14</sub>                               | 98.1896 cis-1,2-Dimethylcyclopentane (liq)        | -41.12   | -172.05   | (4)     |     |
| C <sub>7</sub> H <sub>14</sub>                               | 98.1896 trans-1,2-Dimethylcyclopentane (liq)      | -39.50   | -165.27   | (4)     |     |
| C <sub>7</sub> H <sub>14</sub>                               | 98.1896 cis-1,3-Dimethylcyclopentane (liq)        | -40.92   | -171.21   | (4)     |     |
| C <sub>7</sub> H <sub>14</sub>                               | 98.1896 trans-1,3-Dimethylcyclopentane (liq)      | 40.17    | -168.07   | (4)     |     |
| C <sub>7</sub> H <sub>14</sub>                               | 98.1896 Ethylcyclopentane (liq)                   | -40.66   | -170.12   | (4)     |     |
| C <sub>7</sub> H <sub>14</sub>                               | 98.1896 Methylcyclohexane (liq)                   | -39.06   | -163.43   | (4)     |     |
| C <sub>7</sub> H <sub>14</sub>                               | 98.1896 Methylcyclohexane (liq)                   | -45.43   | -190.08   | (4)     |     |
| C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> | 174.2012 Glycylvaline (c)                         | -200.0   | -836.8  | (1)     |     |
| C <sub>7</sub> H <sub>14</sub> O <sub>3</sub>                | n-Heptaldehyde (liq)                              | 114.1890 | -74.4   | (1)     |     |
| C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>                | Enanthic acid (liq)                               | 130.1884 | -145.75   | (1)     |     |
| C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>                | Methyl caproate (liq)                             | 130.1884 | -129.10   | (1)     |     |
| C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>                | 194.1860 $\beta$ -Methyl-D-glucofuranoside (liq)  | -287.5   | -1202.9   | (1)     |     |
| C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>                | 194.1860 $\alpha$ -Methyl-D-glucopyranoside (c)   | -294.8   | -1233.4   | (1)     |     |
| C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>                | 194.1860 $\beta$ -Methyl-D-glucopyranoside (c)    | -295.8   | -1237.6   | (1)     |     |
| C <sub>7</sub> H <sub>14</sub> O <sub>7</sub>                | 210.1854 D-Glucos- $\alpha$ -heptose (c)          | -353.5   | -1479.0   | (1)     |     |
| C <sub>7</sub> H <sub>15</sub> N <sub>9</sub> O <sub>2</sub> | $\zeta$ -Aminoanthyllic acid (c)                  | 145.2031 | -159.6  | (1)     |     |
| C <sub>7</sub> H <sub>16</sub>                               | 2,2-Dimethylpentane (liq)                         | 100.2056 | -57.03  | (4)     |     |
| C <sub>7</sub> H <sub>16</sub>                               | 2,3-Dimethylpentane (liq)                         | 100.2056 | -55.79  | (1)     |     |
| C <sub>7</sub> H <sub>16</sub>                               | 2,4-Dimethylpentane (liq)                         | 100.2056 | -56.15  | (4)     |     |
| C <sub>7</sub> H <sub>16</sub>                               | 3,3-Dimethylpentane (liq)                         | 100.2056 | -234.93   | (4)     |     |
|  |   |          | -56.05  | -234.51 | (4) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula   | Formula Weight | Name (state)                            | Inenthalpy of Formation<br>kcal mol <sup>-1</sup> | Inenthalpy of Formation<br>kJ mol <sup>-1</sup> | Ref |
|---|----------------|---|---|---|-----|
| C <sub>7</sub> H <sub>16</sub>                              | 100.2056       | 3-Ethylpentane (liq)                    | -53.75  | -224.89   | (4) |
| C <sub>7</sub> H <sub>16</sub>                              | 100.2056       | n-Heptane (liq)                         | -53.61  | -224.30   | (4) |
| C <sub>7</sub> H <sub>16</sub>                              | 100.2056       | 2-Methylhexane (liq)                    | -54.91  | -229.74   | (4) |
| C <sub>7</sub> H <sub>16</sub>                              | 100.2056       | 3-Methylhexane (liq)                    | -54.33  | -227.32   | (4) |
| C <sub>7</sub> H <sub>16</sub>                              | 100.2056       | 2,2,3-Tri-methylbutane (liq)            | -56.61  | -236.86   | (4) |
| C <sub>7</sub> H <sub>16</sub> O <sub>7</sub>               | 212.2014       | D-Glucos-a-heptose (c)                  | -364.5  | -1525.1   | (1) |
| C <sub>7</sub> H <sub>16</sub> O <sub>7</sub>               | 212.2014       | D-Persicitol (c)                        | -369.7  | -1546.8   | (1) |
| C <sub>8</sub> H <sub>5</sub> N <sub>2</sub> O <sub>2</sub> | 147.1346       | Isatin (c)                              | -62.7   | -262.3  | (1) |
| C <sub>8</sub> H <sub>6</sub> N <sub>4</sub> O <sub>6</sub> | 254.1602       | Hydourilic acid (c)                     | -299.2  | -1251.9   | (1) |
| C <sub>8</sub> H <sub>6</sub> N <sub>6</sub>                | 186.1772       | 3-Azido-5-phenyl-s-triazole (c)         | +127.1  | +531.8  | (1) |
| C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>                | 150.1352       | Phenylglyoxylic acid (c)                | -115.3  | -482.4  | (1) |
| C <sub>8</sub> H <sub>6</sub> O <sub>4</sub>                | 166.1346       | m-Phthalic acid (c)                     | -191.91   | -802.95   | (1) |
| C <sub>8</sub> H <sub>6</sub> O <sub>4</sub>                | 166.1346       | o-Phthalic acid (c)                     | -186.91   | -732.03   | (1) |
| C <sub>8</sub> H <sub>6</sub> O <sub>4</sub>                | 166.1346       | p-Phthalic acid (c)                     | -195.05   | -816.09   | (1) |
| C <sub>8</sub> H <sub>7</sub> N                             | 117.5117       | Indole (c)                              | +29.8   | +124.7  | (1) |
| C <sub>8</sub> H <sub>7</sub> N <sub>2</sub> O              | 133.1511       | 6-Indole (c)                            | -41.2   | -172.4  | (1) |
| C <sub>8</sub> H <sub>7</sub> N <sub>2</sub> O <sub>2</sub> | 149.1505       | Dioxindole (c)                          | -76.9   | -321.7  | (1) |
| C <sub>8</sub> H <sub>7</sub> N <sub>7</sub>                | 201.1919       | 4-Amino-3-azido-5-phenyl-s-triazole (c) | +159.5  | +667.3  | (1) |
| C <sub>8</sub> H <sub>8</sub>                               | 104.1530       | Ethenylbenzene (liq)                    | +24.84  | +103.93   | (4) |
| C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> | 164.1652       | Phthalimide (c)                         | -104.4  | -436.8  | (1) |
| C <sub>8</sub> H <sub>8</sub> N <sub>4</sub>                | 160.1798       | 1-Methyl-5-phenyltetrazole (c)          | +69.9   | +292.5  | (1) |
| C <sub>8</sub> H <sub>8</sub> N <sub>4</sub>                | 160.1798       | 1-Phenyl-5-methyltetrazole (c)          | +69.9   | +292.5  | (1) |
| C <sub>8</sub> H <sub>8</sub> N <sub>4</sub>                | 160.1798       | 2-Phenyl-5-methyltetrazole (c)          | +65.7   | +274.9  | (1) |
| C <sub>8</sub> H <sub>8</sub> N <sub>6</sub> O <sub>6</sub> | 284.1896       | Murexide (c)                            | -289.7  | -1212.1   | (1) |
| C <sub>8</sub> H <sub>8</sub> O                             | 120.1524       | Acetophenone (liq)                      | -34.07  | -142.55   | (1) |
| C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>                | 136.1518       | Methyl benzoate (liq)                   | -79.8   | -333.9  | (1) |
| C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>                | 136.1518       | Phenylacetic acid (c)                   | -95.3   | -398.7  | (1) |
| C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>                | 152.1512       | DL-Mandelic acid (c)                    | -138.5  | -579.5  | (1) |
| C <sub>8</sub> H <sub>9</sub> N <sub>6</sub> O              | 152.1512       | L-Mandelic acid (c)                     | -138.8  | -580.7  | (1) |
| C <sub>8</sub> H <sub>9</sub> O <sub>3</sub>                | 152.1512       | Methyl salicylate (liq)                 | -127.1  | -531.9  | (1) |
| C <sub>8</sub> H <sub>9</sub> O <sub>3</sub>                | 152.1512       | Phenoxyacetic acid (c)                  | -122.8  | -513.8  | (1) |
| C <sub>8</sub> H <sub>9</sub> N <sub>6</sub> O              | 135.1670       | Acetanilide (c)                         | -50.3   | -210.5  | (1) |
| C <sub>8</sub> H <sub>9</sub> N <sub>6</sub> O <sub>2</sub> | 151.1664       | $\alpha$ -Phenyl glycine (c)            | -103.2  | -431.8  | (1) |
| C <sub>8</sub> H <sub>9</sub> N <sub>6</sub> O <sub>2</sub> | 151.1664       | N-Phenyl glycine (c)                    | -96.2   | -402.5  | (1) |
| C <sub>8</sub> H <sub>10</sub>                              | 106.1689       | Ethylbenzene (liq)                      | -12.34  | -2.95   | (4) |
| C <sub>8</sub> H <sub>10</sub>                              | 106.1689       | m-Xylene (liq)                          | -25.36  | (4)   |     |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula   | Formula Weight | Name (state)  | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Enthalpy of Formation<br>kJ mol <sup>-1</sup> | Ref |
|---|----------------|---|---|---|-----|
| C <sub>8</sub> H <sub>10</sub>                                | 106.1689       | o-Xylene (liq)  | -5.82   | -24.35  | (4) |
| C <sub>8</sub> H <sub>10</sub>                                | 106.1689       | p-Xylene (liq)  | -5.82   | -24.35  | (4) |
| C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub>  | 194.1945       | Caffeine (c)  | -76.2   | -318.8  | (1) |
| C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>10</sub> | 322.1897       | All oxantin dihydrate (c)   | -510.3  | -2135.1                                       | (1) |
| C <sub>8</sub> H <sub>10</sub> O                              | 122.1683       | 2-Ethylphenol (c)   | -49.91  | -208.82                                       | (1) |
| C <sub>8</sub> H <sub>10</sub> O                              | 122.1683       | 3-Ethylphenol (c)   | -51.21  | -214.26                                       | (1) |
| C <sub>8</sub> H <sub>10</sub> O                              | 122.1683       | 4-Ethylphenol (c)   | -53.63  | -244.39                                       | (1) |
| C <sub>8</sub> H <sub>11</sub> N                              | 121.1836       | N,N-Dimethylaniline (liq)   | +8.2  | +34.3   | (1) |
| C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>  | 184.1964       | Diethylbarbituric acid (c)  | -178.7  | -747.7  | (1) |
| C <sub>8</sub> H <sub>12</sub> Pb                             | 315.3748       | Tetravinyl lead (liq)   | +213.   | +891.   | (2) |
| C <sub>8</sub> H <sub>12</sub> Sn                             | 226.8748       | Tetravinyl tin (liq)  | +72.  | +301.   | (2) |
| C <sub>8</sub> H <sub>14</sub>                                | 110.2008       | 1-Etynyl (g)  | +19.73  | +82.55  | (4) |
| C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>  | 170.2130       | Vallylalanyl anhydride (c)  | -123.3  | -515.9  | (1) |
| C <sub>8</sub> H <sub>14</sub> N <sub>4</sub> O <sub>5</sub>  | 246.2246       | Triglycylglycine (c)  | -284.7  | -1191.2                                       | (1) |
| C <sub>8</sub> H <sub>14</sub> O <sub>4</sub>                 | 174.1984       | Dimethyl adipate (liq)  | -211.9  | -886.6  | (1) |
| C <sub>8</sub> H <sub>14</sub> O <sub>4</sub>                 | 174.1984       | Erythritol diacet al (c)  | -182.   | -761.   | (1) |
| C <sub>8</sub> H <sub>14</sub> O <sub>8</sub>                 | 238.1960       | D-Gluco- $\alpha$ , $\alpha$ -octonic acid- $\gamma$ -lactone (c) | -394.2  | -1649.3                                       | (1) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | Cyclooctane (liq)   | -40.56  | -169.79                                       | (1) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | 1-Octene (g)  | -19.80  | -82.84  | (4) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | 1,1-Dimethylcyclohexane (liq)                                     | -52.28  | -218.74                                       | (4) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | cis-1,2-Dimethylcyclohexane (liq)                                 | -50.62  | -211.79                                       | (4) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | trans-1,2-Dimethylcyclohexane (liq)                               | -52.16  | -218.24                                       | (4) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | cis-1,3-Dimethylcyclohexane (liq)                                 | -53.27  | -222.88                                       | (4) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | trans-1,3-Dimethylcyclohexane (liq)                               | -51.55  | -215.69                                       | (4) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | cis-1,4-Dimethylcyclohexane (liq)                                 | -51.53  | -215.60                                       | (4) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | trans-1,4-Dimethylcyclohexane (liq)                               | -53.15  | -222.38                                       | (4) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | Ethylcyclohexane (liq)  | -50.70  | -212.13                                       | (4) |
| C <sub>8</sub> H <sub>16</sub>                                | 112.2167       | n-Propylcyclopentane (liq)  | -45.19  | -189.07                                       | (4) |
| C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>  | 188.2283       | DL-Leucylglycine (c)  | -205.07   | -853.01                                       | (1) |
| C <sub>8</sub> H <sub>16</sub> O                              | 128.2161       | n-Octaldehyde (liq)   | -80.0   | -334.7  | (1) |
| C <sub>8</sub> H <sub>16</sub> O                              | 144.2155       | Caprylic acid (liq)   | -151.93   | -635.68                                       | (1) |
| C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>                 | 144.2155       | Methyl enanthate (liq)  | -135.53   | -567.06                                       | (1) |
| C <sub>8</sub> H <sub>17</sub> N                              | 127.2314       | Coraine (liq)   | -57.6   | -241.0  | (1) |
| C <sub>8</sub> H <sub>18</sub>                                | 114.2327       | 2,2-Dimethylhexane (liq)  | -62.60  | -251.92                                       | (4) |
| C <sub>8</sub> H <sub>18</sub>                                | 114.2327       | 2,3-Dimethylhexane (liq)  | -60.38  | -252.63                                       | (4) |
| C <sub>8</sub> H <sub>18</sub>                                | 114.2327       | 2,4-Dimethylhexane (liq)  | -61.44  | -257.06                                       | (4) |

TABLE I-a

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Name (state) | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Formation<br>kJ mol <sup>-1</sup> | Ref |
|--|--------------|---|-----------------------------------|-----|
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -62.24  | -260.41                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -61.56  | -257.57                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -60.20  | -251.98                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -59.85  | -250.41                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -59.66  | -249.52                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -60.44  | -252.88                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -60.96  | -255.06                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -60.32  | -252.38                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -60.15  | -251.37                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -59.71  | -249.33                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -64.21  | -268.65                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -61.41  | -256.94                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -61.95  | -259.20                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -60.60  | -253.55                           | (4) |
| C <sub>8</sub> H <sub>18</sub>                 | 114.2327     | -60.96  | -255.06                           | (4) |
| C <sub>8</sub> H <sub>20</sub> G <sup>o</sup>  | 188.8386     | -49.5   | -207.1                            | (2) |
| C <sub>8</sub> H <sub>20</sub> Pb              | 323.4386     | +26.19  | +109.58                           | (2) |
| C <sub>8</sub> H <sub>20</sub> Pb              | 323.4386     | +12.6   | +52.7                             | (2) |
| C <sub>8</sub> H <sub>20</sub> Si              | 208.3322     | -334.   | -1397.                            | (1) |
| C <sub>8</sub> H <sub>20</sub> Si              | 144.3346     | -68.  | -285.                             | (2) |
| C <sub>8</sub> H <sub>20</sub> Sn              | 234.9386     | -10.9   | -45.6                             | (2) |
| C <sub>8</sub> H <sub>20</sub> Sn              | 234.9386     | -22.9   | -95.9                             | (2) |
| C <sub>9</sub> H <sub>7</sub> N                | 129.1628     | +37.9   | +158.6                            | (1) |
| C <sub>9</sub> H <sub>7</sub> N                | 129.1628     | +37.3   | +156.1                            | (1) |
| C <sub>9</sub> H <sub>7</sub> NO               | 145.1622     | -19.9   | -83.3                             | (1) |
| C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> O | 160.1769     | -4.7  | -19.7                             | (1) |
| C <sub>9</sub> H <sub>9</sub> N                | 131.1788     | +14.5   | +60.7                             | (1) |
| C <sub>9</sub> H <sub>9</sub> N                | 131.1788     | +16.3   | +68.2                             | (1) |
| C <sub>9</sub> H <sub>9</sub> NO <sub>3</sub>  | 179.1770     | -145.63   | -609.32                           | (1) |
| C <sub>9</sub> H <sub>10</sub> O <sub>4</sub>  | 182.1777     | -178.5  | -746.8                            | (1) |
| C <sub>9</sub> H <sub>10</sub> N <sub>2</sub>  | 146.1934     | +31.4   | +131.4                            | (1) |
| C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub> | 165.1935     | -111.9  | -468.2                            | (1) |
| C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub> | 165.1935     | -111.9  | -468.2                            | (1) |
| C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub> | 181.1929     | -163.4  | -683.7                            | (1) |
| C <sub>9</sub> H <sub>12</sub>                 | 120.1960     | -9.83   | -41.13                            | (4) |
| C <sub>9</sub> H <sub>12</sub>                 | 120.1960     | -11.09  | -46.40                            | (4) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Formula<br>Weight | Name (state)                                  | Enthalpy of Formation<br>kcal mol <sup>-1</sup><br>kJ mol <sup>-1</sup> | Ref         |
|--|-------------------|---|---|-------------|
| C <sub>9</sub> H <sub>12</sub>                               | 120.1960          | 1-Methyl-3-ethylbenzene (liq)                 | -11.64  | -48.70 (4)  |
| C <sub>9</sub> H <sub>12</sub>                               | 120.1960          | 1-Methyl-4-ethylbenzene (liq)                 | -11.90  | -49.79 (4)  |
| C <sub>9</sub> H <sub>12</sub>                               | 120.1960          | n-Propylbenzene (liq)                         | -9.16   | -38.33 (4)  |
| C <sub>9</sub> H <sub>12</sub>                               | 120.1960          | 1,2,3-Trimethylbenzene (liq)                  | -13.99  | -58.53 (4)  |
| C <sub>9</sub> H <sub>12</sub>                               | 120.1960          | 1,2,4-Triethylbenzene (liq)                   | -14.77  | -61.80 (4)  |
| C <sub>9</sub> H <sub>12</sub>                               | 120.1960          | 1,3,5-Triisopropylbenzene (liq)               | -15.16  | -63.43 (4)  |
| C <sub>9</sub> H <sub>14</sub> O <sub>6</sub>                | 218.2083          | Glyceryl triacetate (liq)                     | -318.3  | -1331.8 (1) |
| C <sub>9</sub> H <sub>14</sub> O <sub>6</sub>                | 218.2083          | Mannitol triformate (c)                       | -242.   | -1013. (1)  |
| C <sub>9</sub> H <sub>15</sub> N                             | 137.2266          | Phyllotyrrrole (c)                            | -20.4   | -85.4 (1)   |
| C <sub>9</sub> H <sub>16</sub>                               | 124.2279          | 1-Nonyne (g)                                  | *14.80  | *61.92 (4)  |
| C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> | 232.2383          | α-Carbethoxyglycylglycine ethyl ester (c)     | -275.3  | -1151.9 (1) |
| C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> | 232.2383          | β-Carbethoxyglycylglycine ethyl ester (c)     | -303.5  | -1259.8 (1) |
| C <sub>9</sub> H <sub>18</sub>                               | 126.2438          | 1-Nonene (g)                                  | -24.71  | -103.39 (4) |
| C <sub>9</sub> H <sub>18</sub>                               | 126.2438          | n-Propylcyclohexane (liq)                     | -56.95  | -238.28 (4) |
| C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>                | 158.2426          | Methyl caprylate (liq)                        | -141.07   | -590.24 (1) |
| C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>                | 158.2426          | Pelargonic acid (liq)                         | -157.67   | -659.69 (1) |
| C <sub>9</sub> H <sub>19</sub> Nd <sub>2</sub>               | 173.2573          | ω-Aminopalemonic acid (c)                     | -174.1  | -728.4 (1)  |
| C <sub>9</sub> H <sub>20</sub>                               | 128.2598          | n-Nonane (liq)                                | -65.81  | -275.35 (4) |
| C <sub>9</sub> H <sub>21</sub> N                             | 143.2744          | Tri-n-propylamine (liq)                       | -49.51  | -207.15 (1) |
| C <sub>9</sub> H <sub>21</sub> O <sub>4</sub> P              | 224.2391          | Tri-n-propyl phosphite (liq)                  | -315.   | -1318. (1)  |
| C <sub>10</sub> H <sub>8</sub>                               | 128.1753          | Naphthalene (c)                               | *18.0   | *75.3 (1)   |
| C <sub>10</sub> H <sub>8</sub>                               | 128.1753          | Naphthalene (g)                               | *35.6   | *149.0 (1)  |
| C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> | 188.1875          | 4-Phenyluracil (c)                            | -81.7   | -341.8 (1)  |
| C <sub>10</sub> H <sub>9</sub> N                             | 143.1899          | α-Phenylpyrrole (c)                           | *34.5   | *144.3 (1)  |
| C <sub>10</sub> H <sub>9</sub> N                             | 143.1899          | N-Phenylpyrrole (c)                           | *38.1   | *159.4 (1)  |
| C <sub>10</sub> H <sub>9</sub> N                             | 143.1899          | Quinaldine (c)                                | *39.3   | *164.4 (1)  |
| C <sub>10</sub> H <sub>9</sub> NO <sub>3</sub>               | 191.1881          | Phenylalanine-N-carboxylic acid anhydride (c) | -132.3  | -553.5 (1)  |
| C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>               | 194.1888          | Dimethyl m-phthalate (c)                      | -711.   | -715. (1)   |
| C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>               | 194.1888          | Dimethyl o-phthalate (liq)                    | -162.   | -678. (1)   |
| C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>               | 194.1888          | Dimethyl p-phthalate (c)                      | -170.   | -711. (1)   |
| C <sub>10</sub> H <sub>11</sub> NO <sub>3</sub>              | 193.2041          | DL-Benzoylalanine (c)                         | -147.9  | -618.8 (1)  |
| C <sub>10</sub> H <sub>11</sub> NO <sub>3</sub>              | 193.2041          | Benzoyl sarcosine (c)                         | -135.7  | -567.8 (1)  |
| C <sub>10</sub> H <sub>11</sub> NO <sub>3</sub>              | 193.2041          | Phenaceturic acid (c)                         | -151.0  | -631.8 (1)  |
| C <sub>10</sub> H <sub>11</sub> NO <sub>3</sub>              | 193.2041          | m-Tolyl glycine (c)                           | -148.8  | -622.6 (1)  |
| C <sub>10</sub> H <sub>11</sub> NO <sub>3</sub>              | 193.2041          | o-Tolyl glycine (c)                           | -148.3  | -620.5 (1)  |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Formula<br>Weight | Name (state)  | Ref | Enthalpy of Formation<br>kcal mol <sup>-1</sup><br>kJ mol <sup>-1</sup> |
|--|-------------------|---|-----|---|
| C <sub>10</sub> H <sub>11</sub> N <sup>0</sup> <sub>3</sub>              | 193.2041          | p-Toluyl glycine (c)  | (1) | -148.5<br>-180.9  |
| C <sub>10</sub> H <sub>11</sub> N <sup>0</sup> <sub>4</sub>              | 209.2035          | Anisoyl glycine (c)   | (1) | -756.9  |
| C <sub>10</sub> H <sub>12</sub> <sup>0</sup> <sub>4</sub>                | 196.2047          | Glyceryl-1-benzoate (c)                                     | (1) | -185.80   |
| C <sub>10</sub> H <sub>12</sub> <sup>0</sup> <sub>4</sub>                | 196.2047          | Glyceryl-2-benzoate (c)                                     | (1) | -184.71   |
| C <sub>10</sub> H <sub>13</sub> N <sup>0</sup> <sub>2</sub>              | 179.2206          | Phenacetin (c)  | (1) | -101.1  |
| C <sub>10</sub> H <sub>14</sub> N <sup>0</sup> <sub>2</sub>              | 162.2365          | Nicotine (liq)  | (1) | +9.4<br>+39.3   |
| C <sub>10</sub> H <sub>14</sub> N <sup>0</sup> <sub>2</sub>              | 292.2476          | Ethylenediaminetetraacetic acid (c)                         | (1) | -423.0<br>-420.5  |
| C <sub>10</sub> H <sub>16</sub> N <sup>0</sup> <sub>2</sub> <sup>+</sup> | 168.2378          | Dehydro- $\beta$ -campholenolactone (c)<br>(dextrorotatory) | (1) | -1759.4<br>-554.  |
| C <sub>10</sub> H <sub>16</sub> <sup>0</sup> <sub>2</sub>                | 168.2378          | Dehydro- $\beta$ -campholenolactone (c)<br>(Inactive)       | (1) | -130.<br>-137.  |
| C <sub>10</sub> H <sub>16</sub> <sup>0</sup> <sub>3</sub>                | 184.2372          | Methyl ethyl heptane lactone (c)<br>(racemic)               | (1) | -573.<br>-183.5   |
| C <sub>10</sub> H <sub>18</sub>  | 138.2550          | 1-Decyne (g)  | (1) | +9.88<br>-29.64   |
| C <sub>10</sub> H <sub>19</sub> N <sup>0</sup> <sub>4</sub>              | 245.2806          | Leucylglycylglycine (c)                                     | (4) | -1086.2<br>+41.34   |
| C <sub>10</sub> H <sub>20</sub>  | 140.2709          | 1-Decene (g)  | (1) | -124.01   |
| C <sub>10</sub> H <sub>20</sub> <sup>0</sup> <sub>2</sub>                | 172.2697          | Capric acid (c)   | (1) | -170.59<br>-163.6   |
| C <sub>10</sub> H <sub>20</sub> <sup>0</sup> <sub>2</sub>                | 172.2697          | Capric acid (liq)   | (1) | -684.5  |
| C <sub>10</sub> H <sub>20</sub> <sup>0</sup> <sub>2</sub>                | 172.2697          | Methyl pelargonate (liq)                                    | (1) | -147.29   |
| C <sub>10</sub> H <sub>22</sub>  | 142.2868          | n-Decane (liq)  | (1) | -71.92<br>-165.78   |
| C <sub>10</sub> H <sub>22</sub> <sup>0</sup> <sub>2</sub>                | 174.2856          | 1,10-Decanediol (c)   | (1) | -693.62   |
| C <sub>10</sub> H <sub>22</sub> <sup>0</sup> <sub>7</sub>                | 254.2826          | Dipenterythritol (c)  | (1) | -376.9<br>-1576.9   |
| C <sub>11</sub> H <sub>12</sub> N <sup>0</sup> <sub>2</sub>              | 204.2305          | Glycyphenylalanyl anhydride (c)                             | (1) | -82.9<br>-99.8  |
| C <sub>11</sub> H <sub>12</sub> N <sup>0</sup> <sub>2</sub>              | 204.2305          | L-Tryptophane (c)   | (1) | -99.8<br>-122.8   |
| C <sub>11</sub> H <sub>12</sub> N <sup>0</sup> <sub>3</sub>              | 220.2299          | Glycytyrosyl anhydride (c)                                  | (1) | -513.8  |
| C <sub>11</sub> H <sub>12</sub> N <sup>0</sup> <sub>4</sub>              | 236.2293          | Hippurylglycine (c)   | (1) | -198.54<br>-156.5   |
| C <sub>11</sub> H <sub>13</sub> N <sup>0</sup> <sub>3</sub>              | 207.2312          | $\alpha$ -Toluyl alanine (c)                                | (1) | -159.0<br>-159.0  |
| C <sub>11</sub> H <sub>13</sub> N <sup>0</sup> <sub>3</sub>              | 207.2312          | p-Toluyl alanine (c)  | (1) | -163.9<br>-830.69   |
| C <sub>11</sub> H <sub>14</sub> N <sup>0</sup> <sub>3</sub>              | 222.2458          | Glycylphenylalanine (c)                                     | (1) | -685.8  |
| C <sub>11</sub> H <sub>20</sub>  | 152.2820          | 1-Undecyne (g)  | (4) | +4.96<br>+20.75   |
| C <sub>11</sub> H <sub>20</sub> N <sup>0</sup> <sub>2</sub>              | 212.2943          | Valylleucyl anhydride (c)                                   | (1) | -150.1<br>-138.   |
| C <sub>11</sub> H <sub>20</sub> <sup>0</sup> <sub>2</sub>                | 184.2809          | Undecyl-10-ene-1-oic acid (c)                               | (1) | -628.0<br>-577.   |
| C <sub>11</sub> H <sub>22</sub>  | 154.2980          | 1-Undecene (g)  | (4) | -144.57   |
| C <sub>11</sub> H <sub>22</sub> <sup>0</sup> <sub>2</sub>                | 186.2968          | Methyl caprate (liq)  | (1) | -153.07<br>-640.44  |
| C <sub>11</sub> H <sub>24</sub>  | 156.3139          | n-Undecane (liq)  | (4) | -326.44   |
| C <sub>12</sub> H <sub>8</sub> N <sub>2</sub>                            | 180.2110          | Phenazine (c)   | (1) | +56.4<br>+236.0   |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula   | Formula Weight | Name (state)  | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Ref |
|---|----------------|---|---|-----|
| C <sub>12</sub> H <sub>9</sub> N                              | 167.2122       | Carbazole (c)   | +30.3   | (1) |
| C <sub>12</sub> H <sub>10</sub> S                             | 186.2775       | Diphenyl sulfide (c)  | +39.1   | (1) |
| C <sub>12</sub> H <sub>10</sub> S <sub>2</sub>                | 218.3415       | Diphenyl disulfide (c)  | +35.8   | (1) |
| C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> | 218.2576       | Alanylphenylalanyl anhydride (c)  | -89.3   | (1) |
| C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>6</sub> | 310.2686       | Desoxyamalic acid (c)   | -285.7  | (1) |
| C <sub>12</sub> H <sub>14</sub> N <sub>4</sub> O <sub>6</sub> | 342.2674       | Amalic acid (c)   | -367.0  | (1) |
| C <sub>12</sub> H <sub>15</sub> N <sub>2</sub> O <sub>4</sub> | 237.2577       | DL-Phenylalanine-N-carboxylic acid<br>dimethyl ester (c)                | -184.3  | (1) |
| C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> | 236.2729       | Alanylphenylalanine (c)   | -170.2  | (1) |
| C <sub>12</sub> H <sub>16</sub> O <sub>8</sub>                | 288.2565       | Levoglucosan triacetate (c)   | -371.3  | (1) |
| C <sub>12</sub> H <sub>18</sub> O <sub>2</sub>                | 197.2761       | 3(a)-Hydroxy-trans-decalin-2(a)-acetic<br>acid lactone (c) (boat form)  | -133.09   | (1) |
| C <sub>12</sub> H <sub>18</sub> O <sub>2</sub>                | 194.2761       | 3(e)-Hydroxy-trans-decalin-2(e)-acetic<br>acid lactone (c) (chair form) | -137.26   | (1) |
| C <sub>12</sub> H <sub>18</sub> O <sub>8</sub>                | 290.2725       | 1,2-Anhydroglucose-3,5,6-triacetate (c)                                 | -411.7  | (1) |
| C <sub>12</sub> H <sub>18</sub> O <sub>8</sub>                | 260.2896       | Mannitol triacetal (c)  | -275.   | (1) |
| C <sub>12</sub> H <sub>22</sub>                               | 166.3091       | 1-Dodecene (g)  | +0.03   | (4) |
| C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> | 226.3213       | Leucine anhydride (c)   | -160.0  | (1) |
| C <sub>12</sub> H <sub>22</sub> O <sub>6</sub>                | 262.3055       | 1,2,5,6-Diacetonomannitol (c)   | -350.   | (1) |
| C <sub>12</sub> H <sub>22</sub> O <sub>6</sub>                | 342.3025       | Cellobiose (c)  | -532.5  | (1) |
| C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>               | 342.3025       | $\beta$ -Lactose (c)  | -530.1  | (1) |
| C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>               | 342.3025       | Maltose (c)   | -530.8  | (1) |
| C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>               | 342.3025       | Sucrose (c)   | -531.9  | (1) |
| C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>               | 342.3025       | Trehalose (c)   | -531.3  | (1) |
| C <sub>12</sub> H <sub>24</sub>                               | 168.32251      | 1-Dodecene (g)  | -39.48  | (4) |
| C <sub>12</sub> H <sub>24</sub>                               | 200.32239      | Lauric acid (c)   | -185.14   | (1) |
| C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>                | 200.32239      | Lauric acid (liq)   | -176.4  | (1) |
| C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>                | 200.32239      | Methyl undecylate (liq)   | -158.97   | (1) |
| C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>                | 360.3179       | $\alpha$ -Lactose monohydrate (c)                                       | -602.   | (1) |
| C <sub>12</sub> H <sub>24</sub> O <sub>12</sub>               | 360.3179       | $\beta$ -Maltose monohydrate (c)  | -606.   | (1) |
| C <sub>12</sub> H <sub>26</sub>                               | 170.3410       | n-Dodecane (liq)  | -84.12  | (4) |
| C <sub>12</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> | 262.3520       | Hexamethylene-1,6-diamine-adipic acid<br>Adduct (c)                     | -305.5  | (1) |
| C <sub>12</sub> H <sub>26</sub> O <sub>13</sub>               | 378.3332       | Trehalose dihydrate (c)   | -676.1  | (1) |
| C <sub>12</sub> H <sub>27</sub> O <sub>P</sub>                | 218.3222       | Tri-n-butyl phosphine oxide (c)   | -110.   | (1) |

-1278.2  
-2828.3  
-460.

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Name (state) | Enthalpy of formation<br>kcal mol <sup>-1</sup>    | Ref                        |
|--|--------------|--|----------------------------|
| Formula<br>Weight  |              | kJ mol <sup>-1</sup>                               |                            |
| C <sub>12</sub> H <sub>27</sub> O <sub>2</sub> P               | 234.3216     | a-Butyl ester of di-n-butyl phosphinic acid (liq)  | -183.<br>-183.<br>(1)      |
| C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P               | 266.3204     | Triisobutyl phosphate (liq)                        | -346.<br>-1448.<br>(1)     |
| C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P               | 266.3204     | Tri-n-butyl phosphate (liq)                        | -348.<br>-1456.<br>(1)     |
| C <sub>13</sub> H <sub>9</sub> N                               | 179.2234     | Acridine (c)                                       | +44.8<br>+187.4<br>(1)     |
| C <sub>13</sub> H <sub>10</sub> O                              | 182.2241     | Benzophenone (c)                                   | -8.0<br>-33.5<br>(1)       |
| C <sub>13</sub> H <sub>11</sub> NO                             | 197.2387     | Benzanilide (c)                                    | -22.3<br>-93.3<br>(1)      |
| C <sub>13</sub> H <sub>24</sub>                                | 180.3362     | 1-Tridecyne (g)                                    | -4.89<br>-20.46<br>(4)     |
| C <sub>13</sub> H <sub>26</sub>                                | 182.3522     | 1-Tridecene (g)                                    | -44.41<br>-185.81<br>(4)   |
| C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>                 | 214.3510     | Methyl laurate (liq)                               | -165.66<br>-693.12<br>(1)  |
| C <sub>13</sub> H <sub>26</sub> O <sub>4</sub>                 | 246.3498     | Glyceryl-1-caprate (c)                             | -265.05<br>-1108.97<br>(1) |
| C <sub>13</sub> H <sub>26</sub> O <sub>4</sub>                 | 246.3498     | Glyceryl-2-caprate (c)                             | -261.90<br>-1095.79<br>(1) |
| C <sub>13</sub> H <sub>28</sub>                                | 184.3681     | n-Tridecane (liq)                                  | -90.22<br>-377.48<br>(4)   |
| C <sub>14</sub> H <sub>10</sub>                                | 178.2358     | Anthracene (c)                                     | +29.0<br>+121.3<br>(1)     |
| C <sub>14</sub> H <sub>10</sub>                                | 178.2358     | Anthracene (g)                                     | +53.7<br>+224.7<br>(1)     |
| C <sub>14</sub> H <sub>10</sub>                                | 178.2358     | Phenanthrene (c)                                   | +27.3<br>+114.2<br>(1)     |
| C <sub>14</sub> H <sub>10</sub>                                | 178.2358     | Phenanthrene (g)                                   | +48.4<br>+202.5<br>(1)     |
| C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>  | 246.3118     | Vallylphenylalanyl anhydride (c)                   | -94.3<br>-394.6<br>(1)     |
| C <sub>14</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>  | 293.3252     | Glycylalanyl phenylalanine (c)                     | -222.0<br>-928.8<br>(1)    |
| C <sub>14</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>  | 264.3271     | Vallylphenylalanine (c)                            | -183.5<br>-767.8<br>(1)    |
| C <sub>14</sub> H <sub>20</sub> O <sub>9</sub>                 | 332.3101     | Rhamnose triacetate (c)                            | -455.4<br>-1905.4<br>(1)   |
| C <sub>14</sub> H <sub>23</sub> N <sub>3</sub> O <sub>10</sub> | 393.3535     | Diethylenetriaminepentaacetic acid (c)             | -531.8<br>-2225.1<br>(1)   |
| C <sub>14</sub> H <sub>26</sub>                                | 194.3633     | 1-Tetradecyne (g)                                  | -9.82<br>-41.09<br>(4)     |
| C <sub>14</sub> H <sub>26</sub>                                | 196.3793     | 1-Tetradecene (g)                                  | -49.33<br>-206.40<br>(4)   |
| C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>                 | 228.3781     | Methyl tridecylate (liq)                           | -171.56<br>-717.81<br>(1)  |
| C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>                 | 228.3781     | Myristic acid (c)                                  | -199.21<br>-833.49<br>(1)  |
| C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>                 | 228.3781     | Myristic acid (liq)                                | -188.5<br>-788.7<br>(1)    |
| C <sub>14</sub> H <sub>30</sub>                                | 198.3952     | n-Tetradecane (liq)                                | -96.33<br>-403.04<br>(4)   |
| C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub>  | 290.4062     | Tetramethylene-1,4-diamine-sebacic acid adduct (c) | -317.9<br>-1330.1<br>(1)   |
| C <sub>15</sub> H <sub>20</sub> O <sub>6</sub>                 | 296.3231     | Tricyclobutyin (liq)                               | -247.<br>-1033.<br>(1)     |
| C <sub>15</sub> H <sub>26</sub> O <sub>6</sub>                 | 302.3709     | Glyceryl tributyrate (liq)                         | -356.<br>-1490.<br>(1)     |
| C <sub>15</sub> H <sub>28</sub>                                | 208.3904     | 1-Pentadecyne (g)                                  | -14.74<br>-61.67<br>(4)    |
| C <sub>15</sub> H <sub>30</sub>                                | 210.4064     | 1-Pentadecene (g)                                  | -54.26<br>-227.02<br>(4)   |
| C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>                 | 242.4051     | Methyl myristate (liq)                             | -177.80<br>-743.92<br>(1)  |
| C <sub>15</sub> H <sub>30</sub> O <sub>4</sub>                 | 274.4040     | Glyceryl-1-lauroate (c)                            | -277.46<br>-1160.89<br>(1) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC COMPOUNDS AT 298.15 K

| Formula   | Formula<br>Weight | Name (state)   | Enthalpy of<br>Formation<br>kcal mol <sup>-1</sup><br>kJ mol <sup>-1</sup> | Ref      |     |
|---|-------------------|--|--|----------|-----|
| C <sub>15</sub> H <sub>30</sub> O <sub>4</sub>                | 274.4040          | Glyceryl-2-laurate (c)                                 | -275.48  | (1)      |     |
| C <sub>15</sub> H <sub>32</sub>                               | 212.4223          | n-Pentadecane (liq)                                    | -102.44  | (4)      |     |
| C <sub>16</sub> H <sub>10</sub>                               | 202.2581          | Fluoranthene (c)                                       | +45.75   | +191.42  | (1) |
| C <sub>16</sub> H <sub>10</sub>                               | 202.2581          | Pyrene (c)   | +27.44   | +114.81  | (1) |
| C <sub>16</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> | 262.2703          | Indigotin (c)  | -32.   | -134.    | (1) |
| C <sub>16</sub> H <sub>11</sub> N <sub>2</sub> O <sub>2</sub> | 249.2716          | Benzalhippuric acid azlactone (c)                      | -30.5  | -127.6   | (1) |
| C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> | 296.2850          | Isovalide (c)  | -139.  | -532.    | (1) |
| C <sub>16</sub> H <sub>13</sub> NO <sub>3</sub>               | 267.2869          | Benzalhippuric acid (c)                                | -102.6   | -429.3   | (1) |
| C <sub>16</sub> H <sub>15</sub> NO <sub>3</sub>               | 269.3029          | Benzoylphenylalanine (c)                               | -129.6   | -542.2   | (1) |
| C <sub>16</sub> H <sub>22</sub> O <sub>2</sub>                | 390.3471          | Galactose pentaacetate (c)                             | -532.8   | -2229.2  | (1) |
| C <sub>16</sub> H <sub>22</sub> O <sub>2</sub>                | 390.3471          | Glucose pentaacetate (c)                               | -532.1   | -2226.3  | (1) |
| C <sub>16</sub> H <sub>30</sub>                               | 222.4175          | 1-Hexadecyne (g)                                       | -19.56   | -81.84   | (4) |
| C <sub>16</sub> H <sub>32</sub>                               | 224.4334          | 1-Hexadecene (g)                                       | -59.18   | -247.61  | (4) |
| C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>                | 256.4322          | Methyl pentadecylate (liq)                             | -184.35  | -771.32  | (1) |
| C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>                | 256.4322          | Palmitic acid (c)                                      | -213.10  | -891.61  | (1) |
| C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>                | 256.4322          | Palmitic acid (liq)                                    | -200.4   | -838.5   | (1) |
| C <sub>16</sub> H <sub>34</sub>                               | 226.4494          | n-Hexadecane (liq)                                     | -108.53  | -454.09  | (4) |
| C <sub>17</sub> H <sub>19</sub> NO <sub>2</sub>               | 269.3465          | Ethyl $\beta$ -anilino- $\beta$ -phenyl propionate (c) | -82.8  | -346.4   | (1) |
| C <sub>17</sub> H <sub>21</sub> NO <sub>2</sub>               | 303.3612          | Morphine monohydrate (c)                               | -170.1   | -711.7   | (1) |
| C <sub>17</sub> H <sub>34</sub> O <sub>4</sub>                | 302.4581          | Glyceryl-1-myristate (c)                               | -292.31  | -1223.03 | (1) |
| C <sub>17</sub> H <sub>34</sub> O <sub>4</sub>                | 302.4581          | Glyceryl-2-myristate (c)                               | -289.89  | -1212.90 | (1) |
| C <sub>17</sub> H <sub>32</sub>                               | 236.4446          | 1-Heptadecyne (g)                                      | -24.59   | -102.38  | (4) |
| C <sub>17</sub> H <sub>34</sub>                               | 238.4605          | 1-Heptadecene (g)                                      | -64.09   | -268.15  | (4) |
| C <sub>17</sub> H <sub>36</sub>                               | 240.4765          | n-Heptadecane (liq)                                    | -114.64  | -479.65  | (4) |
| C <sub>18</sub> H <sub>12</sub>                               | 228.2963          | 1,2-Benzanthracene (c)                                 | +41.2  | +172.4   | (1) |
| C <sub>18</sub> H <sub>12</sub>                               | 228.2963          | 3,4-Benzphenanthrene (c)                               | +4.5   | +186.2   | (1) |
| C <sub>18</sub> H <sub>12</sub>                               | 228.2963          | Chrysene (c)   | +35.0  | +146.4   | (1) |
| C <sub>18</sub> H <sub>12</sub>                               | 228.2963          | Naphthacene (c)  | +38.3  | +160.2   | (1) |
| C <sub>18</sub> H <sub>12</sub>                               | 228.2963          | Triphenylene (c)                                       | +33.72   | +141.08  | (1) |
| C <sub>18</sub> H <sub>15</sub> O <sub>4</sub> P              | 326.2916          | Triphenyl phosphate (c)                                | -181.  | -757.    | (1) |
| C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> | 294.3564          | Phenylalanyl anhydride (c)                             | -69.3  | -290.0   | (1) |
| C <sub>18</sub> H <sub>23</sub> NO <sub>2</sub>               | 317.3883          | Codeline monohydrate (c)                               | -151.2   | -632.6   | (1) |
| C <sub>18</sub> H <sub>26</sub> O <sub>4</sub>                | 338.4043          | Tricyclovalerin (liq)                                  | -270.  | -1130.   | (1) |
| C <sub>18</sub> H <sub>32</sub> O <sub>16</sub>               | 504.4461          | Melezitose (c)   | -815.  | -3410.   | (1) |
| C <sub>18</sub> H <sub>32</sub> O <sub>16</sub>               | 504.4461          | Raffinose (c)  | -761.  | -3184.   | (1) |
| C <sub>18</sub> H <sub>34</sub>                               | 250.4717          | 1-octadecyne (g)                                       | -29.50   | -123.43  | (4) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula  | Formula Weight | Name (state)                                    | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | kJ mol <sup>-1</sup> | Ref |
|--|----------------|---|---|----------------------|-----|
| C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>                 | 282.4705       | Elaelic acid (c)                                | -217.7  | -910.9               | (1) |
| C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>                 | 282.4705       | Oleic acid (c)                                  | -187.2  | -783.2               | (1) |
| C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>                 | 282.4705       | Oleic acid (liq)                                | -178.9  | -748.5               | (1) |
| C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>                 | 252.4876       | 1- $\omega$ -Octadecene (g)                     | -69.02  | -288.78              | (4) |
| C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>                 | 284.4864       | Stearic acid (c)                                | -226.47   | -947.55              | (1) |
| C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>                 | 284.4864       | Stearic acid (liq)                              | -212.5  | -889.1               | (1) |
| C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>                 | 254.5036       | n-Octadecane (liq)                              | -120.74   | -505.18              | (4) |
| C <sub>18</sub> H <sub>42</sub> O <sub>2</sub>                 | 594.5228       | Raffinose pentahydrate (c)                      | -1122.  | -4694.               | (1) |
| C <sub>19</sub> H <sub>21</sub> N <sub>6</sub> O <sub>3</sub>  | 311.3841       | Theanine (c)                                    | +63.0   | +253.6               | (1) |
| C <sub>19</sub> H <sub>22</sub> N <sub>6</sub> O <sub>3</sub>  | 294.4000       | Cinchonidine (c)                                | +7.1  | +29.7                | (1) |
| C <sub>19</sub> H <sub>22</sub> N <sub>6</sub> O <sub>3</sub>  | 294.4000       | Cinchonine (c)                                  | +7.4  | +31.0                | (1) |
| C <sub>19</sub> H <sub>24</sub> N <sub>6</sub> O <sub>3</sub>  | 296.4159       | Cinchonamine (c)                                | +10.4   | +43.5                | (1) |
| C <sub>19</sub> H <sub>25</sub> N <sub>6</sub> O <sub>4</sub>  | 359.4288       | Cinchonamine nitrate (c)                        | -79.9   | -334.3               | (1) |
| C <sub>19</sub> H <sub>26</sub> O <sub>2</sub>                 | 286.4179       | $\Delta_4$ -Androstone-3,17-dione (c)           | -103.   | -431.                | (1) |
| C <sub>19</sub> H <sub>28</sub> O <sub>2</sub>                 | 268.4338       | 5 $\alpha$ -Androstan-3,17-dione (c)            | -130.   | -544.                | (1) |
| C <sub>19</sub> H <sub>28</sub> O <sub>2</sub>                 | 288.4338       | $\Delta_5$ -Androstone-3 $\beta$ -ol-17-one (c) | -107.   | -448.                | (1) |
| C <sub>19</sub> H <sub>28</sub> O <sub>2</sub>                 | 288.4338       | $\Delta_4$ -Androstone-3-one-17 $\beta$ -ol (c) | -94.  | -393.                | (1) |
| C <sub>19</sub> H <sub>30</sub> O <sub>2</sub>                 | 290.4498       | 5 $\alpha$ -Androstan-3 $\alpha$ -ol-17-one (c) | -162.   | -678.                | (1) |
| C <sub>19</sub> H <sub>30</sub> O <sub>2</sub>                 | 290.4498       | 5 $\alpha$ -Androstan-3 $\beta$ -ol-17-one (c)  | -152.   | -636.                | (1) |
| C <sub>19</sub> H <sub>30</sub> O <sub>2</sub>                 | 290.4498       | 5 $\alpha$ -Androstan-3-one-17 $\beta$ -ol (c)  | -120.   | -502.                | (1) |
| C <sub>19</sub> H <sub>32</sub>                                | 260.4569       | 5 $\alpha$ -Androstanone (c)                    | -75.  | -314.                | (1) |
| C <sub>19</sub> H <sub>36</sub>                                | 264.4988       | 1-Nonadecyne (g)                                | -34.43  | -144.06              | (4) |
| C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>                 | 296.4976       | Methyl elaidate (liq)                           | -175.8  | -735.5               | (1) |
| C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>                 | 296.4976       | Methyl oleate (liq)                             | -174.2  | -728.9               | (1) |
| C <sub>19</sub> H <sub>38</sub>                                | 266.5147       | 1-Nonadecene (g)                                | -73.94  | -309.36              | (4) |
| C <sub>19</sub> H <sub>38</sub> O <sub>2</sub>                 | 330.5123       | Glyceryl-1-palmitate (c)                        | -306.28   | -1281.48             | (1) |
| C <sub>19</sub> H <sub>38</sub> O <sub>4</sub>                 | 330.5123       | Glyceryl-2-palmitate (c)                        | -303.23   | -1268.71             | (1) |
| C <sub>19</sub> H <sub>40</sub>                                | 268.5306       | n-Nonadecane (liq)                              | -126.84   | -530.70              | (4) |
| C <sub>20</sub> H <sub>12</sub>                                | 252.3186       | Perylene (c)                                    | +43.69  | +182.3               | (1) |
| C <sub>20</sub> H <sub>21</sub> N <sub>6</sub> O <sub>4</sub>  | 339.3947       | Papaverine (c)                                  | -120.2  | -502.9               | (1) |
| C <sub>20</sub> H <sub>24</sub> N <sub>6</sub> O <sub>2</sub>  | 324.4265       | Quinidine (c)                                   | -38.3   | -160.2               | (1) |
| C <sub>20</sub> H <sub>24</sub> N <sub>6</sub> O <sub>2</sub>  | 324.4265       | Quinine (c)                                     | -37.1   | -155.2               | (1) |
| C <sub>20</sub> H <sub>27</sub> N <sub>6</sub> O <sub>11</sub> | 457.4383       | Amygdaalin (c)                                  | -455.   | -1904.               | (1) |
| C <sub>20</sub> H <sub>38</sub>                                | 278.5259       | 1-Eicosyne (g)                                  | -39.36  | -164.69              | (4) |
| C <sub>20</sub> H <sub>40</sub>                                | 280.5418       | 1-Eicosene (g)                                  | -78.87  | -329.09              | (4) |
| C <sub>20</sub> H <sub>40</sub> O <sub>2</sub>                 | 312.5406       | Arachidic acid (c)                              | -241.82   | -1011.77             | (1) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula   | Formula Weight | Name (state)   | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Ref |
|---|----------------|--|---|-----|
| C <sub>20</sub> H <sub>40</sub> O <sub>2</sub>                | 312.5406       | Arachidic acid (liq)                                     | -224.6  | (1) |
| C <sub>20</sub> H <sub>42</sub>                               | 282.5577       | n-Eicosane (liq)   | -132.94   | (4) |
| C <sub>21</sub> H <sub>16</sub> N <sub>2</sub>                | 188.2747       | Lophine (c)  | +65.  | (1) |
| C <sub>21</sub> H <sub>18</sub> N <sub>2</sub>                | 298.3910       | Amarine (c)  | +63.  | (1) |
| C <sub>21</sub> H <sub>19</sub> N <sub>2</sub> O <sub>5</sub> | 307.3987       | Amarine hemihydrate (c)                                  | +29.  | (1) |
| C <sub>21</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub> | 334.4217       | Strychnine (c)   | -41.0   | (1) |
| C <sub>21</sub> H <sub>28</sub> O <sub>5</sub>                | 360.4543       | Δ <sub>4</sub> -Pregnene-3,11,20-trione-17α,21-diol (c)  | -255.   | (1) |
| C <sub>21</sub> H <sub>30</sub> O <sub>2</sub>                | 314.4721       | Δ <sub>4</sub> -Pregnene-3,20-dione (c)                  | -132.   | (1) |
| C <sub>21</sub> H <sub>30</sub> O <sub>3</sub>                | 330.4715       | Δ <sub>4</sub> -Pregnene-3,20-dione-21-ol (c)            | -124.   | (1) |
| C <sub>21</sub> H <sub>30</sub> O <sub>5</sub>                | 362.4703       | Δ <sub>4</sub> -Pregnene-3,20-dione-11β,17α,21-triol (c) | -256.   | (1) |
| C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>                | 358.5665       | Glyceryl-1-stearate (c)                                  | -319.64   | (1) |
| C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>                | 358.5665       | Glyceryl-2-stearate (c)                                  | -315.80   | (1) |
| C <sub>22</sub> H <sub>23</sub> N <sub>0</sub> 7              | 413.4311       | Narcotine (c)  | -210.9  | (1) |
| C <sub>22</sub> H <sub>42</sub> O <sub>2</sub>                | 338.5788       | Brassidiic acid (c)                                      | -214.   | (1) |
| C <sub>22</sub> H <sub>42</sub> O <sub>2</sub>                | 338.5788       | Fructic acid (c)   | -207.   | (1) |
| C <sub>22</sub> H <sub>44</sub> O <sub>2</sub>                | 340.5948       | Betonic acid (c)   | -235.   | (1) |
| C <sub>22</sub> H <sub>44</sub> O <sub>4</sub>                | 372.5936       | 13,14-Dihydroxy behenic acid (c)                         | -337.   | (1) |
| C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> | 394.4747       | Brucine (c)  | -118.6  | (1) |
| C <sub>23</sub> H <sub>31</sub> N <sub>0</sub> 10             | 481.5042       | Narcotine dihydrate (c)                                  | -421.2  | (1) |
| C <sub>24</sub> H <sub>20</sub> O <sub>6</sub>                | 404.4234       | Glyceryl tribenzoate (c)                                 | -214.   | (1) |
| C <sub>24</sub> H <sub>24</sub> N <sub>2</sub> O <sub>5</sub> | 388.4705       | Anisidine (c)  | -51.  | (1) |
| C <sub>24</sub> H <sub>40</sub> O <sub>20</sub>               | 648.5744       | Diamylose (c)  | -850.   | (1) |
| C <sub>24</sub> H <sub>42</sub> O <sub>6</sub>                | 426.5987       | 5β-Cholan-24-oic acid-3α,7α,12α-triol monohydrate (c)    | -288.   | (1) |
| C <sub>24</sub> H <sub>42</sub> O <sub>21</sub>               | 666.5897       | Stachyose (c)  | -987.   | (1) |
| C <sub>27</sub> H <sub>46</sub> O                             | 386.6671       | Δ <sub>5</sub> -Cholestone-3β-ol (c)                     | -133.   | (1) |
| C <sub>28</sub> H <sub>38</sub> O <sub>19</sub>               | 678.6037       | Celllobiose octaacetate (c)                              | -902.5  | (1) |
| C <sub>28</sub> H <sub>38</sub> O <sub>19</sub>               | 678.6037       | Lactose octaacetate (c)                                  | -906.0  | (1) |
| C <sub>28</sub> H <sub>38</sub> O <sub>19</sub>               | 678.6037       | Maltose octaacetate (c)                                  | -904.5  | (1) |
| C <sub>28</sub> H <sub>38</sub> O <sub>19</sub>               | 678.6037       | Sucrose octaacetate (c)                                  | -901.9  | (1) |
| C <sub>28</sub> H <sub>38</sub> O <sub>19</sub>               | 400.6942       | Δ <sub>5</sub> -Cholestone-3β-yl methyl ether (c)        | -155.9  | (1) |
| C <sub>28</sub> H <sub>48</sub> O                             | 400.6942       | 3:5-Cyclocholestan-6β-yl methyl ether (c)                | -150.3  | (1) |
| C <sub>32</sub> H <sub>36</sub> N <sub>4</sub> O <sub>2</sub> | 508.6693       | Pyrroporphyrin (XV) monomethyl ester (c)                 | +88.6   | (1) |
|   |                |  | -370.7  | (1) |

TABLE I-A

| Formula  | Formula Weight | Name (state)  | Enthalpy of Formation<br>kcal mol <sup>-1</sup> | Enthalpy of Formation<br>kJ mol <sup>-1</sup> | Ref |
|--|----------------|---|---|---|-----|
| C <sub>32</sub> H <sub>38</sub> N <sub>4</sub>                 | 478.6865       | Aetioporphyrin (I) (c)  | -1.8  | -7.5  | (1) |
| C <sub>32</sub> H <sub>38</sub> N <sub>4</sub>                 | 478.6865       | Aetioporphyrin (II) (c)   | +4.4  | +18.4   | (1) |
| C <sub>33</sub> H <sub>38</sub> N <sub>4</sub> O <sub>2</sub>  | 522.6964       | γ-Pheophytin monomethyl ester (c)   | -87.3   | -365.3  | (1) |
| C <sub>34</sub> H <sub>34</sub> N <sub>4</sub> O <sub>4</sub>  | 562.6745       | Protoporphyrin (c)  | -120.6  | -504.6  | (1) |
| C <sub>34</sub> H <sub>36</sub> N <sub>4</sub> O <sub>3</sub>  | 548.6910       | Phylloerythrin monomethyl ester (c)   | -83.2   | -348.1  | (1) |
| C <sub>34</sub> H <sub>36</sub> N <sub>4</sub> O <sub>3</sub>  | 548.6910       | Pheophorbide a monomethyl ester (c)   | -84.8   | -354.8  | (1) |
| C <sub>34</sub> H <sub>36</sub> N <sub>4</sub> O <sub>3</sub>  | 548.6910       | Pheophytin dimethyl ester (c)   | -143.3  | -599.6  | (1) |
| C <sub>34</sub> H <sub>36</sub> N <sub>4</sub> O <sub>4</sub>  | 564.6904       | Vardoporphyrin 18 monomethyl ester (c)  | -230.8  | -965.7  | (1) |
| C <sub>34</sub> H <sub>36</sub> N <sub>4</sub> O <sub>5</sub>  | 580.6898       | Pheopurpurin 18 monomethyl ester (c)  | -   | -   |     |
| C <sub>34</sub> H <sub>38</sub> N <sub>4</sub> O <sub>2</sub>  | 534.7076       | Desoxypyphylloerythrin monomethyl ester (c)   | -38.9   | -162.8  | (1) |
| C <sub>34</sub> H <sub>38</sub> N <sub>4</sub> O <sub>4</sub>  | 566.7064       | Rhodoporphyrin (XV) dimethyl ester (c)  | -122.2  | -511.3  | (1) |
| C <sub>34</sub> H <sub>38</sub> N <sub>4</sub> O <sub>4</sub>  | 566.7064       | Rhodoporphyrin (XXI) dimethyl ester (c)   | -123.9  | -518.4  | (1) |
| C <sub>35</sub> H <sub>38</sub> N <sub>4</sub> O <sub>5</sub>  | 594.7169       | Chloroporphyrin e <sub>5</sub> dimethyl ester (c)   | -103.3  | -432.2  | (1) |
| C <sub>35</sub> H <sub>40</sub> N <sub>4</sub> O <sub>4</sub>  | 580.7335       | Chlorin e <sub>4</sub> dimethyl ester (c)   | -144.9  | -606.3  | (1) |
| C <sub>35</sub> H <sub>40</sub> N <sub>4</sub> O <sub>4</sub>  | 580.7335       | Chloroporphyrin e <sub>4</sub> dimethyl ester (c)   | -154.2  | -645.2  | (1) |
| C <sub>36</sub> H <sub>36</sub> N <sub>4</sub> O <sub>6</sub>  | 620.7115       | Methyl pheophorbide b (c)   | -200.7  | -833.7  | (1) |
| C <sub>36</sub> H <sub>38</sub> N <sub>4</sub> O <sub>4</sub>  | 590.7287       | Proto porphyrin dimethyl ester (c)  | -122.1  | -510.9  | (1) |
| C <sub>36</sub> H <sub>38</sub> N <sub>4</sub> O <sub>5</sub>  | 606.7281       | Methyl pheophorbide a (c)   | -156.1  | -653.1  | (1) |
| C <sub>36</sub> H <sub>38</sub> N <sub>4</sub> O <sub>5</sub>  | 606.7281       | Pheoporphyrin a <sub>5</sub> dimethyl ester (c)   | -164.3  | -687.4  | (1) |
| C <sub>36</sub> H <sub>40</sub> N <sub>4</sub> O <sub>6</sub>  | 624.7434       | Chlorin P <sub>6</sub> trimethyl ester (c)  | -292.0  | -1221.7                                       | (1) |
| C <sub>36</sub> H <sub>42</sub> N <sub>4</sub> O <sub>4</sub>  | 594.7605       | Mesoporphyrin (IX) dimethyl ester (c)   | -196.4  | -821.7  | (1) |
| C <sub>36</sub> H <sub>44</sub> N <sub>2</sub> O <sub>10</sub> | 664.7595       | L(+)-Leucine methyl ester salt of (+)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3') (c) | -540.   | -2259.  |     |
| C <sub>36</sub> H <sub>44</sub> N <sub>2</sub> O <sub>10</sub> | 664.7595       | L(-)-Leucine methyl ester salt of (-)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3') (c) | -531.   | -2222.  |     |
| C <sub>36</sub> H <sub>46</sub> N <sub>4</sub>                 | 534.7948       | Octethylporphyrin (c)   | -39.9   | -166.9  | (1) |
| C <sub>36</sub> H <sub>60</sub> O <sub>30</sub>                | 972.8616       | α-Tetramylose (c)   | -1360.  | -5690.  | (1) |
| C <sub>37</sub> H <sub>40</sub> N <sub>4</sub> O <sub>7</sub>  | 652.7540       | Diethyl pheophytin 7 (c)  | -245.8  | -1028.4                                       | (1) |
| C <sub>37</sub> H <sub>42</sub> N <sub>4</sub> O <sub>6</sub>  | 638.7705       | Chlorin e <sub>6</sub> trimethyl ester (c)  | -221.4  | -926.3  | (1) |
| C <sub>37</sub> H <sub>42</sub> N <sub>4</sub> O <sub>6</sub>  | 638.7705       | Chloroporphyrin e <sub>6</sub> trimethyl ester (c)  | -230.3  | -963.6  | (1) |
| C <sub>39</sub> H <sub>74</sub> O <sub>6</sub>                 | 639.0210       | Glyceryl tri laurate (c)  | -489.   | -2046.  | (1) |
| C <sub>40</sub> H <sub>46</sub> N <sub>4</sub> O <sub>8</sub>  | 710.8346       | Coproporphyrin (II) tetra methyl ester (c)  | -348.3  | -1457.3                                       | (1) |
| C <sub>45</sub> H <sub>86</sub> O <sub>6</sub>                 | 723.1836       | Glyceryl trimyristate (c)   | -520.   | -2176.  | (1) |
| C <sub>47</sub> H <sub>88</sub> O <sub>5</sub>                 | 733.2224       | Glyceryl dibasicate (c)   | -472.   | -1975.  | (1) |

TABLE I-A

ENTHALPIES OF FORMATION OF SOME ORGANIC COMPOUNDS AND INORGANIC CARBON COMPOUNDS AT 298.15 K

| Formula<br>Weight   | Formula<br>Name (state)   | Enthalpy of<br>Formation<br>kcal mol <sup>-1</sup>                        | Formation<br>kJ mol <sup>-1</sup>  | Ref                                   |                          |
|---|---|---|------------------------------------|---------------------------------------|--------------------------|
| C <sub>47</sub> H <sub>88</sub> O <sub>5</sub><br>C <sub>48</sub> H <sub>54</sub> N <sub>4</sub> O <sub>16</sub>                                      | 733.2224 Glyceryl dierucate (c)<br>942.9828 Iso-uroporphyrin (II) octamethyl ester<br>(c) | -447.<br>-1870.   | -447.<br>-1870.                    | (1)                                   |                          |
| C <sub>48</sub> H <sub>80</sub> O <sub>40</sub><br>C <sub>69</sub> H <sub>128</sub> O <sub>6</sub><br>C <sub>69</sub> H <sub>128</sub> O <sub>6</sub> | 1297.1488<br>1053.7859<br>1053.7859   | β-Hexamyolose (c)<br>Glyceryl tribراسidate (c)<br>Glyceryl trierucate (c) | -620.1<br>-1853.<br>-625.<br>-596. | -2594.5<br>-7753.<br>-2615.<br>-2494. | (1)<br>(1)<br>(1)<br>(1) |

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25.3 TABLE I-R COMPOUND NAME-FORMULA INDEX

|                                |                    |
|--------------------------------|--------------------|
| Acetaldehyde                   | $C_2H_4$           |
| Acetamide                      | $C_2H_5N$          |
| Acetamidoquandiline nitrate    | $C_3H_9N_5O_4$     |
| 1-Acetamido-2-nitroguanidine   | $C_3H_7N_5O_3$     |
| 5-Acetamido-tetrazole          | $C_3H_5N_6$        |
| Acetanilide                    | $C_8H_9N$          |
| Acetic acid                    | $C_2H_4O_2$        |
| Acetic anhydride               | $C_4H_6O_3$        |
| Acetone                        | see: Propanone     |
| Acetone glyceraldehyde         | $C_6H_{10}O_3$     |
| Acetone glycerol               | $C_6H_{12}O_3$     |
| Acetophenone                   | $C_8H_8$           |
| Acetyl bromide                 | $C_2H_3BrO$        |
| Acetyl chloride                | $C_2H_3ClO$        |
| Acetylene                      | $C_2H_2$           |
| Acetyl fluoride                | $C_2H_3F_3$        |
| Acetyl iodide                  | $C_2H_3I$          |
| cis-Aconitic acid              | $C_6H_6O_6$        |
| trans-Aconitic acid            | $C_6H_6O_6$        |
| Acridine                       | $C_13H_9N$         |
| Acrylic acid                   | $C_3H_6O_2$        |
| Adenine                        | $C_5H_5N_5$        |
| Adipic acid                    | $C_6H_{10}O_4$     |
| Aetioporphyrin (I)             | $C_{32}H_{38}N_4$  |
| Aetioporphyrin (III)           | $C_{32}H_{38}N_4$  |
| DL-Alanine                     | $C_3H_7N_2O_2$     |
| L-Alanine                      | $C_3H_7N_2O_2$     |
| Alanine anhydride              | $C_6H_10N_2O_2$    |
| DL-Alanyl glycine              | $C_6H_10N_2O_2$    |
| Alanylphenylalanine            | $C_12H_{16}N_2O_3$ |
| Alanylphenylalanyl anhydride   | $C_12H_{14}N_2O_2$ |
| Allantoin                      | $C_6H_6N_4O_3$     |
| Allene                         | see: Propadiene    |
| Allomeric acid                 | $C_6H_{10}O_8$     |
| Alloxan monohydrate            | $C_4H_4N_2O_5$     |
| Alloxanthin dihydrate          | $C_9H_{10}N_4O_10$ |
| 1-Allyl-5-allylamino-tetrazole | $C_7H_11N_5$       |
| 1-Allyl-5-amino-tetrazole      | $C_4H_7N_5$        |
| 2-Allyl-5-amino-triazole       | $C_4H_7N_5$        |
| Aluminum triacetate            | $C_6H_9Al(O_2)_6$  |
| Amalic acid                    | $C_{12}H_4N_4O_8$  |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|  |  |
|--|--|
| Amarine                                      | $C_2H_{18}N_2$                                   |
| Amarine hemihydrate                          | $C_2H_{19}N_2O_0.5$                              |
| 4-Amino-3-azido-5-ethyl- $\alpha$ -triazole  | $C_4H_7N_7$                                      |
| 4-Amino-3-azido-5-methyl- $\alpha$ -triazole | $C_5H_5N_7$                                      |
| 4-Amino-3-azido-5-phenyl- $\beta$ -triazole  | $C_8H_7N_7$                                      |
| 4-Amino-3-azido- $\beta$ -triazole           | $C_2H_3N_7$                                      |
| 5-Aminobarbituric acid                       | see: Uramal                                      |
| m-Aminobenzoic acid                          | $C_7H_7N_2$                                      |
| o-Aminobenzoic acid                          | $C_7H_7N_2$                                      |
| p-Aminobenzoic acid                          | $C_7H_7N_2$                                      |
| $\gamma$ -Aminobutyric acid                  | $C_6H_{13}N_2$                                   |
| $\alpha$ -Aminocaproic acid                  | $C_6H_9N_2$                                      |
| $\gamma$ -Aminocaproic acid                  | $C_6H_{13}N_2$                                   |
| $\delta$ -Aminocaproic acid                  | $C_6H_{13}N_2$                                   |
| $\epsilon$ -Aminocaproic acid                | $C_6H_{13}N_2$                                   |
| S-Aminoanthyllic acid                        | $C_7H_{15}N_2$                                   |
| 2-Aminoethane-1-sulfonic acid                | $C_2H_7N_3S$                                     |
| 3-Amino-5-methyl-1,2,4-triazole nitrate      | $C_3H_7N_5O_3$                                   |
| $\omega$ -Aminopelargonic acid               | $C_9H_{19}N_2$                                   |
| 5-Aminotetrazole                             | $CH_3N_5$  |
| 5-Aminotetrazole nitrate                     | $CH_4N_6O_3$                                     |
| 3-Amino-1,2,4-triazole                       | $C_2H_4N_4$                                      |
| 3-Amino-1,2,4-triazole nitrate               | $C_2H_5N_5O_3$                                   |
| 6-Aminovaleric acid                          | $C_5H_{11}N_2$                                   |
| Amygdalin                                    | $C_20H_{27}N_8O_{11}$                            |
| 5 $\alpha$ -Androstanone                     | $C_19H_{32}$                                     |
| 5 $\alpha$ -Androstan-3,17-dione             | $C_19H_{28}O_2$                                  |
| 5 $\alpha$ -Androstan-3 $\alpha$ -ol-17-one  | $C_19H_{30}O_2$                                  |
| 5 $\alpha$ -Androstan-3 $\beta$ -ol-17-one   | $C_19H_{30}O_2$                                  |
| 5 $\alpha$ -Androstan-3-one-17 $\beta$ -ol   | $C_19H_{30}O_2$                                  |
| $\Delta_4$ -Androstan-3-one-17 $\beta$ -ol   | $C_19H_{28}O_2$                                  |
| $\Delta_4$ -Androstan-3,17-dione             | $C_19H_{26}O_2$                                  |
| $\Delta_5$ -Androstan-3 $\beta$ -ol-17-one   | $C_19H_{28}O_2$                                  |
| Androsterone                                 | see: 5 $\alpha$ -Androstan-3 $\alpha$ -ol-17-one |
| Angelic acid                                 | $C_5H_8O_2$                                      |
| 1,2-Anhydroglucos-3,5,6-triacetate           | $C_{12}H_{18}O_8$                                |
| Ariline                                      | $C_6H_7N$  |
| Aniline nitrate                              | $C_6H_8N_2O_3$                                   |
| Anisine                                      | $C_{24}H_{24}N_2O_3$                             |
| Anisoyl glycine                              | $C_{10}H_{11}NO_4$                               |
| Anthracene                                   | $C_{14}H_{10}$                                   |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|   |   |
|---|---|
| $\beta$ -D-Arabinose                    | C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>                 |
| $\beta$ -L-Arabinose                    | C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>                 |
| L-Arabitol                              | C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>                 |
| D-Arabinic acid- $\gamma$ -lactone      | C <sub>5</sub> H <sub>12</sub> O <sub>5</sub>                 |
| Arachidic acid                          | C <sub>5</sub> H <sub>8</sub> O <sub>5</sub>                  |
| L-Arginine                              | C <sub>20</sub> H <sub>40</sub> N <sub>2</sub>                |
| L-Ascorbic acid                         | C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>  |
| L-Asparagine                            | C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>   |
| L-Asparagine monohydrate                | C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>   |
| L-Aspartic acid                         | C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub>  |
| 3-Azido-5-ethyl-s-triazole              | C <sub>4</sub> H <sub>7</sub> N <sub>3</sub>                  |
| 3-Azido-5-methyl-s-triazole             | C <sub>4</sub> H <sub>6</sub> N <sub>6</sub>                  |
| 3-Azido-5-phenyl-s-triazole             | C <sub>7</sub> H <sub>4</sub> N <sub>6</sub>                  |
| 3-Azido-s-triazole                      | C <sub>2</sub> H <sub>2</sub> N <sub>6</sub>                  |
| Azodicarbamide                          | C <sub>2</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>   |
| Barbituric acid                         | C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>   |
| Benelic acid                            | C <sub>22</sub> H <sub>44</sub> O <sub>2</sub>                |
| Benzaldehyde                            | C <sub>7</sub> H <sub>6</sub> O                               |
| Benzalhippuric acid                     | C <sub>15</sub> H <sub>13</sub> N <sub>5</sub> O <sub>3</sub> |
| Benzalhippuric acid azlactone           | C <sub>16</sub> H <sub>11</sub> N <sub>1</sub> O <sub>2</sub> |
| Benzamide                               | C <sub>7</sub> H <sub>7</sub> N <sub>3</sub>                  |
| Benzanilide                             | C <sub>13</sub> H <sub>11</sub> N <sub>3</sub>                |
| 1,2-Benzanthracene                      | C <sub>18</sub> H <sub>12</sub>                               |
| Benzene                                 | C <sub>6</sub> H <sub>6</sub>                                 |
| Benzenthiol                             | C <sub>6</sub> H <sub>6</sub> S                               |
| Benzoic acid                            | C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>                  |
| Benzophenone                            | C <sub>13</sub> H <sub>10</sub> O                             |
| Benzotriazole                           | C <sub>6</sub> H <sub>5</sub> N <sub>3</sub>                  |
| DL-Benzoylalanine                       | C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> |
| Benzylophenylalanine                    | C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub> |
| Senzylo sarcosine                       | C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>3</sub> |
| 3,4-Benzphenanthrene                    | C <sub>18</sub> H <sub>12</sub>                               |
| Benzyl mercaptan                        | C <sub>7</sub> H <sub>8</sub> S                               |
| Brassidiac acid                         | C <sub>22</sub> H <sub>42</sub> O <sub>2</sub>                |
| Bromal                                  | C <sub>2</sub> H <sub>3</sub> Br <sub>3</sub> O               |
| Bromal hydrate                          | C <sub>2</sub> H <sub>3</sub> Br <sub>3</sub> O <sub>2</sub>  |
| 1-Bromo-1,1-difluoro-2,2-dichloroethane | C <sub>2</sub> HBrCl <sub>2</sub> F <sub>2</sub>              |
| Bromoform                               | CHBr <sub>3</sub>   |
| 1-Bromo-2-iodoethane                    | C <sub>2</sub> H <sub>4</sub> BrI                             |
| Bromotrifluoroethane                    | CBrF <sub>3</sub>   |
| Brucine                                 | C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>6</sub> |

TABLE I-B COMPOUND NAME-Formula INDEX

|                                       |  |
|---------------------------------------|--|
| 1,2-Butadiene                         | C <sub>4</sub> H <sub>6</sub>                                |
| 1,3-Butadiene                         | C <sub>4</sub> H <sub>6</sub>                                |
| 1-Butanal                             | see: n-Butyraldehyde   |
| n-Butane                              | C <sub>4</sub> H <sub>10</sub>                               |
| 1,2-Butanediamine                     | C <sub>4</sub> H <sub>12</sub> N <sub>2</sub>                |
| 2,3-Butanediol                        | C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>                 |
| 1,4-Butanedithiol                     | C <sub>4</sub> H <sub>10</sub> S <sub>2</sub>                |
| meso-1,2,3,4-Butanetetrol             | C <sub>4</sub> H <sub>10</sub> O <sub>4</sub>                |
| 1-Butanethiol                         | C <sub>4</sub> H <sub>10</sub> S                             |
| Butanoic acid                         | see: Butyric acid  |
| 1-Butanol                             | C <sub>4</sub> H <sub>10</sub> O                             |
| 2-Butanol                             | C <sub>4</sub> H <sub>10</sub> O                             |
| Butanone                              | C <sub>4</sub> H <sub>8</sub> O                              |
| 1-Butene                              | C <sub>4</sub> H <sub>8</sub>                                |
| cis-2-Butene                          | C <sub>4</sub> H <sub>8</sub>                                |
| trans-2-Butene                        | C <sub>4</sub> H <sub>8</sub>                                |
| n-Butylamine                          | C <sub>4</sub> H <sub>11</sub> N                             |
| sec.-Butylamine                       | C <sub>4</sub> H <sub>11</sub> N                             |
| tert.-Butylamine                      | C <sub>4</sub> H <sub>11</sub> N                             |
| n-Butyl di-n-butyl phosphinate        | see: n-Butyl ester of di-n-butyl phosphinic acid             |
| 1-Butyne                              | C <sub>12</sub> H <sub>27</sub> O <sub>2</sub> P             |
| 2-Butyne                              | C <sub>4</sub> H <sub>6</sub>                                |
| n-Butyraldehyde                       | C <sub>4</sub> H <sub>8</sub> O                              |
| n-Butyramide                          | C <sub>4</sub> H <sub>9</sub> NO                             |
| Butyric acid                          | C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>                 |
| Cadmium oxalate                       | C <sub>2</sub> CaO <sub>4</sub>                              |
| Caffeine                              | C <sub>8</sub> H <sub>10</sub> N <sub>4</sub> O <sub>2</sub> |
| Caprylic acid                         | C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>               |
| Caproic acid                          | C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>                |
| ε-Caprolactam                         | C <sub>6</sub> H <sub>11</sub> NO                            |
| Caprylic acid                         | C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>                |
| Carbazole                             | C <sub>12</sub> H <sub>9</sub> N                             |
| α-Carbethoxyglycylglycine ethyl ester | C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> |
| β-Carbethoxyglycylglycine ethyl ester | C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> |
| Carbon tetrabromide                   | CHBr <sub>4</sub>  |
| Carbon tetrachloride                  | CCl <sub>4</sub>   |
| Carbon tetrafluoride                  | CF <sub>4</sub>  |
| Carbon tribromide                     | CHBr <sub>3</sub>  |
| Carbon trichloride                    | CCl <sub>3</sub>   |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|  |  |
|--|--|
| Carbon trifluoride   | $\text{CF}_3$  |
| Carbonyl borane  | $\text{CH}_3\text{Be}$   |
| Carbonyl dibromide   | $\text{CBr}_2\text{O}$   |
| Carbonyl dichloride  | $\text{CCl}_2\text{O}$   |
| Carbonyl difluoride  | $\text{CF}_2\text{O}$  |
| Cellobiose   | $\text{C}_{12}\text{H}_{22}\text{O}_{11}$  |
| Cellobiose octaacetate   | $\text{C}_{28}\text{H}_{38}\text{O}_{19}$  |
| Chloral  | $\text{C}_2\text{HCl}_3\text{O}$   |
| Chloral hydrate  | $\text{C}_2\text{H}_3\text{Cl}_3\text{O}_2$  |
| Chlorin e <sub>4</sub> dimethyl ester  | $\text{C}_{35}\text{H}_{40}\text{N}_4\text{O}_4$   |
| Chlorin e <sub>6</sub> trimethyl ester   | $\text{C}_{37}\text{H}_{42}\text{N}_4\text{O}_6$   |
| Chlorin p <sub>6</sub> trimethyl ester   | $\text{C}_{36}\text{H}_{40}\text{N}_4\text{O}_6$   |
| Chloroacetyl chloride  | $\text{C}_2\text{H}_2\text{Cl}_2\text{H}$  |
| Chloroform   | $\text{CHCl}_3$  |
| Chloroporphyrin e <sub>4</sub> dimethyl ester  | $\text{C}_{35}\text{H}_{40}\text{N}_4\text{O}_4$   |
| Chloroporphyrin e <sub>5</sub> dimethyl ester  | $\text{C}_{35}\text{H}_{38}\text{N}_4\text{O}_5$   |
| Chloroporphyrin e <sub>6</sub> trimethyl ester                                       | $\text{C}_{37}\text{H}_{42}\text{N}_4\text{O}_6$   |
| Chlorotrifluoroethylene  | $\text{C}_2\text{ClF}_3$   |
| Chlorotrifluoroethane  | $\text{CCL}_2\text{F}_3$   |
| 5 $\beta$ -Cholan-24-oic acid-3 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -triol monohydrate | $\text{C}_{24}\text{H}_{42}\text{O}_6$<br>$\text{C}_{27}\text{H}_{46}\text{O}$<br>$\text{C}_{28}\text{H}_{48}\text{O}$ |
| 5 $\beta$ -Cholestene-3 $\beta$ -ol  | see: 5 $\beta$ -cholestene-3 $\beta$ -ol   |
| 5 $\beta$ -Cholestene-3 $\beta$ -yl methyl ether                                     | see: 5 $\beta$ -Cholestene-3 $\beta$ -methyl ether   |
| Cholestryl methyl ether  | see: 5 $\beta$ -cholen-24-oic acid-3 $\alpha$ ,7 $\alpha$ ,12 $\alpha$ -triol monohydrate                              |
| Cholic acid monohydrate  |  |
| Chromium hexacarbonyl  | $\text{C}_6\text{CrO}_6$   |
| Chrysene   | $\text{C}_{18}\text{H}_{12}$   |
| Cinchonamine   | $\text{C}_{19}\text{H}_{24}\text{N}_2\text{O}$   |
| Cinchonamine nitrate   | $\text{C}_{19}\text{H}_{25}\text{N}_2\text{O}_4$   |
| Cinchonidine   | $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}$   |
| Cinchonine   | $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}$   |
| Citraconic acid  | $\text{C}_5\text{H}_6\text{O}_4$   |
| Citric acid, anhydrous   | $\text{C}_6\text{H}_8\text{O}_7$   |
| Citric acid monohydrate  | $\text{C}_6\text{H}_{10}\text{O}_8$  |
| Cobalt carbonate   | $\text{CoCO}_3$  |
| Cobaltous formate  | $\text{C}_2\text{H}_2\text{CoO}_4$   |
| Cobalt oxalate   | $\text{C}_2\text{CoO}_4$   |
| Codeine monohydrate  | $\text{C}_{18}\text{H}_{23}\text{NO}_4$  |
| Conine   | $\text{C}_8\text{H}_{17}\text{N}$  |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|   |  |
|---|--|
| Coproporphyrin (II) tetraethyl ester                    | $C_40H_{46}N_4O_8$                                   |
| Copper (II) acetate                                     | $C_4H_6CuO_4$  |
| Copper (II) formate                                     | $C_2H_4CuO_4$  |
| Copper (II) glycollate                                  | $C_4H_6CuO_6$  |
| Cortexone   | $C_4H_6$   |
| Cortisol  | $C_21H_{32}$   |
| Cortisone   | $C_21H_{30}$   |
| Creatine  | $C_7H_{16}$  |
| Creatine hydrate  | $C_7H_{16}O_2$                                       |
| Creatinine  | $C_7H_{16}NO_3$                                      |
| m-Cresol  | $C_7H_8O$  |
| o-Cresol  | $C_7H_8O$  |
| p-Cresol  | $C_7H_8O$  |
| cis-Crotonic acid                                       | $C_4H_6O_2$  |
| trans-Crotonic acid                                     | $C_4H_6O_2$  |
| 3-Cyanopyridine   | $C_6H_5N$  |
| 5-Cyanotetrazole  | $C_2H_5N_5$  |
| 4-Cyanothiazole   | $C_4H_2N_2S$   |
| Cyclobutane   | $C_4H_8$   |
| 3:5-Cyclocholestan-6 $\beta$ -yl methyl ether           | $C_28H_{48}O$  |
| Cycloheptane  | $C_7H_{14}$  |
| Cyclohexane   | $C_6H_{12}$  |
| Cyclooctane   | $C_8H_{16}$  |
| Cyclpentane   | $C_5H_{10}$  |
| Cyclopropane  | $C_3H_6$   |
| L-Cysteine  | $C_3H_7NO_2S$  |
| L-Cystine   | $C_6H_{12}N_2O_4S_2$                                 |
| n-Decane  | $C_{10}H_{22}$                                       |
| 1,10-Decanediol   | $C_{10}H_{22}O_2$                                    |
| Decanoic acid   | see: Capric acid                                     |
| 1-Decene  | $C_{10}H_{20}$                                       |
| 1-Decyne  | $C_{10}H_{18}$                                       |
| trans-Dydroandrosterone                                 | see: $\Delta_5$ -Androstone-3 $\beta$ -ol-17-one     |
| Dehydro- $\beta$ -campholenolactone<br>(dextrorotatory) | $C_{10}H_{16}O_2$                                    |
| Dehydro- $\beta$ -campholenolactone<br>(inactive)       | $C_{10}H_{16}O_2$                                    |
| Desoxyamalic acid                                       | $C_{12}H_{14}N_4O_6$                                 |
| Desoxycorticosterone                                    | see: $\Delta_4$ -Pregnene-3 $\alpha$ ,20-dione-21-ol |
| Desoxyphyalloerythrin monomethyl ester                  | $C_{34}H_{38}N_4O_2$                                 |
| Diacetamide   | $C_4H_7N_2$  |
| 1,2,5,6-Diacetone mannitol                              | $C_{12}H_{22}O_6$                                    |
| Diacetyl  | see: 2,3-Butanedione                                 |
| 5-Diallylaminotetrazole                                 | $C_7H_{11}N_5$                                       |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|                                       |                         |
|---------------------------------------|-------------------------|
| Dialuric acid                         | $C_4H_4N_2O_4$          |
| sym-Diaminoguanidine nitrate          | $CH_8N_6O_3$            |
| 2,6-Diaminopyridine                   | $C_5H_7N_3$             |
| Diamylose                             | $C_24H_{40}O_2$         |
| 1,2-Dibromo-1,2-dichloroethane        | $C_2H_2Br_2Cl_2$        |
| 1,2-Dibromoethane                     | $C_2H_4Br_2$            |
| 1,2-Dibromo-1,1,2,2-tetrafluoroethane | $CH_2F_4$               |
| Dichloroacetic acid                   | $C_2H_2ClO_2$           |
| Dichloroacetyl chloride               | $C_2HCl_3O$             |
| 1,2-Dichluro-1,2-difluoroethylene     | $C_2Cl_2F_2$            |
| Dichlorodifluoromethane               | $C_2Cl_2F_2$            |
| 1,1-Dichluroethane                    | $C_2H_4Cl_2$            |
| 1,2-Dichlurothane                     | $C_2H_4Cl_2$            |
| 1,1-Dichloroethylene                  | $C_2Cl_2$               |
| cis-1,2-Dichloroethylene              | $C_2H_2Cl_2$            |
| trans-1,2-Dichloroethylene            | $C_2H_2Cl_2$            |
| Diethylamine                          | $C_4H_11N$              |
| Diethylamine nitrate                  | $C_4H_12N_2O_3$         |
| 2,2'-Dieethyl-5,5'-azotriazole        | $C_6H_{10}N_{10}$       |
| Diethylbarbituric acid                | $C_8H_{12}N_2O_3$       |
| Diethylenetriaminepentaacetic acid    | $C_{14}H_{23}N_5O_{10}$ |
| Diethyl ether                         | $C_4H_{10}O$            |
| Diethyl ketone                        | see: 3-Pentanone        |
| Diethyl mercury                       | $C_4H_{10}Hg$           |
| Diethyl tin                           | $C_4H_{12}Sn$           |
| Diethyl zinc                          | $C_4H_{10}Zn$           |
| Diffluoroacetic acid                  | $C_2H_2F_2O_2$          |
| 1,1-Difluoro-2-chloroethylene         | $C_2HClF_2$             |
| 1,1-Difluoroethane                    | $C_2H_4F_2$             |
| 2,2-Difluoroethanol                   | $C_2H_4F_2O$            |
| 1,1-Difluoroethylene                  | $C_2H_2F_2$             |
| Diglycolamidic acid                   | $C_4H_7NO_4$            |
| Diglycyldiglycine                     | $C_6H_{11}N_3O_4$       |
| Dihydropyran. 4-H                     | $C_5H_8O$               |
| 13,14-Dihydroxybenenic acid           | $C_{22}H_{44}O_4$       |
| 1,2-Dihydroxybenzene                  | see: Pyrocatechol       |
| 1,3-Dihydroxybenzene                  | see: Resorcinol         |
| 1,4-Dihydroxybenzene                  | see: Hydroquinone       |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|   |   |
|---|---|
| 1,2-Diiodoethane                                | $C_2H_4I_2$                                     |
| Diketene  | see: $\beta$ -Methylene- $\beta$ -propiolactone |
| Dimethoxyborane                                 | $C_2H_7Re_2$                                    |
| 1,2-Dimethoxyethane                             | $C_4H_{10}O_2$                                  |
| Dimethylacetylene                               | see: 2-Butyne                                   |
| cis- $\alpha$ , $\beta$ -Dimethylacrylic acid   | see: Tigliic acid                               |
| trans- $\alpha$ , $\beta$ -Dimethylacrylic acid | see: Angelic acid                               |
| Dimethyl adipate                                | $C_8H_{14}O_4$                                  |
| Dimethylamine                                   | $C_2H_7N$                                       |
| Dimethylamine nitrate                           | $C_2H_8N_2O_3$                                  |
| 5-Dimethylaminotetrazole                        | $C_3H_7N_5$                                     |
| N,N-Dimethylalaniline                           | $C_8H_{11}N$                                    |
| cis-1,1'-Dimethyl-5,5'-azotetrazole             | $C_4H_6N_{10}$                                  |
| trans-1,1'-Dimethyl-5,5'-azotetrazole           | $C_4H_6N_{10}$                                  |
| 2,2'-Dimethyl-5,5'-azotetrazole                 | $C_4H_6N_{10}$                                  |
| 2,2'-Dimethylbutane                             | $C_6H_{14}$                                     |
| 2,3-Dimethylbutane                              | $C_6H_{14}$                                     |
| Dimethyl cadmium                                | $C_2H_6Cd$                                      |
| 1,1-Dimethylcyclohexane                         | $C_8H_{16}$                                     |
| cis-1,2-Dimethylcyclohexane                     | $C_9H_{16}$                                     |
| trans-1,2-Dimethylcyclohexane                   | $C_9H_{16}$                                     |
| cis-1,3-Dimethylcyclohexane                     | $C_9H_{16}$                                     |
| trans-1,3-Dimethylcyclohexane                   | $C_9H_{16}$                                     |
| cis-1,4-Dimethylcyclohexane                     | $C_9H_{16}$                                     |
| trans-1,4-Dimethylcyclohexane                   | $C_8H_{16}$                                     |
| 1,1-Dimethylcyclopentane                        | $C_7H_{14}$                                     |
| cis-1,2-Dimethylcyclopentane                    | $C_7H_{14}$                                     |
| trans-1,2-Dimethylcyclopentane                  | $C_7H_{14}$                                     |
| cis-1,3-Dimethylcyclopentane                    | $C_7H_{14}$                                     |
| trans-1,3-Dimethylcyclopentane                  | $C_7H_{14}$                                     |
| Dimethyl disulfide                              | see: 2,3-Dithiabutane                           |
| Dimethyl ether                                  | $C_2H_6O$                                       |
| N,N-Dimethylformamide                           | $C_3H_7N_5$                                     |
| Dimethyl fumarate                               | $C_6H_8O_4$                                     |
| Dimethyl glutarate                              | $C_7H_{12}O_4$                                  |
| 2,2-Dimethylhexane                              | $C_9H_{18}$                                     |
| 2,3-Dimethylhexane                              | $C_8H_{16}$                                     |
| 2,4-Dimethylhexane                              | $C_8H_{18}$                                     |
| 2,5-Dimethylhexane                              | $C_8H_{18}$                                     |
| 3,3-Dimethylhexane                              | $C_8H_{18}$                                     |
| 3,4-Dimethylhexane                              | $C_8H_{18}$                                     |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|   |                           |
|---|---------------------------|
| 5,5-Dimethylhydantoin                   | $C_5H_8N_2O_2$            |
| 1,3-Dimethyl-5-iminotetrazole nitrate   | $C_3H_8N_6O_3$            |
| Dimeethyl isophthalate                  | see: Dimethyl m-phthalate |
| Dimeethyl maleate                       | $C_6H_8O_4$               |
| Dimeethyl malonate                      | $C_5H_8O_4$               |
| Dimeethyl mercury                       | $C_2H_6Hg$                |
| Dimeethyl oxalate                       | $C_4H_6O_4$               |
| Dimeethyl parabanic acid                | $C_5H_6N_2O_3$            |
| 2,2-Dimethylpentane                     | $C_7H_{16}$               |
| 2,3-Dimethylpentane                     | $C_7H_{16}$               |
| 2,4-Dimethylpentane                     | $C_7H_{16}$               |
| 3,3-Dimethylpentane                     | $C_7H_{16}$               |
| Dimeethylpurpurin 7                     | $C_37H_{40}N_4O_7$        |
| Dimeethyl phthalate                     | see: Dimethyl o-phthalate |
| Dimeethyl m-phthalate                   | $C_{10}H_{10}O_4$         |
| Dimeethyl o-phthalate                   | $C_{10}H_{10}O_4$         |
| Dimeethyl p-phthalate                   | $C_{10}H_{10}O_4$         |
| 2,2-Dimethylpropane                     | $C_5H_{12}$               |
| 2,3-Dimethylpyridine                    | $C_7H_9N$                 |
| 2,4-Dimethylpyridine                    | $C_7H_9N$                 |
| 2,5-Dimethylpyridine                    | $C_7H_9N$                 |
| 2,6-Dimethylpyridine                    | $C_7H_9N$                 |
| 3,4-Dimethylpyridine                    | $C_7H_9N$                 |
| 3,5-Dimethylpyridine                    | $C_7H_9N$                 |
| Dimeethyl tin                           | $C_2H_8Sn$                |
| Dimeethyl succinate                     | $C_6H_{10}O_4$            |
| Dimeethyl terephthalate                 | see: Dimethyl p-phthalate |
| 1,4-Dimethyl-5-tetrazolone              | $C_3H_6N_4$               |
| 1,5-Dimethyltetrazole                   | $C_3H_6N_4$               |
| Dimethyl zinc                           | $C_2H_6Zn$                |
| 1,3-Dioxane                             | $C_4H_8O_2$               |
| 1,4-Dioxane                             | $C_4H_8O_2$               |
| Dioxindole                              | $C_8H_7N_2O_2$            |
| Dipentaerythritol                       | $C_{10}H_{22}O_7$         |
| Diphenyl disulfide                      | $C_{12}H_{10}S_2$         |
| Diphenyl sulfide                        | $C_{12}H_{10}S$           |
| Di- $\alpha$ -pyrrylketone              | $C_9H_8O_2$               |
| Dipyrrylmethane                         | $C_9H_{10}N_2$            |
| 1,2-Di-(5-tetrazolyl)ethane             | $C_4H_6N_8$               |
| 2,3-Dithiabutane                        | $C_2H_6S_2$               |
| $\beta$ , $\beta'$ -Dithiodilactic acid | $C_6H_{10}O_4S_2$         |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|                                    |   |
|------------------------------------|---|
| Docosanoic acid                    | Behenic acid  |
| n-Dodecane                         | C <sub>12</sub> H <sub>26</sub>                             |
| Dodecanoic acid                    | see: Lauric acid  |
| i-Dodecene                         | C <sub>12</sub> H <sub>24</sub>                             |
| 1-Dodecyne                         | C <sub>12</sub> H <sub>22</sub>                             |
| Dulcitol                           | C <sub>6</sub> H <sub>14</sub> O <sub>6</sub>               |
| n-Eicosane                         | C <sub>20</sub> H <sub>42</sub>                             |
| Eicosanoic acid                    | see: Arachidic acid   |
| 1-Eicosene                         | C <sub>20</sub> H <sub>40</sub>                             |
| 1-Eicosyne                         | C <sub>20</sub> H <sub>38</sub>                             |
| Elaidic acid                       | C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>              |
| Enanthic acid                      | C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>               |
| S-Enantholactam                    | C <sub>7</sub> H <sub>13</sub> N <sub>0</sub>               |
| Epiandrosterone                    | see: 5α-Androstan-3β-ol-17-one                              |
| Erucic acid                        | C <sub>22</sub> H <sub>42</sub> O <sub>2</sub>              |
| meso-Erythritol                    | see: meso-1,2,3,4-Butanetetrol                              |
| Erythritol diacetal                | C <sub>8</sub> H <sub>14</sub> O <sub>4</sub>               |
| Erythritol diformal                | C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>               |
| Ethanal                            | see: Acetaldehyde   |
| Ethane                             | C <sub>2</sub> H <sub>6</sub>                               |
| 1,2-Ethanediol                     | C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>                |
| 1,2-Ethanedithiol                  | C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>                |
| Ethanethiol                        | C <sub>2</sub> H <sub>6</sub> S                             |
| Ethanoic acid                      | see: Acetic acid  |
| Ethanol                            | C <sub>2</sub> H <sub>6</sub> O                             |
| Ethenylbenzene                     | C <sub>8</sub> H <sub>8</sub>                               |
| Ethylacetylene                     | see: 1-Butyne   |
| Ethyl alcohol                      | see: Ethanol  |
| Ethylamine                         | C <sub>2</sub> H <sub>7</sub> N                             |
| Ethyldiamine nitrate               | C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> |
| Ethyl β-anilino-β-phenyl proponate | C <sub>17</sub> H <sub>19</sub> N <sub>0</sub> <sub>2</sub> |
| Ethylbenzene                       | C <sub>8</sub> H <sub>10</sub>                              |
| Ethyl bromide                      | C <sub>2</sub> H <sub>5</sub> Br                            |
| Ethyl carbamate                    | C <sub>3</sub> H <sub>7</sub> N <sub>0</sub> <sub>2</sub>   |
| Ethyl chloride                     | C <sub>2</sub> H <sub>5</sub> Cl                            |
| Ethylcyclohexane                   | C <sub>8</sub> H <sub>16</sub>                              |
| Ethylcyclopentane                  | C <sub>7</sub> H <sub>14</sub>                              |
| Ethylene                           | C <sub>2</sub> H <sub>4</sub>                               |
| Ethylene carbonate                 | C <sub>3</sub> H <sub>4</sub> O <sub>3</sub>                |
| Ethylene chlorohydrin              | C <sub>2</sub> H <sub>5</sub> ClO                           |
| Ethylenediamine                    | C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>                |

TABLE I-B COMPOUND NAME-Formula INDEX

|   |   |
|---|---|
| Ethylenediamine dinitrate                         | C <sub>2</sub> H <sub>10</sub> N <sub>4</sub> O <sub>6</sub>  |
| Ethylenediaminetetraacetic acid                   | C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>8</sub> |
| Ethylene glycol                                   | see : 1,2-Ethanediol  |
| Ethylenimine                                      | C <sub>2</sub> H <sub>5</sub> N                               |
| Ethyl glycylglycinat <sup>e</sup>                 | C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>  |
| 3-Ethylhexane                                     | C <sub>8</sub> H <sub>18</sub>                                |
| Ethyl iodide                                      | C <sub>2</sub> H <sub>5</sub> I                               |
| 3-Ethylpentane                                    | C <sub>7</sub> H <sub>16</sub>                                |
| 2-Ethylphenol                                     | C <sub>8</sub> H <sub>10</sub> O                              |
| 3-Ethylphenol                                     | C <sub>8</sub> H <sub>10</sub> O                              |
| 4-Ethylphenol                                     | C <sub>8</sub> H <sub>10</sub> O                              |
| 2-Ethylpyridine                                   | C <sub>7</sub> H <sub>9</sub> N                               |
| Fluoranthene                                      | C <sub>16</sub> H <sub>10</sub>                               |
| Fluoroacetic acid                                 | C <sub>2</sub> H <sub>3</sub> FO <sub>2</sub>                 |
| 2-Fluoroethanol                                   | C <sub>2</sub> H <sub>5</sub> F                               |
| Fluoroform  | CHF <sub>3</sub>  |
| Fluorotrichloromethane                            | CCl <sub>3</sub> F  |
| Formaldehyde                                      | CH <sub>2</sub> O   |
| Formamide   | CH <sub>3</sub> NO  |
| 1-Formamido-2-nitroguanidine                      | C <sub>2</sub> H <sub>5</sub> N <sub>5</sub> O <sub>3</sub>   |
| Formanilide                                       | C <sub>7</sub> H <sub>7</sub> NO                              |
| Formic acid                                       | CH <sub>2</sub> O <sub>2</sub>                                |
| N-Formyl-DL-leucine                               | C <sub>7</sub> H <sub>13</sub> NO <sub>3</sub>                |
| Formylurea  | C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>   |
| $\beta$ -D-Fructose                               | C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                 |
| D-Fucose  | C <sub>6</sub> H <sub>12</sub> O <sub>5</sub>                 |
| Fumaric acid                                      | C <sub>4</sub> H <sub>4</sub> O <sub>4</sub>                  |
| Furan   | C <sub>4</sub> H <sub>4</sub> O                               |
| Furfural  | C <sub>5</sub> H <sub>4</sub> O <sub>2</sub>                  |
| Furfuryl alcohol                                  | C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>                  |
| 2-Furoic acid                                     | C <sub>5</sub> H <sub>4</sub> O <sub>3</sub>                  |
| D-Galactonic acid                                 | C <sub>6</sub> H <sub>12</sub> O <sub>7</sub>                 |
| D-Galactonic acid- $\gamma$ -lactone              | C <sub>6</sub> H <sub>10</sub> O <sub>5</sub>                 |
| $\alpha$ -D-Galactose                             | C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                 |
| Galactose pentaacetate                            | C <sub>16</sub> H <sub>22</sub> O <sub>11</sub>               |
| D-Glucaric acid-1,4-lactone                       | C <sub>5</sub> H <sub>8</sub> O <sub>7</sub>                  |
| D-Glucaric acid-3,6-lactone                       | C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>                  |
| D-Glucuo-D-gulonoheptonic acid- $\gamma$ -lactone | C <sub>7</sub> H <sub>12</sub> O <sub>7</sub>                 |
| D-Glucuo- $\alpha$ -heptite                       | C <sub>7</sub> H <sub>14</sub> O <sub>7</sub>                 |
| D-Glucuo- $\alpha$ -heptose                       | C <sub>6</sub> H <sub>12</sub> O <sub>7</sub>                 |
| D-Gluconic acid                                   |   |

TABLE I-B COMPOUND NAME-<sup>a</sup>FORMULA INDEX

|  |  |
|--|--|
| D-Gluconic acid- $\delta$ -lactone                             | C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>                |
| D-Glucos- $\alpha$ , $\alpha$ -octonic acid- $\gamma$ -lactone | C <sub>8</sub> H <sub>14</sub> O <sub>8</sub>                |
| $\alpha$ -D-Glucose  | C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                |
| $\beta$ -D-Glucose   | C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                |
| $\alpha$ -D-Glucose hydrate                                    | C <sub>6</sub> H <sub>14</sub> O <sub>7</sub>                |
| Glucose pentaacetate   | C <sub>16</sub> H <sub>22</sub> O <sub>11</sub>              |
| L-Glutamic acid  | C <sub>5</sub> H <sub>9</sub> N <sub>4</sub>                 |
| L-Glutamine  | C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> |
| Glutaric acid  | C <sub>5</sub> H <sub>8</sub> O <sub>4</sub>                 |
| Glyceraldehyde   | C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>                 |
| Glycerol   | see: 1,2,3-Propanetriol                                      |
| Glyceryl-1-acetate   | C <sub>5</sub> H <sub>10</sub> O <sub>4</sub>                |
| Glyceryl-1-benzoate  | C <sub>10</sub> H <sub>12</sub> O <sub>4</sub>               |
| Glyceryl-2-benzoate  | C <sub>10</sub> H <sub>12</sub> O <sub>4</sub>               |
| Glyceryl-1-caprate   | C <sub>13</sub> H <sub>26</sub> O <sub>4</sub>               |
| Glyceryl-2-caprate   | C <sub>13</sub> H <sub>26</sub> O <sub>4</sub>               |
| Glyceryl-1,3-diacetate   | C <sub>7</sub> H <sub>12</sub> O <sub>5</sub>                |
| Glyceryl dibassidate   | C <sub>4</sub> H <sub>8</sub> O <sub>5</sub>                 |
| Glyceryl dierucate   | C <sub>4</sub> H <sub>8</sub> O <sub>5</sub>                 |
| Glyceryl-1-lauroate  | C <sub>15</sub> H <sub>30</sub> O <sub>4</sub>               |
| Glyceryl-2-lauroate  | C <sub>15</sub> H <sub>30</sub> O <sub>4</sub>               |
| Glyceryl-1-myristate   | C <sub>17</sub> H <sub>34</sub> O <sub>4</sub>               |
| Glyceryl-2-myristate   | C <sub>17</sub> H <sub>34</sub> O <sub>4</sub>               |
| Glyceryl-1-palmitate   | C <sub>19</sub> H <sub>38</sub> O <sub>4</sub>               |
| Glyceryl-2-palmitate   | C <sub>19</sub> H <sub>38</sub> O <sub>4</sub>               |
| Glyceryl-1-stearate  | C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>               |
| Glyceryl-2-stearate  | C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>               |
| Glyceryl triacetate  | C <sub>9</sub> H <sub>14</sub> O <sub>6</sub>                |
| Glyceryl tribenzoate   | C <sub>24</sub> H <sub>20</sub> O <sub>6</sub>               |
| Glyceryl tribassidate  | C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                |
| Glyceryl tributyrate   | C <sub>15</sub> H <sub>26</sub> O <sub>6</sub>               |
| Glyceryl trilaurate  | C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>                |
| Glyceryl triacetate  | C <sub>39</sub> H <sub>74</sub> O <sub>6</sub>               |
| Glyceryl triauroate  | C <sub>45</sub> H <sub>86</sub> O <sub>6</sub>               |
| Glyceryl trimyristate  | C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>                |
| Glycine  | C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>  |
| Glycine anhydride  | C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>  |
| Glycine nitrate  | C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>                 |
| Glycol acetal  | C <sub>2</sub> H <sub>4</sub> O <sub>3</sub>                 |
| Glycolic acid  | C <sub>1</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> |
| Glycylalanyl phenylalanine                                     | C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>  |
| Glycylglycine  |  |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|  |   |
|--|---|
| Glycylglycine-N-carboxylic acid              | C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>5</sub>   |
| Glycylphenylalanine                          | C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> |
| Glycylphenylalanyl anhydride                 | C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> |
| Glycyltyrosyl anhydride                      | C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> |
| Glycylvaline                                 | C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>  |
| Glycylvalyl anhydride                        | C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>  |
| Glyoxal                                      | C <sub>2</sub> H <sub>2</sub> O                               |
| Glyoxylic acid                               | C <sub>2</sub> H <sub>2</sub> O <sub>2</sub>                  |
| Guanidine                                    | C <sub>2</sub> H <sub>4</sub> N <sub>3</sub>                  |
| Guanidine carbonate                          | C <sub>3</sub> H <sub>12</sub> N <sub>6</sub> O <sub>3</sub>  |
| Guanidine nitrate                            | C <sub>3</sub> H <sub>12</sub> N <sub>6</sub> O <sub>3</sub>  |
| Guanine                                      | C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O                |
| 5-Guanylaminotetrazole                       | C <sub>2</sub> H <sub>5</sub> N <sub>7</sub>                  |
| Guanylurea nitrate                           | C <sub>2</sub> H <sub>7</sub> N <sub>5</sub> O <sub>4</sub>   |
| L-Gulonic acid- $\gamma$ -lactone            | C <sub>6</sub> H <sub>10</sub> O <sub>6</sub>                 |
| n-Heptadecane                                | C <sub>17</sub> H <sub>36</sub>                               |
| 1-Heptadecene                                | C <sub>17</sub> H <sub>34</sub>                               |
| 1-Heptadecyne                                | C <sub>17</sub> H <sub>32</sub>                               |
| n-Heptaldehyde                               | C <sub>7</sub> H <sub>14</sub> O                              |
| 1-Heptanal                                   | see: n-Heptaldehyde   |
| n-Heptane                                    |   |
| Heptanoic acid                               | C <sub>7</sub> H <sub>16</sub>                                |
| 1-Heptene                                    | C <sub>7</sub> H <sub>14</sub>                                |
| 1-Hentyne                                    | C <sub>7</sub> H <sub>12</sub>                                |
| Hexachloroethane                             | C <sub>2</sub> Cl <sub>6</sub>                                |
| n-Hexadecane                                 | C <sub>16</sub> H <sub>34</sub>                               |
| Hexadecanolic acid                           | see: Palmitic acid  |
| 1-Hexadecene                                 |   |
| 1-Hexadecyne                                 | C <sub>16</sub> H <sub>32</sub>                               |
| Hexa-2-ene-1,6-dioic acid                    | C <sub>16</sub> H <sub>30</sub>                               |
| Hexa-3-ene-1,6-dioic acid                    | C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>                  |
| Hexafluoroethane                             | C <sub>6</sub> H <sub>8</sub> O <sub>4</sub>                  |
| Hexamethyl dialuminum                        | C <sub>2</sub> F <sub>6</sub>                                 |
| Hexamethyl disiloxane                        | C <sub>6</sub> H <sub>18</sub> Al <sub>2</sub>                |
| Hexamethyl ditin                             | C <sub>6</sub> H <sub>18</sub> Sn <sub>2</sub>                |
| Hexamethylene-1,6-diamino-adipic acid adduct | C <sub>12</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> |
| Hexamethylenetetramine                       | C <sub>6</sub> H <sub>12</sub> N <sub>4</sub>                 |
| Hexaneethylenetetramine dinitrate            | C <sub>6</sub> H <sub>14</sub> N <sub>6</sub> O <sub>6</sub>  |
| $\beta$ -Hexanoylase                         | C <sub>48</sub> H <sub>80</sub> O <sub>40</sub>               |
| n-Hexane                                     | C <sub>6</sub> H <sub>14</sub>                                |
| 1-Hexanethiol                                | C <sub>6</sub> H <sub>14</sub> S                              |

TABLE I-B COMPOUND NAME- $\mu$ FORMULA INDEX

|  |   |
|--|---|
| Hexanoic acid  | see: Caproic acid   |
| 1-Hexanol  | C <sub>6</sub> H <sub>14</sub> O                              |
| 1-Hexene   | C <sub>6</sub> H <sub>12</sub>                                |
| 1-Hexyne   | C <sub>6</sub> H <sub>10</sub>                                |
| n-Hexyl alcohol  | see: i-Hexanol  |
| Hippuric acid  | C <sub>9</sub> H <sub>9</sub> NO <sub>3</sub>                 |
| Hippurylglycine  | C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> |
| Hydantoic acid   | C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub>   |
| Hydantoin  | C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>   |
| Hydrazodicarbamide   | C <sub>2</sub> H <sub>6</sub> N <sub>4</sub> O <sub>2</sub>   |
| 5,5'-'Hydrazotetrazole   | C <sub>2</sub> H <sub>4</sub> N <sub>10</sub>                 |
| Hydroquinone   | C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>                  |
| Hydroxosuccinic acid   | C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>                 |
| Hydroxyacetic acid   | see: Glycolic acid  |
| DL- $\beta$ -Hydroxybutyric acid   | C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>                  |
| 3( $\alpha$ )-Hydroxy-trans-decalin-2( $\alpha$ ) acetic acid lactone (boat form)      | C <sub>12</sub> H <sub>18</sub> O <sub>2</sub>                |
| 3( $\epsilon$ )-Hydroxy-trans-decalin-2( $\epsilon$ ) acetic acid lactone (chair form) | C <sub>12</sub> H <sub>18</sub> O <sub>2</sub>                |
| Hydroxyisobutyric acid   | C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>                  |
| 5-Hydroxy-1-pentanal   | C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>                 |
| L-Hydroxyproline   | C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>                 |
| 8-Hydroxyquinaline   | C <sub>9</sub> H <sub>7</sub> NO                              |
| 5-Hydroxytetrazole   | C <sub>4</sub> H <sub>2</sub> N <sub>2</sub> O                |
| Hydurilic acid   | C <sub>8</sub> H <sub>6</sub> N <sub>4</sub> O <sub>6</sub>   |
| Hypoxanthine   | C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O                |
| Indazole   | C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>                  |
| Indigotin  | C <sub>16</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> |
| Indole   | C <sub>8</sub> H <sub>7</sub> N                               |
| Iodoform   | CHI <sub>3</sub>  |
| Iron (II) carbonate  | CFeO <sub>3</sub>   |
| Iron pentacarbonyl   | C <sub>5</sub> Fe(CO) <sub>5</sub>                            |
| Isatide  | C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> |
| Isatin   | C <sub>8</sub> H <sub>5</sub> NO <sub>2</sub>                 |
| Isobutene  | see: 2-Methyl propene   |
| Isobutyl alcohol   | see: 2-Methyl-1-propanol                                      |
| Isobutylamine  | C <sub>4</sub> H <sub>11</sub> N                              |
| DL-Isoleucine  | C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>                |
| L-Isoleucine   | C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>                |
| Isopentane   | see: 2-Methylbutane   |
| Isophthalic acid   | see: m-Phthalic acid  |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|  |  |
|--|--|
| Isopropyl alcohol  | see: 2-Propanol  |
| Isopropylamine   | C <sub>3</sub> H <sub>9</sub> N  |
| Isopropylbenzene   | C <sub>9</sub> H <sub>12</sub>   |
| Isoquolinoline   | C <sub>9</sub> H <sub>7</sub> N  |
| L-Isoserine  | C <sub>3</sub> H <sub>7</sub> NH <sub>3</sub>                                |
| Isouric acid   | C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>                  |
| Iso-uroporphyrin (II) octamethyl ester   | C <sub>4</sub> H <sub>8</sub> H <sub>54</sub> N <sub>4</sub> O <sub>16</sub> |
| Itaconic acid  | C <sub>5</sub> H <sub>6</sub> O <sub>4</sub>                                 |
| $\alpha$ -Ketoglutaric acid  | C <sub>5</sub> H <sub>6</sub> O <sub>5</sub>                                 |
| $\gamma$ -Ketovaleric acid   | see: Levulinic acid  |
| D-Lactic acid  | C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>                                 |
| DL-Lactic acid   | C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>                                 |
| Lactide  | C <sub>3</sub> H <sub>6</sub> O <sub>4</sub>                                 |
| $\beta$ -Lactose   | C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>                              |
| $\alpha$ -Lactose monohydrate  | C <sub>12</sub> H <sub>24</sub> O <sub>12</sub>                              |
| Lactose octaacetate  | C <sub>28</sub> H <sub>38</sub> O <sub>19</sub>                              |
| Lauric acid  | C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>                               |
| Lead acetate   | C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> Pb                              |
| Lead formate   | C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> Pb                              |
| D-Leucine  | C <sub>6</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>                 |
| DL-Leucine   | C <sub>6</sub> H <sub>13</sub> NH <sub>2</sub>                               |
| L-Leucine  | C <sub>6</sub> H <sub>13</sub> NH <sub>2</sub>                               |
| Leucine anhydride  | C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub>                |
| L(+) -Leucine methyl ester salt of (-)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3') | C <sub>36</sub> H <sub>44</sub> N <sub>2</sub> O <sub>10</sub>               |
| L(+) -Leucine methyl ester salt of (+)-1,1'-dinaphthyl-2,2'-dihydroxy carboxylic acid-(3,3') | C <sub>36</sub> H <sub>44</sub> N <sub>2</sub> O <sub>10</sub>               |
| DL-Leucylglycine   | C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>                 |
| Leucylglycylglycine  | C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>                |
| Levoglucosan   | C <sub>6</sub> H <sub>10</sub> O <sub>5</sub>                                |
| Levoglucosan triacetate  | C <sub>12</sub> H <sub>16</sub> O <sub>8</sub>                               |
| Levulinic acid   | C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>                                 |
| Levulinic lactone  | C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>                                 |
| Lophine  | C <sub>21</sub> H <sub>16</sub> N <sub>2</sub>                               |
| DL-Lysine  | C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>                 |
| Maleic acid  | C <sub>4</sub> H <sub>4</sub> O <sub>4</sub>                                 |
| Maleic anhydride   | C <sub>4</sub> H <sub>2</sub> O <sub>3</sub>                                 |
| DL-Malic acid  | C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>                                 |
| L-Malic acid   | C <sub>4</sub> H <sub>6</sub> O <sub>5</sub>                                 |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|                                    |                    |
|------------------------------------|--------------------|
| Malonamide                         | $C_3H_6N_2O_2$     |
| Malonic acid                       | $C_3H_4O_4$        |
| Maltose                            | $C_{12}H_{22}O_11$ |
| $\beta$ -Maltose monohydrate       | $C_{12}H_{24}O_12$ |
| Maltose octaacetate                | $C_{28}H_{38}O_19$ |
| DL-Mandellic acid                  | $C_9H_8O_3$        |
| L-Mandellic acid                   | $C_9H_8O_3$        |
| Manganese acetate                  | $C_4H_6MnO_4$      |
| Manganese carbonate                | $C_3MnO_3$         |
| Manganese formate                  | $C_2H_2MnO_4$      |
| D-Mannitol                         | $C_6H_{14}O_6$     |
| Mannitol triacetate                | $C_{12}H_{20}O_6$  |
| Mannitol triformal                 | $C_9H_{14}O_6$     |
| D-Mannonic-1,4-3,6-dilactone       | $C_6H_6O_6$        |
| D-Mannonic acid- $\gamma$ -lactone | $C_6H_{10}O_6$     |
| D-Mannose                          | $C_6H_{12}O_6$     |
| Melanine                           | $C_3H_6N_6$        |
| Melanzitose                        | $C_{18}H_{32}O_16$ |
| Mesaconic acid                     | $C_5H_6O_4$        |
| Mesoporphyrin (IX) dimethyl ester  | $C_36H_{42}N_4O_4$ |
| Mesoxyalic acid                    | $C_3H_4O_6$        |
| Methanal                           | $CH_4$             |
| Methane                            | $CH_4$             |
| Methanethiol                       | $CH_3S$            |
| Methanolic acid                    | see: Formic acid   |
| Methanol                           | $CH_4O$            |
| L-Methionine                       | $C_5H_{11}NO_2S$   |
| 5-Methoxytetrazole                 | $C_2H_4N_4O$       |
| Methyl acetate                     | $C_3H_6O_2$        |
| Methylacetylene                    | see: Propyne       |
| Methyl alcohol                     | see: Methanol      |
| Methyl allantoin                   | $C_5H_8N_4O_3$     |
| Methylamine                        | $CH_3N$            |
| Methylamine nitrate                | $CH_6N_2O_3$       |
| 1-Methyl-5-aminotetrazole          | $C_2H_5N_5$        |
| 2-Methyl-5-aminotetrazole          | $C_2H_5N_5$        |
| 5-Methylaminotetrazole             | $C_7H_9N$          |
| N-Methylaniline                    | see: Toluene       |
| Methylbenzene                      | $C_8H_8$           |
| Methyl benzoate                    | $C_8H_7Br_2$       |
| Methyl bromide                     |                    |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|   |  |
|---|--|
| 2-Methyl-1,3-butadiene                      | C <sub>5</sub> H <sub>6</sub>                                |
| 2-Methylbutane                              | C <sub>5</sub> H <sub>12</sub>                               |
| 2-Methyl-1-butene                           | C <sub>5</sub> H <sub>10</sub>                               |
| 2-Methyl-1-2-butene                         | C <sub>5</sub> H <sub>10</sub>                               |
| 3-Methyl-1-butene                           | C <sub>5</sub> H <sub>10</sub>                               |
| 3-Methyl-1-butyne                           | C <sub>5</sub> H <sub>8</sub>                                |
| Methyl caprate                              | C <sub>11</sub> H <sub>22</sub> O <sub>2</sub>               |
| Methyl caproate                             | C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>                |
| N-Methylcaprolactam                         | C <sub>7</sub> H <sub>13</sub> N <sup>t</sup>                |
| S-Methylcaprolactam                         | C <sub>7</sub> H <sub>13</sub> N <sup>d</sup>                |
| 7-Methylcaprylate                           | C <sub>7</sub> H <sub>13</sub> N <sup>d</sup>                |
| Methyl caprylate                            | C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>                |
| Methyl chloride                             | CH <sub>3</sub> Cl   |
| Methylcyclohexane                           | C <sub>7</sub> H <sub>14</sub>                               |
| Methylcyclopentane                          | C <sub>6</sub> H <sub>12</sub>                               |
| Methyl elaidate                             | C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>               |
| Methyl enanthate                            | C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>                |
| Methylene dichloride                        | CH <sub>2</sub> Cl <sub>2</sub>                              |
| Methylene difluoride                        | CH <sub>2</sub> F <sub>2</sub>                               |
| Methylene diiodide                          | CH <sub>2</sub> I <sub>2</sub>                               |
| $\beta$ -Methylene- $\beta$ -propiolactone  | C <sub>4</sub> H <sub>4</sub> O <sub>2</sub>                 |
| 1-Methyl-2-ethylbenzene                     | C <sub>9</sub> H <sub>12</sub>                               |
| 1-Methyl-3-ethylbenzene                     | C <sub>9</sub> H <sub>12</sub>                               |
| 1-Methyl-4-ethylbenzene                     | C <sub>9</sub> H <sub>12</sub>                               |
| Methyl ethyl ether                          | C <sub>3</sub> H <sub>8</sub>                                |
| Methyl ethyl heptanone lactone<br>(racemic) | C <sub>10</sub> H <sub>16</sub> O <sub>3</sub>               |
| 5-Methyl-5-ethylhydantoin                   | C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> |
| Methyl ethyl ketone                         | see: Butanone  |
| Methyl ethyl mercury                        | C <sub>3</sub> H <sub>8</sub> Hg                             |
| 2-Methyl-3-ethyl pentane                    | C <sub>8</sub> H <sub>18</sub>                               |
| 3-Methyl-3-ethyl pentane                    | C <sub>8</sub> H <sub>18</sub>                               |
| Methyl formate                              | C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>                 |
| $\alpha$ -Methyl-D-glucofuranoside          | C <sub>7</sub> H <sub>14</sub> O <sub>5</sub>                |
| $\beta$ -Methyl-D-glucopyranoside           | C <sub>7</sub> H <sub>14</sub> O <sub>6</sub>                |
| 2-Methylheptane                             | C <sub>8</sub> H <sub>18</sub>                               |
| 3-Methylheptane                             | C <sub>8</sub> H <sub>18</sub>                               |
| 4-Methylheptane                             | C <sub>8</sub> H <sub>18</sub>                               |
| 2-Methylhexane                              | C <sub>7</sub> H <sub>16</sub>                               |
| 3-Methylhexane                              | C <sub>7</sub> H <sub>16</sub>                               |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|                             |   |
|-----------------------------|---|
| 5-Methylhydrastin           | C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>   |
| 4-Methylhydouracil          | C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>   |
| 7-Methylhypoxanthine        | C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O                |
| Methyl iodide               | CH <sub>3</sub> I   |
| $\alpha$ -Methyl indole     | C <sub>9</sub> H <sub>9</sub> N                               |
| $\beta$ -Methyl indole      | see: Skatole  |
| Methyl laurate              | C <sub>13</sub> H <sub>26</sub> O <sub>2</sub>                |
| Methyl mercury              | CH <sub>3</sub> Hg  |
| Methyl myristate            | C <sub>15</sub> H <sub>30</sub> O <sub>2</sub>                |
| Methyl oleate               | C <sub>19</sub> H <sub>36</sub> O <sub>2</sub>                |
| Methyl pelargonate          | C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>                |
| Methyl pentadecylate        | C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>                |
| 2-Methylpentane             | C <sub>6</sub> H <sub>14</sub>                                |
| 3-Methylpentane             | C <sub>6</sub> H <sub>14</sub>                                |
| 2-Methyl phenol             | see: o-Cresol   |
| 3-Methyl phenol             | see: m-Cresol   |
| 4-Methyl phenol             | see: p-Cresol   |
| 1-Methyl-5-phenyltetrazole  | C <sub>8</sub> H <sub>8</sub> N <sub>4</sub>                  |
| Methylpheophorbide a        | C <sub>36</sub> H <sub>38</sub> N <sub>4</sub> O <sub>5</sub> |
| Methylpheophorbide b        | C <sub>36</sub> H <sub>36</sub> N <sub>4</sub> O <sub>6</sub> |
| N-Methylpiperidone          | C <sub>6</sub> H <sub>11</sub> NO                             |
| 2-Methylpropene             | C <sub>4</sub> H <sub>8</sub>                                 |
| 2-Methyl-1,2-propanediamine | C <sub>4</sub> H <sub>12</sub> N <sub>2</sub>                 |
| 2-Methyl-1-propanol         | C <sub>4</sub> H <sub>10</sub> O                              |
| 2-Methyl-2-propanol         | C <sub>4</sub> H <sub>10</sub> O                              |
| Methyl n-propyl ketone      | see: 2-Pentanone  |
| 7-Methylpurine              | C <sub>6</sub> H <sub>6</sub> N <sub>4</sub>                  |
| 2-Methylpyridine            | C <sub>5</sub> H <sub>7</sub> N                               |
| 3-Methylpyridine            | C <sub>6</sub> H <sub>7</sub> N                               |
| 4-Methylpyridine            | C <sub>6</sub> H <sub>7</sub> N                               |
| N-Methylpyrrolidone         | C <sub>5</sub> H <sub>9</sub> NO                              |
| $\alpha$ -Methylquinoline   | see: Quinaldine   |
| Methyl theobromine          | see: Caffeine   |
| Methyl salicylate           | C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>                  |
| 4-Methylthiazole            | C <sub>4</sub> H <sub>5</sub> NS                              |
| 2-Methylthiophene           | C <sub>5</sub> H <sub>6</sub> S                               |
| 3-Methylthiophene           | C <sub>5</sub> H <sub>6</sub> S                               |
| Methyl tridecylate          | C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>                |
| Methyl undecylate           | C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>                |
| 4-Methyl uracil             | C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>   |
| 5-Methyl uracil             | see: Thymine  |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|                          |                        |
|--------------------------|------------------------|
| Methyl valerate          | $C_6H_{12}O_2$         |
| Molybdenum hexacarbonyl  | $C_6Mo_6$              |
| Monochloroacetic acid    | $C_2Cl_3Cl_6$          |
| Monochloroacetaldehyde   | $C_2H_3Cl_6$           |
| Morphine monohydrate     | $C_17H_{21}NO_4$       |
| Mucic acid               | $C_6H_{10}O_8$         |
| Murexide                 | $C_9H_8N_6O_6$         |
| Myristic acid            | $C_{14}H_{28}O_2$      |
| Naphthacene              | $C_{18}H_{12}$         |
| Naphthalene              | $C_{10}H_8$            |
| Narceline dihydrate      | $C_{23}H_{31}NO_10$    |
| Narcotine                | $C_{22}H_{23}N^{+}I^-$ |
| Neopentane               |                        |
| Nickel carbonyl          | $C_4NiO_4$             |
| Nickel formate           | $C_2H_2NiO_4$          |
| Nickel oxalate           | $C_2NiO_4$             |
| Nicotine                 | $C_{10}H_{14}N_2$      |
| Nitrotriethylacetic acid | $C_6H_9NO_6$           |
| Nitrosoaminoquinidine    | $CH_5N_5O_2$           |
| n-Nonenecane             | $C_{19}H_{40}$         |
| 1-Nonadecene             | $C_{19}H_{38}$         |
| 1-Nonadecyne             | $C_{19}H_{36}$         |
| n-Nonane                 | $C_9H_{20}$            |
| Nonanoic acid            |                        |
| 1-Nonene                 | $C_9H_{18}$            |
| 1-Nonyne                 | $C_9H_{16}$            |
| Norleucine               |                        |
| n-Octadecane             |                        |
| Octadecanolic acid       |                        |
| 1-Octadecene             | $C_{18}H_{38}$         |
| 1-Octadecyne             | $C_{18}H_{34}$         |
| 1-Octene                 | $C_8H_{16}$            |
| Octethylporphyrin        | $C_{36}H_{46}N_4$      |
| n-Octaldehyde            | $C_8H_{16}O$           |
| 1-Octanal                |                        |
| n-Octane                 | $C_8H_{18}$            |
| Octanoic acid            |                        |
| 1-Octyne                 |                        |
| Oleic acid               |                        |
| DL-Djenkithine           | $C_5H_{12}N_2O_2$      |
| Oxacyclobutane           | $C_3H_6O$              |

TABLE I-B COMPOUND NAME-Formula INDEX

|                                |                      |
|--------------------------------|----------------------|
| $\alpha$ - $\beta$ -xalic acid | $C_2H_2O_4$          |
| $\beta$ - $\delta$ -xalic acid | $C_2H_2O_4$          |
| $\delta$ xalic acid dihydrate  | $C_2H_2O_4$          |
| Oxamic acid                    | $C_2H_6O_6$          |
| Oxamide                        | $C_2H_3NO_3$         |
| Oxindole                       | $C_2H_4N_2O_2$       |
| 6-Oxyxipurine                  | $C_8H_7N_6$          |
| 8-Oxyxipurine                  | see: Hypoxanthine    |
| Palmitic acid                  | $C_5H_{10}O_6$       |
| Papaverine                     | $C_{16}H_{32}O_2$    |
| Parabanic acid                 | $C_{20}H_{21}NO_4$   |
| Paraldehyde                    | $C_3H_2N_2O_3$       |
| Pelargonic acid                | $C_6H_{12}O_3$       |
| Pentachloroethane              | $C_9H_{18}Cl_2$      |
| n-Pentadecane                  | $C_2HCl_5$           |
| 1-Pentadecene                  | $C_{15}H_{32}$       |
| 1-Pentadecyne                  | $C_{15}H_{30}$       |
| 1,2-Pentadiene                 | $C_{15}H_{28}$       |
| 1,2-trans-3-Pentadiene         | $C_5H_8$             |
| 1,4-Pentadiene                 | $C_5H_8$             |
| 2,3-Pentadiene                 | $C_5H_8$             |
| Pentaerythritol                | $C_5H_{12}O_4$       |
| 1-Pentanal                     | see: n=Valeraldehyde |
| n-Pentane                      | $C_5H_{12}$          |
| 1-Pentanethiol                 | $C_5H_{12}S$         |
| Pentanoic acid                 | see: Valeric acid    |
| 1-Pentanol                     | $C_5H_{12}O$         |
| 2-Pentanone                    | $C_5H_{10}O$         |
| 3-Pentanone                    | $C_5H_{10}O$         |
| 1-Pentene                      | $C_5H_{10}$          |
| 1s-2-Pentene                   | $C_5H_{10}$          |
| trans-2-Pentene                | $C_5H_{10}$          |
| 1-Pentyne                      | $C_5H_8$             |
| 2-Pentyne                      | $C_5H_8$             |
| D-Perseltol                    | $C_7H_{16}O_7$       |
| Perylene                       | $C_{20}H_{12}$       |
| Phenacetin                     | $C_{10}H_{13}NO_2$   |
| Phenaceturic acid              | $C_{10}H_{11}NO_3$   |
| Phenanthrene                   | $C_{14}H_{10}$       |
| Phenazine                      | $C_{12}H_8N_2$       |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|   |                              |
|---|------------------------------|
| phenol  | $C_6H_6O$                    |
| Phenoxyacetic acid                                | $C_8H_8O_3$                  |
| Phenylacetic acid                                 | $C_8H_8O_2$                  |
| DL-Phenylalanine                                  | $C_9H_{11}NO_2$              |
| L-Phenylalanine                                   | $C_9H_{11}NO_2$              |
| Phenylalanyl anhydride                            | $C_{18}H_{18}NO_2$           |
| Phenylalanine N-carboxylic acid anhydride         | $C_{10}H_9NO_3$              |
| DL-Phenylalanine-N-carboxylic acid dimethyl ester | $C_{12}H_{15}NO_4$           |
| 1-Phenyl-5-aminotetrazole                         | $C_7H_7N_5$                  |
| 5-Phenylaminotetrazole                            | $C_7H_7N_5$                  |
| DL-Phenylglyceric acid                            | $C_9H_{10}O_4$               |
| $\alpha$ -Phenyl glycine                          | $C_8H_9NO_2$                 |
| N-Phenyl glycine                                  | $C_8H_9NO_2$                 |
| Phenylglyoxylic acid                              | $C_8H_6O_3$                  |
| 1-Phenyl-5-hydroxytetrazole                       | $C_7H_6N_4O$                 |
| Phenyl methyl sulfide                             | $C_7H_8S$                    |
| 1-Phenyl-5-methyltetrazole                        | $C_9H_8N_4$                  |
| 2-Phenyl-5-methyltetrazole                        | $C_8H_8N_4$                  |
| $\alpha$ -Phenylpyrrole                           | $C_{10}H_9N$                 |
| N-Phenylpyrrole                                   | $C_{10}H_9N$                 |
| 1-Phenyltetrazole                                 | $C_7H_6N_4$                  |
| 5-Phenyltetrazole                                 | $C_7H_6N_4$                  |
| 4-Phenyluracil                                    | $C_{10}H_8N_2O_2$            |
| Pheoporphyrin $\alpha_5$ dimethyl ester           | $C_{36}H_{38}N_4O_5$         |
| Pheopurpurin 18 monomethyl ester                  | $C_{34}H_{36}N_4O_5$         |
| Phthalimide                                       | $C_8H_8N_2O_2$               |
| Phthalic acid                                     | see: $\alpha$ -Phthalic acid |
| m-Phthalic acid                                   | $C_8H_6O_4$                  |
| $\alpha$ -Phthalic acid                           | $C_8H_6O_4$                  |
| p-Phthalic acid                                   | $C_8H_6O_4$                  |
| Phloerythrin monomethyl ester                     | $C_{34}H_{36}N_4O_3$         |
| $\gamma$ -Phylloporphyrin monomethyl ester        | $C_{33}H_{38}N_4O_2$         |
| Phyllopyrrole                                     | $C_9H_{15}N$                 |
| Picolinic acid                                    | $C_6H_5NO_2$                 |
| Piperazine  | $C_4H_{10}N_2$               |
| Piperazine hexahydrate                            | $C_4H_{22}N_2O_6$            |
| Piperidine  | $C_5H_{11}N$                 |
| $\alpha$ -Piperidone                              | $C_5H_9NO$                   |
| $\Delta_4$ -Pregnene-3,20-dione                   | $C_{21}H_{30}O_2$            |
| $\Delta_4$ -Pregnene-3,20-dione-21-ol             | $C_{21}H_{30}O_3$            |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|   |   |
|---|---|
| $\Delta_4$ -Pregnene-3,20-dione-11 $\beta$ ,17 $\alpha$ ,21-triol | C <sub>21</sub> H <sub>30</sub> O <sub>5</sub>                |
| $\Delta_4$ -Pregnene-3,11,20-trione-17 $\beta$ ,21-diol           | C <sub>21</sub> H <sub>28</sub> O <sub>5</sub>                |
| Progesterone  | see: $\Delta_4$ -Pregnene-3,20-dione                          |
| DL-Proline  | C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>                 |
| Propadiene  | C <sub>4</sub> H <sub>6</sub>                                 |
| 1-Propenal  | n-Propionaldehyde   |
| Propane   | C <sub>3</sub> H <sub>8</sub>                                 |
| 1,2-Propanediamine  | C <sub>3</sub> H <sub>10</sub> N <sub>2</sub>                 |
| 1,2-Propanediol   | C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>                  |
| 1,3-Propanediol   | C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>                  |
| 1,3-Propanedithiol  | C <sub>3</sub> H <sub>8</sub> S <sub>2</sub>                  |
| 1-Propanethiol  | C <sub>3</sub> H <sub>8</sub> S                               |
| 1,2,3-Propanetriol  | C <sub>3</sub> H <sub>8</sub> O <sub>3</sub>                  |
| Propanoic acid  | see: Propionic acid   |
| 1-Propanol  | C <sub>3</sub> H <sub>8</sub> O                               |
| 2-Propanol  | C <sub>3</sub> H <sub>8</sub> O                               |
| Propanone   | C <sub>3</sub> H <sub>6</sub> O                               |
| Propene   | C <sub>3</sub> H <sub>6</sub>                                 |
| $\beta$ -Propiolactone  | C <sub>3</sub> H <sub>4</sub> O <sub>2</sub>                  |
| n-Propionaldehyde   | C <sub>3</sub> H <sub>6</sub> O                               |
| Propionamide  | C <sub>3</sub> H <sub>7</sub> NO                              |
| Propionic acid  | C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>                  |
| n-Propyl alcohol  | C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>                  |
| n-Propylamine   | C <sub>3</sub> H <sub>9</sub> N                               |
| n-Propylbenzene   | C <sub>9</sub> H <sub>12</sub>                                |
| n-Propylcyclohexane   | C <sub>9</sub> H <sub>18</sub>                                |
| n-Propylcyclopentane  | C <sub>8</sub> H <sub>16</sub>                                |
| Propylene   | see: Propene  |
| Propylene glycol  | see: 1,2- and 1,3-Propanediol                                 |
| Propyne   | C <sub>3</sub> H <sub>4</sub>                                 |
| Protoporphyrin  | C <sub>34</sub> H <sub>34</sub> N <sub>4</sub> O <sub>4</sub> |
| Protoporphyrin dimethyl ester                                     | C <sub>36</sub> H <sub>38</sub> N <sub>4</sub> O <sub>4</sub> |
| Pseudouric acid   | C <sub>5</sub> H <sub>6</sub> N <sub>4</sub> O <sub>4</sub>   |
| Pyrazine  | C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>                  |
| Pyrazole  | C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>                  |
| Pyrene  | C <sub>16</sub> H <sub>10</sub>                               |
| Pyridazine  | C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>                  |
| Pyridine  | C <sub>5</sub> H <sub>5</sub> N                               |
| Pyrimidine  | C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>                  |
| Pyrocatechol  | C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>                  |
| Pyromucic acid  | see: 2-Furoic acid  |

TABLE I-B COMPOUND NAME- $\text{I}^{\text{C}}$  FORMULA INDEX

|  |  |
|--|--|
| Pyropheophorbide $\alpha$ monomethyl ester | $\text{C}_{34}\text{H}_{36}\text{N}_4\text{O}_3$ |
| Pyrrolaldehyde                             | $\text{C}_5\text{H}_5\text{N}$                   |
| Pyrrolaldoxime                             | $\text{C}_5\text{H}_6\text{N}_2\text{O}$         |
| Pyrrole                                    | $\text{C}_4\text{H}_5\text{N}$                   |
| Pyrrolidine                                | $\text{C}_4\text{H}_9\text{N}$                   |
| $\alpha$ -Pyrrolidone                      | $\text{C}_4\text{H}_7\text{NH}$                  |
| Pyrrorphyrin (XV) monomethyl ester         | $\text{C}_{32}\text{H}_{36}\text{N}_4\text{O}_2$ |
| Pyruvic acid                               | $\text{C}_{3}\text{H}_4\text{O}_3$               |
| Pyurilic acid                              | see: Methyl allantoin                            |
| Quinaldine                                 | $\text{C}_1\text{H}_9\text{N}$                   |
| Ouinidine                                  | $\text{C}_{20}\text{H}_{24}\text{N}_2\text{O}_2$ |
| Quinine                                    | $\text{C}_{20}\text{H}_{24}\text{N}_2\text{O}_2$ |
| Quinoline                                  | $\text{C}_9\text{H}_7\text{N}$                   |
| Raffinose                                  | $\text{C}_{18}\text{H}_{32}\text{O}_16$          |
| Raffinose pentahydrate                     | $\text{C}_{18}\text{H}_{42}\text{O}_{21}$        |
| Resorcinol                                 | $\text{C}_6\text{H}_6\text{O}_2$                 |
| $\beta$ -L-Rhamnose                        | $\text{C}_6\text{H}_{12}\text{O}_5$              |
| $\alpha$ -L-Rhamnose monohydrate           | $\text{C}_6\text{H}_{14}\text{O}_6$              |
| Rhamnose trilacetate                       | $\text{C}_{14}\text{H}_{20}\text{O}_9$           |
| Rhodoporphyrin (XV) dimethyl ester         | $\text{C}_{34}\text{H}_{38}\text{N}_4\text{O}_4$ |
| Rhodoporphyrin (XXI) dimethyl ester        | $\text{C}_{34}\text{H}_{38}\text{N}_4\text{O}_4$ |
| $\beta$ -D-Ribose                          | $\text{C}_5\text{H}_{10}\text{O}_5$              |
| Saccharinic acid lactone                   | $\text{C}_6\text{H}_{10}\text{O}_5$              |
| Salicylaldehyde                            | $\text{C}_7\text{H}_6\text{O}_2$                 |
| Salicylic acid                             | $\text{C}_7\text{H}_6\text{O}_3$                 |
| Sarcosine                                  | $\text{C}_3\text{H}_7\text{NO}_2$                |
| Sarcosine-N-carboxylic acid anhydride      | $\text{C}_4\text{H}_5\text{NO}_3$                |
| L-Serine                                   | $\text{C}_3\text{H}_7\text{NO}_3$                |
| Serine anhydride                           | $\text{C}_6\text{H}_{10}\text{N}_2\text{O}_4$    |
| Serylserine                                | $\text{C}_6\text{H}_{12}\text{N}_2\text{O}_5$    |
| Skatole                                    | $\text{C}_9\text{H}_9\text{N}$                   |
| Silver acetate                             | $\text{C}_2\text{H}_3\text{A}_2\text{O}_2$       |
| Silver carbonate                           | $\text{C}_4\text{E}_2\text{O}_3$                 |
| Silver oxalate                             | $\text{C}_2\text{Ag}_2\text{O}_4$                |
| Sorbitic acid                              | $\text{C}_6\text{H}_8\text{O}_2$                 |
| L-Sorbose                                  | $\text{C}_6\text{H}_{12}\text{O}_6$              |
| Spiropentane                               | $\text{C}_5\text{H}_8$                           |
| Stachyose                                  | $\text{C}_{24}\text{H}_{42}\text{O}_{21}$        |
| Stearic acid                               | $\text{C}_{18}\text{H}_{36}\text{O}_2$           |
| Strychnine                                 | $\text{C}_{21}\text{H}_{22}\text{N}_2\text{O}_2$ |
| Styrene                                    | see: Ethenylbenzene                              |

TABLE I-B COMPOUND NAME-Formula INDEX

|   |  |
|---|--|
| Succinamide                                 | $C_4H_8N_2O_2$                                   |
| Succinic acid                               | $C_4H_6O_4$                                      |
| Succinic anhydride                          | $C_4H_4O_3$                                      |
| Sucrose                                     | $C_{12}H_{22}O_11$                               |
| Sucrose octaacetate                         | $C_{28}H_{38}O_19$                               |
| DL-Tartaric acid                            | $C_4H_6O_6$                                      |
| L-Tartaric acid                             | $C_4H_6O_6$                                      |
| meso-Tartaric acid                          | $C_4H_6O_6$                                      |
| DL-Tartaric acid monohydrate                | $C_4H_5O_6$                                      |
| L-Tartramide                                | $C_4H_8N_2O_4$                                   |
| meso-Tartramide                             | $C_4H_8N_2O_4$                                   |
| Taurine                                     | see: 2-Aminoethane-1-sulfonic acid               |
| Terebic acid                                | $C_7H_{10}O_4$                                   |
| Terephthalic acid                           | see: p-Phthalic acid                             |
| Testosterone                                | see: $\Delta_4$ -Androstone-3-one-17 $\beta$ -ol |
| Tetracene                                   | see: Naphthacene                                 |
| 1,1,1,2-Tetrachloro-2,2-difluoroethane      | $C_2Cl_4F_2$                                     |
| 1,1,2,2-Tetrachloroethane                   | $C_2H_2Cl_4$                                     |
| Tetrachloroethylene                         | $C_2Cl_4$  |
| Tetraconic acid                             | $C_7H_{10}O_4$                                   |
| n-Tetradecane                               | $C_{14}H_{30}$                                   |
| Tetradecanoic acid                          | see: Myristic acid                               |
| 1-Tetradecene                               | $C_{14}H_{28}$                                   |
| 1-Tetradecyne                               | $C_{14}H_{26}$                                   |
| Tetraethoxysilane                           | $C_8H_{20}O_4Si$                                 |
| Tetraethyl germanium                        | $C_8H_{20}Ge$                                    |
| Tetraethyl lead                             | $C_8H_{20}Pb$                                    |
| Tetraethylsilane                            | $C_8H_{20}Si$                                    |
| Tetraethyl tin                              | $C_8H_{20}Sn$                                    |
| 1,1,2,2-Tetrafluorobromoethane              | $C_2HBrF_4$                                      |
| 1,1,2,2-Tetrafluoro-1,2-dichloroethane      | $C_2Cl_2F_4$                                     |
| Tetrafluoroethylene                         | $C_2F_4$   |
| Tetrahydrofuran                             | $C_4H_8O$  |
| Tetrahydrofurfuryl alcohol                  | $C_5H_{10}O_2$                                   |
| Tetrahydropyran                             | $C_6H_{10}O_2$                                   |
| 1,2,5,6-Tetrahydropyridine                  | $C_5H_9N$  |
| Tetraiodoethylene                           | $C_2I_4$   |
| Tetrame thoxysilane                         | $C_4H_{12}O_4Si$                                 |
| Tetramethyl-1,4-diamine-sebacic acid adduct | $C_{14}H_{30}N_2O_4$                             |
| Tetramethyl lead                            | $C_4H_{12}Pb$                                    |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|  |                    |
|--|--------------------|
| Tetramethylsilane                                  | $C_4H_{12}Si$      |
| Tetramethylthiuram disulfide                       | $C_6H_{12}N_2S_4$  |
| Tetra-methylthiuram monosulfide                    | $C_6H_{12}N_2S_3$  |
| Tetramethyl tin                                    | $C_4H_{12}Sn$      |
| $\alpha$ -Tetamylose                               | $C_3H_{60}O_6$     |
| Tetravinyl lead                                    | $C_8H_{12}Pb$      |
| Tetravinyl tin                                     | $C_9H_{12}Sn$      |
| Tetrazole  | $CR_2N_4$          |
| 1-(5-Tetrazoyl)-4-guananyl tetrazenone monohydrate | $C_2H_8N_{10}O$    |
| 5-Tetrazaylurethane                                | $C_4H_{7.5}O_2$    |
| Thallium acetate                                   | $C_2H_3O_2Tl$      |
| Thallium carbonate                                 | $C_6H_3O_2Tl$      |
| Thallium ethoxide                                  | $C_2H_5O_2Tl$      |
| Thallium methoxide                                 | $CH_3O_2Tl$        |
| Thebuine   | $C_19H_{21}N^4_3$  |
| Theobromine  | $C_7H_8N_4O_2$     |
| Thiacyclobutane                                    | $C_3H_6S$          |
| Thiacyclohexane                                    | $C_5H_{10}S$       |
| Thiacyclopentane                                   | $C_4H_8S$          |
| Thiacyclopropane                                   | $C_2H_4S$          |
| 2-Thiapropane                                      | $C_2H_6S$          |
| Thiohydantoinic acid                               | $C_3H_6N_2O_2S$    |
| Thiohydantoin                                      | $C_3H_4N_2O_2S$    |
| Thiolactic acid                                    | $C_2H_4O_2S$       |
| $\beta$ -Thiolactic acid                           | $C_3H_6O_2S$       |
| Thiophene  | $C_4H_4S$          |
| Thiourea   | $CH_4N_2S$         |
| DL-Threonine                                       | $C_4H_9N_2O_3$     |
| L-Threonine  | $C_4H_9N_2O_3$     |
| Thymine  | $C_5H_6N_2O_2$     |
| Tiglic acid  | $C_5H_8O_2$        |
| Toluene  | $C_7H_8$           |
| $\alpha$ -Toluyl alanine                           | $C_{11}H_{13}NO_3$ |
| p-Toluyl alanine                                   | $C_{11}H_{13}NO_3$ |
| m-Toluyl glycine                                   | $C_{10}H_{11}NO_3$ |
| $\alpha$ -Toluyl glycine                           | $C_{10}H_{11}NO_3$ |
| p-Toluyl glycine                                   | $C_{10}H_{11}NO_3$ |
| Trehalose  | $C_{12}H_{22}O_11$ |
| Trehalose dihydrate                                | $C_{12}H_{26}O_13$ |
| Tri-n-butyl phosphate                              | $C_{12}H_{27}O_4P$ |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|                                       |   |
|---------------------------------------|---|
| Tri- <i>n</i> -butyl phosphine oxide  | C <sub>12</sub> H <sub>27</sub> OP  |
| Trichloroacetic acid                  | C <sub>2</sub> HCl <sub>3</sub> O <sub>2</sub>                            |
| Trichloroacetyl chloride              | C <sub>2</sub> Cl <sub>4</sub> O  |
| 1,1,2-Trichloroethane                 | C <sub>2</sub> HCl <sub>3</sub>   |
| Trichloroethylene                     | C <sub>2</sub> HCl <sub>3</sub>   |
| 1,1,2-Trichloro-2,2,1-trifluoroethane | C <sub>2</sub> Cl <sub>3</sub> F <sub>3</sub>                             |
| Tricyclobutyryl                       | C <sub>15</sub> H <sub>20</sub> O <sup>d</sup> <sub>6</sub>               |
| Tricyclovalerin                       | C <sub>18</sub> H <sub>26</sub> O <sub>6</sub>                            |
| <i>n</i> -Tridecane                   | C <sub>13</sub> H <sub>28</sub>   |
| 1-Tridecene                           | C <sub>13</sub> H <sub>26</sub>   |
| 1-Tridecyne                           | C <sub>13</sub> H <sub>24</sub>   |
| Triethoxyborane                       | C <sub>6</sub> H <sub>15</sub> B(O) <sub>3</sub>                          |
| Triethoxysilane                       | C <sub>6</sub> H <sub>16</sub> O <sub>3</sub> Si                          |
| Triethylamine                         | C <sub>6</sub> H <sub>15</sub> N  |
| Triethylamine nitrate                 | C <sub>6</sub> H <sub>16</sub> N <sup>d</sup> <sub>2</sub> 3              |
| Triethylboron                         | C <sub>6</sub> H <sub>15</sub> B  |
| Triethylenediamine                    | C <sub>6</sub> H <sub>12</sub> N <sub>2</sub>                             |
| Triethyl phosphate                    | C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P                           |
| Triethylsilane                        | C <sub>6</sub> H <sub>16</sub> Si   |
| 1,1,1-Trifluoroethane                 | C <sub>2</sub> H <sub>3</sub> F <sub>3</sub>                              |
| 1,1,2-Trifluoromethane                | C <sub>2</sub> H <sub>3</sub> F <sub>3</sub>                              |
| 2,2,2-Trifluoroethanol                | C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O                            |
| Triacylglycine                        | C <sub>8</sub> H <sub>14</sub> N <sup>d</sup> <sub>5</sub>                |
| DL-Trihydroxyglutaric acid            | C <sub>5</sub> H <sub>8</sub> O <sub>7</sub>                              |
| Trisobutyl phosphate                  | C <sub>12</sub> H <sub>27</sub> O <sub>4</sub> P                          |
| Trimethoxysilane                      | C <sub>3</sub> H <sub>9</sub> BO <sub>3</sub>                             |
| Trimethylaluminum                     | C <sub>3</sub> H <sub>10</sub> O <sub>3</sub> Si                          |
| Trimethylamine                        | C <sub>3</sub> H <sub>9</sub> N   |
| Trimethylamine nitrate                | C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> O <sup>d</sup> <sub>3</sub> |
| 1,2,3-Trimethylbenzene                | C <sub>9</sub> H <sub>12</sub>  |
| 1,2,4-Trimethylbenzene                | C <sub>9</sub> H <sub>12</sub>  |
| 1,3,5-Trimethylbenzene                | C <sub>9</sub> H <sub>12</sub>  |
| Trimethyl boron                       | C <sub>3</sub> H <sub>9</sub> B   |
| 2,2,3-Trimethylbutane                 | C <sub>7</sub> H <sub>16</sub>  |
| Trimethylene oxide                    | see: Oxacyclobutane   |
| 2,4,5-Trimethyl-3-ethylpyrrole        | see: Phyllotopyrrole  |
| Trimethyl gallium                     | C <sub>3</sub> H <sub>9</sub> Ga  |
| 2,2,3-Trimethylpentane                | C <sub>8</sub> H <sub>18</sub>  |
| 2,2,4-Trimethylpentane                | C <sub>8</sub> H <sub>18</sub>  |
| 2,3,3-Trimethylpentane                | C <sub>8</sub> H <sub>18</sub>  |

TABLE I-B COMPOUND NAME-FORMULA INDEX

|                               |                             |
|-------------------------------|-----------------------------|
| 2,3,4-Trimethylpentane        | $C_8H_{18}$                 |
| Trimethylphosphine            | $C_3H_9P$                   |
| Trimethyl tin                 | $C_3H_{10}Sn$               |
| Triphenylene                  | $C_{18}H_{12}$              |
| Triphenyl phosphate           | $C_{18}H_{15}O_4P$          |
| Tri-n-propylamine             | $C_9H_{21}N$                |
| Tri-n-propyl phosphate        | $C_9H_{21}O_4P$             |
| L-Tryptophane                 | $C_{11}H_{12}N_2O_2$        |
| L-Tyrosine                    | $C_9H_{11}NO_3$             |
| n-Undecane                    | $C_{11}H_{24}$              |
| 1-Undecene                    | $C_{11}H_{22}$              |
| Undecyl-10-ene-1-oic acid     | $C_{11}H_{20}O_2$           |
| Uramil                        | $C_4H_5N_3O_3$              |
| 1-Undecyne                    | $C_{11}H_{20}$              |
| Urea                          | $CH_4N_2H$                  |
| Urea nitrate                  | $CH_5N_3O_4$                |
| Ureidoacetic acid             | see: Hydantoinic acid       |
| Urethane                      | see: Ethyl carbamate        |
| Uric acid                     | $C_5H_4N_4O_3$              |
| n-Valeraldehyde               | $C_5H_{10}O$                |
| Valeric acid                  | $C_5H_{10}O_2$              |
| D,L-Valine                    | $C_5H_{11}NO_2$             |
| L-Valline                     | $C_5H_{11}NO_2$             |
| Valylalanyl anhydride         | $C_8H_{14}N_2O_2$           |
| Valylleucyl anhydride         | $C_{11}H_{20}N_2O_2$        |
| Valylphenylalanine            | $C_{14}H_{20}N_2O_3$        |
| Valylphenylalanyl anhydride   | $C_{14}H_{18}N_2O_2$        |
| Verdoporphyrin dimethyl ester | $C_{34}H_{36}N_4O_4$        |
| Veronal                       | see: Diethylbarbituric acid |
| Vinyl bromide                 | $C_2H_3Br$                  |
| Vinyl chloride                | $C_2H_3Cl$                  |
| 2-Vinylpyridine               | $C_7H_7N$                   |
| Vinylsilane                   | $C_2H_6Si$                  |
| Xanthine                      | $C_5H_4N_4O_2$              |
| m-Xylene                      | $C_8H_{10}$                 |
| o-Xylene                      | $C_8H_{10}$                 |
| p-Xylene                      | $C_8H_{10}$                 |
| Xylitol                       | $C_5H_{12}O_5$              |
| $\alpha$ -D-Xylose            | $C_5H_{10}O_5$              |
| Zinc acetate                  | $C_4H_6O_4Zn$               |
| Zinc carbonate                | $C_3Zn$                     |
| Zinc formate                  | $C_2H_2O_4Zn$               |
| Zinc glycollate               | $C_4H_6O_4Zn$               |

25.4 Table II. Enthalpies of Formation of Organic Polymers at 298.15 K

| formula<br>(repeating unit)                                     | formula<br>(g mol <sup>-1</sup> ) | name (state)                        | Enthalpy of formation<br>kcal <sup>-1</sup><br>mol <sup>-1</sup> | Ref.            |
|---|-----------------------------------|-------------------------------------|--|-----------------|
| [-CH <sub>1.891-</sub> ] <sub>n</sub>                           | 13.9172                           | Mineral oil (liq)                   | -5.5   | [1]             |
| [-CH <sub>2-</sub> ] <sub>n</sub>                               | 14.0271                           | Polymethylene (s)                   | -6.99  | -29.25 [2]      |
| [-CH <sub>2O-</sub> ] <sub>n</sub>                              | 30.0265                           | Polyoxymethylene (s)                | -40.93   | -171.25 [2]     |
| [-C <sub>2H<sub>2</sub>Cl<sub>2</sub>-</sub> ] <sub>n</sub>     | 96.9442                           | Poly-1,1-dichloroethylene (s)       | -24.0  | -100.4 [3]      |
| [-C <sub>2H<sub>2</sub>F<sub>2</sub>-</sub> ] <sub>n</sub>      | 64.0350                           | Polyvinylidene fluoride             | -114.58  | -479.40 [4]     |
| [-C <sub>2H<sub>3</sub>Cl-</sub> ] <sub>n</sub>                 | 62.4992                           | Polyvinylchloride (s)               | -22.5  | -94.1 [3]       |
| [-CF <sub>2</sub> CF <sub>2</sub> -] <sub>n</sub>               | 100.0159                          | Teflon, polytetrafluoroethylene (s) | -197.82  | -827.68 [5]     |
| [-CH <sub>2</sub> CH <sub>2</sub> -] <sub>n</sub>               | 28.0542                           | Polyethylene (s)                    | -13.50   | -56.48 [2, 6]   |
| [-C <sub>3</sub> O <sub>2-</sub> ] <sub>n</sub>                 | 68.0322                           | Poly(carbon suboxide) (s)           | -56.6  | -236.8 [7]      |
| [-C <sub>3</sub> H <sub>5</sub> NO-] <sub>n</sub>               | 71.0794                           | Sarcosine polypeptide (s)           | -53.2  | -222.6 [8]      |
| [-C <sub>3</sub> H <sub>6</sub> -] <sub>n</sub>                 | 42.0813                           | Polypropylene (s)                   | -20.02   | -83.76 [6]      |
| [-C <sub>3</sub> H <sub>6</sub> O-] <sub>n</sub>                | 58.0807                           | Polyvinyl methyl ether (s)          | -48.92   | -204.68 [22]    |
| [-C <sub>4</sub> H <sub>6</sub> O-] <sub>n</sub>                | 54.0924                           | Polybutadiene (s)                   | +3.3   | +13.8 [9]       |
| [-C <sub>4</sub> H <sub>8-</sub> ] <sub>n</sub>                 | 56.1084                           | Poly(butene-1) (s)                  | -24.68   | -103.26 [6]     |
| [-C <sub>4</sub> H <sub>8-</sub> ] <sub>n</sub>                 | 56.1084                           | Polyisobutylene (s)                 | -21.18   | -88.62 [10, 11] |
| [-C <sub>4</sub> H <sub>8</sub> O-] <sub>n</sub>                | 72.1078                           | Polyvinyl ethyl ether (s)           | -56.92   | -238.15 [22]    |
| [-C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S-] <sub>n</sub> | 120.1712                          | But-1-ene polysulfone (s)           | -100.08  | -418.73 [12]    |
| [-C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S-] <sub>n</sub> | 120.1712                          | Isobutene polysulfone (s)           | -100.46  | -420.32 [12]    |
| [-C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S-] <sub>n</sub> | 120.1712                          | cis-But-2-ene polysulfone (s)       | -101.50  | -424.68 [12]    |
| [-C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S-] <sub>n</sub> | 120.1712                          | trans-But-2-ene polysulfone (s)     | -101.36  | -424.09 [12]    |
| [-C <sub>5</sub> H <sub>8-</sub> ] <sub>n</sub>                 | 68.1195                           | Polyisoprene, purified rubber (s)   | -6.24  | -26.11 [23, 24] |
| [-C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> -] <sub>n</sub> | 162.1436                          | Cellulose (s)                       | -229.7   | -961.1 [13]     |
| [-C <sub>6</sub> H <sub>10</sub> O <sub>5-</sub> ] <sub>n</sub> | 162.1436                          | Glycogen (s)                        | -225.  | -941. [15, 16]  |

## Enthalpies of Formation of Organic Polymers at 298.15 K (Cont'd)

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| formula<br>(repeating unit) | formula<br>weight<br>(g mol <sup>-1</sup> ) | name (state)  | Enthalpy of formation<br>kcal<br>mol <sup>-1</sup> | Enthalpy of formation<br>kJ<br>mol <sup>-1</sup> | Ref.    |
|-----------------------------|---|---|--|--|---------|
| $[-C_6H_7N_3O_{11}-]_n$     | 297.1362                                    | Trinitrocellulose (s)   | -155.7   | -651.4   | [13]    |
| $[-C_6H_8N_2O_9-]_n$        | 252.1387                                    | Dinitrocellulose (s)  | -179.9   | -752.7   | [13]    |
| $[-C_6H_9NO_7-]_n$          | 207.1411                                    | Mononitrocellulose (s)  | -205.  | -858.  | [14]    |
| $[-C_8H_8-]_n$              | 104.1530                                    | Polystyrene (s) (isotactic, 40% crystalline)  | +7.09  | +29.66   | [6]     |
| $[-C_8H_8-]_n$              | 104.1530                                    | Polystyrene (s) (isotactic, amorphous)  | +7.99  | +33.43   | [6]     |
| $[-C_8H_8-]_n$              | 104.1530                                    | Polystyrene (s) (atactic, amorphous)  | +8.25  | +34.52   | [6,17]  |
| $[-C_8H_8O-]_n$             | 120.1524                                    | Poly(2,6-dimethylphenylene ether) (s)   | -31.88   | -133.39  | [6]     |
| $[-C_8H_{12}O_6-]_n$        | 204.1812                                    | Cellulose monoacetate (s)   | -278.  | -1163.   | [19]    |
| $[-C_9H_{10}-]_n$           | 118.1800                                    | Poly( $\alpha$ -methylstyrene) (s)  | +7.88  | +32.97   | [6]     |
| $[-C_9H_9NO-]_n$            | 147.1782                                    | Phenylalanine polypeptide (s)<br>(benzene soluble)                                    | -49.6  | -207.5   | [8]     |
| $[-C_9H_9NO-]_n$            | 147.1782                                    | Phenylalanine polypeptide (s)<br>(benzene insoluble)                                  | -53.1  | -222.2   | [8]     |
| $[-C_{10}H_8O_4-]_n$        | 192.1729                                    | Mylar, Melinex, Terylene film, polyester of ethylene glycol and terephthalic acid (s) | -161.1   | -674.0   | [20,21] |
| $[-C_{10}H_{14}O_7-]_n$     | 246.2189                                    | Cellulose diacetate (s)   | -326.  | -1364.   | [18]    |
| $[-C_{12}H_8-]_n$           | 152.1976                                    | Polyacenaphthylene (s)  | +27.13   | +113.51  | [6]     |
| $[-C_{12}H_{16}O_8-]_n$     | 288.2565                                    | Cellulose triacetate (s)  | -377.  | -1577.   | [18]    |
| $[-C_{16}H_{14}O_3-]_n$     | 254.2882                                    | Poly(4,4'-dioxydiphenyl-2,2-propane carbonate) (s)                                    | -103.26  | -432.04  | [6]     |

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25.5 Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K

| formula<br>(state)                                | formula<br>weight<br>(g mol <sup>-1</sup> ) | name                                | Enthalpy of formation, ΔH <sub>f</sub> <sup>°</sup><br>kcal mol <sup>-1</sup> | Enthalpy of formation, ΔH <sub>f</sub> <sup>°</sup><br>kJ mol <sup>-1</sup> | Ref. |
|---|---|-------------------------------------|---|---|------|
| Ag <sub>2</sub> O (c)                             | 231.7394                                    | Silver oxide                        | -7.42   | -31.04  | [4]  |
| Ag <sub>2</sub> O <sub>2</sub> (c)                | 247.7388                                    | Silver peroxide                     | -5.8  | -24.3   | [4]  |
| Ag <sub>2</sub> O <sub>3</sub> (c)                | 263.7382                                    | Silver sesquioxide                  | 8.1   | 33.9  | [4]  |
| Al <sub>0</sub> (g)                               | 42.9809                                     | Aluminum monoxide                   | 21.8  | 91.2  | [3]  |
| (AlO) <sub>2</sub> (g)                            | 85.9618                                     | Aluminum monoxide, dimer            | -94.  | -393.   | [3]  |
| Al <sub>2</sub> O (g)                             | 69.9624                                     | Dialuminum monoxide                 | -31.  | -130.   | [3]  |
| Al <sub>2</sub> O <sub>3</sub> (c,α)              | 101.9612                                    | Aluminum oxide, α-Alumina, Corundum | -400.5  | -1675.7   | [3]  |
| Al <sub>2</sub> O <sub>3</sub> (c,γ)              | 101.9612                                    | Aluminum oxide, γ-Alumina           | -395.   | -1653.  | [3]  |
| Al <sub>2</sub> O <sub>3</sub> (c,δ)              | 101.9612                                    | Aluminum oxide, δ-Alumina           | -398.   | -1665.  | [3]  |
| Al <sub>2</sub> O <sub>3</sub> (c,κ)              | 101.9612                                    | Aluminum oxide, κ-Alumina           | -397.   | -1661.  | [3]  |
| Al <sub>2</sub> O <sub>3</sub> (c,ρ)              | 101.9612                                    | Aluminum oxide, ρ-Alumina           | -391.   | -1636.  | [3]  |
| Al <sub>2</sub> O <sub>3</sub> (amorp)            | 101.9612                                    | Aluminum oxide                      | -390.   | -1632.  | [3]  |
| As <sub>0</sub> (g)                               | 90.9210                                     | Arsenic monoxide                    | 16.72   | 69.96   | [3]  |
| As <sub>2</sub> O <sub>4</sub> (c)                | 213.8408                                    | Diarsenic tetroxide                 | -189.72   | -793.79   | [3]  |
| As <sub>2</sub> O <sub>5</sub> (c)                | 229.8402                                    | Arsenic pentoxide                   | -221.05   | -924.87   | [3]  |
| As <sub>4</sub> O <sub>6</sub> (g)                | 395.6828                                    | Arsenic trioxide                    | -289.0  | -1209.2   | [3]  |
| As <sub>4</sub> O <sub>6</sub> (c,<br>octahedral) | 395.6828                                    | Arsenic trioxide, Arsenolite        | -314.04   | -1313.94  | [3]  |
| As <sub>4</sub> O <sub>6</sub> (c,<br>monoclinic) | 395.6828                                    | Arsenic trioxide, Claudetite        | -313.0  | -1309.6   | [3]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                    | formula<br>weight<br>(g mol <sup>-1</sup> ) | name                      | Enthalpy of formation, ΔH <sub>f</sub><br>kcal mol <sup>-1</sup> | Enthalpy of formation, ΔH <sub>f</sub><br>kJ mol <sup>-1</sup> | Ref. |
|---------------------------------------|---|---------------------------|--|--|------|
| B0 (g)                                | 26.8104                                     | Boron monoxide            | 6.   | 25.  | [3]  |
| BO <sub>2</sub> (g)                   | 42.8098                                     | Boron dioxide             | -71.8  | -300.4   | [3]  |
| B <sub>2</sub> O <sub>2</sub> (g)     | 53.6208                                     | Diboron dioxide           | -108.7   | -454.8   | [3]  |
| B <sub>2</sub> O <sub>3</sub> (g)     | 69.6202                                     | Boric oxide               | -201.67  | -843.79  | [3]  |
| B <sub>2</sub> O <sub>3</sub> (c)     | 69.6202                                     | Boric oxide               | -304.20  | -1272.77   | [3]  |
| B <sub>2</sub> O <sub>3</sub> (amorp) | 69.6202                                     | Boric oxide               | -299.84  | -1254.53   | [3]  |
| BaO (g)                               | 153.339                                     | Barium oxide              | -28.   | -117.  | [6]  |
| BaO (c)                               | 153.339                                     | Barium oxide              | -132.3   | -553.5   | [6]  |
| BaO <sub>2</sub> (c)                  | 169.339                                     | Barium peroxide           | -151.6   | -634.3   | [6]  |
| Ba <sub>2</sub> O (g)                 | 290.679                                     | Dibarium monoxide         | -72.   | -301.  | [6]  |
| Ba <sub>2</sub> O (c)                 | 290.679                                     | Dibarium monoxide         | -147.1   | -615.5   | [6]  |
| Ba <sub>2</sub> O <sub>2</sub> (g)    | 306.679                                     | Dibarium dioxide          | -135.  | -565.  | [6]  |
| BeO (g)                               | 25.0116                                     | Beryllium oxide           | 28.  | 117.   | [6]  |
| BeO (c)                               | 25.0116                                     | Beryllium oxide           | -145.7   | -609.6   | [6]  |
| Be <sub>2</sub> O (g)                 | 34.0238                                     | Diberyllium monoxide      | -20.   | -84.   | [6]  |
| (BeO) <sub>2</sub> (g)                | 50.0232                                     | Beryllium oxide, dimer    | -103.  | -431.  | [6]  |
| (BeO) <sub>3</sub> (g)                | 75.0348                                     | Beryllium oxide, trimer   | -260.  | -1088.   | [6]  |
| (BeO) <sub>4</sub> (g)                | 100.0464                                    | Beryllium oxide, tetramer | -391.  | -1636.   | [6]  |
| (BeO) <sub>5</sub> (g)                | 125.0580                                    | Beryllium oxide, pentamer | -518.  | -2167.   | [6]  |
| (BeO) <sub>6</sub> (g)                | 150.0696                                    | Beryllium oxide, hexamer  | -651.  | -2724.   | [6]  |
| Bi <sub>2</sub> O <sub>3</sub> (c)    | 465.9582                                    | Bismuth trioxide, Bismite | -137.16  | -573.88  | [3]  |
| BrO (g)                               | 95.9084                                     | Bromine monoxide          | 30.06  | 125.77   | [3]  |
| BrO <sub>2</sub> (c)                  | 111.9078                                    | Bromine dioxide           | 11.6   | 48.5   | [3]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                                 | formula<br>weight<br>(g mol <sup>-1</sup> ) | name   | Enthalpy of formation, ΔHf°<br>kcal mol <sup>-1</sup> | Enthalpy of formation, ΔHf°<br>kJ mol <sup>-1</sup> | Ref. |
|--|---|--|---|---|------|
| CO (g)   | 28.0106                                     | Carbon monoxide  | -26.416   | -110.524  | [3]  |
| CO <sub>2</sub> (g)                                | 44.0100                                     | Carbon dioxide   | -94.051   | -393.509  | [3]  |
| C <sub>3</sub> O <sub>2</sub> (g)                  | 68.0323                                     | Carbon suboxide  | -22.38  | -93.64  | [7]  |
| C <sub>3</sub> O <sub>2</sub> (liq)                | 68.0323                                     | Carbon suboxide  | -28.03  | -117.28   | [7]  |
| CaO (c)  | 56.079                                      | Calcium oxide  | -151.79   | -635.09   | [6]  |
| CaO <sub>2</sub> (c)                               | 72.079                                      | Calcium peroxide                                       | -156.0  | -652.7  | [6]  |
| CdO (c)  | 128.399                                     | Cadmium oxide, Montepponite                            | -61.7   | -258.2  | [3]  |
| CeO <sub>2</sub> (c)                               | 172.119                                     | Cerium dioxide, Cerium (IV) oxide,<br>Cerianite, Ceria | -260.2  | -1088.7   | [12] |
| Ce <sub>2</sub> O <sub>3</sub> (c, hexago-<br>nal) | 328.238                                     | Cerium trioxide, Cerium (III) oxide                    | -428.4  | -1792.4   | [12] |
| ClO (g)  | 51.4524                                     | Chlorine monoxide                                      | 24.34   | 101.84  | [3]  |
| ClO <sub>2</sub> (g)                               | 67.4518                                     | Chlorine dioxide                                       | 24.5  | 102.5   | [3]  |
| ClO <sub>3</sub> (g)                               | 83.4512                                     | Chlorine trioxide                                      | 37.   | 155.  | [3]  |
| Cl <sub>2</sub> O (g)                              | 86.9054                                     | Dichlorine monoxide                                    | 19.2  | 80.3  | [3]  |
| Cl <sub>2</sub> O <sub>7</sub> (g)                 | 182.9018                                    | Chlorine heptoxide                                     | 65.0  | 272.0   | [3]  |
| Cl <sub>2</sub> O <sub>7</sub> (liq)               | 182.9018                                    | Chlorine heptoxide                                     | 56.9  | 238.1   | [3]  |
| CoO (c)  | 74.9326                                     | Cobaltous oxide, Cobalt (II) oxide                     | -56.87  | -237.94   | [4]  |
| Co <sub>3</sub> O <sub>4</sub> (c)                 | 240.7972                                    | Cobalt (II, III) oxide                                 | -213.   | -891.   | [4]  |
| CrO <sub>2</sub> (c)                               | 83.9948                                     | Chromium dioxide                                       | -143.   | -598.   | [4]  |
| CrO <sub>3</sub> (g)                               | 99.9942                                     | Chromium trioxide, Chromic anhydride<br>"Chromic acid" | -92.2   | -385.8  | [4]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                                  | formula<br>weight-<br>(g mol <sup>-1</sup> ) | name   | Enthalpy of formation, ΔH <sub>f</sub> <sup>°</sup><br>kJ mol <sup>-1</sup> | Ref.         |
|---|--|--|---|--------------|
| CrO <sub>3</sub> (c)                                | 99.9942                                      | Chromium trioxide, chromic anhydride<br>"chromic acid" | -140.9  | -589.5 [4]   |
| Cr <sub>2</sub> O <sub>3</sub> (c)                  | 151.9902                                     | Chromium sesquioxide, Eskolaite                        | -272.4  | -1139.7 [4]  |
| Cr <sub>3</sub> O <sub>4</sub> (c)                  | 219.9856                                     | Chromium (II, III) oxide                               | -366.   | -1531. [4]   |
| Cs <sub>2</sub> O (c)                               | 281.8094                                     | Dicesium oxide   | -75.9   | -317.6 [2]   |
| Cs <sub>2</sub> O <sub>2</sub> (c)                  | 297.8088                                     | Dicesium dioxide                                       | -96.2   | -402.5 [2]   |
| Cs <sub>2</sub> O <sub>3</sub> (c)                  | 313.8082                                     | Dicesium trioxide                                      | -111.2  | -465.3 [2]   |
| Cs <sub>2</sub> O <sub>4</sub> (c)                  | 329.8076                                     | Dicesium tetroxide                                     | -124.2  | -519.6 [2]   |
| CuO (c)   | 79.539                                       | Cupric oxide, Copper (II) oxide                        | -37.6   | -157.3 [4]   |
| Cu <sub>2</sub> O (liq)                             | 143.0794                                     | Tenorite<br>Cuprous oxide                              | -32.0   | -133.9 [7]   |
| Cu <sub>2</sub> O (c)                               | 143.079                                      | Cuprous oxide, Copper (I) oxide<br>Cuprite             | -40.3   | -168.6 [4]   |
| Dy <sub>2</sub> O <sub>3</sub> (c, cubic)           | 372.998                                      | Dysprosium trioxide, Dysprosium<br>(III) oxide         | -446.8  | -1869.4 [12] |
| Er <sub>2</sub> O <sub>3</sub> (c, cubic)           | 382.518                                      | Erbium trioxide, Erbium (III) oxide                    | -453.6  | -1897.9 [12] |
| Eu <sub>2</sub> O <sub>3</sub> (c, cubic)           | 351.918                                      | Europium trioxide, Europium (III)<br>oxide             | -389.6  | -1630.1 [12] |
| Eu <sub>2</sub> O <sub>3</sub> (c, mono-<br>clinic) | 351.918                                      | Europium trioxide, Europium (III)<br>oxide             | -393.9  | -1648.1 [12] |
| F <sub>0</sub> (g)                                  | 34.9978                                      | Fluorine monoxide                                      | 41.   | 171. [3]     |
| F <sub>2</sub> O (g)                                | 53.9962                                      | Oxygen difluoride, Difluorine oxide                    | -5.2  | -21.8 [3]    |
| F <sub>2</sub> O <sub>2</sub> (g)                   | 69.9956                                      | Dioxygen difluoride, Fluorine dioxide                  | 4.3   | 18.0 [3]     |
| F <sub>2</sub> O <sub>3</sub> (g)                   | 85.9950                                      | Difluorine trioxide                                    | 3.8   | 15.9 [3]     |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                                  | formula<br>weight<br>(g mol <sup>-1</sup> ) | name   | Enthalpy of formation, ΔH <sub>f</sub> <sup>°</sup><br>kcal mol <sup>-1</sup> | Ref. |
|---|---|--|---|------|
| Fe <sub>0.9470</sub> (c)                            | 68.8865                                     | Ferrous oxide, Wustite                         | -63.64  | [4]  |
| FeO (c)   | 71.8464                                     | Ferrous oxide, Iron (II) oxide,<br>(Fictive)   | -65.0   | [4]  |
| Fe <sub>2</sub> O <sub>3</sub> (c)                  | 159.6922                                    | Ferric oxide, Iron (III) oxide,<br>Hematite    | -197.0  | [4]  |
| Fe <sub>3</sub> O <sub>4</sub> (c)                  | 231.5386                                    | Iron (II, III) oxide, Magnetite                | -267.3  | [4]  |
| GaO (g)   | 85.7119                                     | Gallium monoxide                               | 66.8  | [3]  |
| Ga <sub>2</sub> O (g)                               | 155.439                                     | Digallium monoxide                             | -21.  | [3]  |
| Ga <sub>2</sub> O (c)                               | 155.439                                     | Digallium monoxide                             | -85.  | [3]  |
| Ga <sub>2</sub> O <sub>3</sub> (c)                  | 187.438                                     | Gallium sesquioxide                            | -260.3  | [3]  |
| Gd <sub>2</sub> O <sub>3</sub> (c, mono-<br>clinic) | 362.498                                     | Gadolinium trioxide, Gadolinium<br>(III) oxide | -434.9  | [12] |
| GeO (g)   | 88.589                                      | Germanium monoxide                             | -11.04  | [3]  |
| GeO (c, brown)                                      | 88.589                                      | Germanium monoxide                             | -50.7   | [3]  |
| GeO (c, hexago-<br>nal)                             | 104.589                                     | Germanium dioxide                              | -131.7  | [3]  |
| GeO <sub>2</sub> (amorp)                            | 104.589                                     | Germanium dioxide                              | -128.4  | [3]  |
| Ge <sub>2</sub> O <sub>2</sub> (g)                  | 177.179                                     | Digermanium dioxide                            | -112.   | [3]  |
| Ge <sub>3</sub> O <sub>3</sub> (g)                  | 265.768                                     | Trigermanium trioxide                          | -212.   | [3]  |
| HO (g)  | 17.0074                                     | Hydroxyl                                       | 9.31  | [3]  |
| HO <sub>2</sub> (g)                                 | 33.00668                                    | Hydroperoxy1                                   | 5.  | [3]  |
| H <sub>2</sub> O (g)                                | 18.0153                                     | Water  | -57.796   | [3]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                        | formula<br>weight<br>(g mol <sup>-1</sup> ) | name  | Enthalpy of formation, ΔHf <sup>o</sup><br>kcal mol <sup>-1</sup> | Enthalpy of formation, ΔHf <sup>o</sup><br>kJ mol <sup>-1</sup> | Ref. |
|---|---|---|---|---|------|
| H <sub>2</sub> O (liq)                    | 18.0153                                     | Water   | -68.315   | -285.830  | [3]  |
| H <sub>2</sub> O (c)                      | 18.0153                                     | Water (ice, metastable)                         | -66.879   | -279.822  | [1]  |
| H <sub>2</sub> O <sub>2</sub> (g)         | 37.0147                                     | Hydrogen peroxide                               | -32.58  | -136.31   | [3]  |
| H <sub>2</sub> O <sub>2</sub> (liq)       | 34.0147                                     | Hydrogen peroxide                               | -44.88  | -187.78   | [3]  |
| HfO (g)                                   | 194.489                                     | Hafnium monoxide                                | 12.   | 50.   | [5]  |
| HfO <sub>2</sub> (c)                      | 210.489                                     | Hafnium dioxide, Hafnia                         | -273.6  | -1144.7   | [5]  |
| HgO (c, hexagonal)                        | 216.589                                     | Mercuric oxide, Mercury (II) oxide              | -21.4   | -89.5   | [4]  |
| HgO (c, red, orthorhombic)                | 216.589                                     | Mercuric oxide, Mercury (II) oxide, Montroydite | -21.71  | -90.83  | [4]  |
| HgO (c, yellow, orthorhombic)             | 216.589                                     | Mercuric oxide, Mercury (II) oxide, Montroydite | -21.62  | -90.46  | [4]  |
| Ho <sub>2</sub> O <sub>3</sub> (c, cubic) | 377.8582                                    | Holmium trioxide, Holmium (III) oxide           | -449.5  | -1880.7   | [12] |
| I <sub>2</sub> O (g)                      | 142.9038                                    | Iodine monoxide                                 | 41.84   | 175.06  | [3]  |
| I <sub>2</sub> O <sub>5</sub> (c)         | 333.8058                                    | Iodine pentoxide                                | -37.78  | -158.07   | [3]  |
| InO (g)                                   | 130.819                                     | Indium monoxide                                 | 92.5  | 387.0   | [3]  |
| In <sub>2</sub> O <sub>3</sub> (c)        | 277.638                                     | Indium sesquioxide                              | -221.27   | -925.79   | [3]  |
| IrO <sub>2</sub> (c)                      | 224.20                                      | Iridium dioxide                                 | -65.5   | -274.0  | [4]  |
| IrO <sub>3</sub> (g)                      | 240.20                                      | Iridium trioxide                                | 1.9   | 7.9   | [4]  |
| KO <sub>2</sub> (c)                       | 71.1008                                     | Potassium superoxide                            | -68.0   | -284.5  | [8]  |
| K <sub>2</sub> O (c)                      | 94.2034                                     | Potassium oxide                                 | -86.8   | -363.2  | [7]  |
| K <sub>2</sub> O <sub>2</sub> (c)         | 110.2028                                    | Potassium peroxide                              | -118.5  | -495.8  | [7]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                                 | formula<br>weight-<br>(g mol <sup>-1</sup> ) | name  | Enthalpy of formation, ΔH <sub>f</sub> <sup>o</sup><br>kcal mol <sup>-1</sup> | Enthalpy of formation, ΔH <sub>f</sub> <sup>o</sup><br>kJ mol <sup>-1</sup> | Ref. |
|--|--|---|---|---|------|
| La <sub>2</sub> O (g)                              | 293.819                                      | Dilanthanum monoxide                                    | -3.2  | -13.4   | [12] |
| La <sub>2</sub> O <sub>2</sub> (g)                 | 309.819                                      | Dilanthanum dioxide                                     | -146.6  | -613.4  | [12] |
| La <sub>2</sub> O <sub>3</sub> (c, hexago-<br>nal) | 325.818                                      | Lanthanum trioxide, Lanthanum (III)<br>oxide            | -428.7  | -1793.7   | [12] |
| Li <sub>2</sub> O (g)                              | 29.8774                                      | Lithium oxide   | -39.9   | -166.9  | [7]  |
| Li <sub>2</sub> O (c)                              | 29.8774                                      | Lithium oxide   | -143.1  | -598.7  | [7]  |
| Li <sub>2</sub> O <sub>2</sub> (c)                 | 45.8768                                      | Lithium peroxide  | -151.2  | -632.6  | [7]  |
| Lu <sub>2</sub> O <sub>3</sub> (c, cubic)          | 397.938                                      | Lutetium trioxide, Lutetium (III)<br>oxide              | -448.9  | -1878.2   | [12] |
| MgO (c, macro-<br>crystal)                         | 40.3114                                      | Magnesium oxide, Periclase                              | -143.81   | -601.70   | [6]  |
| MgO (c, micro-<br>crystal)                         | 40.3114                                      | Magnesium oxide   | -142.92   | -597.98   | [6]  |
| MnO (g)  | 70.9374                                      | Manganese (II) oxide, Manganosite                       | 29.6  | 123.8   | [4]  |
| MnO (c)  | 70.9374                                      | Manganese (II) oxide, Manganosite                       | -92.07  | -385.22   | [4]  |
| MnO <sub>2</sub> (c)                               | 86.9368                                      | Manganese dioxide, Pyrolusite                           | -124.29   | -520.03   | [4]  |
| Mn <sub>2</sub> O <sub>3</sub> (c)                 | 157.8742                                     | Manganese sesquioxide, Braunitite,<br>Bixbyite          | -229.2  | -959.0  | [4]  |
| Mn <sub>3</sub> O <sub>4</sub> (c)                 | 228.8116                                     | Manganese (II,III) oxide, Hausmannite                   | -331.7  | -1387.8   | [4]  |
| MoO (g)  | 111.939                                      | Molybdenum monoxide                                     | 101.  | 422.  | [4]  |
| MoO <sub>2</sub> (g)                               | 127.939                                      | Molybdenum dioxide                                      | 3.  | 13.   | [4]  |
| MoO <sub>2</sub> (c)                               | 127.939                                      | Molybdenum dioxide                                      | -140.76   | -588.94   | [4]  |
| MoO <sub>3</sub> (g)                               | 143.939                                      | Molybdenum trioxide, Molybdic anhy-<br>dride, Molybdate | -78.  | -326.   | [4]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                   | formula<br>weight<br>(g mol <sup>-1</sup> ) | name   | Enthalpy of formation, ΔHf°<br>kcal mol <sup>-1</sup> | Enthalpy of formation, ΔHf°<br>kJ mol <sup>-1</sup> | Ref. |
|--------------------------------------|---|--|---|---|------|
| MoO <sub>3</sub> (c)                 | 143.939                                     | Molybdenum trioxide, Molybdite<br>anhydride, Molybdate | -178.08   | -745.09   | [4]  |
| (MoO <sub>3</sub> ) <sub>2</sub> (g) | 287.876                                     | Molybdenum trioxide, dimer                             | -271.   | -1134.  | [4]  |
| (MoO <sub>3</sub> ) <sub>3</sub> (g) | 431.815                                     | Molybdenum trioxide, trimer                            | -451.   | -1887.  | [4]  |
| (MoO <sub>3</sub> ) <sub>4</sub> (g) | 575.753                                     | Molybdenum trioxide, tetramer                          | -618.   | -2586.  | [4]  |
| (MoO <sub>3</sub> ) <sub>5</sub> (g) | 719.691                                     | Molybdenum trioxide, pentamer                          | -783.   | -3276.  | [4]  |
| NO (g)                               | 30.0061                                     | Nitric oxide   | 21.57   | 90.25   | [3]  |
| NO <sub>2</sub> (g)                  | 46.0055                                     | Nitrogen dioxide, Nitrogen peroxide                    | 7.93  | 33.18   | [3]  |
| N <sub>2</sub> O (g)                 | 44.0128                                     | Nitrous oxide  | 19.61   | 82.05   | [3]  |
| N <sub>2</sub> O <sub>3</sub> (g)    | 76.0116                                     | Dinitrogen trioxide, Nitrous anhydride                 | 20.01   | 83.72   | [3]  |
| N <sub>2</sub> O <sub>3</sub> (liq)  | 76.0116                                     | Dinitrogen trioxide, Nitrous anhydride                 | 12.02   | 50.29   | [3]  |
| N <sub>2</sub> O <sub>4</sub> (g)    | 92.0110                                     | Dinitrogen tetroxide                                   | 2.19  | 9.16  | [3]  |
| N <sub>2</sub> O <sub>4</sub> (liq)  | 92.0110                                     | Dinitrogen tetroxide                                   | -4.66   | -19.50  | [3]  |
| N <sub>2</sub> O <sub>5</sub> (g)    | 108.0104                                    | Nitrogen pentoxide, Nitric anhydride                   | 2.7   | 11.3  | [3]  |
| N <sub>2</sub> O <sub>5</sub> (c)    | 108.0104                                    | Nitrogen pentoxide, Nitric anhydride                   | -10.3   | -43.1   | [3]  |
| NaO <sub>2</sub> (c)                 | 54.9886                                     | Sodium superoxide                                      | -62.3   | -260.7  | [7]  |
| Na <sub>2</sub> O (c)                | 61.9790                                     | Sodium oxide   | -99.9   | -418.0  | [7]  |
| Na <sub>2</sub> O <sub>2</sub> (c)   | 77.9784                                     | Sodium peroxide  | -122.66   | -513.21   | [7]  |
| NbO (g)                              | 108.9054                                    | Niobium monoxide                                       | 51.   | 213.  | [5]  |
| NbO (c)                              | 108.9054                                    | Niobium monoxide                                       | -97.0   | -405.8  | [5]  |
| NbO <sub>2</sub> (g)                 | 124.9048                                    | Niobium dioxide  | -51.3   | -214.6  | [5]  |
| NbO <sub>2</sub> (c)                 | 124.9048                                    | Niobium dioxide  | -190.3  | -796.2  | [5]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                            | formula<br>weight<br>(g mol <sup>-1</sup> ) | name  | Enthalpy of formation, ΔHf°<br>kJ mol <sup>-1</sup> | Ref. |
|---|---|---|---|------|
| Nb <sub>2</sub> O <sub>5</sub> (c)            | 265.809                                     | Niobium pentoxide                           | -454.0  | [5]  |
| Nd <sub>2</sub> O <sub>3</sub> (c, hexagonal) | 336.478                                     | Neodymium trioxide, Neodymium (III) oxide   | -432.36   | [12] |
| NiO (c)                                       | 74.709                                      | Nickel monoxide, Bunsenite                  | -57.3   | [4]  |
| Ni <sub>2</sub> O <sub>3</sub> (c)            | 165.418                                     | Nickel sesquioxide, Nickel (III) oxide      | -117.0  | [4]  |
| NP <sub>2</sub> (c)                           | (269.0488) <sup>a</sup>                     | Neptunium dioxide                           | -256.7  | [9]  |
| O (g)   | 15.9994                                     | Oxygen, monatomic                           | 59.553  | [3]  |
| O <sub>2</sub> (g)                            | 31.9988                                     | Oxygen                                      | 0   | [3]  |
| O <sub>3</sub> (g)                            | 47.9982                                     | Ozone                                       | 34.1  | [3]  |
| OsO <sub>3</sub> (g)                          | 238.20                                      | Osmium trioxide                             | -67.8   | [4]  |
| OsO <sub>4</sub> (g)                          | 254.20                                      | Osmium tetroxide                            | -80.6   | [4]  |
| OsO <sub>4</sub> (c, white)                   | 254.20                                      | Osmium tetroxide                            | -92.2   | [4]  |
| OsO <sub>4</sub> (c, yellow)                  | 254.20                                      | Osmium tetroxide                            | -94.2   | [4]  |
| P <sub>4</sub> O <sub>6</sub> (g)             | 219.8916                                    | Phosphorus sesquioxide, Phosphorus trioxide | -512.5  | [7]  |
| P <sub>4</sub> O <sub>6</sub> (c)             | 219.8916                                    | Phosphorus trioxide, Phosphorous anhydride  | -392.0  | [3]  |
| P <sub>4</sub> O <sub>10</sub> (g)            | 283.8892                                    | Phosphorus pentoxide, Phosphoric anhydride  | -677.4  | [7]  |
| P <sub>4</sub> O <sub>10</sub> (c)            | 283.8892                                    | Phosphorus pentoxide, Phosphoric anhydride  | -713.2  | [3]  |

<sup>a</sup>Enthalpy of formation and formula weight are based on an atomic weight of 237.05 for Np, as used by the authors of reference [9].

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                     | formula<br>weight<br>(g<br>mol <sup>-1</sup> ) | name                                       | Enthalpy of formation, ΔH <sub>f</sub><br>kJ<br>mol <sup>-1</sup> | Ref. |
|--|--|--|---|------|
| P <sub>4</sub> O <sub>10</sub> (amorp) | 283.8892                                       | Phosphorus pentoxide, Phosphoric anhydride | -727.   | [3]  |
| PbO (g)                                | 223.189  | Lead monoxide                              | -11.48  | [7]  |
| PbO (c, red)                           | 223.189  | Lead monoxide, Litharge                    | -52.34  | [3]  |
| PbO (c, yellow)                        | 223.189  | Lead monoxide, Massicot                    | -51.94  | [3]  |
| PbO <sub>2</sub> (c)                   | 239.189  | Lead dioxide, Plattnerite                  | -66.3   | [3]  |
| Pb <sub>3</sub> O <sub>4</sub> (c)     | 685.568  | Lead oxide, Minium                         | -171.7  | [3]  |
| PdO (g)                                | 122.40   | Palladium monoxide                         | 83.4  | [4]  |
| PdO (c)                                | 122.40   | Palladium monoxide                         | -20.4   | [4]  |
| PtO <sub>2</sub> (g)                   | 227.089  | Platinum dioxide                           | 41.0  | [4]  |
| Pt <sub>3</sub> O <sub>4</sub> (c)     | 649.268  | Platinum (II, III) oxide                   | -39.  | [4]  |
| PuO <sub>2</sub> (c)                   | (271.0998) <sup>b</sup>                        | Plutonium dioxide                          | -252.87   | [10] |
| RaO (c)                                | 242.019  | Radium oxide                               | -125.   | [6]  |
| Rb <sub>2</sub> O (c)                  | 186.939  | Rubidium oxide                             | -78.9   | [2]  |
| Rb <sub>2</sub> O <sub>2</sub> (c)     | 202.939  | Dirubidium dioxide                         | -101.7  | [2]  |
| Rb <sub>2</sub> O <sub>3</sub> (c)     | 218.938  | Dirubidium trioxide                        | -116.7  | [2]  |
| Rb <sub>2</sub> O <sub>4</sub> (c)     | 234.938  | Dirubidium tetroxide                       | -126.2  | [2]  |
| ReO <sub>3</sub> (c)                   | 234.20   | Rhenium trioxide                           | -144.6  | [4]  |
| Re <sub>2</sub> O <sub>7</sub> (g)     | 484.40   | Rhenium heptoxide                          | -263.   | [4]  |
| Re <sub>2</sub> O <sub>7</sub> (c)     | 484.40   | Rhenium heptoxide                          | -296.4  | [4]  |
| RhO (g)                                | 118.9044                                       | Rhodium monoxide                           | 92.   | [4]  |
| RhO <sub>2</sub> (g)                   | 134.9038                                       | Rhodium dioxide                            | 44.   | [4]  |

<sup>b</sup> Enthalpy of formation and formula weight are based on an atomic weight of 239.1 for Pu, as used by the authors of reference [10].

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                                  | formula<br>weight<br>(g mol <sup>-1</sup> ) | name                            | Enthalpy of formation, ΔH <sub>f</sub> <sup>o</sup><br>kJ mol <sup>-1</sup> | Ref. |
|---|---|---------------------------------|---|------|
| Rh <sub>2</sub> O <sub>3</sub> (c)                  | 253.8082                                    | Rhodium sesquioxide             | -82.  | [4]  |
| RuO <sub>2</sub> (c)                                | 133.069                                     | Ruthenium dioxide               | -72.9   | [4]  |
| RuO <sub>3</sub> (g)                                | 149.068                                     | Ruthenium trioxide              | -18.7   | [4]  |
| RuO <sub>4</sub> (g)                                | 165.068                                     | Ruthenium tetroxide             | -44.0   | [4]  |
| RuO <sub>4</sub> (liq)                              | 165.068                                     | Ruthenium tetroxide             | -54.6   | [4]  |
| RuO <sub>4</sub> (c)                                | 165.068                                     | Ruthenium tetroxide             | -57.2   | [4]  |
| SO (g)  | 48.0634                                     | Sulfur monoxide                 | 1.496   | [3]  |
| SO <sub>2</sub> (g)                                 | 64.0628                                     | Sulfur dioxide                  | -70.944   | [3]  |
| SO <sub>2</sub> (liq)                               | 64.0628                                     | Sulfur dioxide                  | -76.6   | [3]  |
| SO <sub>3</sub> (g)                                 | 80.0622                                     | Sulfur trioxide                 | -94.58  | [3]  |
| SO <sub>3</sub> (liq)                               | 80.0622                                     | Sulfur trioxide                 | -105.41   | [3]  |
| SO <sub>3</sub> (c)                                 | 80.0622                                     | Sulfur trioxide                 | -108.63   | [3]  |
| SbO (g)   | 137.749                                     | Antimony monoxide               | 47.67   | [3]  |
| Sb <sub>2</sub> O <sub>4</sub> (c)                  | 307.498                                     | Antimony tetroxide, Cerrantite  | -216.9  | [3]  |
| Sb <sub>2</sub> O <sub>5</sub> (c)                  | 323.497                                     | Antimony pentoxide              | -232.3  | [3]  |
| Sb <sub>4</sub> O <sub>6</sub> (c, cubic)           | 582.996                                     | Antimony trioxide, Senarmontite | -344.3  | [3]  |
| Sb <sub>4</sub> O <sub>6</sub> (c,<br>orthorhombic) | 582.996                                     | Antimony trioxide, Valentinite  | -338.7  | [3]  |
| Sb <sub>6</sub> O <sub>13</sub> (c)                 | 938.492                                     | Antimony (III, IV) oxide        | -670.6  | [3]  |
| ScO (g)   | 60.955                                      | Scandium monoxide               | -13.68  | [5]  |
| Sc <sub>2</sub> O (g)                               | 105.911                                     | Discandium monoxide             | -6.9  | [5]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                                  | formula<br>weight<br>(g mol <sup>-1</sup> ) | name  | Enthalpy of formation, ΔH <sub>f</sub> <sup>o</sup><br>kcal mol <sup>-1</sup> | Enthalpy of formation, ΔH <sub>f</sub> <sup>o</sup><br>kJ mol <sup>-1</sup> | Ref. |
|---|---|---|---|---|------|
| Sc <sub>2</sub> O <sub>3</sub> (c)                  | 137.910                                     | Scandium trioxide, Scandia,<br>Scandium sesquioxide | -456.22   | -1908.82  | [5]  |
| SeO (g)   | 94.959                                      | Selenium monoxide                                   | 12.75   | 53.35   | [3]  |
| SeO <sub>2</sub> (c)                                | 110.959                                     | Selenium dioxide                                    | -53.86  | -225.35   | [3]  |
| SeO <sub>3</sub> (c)                                | 126.958                                     | Selenium trioxide                                   | -39.9   | -166.9  | [3]  |
| Se <sub>2</sub> O <sub>5</sub> (c)                  | 237.917                                     | Diselenium pentoxide                                | -97.6   | -408.4  | [3]  |
| SiO (g)   | 44.0854                                     | Silicon monoxide                                    | -23.8   | -99.6   | [3]  |
| SiO <sub>2</sub> (g)                                | 60.0848                                     | Silicon dioxide                                     | -77.  | -322.   | [3]  |
| SiO <sub>2</sub> (c, crysto-<br>balite)             | 60.0848                                     | Silicon dioxide, Crystobalite                       | -217.37   | -909.48   | [3]  |
| SiO <sub>2</sub> (c, quartz)                        | 60.0848                                     | Silicon dioxide, Quartz                             | -217.72   | -910.94   | [3]  |
| SiO <sub>2</sub> (c, tri-<br>dymite)                | 60.0848                                     | Silicon dioxide, Tridymite                          | -217.27   | -909.06   | [3]  |
| SiO <sub>2</sub> (c)                                | 60.0848                                     | Silicon dioxide, Coesite                            | -216.44   | -905.58   | [1]  |
| SiO <sub>2</sub> (c)                                | 60.0848                                     | Silicon dioxide, Stishovite                         | -205.86   | -861.32   | [1]  |
| SiO <sub>2</sub> (amorp)                            | 60.0848                                     | Silicon dioxide, Silica glass                       | -215.94   | -903.49   | [3]  |
| Sm <sub>2</sub> O <sub>3</sub> (c, mono-<br>clinic) | 348.698                                     | Samarium trioxide, Samarium (III)<br>oxide          | -433.7  | -1814.6   | [12] |
| Tin (SnO) (c)                                       | 134.689                                     | Tin monoxide  | -68.3   | -285.8  | [3]  |
| Tin dioxide (SnO <sub>2</sub> ) (c)                 | 150.689                                     | Tin dioxide, Cussiterite                            | -138.8  | -580.7  | [3]  |
| SrO (g)   | 103.619                                     | Strontium monoxide                                  | -2.   | -8.   | [6]  |
| SrO (c)   | 103.619                                     | Strontium monoxide                                  | -141.5  | -592.0  | [6]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                        | formula<br>weight<br>(g mol <sup>-1</sup> ) | name                                  | Enthalpy of formation, ΔH <sub>f</sub> <sup>o</sup><br>kcal mol <sup>-1</sup> | Enthalpy of formation, ΔH <sub>f</sub> <sup>o</sup><br>kJ mol <sup>-1</sup> | Ref. |
|---|---|---------------------------------------|---|---|------|
| SrO <sub>2</sub> (c)                      | 119.619                                     | Strontium peroxide                    | -151.4  | -633.5  | [6]  |
| Sr <sub>2</sub> O (g)                     | 191.239                                     | Distorontium monoxide                 | -56.  | -234.   | [6]  |
| Sr <sub>2</sub> O (c)                     | 191.239                                     | Distorontium monoxide                 | -154.7  | -647.3  | [6]  |
| TaO (g)                                   | 196.9474                                    | Tantalum monoxide                     | 60.   | 251.  | [5]  |
| TaO <sub>2</sub> (g)                      | 212.9468                                    | Tantalum tetroxide                    | -41.  | -172.   | [5]  |
| Ta <sub>2</sub> O <sub>5</sub> (c,β)      | 441.8930                                    | Tantalum pentoxide                    | -489.0  | -2046.0   | [5]  |
| TbO <sub>2</sub> (c)                      | 190.9228                                    | Terbium dioxide, Terbium (IV) oxide   | -232.2  | -971.5  | [12] |
| Tb <sub>2</sub> O <sub>3</sub> (c, cubic) | 365.8462                                    | Terbium trioxide, Terbium (III) oxide | -445.2  | -1862.7   | [12] |
| Tc <sub>2</sub> O <sub>7</sub> (c)        | 309.8078                                    | Technetium heptoxide                  | -266.   | -1113.  | [4]  |
| TeO (g)                                   | 143.599                                     | Tellurium monoxide                    | 15.6  | 65.3  | [3]  |
| TeO <sub>2</sub> (c)                      | 159.599                                     | Tellurium dioxide, Tellurite          | -77.1   | -322.6  | [3]  |
| ThO <sub>2</sub> (c)                      | 264.0368                                    | Thorium dioxide, Thorianite, Thoria   | -293.20   | -1226.75  | [1]  |
| TlO (g)                                   | 63.899                                      | Titanium monoxide                     | 4.  | 17.   | [5]  |
| TiO (c,α)                                 | 63.899                                      | Titanium monoxide                     | -124.2  | -519.6  | [5]  |
| TiO <sub>2</sub> (g)                      | 79.899                                      | Titanium dioxide                      | -60.  | -251.   | [5]  |
| TiO <sub>2</sub> (c)                      | 79.899                                      | Titanium dioxide, Anatase Octahedrite | -224.6  | -939.7  | [5]  |
| TiO <sub>2</sub> (c)                      | 79.899                                      | Titanium dioxide, Brookite            | -225.1  | -941.8  | [5]  |
| TiO <sub>2</sub> (c)                      | 79.899                                      | Titanium dioxide, Rutile              | -225.8  | -944.7  | [5]  |
| TiO <sub>2</sub> (amorp)                  | 79.899                                      | Titanium dioxide                      | -210.   | -879.   | [5]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>state)                         | formula<br>weight<br>(g mol <sup>-1</sup> ) | name  | Enthalpy of formation, ΔH <sup>o</sup><br>kcal mol <sup>-1</sup> | Enthalpy of formation, ΔH <sup>o</sup><br>kJ mol <sup>-1</sup> | Ref. |
|---|---|---|--|--|------|
| Ti <sub>2</sub> O <sub>3</sub> (c)        | 143.798                                     | Titanium sesquioxide                                  | -363.5   | -1520.9  | [5]  |
| Ti <sub>3</sub> O <sub>5</sub> (c)        | 223.697                                     | Titanium pentoxide                                    | -587.8   | -2459.4  | [5]  |
| Tl <sub>2</sub> O (c)                     | 424.7394                                    | Thallous oxide, Thallium (I) oxide                    | -42.7  | -178.7   | [3]  |
| Tm <sub>2</sub> O <sub>3</sub> (c, cubic) | 385.8662                                    | Thulium trioxide, Thulium (III) oxide                 | -451.4   | -1888.7  | [12] |
| UO <sub>2</sub> (c)                       | 270.029                                     | Uranium dioxide, Uraninite                            | -259.20  | -1084.49   | [1]  |
| UO <sub>3</sub> (c, α)                    | 286.0282                                    | Uranium trioxide                                      | -291.3   | -1218.8  | [11] |
| UO <sub>3</sub> (c, β)                    | 286.0282                                    | Uranium trioxide                                      | -292.0   | -1221.7  | [11] |
| UO <sub>3</sub> (c, γ)                    | 286.0282                                    | Uranium trioxide                                      | -292.0   | -1225.9  | [11] |
| U <sub>3</sub> O <sub>7</sub> (c, β)      | 826.0858                                    | Triuranium heptoxide                                  | -819.1   | -3427.1  | [11] |
| U <sub>3</sub> O <sub>8</sub> (c)         | 842.0852                                    | Triuranium octoxide, Pitchblende                      | -854.4   | -3574.8  | [11] |
| U <sub>4</sub> O <sub>9</sub> (c)         | 1094.1146                                   | Tetrauranium nonoxide                                 | -1078.0  | -4510.4  | [11] |
| VO (g)                                    | 66.9414                                     | Vanadium monoxide                                     | 25.  | 105.   | [5]  |
| VO (c)                                    | 66.9414                                     | Vanadium monoxide                                     | -103.2   | -431.8   | [5]  |
| VO <sub>2</sub> (g)                       | 82.9408                                     | Vanadium dioxide                                      | -57.   | -238.  | [5]  |
| V <sub>2</sub> O <sub>3</sub> (c)         | 149.8822                                    | Vanadium sesquioxide, Vanadium tri-oxide, Karelianite | -293.5   | -1228.0  | [5]  |
| V <sub>2</sub> O <sub>4</sub> (c, α)      | 165.8816                                    | Vanadium tetroxide                                    | -341.1   | -1427.2  | [5]  |
| V <sub>2</sub> O <sub>5</sub> (c)         | 181.8810                                    | Vanadium pentoxide                                    | -370.6   | -1550.6  | [5]  |
| V <sub>3</sub> O <sub>5</sub> (c)         | 232.8230                                    | Trivanadium pentoxide                                 | -465.  | -1946.   | [5]  |
| V <sub>4</sub> O <sub>7</sub> (c)         | 315.7638                                    | Tetravanadium heptoxide                               | -635.  | -2657.   | [5]  |
| V <sub>6</sub> O <sub>13</sub> (c)        | 513.6442                                    | Hexavanadium tridecaoxide                             | -1062.   | -4443.   | [5]  |

Table III. Enthalpies of Formation of Inorganic Oxides at 298.15 K (Cont'd)

| formula<br>(state)                              | formula<br>weight<br>(g mol <sup>-1</sup> ) | name   | Enthalpy of formation, $\Delta H_f^\circ$<br>kcal mol <sup>-1</sup> | Enthalpy of formation, $\Delta H_f^\circ$<br>kJ mol <sup>-1</sup> | Ref. |
|---|---|--|---|---|------|
| W <sub>0</sub> (g)                              | 199.849                                     | Tungsten monoxide                                    | 108.  | 452.  | [4]  |
| W <sub>0</sub> <sub>2</sub> (g)                 | 215.849                                     | Tungsten dioxide                                     | 11.   | 46.   | [4]  |
| W <sub>0</sub> <sub>2</sub> (c)                 | 215.849                                     | Tungsten dioxide                                     | -140.94   | -589.69   | [4]  |
| W <sub>0</sub> <sub>3</sub> (g)                 | 231.848                                     | Tungsten trioxide                                    | -71.  | -297.   | [4]  |
| W <sub>0</sub> <sub>3</sub> (c)                 | 231.848                                     | Tungsten trioxide, Wolframite                        | -201.45   | -842.87   | [4]  |
| (W <sub>0</sub> <sub>3</sub> ) <sub>2</sub> (g) | 463.696                                     | Tungsten trioxide, dimer                             | -277.   | -1159.  | [4]  |
| (W <sub>0</sub> <sub>3</sub> ) <sub>3</sub> (g) | 695.545                                     | Tungsten trioxide, trimer                            | -468.   | -1958.  | [4]  |
| (W <sub>0</sub> <sub>3</sub> ) <sub>4</sub> (g) | 927.393                                     | Tungsten trioxide, tetramer                          | -649.   | -2715.  | [4]  |
| Yb <sub>2</sub> O <sub>3</sub> (c, cubic)       | 394.078                                     | Ytterbium trioxide, Ytterbium (III) oxide            | -433.7  | -1814.6   | [12] |
| Y <sub>0</sub> (g)                              | 104.9044                                    | Yttrium monoxide                                     | -9.3  | -38.9   | [5]  |
| Y <sub>2</sub> <sup>0</sup> (g)                 | 193.8094                                    | Diyttrium monoxide                                   | 1.0   | 4.2   | [5]  |
| Y <sub>2</sub> O <sub>2</sub> (g)               | 209.8088                                    | Diyttrium dioxide                                    | -127.4  | -533.0  | [5]  |
| Y <sub>2</sub> O <sub>3</sub> (c)               | 225.8082                                    | Yttrium trioxide, Yttria                             | -455.38   | -1095.31  | [5]  |
| ZnO (c)   | 81.369                                      | Zinc oxide, Zincite                                  | -83.24  | -348.28   | [3]  |
| ZrO (g)   | 107.219                                     | Zirconium monoxide, Zirconium (II) oxide             | 15.   | 63.   | [5]  |
| ZrO <sub>2</sub> (g)                            | 123.219                                     | Zirconium dioxide, Zirconium (IV) oxide              | -75.  | -314.   | [5]  |
| ZrO <sub>2</sub> (c, $\alpha$ monoclinic)       | 123.219                                     | Zirconium dioxide, Zirconium (IV) oxide, Baddeleyite | -263.04   | -1100.56  | [5]  |

## References to Table III

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- [6] Parker, V. B., Wagman, D. D. and Evans, W. H., NBS Tech. Note 270-6, November 1971.
- [7] Stull, D. R., and Prophet, H., et al., JANAF Thermochemical Tables, 2nd Edition, NSRDS-NBS-37, 1141 pp. (June 1971), (U. S. Government Printing Office, Washington, D. C. 20402).
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26.0 Appendix26.1 Symbols for Thermodynamic Quantities, (IUPAC). (1) (2)

|        |  |
|--------|--|
| T      | thermodynamic temperature (absolute temperature)               |
| t, θ   | Celsius temperature  |
| R      | molar gas constant   |
| k      | Boltzmann constant   |
| q, Q   | heat   |
| w, W   | work   |
| U, (E) | internal energy  |
| H      | enthalpy: $H = U + pV$   |
| S      | entropy  |
| A      | Helmholtz energy: $A = U - TS$                                 |
| J      | Massieu function: $J = -A/T$                                   |
| G      | Gibbs energy: $G = H - TS$ , (3) (see footnote (3), page 202 ) |
| Y      | Planck function: $Y = -G/T$                                    |
| Z      | compressibility factor: $Z = pV/nRT$                           |
| C      | heat capacity  |
| c      | specific heat capacity (heat capacity divided by mass)         |
| γ, (k) | heat capacity ratio: $C_p/C_v$                                 |
| μ      | Joule-Thomson coefficient                                      |
| λ, k   | thermal conductivity   |
| a      | thermal diffusivity: $a = \lambda/\rho C_p$                    |

(1) Symbols adopted by the International Union of Pure and Applied Chemistry (IUPAC), 1969.

(2) Symbols in parentheses are alternates, accepted but not recommended by IUPAC. See Section 25.2 for other commonly used symbols and names of quantities not accepted by IUPAC.

|             |  |
|-------------|--|
| $h$         | coefficient of heat transfer   |
| $\alpha$    | cubic expansion coefficient: $\alpha = (\partial V / \partial T)_P / V$                  |
| $k$         | isothermal compressibility: $k = -(\partial V / \partial P)_T / V$                       |
| $\beta$     | pressure coefficient: $\beta = (\partial P / \partial T)_V$                              |
| $\mu_B$     | chemical potential of substance B  |
| $\lambda_B$ | absolute activity of substance B: $\lambda_B = \exp(\mu_B / RT)$                         |
| $f, (p^*)$  | fugacity   |
| $\Pi$       | osmotic pressure   |
| $I$         | ionic strength: $I = \frac{1}{2} \sum_i m_i z_i^2$ or $I = \frac{1}{2} \sum_i c_i z_i^2$ |
| $a_B$       | activity, relative activity of substance B   |
| $f_B$       | activity coefficient, mole fraction basis  |
| $\gamma_B$  | activity coefficient, molality basis   |
| $y_B$       | activity coefficient, concentration basis  |
| $\phi$      | osmotic coefficient  |

- (3) The Gibbs energy is frequently called free energy, Gibbs free energy, or Gibbs function. The commonly encountered term free energy in American work on thermodynamics almost invariably refers to Gibbs energy. This usage of the term free energy and the symbol F are being discouraged by the IUPAC because of confusion with the Helmholtz energy and the common European usage of F for the latter.

## 26.2 Selected Symbols for Other Quantities needed in Thermodynamics

(IUPAC)<sup>(1)</sup> (see footnote (1), page 201)

|        |        |
|--------|--------|
| $A, S$ | area   |
| $V$    | volume |
| $t$    | time   |
| $m$    | mass   |

|   |   |
|---|---|
| $\rho$  | density (mass divided by volume)  |
| P   | pressure  |
| $A_r$   | relative atomic mass (also called "atomic weight")  |
| $M_r$   | relative molecular mass (also called "molecular weight")                                      |
| $L, N_A$  | Avogadro constant   |
| N   | number of molecules   |
| n, ( $\nu$ )  | amount of substance   |
| $x_B, y_B$  | mole fraction of substance B: $x_B = n_B / \sum_i n_i$  |
| $w_B$   | mass fraction of substance B  |
| $\phi_B$  | volume fraction of substance B  |
| $m_B$   | molality of solute substance B (amount of B divided<br>by the mass of solvent)                |
| $c_B, [B]$  | concentration of substance B (amount of B divided by<br>the volume of the solution)           |
| $\rho_B$  | mass concentration of substance B (mass of B divided<br>by the volume of the solution)        |
| $\nu_B$   | stoichiometric coefficient of substance B (negative<br>for reactants, positive for products). |
| (The general equation for a chemical reaction is --                                       |   |
| $\sum_B \nu_B = 0$ , [Example: for the reaction $H_2O \rightarrow H_2 + \frac{1}{2}O_2$ , |   |
| $H_2 + \frac{1}{2}O_2 - H_2O = 0$ ]   |   |
| $\zeta$   | extent of reaction: $(d\zeta = dn_B / \nu_B)$   |
| K   | equilibrium constant  |
| $\alpha$  | degree of dissociation  |
| $z_B$   | charge number of an ion B (positive for cations, negative<br>for anions)                      |

### 26.3 Units of Measurement - International System (SI)

#### SI - Base Units and Supplementary Units

| quantity            | name of unit | symbol |
|---------------------|--------------|--------|
| length              | metre        | m      |
| mass                | kilogram     | kg     |
| time                | second       | s      |
| temperature         | kelvin       | K      |
| electric current    | ampere       | A      |
| luminous intensity  | candela      | cd     |
| amount of substance | mole         | mol    |
| plane angle         | radian       | rad    |
| solid angle         | steradian    | sr     |

### 26.4 Definitions of the SI Base Units

**metre:** The metre is the length equal to 1 650 763.73 wavelengths in vacuum of the radiation corresponding to the transition between the levels  $2p_{10}$  and  $5d_5$  of the krypton -86 atom.

**kilogram:** The kilogram is equal to the mass of the international prototype of the kilogram.

**second:** The second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium-133 atom.

kelvin: The kelvin is the fraction 1/273.16 of the thermodynamic temperature of the triple point of water. The kelvin is used both for thermodynamic temperature and for thermodynamic temperature interval.

ampere: The ampere is that constant current which, if maintained in two straight parallel conductors of infinite length, of negligible cross-section, and placed 1 metre apart in vacuum, would produce between these conductors a force equal to  $2 \times 10^{-7}$  newton per metre of length.

candela: The candela is the luminous intensity, in the perpendicular direction, of a surface of 1/600 000 square metre of a black body at the temperature of freezing platinum under a pressure of 101 325 newtons per square metre.

mole: The mole is the amount of substance of a system which contains as many elementary entities as there are carbon atoms in 0.012 kilogram of carbon-12.

Note: The elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.

26.5 Prefixes

| <u>SI Symbol</u> | <u>Prefix name</u> | <u>Multiplication factor</u> |
|------------------|--------------------|------------------------------|
| T                | tera               | $10^{12}$                    |
| G                | giga               | $10^9$                       |
| M                | mega               | $10^6$                       |
| k                | kilo               | $10^3$                       |
| h                | hecto              | $10^{+2}$                    |
| d <sub>a</sub>   | deka               | $10^{+1}$                    |
| d                | deci               | $10^{-1}$                    |
| c                | centi              | $10^{-2}$                    |
| m                | milli              | $10^{-3}$                    |
| $\mu$            | micro              | $10^{-6}$                    |
| n                | nano               | $10^{-9}$                    |
| p                | pico               | $10^{-12}$                   |
| f                | femto              | $10^{-15}$                   |
| a                | atto               | $10^{-18}$                   |

## 26.6 SI Derived Units (partial listing)

|                               | Symbol<br>for SI unit | Definition<br>of SI unit | Other<br>Definitions   |
|-------------------------------|-----------------------|--------------------------|--|
| force                         | newton                | N                        | $\text{m} \cdot \text{kg} \cdot \text{s}^{-2}$                         |
| pressure                      | pascal                | $\text{Pa}$              | $\text{N} \cdot \text{m}^{-2}$   |
| energy                        | joule                 | J                        | $\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2}$                       |
| power                         | watt                  | W                        | $\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-3}$                       |
| electric charge               | coulomb               | C                        | $\text{A} \cdot \text{s}$  |
| electric potential difference | volt                  | V                        | $\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-3} \cdot \text{A}^{-1}$   |
| electric resistance           | ohm                   | $\Omega$                 | $\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-3} \cdot \text{A}^{-2}$   |
| electric conductance          | siemens               | S                        | $\text{m}^{-2} \cdot \text{kg}^{-1} \cdot \text{s}^3 \cdot \text{A}^2$ |
| electric capacitance          | farad                 | F                        | $\text{m}^{-2} \cdot \text{kg}^{-1} \cdot \text{s}^4 \cdot \text{A}^2$ |
| magnetic flux                 | weber                 | Wb                       | $\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{A}^{-1}$   |
| inductance                    | henry                 | H                        | $\text{m}^2 \cdot \text{kg} \cdot \text{s}^{-2} \cdot \text{A}^{-2}$   |
| magnetic flux density         | tesla                 | T                        | $\text{kg} \cdot \text{s}^{-2} \cdot \text{A}^{-1}$                    |
| luminous flux                 | lumen                 | lm                       | $\text{cd} \cdot \text{sr}$  |
| illumination                  | lux                   | lx                       | $\text{m}^{-2} \cdot \text{cd} \cdot \text{sr}$                        |
| frequency                     | hertz                 | Hz                       | $\text{s}^{-1}$  |

26.7 Other Units Exactly Defined in Terms of SI Units (partial listing)

| <u>Quantity</u>                | <u>Name</u>               | <u>Symbol</u>     | <u>Definition</u>   |
|--------------------------------|---------------------------|-------------------|---|
| length                         | inch                      | in.               | $2.54 \times 10^{-2} \text{ m}$                                       |
| mass                           | pound (av.)               | lb                | 0.453 592 37 kg   |
| force                          | kilogram force            | kgf               | 9.806 65 N  |
| pressure                       | atmosphere                | atm               | $101\ 325 \text{ N} \cdot \text{m}^{-2}$                              |
| pressure                       | torr                      | Torr              | $(101\ 325/760) \text{ N} \cdot \text{m}^{-2}$                        |
| pressure                       | millimetre of mercury     | mmHg              | $13.5951 \times 980.665 \times 10^{-2} \text{ N} \cdot \text{m}^{-2}$ |
| energy                         | kilowatt-hour             | kWh               | $3.6 \times 10^6 \text{ J}$   |
| energy                         | thermochemical calorie*** | cal <sub>th</sub> | 4.184 J   |
| energy                         | IT calorie**              | cal <sub>IT</sub> | 4.1868 J  |
| energy                         | IT British thermal unit** | Btu <sub>IT</sub> | 1055.06 J*  |
| temperature<br>(thermodynamic) | degree Rankine            | °R                | $5/9 \text{ K}^{****}$  |
| temperature                    | degree Celsius            | °C                | K*****  |
| temperature                    | degree Fahrenheit         | °F                | $5/9 \text{ K}^{*****}$   |
| volume                         | litre                     | l                 | $10^{-3} \text{ m}^3$   |

\* The exact relationship is:  $1 \text{ Btu}_{\text{IT}} = (4.1868/1.8) \times 435.592\ 37 \text{ J}$ .

\*\* IT refers to International Tables (International Steam Tables)

\*\*\* The thermochemical calorie is used in tables in this monograph.

\*\*\*\*  $[T(\text{°R}) = 1.8T(\text{K})]; [T(\text{°R}) = t(\text{°F}) + 459.67]; [T(\text{°R}) = 1.8t(\text{°C}) + 491.67]$

\*\*\*\*\*  $[t(\text{°C}) = T(\text{K}) - 273.15]$

\*\*\*\*\*  $[t(\text{°F}) = 1.8t(\text{°C}) + 32]$

## 26.8 Physical Constants

| Constant                     | Symbol         | Value       | Error Limit | Units (SI)  |
|------------------------------|----------------|-------------|-------------|---|
| Speed of light in vacuum     | c              | 2.997 925   | 3           | x10 <sup>-8</sup> m·s <sup>-1</sup>                   |
| Elementary charge            | e              | 1.602 10    | 7           | 10 <sup>19</sup> C                                    |
| Avogadro constant            | N <sub>A</sub> | 6.022 52    | 28          | 10 <sup>23</sup> mol <sup>-1</sup>                    |
| Electron rest mass           | m <sub>e</sub> | 9.109 1     | 4           | 10 <sup>-31</sup> kg                                  |
| Proton rest mass             | m <sub>p</sub> | 1.672 52    | 8           | 10 <sup>-27</sup> kg                                  |
| Neutron rest mass            | m <sub>n</sub> | 1.674 82    | 8           | 10 <sup>-27</sup> kg                                  |
| Faraday constant             | F              | 9.648 70    | 16          | 10 <sup>4</sup> mol <sup>-1</sup>                     |
| Planck constant              | h              | 6.625 6     | 5           | 10 <sup>-34</sup> J·s                                 |
| Rydberg constant             | R <sub>∞</sub> | 1.097 373 1 | 3           | 10 <sup>-11</sup> m                                   |
| Bohr radius                  | a <sub>0</sub> | 5.291 67    | 7           | 10 <sup>-15</sup> m                                   |
| Electron radius              | r <sub>e</sub> | 2.817 77    | 11          | 10 <sup>0</sup> J·K <sup>-1</sup> ·mol <sup>-1</sup>  |
| Gas constant                 | R              | 8.314 3     | 12          | 10 <sup>-2</sup> J·K <sup>-1</sup> ·mol <sup>-1</sup> |
| Normal volume perfect gas    | V <sub>o</sub> | 2.241 36    | 30          | 10 <sup>-3</sup> m <sup>3</sup> ·mol <sup>-1</sup>    |
| Boltzmann constant           | k              | 1.380 54    | 18          | 10 <sup>-23</sup> J·K <sup>-1</sup>                   |
| First radiation constant     | c <sub>1</sub> | 3.741 5     | 3           | 10 <sup>-16</sup> W·m <sup>2</sup>                    |
| Second radiation constant    | c <sub>2</sub> | 1.438 79    | 19          | 10 <sup>-2</sup> m·K                                  |
| Wien displacement constant   | b              | 2.897 8     | 4           | 10 <sup>-3</sup> m·K                                  |
| Stefan-Boltzmann constant    | σ              | 5.669 7     | 29          | 10 <sup>-8</sup> W·m <sup>-2</sup> ·K <sup>-4</sup>   |
| Energy associated with -     |                |             |             |   |
| Electron volt                | eV             | 1.602 10    | 7           | x10 <sup>-19</sup> J·(eV) <sup>-1</sup>               |
| Frequency (electromagnetic)  | e/h            | 2.418 04    | 7           | 10 <sup>14</sup> Hz·(eV) <sup>-1</sup>                |
| Wavelength (electromagnetic) | ch/e           | 1.239 81    | 4           | 10 <sup>-6</sup> eV·m                                 |
| Wave number                  | e/ch           | 8.065 73    | 23          | 10 <sup>5</sup> m <sup>-1</sup> ·(eV) <sup>-1</sup>   |
| Kelvin                       | e/k            | 1.160 49    | 16          | 10 <sup>4</sup> K·(eV) <sup>-1</sup>                  |

These physical constants are excerpted from a list recommended by the National Academy of Sciences and adopted by the National Bureau of Standards. The complete list is found in National Bureau of Standards Technical News Bulletin, October, 1963.

- ± Error limits are approximately 3 standard deviations and apply to last digits of the value.

26.9 Atomic Weights (Relative Atomic Masses) of the Elements

| Name        | Symbol | Atomic number | Atomic weight         |
|-------------|--------|---------------|-----------------------|
| Actinium    | Ac     | 89            | .....                 |
| Aluminum    | Al     | 13            | 26.9815               |
| Americium   | Am     | 95            | .....                 |
| Antimony    | Sb     | 51            | 121.75                |
| Argon       | Ar     | 18            | 39.948                |
| Arsenic     | As     | 33            | 74.9216               |
| Astatine    | At     | 85            | .....                 |
| Barium      | Ba     | 56            | 137.34                |
| Berkelium   | Bk     | 97            | .....                 |
| Beryllium   | Be     | 4             | 9.0122                |
| Bismuth     | Bi     | 83            | 208.980               |
| Boron       | B      | 5             | 10.811 <sup>a</sup>   |
| Bromine     | Br     | 35            | 79.909 <sup>b</sup>   |
| Cadmium     | Cd     | 48            | 112.40                |
| Calcium     | Ca     | 20            | 40.08                 |
| Californium | Cf     | 98            | .....                 |
| Carbon      | C      | 6             | 12.01115 <sup>a</sup> |
| Cerium      | Ce     | 58            | 140.12                |
| Cesium      | Cs     | 55            | 132.905               |
| Chlorine    | Cl     | 17            | 35.453 <sup>b</sup>   |
| Chromium    | Cr     | 24            | 51.996 <sup>b</sup>   |
| Cobalt      | Co     | 27            | 58.9332               |
| Copper      | Cu     | 29            | 63.54                 |
| Curium      | Cm     | 96            | .....                 |
| Dysprosium  | Dy     | 66            | 162.50                |
| Einsteinium | Es     | 99            | .....                 |
| Erbium      | Er     | 68            | 167.26                |
| Europium    | Eu     | 63            | 151.96                |
| Fermium     | Fm     | 100           | .....                 |
| Fluorine    | F      | 9             | 18.9984               |
| Francium    | Fr     | 87            | .....                 |
| Gadolinium  | Gd     | 64            | 157.25                |

| Name        | Symbol | Atomic number | Atomic weight        |
|-------------|--------|---------------|----------------------|
| Gallium     | Ga     | 31            | 69.72                |
| Germanium   | Ge     | 32            | 72.59                |
| Gold        | Au     | 79            | 196.967              |
| Hafnium     | Hf     | 72            | 178.49               |
| Helium      | He     | 2             | 4.0026               |
| Holmium     | Ho     | 67            | 164.930              |
| Hydrogen    | H      | 1             | 1.00797 <sup>a</sup> |
| Indium      | In     | 49            | 114.82               |
| Iodine      | I      | 53            | 126.9044             |
| Iridium     | Ir     | 77            | 192.2                |
| Iron        | Fe     | 26            | 55.847 <sup>b</sup>  |
| Krypton     | Kr     | 36            | 83.80                |
| Lanthanum   | La     | 57            | 138.91               |
| Lead        | Pb     | 82            | 207.19               |
| Lithium     | Li     | 3             | 6.939                |
| Lutetium    | Lu     | 71            | 174.97               |
| Magnesium   | Mg     | 12            | 24.312               |
| Manganese   | Mn     | 25            | 54.9380              |
| Mendelevium | Md     | 101           | .....                |
| Mercury     | Hg     | 80            | 200.59               |
| Molybdenum  | Mo     | 42            | 95.94                |
| Neodymium   | Nd     | 60            | 144.24               |
| Neon        | Ne     | 10            | 20.183               |
| Neptunium   | Np     | 93            | .....                |
| Nickel      | Ni     | 28            | 58.71                |
| Niobium     | Nb     | 41            | 92.906               |
| Nitrogen    | N      | 7             | 14.0067              |
| Nobelium    | No     | 102           | .....                |
| Osmium      | Os     | 76            | 109.2                |
| Oxygen      | O      | 8             | 15.9994 <sup>a</sup> |
| Palladium   | Pd     | 46            | 106.4                |
| Phosphorus  | P      | 15            | 30.9738              |
| Platinum    | Pt     | 78            | 195.09               |
| Plutonium   | Pu     | 94            | .....                |

| Name         | Symbol | Atomic number | Atomic weight        |
|--------------|--------|---------------|----------------------|
| Polonium     | Po     | 84            | .....                |
| Potassium    | K      | 19            | 39.102               |
| Praseodymium | Pr     | 59            | 140.907              |
| Promethium   | Pm     | 61            | .....                |
| Protactinium | Pa     | 91            | .....                |
| Radium       | Ra     | 88            | .....                |
| Radon        | Rn     | 86            | .....                |
| Rhenium      | Re     | 75            | 186.2                |
| Rhodium      | Rh     | 45            | 102.905              |
| Rubidium     | Rb     | 37            | 85.47                |
| Ruthenium    | Ru     | 44            | 101.07               |
| Samarium     | Sm     | 62            | 150.35               |
| Scandium     | Sc     | 21            | 44.956               |
| Selenium     | Se     | 34            | 78.96                |
| Silicon      | Si     | 14            | 28.086 <sup>a</sup>  |
| Silver       | Ag     | 47            | 107.870 <sup>b</sup> |
| Sodium       | Na     | 11            | 22.9898              |
| Strontium    | Sr     | 38            | 87.62                |
| Sulfur       | S      | 16            | 32.064 <sup>a</sup>  |
| Tantalum     | Ta     | 73            | 180.948              |
| Technetium   | Tc     | 43            | .....                |
| Tellurium    | Te     | 52            | 127.60               |
| Terbium      | Tb     | 65            | 158.924              |
| Thallium     | Tl     | 81            | 204.37               |
| Thorium      | Th     | 90            | 232.038              |
| Thulium      | Tm     | 69            | 168.934              |
| Tin          | Sn     | 50            | 118.69               |
| Titanium     | Ti     | 22            | 47.90                |
| Tungsten     | W      | 74            | 183.85               |
| Uranium      | U      | 92            | 238.03               |
| Vanadium     | V      | 23            | 50.942               |
| Xenon        | Xe     | 54            | 131.30               |
| Ytterbium    | Yb     | 70            | 173.04               |

| Name      | Symbol | Atomic number | Atomic weight |
|-----------|--------|---------------|---------------|
| Zinc      | Zn     | 30            | 65.37         |
| Zirconium | Zr     | 40            | 91.22         |

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A. E. Cameron and E. Wichers, J. Am. Chem. Soc. 84, 4175-4197 (1962).  
The element symbols, names, and atomic weights (relative atomic masses) are those recommended by the International Union of Pure and Applied Chemistry (1961). The atomic mass unit is 1/12 the mass of the carbon isotope carbon-12.



