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CET93 and CETPC: An Interim Updated Version of the NASA Lewis Computer Program for Calculating Complex Chemical Equilibria With Applications

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Introduction

For more than 40 years the NASA Lewis Research Center has been involved in developing methods and computer programs for calculating complex chemical equilibrium compositions and thermodynamic and transport properties of the equilibrium mixtures and for applying these properties to a number of problems. The latest version of these programs is documented in Gordon et al. (1976, 1984, 1988). Prior to this report the source code has been known most recently as CET89. Two new options have been added to CET89, and the thermodynamic data for many species have been updated. The code containing these changes is now called CET93. The CET93 code, with smaller arrays, has been compiled for use on an IBM or IBM-compatible personal computer and is called CETPC. The source code for CET93 and/or a CETPC diskette of the compiled PC code may be obtained for a fee from COSMIC, 382 E. Broad Street, University of Georgia, Athens, GA 30602 (Tel: 706–542–3265).

This report is intended to be primarily a users manual for CET93 and CETPC. It does not repeat the more complete documentation of the previously mentioned reports, which cover details of capabilities, assumptions, options, and mathematical equations for obtaining chemical equilibrium compositions, mixture properties, rocket performance, shock parameters, and Chapman-Jouguet detonations. However, a brief summary of some of these topics is given.

The discussion in this report covers primarily input and output files, the two new options (ONLY and comments), and implementation of CETPC. The ONLY option permits equilibrium composition calculations to be made that consider only those species which are specified in the input. The comments option permits the user to provide comments in the input and output. The thermodynamic data file includes updated data for many species, such as the reference elements (McBride et al., 1993a) and species in the carbon-hydrogen-oxygen-nitrogen (C–H–O–N) chemical system (McBride et al., 1993b). Input files for 13 example problems are also included with CET93 and CETPC for testing and illustrating some features of the program.

Program Capabilities

Thermodynamic and Thermal Transport Mixture Properties

Chemical equilibrium compositions are obtained by the method of free energy minimization. A thermodynamic state is characterized by two independent state variables, such as temperature and pressure. If pressure is one of the state variables, Gibbs energy is minimized. This is the case for the following combination of variables permitted to be assigned by the program: temperature and pressure (tp), enthalpy and pressure (hp), and entropy and pressure (sp). If volume (or density) is one of the state variables, Helmholtz energy is minimized. This is the case for the following combination of variables permitted by the program: temperature and volume (or density) (tv), internal energy and volume (or density) (uv), and entropy and volume (or density) (sv).

It is assumed that all gases are ideal and that interactions among phases can be neglected. An ideal-gas equation of state is used to represent the mixture and is assumed to be correct even when small amounts of condensed phases are present. Equilibrium properties of plasmas (mixtures containing ionized species) may also be calculated if the plasma is considered to be ideal, that is, if columbic interactions are not considered.

Thermodynamic properties of mixtures include the contribution of condensed as well as gaseous phases. However, thermal transport mixture properties include the contributions of gas-phase species only. If condensed phases are present, mole fractions for the gas-phase species are first normalized to gases only prior to calculating thermal transport mixture properties. The thermodynamic and thermal transport mixture properties calculated by the program are discussed in the section Output.

Rocket, Shock, and Detonation Problems

In addition to calculating equilibrium compositions and mixture properties for the assigned thermodynamic states

previously discussed, CETPC is capable of calculating theoretical rocket performance, shock parameters, and Chapman-Jouguet detonation parameters. Some input options for these application problems are given in the section General Input Instructions. The following is a brief summary of some additional aspects of these calculations.

Rocket performance.—Options are provided for two rocket models—one with an infinite-area combustor (IAC) and the other with a finite-area combustor (FAC) (Gordon et al., 1976, 1984). The IAC model permits both equilibrium and frozen performance. Equilibrium performance assumes that the combustion gases attain instantaneous chemical equilibrium as they flow through the nozzle. Frozen performance assumes that the combustion products remain constant after some specified station in the rocket, such as at the combustor, the throat, or some assigned exit point downstream of the throat. The FAC model permits equilibrium performance only.

Shock parameters.—Options are provided for calculating incident and reflected shocks in a constant-area duct, such as a shock tube. Reactants are limited to gas phase only. Options are also provided for the assumption of equilibrium or frozen composition during the flow of the shocked gases.

Chapman-Jouguet detonations.—Chapman-Jouguet detonations are characterized by the condition that the difference in flow velocity of the shock and flame fronts is the velocity of sound in the burned gases. Reactants are limited to gas phase only.

Initial Estimates, Iteration, and Convergence

Various iteration techniques are used for obtaining equilibrium compositions and solutions to the application problems. Iterations are continued until specified convergence criteria are met.

Equilibrium compositions.—An extremely simple method is used for estimating the first assigned point in any schedule of points. For all points after the first the results of a preceding point serve as initial estimates. A Newton-Raphson iteration procedure is used to obtain corrections to compositions. A control factor, based on several criteria, is used to limit the size of the corrections in order to avoid overcorrecting and ensure convergence. The maximum number of iterations permitted to obtain convergence is initially set by the number of possible species in the chemical system being considered. This maximum number may be modified during the calculations if singularities occur or if the TRACE option (to consider trace species) has been specified in the input. After each composition convergence the program checks for the possible addition or removal of condensed species.

Rocket performance.—Various iteration procedures are used to converge to assigned pressures (or pressure ratios), throat area, assigned area ratios, and, for the FAC model, to contraction ratios or mass flow rate per unit area. For each condition special methods are used to obtain excellent initial estimates in order to minimize the number of iterations required for a solution. In addition, because of these excellent initial estimates, control factors are not needed to limit the size of the iteration corrections.

Shock parameters.—The shock problem in CETPC is limited to gaseous state reactants only. Special procedures are used to obtain excellent initial estimates of temperature and pressure for the incident shock conditions. A control factor is used to limit the size of the iteration corrections. The initial estimate for the reflected shock temperature is simply twice the incident shock temperature. The initial estimate for the reflected shock pressure is obtained from a special formula. Except for high Mach numbers, convergence is often obtained in three to five iterations.

Chapman-Jouguet detonations.—The detonation problem in CETPC is limited to gaseous state reactants only. Special procedures are used to obtain initial estimates for temperature and pressure. A recursion formula is used to improve these estimates in order to provide generally excellent initial estimates prior to the final iteration procedure.

General Input Instructions

Input consists of two general data files and a file for the set of particular problems to be solved. One of the general files contains thermodynamic data for reaction or reactant species (currently 1136 species). The other general file contains thermal transport mixture property data for some of the reaction species (currently 155 species). The thermodynamic and thermal transport data files are in text form for CET93. The program reads these data files and stores the data in binary form (unformatted). See the subsection Outline of Input Preparation for additional input information. For CETPC these data are already in binary form. Three binary files are linked to input/output (I/O) units with OPEN and PARAMETER statements in the source program: thermodynamic data are linked with I/O unit 4; thermal transport data are linked with I/O unit 8; I/O unit 3 is a scratch unit used in processing these data.

Thermodynamic and Thermal Transport Mixture Properties

The thermodynamic data are in the form of least-squares coefficients, which are generated by fitting heat capacity, enthalpy, and entropy simultaneously. Heat capacity is represented by a fourth degree polynomial in temperature. In addition to the coefficients for heat capacity, integration constants are provided to obtain enthalpy and entropy. The temperature range over which the data have been fitted is not the same for all species. For most of the gaseous species in the C–H–O–N

chemical system and for the noble gases the temperature range is 200 to 6000 K. For most of the other gaseous species the temperature range is 300 to 5000 K. The temperature range for each condensed species depends on where phase transitions occur for that species. The names of the 1136 species for which thermodynamic data are provided with the program are listed in appendix A. The sources for these data and a listing of their least-squares coefficients are given in McBride et al. (1993b). When using the ONLY, OMIT, or INSERT options, the names of the species appearing on these records must be exactly as given in appendix A. A maximum of 15 characters is permitted for the name of each species, resulting in the names of a few species being chopped off.

The thermal transport properties (viscosity and thermal conductivity) for the gaseous species are also in the form of least-squares coefficients. The temperature range for these properties is 300 to 5000 K. The equation used to represent the properties and the sources of the data are given in Gordon et al. (1984). The coefficients are given in McBride et al. (1993b).

Outline of Input Preparation

The program permits solving for chemical equilibrium compositions for assigned thermodynamic states, obtaining thermodynamic mixture properties, and applying these properties to the solution of problems such as rocket performance, shocks, and detonations. Some types of input are required for all problems, but other types depend on what options are specified. The following outline is intended to assist the user in preparing input data files. Thirteen example problems are given in appendix B that illustrate some of the many possible options presented in this outline.

I. Comments records
   - A. A "#" is required in column 1.
   - B. Length is limited to 80 characters.
   - C. These records may appear anywhere except within namelist input.

II. Input code records
   - A. An alphameric variable is used to identify the input that follows it.
   - B. Codes are all capital letters starting in column 1.
   - C. Only the first four letters are checked by the program.
   - D. Acceptable codes are as follows (input described more fully below):
     1. THERMO (or THER)—precedes formatted thermodynamic data file.
     2. TRANSPORT (or TRAN)—precedes formatted thermal transport property file.
     3. REACTANTS (or REAC)—precedes set of reactants data.
     4. INSERT (or INSE)—precedes set of names of condensed combustion products to be considered with initial calculations.
     5. ONLY—precedes set of names of species products to be considered. Other possible species in the thermodynamic data file will be ignored.
     6. OMIT—precedes set of names of species to be omitted from consideration.
     7. NAMELISTS (or NAME)—precedes namelist-directed input.

III. Order of input records
   - A. For CET93, text files of thermodynamic and thermal transport properties must be read in first, either by themselves or just ahead of the individual problems. CET93 processes these data and stores the information in binary files. For CETPC this step is unnecessary because the binary files are already available.
   - B. Problems start with a set of reactants records.
   - C. If there are OMIT, ONLY, or INSERT records, they follow reactants.
   - D. Namelist input is next and includes, in order, the NAMELISTS record and the "inpt2" namelist. This is followed by the "rktinp" namelist for rocket problems and the "shkinp" namelist for shock problems.
   - E. The previous records may be followed by the input sets for any number of cases. If the reactants records are the same for two adjacent problems, the second set of reactants may be omitted.

IV. Thermodynamic data files
   - A. Text (formatted) data are read by CET93 from standard input. The first record starts with "THER" and the final record starts with "END."
   - B. The data file is converted by CET93 to binary (unformatted) data, which are stored on I/O unit 4.
   - C. For any particular problem CET93 or CETPC selects the appropriate data from I/O unit 4.

V. Thermal transport property data files
   - A. Text (formatted) data are read by CET93 from standard input. The first record starts with "TRAN" and the final record starts with "LAST."
   - B. The data file is converted by CET93 to binary (unformatted) data, which are stored on I/O unit 8.
   - C. For any particular problem CET93 or CETPC selects the appropriate data from I/O unit 8.

VI. Reactants data
   - A. The first record starts with "REAC" and the final record is blank.
   - B. After the first record, one record of information is required for each reactant according to the following format:

Column	Format	Contents
1–45	5(A2,F7.5)	Chemical formula. Symbols for chemical elements (two columns; first character upper case) start in columns 1, 10, 19, 28, and 37. The numerical values that follow must include decimal points. Note that zeros in columns 37 and 38 cause the program to calculate the enthalpy or internal energy of the species from the thermodynamic data file.
46–52	F7.5	Either number of moles or relative weight of total fuel or oxidant. (Note that all reactants must be either moles or relative weights)
53	A1	"M" if previous number refers to moles; blank if previous number refers to weight. (Reactants for the current problem must have either all blanks or all M's in this column.)
54–62	F9.5	Enthalpy (if "hp" or "rkt" problem) or internal energy (if "uv" problem) in units of calories per mole or joules per mole (see column 71).
63	A1	Phase of the reactant (e.g., "L" for liquid).
64–70	F7.0	Temperature in kelvin for previous enthalpy or internal energy. (Required for reactants with "00" in columns 37 and 38 and optional otherwise.)
71	A1	"J" if enthalpy or internal energy (columns 54–62) is in joules per mole.
72	A1	"O" if reactant is oxidant; "F" otherwise.

VII. INSERT record (or records)
- A. These records specify which condensed species are to be included as possible products for the first point. Species names must be exactly as given in the thermodynamic data file. The names are listed in appendix A.
- B. These records are usually optional but may be required to obtain convergence.
- C. "INSE" starts in column 1. Species names start in columns 16, 31, 46, and 61.

VIII. OMIT record (or records)
- A. These records specify which product species are to be omitted for the current problem. Species names must be exactly as given in the thermodynamic data file (appendix A).
- B. These records are optional. If no ONLY and no OMIT records are included in the input for the current problem, all species in the thermodynamic data file for the chemical system of the problem will be included as possible products.
- C. "OMIT" starts in column 1. Species names start in columns 16, 31, 46, and 61.

IX. ONLY record (or records)
- A. These records specify the only species from the thermodynamic data file that are to be considered in the current problem. Species names must be exactly as given in the thermodynamic data file (appendix A).
- B. These records are optional. If no ONLY and no OMIT records are included in the input for the current problem, all species in the thermodynamic data file for the chemical system of the problem will be included as possible products.
- C. "ONLY" starts in column 1. Species names start in columns 16, 31, 46, and 61.

X. Namelist-directed input (note that the characters (e.g., &, $, /) used to indicate the beginning and end of a namelist set vary with the Fortran compiler)
- A. Namelist "inpt2" (required for all problems)
  1. Logical variables (set appropriate ones to true)
     - (a) tp—Assigned-temperature-and-pressure problem.
     - (b) hp—Assigned-enthalpy-and-pressure problem.
     - (c) sp—Assigned-entropy-and-pressure problem.
     - (d) tv—Assigned-temperature-and-volume (or density) problem.
     - (e) uv—Assigned-internal-energy-and-volume (or density) problem.
     - (f) sv—Assigned-entropy-and-volume (or density) problem.
     - (g) rkt—Rocket problem.
     - (h) shock—Shock problem.
     - (i) detn—Detonation problem.
     - (j) ions—Ionized species are considered.
     - (k) trnspt—Thermal transport properties are calculated.
     - (l) of—Values in "mix" array are oxidant-to-fuel weight ratios.
     - (m) fa—Values in "mix" array are fuel-to-oxidant weight ratios.
     - (n) fpct—Values in "mix" array are percentage of fuel by weight.
     - (o) phi—Values in "mix" array are equivalence ratios defined as ratio of fla to $(fla)_{stoich}$.
     - (p) eratio—Values in "mix" array are equivalence ratios defined in terms of chemical valences.
     - (q) bar—Values in "p" array are in bars.
     - (r) atm—Values in "p" array are in atmospheres.

(s) psia—Values in "p" array are in pounds per square inch absolute.
(t) nsqm—Values in "p" array are in newtons per square meter.
(u) mmhg—Values in "p" array are in millimeters of mercury.
(v) inhg—Values in "p" array are in inches of mercury.
(w) siunit—Output is printed in SI units.

2. Real variables
(a) p—Assigned pressures (1–26 values); for "rkt" problems, assigned chamber pressures.
(b) t—Assigned temperatures (1–26 values) in units of kelvin.
(c) v—Assigned volumes (1–26 values) in units of cubic centimeters per gram.
(d) rho—Assigned densities (1–26 values) in units of grams per cubic centimeter.
(e) mix—Assigned reactant mixture ratios (1–26 values) corresponding to the logical variable set to true (of, fa, fpct, phi, or eratio).
(f) trace—Option to print compositions of species with mole fractions greater than or equal to the assigned trace value.
(g) hr—Assigned enthalpy divided by the universal gas constant R in units of kelvin per gram of mixture (overrides value from reactants records).
(h) ur—Assigned internal energy/R in units of kelvin per gram of mixture (overrides value from reactants records).
(i) s0—Assigned entropy for "sv" problem in units of calories per gram degree kelvin.

3. Integer variables (optional)
(a) kase—Case number to be printed on output tables (one to four digits).
(b) idebug—Intermediate output to be printed for all points greater than or equal to assigned value.

B. Namelist "shkinp" (for shock problems; follows namelist "inpt2" input)
1. Logical variables (set true or false as required)
(a) incdeq—Calculate incident shock parameters assuming equilibrium compositions (default is true).
(b) incdfz—Calculate incident shock parameters assuming frozen compositions (default is true).
(c) refleq—Calculate reflected shock parameters assuming equilibrium compositions (default is false).
(d) reflfz—Calculate reflected shock parameters assuming frozen compositions (default is false).
(e) shkdbg—Print intermediate output for shock iteration procedure.

2. Real variables (assign values to only one of the following)
(a) u1—Shock velocity (1–13 values) in units of meters per second.
(b) mach1—Ratio of shock velocity to the velocity of sound in the shocked gas (1–13 values).

C. Namelist "rktinp" (for rocket problems; follows namelist "inpt2" input)
1. Logical variables (set true or false as required)
(a) eql—Calculate rocket performance assuming equilibrium composition during expansion (default is true).
(b) froz—Calculate rocket performance assuming frozen composition (not available when fac=true; default is true).
(c) fac—Calculate rocket performance assuming finite-area combustion chamber (default is "iac," infinite-area combustion chamber).
(d) debugf—Print intermediate output for the "fac" chamber and throat iteration procedure.

2. Real variables
(a) pcp—Ratio of chamber pressure to exit pressure (not assignable for chamber and throat; 1–22 values).
(b) subar—Subsonic area ratios (1–13 values).
(c) supar—Supersonic area ratios (1–13 values).
(d) ma—ratio of mass flow rate (mdot) to chamber area in units of kilograms per square centimeter per second (set either "ma" or "acat" with fac=true).
(e) acat—Contraction ratio, ratio of finite chamber area to throat area (set either "ma" or "acat" with fac=true).
(f) tcest—Initial chamber temperature estimate in units of kelvin. The default value is 3800 K. (Setting this variable may be necessary only when a condensed species has been inserted on an INSERT record and 3800 K is outside its temperature range.)

3. Integer variable nfz—Option for freezing composition at throat (nfz=2) or a supersonic area ratio (nfz>2) when froz=true. The output table has

equilibrium properties through point nfz and frozen thereafter. If nfz>2, only ncol–nfz additional exit points are allowed (where ncol is 13 for CET93 and 7 for CETPC).

Example Problems

Thirteen examples are given in appendix B to illustrate various types of problems that can be handled by the program and to illustrate many of the possible input options. Each example starts with a number of comments records, which describe the type of problem being solved and give many details concerning the input. The first two examples are for assigned temperatures. Example 1 is for assigned temperatures and pressures (tp=t); example 2 is for assigned temperatures and volumes (tv=t). The input value for volume in example 2 was calculated from the output of example 1. This was done as a check on the internal consistency of the program by verifying that the same output is obtained for examples 1 and 2 when different but consistent input is used. Note that if the thermodynamic data are changed, the results for the examples may vary. Thus, the input for the second example will have to be adjusted to match the output of the first example in order for the properties to match.

Examples 3 to 5 illustrate combustion problems. Example 3 is for constant-pressure combustion, which requires enthalpy and pressure to be assigned (hp=t). Example 4 is for constant-volume (or density) combustion, which requires internal energy and volume (or density) to be assigned (uv=t). As in the case of examples 1 and 2, examples 3 and 4 serve as a check on the internal consistency of the program. This is accomplished by using the example 3 output of density and internal energy as input for example 4. Some adjustment of units is required as explained in the comments records of example 4. Consistency is verified if the same output is obtained for examples 3 and 4 when different but consistent input is used. Example 5 is another constant-pressure combustion problem that is given to illustrate some additional input options.

Example 6 illustrates a Chapman-Jouguet detonation problem (detn=t); example 7 covers a shock problem (shock=t). Six examples of rocket performance calculations (rkt=t) are given in examples 8 to 13. Examples 8 to 10 are all for the same propellants and operating conditions. They permit comparison of results obtained from the assumptions of a finite-area combustor (examples 9 and 10; fac=t) and an infinite-area combustor (example 8). Examples 9 and 10 serve to further illustrate some additional input options. Additional information on these three examples can be found in Gordon and McBride (1988). Examples 11 and 12 illustrate some additional options, such as the inclusion of ionized species in example 11 and freezing composition at the throat in example 12. Example 13 illustrates a special case (which rarely occurs) of a thermodynamic discontinuity at the nozzle throat due to the presence of two phases of the same species. Note that if the thermodynamic data are changed, the discontinuity may no longer occur at the throat for the same conditions. The details of the procedures used to solve this type of situation and a discussion of unusual derivative values, such as $\gamma_s < 1$ (where γ_s is the isentropic exponent), are given in Gordon (1970).

Output

Details of output are given in Gordon et al. (1976, 1984, 1988). For all problems these include headings, composition, thermodynamic and thermal transport mixture properties, thermodynamic derivatives, optional intermediate output covering details of various iteration procedures, and error messages. In addition, each application problem (rocket, shock, and detonation) has its own set of output parameters. Output files for the 13 example problems discussed in the previous section are provided with CET93 and CETPC for comparison and testing.

CETPC Version of CET93

CETPC was reduced in size relative to CET93 in order to run on basic IBM or IBM-compatible personal computers that have only 640K of random-access memory (RAM). The maximum number of possible reaction species that is permitted in any chemical system was reduced from 600 to 300, and the maximum number of condensed reaction species was reduced from 300 to 200. Experience has shown that these limits are sufficient for most practical chemical systems.

CETPC was developed and tested by using MS–DOS on a 386SX machine with 640K of RAM and no floating-point processor. The test cases ran satisfactorily on the minimum system using one floppy drive. The running time for all 13 test cases was 14 min. This time can be considerably reduced by using a faster processor, a floating-point processor, or a hard disk drive. The Fortran source code for CETPC was compiled by using Microsoft Fortran Version 4.1.

The compiled program and accompanying files are available on a 3.5-in. diskette that contains the following: the CETPC executable file, files for thermodynamic data (for 1136 species) and thermal transport mixture property data (for 155 species) in binary form, input and output files for the 13 example problems, and an instruction file for system operation.

Appendix A

Thermodynamic Data Species List

Species ID.	Code	Formula Used by CETPC	Phase	Temp. Range	Mole. Wt.
Electron gas	L10/92	E 1. 0. 0. 0.	G	200.000 6000.000	5.48579903-4
AL	J 6/83	AL 1. 0. 0. 0.	G	200.000 6000.000	26.98154
AL+	J 6/83	AL 1. E -1. 0. 0.	G	298.150 6000.000	26.98099
AL-	J 6/83	AL 1. E 1. 0. 0.	G	298.150 6000.000	26.98209
ALBO2	J 6/66	AL 1. B 1. O 2. 0.	G	300.000 5000.000	69.79134
ALBr	J 9/79	AL 1. BR 1. 0. 0.	G	300.000 5000.000	106.88554
ALBr3	J 9/79	AL 1. BR 3. 0. 0.	G	300.000 5000.000	266.69354
ALC	J 6/63	AL 1. C 1. 0. 0.	G	300.000 5000.000	38.99254
ALCL	J 9/79	AL 1. CL 1. 0. 0.	G	300.000 5000.000	62.43424
ALCL+	J 6/76	AL 1. CL 1. E -1. 0.	G	300.000 5000.000	62.43369
ALCLF	J 6/76	AL 1. CL 1. F 1. 0.	G	300.000 5000.000	81.43264
ALCLF+	J 6/76	AL 1. CL 1. F 1. E -1.	G	300.000 5000.000	81.43209
ALCLF2	J 6/76	AL 1. CL 1. F 2. 0.	G	300.000 5000.000	100.43105
ALCL2	J 6/76	AL 1. CL 2. 0. 0.	G	300.000 5000.000	97.88694
ALCL2+	J 6/76	AL 1. CL 2. E -1. 0.	G	300.000 5000.000	97.88639
ALCL2-	J 6/76	AL 1. CL 2. E 1. 0.	G	300.000 5000.000	97.88749
ALCL2F	J 6/76	AL 1. CL 2. F 1. 0.	G	300.000 5000.000	116.88584
ALCL3	J 9/79	AL 1. CL 3. 0. 0.	G	300.000 5000.000	133.33964
ALF	J 9/79	AL 1. F 1. 0. 0.	G	300.000 5000.000	45.97994
ALF+	J 6/76	AL 1. F 1. E -1. 0.	G	300.000 5000.000	45.97939
ALF2	J 6/76	AL 1. F 2. 0. 0.	G	300.000 5000.000	64.97835
ALF2+	J 6/76	AL 1. F 2. E -1. 0.	G	300.000 5000.000	64.97780
ALF2-	J 6/76	AL 1. F 2. E 1. 0.	G	300.000 5000.000	64.97889
ALF2O	J 6/76	AL 1. F 2. O 1. 0.	G	300.000 5000.000	80.97775
ALF2O-	J 6/76	AL 1. F 2. O 1. E 1.	G	300.000 5000.000	80.97829
ALF3	J 9/79	AL 1. F 3. 0. 0.	G	200.000 6000.000	83.97675
ALF4-	J 6/76	AL 1. F 4. E 1. 0.	G	300.000 5000.000	102.97570
ALH	J 6/68	AL 1. H 1. 0. 0.	G	300.000 5000.000	27.98948
ALI	J 9/79	AL 1. I 1. 0. 0.	G	200.000 6000.000	153.88601
ALI3	J 9/79	AL 1. I 3. 0. 0.	G	300.000 5000.000	407.69495
ALN	J12/79	AL 1. N 1. 0. 0.	G	300.000 5000.000	40.98828
ALO	J12/79	AL 1. O 1. 0. 0.	G	300.000 5000.000	42.98694
ALO+	J12/79	AL 1. O 1. E -1. 0.	G	300.000 5000.000	42.98639
ALO-	J12/79	AL 1. O 1. E 1. 0.	G	300.000 5000.000	42.98149
ALOCL	J 9/64	AL 1. O 1. CL 1. 0.	G	300.000 5000.000	78.43364
ALOF	J12/75	AL 1. O 1. F 1. 0.	G	300.000 5000.000	61.97934
ALOH	J12/67	AL 1. O 1. H 1. 0.	G	300.000 5000.000	43.98888
ALOH+	J12/67	AL 1. O 1. H 1. E -1.	G	300.000 5000.000	43.98833
ALOH-	J12/67	AL 1. O 1. H 1. E 1.	G	300.000 5000.000	43.98943
ALO2	J12/79	AL 1. O 2. 0. 0.	G	300.000 5000.000	58.98834
ALO2-	J12/79	AL 1. O 2. E 1. 0.	G	300.000 5000.000	58.98889
ALO2H	J12/68	AL 1. O 2. H 1. 0.	G	300.000 5000.000	59.98828
ALS	J12/79	AL 1. S 1. 0. 0.	G	200.000 6000.000	59.04754
AL2	J 6/79	AL 2. 0. 0. 0.	G	300.000 5000.000	53.96300
AL2Br6	J 9/79	AL 2. BR 6. 0. 0.	G	300.000 5000.000	533.38700
AL2CL6	J 9/79	AL 2. CL 6. 0. 0.	G	300.000 5000.000	266.67928
AL2F6	J 9/79	AL 2. F 6. 0. 0.	G	300.000 5000.000	167.95350
AL2I6	J 9/79	AL 2. I 6. 0. 0.	G	300.000 5000.000	815.38990
AL2O	J12/79	AL 2. O 1. 0. 0.	G	300.000 5000.000	69.96248
AL2O+	J12/79	AL 2. O 1. E -1. 0.	G	300.000 5000.000	69.96193
AL2O2	J12/79	AL 2. O 2. 0. 0.	G	300.000 5000.000	85.96188
AL2O2+	J12/79	AL 2. O 2. E -1. 0.	G	300.000 5000.000	85.96133
Ar	L 6/88	AR 1. 0. 0. 0.	G	200.000 6000.000	39.94800
Ar+	L10/92	AR 1. E -1. 0. 0.	G	298.150 6000.000	39.94745
B	J 6/83	B 1. 0. 0. 0.	G	200.000 6000.000	10.81100
B+	J 6/83	B 1. E -1. 0. 0.	G	298.150 6000.000	10.81045
B-	J 6/83	B 1. E 1. 0. 0.	G	298.150 6000.000	10.81155
BCL	J12/64	B 1. CL 1. 0. 0.	G	300.000 5000.000	46.26370
BCL+	J 6/68	B 1. CL 1. E -1. 0.	G	300.000 5000.000	46.26315
BCLF	J12/64	B 1. CL 1. F 1. 0.	G	300.000 5000.000	65.26210
BCL2	J 6/72	B 1. CL 2. 0. 0.	G	300.000 5000.000	81.71640
BCL2+	J12/70	B 1. CL 2. E -1. 0.	G	300.000 5000.000	81.71585
BCL2-	J 6/72	B 1. CL 2. E 1. 0.	G	300.000 5000.000	81.71695
BCL3	J12/64	B 1. CL 3. 0. 0.	G	300.000 5000.000	117.16910
BF	J12/64	B 1. F 1. 0. 0.	G	300.000 5000.000	29.80940
BF2	J 6/72	B 1. F 2. 0. 0.	G	300.000 5000.000	48.80781
BF2+	J12/70	B 1. F 2. E -1. 0.	G	300.000 5000.000	48.80726
BF2-	J 6/72	B 1. F 2. E 1. 0.	G	300.000 5000.000	48.80835
BF3	J 6/69	B 1. F 3. 0 0. 0.	G	300.000 5000.000	67.80621
BH	J12/64	B 1. H 1. 0. 0.	G	300.000 5000.000	11.81894

Species ID.	Code	Formula Used by CETPC						Phase		Temp. Range		Mole. Wt.
BHF2	J12/65	B	1.	H	1.	F	2.	0.	G	300.000	5000.000	49.81575
BH2	J12/64	B	1.	H	2.		0.	0.	G	300.000	5000.000	12.82685
BH3	J12/64	B	1.	H	3.		0.	0.	G	300.000	5000.000	13.83482
BN	J 6/66	B	1.	N	1.		0.	0.	G	300.000	5000.000	24.81774
BO	J 6/68	B	1.	O	1.		0.	0.	G	300.000	5000.000	26.81046
BOCL	J12/65	B	1.	O	1.	CL	1.	0.	G	300.000	5000.000	62.26316
BOF	J12/65	B	1.	O	1.	F	1.	0.	G	200.000	6000.000	45.80886
BOF2	J12/66	B	1.	O	1.	F	2.	0.	G	300.000	5000.000	64.80721
BO2	J 6/68	B	1.	O	2.		0.	0.	G	300.000	5000.000	42.80986
BO2-	J12/68	B	1.	O	2.	E	1.	0.	G	300.000	5000.000	42.81036
BS	J 6/72	B	1.	S	1.		0.	0.	G	300.000	5000.000	42.87706
B2	J 3/79	B	2.		0.		0.	0.	G	200.000	6000.000	21.62206
B2O	J 6/68	B	2.	O	1.		0.	0.	G	300.000	5000.000	37.62146
B2O2	J12/64	B	2.	O	2.		0.	0.	G	300.000	5000.000	53.62086
B2O3	J 6/71	B	2.	O	3.		0.	0.	G	300.000	5000.000	69.62026
B3O3CL3	J 3/65	B	3.	O	3.	CL	3.	0.	G	300.000	5000.000	186.78936
B3O3F3	J 3/65	B	3.	O	3.	F	3.	0.	G	300.000	5000.000	137.42641
B3O3H3	J 3/65	B	3.	O	3.	H	3.	0.	G	200.000	6000.000	83.45502
Ba	J12/70	BA	1.		0.		0.	0.	G	300.000	5000.000	137.32706
BaBr	J12/74	BA	1.	BR	1.		0.	0.	G	300.000	5000.000	217.23106
BaBr2	J12/74	BA	1.	BR	2.		0.	0.	G	300.000	5000.000	297.13506
BaCL	J12/72	BA	1.	CL	1.		0.	0.	G	300.000	5000.000	172.77976
BaCL2	J12/72	BA	1.	CL	2.		0.	0.	G	300.000	5000.000	208.23246
BaF	J12/72	BA	1.	F	1.		0.	0.	G	300.000	5000.000	156.32546
BaF+	J12/72	BA	1.	F	1.	E	-1.	0.	G	300.000	5000.000	156.32486
BaF2	J12/72	BA	1.	F	2.		0.	0.	G	300.000	5000.000	175.32381
BaOH	J12/75	BA	1.	O	1.	H	1.	0.	G	300.000	5000.000	154.33434
BaOH+	J 6/76	BA	1.	O	1.	H	1.	E -1.	G	300.000	5000.000	154.33376
BaO2H2	J12/75	BA	1.	O	2.	H	2.	0.	G	300.000	5000.000	171.34166
BaS	J 9/77	BA	1.	S	1.		0.	0.	G	300.000	5000.000	169.39306
Be	J 9/83	BE	1.		0.		0.	0.	G	200.000	6000.000	9.01216
Be+	J 9/83	BE	1.	E	-1.		0.	0.	G	298.150	6000.000	9.01163
BeBO2	J 6/66	BE	1.	B	1.	O	2.	0.	G	300.000	5000.000	51.82196
BeBr	J 6/75	BE	1.	BR	1.		0.	0.	G	300.000	5000.000	88.91616
BeBr2	J 6/75	BE	1.	BR	2.		0.	0.	G	300.000	5000.000	168.82016
BeCL	J 9/66	BE	1.	CL	1.		0.	0.	G	300.000	5000.000	44.46486
BeCL+	J 6/68	BE	1.	CL	1.	E	-1.	0.	G	300.000	5000.000	44.46433
BeCLF	J 6/65	BE	1.	CL	1.	F	1.	0.	G	300.000	5000.000	63.46325
BeCL2	J 6/65	BE	1.	CL	2.		0.	0.	G	300.000	5000.000	79.91756
BeF	J12/71	BE	1.	F	1.		0.	0.	G	300.000	5000.000	28.01055
BeF2	J 6/70	BE	1.	F	2.		0.	0.	G	300.000	5000.000	47.00895
BeH	J 3/63	BE	1.	H	1.		0.	0.	G	300.000	5000.000	10.02012
BeH+	J 9/66	BE	1.	H	1.	E	-1.	0.	G	300.000	5000.000	10.01957
BeI	J12/75	BE	1.	I	1.		0.	0.	G	300.000	5000.000	135.91666
BeI2	J12/75	BE	1.	I	2.		0.	0.	G	300.000	5000.000	262.82112
BeN	J 6/63	BE	1.	N	1.		0.	0.	G	300.000	5000.000	23.01892
BeO	J12/74	BE	1.	O	1.		0.	0.	G	200.000	6000.000	25.01156
BeOH	J12/75	BE	1.	O	1.	H	1.	0.	G	300.000	5000.000	26.01952
BeOH+	J12/75	BE	1.	O	1.	H	1.	E -1.	G	300.000	5000.000	26.01897
BeO2H2	J12/75	BE	1.	O	2.	H	2.	0.	G	300.000	5000.000	43.02686
BeS	J 9/77	BE	1.	S	1.		0.	0.	G	300.000	5000.000	41.07816
Be2O	J 9/63	BE	2.	O	1.		0.	0.	G	300.000	5000.000	34.02376
Be2OF2	J 6/66	BE	2.	O	1.	F	2.	0.	G	300.000	5000.000	72.02057
Be2O2	J 9/63	BE	2.	O	2.		0.	0.	G	300.000	5000.000	50.02316
Be3O3	J 9/63	BE	3.	O	3.		0.	0.	G	300.000	5000.000	75.03476
Be4O4	J 9/63	BE	4.	O	4.		0.	0.	G	300.000	5000.000	100.04633
Br	J 6/82	BR	1.		0.		0.	0.	G	200.000	6000.000	79.90408
Br2	TPIS89	BR	2.		0.		0.	0.	G	200.000	6000.000	159.80806
C	L11/88	C	1.		0.		0.	0.	G	200.000	6000.000	12.01106
C+	L 7/88	C	1.	E	-1.		0.	0.	G	298.150	6000.000	12.01045
C-	TPIS91	C	1.	E	1.		0.	0.	G	298.150	6000.000	12.01155
CCL	J12/69	C	1.	CL	1.		0.	0.	G	300.000	5000.000	47.46376
CCLF3	L12/77	C	1.	CL	1.	F	3.	0.	G	298.150	5000.000	104.45891
CCL2	J12/68	C	1.	CL	2.		0.	0.	G	300.000	5000.000	82.91646
CCL2F2	L12/77	C	1.	CL	2.	F	2.	0.	G	298.150	5000.000	120.91321
CCL3	J 6/70	C	1.	CL	3.		0.	0.	G	300.000	5000.000	118.36916
CCL3F	L12/77	C	1.	CL	3.	F	1.	0.	G	298.150	5000.000	137.36756
CCL4	L12/81	C	1.	CL	4.		0.	0.	G	298.150	5000.000	153.82186
CF	J 6/70	C	1.	F	1.		0.	0.	G	300.000	5000.000	31.00946
CF+	J12/70	C	1.	F	1.	E	-1.	0.	G	200.000	6000.000	31.00886
CF2	J 6/70	C	1.	F	2.		0.	0.	G	300.000	5000.000	50.00781
CF2+	J12/70	C	1.	F	2.	E	-1.	0.	G	300.000	5000.000	50.00726
CF3	J 6/69	C	1.	F	3.		0.	0.	G	300.000	5000.000	69.00621
CF3+	J12/71	C	1.	F	3.	E	-1.	0.	G	300.000	5000.000	69.00566
CF4	L 6/83	C	1.	F	4.		0.	0.	G	200.000	6000.000	88.00461

Species ID.	Code	Formula Used by CETPC								Phase	Temp. Range		Mole. Wt.
CH	TPIS79	C	1.	H	1.		0.		0.	G	200.000	6000.000	13.01894
CH+	TPIS91	C	1.	H	1.	E	-1.		0.	G	298.150	6000.000	13.01839
CHCL	TPIS79	C	1.	H	1.	CL	1.		0.	G	298.150	5000.000	48.47164
CHCLF2	L12/77	C	1.	H	1.	CL	1.	F	2.	G	298.150	5000.000	86.46845
CHCL2F	L12/77	C	1.	H	1.	CL	2.	F	1.	G	298.150	5000.000	102.92274
CHCL3	X 6/81	C	1.	H	1.	CL	3.		0.	G	298.150	5000.000	119.37704
CHF3	L 6/81	C	1.	H	1.	F	3.		0.	G	298.150	5000.000	70.01416
CH2	L11/89	C	1.	H	2.		0.		0.	G	200.000	6000.000	14.02686
CH2CLF	L12/77	C	1.	H	2.	CL	1.	F	1.	G	298.150	5000.000	68.47796
CH2CL2	L12/81	C	1.	H	2.	CL	2.		0.	G	298.150	5000.000	84.93226
CH2F2	L 6/81	C	1.	H	2.	F	2.		0.	G	298.150	5000.000	52.02369
CH3	L11/89	C	1.	H	3.		0.		0.	G	200.000	6000.000	15.03482
CH3CL	L12/81	C	1.	H	3.	CL	1.		0.	G	298.150	5000.000	50.48752
CH3F	L 6/81	C	1.	H	3.	F	1.		0.	G	298.150	5000.000	34.03322
CH2OH	L12/92	C	1.	H	3.	O	1.		0.	G	200.000	6000.000	31.03422
CH3O	L10/92	C	1.	H	3.	O	1.		0.	G	200.000	6000.000	31.03422
CH4	L 8/88	C	1.	H	4.		0.		0.	G	200.000	6000.000	16.04276
CH3OH	L 8/88	C	1.	H	4.	O	1.		0.	G	200.000	6000.000	32.04216
CN	TPIS91	C	1.	N	1.		0.		0.	G	200.000	6000.000	26.01774
CN+	TPIS91	C	1.	N	1.	E	-1.		0.	G	298.150	6000.000	26.01719
CN-	L10/92	C	1.	N	1.	E	1.		0.	G	298.150	6000.000	26.01829
CNN	L12/89	C	1.	N	2.		0.		0.	G	200.000	6000.000	40.02446
CO	TPIS79	C	1.	O	1.		0.		0.	G	200.000	6000.000	28.01046
CO+	TPIS91	C	1.	O	1.	E	-1.		0.	G	298.150	6000.000	28.00986
COCL	J12/65	C	1.	O	1.	CL	1.		0.	G	300.000	5000.000	63.46316
COCLF	J 6/61	C	1.	O	1.	CL	1.	F	1.	G	300.000	5000.000	82.46156
COCL2	TPIS91	C	1.	O	1.	CL	2.		0.	G	200.000	6000.000	98.91586
COF	J12/65	C	1.	O	1.	F	1.		0.	G	300.000	5000.000	47.00886
COF2	TPIS91	C	1.	O	1.	F	2.		0.	G	200.000	6000.000	66.00721
COS	J 3/61	C	1.	O	1.	S	1.		0.	G	300.000	5000.000	60.07646
CO2	L 7/88	C	1.	O	2.		0.		0.	G	200.000	6000.000	44.00986
CO2+	L10/92	C	1.	O	2.	E	-1.		0.	G	298.150	6000.000	44.00926
COOH	TPIS91	C	1.	O	2.	H	1.		0.	G	200.000	6000.000	45.01774
CP	L 9/93	C	1.	P	1.		0.		0.	G	200.000	6000.000	42.98476
CS	J12/76	C	1.	S	1.		0.		0.	G	300.000	5000.000	44.07706
CS2	J12/76	C	1.	S	2.		0.		0.	G	300.000	5000.000	76.14306
C2	TPIS91	C	2.		0.		0.		0.	G	200.000	6000.000	24.02206
C2+	TPIS91	C	2.	E	-1.		0.		0.	G	298.150	6000.000	24.02146
C2-	TPIS91	C	2.	E	1.		0.		0.	G	298.150	6000.000	24.02256
C2CL2	J12/68	C	2.	CL	2.		0.		0.	G	300.000	5000.000	94.92746
C2CL4	L10/87	C	2.	CL	4.		0.		0.	G	298.150	5000.000	165.83286
C2CL6	L10/87	C	2.	CL	6.		0.		0.	G	298.150	5000.000	236.73826
C2F2	J12/67	C	2.	F	2.		0.		0.	G	300.000	5000.000	62.01881
C2F4	J 6/69	C	2.	F	4.		0.		0.	G	300.000	5000.000	100.01561
C2H	L 1/91	C	2.	H	1.		0.		0.	G	200.000	6000.000	25.02994
C2HCL	TPIS91	C	2.	H	1.	CL	1.		0.	G	298.150	5000.000	60.48264
C2HF	J12/67	C	2.	H	1.	F	1.		0.	G	300.000	5000.000	44.02834
CHCO,ketyl	L 6/89	C	2.	H	1.	O	1.		0.	G	200.000	6000.000	41.02934
C2H2	L 1/91	C	2.	H	2.		0.		0.	G	200.000	6000.000	26.03788
C2H2,vinylidene	L12/89	C	2.	H	2.		0.		0.	G	200.000	6000.000	26.03788
CH2CO,ketene	L 5/90	C	2.	H	2.	O	1.		0.	G	200.000	6000.000	42.03728
C2H3,vinyl	L 2/92	C	2.	H	3.		0.		0.	G	200.000	6000.000	27.04582
CH3CN	L12/92	C	2.	H	3.	N	1.		0.	G	200.000	6000.000	41.05256
CH3CO,acetyl	BUR 84	C	2.	H	3.	O	1.		0.	G	300.000	5000.000	43.04522
C2H4	L 1/91	C	2.	H	4.		0.		0.	G	200.000	6000.000	28.05376
C2H4O,ethylen o	L 8/88	C	2.	H	4.	O	1.		0.	G	200.000	6000.000	44.05316
CH3CHO,ethanal	L 8/88	C	2.	H	4.	O	1.		0.	G	200.000	6000.000	44.05316
CH3COOH	L 8/88	C	2.	H	4.	O	2.		0.	G	200.000	6000.000	60.05256
(HCOOH)2	BUR 92	C	2.	H	4.	O	4.		0.	G	300.000	5000.000	92.05136
C2H5	L12/92	C	2.	H	5.		0.		0.	G	200.000	6000.000	29.06176
C2H6	L 8/88	C	2.	H	6.		0.		0.	G	200.000	6000.000	30.06964
CH3N2CH3	L 8/88	C	2.	H	6.	N	2.		0.	G	200.000	6000.000	58.08312
CH3OCH3	L12/92	C	2.	H	6.	O	1.		0.	G	200.000	6000.000	46.06904
C2H5OH	L 8/88	C	2.	H	6.	O	1.		0.	G	200.000	6000.000	46.06904
CCN	L12/92	C	2.	N	1.		0.		0.	G	200.000	6000.000	38.02874
CNC	TPIS91	C	2.	N	1.		0.		0.	G	200.000	6000.000	38.02874
C2N2	TPIS79	C	2.	N	2.		0.		0.	G	200.000	6000.000	52.03548
C2O	L12/89	C	2.	O	1.		0.		0.	G	200.000	6000.000	40.02146
C3	TPIS79	C	3.		0.		0.		0.	G	200.000	6000.000	36.03306
C3H3,propargyl	BUR 92	C	3.	H	3.		0.		0.	G	200.000	6000.000	39.05682
C3H4,allene	L12/92	C	3.	H	4.		0.		0.	G	200.000	6000.000	40.06476
C3H4,propyne	L12/92	C	3.	H	4.		0.		0.	G	200.000	6000.000	40.06476
C3H4,cyclo-	L 5/90	C	3.	H	4.		0.		0.	G	200.000	6000.000	40.06476
C3H5,allyl	BUR 92	C	3.	H	5.		0.		0.	G	200.000	6000.000	41.07276
C3H6,propylene	L 7/90	C	3.	H	6.		0.		0.	G	200.000	6000.000	42.08064

Species ID.	Code	Formula Used by CETPC						Phase	Temp. Range		Mole. Wt.
C3H6,cyclo-	L 1/93	C	3.	H	6.		0.	0. G	200.000	6000.000	42.08064
C3H6O	L 6/90	C	3.	H	6.	O	1.	0. G	200.000	6000.000	58.08004
C3H7,n-propyl	L 6/90	C	3.	H	7.		0.	0. G	200.000	6000.000	43.08858
C3H7,i-propyl	L 9/85	C	3.	H	7.		0.	0. G	200.000	6000.000	43.08858
C3H8	L 6/90	C	3.	H	8.		0.	0. G	200.000	6000.000	44.09652
C3H8O,1propanol	L 9/88	C	3.	H	8.	O	1.	0. G	200.000	6000.000	60.09592
C3H8O,2propanol	L 9/88	C	3.	H	8.	O	1.	0. G	200.000	6000.000	60.09592
C3O2	L 7/88	C	3.	O	2.		0.	0. G	200.000	6000.000	68.03180
C4	L 7/88	C	4.		0.		0.	0. G	200.000	6000.000	48.04400
C4H2	L 2/93	C	4.	H	2.		0.	0. G	200.000	6000.000	50.05988
C4H4,1,3-cyclo-	L 5/90	C	4.	H	4.		0.	0. G	200.000	6000.000	52.07576
C4H6,butadiene	X10/92	C	4.	H	6.		0.	0. G	200.000	6000.000	54.09164
C4H6,2-butyne	X10/88	C	4.	H	6.		0.	0. G	200.000	6000.000	54.09164
C4H6,cyclo-	L 5/90	C	4.	H	6.		0.	0. G	200.000	6000.000	54.09164
C4H8,1-butene	X 4/88	C	4.	H	8.		0.	0. G	200.000	6000.000	56.10752
C4H8,cis2-buten	X 4/88	C	4.	H	8.		0.	0. G	200.000	6000.000	56.10752
C4H8,tr2-butene	X 4/88	C	4.	H	8.		0.	0. G	200.000	6000.000	56.10752
C4H8,isobutene	X 4/88	C	4.	H	8.		0.	0. G	200.000	6000.000	56.10752
C4H8,cyclo-	L 5/90	C	4.	H	8.		0.	0. G	200.000	6000.000	56.10752
(CH3COOH)2	L 6/90	C	4.	H	8.	O	4.	0. G	200.000	6000.000	120.10512
C4H9,n-butyl	X10/84	C	4.	H	9.		0.	0. G	200.000	6000.000	57.11546
C4H9,i-butyl	X10/84	C	4.	H	9.		0.	0. G	200.000	6000.000	57.11546
C4H9,s-butyl	L 1/93	C	4.	H	9.		0.	0. G	200.000	6000.000	57.11546
C4H9,t-butyl	L 1/93	C	4.	H	9.		0.	0. G	200.000	6000.000	57.11546
C4H10,isobutane	L 6/90	C	4.	H	10.		0.	0. G	200.000	6000.000	58.12340
C4H10,n-butane	L 6/90	C	4.	H	10.		0.	0. G	200.000	6000.000	58.12340
C4N2	J 3/61	C	4.	N	2.		0.	0. G	200.000	6000.000	76.05748
C5	L 7/88	C	5.		0.		0.	0. G	200.000	6000.000	60.05500
C5H6,1,3cyclo-	L 5/90	C	5.	H	6.		0.	0. G	200.000	6000.000	66.10264
C5H8,cyclo-	L 1/93	C	5.	H	8.		0.	0. G	200.000	6000.000	68.11852
C5H10,1-pentene	X 4/87	C	5.	H	10.		0.	0. G	200.000	6000.000	70.13440
C5H10,cyclo-	L 6/90	C	5.	H	10.		0.	0. G	200.000	6000.000	70.13440
C5H11,pentyl	X10/84	C	5.	H	11.		0.	0. G	200.000	6000.000	71.14234
C5H11,t-pentyl	L 1/93	C	5.	H	11.		0.	0. G	200.000	6000.000	71.14234
C5H12,n-pentane	X10/85	C	5.	H	12.		0.	0. G	298.150	5000.000	72.15028
C5H12,i-pentane	X10/85	C	5.	H	12.		0.	0. G	298.150	5000.000	72.15028
CH3C(CH3)2CH3	X10/85	C	5.	H	12.		0.	0. G	298.150	5000.000	72.15028
C6H2	L 2/93	C	6.	H	2.		0.	0. G	200.000	6000.000	74.08188
C6H5,phenyl	L 1/91	C	6.	H	5.		0.	0. G	200.000	6000.000	77.10570
C6D6	L12/84	C	6.	D	6.		0.	0. G	300.000	5000.000	82.13651
C6H5O,phenoxy	L 6/90	C	6.	H	5.	O	1.	0. G	200.000	6000.000	93.10510
C6H6	L 1/91	C	6.	H	6.		0.	0. G	200.000	6000.000	78.11364
C6D6	L12/84	C	6.	D	6.		0.	0. G	300.000	5000.000	84.15061
C6H5OH,phenol	L 6/90	C	6.	H	6.	O	1.	0. G	200.000	6000.000	94.11304
C6H10,cyclo-	L 1/93	C	6.	H	10.		0.	0. G	200.000	6000.000	82.14548
C6H12,1-hexene	X 4/87	C	6.	H	12.		0.	0. G	200.000	6000.000	84.16128
C6H12,cyclo-	L 6/90	C	6.	H	12.		0.	0. G	200.000	6000.000	84.16128
C6H13,n-hexyl	X10/83	C	6.	H	13.		0.	0. G	200.000	6000.000	85.16922
C7H7,benzyl	L 1/93	C	7.	H	7.		0.	0. G	200.000	6000.000	91.13258
C7H8	L 1/93	C	7.	H	8.		0.	0. G	200.000	6000.000	92.14052
C7H8O,cresol mx	L 1/93	C	7.	H	8.	O	1.	0. G	200.000	6000.000	108.13992
C7H14,1-heptene	X 4/87	C	7.	H	14.		0.	0. G	200.000	6000.000	98.18816
C7H15,n-heptyl	X10/83	C	7.	H	15.		0.	0. G	200.000	6000.000	99.19610
C7H16,n-heptane	X10/85	C	7.	H	16.		0.	0. G	200.000	6000.000	100.20404
C8H8,styrene	X 4/89	C	8.	H	8.		0.	0. G	200.000	6000.000	104.15152
C8H10,ethylbenz	X10/86	C	8.	H	10.		0.	0. G	200.000	6000.000	106.16740
C8H16,1-octene	X 4/87	C	8.	H	16.		0.	0. G	200.000	6000.000	112.21504
C8H17,n-octyl	X10/83	C	8.	H	17.		0.	0. G	200.000	6000.000	113.22298
C8H18,isooctane	X 4/85	C	8.	H	18.		0.	0. G	200.000	6000.000	114.23092
C8H18,n-octane	X 4/85	C	8.	H	18.		0.	0. G	200.000	6000.000	114.23092
C9H19,n-nonyl	X10/83	C	9.	H	19.		0.	0. G	298.150	5000.000	127.24986
C10H8,naphthale	L 8/93	C	10.	H	8.		0.	0. G	200.000	6000.000	128.17352
C10H21,n-decyl	X10/83	C	10.	H	21.		0.	0. G	298.150	5000.000	141.27674
C12H9,o-bipheny	L12/84	C	12.	H	9.		0.	0. G	200.000	6000.000	153.20346
O-C12D9	L12/84	C	12.	D	9.		0.	0. G	300.000	5000.000	162.25892
C12H10,biphenyl	L12/84	C	12.	H	10.		0.	0. G	200.000	6000.000	154.21140
C12D10	L12/84	C	12.	D	10.		0.	0. G	300.000	5000.000	164.27302
Jet-A(g)	L 6/88	C	12.	H	23.		0.	0. G	273.150	5000.000	167.31462
Ca	L 3/93	CA	1.		0.		0.	0. G	200.000	6000.000	40.07800
Ca+	J 9/83	CA	1.	E	-1.		0.	0. G	298.150	6000.000	40.07745
CaBr	J12/74	CA	1.	BR	1.		0.	0. G	300.000	5000.000	119.98200
CaBr2	J 6/74	CA	1.	BR	2.		0.	0. G	300.000	5000.000	199.88600
CaCL	J 6/70	CA	1.	CL	1.		0.	0. G	300.000	5000.000	75.53070
CaCL2	J 6/70	CA	1.	CL	2.		0.	0. G	300.000	5000.000	110.98340

Species ID.	Code	Formula Used by CETPC							Phase	Temp. Range		Mole. Wt.
CaF	J12/68	CA	1.	F	1.		0.	0.	G	300.000	5000.000	59.07640
CaF2	J12/68	CA	1.	F	2.		0.	0.	G	300.000	5000.000	78.07481
CaI	J 6/74	CA	1.	I	1.		0.	0.	G	300.000	5000.000	166.98247
CaI2	J 6/74	CA	1.	I	2.		0.	0.	G	300.000	5000.000	293.88694
CaO	J12/74	CA	1.	O	1.		0.	0.	G	300.000	5000.000	56.07740
CaOH	J12/75	CA	1.	O	1.	H	1.	0.	G	300.000	5000.000	57.08534
CaOH+	J12/75	CA	1.	O	1.	H	1.	E -1.	G	300.000	5000.000	57.08479
CaO2H2	J12/75	CA	1.	O	2.	H	2.	0.	G	300.000	5000.000	74.09268
CaS	J 9/77	CA	1.	S	1.		0.	0.	G	298.150	5000.000	72.14400
Ca2	J 9/83	CA	2.		0.		0.	0.	G	200.000	6000.000	80.15600
CL	J 6/82	CL	1.		0.		0.	0.	G	200.000	6000.000	35.45270
CL+	J 6/82	CL	1.	E	-1.		0.	0.	G	298.150	6000.000	35.45215
CL-	J 6/82	CL	1.	E	1.		0.	0.	G	298.150	6000.000	35.45325
CLCN	J 6/66	CL	1.	C	1.	N	1.	0.	G	300.000	5000.000	61.47044
CLF	J 6/77	CL	1.	F	1.		0.	0.	G	300.000	5000.000	54.45110
CLF3	J 9/65	CL	1.	F	3.		0.	0.	G	300.000	5000.000	92.44791
CLO	J 6/61	CL	1.	O	1.		0.	0.	G	300.000	5000.000	51.45210
CLO2	L 7/93	CL	1.	O	2.		0.	0.	G	200.000	6000.000	67.45150
CL2	TPIS89	CL	2.		0.		0.	0.	G	200.000	6000.000	70.90540
CL2O	J12/65	CL	2.	O	1.		0.	0.	G	300.000	5000.000	86.90480
Cr	J 6/79	CR	1.		0.		0.	0.	G	200.000	6000.000	51.99610
CrN	J12/73	CR	1.	N	1.		0.	0.	G	300.000	5000.000	66.00284
CrO	J12/73	CR	1.	O	1.		0.	0.	G	300.000	5000.000	67.99550
CrO2	J12/73	CR	1.	O	2.		0.	0.	G	300.000	5000.000	83.99490
CrO3	J12/73	CR	1.	O	3.		0.	0.	G	300.000	5000.000	99.99430
Cs	L 3/93	CS	1.		0.		0.	0.	G	200.000	6000.000	132.90543
Cs+	J12/83	CS	1.	E	-1.		0.	0.	G	298.150	6000.000	132.90488
CsCL	J 6/68	CS	1.	CL	1.		0.	0.	G	300.000	5000.000	168.35813
CsF	J 6/68	CS	1.	F	1.		0.	0.	G	300.000	5000.000	151.90383
CsO	J12/68	CS	1.	O	1.		0.	0.	G	300.000	5000.000	148.90483
CsOH	J 6/71	CS	1.	O	1.	H	1.	0.	G	300.000	5000.000	149.91277
CsOH+	J12/71	CS	1.	O	1.	H	1.	E -1.	G	300.000	5000.000	149.91222
Cs2	J12/83	CS	2.		0.		0.	0.	G	200.000	6000.000	265.81086
Cs2CL2	J 6/68	CS	2.	CL	2.		0.	0.	G	300.000	5000.000	336.71626
Cs2F2	J 6/68	CS	2.	F	2.		0.	0.	G	300.000	5000.000	303.80767
Cs2O	J12/68	CS	2.	O	1.		0.	0.	G	300.000	5000.000	281.81026
Cs2O2H2	J 6/71	CS	2.	O	2.	H	2.	0.	G	300.000	5000.000	299.82554
Cs2SO4	J 6/79	CS	2.	S	1.	O	4.	0.	G	300.000	5000.000	361.87446
Cu	J 9/84	CU	1.		0.		0.	0.	G	200.000	6000.000	63.54600
Cu+	J 9/84	CU	1.	E	-1.		0.	0.	G	298.150	6000.000	63.54545
CuCL	J 3/66	CU	1.	CL	1.		0.	0.	G	300.000	5000.000	98.99878
CuF	J12/77	CU	1.	F	1.		0.	0.	G	300.000	5000.000	82.54440
CuF2	J12/77	CU	1.	F	2.		0.	0.	G	300.000	5000.000	101.54281
CuO	J12/77	CU	1.	O	1.		0.	0.	G	300.000	5000.000	79.54540
Cu2	J 9/66	CU	2.		0.		0.	0.	G	300.000	5000.000	127.09200
Cu3CL3	J 3/66	CU	3.	CL	3.		0.	0.	G	300.000	5000.000	296.99610
D	J 3/82	D	1.		0.		0.	0.	G	200.000	6000.000	2.01410
D+	J 3/82	D	1.	E	-1.		0.	0.	G	298.150	6000.000	2.01355
D-	J 3/82	D	1.	E	1.		0.	0.	G	298.150	6000.000	2.01465
DCL	J 6/77	D	1.	CL	1.		0.	0.	G	300.000	5000.000	37.46680
DF	J 6/77	D	1.	F	1.		0.	0.	G	300.000	5000.000	21.01251
DOCL	J 3/79	D	1.	O	1.	CL	1.	0.	G	300.000	5000.000	53.46620
D2	TPIS89	D	2.		0.		0.	0.	G	200.000	6000.000	4.02820
D2+	J 9/77	D	2.	E	-1.		0.	0.	G	300.000	5000.000	4.02766
D2-	J 9/77	D	2.	E	1.		0.	0.	G	300.000	5000.000	4.02875
D2O	J 6/77	D	2.	O	1.		0.	0.	G	300.000	5000.000	20.02760
D2S	J 6/77	D	2.	S	1.		0.	0.	G	300.000	5000.000	36.09420
F	J 6/82	F	1.		0.		0.	0.	G	200.000	6000.000	18.99840
F+	J 6/82	F	1.	E	-1.		0.	0.	G	298.150	6000.000	18.99785
F-	J 6/82	F	1.	E	1.		0.	0.	G	298.150	6000.000	18.99895
FCN	J 6/69	F	1.	C	1.	N	1.	0.	G	300.000	5000.000	45.01614
FO	J12/66	F	1.	O	1.		0.	0.	G	300.000	5000.000	34.99780
FO2	J 9/66	F	1.	O	2.		0.	0.	G	300.000	5000.000	50.99720
F2	TPIS89	F	2.		0.		0.	0.	G	200.000	6000.000	37.99681
F2O	J12/69	F	2.	O	1.		0.	0.	G	300.000	5000.000	53.99621
FS2F,fluorodisu	J 6/76	F	2.	S	2.		0.	0.	G	200.000	6000.000	182.11681
Fe	J 3/78	FE	1.		0.		0.	0.	G	200.000	6000.000	55.84700
Fe+	J 6/84	FE	1.	E	-1.		0.	0.	G	298.150	6000.000	55.84645
Fe-	J 6/84	FE	1.	E	1.		0.	0.	G	298.150	6000.000	55.84755
FeC5O5	J 3/78	FE	1.	C	5.	O	5.	0.	G	300.000	5000.000	195.89900
FeCL	J 6/65	FE	1.	CL	1.		0.	0.	G	300.000	5000.000	91.29978
FeCL2	J12/70	FE	1.	CL	2.		0.	0.	G	300.000	5000.000	126.75246
FeCL3	J 6/65	FE	1.	CL	3.		0.	0.	G	300.000	5000.000	162.20514
FeO	J 9/66	FE	1.	O	1.		0.	0.	G	300.000	5000.000	71.84644

Species ID.	Code	Formula Used by CETPC								Phase	Temp. Range		Mole. Wt.
Fe(OH)2	J12/66	FE	1.	O	2.	H	2.		0.	G	200.000	6000.000	89.86168
Fe2CL4	J12/70	FE	2.	CL	4.		0.		0.	G	300.000	5000.000	253.50488
Fe2CL6	J 6/65	FE	2.	CL	6.		0.		0.	G	200.000	6000.000	324.41028
H	L 5/93	H	1.		0.		0.		0.	G	200.000	6000.000	1.00794
H+	L 7/88	H	1.	E	-1.		0.		0.	G	298.150	6000.000	1.00739
H-	L/7/88	H	1.	E	1.		0.		0.	G	298.150	6000.000	1.00849
HALO	J 3/64	H	1.	AL	1.	O	1.		0.	G	300.000	5000.000	43.98886
HBO	J12/75	H	1.	B	1.	O	1.		0.	G	300.000	5000.000	27.81834
HBO+	J12/75	H	1.	B	1.	O	1.	E	-1.	G	300.000	5000.000	27.81779
HBO-	J12/75	H	1.	B	1.	O	1.	E	1.	G	300.000	5000.000	27.81889
HBO2	J12/64	H	1.	B	1.	O	2.		0.	G	300.000	5000.000	43.81774
HBS	J12/75	H	1.	B	1.	S	1.		0.	G	300.000	5000.000	43.88494
HBS+	J12/75	H	1.	B	1.	S	1.	E	-1.	G	300.000	5000.000	43.88439
HBr	J 9/65	H	1.	BR	1.		0.		0.	G	300.000	5000.000	80.91194
HCN	L 7/88	H	1.	C	1.	N	1.		0.	G	200.000	6000.000	27.02568
HCO	L12/89	H	1.	C	1.	O	1.		0.	G	200.000	6000.000	29.01834
HCO+	J12/70	H	1.	C	1.	O	1.	E	-1.	G	300.000	5000.000	29.01779
HCCN	TPIS91	H	1.	C	2.	N	1.		0.	G	200.000	6000.000	39.03668
HCL	J 9/64	H	1.	CL	1.		0.		0.	G	300.000	5000.000	36.46064
HD	J 6/77	H	1.	D	1.		0.		0.	G	300.000	5000.000	3.02204
HD+	J 9/77	H	1.	D	1.	E	-1.		0.	G	300.000	5000.000	3.02149
HD-	J 9/77	H	1.	D	1.	E	1.		0.	G	300.000	5000.000	3.02259
HDO	J 6/77	H	1.	D	1.	O	1.		0.	G	300.000	5000.000	19.02144
HF	J 6/77	H	1.	F	1.		0.		0.	G	300.000	5000.000	20.00634
HI	J 9/61	H	1.	I	1.		0.		0.	G	300.000	5000.000	127.91241
HNC	L11/92	H	1.	N	1.	C	1.		0.	G	200.000	6000.000	27.02568
HNCO	J12/70	H	1.	N	1.	C	1.	O	1.	G	200.000	6000.000	43.02508
HNO	L12/89	H	1.	N	1.	O	1.		0.	G	200.000	6000.000	31.01408
HNO2	TPIS89	H	1.	N	1.	O	2.		0.	G	200.000	6000.000	47.01348
HNO3	L 4/90	H	1.	N	1.	O	3.		0.	G	200.000	6000.000	63.01288
HOCL	J 3/79	H	1.	O	1.	CL	1.		0.	G	300.000	5000.000	52.46004
HOF	J12/72	H	1.	O	1.	F	1.		0.	G	300.000	5000.000	36.00574
HO2	L 5/89	H	1.	O	2.		0.		0.	G	200.000	6000.000	33.00674
HSO3F	J 6/72	H	1.	S	1.	O	3.	F	1.	G	300.000	5000.000	100.07054
H2	TPIS78	H	2.		0.		0.		0.	G	200.000	6000.000	2.01588
H2+	TPIS78	H	2.	E	-1.		0.		0.	G	298.150	6000.000	2.01533
H2-	J 9/77	H	2.	E	1.		0.		0.	G	300.000	5000.000	2.01643
HCHO,formaldehy	L 8/88	H	2.	C	1.	O	1.		0.	G	200.000	6000.000	30.02628
HCOOH	L 8/88	H	2.	C	1.	O	2.		0.	G	200.000	6000.000	46.02568
H2F2	J 6/77	H	2.	F	2.		0.		0.	G	300.000	5000.000	40.01269
H2O	L 8/89	H	2.	O	1.		0.		0.	G	200.000	6000.000	18.01528
H2O+	TPIS89	H	2.	O	1.	E	-1.		0.	G	298.150	6000.000	18.01473
H2O2	L 2/93	H	2.	O	2.		0.		0.	G	200.000	6000.000	34.01468
H2S	J 6/77	H	2.	S	1.		0.		0.	G	300.000	5000.000	34.08188
H2SO4	J 9/77	H	2.	S	1.	O	4.		0.	G	300.000	5000.000	98.07948
H3B3O6	J12/64	H	3.	B	3.	O	6.		0.	G	300.000	5000.000	131.45322
H3F3	J 6/77	H	3.	F	3.		0.		0.	G	300.000	5000.000	60.01983
H3O+	TPIS89	H	3.	O	1.	E	-1.		0.	G	298.150	6000.000	19.02267
(HCOOH)2	L 8/88	H	4.	C	2.	O	4.		0.	G	200.000	6000.000	92.05136
H4F4	J 6/77	H	4.	F	4.		0.		0.	G	200.000	6000.000	80.02537
H5F5	J 6/77	H	5.	F	5.		0.		0.	G	300.000	5000.000	100.03172
H6F6	J 6/77	H	6.	F	6.		0.		0.	G	300.000	5000.000	120.03806
H7F7	J 6/77	H	7.	F	7.		0.		0.	G	300.000	5000.000	140.04440
He	L10/90	HE	1.		0.		0.		0.	G	200.000	6000.000	4.00260
He+	L10/92	HE	1.	E	-1.		0.		0.	G	298.150	6000.000	4.00205
Hg	J 9/84	HG	1.		0.		0.		0.	G	200.000	6000.000	200.59000
HgBr2	J 3/62	HG	1.	BR	2.		0.		0.	G	300.000	5000.000	360.39800
I	J 6/82	I	1.		0.		0.		0.	G	200.000	6000.000	126.90447
I2	TPIS89	I	2.		0.		0.		0.	G	200.000	6000.000	253.80894
K	L 4/93	K	1.		0.		0.		0.	G	200.000	6000.000	39.09830
K+	J12/83	K	1.	E	-1.		0.		0.	G	298.150	6000.000	39.09775
KBO2	J 6/71	K	1.	B	1.	O	2.		0.	G	300.000	5000.000	81.90810
KCN	J 3/66	K	1.	C	1.	N	1.		0.	G	300.000	5000.000	65.11604
KCL	J 3/66	K	1.	CL	1.		0.		0.	G	300.000	5000.000	74.55100
KF	J 6/69	K	1.	F	1.		0.		0.	G	300.000	5000.000	58.09670
KF2-	J12/68	K	1.	F	2.	E	1.		0.	G	300.000	5000.000	77.09565
KH	J 3/63	K	1.	H	1.		0.		0.	G	300.000	5000.000	40.10624
KO	J12/67	K	1.	O	1.		0.		0.	G	300.000	5000.000	55.09770
KO-	J12/67	K	1.	O	1.	E	1.		0.	G	300.000	5000.000	55.09825
KOH	J12/70	K	1.	O	1.	H	1.		0.	G	300.000	5000.000	56.10564
KOH+	J12/71	K	1.	O	1.	H	1.	E	-1.	G	300.000	5000.000	56.10509
K2	J12/83	K	2.		0.		0.		0.	G	200.000	6000.000	78.19660
K2C2N2	J 3/66	K	2.	C	2.	N	2.		0.	G	300.000	5000.000	130.23208

Species ID.	Code	Formula Used by CETPC							Phase	Temp. Range		Mole. Wt.
K2CL2	J 3/66	K	2.	CL	2.		Ø.	Ø.	G	300.000	5000.000	149.10206
K2F2	J 6/69	K	2.	F	2.		Ø.	Ø.	G	300.000	5000.000	116.19341
K2O2H2	J12/70	K	2.	O	2.	H	2.	Ø.	G	300.000	5000.000	112.21128
K2SO4	J 6/78	K	2.	S	1.	O	4.	Ø.	G	300.000	5000.000	174.26026
Kr	L10/90	KR	1.		Ø.			Ø.	G	200.000	6000.000	83.80006
Kr+	L10/92	KR	1.	E	-1.			Ø.	G	298.150	6000.000	83.79945
Li	J12/83	LI	1.		Ø.			Ø.	G	200.000	6000.000	6.94106
Li+	J12/83	LI	1.	E	-1.			Ø.	G	298.150	6000.000	6.94045
LiALF4	J12/79	LI	1.	AL	1.	F	4.	Ø.	G	300.000	5000.000	109.91618
LiBO2	J 6/71	LI	1.	B	1.	O	2.	Ø.	G	300.000	5000.000	49.75606
LiCL	J 6/62	LI	1.	CL	1.			Ø.	G	300.000	5000.000	42.39376
LiF	J12/68	LI	1.	F	1.			Ø.	G	300.000	5000.000	25.93946
LiFO	J 9/65	LI	1.	F	1.	O	1.	Ø.	G	300.000	5000.000	41.93886
LiF2-	J12/68	LI	1.	F	2.	E	1.	Ø.	G	300.000	5000.000	44.93835
LiH	J 9/67	LI	1.	H	1.			Ø.	G	300.000	5000.000	7.94894
LiN	J12/66	LI	1.	N	1.			Ø.	G	300.000	5000.000	20.94774
LiO	J 3/64	LI	1.	O	1.			Ø.	G	300.000	5000.000	22.94646
LiO-	J12/67	LI	1.	O	1.	E	1.	Ø.	G	300.000	5000.000	22.94589
LiOH	J 6/71	LI	1.	O	1.	H	1.	Ø.	G	300.000	5000.000	23.94834
LiOH+	J12/71	LI	1.	O	1.	H	1.	E -1.	G	300.000	5000.000	23.94775
LiON	J 9/66	LI	1.	O	1.	N	1.	Ø.	G	300.000	5000.000	36.94714
Li2	J12/83	LI	2.		Ø.			Ø.	G	200.000	6000.000	13.88206
Li2CL2	J 6/62	LI	2.	CL	2.			Ø.	G	300.000	5000.000	84.78746
Li2F2	J12/68	LI	2.	F	2.			Ø.	G	300.000	5000.000	51.87881
Li2O	J 3/64	LI	2.	O	1.			Ø.	G	300.000	5000.000	29.88146
Li2O2	J 3/64	LI	2.	O	2.			Ø.	G	300.000	5000.000	45.88886
Li2O2H2	J 6/71	LI	2.	O	2.	H	2.	Ø.	G	300.000	5000.000	47.89666
Li2SO4	J12/78	LI	2.	S	1.	O	4.	Ø.	G	300.000	5000.000	109.94566
Li3CL3	J 6/62	LI	3.	CL	3.			Ø.	G	300.000	5000.000	127.18116
Li3F3	J12/68	LI	3.	F	3.			Ø.	G	300.000	5000.000	77.81821
Mg	J 9/83	MG	1.		Ø.			Ø.	G	200.000	6000.000	24.30506
Mg+	J 9/83	MG	1.	E	-1.			Ø.	G	298.150	6000.000	24.30445
MgBr	J 6/75	MG	1.	BR	1.			Ø.	G	300.000	5000.000	104.20906
MgBr2	J 6/74	MG	1.	BR	2.			Ø.	G	300.000	5000.000	184.11386
MgCL	J 3/66	MG	1.	CL	1.			Ø.	G	300.000	5000.000	59.75776
MgCL+	J 6/68	MG	1.	CL	1.	E	-1.	Ø.	G	300.000	5000.000	59.75715
MgCLF	J 3/66	MG	1.	CL	1.	F	1.	Ø.	G	200.000	6000.000	78.75616
MgCL2	J12/69	MG	1.	CL	2.			Ø.	G	300.000	5000.000	95.21646
MgF	J 6/76	MG	1.	F	1.			Ø.	G	300.000	5000.000	43.30346
MgF+	J12/75	MG	1.	F	1.	E	-1.	Ø.	G	300.000	5000.000	43.30285
MgF2	J 6/75	MG	1.	F	2.			Ø.	G	300.000	5000.000	62.30181
MgF2+	J12/75	MG	1.	F	2.	E	-1.	Ø.	G	300.000	5000.000	62.30126
MgH	J12/66	MG	1.	H	1.			Ø.	G	300.000	5000.000	25.31294
MgI	J12/74	MG	1.	I	1.			Ø.	G	200.000	6000.000	151.20947
MgI2	J12/74	MG	1.	I	2.			Ø.	G	300.000	5000.000	278.11394
MgN	J 3/64	MG	1.	N	1.			Ø.	G	300.000	5000.000	38.31174
MgO	J12/74	MG	1.	O	1.			Ø.	G	300.000	5000.000	40.30446
MgOH	J12/75	MG	1.	O	1.	H	1.	Ø.	G	300.000	5000.000	41.31234
MgOH+	J12/75	MG	1.	O	1.	H	1.	E -1.	G	300.000	5000.000	41.31175
MgO2H2	J12/75	MG	1.	O	2.	H	2.	Ø.	G	300.000	5000.000	58.31966
MgS	J 9/77	MG	1.	S	1.			Ø.	G	300.000	5000.000	56.37106
Mg2	J 9/83	MG	2.		Ø.			Ø.	G	200.000	6000.000	48.61006
Mg2F4	J12/75	MG	2.	F	4.			Ø.	G	300.000	5000.000	124.60361
MoO3	TPIS82	MO	1.	O	3.			Ø.	G	298.150	5000.000	143.93826
Mo2O6	TPIS82	MO	2.	O	6.			Ø.	G	298.150	5000.000	287.87646
Mo3O9	TPIS82	MO	3.	O	9.			Ø.	G	298.150	5000.000	431.81466
Mo4O12	TPIS82	MO	4.	O	12.			Ø.	G	298.150	5000.000	575.75286
Mo5O15	TPIS82	MO	5.	O	15.			Ø.	G	298.150	5000.000	719.69106
N	L 6/88	N	1.		Ø.			Ø.	G	200.000	6000.000	14.00674
N+	L 7/88	N	1.	E	-1.			Ø.	G	298.150	6000.000	14.00615
N-	L 7/88	N	1.	E	1.			Ø.	G	298.150	6000.000	14.00729
NCO	L12/89	N	1.	C	1.	O	1.	Ø.	G	200.000	6000.000	42.01714
ND	J 6/77	N	1.	D	1.			Ø.	G	298.150	5000.000	15.02084
ND2	J 6/77	N	1.	D	2.			Ø.	G	298.150	5000.000	18.03494
ND3	J 6/77	N	1.	D	3.			Ø.	G	298.150	5000.000	20.04905
NF	TPIS89	N	1.	F	1.			Ø.	G	200.000	6000.000	33.00516
NF2	TPIS78	N	1.	F	2.			Ø.	G	298.150	5000.000	52.00356
NF3	L12/86	N	1.	F	3.			Ø.	G	298.150	5000.000	71.00195
NH	L11/89	N	1.	H	1.			Ø.	G	200.000	6000.000	15.01466
NH+	L 2/89	N	1.	H	1.	E	-1.	Ø.	G	298.150	6000.000	15.01413
NHF	TPIS78	N	1.	H	1.	F	1.	Ø.	G	298.150	5000.000	34.01306
NHF2	TPIS78	N	1.	H	1.	F	2.	Ø.	G	298.150	5000.000	53.01145
NH2	L12/89	N	1.	H	2.			Ø.	G	200.000	6000.000	16.02262
NH2F	TPIS78	N	1.	H	2.	F	1.	Ø.	G	298.150	5000.000	35.02102

Species ID.	Code	Formula Used by CETPC							Phase		Temp. Range		Mole. Wt.
NH3	TPIS89	N	1.	H	3.		0.		0.	G	200.000	6000.000	17.03056
NH2OH	TPIS89	N	1.	H	3.	O	1.		0.	G	200.000	6000.000	33.02996
NH4+	TPIS89	N	1.	H	4.	E	-1.		0.	G	298.150	6000.000	18.03795
NO	TPIS89	N	1.	O	1.		0.		0.	G	200.000	6000.000	30.00614
NO+	TPIS89	N	1.	O	1.	E	-1.		0.	G	298.150	6000.000	30.00559
NOCL	L12/86	N	1.	O	1.	CL	1.		0.	G	298.150	5000.000	65.45884
NOF	TPIS78	N	1.	O	1.	F	1.		0.	G	298.150	5000.000	49.00454
NOF3	TPIS78	N	1.	O	1.	F	3.		0.	G	298.150	5000.000	87.00135
NO2	L 7/88	N	1.	O	2.		0.		0.	G	200.000	6000.000	46.00554
NO2-	TPIS89	N	1.	O	2.	E	1.		0.	G	298.150	6000.000	46.00609
NO2CL	L12/86	N	1.	O	2.	CL	1.		0.	G	298.150	5000.000	81.45824
NO2F	L12/86	N	1.	O	2.	F	1.		0.	G	298.150	5000.000	65.00394
NO3	J12/64	N	1.	O	3.		0.		0.	G	200.000	6000.000	62.00494
NO3-	TPIS89	N	1.	O	3.	E	1.		0.	G	298.150	6000.000	62.00549
NO3F	L12/86	N	1.	O	3.	F	1.		0.	G	298.150	5000.000	81.00334
N2	TPIS78	N	2.		0.		0.		0.	G	200.000	6000.000	28.01348
N2+	TPIS89	N	2.	E	-1.		0.		0.	G	298.150	6000.000	28.01293
N2-	J 9/77	N	2.	E	1.		0.		0.	G	298.150	5000.000	28.01403
NCN	L12/89	N	2.	C	1.		0.		0.	G	200.000	6000.000	40.02448
cis-N2D2	J 6/77	N	2.	D	2.		0.		0.	G	200.000	6000.000	32.04160
N2F2	L12/86	N	2.	F	2.		0.		0.	G	298.150	5000.000	66.01029
N2F4	L12/86	N	2.	F	4.		0.		0.	G	298.150	5000.000	104.00709
N2H2	L 5/90	N	2.	H	2.		0.		0.	G	200.000	6000.000	30.02936
NH2NO2	TPIS89	N	2.	H	2.	O	2.		0.	G	200.000	6000.000	62.02816
N2H4	L 5/90	N	2.	H	4.		0.		0.	G	200.000	6000.000	32.04524
N2O	L 7/88	N	2.	O	1.		0.		0.	G	200.000	6000.000	44.01288
N2O+	J12/70	N	2.	O	1.	E	-1.		0.	G	298.150	6000.000	44.01233
N2O3	L 4/90	N	2.	O	3.		0.		0.	G	200.000	6000.000	76.01168
N2O4	TPIS89	N	2.	O	4.		0.		0.	G	200.000	6000.000	92.01108
N2O5	L 4/90	N	2.	O	5.		0.		0.	G	200.000	6000.000	108.01048
N3	TPIS89	N	3.		0.		0.		0.	G	200.000	6000.000	42.02022
N3H	L 7/88	N	3.	H	1.		0.		0.	G	200.000	6000.000	43.02816
Na	L 4/93	NA	1.		0.		0.		0.	G	200.000	6000.000	22.98977
Na+	J12/83	NA	1.	E	-1.		0.		0.	G	298.150	6000.000	22.98922
NaALF4	J12/79	NA	1.	AL	1.	F	4.		0.	G	300.000	5000.000	125.96492
NaBO2	J 6/71	NA	1.	B	1.	O	2.		0.	G	300.000	5000.000	65.79957
NaBr	J 9/64	NA	1.	BR	1.		0.		0.	G	300.000	5000.000	102.89377
NaCN	J3/66	NA	1.	C	1.	N	1.		0.	G	300.000	5000.000	49.00751
NaCL	J12/64	NA	1.	CL	1.		0.		0.	G	300.000	5000.000	58.44247
NaF	J12/68	NA	1.	F	1.		0.		0.	G	200.000	6000.000	41.98817
NaF2-	J12/68	NA	1.	F	2.	E	1.		0.	G	300.000	5000.000	60.98712
NaH	J 3/63	NA	1.	H	1.		0.		0.	G	300.000	5000.000	23.99771
NaI	L 6/72	NA	1.	I	1.		0.		0.	G	300.000	5000.000	149.89424
NaO	J12/67	NA	1.	O	1.		0.		0.	G	300.000	5000.000	38.98917
NaO-	J12/67	NA	1.	O	1.	E	1.		0.	G	300.000	5000.000	38.98972
NaOH	J12/70	NA	1.	O	1.	H	1.		0.	G	300.000	5000.000	39.99711
NaOH+	J12/71	NA	1.	O	1.	H	1.	E	-1.	G	300.000	5000.000	39.99656
Na2	J12/83	NA	2.		0.		0.		0.	G	200.000	6000.000	45.97954
Na2C2N2	J 3/66	NA	2.	C	2.	N	2.		0.	G	300.000	5000.000	98.01502
Na2CL2	J12/64	NA	2.	CL	2.		0.		0.	G	300.000	5000.000	116.88494
Na2F2	J12/68	NA	2.	F	2.		0.		0.	G	300.000	5000.000	83.97634
Na2O	L10/74	NA	2.	O	1.		0.		0.	G	300.000	5000.000	61.97894
Na2O2H2	J12/70	NA	2.	O	2.	H	2.		0.	G	300.000	5000.000	79.99422
Na2SO4	J 6/78	NA	2.	S	1.	O	4.		0.	G	300.000	5000.000	142.04314
Nb	J12/73	NB	1.		0.		0.		0.	G	300.000	5000.000	92.90638
NbO	J12/73	NB	1.	O	1.		0.		0.	G	300.000	5000.000	108.90578
NbO2	J12/73	NB	1.	O	2.		0.		0.	G	300.000	5000.000	124.90518
Ne	L10/90	NE	1.		0.		0.		0.	G	200.000	6000.000	20.17970
Ne+	L10/92	NE	1.	E	-1.		0.		0.	G	298.150	6000.000	20.17915
NI	J12/76	NI	1.		0.		0.		0.	G	300.000	5000.000	58.69340
NICL	J 9/77	NI	1.	CL	1.		0.		0.	G	300.000	5000.000	94.14618
NICL2	J 9/77	NI	1.	CL	2.		0.		0.	G	300.000	5000.000	129.59886
NIO	L 2/84	NI	1.	O	1.		0.		0.	G	300.000	5000.000	74.69280
NIS	J12/76	NI	1.	S	1.		0.		0.	G	300.000	5000.000	90.75940
O	L 1/90	O	1.		0.		0.		0.	G	200.000	6000.000	15.99940
O+	L 1/90	O	1.	E	-1.		0.		0.	G	298.150	6000.000	15.99885
O-	TPIS89	O	1.	E	1.		0.		0.	G	298.150	6000.000	15.99995
OD	J 6/77	O	1.	D	1.		0.		0.	G	300.000	5000.000	18.01358
OH	TPIS78	O	1.	H	1.		0.		0.	G	200.000	6000.000	17.00734
OH+	TPIS78	O	1.	H	1.	E	-1.		0.	G	298.150	6000.000	17.00679
OH-	L 3/93	O	1.	H	1.	E	1.		0.	G	298.150	6000.000	17.00789
O2	TPIS89	O	2.		0.		0.		0.	G	200.000	6000.000	31.99880
O2+	TPIS89	O	2.	E	-1.		0.		0.	G	298.150	6000.000	31.99825
O2-	L 4/89	O	2.	E	1.		0.		0.	G	298.150	6000.000	31.99935

Species ID.	Code	Formula Used by CETPC							Phase		Temp. Range		Mole. Wt.
O3	L 5/90	O	3.		0.		0.		0.	G	200.000	6000.000	47.99820
P	J 6/62	P	1.		0.		0.		0.	G	300.000	5000.000	30.97376
P+	L12/66	P	1.	E	-1.		0.		0.	G	300.000	5000.000	30.97321
PCL3	J 6/70	P	1.	CL	3.		0.		0.	G	300.000	5000.000	137.33186
PF	J 6/77	P	1.	F	1.		0.		0.	G	300.000	5000.000	49.97217
PF+	J 6/77	P	1.	F	1.	E	-1.		0.	G	300.000	5000.000	49.97162
PF-	J 6/77	P	1.	F	1.	E	1.		0.	G	300.000	5000.000	49.97271
PF2	J 6/77	P	1.	F	2.		0.		0.	G	300.000	5000.000	68.97057
PF2+	J 6/77	P	1.	F	2.	E	-1.		0.	G	300.000	5000.000	68.97002
PF3	J12/69	P	1.	F	3.		0.		0.	G	300.000	5000.000	87.96897
PF5	J12/69	P	1.	F	5.		0.		0.	G	300.000	5000.000	125.96578
PH	J 6/67	P	1.	H	1.		0.		0.	G	300.000	5000.000	31.98170
PH3	J 6/62	P	1.	H	3.		0.		0.	G	300.000	5000.000	33.99758
PO	J 6/71	P	1.	O	1.		0.		0.	G	300.000	5000.000	46.97316
PO2	J 9/62	P	1.	O	2.		0.		0.	G	300.000	5000.000	62.97256
P2	J 6/61	P	2.		0.		0.		0.	G	300.000	5000.000	61.94752
P4	J 6/61	P	4.		0.		0.		0.	G	300.000	5000.000	123.89505
P4O10	J12/65	P	4.	O	10.		0.		0.	G	300.000	5000.000	283.88905
Pb	J 3/83	PB	1.		0.		0.		0.	G	200.000	6000.000	207.20000
PbBr	J12/73	PB	1.	BR	1.		0.		0.	G	300.000	5000.000	287.10400
PbBr2	J12/73	PB	1.	BR	2.		0.		0.	G	300.000	5000.000	367.00800
PbBr4	J12/73	PB	1.	BR	4.		0.		0.	G	300.000	5000.000	526.81600
PbCL	J 6/73	PB	1.	CL	1.		0.		0.	G	300.000	5000.000	242.65270
PbCL+	J 6/73	PB	1.	CL	1.	E	-1.		0.	G	300.000	5000.000	242.65215
PbCL2	J 6/73	PB	1.	CL	2.		0.		0.	G	300.000	5000.000	278.10540
PbCL2+	J 6/73	PB	1.	CL	2.	E	-1.		0.	G	300.000	5000.000	278.10485
PbCL4	J12/73	PB	1.	CL	4.		0.		0.	G	300.000	5000.000	349.01080
PbF	J12/73	PB	1.	F	1.		0.		0.	G	300.000	5000.000	226.19840
PbF2	J12/73	PB	1.	F	2.		0.		0.	G	300.000	5000.000	245.19681
PbF4	J12/73	PB	1.	F	4.		0.		0.	G	300.000	5000.000	283.19361
PbI	J12/73	PB	1.	I	1.		0.		0.	G	300.000	5000.000	334.10447
PbI2	J12/73	PB	1.	I	2.		0.		0.	G	300.000	5000.000	461.00894
PbI4	J12/73	PB	1.	I	4.		0.		0.	G	300.000	5000.000	714.81788
PbO	J12/71	PB	1.	O	1.		0.		0.	G	300.000	5000.000	223.19940
PbS	J 6/73	PB	1.	S	1.		0.		0.	G	300.000	5000.000	239.26000
Pb2	J 9/63	PB	2.		0.		0.		0.	G	300.000	5000.000	414.40000
S	J 9/82	S	1.		0.		0.		0.	G	200.000	6000.000	32.06000
S+	J 9/82	S	1.	E	-1.		0.		0.	G	298.150	6000.000	32.06545
S-	J 9/82	S	1.	E	1.		0.		0.	G	298.150	6000.000	32.06655
SCL	J 6/78	S	1.	CL	1.		0.		0.	G	300.000	5000.000	67.51870
SCL2	J 6/78	S	1.	CL	2.		0.		0.	G	300.000	5000.000	102.97140
SCL2+	J 6/78	S	1.	CL	2.	E	-1.		0.	G	300.000	5000.000	102.97085
SD	J 6/77	S	1.	D	1.		0.		0.	G	300.000	5000.000	34.08010
SF	J 6/76	S	1.	F	1.		0.		0.	G	300.000	5000.000	51.06440
SF+	J 6/76	S	1.	F	1.	E	-1.		0.	G	300.000	5000.000	51.06385
SF-	J12/76	S	1.	F	1.	E	1.		0.	G	300.000	5000.000	51.06495
SF2	J 6/76	S	1.	F	2.		0.		0.	G	300.000	5000.000	70.06281
SF2+	J12/76	S	1.	F	2.	E	-1.		0.	G	300.000	5000.000	70.06226
SF2-	J12/76	S	1.	F	2.	E	1.		0.	G	300.000	5000.000	70.06335
SF3	J 6/77	S	1.	F	3.		0.		0.	G	300.000	5000.000	89.06121
SF3+	J12/76	S	1.	F	3.	E	-1.		0.	G	300.000	5000.000	89.06066
SF3-	J12/76	S	1.	F	3.	E	1.		0.	G	300.000	5000.000	89.06176
SF4	J 6/76	S	1.	F	4.		0.		0.	G	300.000	5000.000	108.05961
SF4+	J12/76	S	1.	F	4.	E	-1.		0.	G	300.000	5000.000	108.05906
SF4-	J12/76	S	1.	F	4.	E	1.		0.	G	300.000	5000.000	108.06016
SF5	J12/77	S	1.	F	5.		0.		0.	G	300.000	5000.000	127.05802
SF5+	J12/77	S	1.	F	5.	E	-1.		0.	G	300.000	5000.000	127.05747
SF5-	J12/77	S	1.	F	5.	E	1.		0.	G	300.000	5000.000	127.05856
SF6	J 6/76	S	1.	F	6.		0.		0.	G	300.000	5000.000	146.05642
SF6-	J 6/77	S	1.	F	6.	E	1.		0.	G	300.000	5000.000	146.05697
SH	J 6/77	S	1.	H	1.		0.		0.	G	300.000	5000.000	33.07394
SN	J 6/61	S	1.	N	1.		0.		0.	G	300.000	5000.000	46.07274
SO	J 6/77	S	1.	O	1.		0.		0.	G	300.000	5000.000	48.06540
SOF2	J 6/72	S	1.	O	1.	F	2.		0.	G	300.000	5000.000	86.06221
SO2	J 6/61	S	1.	O	2.		0.		0.	G	300.000	5000.000	64.06480
SO2CLF	J 6/71	S	1.	O	2.	CL	1.	F 1.	0.	G	300.000	5000.000	118.51590
SO2CL2	J 6/71	S	1.	O	2.	CL	2.		0.	G	300.000	5000.000	134.97020
SO2F2	J 6/71	S	1.	O	2.	F	2.		0.	G	300.000	5000.000	102.06161
SO3	J 9/65	S	1.	O	3.		0.		0.	G	300.000	5000.000	80.06420
S2	J 9/77	S	2.		0.		0.		0.	G	300.000	5000.000	64.13200
S2CL	J 6/78	S	2.	CL	1.		0.		0.	G	200.000	6000.000	99.58470
S2CL2	L 4/93	S	2.	CL	2.		0.		0.	G	200.000	6000.000	135.03740
S2F2,thiothionyl	J 6/76	S	2.	F	2.		0.		0.	G	200.000	6000.000	102.12881
S2O	J 9/65	S	2.	O	1.		0.		0.	G	300.000	5000.000	80.13140

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S8	J 9/77	S 8.		0.		0.	0.	G	200.000	6000.000	256.52800
Si	J 3/83	SI 1.		0.		0.	0.	G	200.000	6000.000	28.08550
Si+	J 3/83	SI 1.	E -1.			0.	0.	G	298.150	6000.000	28.08495
SiBr	J12/76	SI 1.	BR 1.			0.	0.	G	300.000	5000.000	107.98950
SiBr2	J12/77	SI 1.	BR 2.			0.	0.	G	300.000	5000.000	187.89350
SiBr3	J12/77	SI 1.	BR 3.			0.	0.	G	300.000	5000.000	267.79750
SiBr4	J12/76	SI 1.	BR 4.			0.	0.	G	300.000	5000.000	347.70150
SiC	J 3/67	SI 1.	C 1.			0.	0.	G	300.000	5000.000	40.09650
SiC2	J 3/67	SI 1.	C 2.			0.	0.	G	300.000	5000.000	52.10750
SiC4H12	J12/66	SI 1.	C 4.	H 12.			0.	G	298.150	5000.000	88.22430
SiCL	J12/76	SI 1.	CL 1.			0.	0.	G	300.000	5000.000	63.53820
SiCL2	J12/77	SI 1.	CL 2.			0.	0.	G	300.000	5000.000	98.99090
SiCL3	J12/77	SI 1.	CL 3.			0.	0.	G	300.000	5000.000	134.44360
SiCL4	J12/76	SI 1.	CL 4.			0.	0.	G	300.000	5000.000	169.89630
SiF	J12/76	SI 1.	F 1.			0.	0.	G	300.000	5000.000	47.08390
SiF2	J12/77	SI 1.	F 2.			0.	0.	G	300.000	5000.000	66.08231
SiF3	J12/77	SI 1.	F 3.			0.	0.	G	300.000	5000.000	85.08071
SiF4	J 6/76	SI 1.	F 4.			0.	0.	G	300.000	5000.000	104.07911
SiH	J12/76	SI 1.	H 1.			0.	0.	G	300.000	5000.000	29.09344
SiH+	J12/71	SI 1.	H 1.	E -1.			0.	G	300.000	5000.000	29.09289
SiHBr3	J12/76	SI 1.	H 1.	BR 3.			0.	G	300.000	5000.000	268.80544
SiHCL3	J12/76	SI 1.	H 1.	CL 3.			0.	G	300.000	5000.000	135.45154
SiHF3	J 6/76	SI 1.	H 1.	F 3.			0.	G	300.000	5000.000	86.08865
SiHI3	J12/76	SI 1.	H 1.	I 3.			0.	G	300.000	5000.000	409.80685
SiH2	TPIS79	SI 1.	H 2.			0.	0.	G	298.150	5000.000	30.10138
SiH2Br2	J12/76	SI 1.	H 2.	BR 2.			0.	G	300.000	5000.000	189.90938
SiH2CL2	J12/76	SI 1.	H 2.	CL 2.			0.	G	300.000	5000.000	101.00678
SiH2F2	J 6/76	SI 1.	H 2.	F 2.			0.	G	300.000	5000.000	68.09819
SiH2I2	J12/76	SI 1.	H 2.	I 2.			0.	G	300.000	5000.000	283.91032
SiH3	TPIS79	SI 1.	H 3.			0.	0.	G	298.150	5000.000	31.10932
SiH3Br	J12/76	SI 1.	H 3.	BR 1.			0.	G	300.000	5000.000	111.01332
SiH3CL	J12/76	SI 1.	H 3.	CL 1.			0.	G	300.000	5000.000	66.56202
SiH3F	J 6/76	SI 1.	H 3.	F 1.			0.	G	300.000	5000.000	50.10772
SiH3I	J12/76	SI 1.	H 3.	I 1.			0.	G	300.000	5000.000	158.01379
SiH4	J 6/76	SI 1.	H 4.			0.	0.	G	300.000	5000.000	32.11726
SII	J12/76	SI 1.	I 1.			0.	0.	G	300.000	5000.000	154.98997
SII2	J12/77	SI 1.	I 2.			0.	0.	G	200.000	6000.000	281.89444
SIN	J 3/67	SI 1.	N 1.			0.	0.	G	300.000	5000.000	42.09224
SIO	J 9/67	SI 1.	O 1.			0.	0.	G	300.000	5000.000	44.08496
SIO2	J 9/67	SI 1.	O 2.			0.	0.	G	300.000	5000.000	60.08430
SIS	J12/71	SI 1.	S 1.			0.	0.	G	300.000	5000.000	60.15150
SI2	J 3/67	SI 2.		0.		0.	0.	G	300.000	5000.000	56.17100
SI2C	J 3/67	SI 2.	C 1.			0.	0.	G	300.000	5000.000	68.18200
SI2N	J 3/67	SI 2.	N 1.			0.	0.	G	300.000	5000.000	70.17774
SI3	J 3/67	SI 3.		0.		0.	0.	G	300.000	5000.000	84.25650
Sr	L 4/93	SR 1.		0.		0.	0.	G	200.000	6000.000	87.62000
SrBr	J12/74	SR 1.	BR 1.			0.	0.	G	300.000	5000.000	167.52400
SrCL	J12/72	SR 1.	CL 1.			0.	0.	G	300.000	5000.000	123.07270
SrCL2	J12/72	SR 1.	CL 2.			0.	0.	G	300.000	5000.000	158.52540
SrF	J12/72	SR 1.	F 1.			0.	0.	G	300.000	5000.000	106.61840
SrF+	J12/72	SR 1.	F 1.	E -1.			0.	G	300.000	5000.000	106.61785
SrF2	J12/72	SR 1.	F 2.			0.	0.	G	300.000	5000.000	125.61681
SrI2	J 6/74	SR 1.	I 2.			0.	0.	G	300.000	5000.000	341.42894
SrO	J 6/74	SR 1.	O 1.			0.	0.	G	300.000	5000.000	103.61940
SrOH	J12/75	SR 1.	O 1.	H 1.			0.	G	300.000	5000.000	104.62734
SrOH+	J 6/76	SR 1.	O 1.	H 1.		E -1.		G	300.000	5000.000	104.62679
SrO2H2	J12/75	SR 1.	O 2.	H 2.			0.	G	300.000	5000.000	121.63468
SrS	J 9/77	SR 1.	S 1.			0.	0.	G	300.000	5000.000	119.68600
Ta	J12/72	TA 1.		0.		0.	0.	G	300.000	5000.000	180.94790
TaO	J12/73	TA 1.	O 1.			0.	0.	G	300.000	5000.000	196.94730
TaO2	J12/73	TA 1.	O 2.			0.	0.	G	300.000	5000.000	212.94670
Ti	J 6/79	TI 1.		0.		0.	0.	G	200.000	6000.000	47.88000
Ti+	J 3/84	TI 1.	E -1.			0.	0.	G	298.150	6000.000	47.87945
Ti-	J 3/84	TI 1.	E 1.			0.	0.	G	298.150	6000.000	47.88055
TiCL	J12/68	TI 1.	CL 1.			0.	0.	G	300.000	5000.000	83.33270
TiCL2	J12/68	TI 1.	CL 2.			0.	0.	G	300.000	5000.000	118.78540
TiCL3	J12/68	TI 1.	CL 3.			0.	0.	G	300.000	5000.000	154.23810
TiCL4	J12/67	TI 1.	CL 4.			0.	0.	G	300.000	5000.000	189.69080
TiO	J12/73	TI 1.	O 1.			0.	0.	G	300.000	5000.000	63.87940
TiOCL	J 9/63	TI 1.	O 1.	CL 1.			0.	G	300.000	5000.000	99.33210
TiOCL2	J 9/63	TI 1.	O 1.	CL 2.			0.	G	300.000	5000.000	134.78480
TiO2	J12/73	TI 1.	O 2.			0.	0.	G	300.000	5000.000	79.87880
V	J 6/73	V 1.		0.		0.	0.	G	300.000	5000.000	50.94150
VCL4	L 2/76	V 1.	CL 4.			0.	0.	G	300.000	5000.000	192.75230

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VN	J12/73	V 1.	N 1.			0.	0.	G	300.000	5000.000	64.94824
VO	J12/73	V 1.	O 1.			0.	0.	G	300.000	5000.000	66.94896
VO2	J12/73	V 1.	O 2.			0.	0.	G	300.000	5000.000	82.94836
Xe	L12/91	XE 1.				0.	0.	G	200.000	6000.000	131.29006
Xe+	L10/92	XE 1.	E -1.			0.	0.	G	298.150	6000.000	131.28945
Zn	L 7/93	ZN 1.				0.	0.	G	200.000	6000.000	65.39008
Zn+	L 7/93	ZN 1.	E -1.			0.	0.	G	200.000	6000.000	65.38945
Zn-	J12/78	ZN 1.	E 1.			0.	0.	G	200.000	6000.000	65.39055
Zr	L 7/93	ZR 1.				0.	0.	G	200.000	6000.000	91.22408
ZrN	J 6/63	ZR 1.	N 1.			0.	0.	G	200.000	6000.000	105.23074
ZrO	L 7/93	ZR 1.	O 1.			0.	0.	G	200.000	6000.000	107.22348
ZrO2	J12/65	ZR 1.	O 2.			0.	0.	G	300.000	5000.000	123.22286
AL(cr)	CODA89	AL 1.				0.	0.	C	200.000	933.610	26.98154
AL(L)	CODA89	AL 1.				0.	0.	C	933.610	6000.000	26.98154
ALBr3(s)	J 9/79	AL 1.	BR 3.			0.	0.	C	300.000	370.600	266.69354
ALBr3(L)	J 9/79	AL 1.	BR 3.			0.	0.	C	370.600	5000.000	266.69354
ALCL3(s)	J 9/79	AL 1.	CL 3.			0.	0.	C	300.000	465.700	133.33964
ALCL3(L)	J 9/79	AL 1.	CL 3.			0.	0.	C	465.700	5000.000	133.33964
ALF3(a)	J 9/79	AL 1.	F 3.			0.	0.	C	300.000	728.000	83.97675
ALF3(b)	J 9/79	AL 1.	F 3.			0.	0.	C	728.000	2523.000	83.97675
ALF3(L)	J 9/79	AL 1.	F 3.			0.	0.	C	2523.000	5000.000	83.97675
ALI3(s)	J 9/79	AL 1.	I 3.			0.	0.	C	300.000	464.140	407.69495
ALI3(L)	J 9/79	AL 1.	I 3.			0.	0.	C	464.140	5000.000	407.69495
ALN(s)	J12/79	AL 1.	N 1.			0.	0.	C	300.000	3000.000	40.98826
AL2O3(a)	J12/79	AL 2.	O 3.			0.	0.	C	300.000	2327.000	101.96128
AL2O3(L)	J12/79	AL 2.	O 3.			0.	0.	C	2327.000	6000.000	101.96128
AL2SIO5(an)	J 9/67	AL 2.	SI 1.	O	5.	0.	C	300.000	3000.000	162.04558
AL6SI2O13(s)	J 9/67	AL 6.	SI 2.	O	13.	0.	C	300.000	3000.000	426.05243
B(b)	J 6/83	B 1.				0.	0.	C	200.000	2350.000	10.81106
B(L)	J 6/83	B 1.				0.	0.	C	2350.000	6000.000	10.81106
BN(s)	J 6/66	B 1.	N 1.			0.	0.	C	200.000	6000.000	24.81774
B2O3(L)	J 6/71	B 2.	O 3.			0.	0.	C	300.000	5000.000	69.62022
B3O3H3(cr)	J 3/65	B 3.	O 3.	H	3.	0.	C	298.150	2000.000	83.45502
Ba(cr)	SRD 93	BA 1.				0.	0.	C	298.150	1000.000	137.32706
Ba(L)	SRD 93	BA 1.				0.	0.	C	1000.000	6000.000	137.32706
BaBr2(s)	J12/74	BA 1.	BR 2.			0.	0.	C	300.000	1130.000	297.13508
BaBr2(L)	J12/74	BA 1.	BR 2.			0.	0.	C	1130.000	5000.000	297.13508
BaCL2(a)	J12/72	BA 1.	CL 2.			0.	0.	C	300.000	1198.000	208.23248
BaCL2(b)	J12/72	BA 1.	CL 2.			0.	0.	C	1198.000	1235.000	208.23248
BaCL2(L)	J12/72	BA 1.	CL 2.			0.	0.	C	1235.000	5000.000	208.23248
BaF2(a)	J12/72	BA 1.	F 2.			0.	0.	C	300.000	1480.000	175.32381
BaF2(b,c)	J12/72	BA 1.	F 2.			0.	0.	C	1480.000	1641.000	175.32381
BaF2(L)	J12/72	BA 1.	F 2.			0.	0.	C	1641.000	5000.000	175.32381
BaO(a)	J 6/74	BA 1.	O 1.			0.	0.	C	300.000	2286.000	153.32648
BaO(L)	J 6/74	BA 1.	O 1.			0.	0.	C	2286.000	5000.000	153.32648
BaO2H2(s)	J12/75	BA 1.	O 2.	H	2.	0.	C	300.000	681.150	171.34168
BaO2H2(L)	J12/75	BA 1.	O 2.	H	2.	0.	C	681.150	5000.000	171.34168
BaS(s)	J 9/77	BA 1.	S 1.			0.	0.	C	300.000	3000.000	169.39300
Be(a)	SRD 93	BE 1.				0.	0.	C	298.150	1543.000	9.01218
Be(b)	SRD 93	BE 1.				0.	0.	C	1543.000	1563.000	9.01218
Be(L)	SRD 93	BE 1.				0.	0.	C	1563.000	6000.000	9.01218
BeAL2O4(s)	J12/79	BE 1.	AL 2.	O	4.	0.	C	300.000	2146.000	126.97286
BeAL2O4(L)	J12/79	BE 1.	AL 2.	O	4.	0.	C	2146.000	5000.000	126.97286
BeBr2(s)	J 6/75	BE 1.	BR 2.			0.	0.	C	300.000	1500.000	168.82018
BeCL2(s)	J 6/65	BE 1.	CL 2.			0.	0.	C	300.000	688.000	79.91758
BeCL2(L)	J 6/65	BE 1.	CL 2.			0.	0.	C	688.000	5000.000	79.91758
BeF2(Lqz)	J 6/70	BE 1.	F 2.			0.	0.	C	300.000	500.000	47.00899
BeF2(hqz)	J 6/70	BE 1.	F 2.			0.	0.	C	500.000	825.000	47.00899
BeF2(L)	J 6/70	BE 1.	F 2.			0.	0.	C	825.000	2000.000	47.00899
BeI2(s)	J12/75	BE 1.	I 2.			0.	0.	C	300.000	753.000	262.82112
BeI2(L)	J12/75	BE 1.	I 2.			0.	0.	C	753.000	5000.000	262.82112
BeO(a)	J 6/75	BE 1.	O 1.			0.	0.	C	200.000	2373.001	25.01158
BeO(b)	J 6/75	BE 1.	O 1.			0.	0.	C	2373.001	2821.220	25.01158
BeO(L)	J 6/75	BE 1.	O 1.			0.	0.	C	2821.220	6000.000	25.01158
BeO2H2(b)	J12/75	BE 1.	O 2.	H	2.	0.	C	300.000	1000.000	43.02686
BeS(s)	J 9/77	BE 1.	S 1.			0.	0.	C	300.000	3000.000	41.07818
Be2C(s)	BAR 73	BE 2.	C 1.			0.	0.	C	300.000	2400.000	30.03536
Be2C(L)	BAR 73	BE 2.	C 1.			0.	0.	C	2400.000	5000.000	30.03536
Br2(cr)	L 1/93	BR 2.				0.	0.	C	200.000	265.900	159.80800
Br2(L)	L 1/93	BR 2.				0.	0.	C	265.900	332.503	159.80800
Br2(L)	L 1/93	BR 2.				0.	0.	C	332.503	6000.000	159.80800
C(gr)	X 4/83	C 1.				0.	0.	C	200.000	5000.000	12.01100
C6H6(L)	X10/86	C 6.	H 6.			0.	0.	C	278.680	500.000	78.11364
C7H8(L)	X10/86	C 7.	H 8.			0.	0.	C	178.150	500.000	92.14052

Species ID.	Code	Formula Used by CETPC						Phase	Temp. Range		Mole. Wt.
C8H18(L),n-octa	X10/76	C	8.	H	18.		0.	0. C	220.000	300.000	114.23092
Jet-A(L)	L 6/88	C	12.	H	23.		0.	0. C	220.000	550.000	167.31462
Ca(a)	SRD 93	CA	1.		0.		0.	0. C	298.150	716.000	40.07800
Ca(b)	SRD 93	CA	1.		0.		0.	0. C	716.000	1115.000	40.07800
Ca(L)	SRD 93	CA	1.		0.		0.	0. C	1115.000	6000.000	40.07800
CaBr2(s)	J 6/74	CA	1.	BR	2.		0.	0. C	300.000	1015.000	199.88600
CaBr2(L)	J 6/74	CA	1.	BR	2.		0.	0. C	1015.000	5000.000	199.88600
CaCO3(caL)	BAR 89	CA	1.	C	1.	O	3.	0. C	298.15	1200.000	100.08720
CaCL2(a)	J 6/70	CA	1.	CL	2.		0.	0. C	300.000	1045.000	110.98340
CaCL2(L)	J 6/70	CA	1.	CL	2.		0.	0. C	1045.000	5000.000	110.98340
CaF2(a)	J12/68	CA	1.	F	2.		0.	0. C	300.000	1424.000	78.07481
CaF2(b)	J12/68	CA	1.	F	2.		0.	0. C	1424.000	1691.000	78.07481
CaF2(L)	J12/68	CA	1.	F	2.		0.	0. C	1691.000	6000.000	78.07481
CaO(a)	J 6/73	CA	1.	O	1.		0.	0. C	300.000	3200.000	56.07740
CaO(L)	J 6/73	CA	1.	O	1.		0.	0. C	3200.000	5000.000	56.07740
CaO2H2(a)	J12/75	CA	1.	O	2.	H	2.	0. C	300.000	1000.000	74.09268
CaS(a)	J 9/77	CA	1.	S	1.		0.	0. C	300.000	3000.000	72.14406
CaSO4(a)	BAR 73	CA	1.	S	1.	O	4.	0. C	300.000	5000.000	136.14166
Cr(cr)	J 6/73	CR	1.		0.		0.	0. C	200.000	311.500	51.99610
Cr(cr)	J 6/73	CR	1.		0.		0.	0. C	311.500	2130.000	51.99610
Cr(L)	J 6/73	CR	1.		0.		0.	0. C	2130.000	6000.000	51.99610
CrN(a)	J12/73	CR	1.	N	1.		0.	0. C	300.000	2500.000	66.00284
Cr2N(a)	J12/73	CR	2.	N	1.		0.	0. C	300.000	2500.000	117.99894
Cr2O3(a)	J12/73	CR	2.	O	3.		0.	0. C	300.000	2603.000	151.99040
Cr2O3(L)	J12/73	CR	2.	O	3.		0.	0. C	2603.000	5000.000	151.99040
Cs(cr)	CODA89	CS	1.		0.		0.	0. C	100.000	301.590	132.90543
Cs(L)	CODA89	CS	1.		0.		0.	0. C	301.590	2000.000	132.90543
CsCL(a)	J 6/68	CS	1.	CL	1.		0.	0. C	300.000	743.000	168.35813
CsCL(b)	J 6/68	CS	1.	CL	1.		0.	0. C	743.000	918.000	168.35813
CsCL(L)	J 6/68	CS	1.	CL	1.		0.	0. C	918.000	5000.000	168.35813
CsF(a)	J 6/68	CS	1.	F	1.		0.	0. C	300.000	976.000	151.90383
CsF(L)	J 6/68	CS	1.	F	1.		0.	0. C	976.000	5000.000	151.90383
CsOH(a)	J 6/71	CS	1.	O	1.	H	1.	0. C	298.150	410.000	149.91277
CsOH(b)	J 6/71	CS	1.	O	1.	H	1.	0. C	410.000	493.000	149.91277
CsOH(c)	J 6/71	CS	1.	O	1.	H	1.	0. C	493.000	588.000	149.91277
CsOH(L)	J 6/71	CS	1.	O	1.	H	1.	0. C	588.000	6000.000	149.91277
Cs2SO4(II)	J 6/79	CS	2.	S	1.	O	4.	0. C	300.000	940.000	361.87446
Cs2SO4(I)	J 6/79	CS	2.	S	1.	O	4.	0. C	940.000	1278.000	361.87446
Cs2SO4(L)	J 6/79	CS	2.	S	1.	O	4.	0. C	1278.000	5000.000	361.87446
Cu(cr)	CODA89	CU	1.		0.		0.	0. C	200.000	1358.000	63.54600
Cu(L)	CODA89	CU	1.		0.		0.	0. C	1358.000	6000.000	63.54600
CuF(a)	J12/77	CU	1.	F	1.		0.	0. C	300.000	2000.000	82.54440
CuF2(a)	J12/77	CU	1.	F	2.		0.	0. C	300.000	1109.000	101.54281
CuF2(L)	J12/77	CU	1.	F	2.		0.	0. C	1109.000	5000.000	101.54281
CuO(s)	J12/77	CU	1.	O	1.		0.	0. C	300.000	2000.000	79.54540
CuO2H2(s)	J 6/66	CU	1.	O	2.	H	2.	0. C	300.000	1500.000	97.56068
CuSO4(s)	J 6/66	CU	1.	S	1.	O	4.	0. C	300.000	2000.000	159.60960
Cu2O(s)	J12/77	CU	2.	O	1.		0.	0. C	300.000	1516.720	143.09140
Cu2O(L)	J12/77	CU	2.	O	1.		0.	0. C	1516.720	5000.000	143.09140
Cu2O5S(s)	J 6/66	CU	2.	O	5.	S	1.	0. C	300.000	1500.000	239.15500
Fe(a)	J 3/78	FE	1.		0.		0.	0. C	200.000	1042.000	55.84700
Fe(a)	J 3/78	FE	1.		0.		0.	0. C	1042.000	1184.000	55.84700
Fe(c)	J 3/78	FE	1.		0.		0.	0. C	1184.000	1665.000	55.84700
Fe(d)	J 3/78	FE	1.		0.		0.	0. C	1665.000	1809.000	55.84700
Fe(L)	J 3/78	FE	1.		0.		0.	0. C	1809.000	6000.000	55.84700
FeC5O5(L)	J 3/78	FE	1.	C	5.	O	5.	0. C	300.000	5000.000	195.89900
FeCL2(a)	J12/70	FE	1.	CL	2.		0.	0. C	300.000	950.000	126.75240
FeCL2(L)	J12/70	FE	1.	CL	2.		0.	0. C	950.000	5000.000	126.75240
FeCL3(a)	J 6/65	FE	1.	CL	3.		0.	0. C	200.000	577.000	162.20510
FeCL3(L)	J 6/65	FE	1.	CL	3.		0.	0. C	577.000	6000.000	162.20510
FeO(a)	J 6/65	FE	1.	O	1.		0.	0. C	300.000	1650.000	71.84640
FeO(L)	J 6/65	FE	1.	O	1.		0.	0. C	1650.000	5000.000	71.84640
Fe(OH)2(s)	J 6/66	FE	1.	O	2.	H	2.	0. C	300.000	1500.000	89.86168
Fe(OH)3(s)	J 6/66	FE	1.	O	3.	H	3.	0. C	300.000	1500.000	106.86902
FeS(a)	J 9/77	FE	1.	S	1.		0.	0. C	300.000	411.000	87.91300
FeS(b)	J 9/77	FE	1.	S	1.		0.	0. C	411.000	598.000	87.91300
FeS(c)	J 9/77	FE	1.	S	1.		0.	0. C	598.000	1463.000	87.91300
FeS(L)	J 9/77	FE	1.	S	1.		0.	0. C	1463.000	5000.000	87.91300
FeSO4(s)	J 6/66	FE	1.	S	1.	O	4.	0. C	300.000	2000.000	151.91060
FeS2(s)	J 9/77	FE	1.	S	2.		0.	0. C	300.000	1400.000	119.97900
Fe2O3(s)	J 6/65	FE	2.	O	3.		0.	0. C	300.000	2500.000	159.69220
Fe2S3O12(s)	J 6/66	FE	2.	S	3.	O	12.	0. C	300.000	2000.000	399.88480
Fe3O4(s)	J 6/65	FE	3.	O	4.		0.	0. C	300.000	5000.000	231.53860
H2O(s)	L 8/89	H	2.	O	1.		0.	0. C	200.000	273.150	18.01528

Species ID.	Code	Formula Used by CETPC							Phase	Temp. Range		Mole. Wt.
H2O(L)	L 8/89	H	2.	O	1.			0.	0.	C	273.150	600.000	18.01528
H2SO4(L)	J 9/77	H	2.	S	1.	O	4.	0.	0.	C	300.000	1000.000	98.07948
Hg(cr)	J12/61	HG	1.		0.			0.	0.	C	200.000	234.290	200.59000
Hg(L)	J12/61	HG	1.		0.			0.	0.	C	234.290	2000.000	200.59000
HgBr2(s)	J 3/62	HG	1.	BR	2.			0.	0.	C	300.000	514.000	360.39800
HgBr2(L)	J 3/62	HG	1.	BR	2.			0.	0.	C	514.000	5000.000	360.39800
HgO(s)	J 6/62	HG	1.	O	1.			0.	0.	C	300.000	1000.000	216.58940
I2(cr)	TPIS89	I	2.		0.			0.	0.	C	200.000	386.750	253.80894
I2(L)	TPIS89	I	2.		0.			0.	0.	C	386.750	6000.000	253.80894
K(cr)	CODA89	K	1.		0.			0.	0.	C	200.000	336.860	39.09830
K(L)	CODA89	K	1.		0.			0.	0.	C	336.860	2200.000	39.09830
KCN(s)	J 3/66	K	1.	C	1.	N	1.	0.	0.	C	300.000	895.000	65.11604
KCN(L)	J 3/66	K	1.	C	1.	N	1.	0.	0.	C	895.000	5000.000	65.11604
KCL(s)	J 3/66	K	1.	CL	1.			0.	0.	C	300.000	1044.000	74.55100
KCL(L)	J 3/66	K	1.	CL	1.			0.	0.	C	1044.000	5000.000	74.55100
KF(s)	J 6/69	K	1.	F	1.			0.	0.	C	300.000	1131.000	58.09670
KF(L)	J 6/69	K	1.	F	1.			0.	0.	C	1131.000	5000.000	58.09670
KHF2(a)	J 6/71	K	1.	H	1.	F	2.	0.	0.	C	300.000	469.850	78.10305
KHF2(b)	J 6/71	K	1.	H	1.	F	2.	0.	0.	C	469.850	511.950	78.10305
KHF2(L)	J 6/71	K	1.	H	1.	F	2.	0.	0.	C	511.950	6000.000	78.10305
KOH(a)	J12/70	K	1.	O	1.	H	1.	0.	0.	C	300.000	516.000	56.10564
KOH(b)	J12/70	K	1.	O	1.	H	1.	0.	0.	C	516.000	679.000	56.10564
KOH(L)	J12/70	K	1.	O	1.	H	1.	0.	0.	C	679.000	5000.000	56.10564
KO2(s)	J 6/71	K	1.	O	2.			0.	0.	C	300.000	1500.000	71.09710
K2CO3(s)	J 3/66	K	2.	C	1.	O	3.	0.	0.	C	300.000	1174.000	138.20580
K2CO3(L)	J 3/66	K	2.	C	1.	O	3.	0.	0.	C	1174.000	5000.000	138.20580
K2O(s)	J 6/63	K	2.	O	1.			0.	0.	C	298.150	2000.000	94.19600
K2O2(s)	J 9/63	K	2.	O	2.			0.	0.	C	298.150	2000.000	110.19540
K2S(1)	J 3/78	K	2.	S	1.			0.	0.	C	300.000	1050.000	110.26260
K2S(2)	J 3/78	K	2.	S	1.			0.	0.	C	1050.000	1100.000	110.26260
K2S(3)	J 3/78	K	2.	S	1.			0.	0.	C	1100.000	1221.000	110.26260
K2S(L)	J 3/78	K	2.	S	1.			0.	0.	C	1221.000	5000.000	110.26260
K2SO4(a)	J 6/78	K	2.	S	1.	O	4.	0.	0.	C	300.000	857.000	174.26020
K2SO4(b)	J 6/78	K	2.	S	1.	O	4.	0.	0.	C	857.000	1342.000	174.26020
K2SO4(L)	J 6/78	K	2.	S	1.	O	4.	0.	0.	C	1342.000	5000.000	174.26020
LI(cr)	TPIS82	LI	1.		0.			0.	0.	C	200.000	453.690	6.94100
LI(L)	TPIS82	LI	1.		0.			0.	0.	C	453.690	3000.000	6.94100
LIALO2(s)	J12/79	LI	1.	AL	1.	O	2.	0.	0.	C	300.000	1973.000	65.92134
LIALO2(L)	J12/79	LI	1.	AL	1.	O	2.	0.	0.	C	1973.000	5000.000	65.92134
LICL(s)	J 6/62	LI	1.	CL	1.			0.	0.	C	300.000	883.000	42.39370
LICL(L)	J 6/62	LI	1.	CL	1.			0.	0.	C	883.000	2000.000	42.39370
LIF(s)	J12/68	LI	1.	F	1.			0.	0.	C	300.000	1121.300	25.93940
LIF(L)	J12/68	LI	1.	F	1.			0.	0.	C	1121.300	5000.000	25.93940
LIH(s)	J 9/67	LI	1.	H	1.			0.	0.	C	300.000	961.000	7.94894
LIH(L)	J 9/67	LI	1.	H	1.			0.	0.	C	961.000	5000.000	7.94894
LIOH(s)	J 6/71	LI	1.	O	1.	H	1.	0.	0.	C	300.000	744.300	23.94834
LIOH(L)	J 6/71	LI	1.	O	1.	H	1.	0.	0.	C	744.300	5000.000	23.94834
LI2O(s)	J 3/64	LI	2.	O	1.			0.	0.	C	300.000	1843.000	29.88140
LI2O(L)	J 3/64	LI	2.	O	1.			0.	0.	C	1843.000	5000.000	29.88140
LI2SO4(a)	J12/78	LI	2.	S	1.	O	4.	0.	0.	C	200.000	848.000	109.94560
LI2SO4(b)	J12/78	LI	2.	S	1.	O	4.	0.	0.	C	848.000	1132.000	109.94560
LI2SO4(L)	J12/78	LI	2.	S	1.	O	4.	0.	0.	C	1132.000	6000.000	109.94560
LI3N(s)	J 3/78	LI	3.	N	1.			0.	0.	C	300.000	1300.000	34.82974
Mg(cr)	SRD 93	MG	1.		0.			0.	0.	C	298.150	923.000	24.30500
Mg(L)	SRD 93	MG	1.		0.			0.	0.	C	923.000	6000.000	24.30500
MgAL2O4(s)	J12/79	MG	1.	AL	2.	O	4.	0.	0.	C	300.000	2408.000	142.26568
MgAL2O4(L)	J12/79	MG	1.	AL	2.	O	4.	0.	0.	C	2408.000	5000.000	142.26568
MgBr2(s)	J 6/74	MG	1.	BR	2.			0.	0.	C	300.000	984.000	184.11300
MgBr2(L)	J 6/74	MG	1.	BR	2.			0.	0.	C	984.000	5000.000	184.11300
MgCO3(s)	J12/66	MG	1.	C	1.	O	3.	0.	0.	C	300.000	1000.000	84.31420
MgCL2(s)	J12/65	MG	1.	CL	2.			0.	0.	C	300.000	987.000	95.21040
MgCL2(L)	J12/65	MG	1.	CL	2.			0.	0.	C	987.000	5000.000	95.21040
MgF2(s)	J 6/75	MG	1.	F	2.			0.	0.	C	300.000	1536.000	62.30181
MgF2(L)	J 6/75	MG	1.	F	2.			0.	0.	C	1536.000	5000.000	62.30181
MgI2(s)	J12/74	MG	1.	I	2.			0.	0.	C	300.000	987.000	278.11394
MgI2(L)	J12/74	MG	1.	I	2.			0.	0.	C	987.000	5000.000	278.11394
MgO(s)	J12/74	MG	1.	O	1.			0.	0.	C	300.000	3105.000	40.30440
MgO(L)	J12/74	MG	1.	O	1.			0.	0.	C	3105.000	5000.000	40.30440
MgO2H2(s)	J12/75	MG	1.	O	2.	H	2.	0.	0.	C	300.000	1000.000	58.31968
MgS(s)	J 9/77	MG	1.	S	1.			0.	0.	C	300.000	3000.000	56.37100
MgSO4(s)	L 7/76	MG	1.	S	1.	O	4.	0.	0.	C	300.000	1400.000	120.36860
MgSO4(L)	L 7/76	MG	1.	S	1.	O	4.	0.	0.	C	1400.000	5000.000	120.36860
MgSIO3(I)	J12/67	MG	1.	SI	1.	O	3.	0.	0.	C	300.000	903.000	100.38870
MgSIO3(II)	J12/67	MG	1.	SI	1.	O	3.	0.	0.	C	903.000	1258.000	100.38870

Species ID.	Code	Formula Used by CETPC						Phase		Temp. Range		Mole. Wt.
MgSiO3(III)	J12/67	MG	1.	SI	1.	O	3.	0.	C	1258.000	1850.000	100.38870
MgSiO3(L)	J12/67	MG	1.	SI	1.	O	3.	0.	C	1850.000	5000.000	100.38870
MgTiO3(s)	J 6/67	MG	1.	TI	1.	O	3.	0.	C	300.000	1953.000	120.18320
MgTiO3(L)	J 6/67	MG	1.	TI	1.	O	3.	0.	C	1953.000	5000.000	120.18320
MgTi2O5(s)	J 6/67	MG	1.	TI	2.	O	5.	0.	C	300.000	1963.000	200.06200
MgTi2O5(L)	J 6/67	MG	1.	TI	2.	O	5.	0.	C	1963.000	5000.000	200.06200
Mg2SiO4(s)	J12/67	MG	2.	SI	1.	O	4.	0.	C	300.000	2171.000	140.69310
Mg2SiO4(L)	J12/67	MG	2.	SI	1.	O	4.	0.	C	2171.000	5000.000	140.69310
Mg2TiO4(s)	J 6/67	MG	2.	TI	1.	O	4.	0.	C	300.000	2013.000	160.48760
Mg2TiO4(L)	J 6/67	MG	2.	TI	1.	O	4.	0.	C	2013.000	5000.000	160.48760
Mo(cr)	J 3/78	MO	1.		0.		0.	0.	C	200.000	2896.000	95.94000
Mo(L)	J 3/78	MO	1.		0.		0.	0.	C	2896.000	6000.000	95.94000
NH4CL(a)	BAR 73	N	1.	H	4.	CL	1.	0.	C	298.150	458.000	53.49120
NH4CL(b)	BAR 73	N	1.	H	4.	CL	1.	0.	C	458.000	793.200	53.49120
Na(cr)	CODA89	NA	1.		0.		0.	0.	C	200.000	371.010	22.98977
Na(L)	CODA89	NA	1.		0.		0.	0.	C	371.010	2300.000	22.98977
NaAlO2(a)	J 3/63	NA	1.	AL	1.	O	2.	0.	C	300.000	740.000	81.97011
NaAlO2(b)	J 3/63	NA	1.	AL	1.	O	2.	0.	C	740.000	3000.000	81.97011
NaBr(s)	J 9/64	NA	1.	BR	1.		0.	0.	C	300.000	1020.000	102.89377
NaBr(L)	J 9/64	NA	1.	BR	1.		0.	0.	C	1020.000	5000.000	102.89377
NaCN(s)	J 3/66	NA	1.	C	1.	N	1.	0.	C	300.000	835.000	49.00751
NaCN(L)	J 3/66	NA	1.	C	1.	N	1.	0.	C	835.000	5000.000	49.00751
NaCL(s)	J 9/64	NA	1.	CL	1.		0.	0.	C	300.000	1073.800	58.44247
NaCL(L)	J 9/64	NA	1.	CL	1.		0.	0.	C	1073.800	5000.000	58.44247
NaF(s)	J12/68	NA	1.	F	1.		0.	0.	C	300.000	1269.000	41.98817
NaF(L)	J12/68	NA	1.	F	1.		0.	0.	C	1269.000	3500.000	41.98817
NaI(s)	J 9/63	NA	1.	I	1.		0.	0.	C	300.000	933.000	149.89424
NaI(L)	J 9/63	NA	1.	I	1.		0.	0.	C	933.000	5000.000	149.89424
NaOH(a)	J12/70	NA	1.	O	1.	H	1.	0.	C	300.000	596.000	39.99711
NaOH(L)	J12/70	NA	1.	O	1.	H	1.	0.	C	596.000	2500.000	39.99711
NaO2(s)	J 6/63	NA	1.	O	2.		0.	0.	C	300.000	2000.000	54.98857
Na2CO3(1)	J 3/66	NA	2.	C	1.	O	3.	0.	C	300.000	723.150	105.98874
Na2CO3(2)	J 3/66	NA	2.	C	1.	O	3.	0.	C	723.150	1123.150	105.98874
Na2CO3(L)	J 3/66	NA	2.	C	1.	O	3.	0.	C	1123.150	5000.000	105.98874
Na2O(c)	J 6/68	NA	2.	O	1.		0.	0.	C	300.000	1243.200	61.97894
Na2O(a)	J 6/68	NA	2.	O	1.		0.	0.	C	1243.200	1405.200	61.97894
Na2O(L)	J 6/68	NA	2.	O	1.		0.	0.	C	1405.200	5000.000	61.97894
Na2O2(a)	J 6/68	NA	2.	O	2.		0.	0.	C	300.000	785.000	77.97834
Na2O2(b)	J 6/68	NA	2.	O	2.		0.	0.	C	785.000	5000.000	77.97834
Na2S(1)	J 3/78	NA	2.	S	1.		0.	0.	C	300.000	1276.000	78.04554
Na2S(2)	J 3/78	NA	2.	S	1.		0.	0.	C	1276.000	1445.000	78.04554
Na2S(L)	J 3/78	NA	2.	S	1.		0.	0.	C	1445.000	5000.000	78.04554
Na2SO4(V)	J 6/78	NA	2.	S	1.	O	4.	0.	C	200.000	458.000	142.04314
Na2SO4(IV)	J 6/78	NA	2.	S	1.	O	4.	0.	C	458.000	514.000	142.04314
Na2SO4(I)	J 6/78	NA	2.	S	1.	O	4.	0.	C	514.000	1157.000	142.04314
Na2SO4(L)	J 6/78	NA	2.	S	1.	O	4.	0.	C	1157.000	6000.000	142.04314
Na3ALF6(a)	J12/79	NA	3.	AL	1.	F	6.	0.	C	300.000	836.000	209.94126
Na3ALF6(b)	J12/79	NA	3.	AL	1.	F	6.	0.	C	836.000	1285.000	209.94126
Na3ALF6(L)	J12/79	NA	3.	AL	1.	F	6.	0.	C	1285.000	5000.000	209.94126
Na5AL3F14(a)	J12/79	NA	5.	AL	3.	F	14.	0.	C	300.000	1010.000	461.87110
Na5AL3F14(L)	J12/79	NA	5.	AL	3.	F	14.	0.	C	1010.000	5000.000	461.87110
Nb(cr)	J12/73	NB	1.		0.		0.	0.	C	200.000	2750.000	92.90638
Nb(L)	J12/73	NB	1.		0.		0.	0.	C	2750.000	6000.000	92.90638
NbO(a)	J12/73	NB	1.	O	1.		0.	0.	C	300.000	2210.000	108.90578
NbO(L)	J12/73	NB	1.	O	1.		0.	0.	C	2210.000	5000.000	108.90578
NbO2(I)	J12/73	NB	1.	O	2.		0.	0.	C	200.000	1090.000	124.90518
NbO2(II)	J12/73	NB	1.	O	2.		0.	0.	C	1090.000	1200.000	124.90518
NbO2(III)	J12/73	NB	1.	O	2.		0.	0.	C	1200.000	2175.000	124.90518
NbO2(L)	J12/73	NB	1.	O	2.		0.	0.	C	2175.000	5000.000	124.90518
Nb2O5(s)	J12/72	NB	2.	O	5.		0.	0.	C	300.000	1785.000	265.80976
Nb2O5(L)	J12/72	NB	2.	O	5.		0.	0.	C	1785.000	5000.000	265.80976
Ni(cr)	J12/76	NI	1.		0.		0.	0.	C	200.000	631.000	58.69340
Ni(cr)	J12/76	NI	1.		0.		0.	0.	C	631.000	1728.000	58.69340
Ni(L)	J12/76	NI	1.		0.		0.	0.	C	1728.000	6000.000	58.69340
NiS(b)	J12/76	NI	1.	S	1.		0.	0.	C	300.000	652.000	90.75940
NiS(a)	J12/76	NI	1.	S	1.		0.	0.	C	652.000	1249.000	90.75940
NiS(L)	J12/76	NI	1.	S	1.		0.	0.	C	1249.000	5000.000	90.75940
NiS2(s)	J 3/77	NI	1.	S	2.		0.	0.	C	300.000	1280.000	122.82540
NiS2(L)	J 3/77	NI	1.	S	2.		0.	0.	C	1280.000	5000.000	122.82540
Ni3S2(1)	J12/76	NI	3.	S	2.		0.	0.	C	300.000	829.000	240.21220
Ni3S2(2)	J12/76	NI	3.	S	2.		0.	0.	C	829.000	1062.000	240.21220
Ni3S2(L)	J12/76	NI	3.	S	2.		0.	0.	C	1062.000	5000.000	240.21220
Ni3S4(s)	J 3/77	NI	3.	S	4.		0.	0.	C	300.000	1100.000	304.34420
P(cr)	TPIS89	P	1.		0.		0.	0.	C	195.400	317.300	30.97376

Species ID.	Code	Formula Used by CETPC						Phase	Temp. Range		Mole. Wt.
P(L)	TPIS89	P 1.		0.		0.	0.	C	317.300	6000.000	30.97376
P4O10(s)	J12/65	P 4.	O 10.			0.	0.	C	300.000	1500.000	283.88905
Pb(cr)	TPIS91	PB 1.		0.		0.	0.	C	200.000	600.650	207.20000
Pb(L)	TPIS91	PB 1.		0.		0.	0.	C	600.650	3600.000	207.20000
PbBr2(s)	J12/73	PB 1.	BR 2.			0.	0.	C	300.000	644.000	367.00800
PbBr2(L)	J12/73	PB 1.	BR 2.			0.	0.	C	644.000	5000.000	367.00800
PbCL2(s)	J 6/73	PB 1.	CL 2.			0.	0.	C	300.000	774.000	278.10540
PbCL2(L)	J 6/73	PB 1.	CL 2.			0.	0.	C	774.000	5000.000	278.10540
PbF2(a)	J12/73	PB 1.	F 2.			0.	0.	C	298.150	583.000	245.19681
PbF2(b)	J12/73	PB 1.	F 2.			0.	0.	C	583.000	1103.000	245.19681
PbF2(L)	J12/73	PB 1.	F 2.			0.	0.	C	1103.000	6000.000	245.19681
PbI2(s)	J12/73	PB 1.	I 2.			0.	0.	C	300.000	683.000	461.00894
PbI2(L)	J12/73	PB 1.	I 2.			0.	0.	C	683.000	5000.000	461.00894
PbO(rd)	J12/71	PB 1.	O 1.			0.	0.	C	300.000	762.000	223.19940
PbO(yw)	J12/71	PB 1.	O 1.			0.	0.	C	762.000	1159.000	223.19940
PbO(L)	J12/71	PB 1.	O 1.			0.	0.	C	1159.000	5000.000	223.19940
PbO2(s)	J12/71	PB 1.	O 2.			0.	0.	C	300.000	1200.000	239.19880
PbS(s)	J 6/73	PB 1.	S 1.			0.	0.	C	300.000	1386.500	239.26600
PbS(L)	J 6/73	PB 1.	S 1.			0.	0.	C	1386.500	5000.000	239.26600
Pb3O4(s)	J12/71	PB 3.	O 4.			0.	0.	C	300.000	5000.000	685.59760
S(cr1)	TPIS89	S 1.		0.		0.	0.	C	200.000	368.300	32.06600
S(cr2)	TPIS89	S 1.		0.		0.	0.	C	368.300	388.360	32.06600
S(L)	TPIS89	S 1.		0.		0.	0.	C	388.360	6000.000	32.06600
SCL2(L)	J 6/78	S 1.	CL 2.			0.	0.	C	300.000	5000.000	102.97140
S2CL2(L)	J 6/78	S 2.	CL 2.			0.	0.	C	300.000	5000.000	135.03740
Si(cr)	TPIS91	SI 1.		0.		0.	0.	C	200.000	1690.000	28.08550
SI(L)	TPIS91	SI 1.		0.		0.	0.	C	1690.000	6000.000	28.08550
SIC(b)	J 3/67	SI 1.	C 1.			0.	0.	C	300.000	4000.000	40.09650
SIO2(Lqz)	J 6/67	SI 1.	O 2.			0.	0.	C	200.000	847.000	60.08430
SIO2(hqz)	J 6/67	SI 1.	O 2.			0.	0.	C	847.000	1079.000	60.08430
SiO2(L)	J 6/67	SI 1.	O 2.			0.	0.	C	1696.000	6000.000	60.08430
Si2N2O(s)	L 1/84	SI 2.	N 2.	O	1.	0.	0.	C	298.150	2500.000	100.10380
SI3N4(a)	J 3/67	SI 3.	N 4.			0.	0.	C	300.000	3000.000	140.28340
Sr(a)	SRD 93	SR 1.		0.		0.	0.	C	298.150	820.000	87.62000
Sr(b)	SRD 93	SR 1.		0.		0.	0.	C	820.000	1041.000	87.62000
Sr(L)	SRD 93	SR 1.		0.		0.	0.	C	1041.000	6000.000	87.62000
SrCL2(1)	J12/72	SR 1.	CL 2.			0.	0.	C	300.000	1000.000	158.52540
SrCL2(2)	J12/72	SR 1.	CL 2.			0.	0.	C	1000.000	1147.000	158.52540
SrCL2(L)	J12/72	SR 1.	CL 2.			0.	0.	C	1147.000	5000.000	158.52540
SrF2(s)	J12/72	SR 1.	F 2.			0.	0.	C	300.000	1750.000	125.61681
SrF2(L)	J12/72	SR 1.	F 2.			0.	0.	C	1750.000	5000.000	125.61681
SrO(s)	J12/72	SR 1.	O 1.			0.	0.	C	300.000	2938.000	103.61940
SrO(L)	J12/72	SR 1.	O 1.			0.	0.	C	2938.000	5000.000	103.61940
SrO2H2(s)	J12/75	SR 1.	O 2.	H	2.	0.	0.	C	300.000	783.150	121.63468
SrO2H2(L)	J12/75	SR 1.	O 2.	H	2.	0.	0.	C	783.150	5000.000	121.63468
SrS(s)	J 9/77	SR 1.	S 1.			0.	0.	C	300.000	3000.000	119.68600
Ta(cr)	J12/72	TA 1.		0.		0.	0.	C	200.000	3258.000	180.94790
Ta(L)	J12/72	TA 1.		0.		0.	0.	C	3258.000	6000.000	180.94790
TaC(s)	J12/73	TA 1.	C 1.			0.	0.	C	300.000	4273.000	192.95890
TaC(L)	J12/73	TA 1.	C 1.			0.	0.	C	4273.000	5000.000	192.95890
Ta2O5(s)	J12/72	TA 2.	O 5.			0.	0.	C	300.000	2058.000	441.89280
Ta2O5(L)	J12/72	TA 2.	O 5.			0.	0.	C	2058.000	5000.000	441.89280
TI(a)	CODA89	TI 1.		0.		0.	0.	C	200.000	1156.000	47.88000
TI(b)	CODA89	TI 1.		0.		0.	0.	C	1156.000	1944.000	47.88000
TI(L)	CODA89	TI 1.		0.		0.	0.	C	1944.000	6000.000	47.88000
TIC(s)	J 6/68	TI 1.	C 1.			0.	0.	C	300.000	3298.000	59.89100
TIC(L)	J 6/68	TI 1.	C 1.			0.	0.	C	3298.000	5000.000	59.89100
TICL2(s)	J12/68	TI 1.	CL 2.			0.	0.	C	300.000	2000.000	118.78540
TICL3(s)	J 6/68	TI 1.	CL 3.			0.	0.	C	300.000	5000.000	154.23810
TiCL4(L)	J12/67	TI 1.	CL 4.			0.	0.	C	300.000	5000.000	189.69080
TiN(s)	J 6/68	TI 1.	N 1.			0.	0.	C	300.000	3220.000	61.88674
TIN(L)	J 6/68	TI 1.	N 1.			0.	0.	C	3220.000	5000.000	61.88674
TIO(a)	J12/73	TI 1.	O 1.			0.	0.	C	300.000	1265.000	63.87940
TIO(b)	J12/73	TI 1.	O 1.			0.	0.	C	1265.000	2023.000	63.87940
TIO(L)	J12/73	TI 1.	O 1.			0.	0.	C	2023.000	5000.000	63.87940
TIO2(ru)	J12/73	TI 1.	O 2.			0.	0.	C	300.000	2130.000	79.87880
TIO2(L)	J12/73	TI 1.	O 2.			0.	0.	C	2130.000	5000.000	79.87880
TI2O3(1)	J 6/73	TI 2.	O 3.			0.	0.	C	300.000	470.000	143.75820
TI2O3(2)	J 6/73	TI 2.	O 3.			0.	0.	C	470.000	2115.000	143.75820
TI2O3(L)	J 6/73	TI 2.	O 3.			0.	0.	C	2115.000	5000.000	143.75820
TI3O5(a)	J12/73	TI 3.	O 5.			0.	0.	C	300.000	450.000	223.63760
Ti3O5(b)	J12/73	TI 3.	O 5.			0.	0.	C	450.000	2050.000	223.63760
TI3O5(L)	J12/73	TI 3.	O 5.			0.	0.	C	2050.000	5000.000	223.63760
Ti4O7(s)	J12/73	TI 4.	O 7.			0.	0.	C	300.000	1950.000	303.51580

Species ID.	Code	Formula Used by CETPC						Phase	Temp. Range		Mole. Wt.
TI407(L)	J12/73	TI	4.	O	7.		0.	0.	C	1950.000	5000.000	303.51500
V(cr)	J 6/73	V	1.		0.		0.	0.	C	200.000	2190.000	50.94150
V(L)	J 6/73	V	1.		0.		0.	0.	C	2190.000	6000.000	50.94150
VCL2(s)	L 2/76	V	1.	CL	2.		0.	0.	C	300.000	1300.000	121.84690
VCL3(s)	L 2/76	V	1.	CL	3.		0.	0.	C	300.000	1000.000	157.29960
VCL4(L)	L 2/76	V	1.	CL	4.		0.	0.	C	300.000	2000.000	192.75230
VN(s)	J12/73	V	1.	N	1.		0.	0.	C	300.000	3500.000	64.94824
VO(s)	J12/73	V	1.	O	1.		0.	0.	C	300.000	2063.000	66.94090
VO(L)	J12/73	V	1.	O	1.		0.	0.	C	2063.000	5000.000	66.94090
V203(s)	J12/73	V	2.	O	3.		0.	0.	C	300.000	2340.000	149.88120
V203(L)	J12/73	V	2.	O	3.		0.	0.	C	2340.000	5000.000	149.88120
V204(1)	J 6/73	V	2.	O	4.		0.	0.	C	300.000	340.000	165.88060
V204(2)	J 6/73	V	2.	O	4.		0.	0.	C	340.000	1818.000	165.88060
V204(L)	J 6/73	V	2.	O	4.		0.	0.	C	1818.000	5000.000	165.88060
V205(s)	J 6/73	V	2.	O	5.		0.	0.	C	300.000	943.000	181.88000
V205(L)	J 6/73	V	2.	O	5.		0.	0.	C	943.000	5000.000	181.88000
Zn(cr)	CODA89	ZN	1.		0.		0.	0.	C	200.000	692.730	65.39000
Zn(L)	CODA89	ZN	1.		0.		0.	0.	C	692.730	6000.000	65.39000
ZnSO4(a)	J 3/79	ZN	1.	S	1.	O	4.	0.	C	300.000	540.000	161.45360
ZnSO4(a)	J 3/79	ZN	1.	S	1.	O	4.	0.	C	540.000	1013.000	161.45360
ZnSO4(b)	J 3/79	ZN	1.	S	1.	O	4.	0.	C	1013.000	5000.000	161.45360
Zr(a)	J 6/79	ZR	1.		0.		0.	0.	C	200.000	1135.000	91.22400
Zr(b)	J 6/79	ZR	1.		0.		0.	0.	C	1135.000	2125.000	91.22400
Zr(L)	J 6/79	ZR	1.		0.		0.	0.	C	2125.000	6000.000	91.22400
ZrN(s)	J 6/61	ZR	1.	N	1.		0.	0.	C	300.000	3225.000	105.23074
ZrN(L)	J 6/61	ZR	1.	N	1.		0.	0.	C	3225.000	5000.000	105.23074
ZrO2(a)	J12/65	ZR	1.	O	2.		0.	0.	C	300.000	1478.000	123.22280
ZrO2(b)	J12/65	ZR	1.	O	2.		0.	0.	C	1478.000	2950.000	123.22280
ZrO2(L)	J12/65	ZR	1.	O	2.		0.	0.	C	2950.000	5000.000	123.22280

Appendix B

Example Problems

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#  EXAMPLE 1, case 1:
#      (a)  Assigned-temperature-and-pressure problem (tp=t).
#      (b)  Reactants are H2 and air.
#      (c)  Molar composition of air is taken from Gordon (1982) ("M" in col.53).
#      (d)  Assigned enthalpy for CO2 is given in J/mole ("J" in col. 71).
#      (e)  Calculations are for two equivalence ratios (eratio=t,mix=1,1.5).
#      (f)  Assigned pressures are 1, 0.1, and 0.01 atm (atm=t,p=1,.1,.01).
#      (g)  Assigned temperatures are 3000 and 2000 K (t=3000,2000).
#      (h)  ONLY records are used to restrict possible products.
#      (i)  Transport property calculations are omitted (trnspt=f or default).
#        1         2         3         4         5         6         7         8
#2345678901234567890123456789012345678901234567890123456789012345678901234567890
REACTANTS
H 2.                                        1.     M 0.      G298.15  F
N 2.                                        .78084 M 0.      G298.15  0
O 2.                                        .209476M 0.      G298.15  0
Ar1.                                        .009365M 0.      G298.15  0
C 1.     O 2.                               .000319M-393510. G298.15 J0

ONLY          Ar            C             CO            CO2
ONLY          H             H2            H2O           HNO
ONLY          HO2           HNO2          HNO3          N
ONLY          NH            NO            N2            N2O3
ONLY          O             O2            OH            O3
#
NAMELISTS
 &inpt2 kase=1,tp=t,atm=t,p=1,.1,.01,eratio=t,mix=1,1.5,t=3000,2000, &end


#  EXAMPLE 2, case 2:
#      (a)  Assigned-temperature-and-volume problem (tv=t) including thermal
#           transport properties (trnspt=t).
#      (b)  Reactants are the same as in case 1 but air is given on one record.
#      (c)  Assigned enthalpy for air is given in J/mole ("J" in col. 71).
#      (d)  One mixture and one temperature were taken from example 1 (mix=1,
#           eratio=t,t=3000).
#      (e)  Assigned specific volumes were obtained by first running example 1.
#           The assigned v values are the inverse values of rho printed in
#           example 1.  Composition and properties in examples 1 and 2 should
#           match for these values.
#      (f)  ONLY records are used to restrict possible products.
#        1         2         3         4         5         6         7         8
#2345678901234567890123456789012345678901234567890123456789012345678901234567890
REACTANTS
H 2.                                        100.      0.     G298.15  F
N 1.561680 .419590Ar.009365C .000319        100.   -125.53   G298.15 J0

ONLY          Ar            C             CO            CO2
ONLY          H             H2            H2O           HNO
ONLY          HO2           HNO2          HNO3          N
ONLY          NH            NO            N2            N2O3
ONLY          O             O2            OH            O3
#
NAMELISTS
 &inpt2 kase=2, tv=t,v=10885.9,123640,1513798,eratio=t,mix=1,t=3000,trnspt=t,
       &end
```

```
#  EXAMPLE 3, case 3:
#     (a)  Combustion or assigned-enthalpy-and-pressure problem (hp=t).
#     (b)  Fuels are C7H8(L) and C8H18(L) at 298.15 K and oxidant is air at
#          700 K.
#     (c)  The enthalpies of all the reactants are to be calculated from the
#          product thermodynamic data base (00 in cols. 37 and 38).
#     (d)  Oxidant-to-fuel weight ratio is 17 (of=t,mix=17).
#     (e)  Mixture enthalpy is calculated from reactant values (default).
#     (f)  Many species are omitted from the product data base (OMIT records).
#     (g)  Assigned pressures are 100, 10, and 1 bar (p=100,10,1).
#     (h)  Mixture properties are to be printed in SI units (siunit=t).
#     (i)  Mole fractions > 1.e-15 are to be in e-format (trace=1.e-15).
#
#234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
#        1         2         3         4         5         6         7         8
REACTANTS
N 2.                                  00        .75524          G 700.0  0
O 2.                                  00        .23144          G 700.0  0
Ar1.                                  00        .01286          G 700.0  0
C 1.     O 2.                         00        .00046          G 700.0  0
C 7.     H 8.                         00        .4              L 298.15 F
C 8.     H 18.                        00        .6              L 298.15 F

OMIT          CCN             CNC             C2N2            C2O
OMIT          C3H4,allene     C3H4,propyne    C3H4,cyclo-     C3
OMIT          C3H5,allyl      C3H6,propylene  C3H6,cyclo-     C3H3,propargyl
OMIT          C3H6O           C3H7,n-propyl   C3H7,i-propyl   Jet-A(g)
OMIT          C3O2            C4              C4H2            C3H8O,2propanol
OMIT          C4H4,1,3-cyclo- C4H6,butadiene  C4H6,2-butyne  C3H8O,1propanol
OMIT          C4H8,tr2-buteneC4H8,isobutene   C4H8,cyclo-     C4H6,cyclo-
OMIT          (CH3COOH)2      C4H9,n-butyl    C4H9,i-butyl    C4H8,1-butene
OMIT          C4H9,s-butyl    C4H9,t-butyl    C4H10,isobutaneC4H8,cis2-buten
OMIT          C4H10,n-butane  C4N2            C5              C3H8
OMIT          C5H6,1,3cyclo-  C5H8,cyclo-     C5H10,1-penteneC10H21,n-decyl
OMIT          C5H10,cyclo-    C5H11,pentyl    C5H11,t-pentyl  C12H10,biphenyl
OMIT          C5H12,n-pentaneC5H12,i-pentaneCH3C(CH3)2CH3     C12H9,o-bipheny
OMIT          C6H6            C6H5OH,phenol   C6H10,cyclo-    C6H2
OMIT          C6H12,1-hexene  C6H12,cyclo-    C6H13,n-hexyl   C6H5,phenyl
OMIT          C7H7,benzyl     C7H8            C7H8O,cresol mx C6H5O,phenoxy
OMIT          C7H14,1-heptene C7H15,n-heptyl  C7H16,n-heptaneC10H8,azulene
OMIT          C8H8,styrene    C8H10,ethylbenzC8H16,1-octene   C10H8,napthlene
OMIT          C8H17,n-octyl   C8H18,isooctaneC8H18,n-octane  C9H19,n-nonyl
OMIT          Jet-A(L)        C6H6(L)         H2O(s)          H2O(L)

NAMELISTS
 &inpt2 kase=3,hp=t,p=100,10,1,of=t,mix=17,siunit=t,trace=1.e-15&end
```

```
#  EXAMPLE 4, case 4:
#      (a)  Assigned-internal-energy-and-density problem (uv=t).
#      (b)  Fuel, oxidant, and oxidant-to-fuel weight ratio are the same as in
#           example 3.
#      (c)  Internal energy u was taken from col. 1 of the output of example 3.
#           However, input requires u/R, i.e., u = -375.08 kJ/kg and
#           u/R = -375.08/8.31451 = -45.1115  (ur=-45.1115).
#      (d)  Units for density input are limited to g/cc.  From example 3 point 1,
#           rho = 14.426 kg/m**3 = 0.014426 g/cc (rho=.014426).
#      (e)  Mixture properties are to be printed in SI units (siunit=t).
#      (f)  Mole fractions > 1.e-15 are to be in e-format (trace=1.e-15).
#      (g)  Note that since all parameters for this example are the same as
#           those used for col. 1 of example 3, assigning u and rho from
#           this column should yield the same pressure and temperature assigned
#           for that point in example 3.
#
#234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
#       1         2         3         4         5         6         7         8
REACTANTS
N 2.                                          .75524          G 700.    0
O 2.                                          .23144          G 700.    0
Ar1.                                          .01286          G 700.    0
C 1.     O 2.                                 .00046          G 700.    0
C 7.     H 8.                                 .4              L 298.15 F
C 8.     H 18.                                .6              L 298.15 F

OMIT          CCN             CNC             C2N2            C2O
OMIT          C3H4,allene     C3H4,propyne    C3H4,cyclo-     C3
OMIT          C3H5,allyl      C3H6,propylene  C3H6,cyclo-     C3H3,propargyl
OMIT          C3H6O           C3H7,n-propyl   C3H7,i-propyl   Jet-A(g)
OMIT          C3O2            C4              C4H2            C3H8O,2propanol
OMIT          C4H4,1,3-cyclo-C4H6,butadiene   C4H6,2-butyne   C3H8O,1propanol
OMIT          C4H8,tr2-buteneC4H8,isobutene   C4H8,cyclo-     C4H6,cyclo-
OMIT          (CH3COOH)2      C4H9,n-butyl    C4H9,i-butyl    C4H8,1-butene
OMIT          C4H9,s-butyl    C4H9,t-butyl    C4H10,isobutaneC4H8,cis2-buten
OMIT          C4H10,n-butane  C4N2            C5              C3H8
OMIT          C5H6,1,3cyclo-  C5H8,cyclo-     C5H10,1-penteneC10H21,n-decyl
OMIT          C5H10,cyclo-    C5H11,pentyl    C5H11,t-pentyl  C12H10,biphenyl
OMIT          C5H12,n-pentaneC5H12,i-pentaneCH3C(CH3)2CH3     C12H9,o-bipheny
OMIT          C6H6            C6H5OH,phenol   C6H10,cyclo-    C6H2
OMIT          C6H12,1-hexene  C6H12,cyclo-    C6H13,n-hexyl   C6H5,phenyl
OMIT          C7H7,benzyl     C7H8            C7H8O,cresol mxC6H5O,phenoxy
OMIT          C7H14,1-heptaneC7H15,n-heptyl   C7H16,n-heptaneC10H8,azulene
OMIT          C8H8,styrene    C8H10,ethylbenzC8H16,1-octene   C10H8,napthlene
OMIT          C8H17,n-octyl   C8H18,isooctaneC8H18,n-octane   C9H19,n-nonyl
OMIT          C7H8(L)         C8H18(L),n-octaJet-A(L)         C6H6(L)
OMIT          H2O(s)          H2O(L)
NAMELISTS
 &inpt2 kase=4,uv=t,ur=-45.1115,rho=.014426,of=t,mix=17,siunit=t,
   trace=1.e-15&end
```

```
#  EXAMPLE 5, case 5:
#     (a)  Combustion problem (hp=t) for solid propellant with 5 ingredients.
#     (b)  The assigned enthalpies in cal/mole are given on each reactant
#          record except for MgO(s), which is to be calculated from the
#          product data base (OO in cols. 37 and 38).
#     (c)  The reactants are given in percent by weight (default).
#     (d)  Five pressures are given in units of psia (psia=t,p=500,250,
#          125,50,5,).
#     (e)  AL203(L) is included as a possible combustion species for the first
#          pressure (INSERT record).  Note that the program will remove
#          any condensed species if their inclusion is wrong.
#     (f)  Many species are omitted from the product data base (OMIT records).
#
REACTANTS
N 1.     H 4.     C11.     0 4.                72.06   -70690.  S298.15  0
C 1.     H 1.869550 .031256S .008415          18.58   -2999.082L298.15  F
Al1.                                           9.       0.0     S298.15  F
Mg1.     0 1.                          OO       .2              S298.15  F
H 2.     0 1.                                   .16   -68317.4 L298.15  F

INSERT          AL203(L)
OMIT            COOH            C2              C2H             CHCO,ketyl
OMIT            C2H2,vinylideneCH2CO,ketene     C2H3,vinyl      CH3CO,acetyl
OMIT            C2H4O,ethylen oCH3CHO,ethanal   CH3COOH         (HCOOH)2
OMIT            C2H5            C2H6            CH3N2CH3        CH3OCH3
OMIT            C2H5OH          CCN             CNC             C2N2
OMIT            C2O             C3              C3H3,propargyl  C3H4,allene
OMIT            C3H4,propyne    C3H4,cyclo-     C3H5,allyl      C3H6,propylene
OMIT            C3H6,cyclo-     C3H6O           C3H7,n-propyl   C3H7,i-propyl
OMIT            C3H8            C3H8O,1propanolC3H8O,2propanolC3O2
OMIT            C4              C4H2            C4H4,1,3-cyclo-C4H6,butadiene
OMIT            C4H6,2-butyne   C4H6,cyclo-     C4H8,1-butene   C4H8,cis2-buten
OMIT            C4H8,tr2-buteneC4H8,isobutene   C4H8,cyclo-     (CH3COOH)2
OMIT            C4H9,n-butyl    C4H9,i-butyl    C4H9,s-butyl    C4H9,t-butyl
OMIT            C4H10,isobutaneC4H10,n-butane   C4N2            C5
OMIT            C5H6,1,3cyclo-  C5H8,cyclo-     C5H10,1-penteneC5H10,cyclo-
OMIT            C5H11,pentyl    C5H11,t-pentyl  C5H12,n-pentaneC5H12,i-pentane
OMIT            CH3C(CH3)2CH3   C6H2            C6H5,phenyl     C6H5O,phenoxy
OMIT            C6H6            C6H5OH,phenol   C6H10,cyclo-   C6H12,1-hexene
OMIT            C6H12,cyclo-    C6H13,n-hexyl   C7H7,benzyl     C7H8
OMIT            C7H8O,cresol mxC7H14,1-heptene  C7H15,n-heptyl  C7H16,n-heptane
OMIT            C8H8,styrene    C8H10,ethylbenzC8H16,1-octene   C8H17,n-octyl
OMIT            C8H18,isooctaneC8H18,n-octane   C9H19,n-nonyl   C10H8,naphthale
OMIT            C10H21,n-decyl C12H9,o-biphenyC12H10,biphenylJet-A(g)
OMIT            HNCO            HNO             HNO2            HNO3
OMIT            HCCN            HCHO,formaldehyHCOOH
OMIT            NH              NH2             NH2OH
OMIT            NCN             N2H2            NH2NO2          N2H4
OMIT            H2O2            (HCOOH)2        C6H6(L)         C7H8(L)
OMIT            C8H18(L),n-octaJet-A(L)         H2O(s)          H2O(L)
NAMELISTS
 &inpt2  kase=5,hp=t,psia=t,p=500,250,125,50,5,&end
```

```
#  EXAMPLE 6, case 6:
#      (a)  Chapman-Jouguet detonation problem (detn=t).
#      (b)  The reactants are stoichiometric H2 and 02 gases (eratio=t,mix=1).
#      (c)  The unburned gases are at 298.15 and 500 K and 1 bar (t=298.15,500,
#           bar=t,p=1)
#      (d)  Thermal transport properties are called for (trnspt=t).
#
#234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
#       1         2         3         4         5         6         7         8
REACTANTS
O 2.                                        100.0   0.0       G298.15  0
H 2.                                        100.    0.        G298.15  F

NAMELISTS
 &inpt2 kase=6,detn=t,eratio=t,mix=1,t=298.15,500,bar=t,p=1,trnspt=t, &end
```

```
#  EXAMPLE 7, case 7:
#      (a)  Shock tube problem (shock=t).
#      (b)  Reactants are H2, 02, and Ar gases at 300 K.  Note that for shock
#           problems reactants must be gaseous species in the thermodynamic
#           product data base.  The program calculates properties of the
#           reactants at the temperature given on the records (300 K).
#      (c)  Reactants are given in moles (M in col. 53).
#      (d)  Initial gas pressures are 10 and 20 mm Hg (p=10,20,mmhg=t).
#      (e)  Seven initial gas velocities are assigned (u1=1000,1100,1200,
#           1250,1300,1350,1400,).
#      (f)  Equilibrium calculations are to be performed for incident shock
#           conditions (incdeq=t).
#      (g)  Frozen calculations are to be performed for incident shock
#           conditions (incdfz=t).
#
#234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
#       1         2         3         4         5         6         7         8
REACTANTS
H 2.                                          0.050  M        G 300.00
O 2.                                          0.050  M        G 300.00
Ar1.                                          0.900  M        G 300.00

NAMELISTS
 &inpt2 kase=7,p=10,20,mmhg=t, shock=t,&end
 &shkinp u1=1000,1100,1200,1250,1300,1350,1400,incdeq=t,incdfz=t&end
```

```
#  EXAMPLE 8, case 8 (see Gordon and McBride, 1988):
#      (a)  Rocket problem with an infinite-area combustor (rkt=t).
#      (b)  The fuel is H2(L) at 20.17 K; the oxidant is O2(L) at 90.18 K.
#      (c)  The oxidant-to-fuel ratio is 5.55157 (of=t,mix=5.55157).
#      (d)  The chamber pressure is 53.3172 bars (p=53.3172,bar=t).
#      (e)  Calculations are with equilibrium chemistry only (froz=f)
#      (f)  For exit points there are three pressure ratios (pcp=10,100,1000),
#           one subsonic area ratio (subar=1.58), and three supersonic area
#           ratios (supar=25,50,75).
#
#234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
#        1         2         3         4         5         6         7         8
REACTANTS
H 2.                                        100.    -2154.  L  20.17 F
O 2.                                        100.    -3102.  L  90.18 0

NAMELISTS
 &inpt2 kase=8,rkt=t,p=53.3172,bar=t,of=t,mix=5.55157,siunit=t  &end
 &rktinp froz=f,subar=1.58,pcp=10,100,1000,supar=25,50,75&end



#  EXAMPLE 9, case 9 (see Gordon and McBride, 1988):
#      (a)  Rocket problem with a finite-area combustor (rkt=t,fac=t).
#      (b)  Contraction ratio of 1.58 (acat=1.58) is assigned.
#      (c)  Fuel, oxidant, and the remaining parameters are the same as in
#           example 8.
#
#234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
#        1         2         3         4         5         6         7         8
REACTANTS
H 2.                                        100.    -2154.  L  20.17 F
O 2.                                        100.    -3102.  L  90.18 0

NAMELISTS
 &inpt2 kase=9,rkt=t,p=53.3172,bar=t,of=t,mix=5.55157,siunit=t  &end
 &rktinp fac=t,acat=1.58,pcp=10,100,1000,supar=25,50,75&end



#  EXAMPLE 10, case 10 (see Gordon and McBride, 1988):
#      (a)  Rocket problem with a finite-area combustor (rkt=t,fac=t).
#      (b)  A ratio of mass flow rate to chamber area of 1333.8 (ma=1333.8)
#           is assigned.  This value was calculated from the results
#           of example 9 where a contraction ratio of 1.58 was assigned.
#      (c)  Fuel, oxidant, and the remaining parameters are the same as in
#           examples 8 and 9.
#
#234567890123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
#        1         2         3         4         5         6         7         8
REACTANTS
H 2.                                        100.    -2154.  L  20.17 F
O 2.                                        100.    -3102.  L  90.18 0

NAMELISTS
 &inpt2 kase=10,rkt=t,p=53.3172,bar=t,of=t,mix=5.55157,siunit=t&end
 &rktinp fac=t,ma=1333.8, pcp=10,100,1000,supar=25,50,75&end
```

```
#  EXAMPLE 11, case 11:
#      (a)  Rocket problem with an infinite-area combustor (rkt=t).
#      (b)  Reactants are Li(s) at 298.15 K and F2(L) at 85.02 K.
#      (c)  Relative amounts of reactants are given as moles on the records
#           (M in col. 53).
#      (d)  Chamber pressure is 1000 psia (p=1000,psia=t).
#      (e)  Ionized species are to be included in the products (ions=t).
#      (f)  Only equilibrium calculations are to be performed (froz=f).
#      (g)  For exit points one pressure ratio (pcp=68.0457), one
#           subsonic area ratio (subar=5), and three supersonic area ratios
#           (supar=10,20,100) are to be included.
#
#23456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
#       1         2         3         4         5         6         7         8
REACTANTS
Li1.
F 2.                                          1.   M    0.    S298.15  F
                                             .5556 M-3098.    L 85.02  0

NAMELISTS
 &inpt2 kase=11, rkt=t,p=1000,psia=t,ions=t ,trnspt=f&end
 &rktinp pcp=68.0457,subar=5,supar=10,20,100,froz=f&end



#  EXAMPLE 12, case 12:
#      (a)  Infinite-area rocket problem (rkt=t).
#      (b)  The fuel is monomethyl hydrazine and the oxidant is nitrogen
#           tetroxide, both liquids at 298.15 K.
#      (c)  The oxidant-to-fuel weight ratio is 2.5 (of=t,mix=2.5).
#      (d)  Chamber pressure is 1000 psia (p=1000,psia=t).
#      (e)  Equilibrium and frozen calculations are to be performed with freezing
#           at the throat (nfz=2).
#      (f)  For exit points one pressure ratio (pcp=68.0457) and four supersonic
#           area ratios (supar=10,50,100,200) are to be included.
#
#23456789012345678901234567890123456789012345678901234567890123456789012345678901234567890
#       1         2         3         4         5         6         7         8
REACTANTS
C 1.     H 6.     N 2.                        100.     54000.   L298.15 JF
N 2.     O 4.                                 100.     -19564.  L298.15 JO

ONLY          CO            CO2           H             HNO
ONLY          HNO2          HO2           H2            H2O
ONLY          H2O2          N             NO            NO2
ONLY          N2            N2O           O             OH
ONLY          O2            HCO           NH            CH4
ONLY          NH2           NH3           H2O(L)        C(gr)
NAMELISTS
 &inpt2 kase=12,p=1000,psia=t,of=t,mix=2.5,rkt=t,siunit=t,&end
 &rktinp pcp=68.0457, supar=10,50,100,200, nfz=2, &end
```

```
#  EXAMPLE 13, case 13:
#     (a)  Rocket problem with an infinite-area combustor (rkt=t).  This problem
#          was selected to show singularity at the throat.
#     (b)  Tripropellant.  Fuels are N2H4(L) and Be(L) and oxidant is H202(L),
#          all at 298.15 K.
#     (c)  Reactant mixture is given as 67% fuel by weight (fpct=t,mix=67.).
#     (d)  Chamber pressure is 3000 psia (psia=t,p=3000).
#     (e)  Calculations are to be for equilibrium conditions only (froz=f).
#     (f)  Four exit pressure ratios are assigned (pcp=3,10,30,300).
#     (g)  BeO(L) is included as possible combustion product for combustion
#          chamber (INSERT record).
#     (h)  Mole fractions > 1.e-10 are to be in e-format (trace=1.e-10).
#
#234567890123456789012345678901234567890123456789012345678901234567890123456789012345678
#        1         2         3         4         5         6         7         8
REACTANTS
N 2.     H 4.                                  80.     12050.    L298.15  F
Be1.                                           20.     0.0       S298.15  F
H 2.     O 2.                                  100.    -44880.   L298.15  O

INSERT          BeO(L)
NAMELISTS
 &inpt2 kase=13,fpct=t,mix=67,psia=t,p=3000,trace=1.e-10,rkt=t&end
 &rktinp pcp=3,10,30,300,froz=f &end
```

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13. ABSTRACT (*Maximum 200 words*)

The NASA Lewis chemical equilibrium program with applications continues to be improved and updated. The latest version is CET93. This code, with smaller arrays, has been compiled for use on an IBM or IBM-compatible personal computer and is called CETPC. This report is intended to be primarily a users manual for CET93 and CETPC. It does not repeat the more complete documentation of earlier reports on the equilibrium program. Most of the discussion covers input and output files, two new options (ONLY and comments), example problems, and implementation of CETPC.

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