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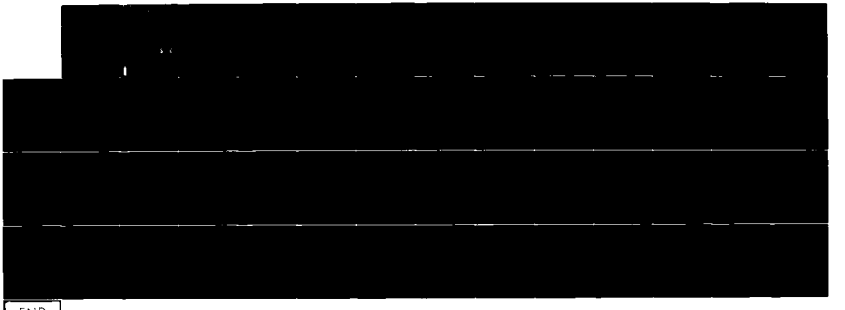

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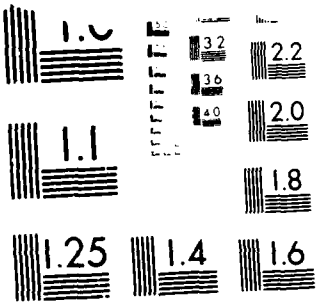

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MELBOURNE, VICTORIA

REPORT

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ABSTRACT

The second order approximation for the estimation of standard enthalpy of formation, entropy of formation and heat capacity of molecules by summation of atomic contributions with nearest neighbour interactions has been incorporated into a Fortran 77 computer programme which currently executes on the IBM P /XT and VAX 11/780 computers. The data base for the programme also includes group corrections for next-to-nearest neighbor interactions and corrections for ring compounds. The programme prompts for the required input, including the symmetry and optical isomers of the molecule, in an interactive manner and allows re-entry and correction of the data after input from a computer terminal.

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C O N T E N T S

THERMODYNAMIC VALUES FROM COMPUTER SUMMATION OF GROUP ADDITIVITY DATA

1. INTRODUCTION

Calculation of equilibrium concentrations in a multi-component system over a range of temperatures requires values for the thermodynamic functions, enthalpy of formation, entropy and heat capacity for each of the species in the equilibrium. The number of species for which these functions have been determined is limited. To supplement the established values, several procedures have been developed for the estimation of these thermodynamic functions. Benson and Buss (1) consider what may be described as zero, first, second, etc order approximations for the estimation of thermodynamic functions. Zero or first order approximations may yield values for the entropy and heat capacity within 4.2 J Mol^{-1} K^{-1} of known values, but second order approximations are required to obtain this precision for the enthalpy of formation. These second order approximations are most readily obtained by consideration of molecules as a combination of groups, from which the thermodynamic functions may be obtained by algebraic summation. Tables of group values for the standard gas phase have been published with a discussion of the procedures used to obtain the values (2). More recently, Alberty (3) showed how a mathematical form of group values could be used to calculate thermodynamic properties of hydrocarbon isomers, in which an isomer group was considered as a whole.

The group values of Benson et al. (2) have been extended and incorporated into a computer programme, CHETAH - Chemical Thermodynamic and Energy Release Evaluation Programme, for Committee E-27 (Hazard Potential of Chemicals) of the American Society for Testing of Materials (4). This programme was written in Fortran IV primarily for mainframe IBM computers. CHETAH will calculate energy hazard potential parameters for compounds based primarily on heat release values. It will also calculate values of the estimated thermodynamic functions and the free energy of reaction for a balanced chemical reaction. The programme and data base is available from ASTM on punched computer cards.

A number of computer programmes have been developed for the calculation of equilibrium concentrations of chemical species using the

thermodynamic functions. The current version of "Thermodata", developed by Turnbull and Wadsley (5), can calculate the equilibrium concentration of up to 100 species. This programme will also output heat balances and has an inbuilt plotting routine. The data base for Thermodata consists of values for the standard enthalpy and entropy of formation of the species and a mathematical function for the variation of the heat capacity with temperature. A routine is available within the Thermodata programme package for adding data to the data base if values for the standard enthalpy and entropy of formation and heat capacity values at several temperatures are available. Thermodata is written in Fortran 77 for the Vax 11/780 computer. It also has been transferred to the IBM PC/XT microcomputer to make use of the graphics capability of the PC/XT display. Currently it is available in Vax compatible tape format and PC/XT floppy disks.

Due to the low unit cost of the IBM PC/XT microcomputer or compatible, a data base originally derived from reference (2) as used in CHETAH has been incorporated into a PC/XT Fortran 77 compatible programme. This programme is designed to be used in an iterative manner with free form "user friendly" terminal input. From an input of the groups in a species it will calculate the thermodynamic values which are required as input for the Thermodata database management programme. These values may be output in machine readable form for direct input into Thermodata.

2. USE OF GROUP ADDITIVITY DATA

The second order approximation for estimation of thermodynamic values is based upon subdivision of a molecular species into a number of groups based upon a central atom in a specified chemical environment which is defined by nearest neighbour interactions (2). In order to obtain a group value, the group must be present in at least one species for which the thermodynamic values are known. When the group is present in more than one species for which thermodynamic values are known, the validity of the group value may be confirmed. In deriving the group values, defined contributions to the known thermodynamic data which were not dependent upon nearest neighbour interactions were algebraically subtracted from the species value. These additional contributions may be considered as pseudo groups and a means of correction for interactions other than nearest neighbour. In all cases these pseudo groups are a means of quantifying non-nearest neighbour symmetry, steric or electronic factors in a species.

2.1 Symmetry Corrections

From statistical mechanics the molar entropy, of a species is given by

$$S = R \ln W$$

where W is the number of distinguishable configurations that the species may have. While these configurations must be weighted by the Boltzmann energy distribution at temperatures of 300K and above, the effect of symmetry elements in a species is to reduce the entropy by R ln σ, where σ is the symmetry number defined as the total number of independent permutations of identical atoms in a molecule that can be arrived at by simple rigid rotations of the entire molecule.

The symmetry number of a species may be further subdivided into an external symmetry number and an internal symmetry number due to "free" internal rotation of symmetrical substitutents The internal symmetry number arises due to "free" rotation of the substituent. Internal rotation around bonds is "free" if the internal energy in the molecule is large compared to the potential energy barrier for rotation of the substituent about the bond. This is true for all unhindered substituents at temperatures of 300 K and above. The entropy contribution of hindered substituents is temperature dependent and not simply included in group contributions based on nearest neighbour interactions. At higher temperatures, even hindered substituents may be considered to have "free" internal rotation. Good agreement between estimated and measured entropy values will be obtained by using the "free" internal rotation model for most single bond substituents. The methyl substitutent is the most common symmetrical substitutent and each has an internal symmetry number of 3. The overall symmetry number is the product of the external symmetry number and the internal symmetry numbers.

External symmetry numbers are most readily obtained from the product of each of the independent symmetry axis. For example, benzene has six two fold symmetry axes and an external symmetry number of 12. SF_6 with six fourfold symmetry axes has an external symmetry number of 24. All normal alkanes have one twofold symmetry axis. With the terminal methyl substitutents each having a internal symmetry number of 3, the overall symmetry number for normal alkanes is 2 x 3 x 3 = 18.

2.2 Optical Isomers

Optical isomers increase the number of possible configurations and thus the molar entropy. The increase in entropy is given by R ln n, where n is the number of optical isomers.

2.3 Correction for Groups in a Ring

Thermodynamic values for non-aromatic ring compounds are obtained by summation of the equivalent non-ring groups with the addition of a ring correction for each ring in the species. This ring correction for the enthalpy may be equated to the destabilization due to ring "strain". This enthalpy correction is greatest for 3 membered rings and almost zero for cyclohexane which can adopt a strain free configuration. Groups in aromatic rings have no non-ring equivalents, so group values for aromatic atoms have any ring correction incorporated in the group value. Ring corrections are not required for aromatic rings. Values for non-aromatic rings are considered as pseudo groups and algebraically summed for each thermodynamic function.

2.4 Steric Corrections

Corrections have been incorporated into the data base for steric interactions with next-nearest neighbour groups. These include alkane and alkene gauche interactions, alkene and ring cis interactions, aromatic ortho interactions and other miscellaneous interactions as listed in sequence numbers 485 to 510 of Tables 1 and 2. These corrections are considered as pseudo groups and algebraically summed with other groups in calculating the thermodynamic values.

2.5 Assignment of Groups in a Species

A group value is required for each "central" atom in a species, where a "central" atom is bonded to more than one other atom. All atoms bonded to other atoms by only one bond are terminal atoms and do not require a group value. (eg. All hydrogen atoms and carbonyl oxygen atoms are in this category). A limited number of atoms bonded to unique atom configurations are considered as pseudo terminal atoms. Atoms in this category include the nitrile carbon ($-C\equiv N$) and the nitrate nitrogen ($-NO_2$). No group values are required for these pseudo terminal atoms. Their effect is contained in the group values of the atom to which they are bonded.

3. PRECISION OF THE GROUP ADDITIVITY ESTIMATES

The group values have been derived from known thermodynamic values for compounds in the standard gas phase. These known values have been used to assign group values for groups based on nearest neighbour interactions. For groups contained in many compounds for which there are a number of reliable experimental measurements, the group value may be considered as the weighted mean of all the measurements. Thermodynamic values estimated from these group values can be considered to yield data which exceeds the precision of single experimental measurements provided there are no interactions in the species other than that with nearest neighbour atoms. This is likely to be the case for the n-alkanes.

Group values which are obtained from experimental values for a single compound will contain the uncertainty of the experimental measurement. In addition, it is more difficult to consider the effect of any interactions other than nearest neighbour. As a general approximation, the validity in the use of group values is likely to decrease as the number of heteroatoms in the species increases. Not only are the groups based on limited numbers of experimental measurements but the probability of significant non-nearest neighbour interaction is greatly increased.

4. USE OF THE COMPUTER PROGRAMME

The computer programme, GROUP.EXE and the data base, GROUP.DAT, are contained on one standard IBM PC 360 Kbyte floppy diskette. The programme may be run from the floppy disk or both programmes copied to a hard disk and run from the hard disk. As the programme reads the data base for each species, the speed of execution is increased for operation from a hard disk. The data base must be on the default directory when the programme is started by typing "GROUP". The programme will readily operate on a standard IBM PC with 192 Kbyte of memory or more.

A terminal dialogue is shown in Appendix 1 for estimation of the thermodynamic values for 2-methylbutane. The input into the programme is shown in bold type. All input may be in either upper or lower case. The first input into the programme is the name of a file to store a copy of the calculated output shown on the terminal. Any PC file name of up to 8 characters and 3 character extension may be used (mydata.txt being used in the example). If the specified file does not exist then it is created else data is appended to the existing file. A blank return by pressing only the <ENTER> key will disable creation of and addition to this type of file.

The second input is for the creation of or addition to a command file for direct input to the CSIRO/NPL "THERMODATA-V" programme "FILER". Any file name may be used. (myfiler.fil is shown in Appendix 1.) The specified file will be created if it does not already exist. A blank return will bypass this step.

For addition to its data base, "FILER" requires a unique formula and a unique name for the species. C5H12 (g) and 2-methylbutane (g) are shown in the example. These entries are added to the "FILER" data base specified in the steps discussed below. The name is also used to describe the output regardless of whether a "FILER" command file is accessed.

As discussed above, the entropy is corrected for the symmetry and the number of optical isomers. 2-methylbutane has a external symmetry number of 1 and each of the 3 terminal methyl groups have an internal symmetry of 3, so the overall symmetry is 27. There are no asymmetric carbon atoms so there is only 1 optical isomer.

The next input is the group sequence number and the number of occurrences of that group in the species. Each group is input on a new line, with a blank line terminating the group input. It is not necessary to input the sequence numbers in numerical order. The group input may be edited during or after input if required. 2-methylbutane has one C-(C)/3-(H) group, one C-(C)/2-(H)/2 and three C-(C)-(H)/3 groups. In addition, it has one alkane gauche interaction in the most stable rotomeric configuration shown in Figure 1. These are input to the programme as a group sequence number (from Table 1 or Table 2) followed by a comma then the number of times the group occurs in the molecule.

```
  6,1
  5,1
  1,3
485,1
```

If the input is satisfactory, the group values are summed and output as shown in Appendix 1. The line following "TOTALS" consists of the standard enthalpy of formation (cal mol^{-1}), standard entropy (cal mol^{-1} K^{-1}) and heat capacity (cal mol^{-1} K^{-1}) at 300K, 400K, 500K, 600K, 800K, 1000K and 1500K. An "*" in the next line under the sum indicates that one or more data values required for that sum from the database are unknown and have been assigned a value of zero. Finally, a line of totals using Joule as the energy unit is output. Following the output, the programme may recycle as shown in Appendix 1.

The data base includes groups for which not all required thermodynamic values are available. The presence of a "*" below a sum indicates that this summation includes a zero assigned to an unknown value. If zero is a reasonable approximation to the unknown value or values, then the summation is valid. This is likely to be the case for alkane gauche interaction, where the only effect is likely to be upon the enthalpy of formation. Thus all sums shown in example in Appendix 1 may be considered to be valid. However, for most groups unknown values cannot be considered to be zero and a summation including an unknown value should be considered invalid. Tables 1 and 2 show dashes "-" for data values which are unknown. Due to the high proportion of the data base groups which do not have values for the heat capacity at 1500K, heat capacity values at 1500K are not included in the data transferred to the "FILER" command file.

The estimate made by GROUP for standard enthalpy of formation and standard entropy at 298K for 2-methylbutane (g) and for its heat capacity at 300K of -36290 cal mol^{-1}, 82.03 cal $mol^{-1}K^{-1}$ and 28.61 cal $mol^{-1}K^{-1}$ may be compared with literature values of -36960 cal mol^{-1}, 82.29 cal $mol^{-1}K^{-1}$ and 28.54 cal $mol^{-1}K^{-1}$ respectively (6).

If a "FILER" command file has been requested, the programme will request an Access Code for the "THERMODATA" programme suite. If Access Code checking has not been selected in your installation of "THERMODATA", this section of the command file will be ignored. The final input is the name of the Thermodata database file to which the data is to be added. The file name must commence with the letters "CPD" followed by any allowed 5 characters without an extension ("FILER" automatically assumes and appends the file extension DAT). When "FILER" is run from "THERMODATA", the estimates from the programme "GROUP" will be added to the named "THERMODATA" database if it already exits or a new database will be created if it does not. It may be noted that if the same "FILER" command file is run more than once, "FILER" will simply overwrite existing data in the database.

A second example is shown in Appendix 2 for n-hexylcyclopentane. The same files names may be used as for the example in Appendix 1, in which case the data will be appended to the files. The molecule has no external symmetry and an internal symmetry number of 3 associated with the internal rotation of the methyl group. Thus the overall symmetry number is 3 and there

is only one optical isomer. The groups present in the molecule are one methyl group, C-(C)-(H)/3, nine methylene groups, C-(C)/2-(H)/2, including both those in the ring and the ring substituent and one tertiary carbon group, C-(C)/3-(H). Correction is made for the cyclopentane ring by including an additional cyclopentane pseudo group. The groups are input to the programme as

```
5,9
6,1
1,1
45,1
```

Values are output by the programme for C_p^o ΔH_f^o and ΔS^o in both calorie and joule units as shown in Appendix 2. Good agreement is obtained between the estimated values of 53.3 cal mol^{-1} K^{-1}, -50230 cal mol^{-1} and 128.2 cal mol^{-1} K^{-1} with the respective values from reference 6 of 53.7 cal mol^{-1} K^{-1}, -50070 cal mol^{-1} and 127.7 cal mol^{-1} K^{-1}. Values are available for all required groups to the temperature of 1500 K, so no "*"s appear below the totals for this example. However, to allow consistency with the bulk of the group data, C_p^o data at 1500 K is not included in the "FILER" myfiler.inp file for calculation of the equation for variation of heat capacity with temperature.

5. FURTHER EXAMPLES OF GROUP ALLOCATIONS

Further examples to illustrate the assignment of groups in a molecule may be considered. Ethylnitrile has a formula of CH_3CH_2CN. As discussed above, the -CN group is considered a pseudo terminal group and does not require a group value. The two groups in the molecule are C-(C)-(H)/3 and C-(C)-(CN)-(H)/2. These are input to the programme as:

```
  1,1
205,1
```

Cis-1,2-dimethylcyclobutane has a formula of C_6H_{12}. There are two C-(C)/2-(H)/2 groups, two C-(C)/3-(H) and two C-(C)-(H)/3 groups. Additional non-nearest neighbour interactions contributing to the final values as pseudo groups are one cyclobutane ring and one alkane cis interaction. The groups inputs to the programme are:

```
  5,2
  6,2
  1,2
 43,1
490,1
```

1,1-dichloro-7-nitro-hept-cis,cis-2,4-diene may be considered as the

final example. The structural formula is $CHCl_2(CH)_4CH_2CH_2NO_2$. The groups in the molecule are:

one C-(C)-(Cl)/2-(H) group
two C/D-(C)-(H) groups
two C/D-(C/D)-(H) groups
one C-(C)-(C/D)-(H)/2 group
one C-(C)-(H)/2-(NO/2) group

In addition there are two cis interactions. These are input to the programme as:

```
238,1
  9,2
 11,2
 18,1
214,1
490,2
```

It may be noted that interaction between the 1,3 diene system is included in the C/D-(C/D)-(H) group. However, there is likely to be additional non-nearest neighbour interaction between the 1,3-diene system with the chlorine atoms and possibly with the nitro group. This interaction is not included in the group values. Any variation between the estimated thermodynamic values and experimental values may be considered a quantitative estimate of this long range interaction.

6. CONCLUSIONS

The computer programme simplifies the estimation of thermodynamic values by the method of Benson et. al. (2) by prompting for the required input and then carrying out the summation of values for each of the groups with correction for symmetry factors. The output listing then allows cross checking that the correct groups have been input into the programme. An optional file may be produced which can be used as direct input to add to the Australian CSIRO/NPL "THERMODATA" database.

Variations between estimated thermodynamic values and experimental values may be be due to inaccuracies in the experimental measurements, inaccuracies in the group values or non-nearest neighbour interactions which are not included in the data base.

The authors welcome correspondence from users of the data base for the programme "GROUP" with respect to group values which may be considered inaccurate or incomplete.

7. REFERENCES

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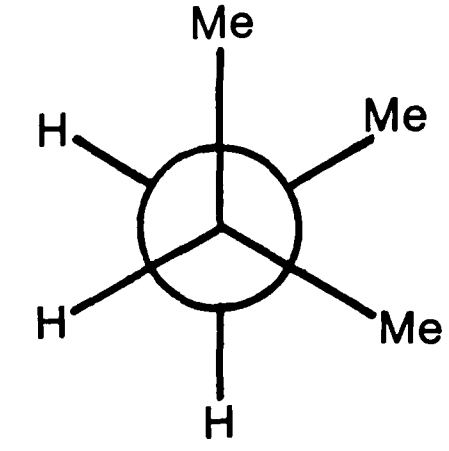
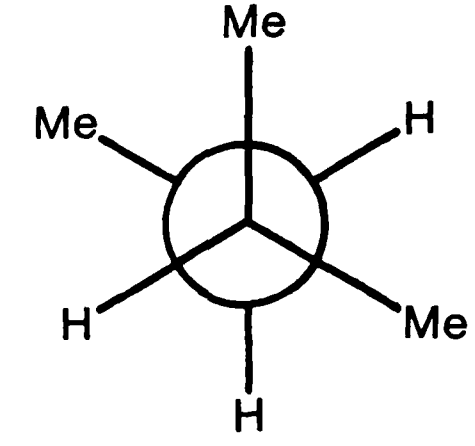
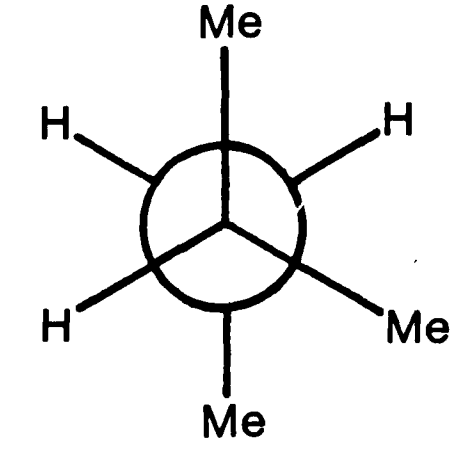


(a) 2 gauche interactions



(b) 1 gauche interaction



(c) 1 gauche interaction

FIGURE 1 Rotomeric Conformations of 2-methylbutane.

GLOSSARY FOR TABLE 1 AND TABLE 2

For each group, the left-most atom is the "Central atom" of the group. The central atom" has at least two bonds to other atoms.

Functional groups which are normally indivisible (such as NO_2 etc.) and are externally linked by only one bond are regarded for the purpose of group additivity as "pseudo-atoms".

All terminal atoms (or "pseudo-atoms") are enclosed in brackets and are separated from each other and from the "central atom" by the dash or hyphen character "-".

A "/" followed by a number is used to indicate a repitition factor for the atom or "pseudo-atom" immediately before it.

For example:- in -(NO/2)- the slash notation indicates that the nitrogen atom has two oxygens bonded to it to form the NITRO terminal "Pseudo-atom"; in -(Cl)/2- the slash notation indicates that the "central atom" has two chlorine atoms bonded to it.

A slash followed by a letter indicates a descriptive environment for the atom preceding it. A list of the notation used is shown below:-

C/B	A benzenoid carbon atom.
C/D	An Alkene carbon atom.
C/T	An Alkyne carbon atom.
C/A	An Allylic carbon atom.
N/I	An Imino nitrogen.
N/A	An Amino nitrogen.

TABLE 1

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
1	C-(C)-(H)/3	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
2	C-(C/B)-(H)/3	-10000.	30.28	6.08	7.99	9.72	11.19	13.49	15.29	-
3	C-(C/D)-(H)/3	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
4	C-(C/T)-(H)/3	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
5	C-(C)/2-(H)/2	-4950.	9.42	5.50	6.95	8.25	9.35	11.07	12.34	14.25
6	C-(C)/3-(H)	-1900.	-12.07	4.54	6.00	7.17	8.05	9.31	10.05	11.17
7	C-(C)/4	500.	-35.10	4.37	6.13	7.36	8.12	8.77	8.76	8.12
8	C/D-(H)/2	6260.	27.61	5.10	6.36	7.51	8.50	10.07	11.27	13.19
9	C/D-(C)-(H)	8590.	7.97	4.16	5.03	5.81	6.50	7.65	8.45	9.62
10	C/D-(C)/2	10340.	-12.70	4.10	4.61	4.99	5.26	5.80	6.08	6.36
11	C/D-(C/D)-(H)	6780.	6.38	4.46	5.79	6.75	7.42	8.35	8.99	9.98
12	C/D-(C)-(C/D)	8880.	-14.60	4.40	5.37	5.93	6.18	6.50	6.62	6.72
13	C/D-(C/B)-(H)	6780.	6.38	4.46	5.79	6.75	7.42	8.35	8.99	9.98
14	C/D-(C)-(C/B)	8640.	-14.60	4.40	5.37	5.93	6.18	6.50	6.62	6.72
15	C/D-(C/T)-(H)	6780.	6.38	4.46	5.79	6.75	7.42	8.35	8.99	9.98
16	C/D-(C/B)/2	8000.	-12.70	-	-	-	-	-	-	-
17	C/D-(C/D)/2	4600.	-8.80	-	-	-	-	-	-	-
18	C-(C)-(C/D)-(H)/2	-4760.	9.80	5.12	6.86	8.32	9.49	11.22	12.48	14.36
19	C-(C/D)/2-(H)/2	-4290.	10.20	4.70	6.80	8.40	9.60	11.30	12.60	14.40
20	C-(C/D)-(C/B)-(H)/2	-4290.	10.20	4.70	6.80	8.40	9.60	11.30	12.60	14.40
21	C-(C)-(C/T)-(H)/2	-4730.	10.30	4.95	6.56	7.93	9.08	10.86	12.19	14.20
22	C-(C)-(C/B)-(H)/2	-4860.	9.34	5.84	7.61	8.98	10.01	11.49	12.54	13.76
23	C-(C)/2-(C/D)-(H)	-1480.	-11.69	4.16	5.91	7.34	8.19	9.46	10.19	11.28
24	C-(C)/2-(C/T)-(H)	-1720.	-11.19	3.99	5.61	6.85	7.78	9.10	9.90	11.12
25	C-(C)/2-(C/B)-(H)	-980.	-12.15	4.88	6.66	7.90	8.75	9.73	10.25	10.68
26	C-(C)/3-(C/D)	1680.	-34.72	3.99	6.04	7.43	8.26	8.92	8.96	8.23
27	C-(C)/3-(C/B)	2810.	-35.18	4.37	6.79	8.09	8.78	9.19	8.96	7.63
28	C/T-(H)	26930.	24.70	5.27	5.99	6.49	6.87	7.47	7.96	8.85
29	C/T-(C)	27550.	6.35	3.13	3.48	3.81	4.09	4.60	4.92	6.35
30	C/T-(C/D)	29200.	6.43	2.57	3.54	3.50	4.92	5.34	5.50	5.80
31	C/T-(C/B)	29200.	6.43	2.57	3.54	3.50	4.92	5.34	5.50	5.80
32	C/B-(H)	3300.	11.53	3.24	4.44	5.46	6.30	7.54	8.41	9.73
33	C/B-(C)	5510.	-7.69	2.67	3.14	3.68	4.15	4.96	5.44	5.98

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
34	C/B-(C/D)	5680.	-7.80	3.59	3.97	4.38	4.72	5.28	5.61	5.75
35	C/B-(C/T)	5680.	-7.80	3.59	3.97	4.38	4.72	5.28	5.61	5.75
36	C/B-(C/B)	4960.	-8.64	3.33	4.22	4.89	5.27	5.76	5.95	6.05
37	C/A	34200.	6.00	3.90	4.40	4.70	5.00	5.30	5.50	5.70
38	C/T-(C/T)	29570.	5.87	-	-	-	-	-	-	-
39	C-(C)/3-(C/T)	460.	-35.00	.08	1.75	3.43	4.77	6.02	6.38	-
40	Cyclopropane Ring	27600.	32.10	-3.05	-2.53	-2.10	-1.90	-1.77	-1.62	-1.52
41	Methylene Cyclopropane Ring	40900.	-	-	-	-	-	-	-	-
42	Cyclopropene Ring	53700.	33.60	-	-	-	-	-	-	-
43	Cyclobutane Ring	26200.	29.80	-4.61	-3.89	-3.14	-2.64	-1.88	-1.38	-.67
44	Cyclobutene Ring	29800.	29.00	-2.53	-2.19	-1.89	-1.68	-1.48	-1.33	-1.22
45	Cyclopentane Ring	6300.	27.30	-6.50	-5.50	-4.50	-3.80	-2.80	-1.93	-.37
46	Cyclopentene Ring	5900.	25.80	-5.98	-5.35	-4.89	-4.14	-2.93	-2.26	-1.08
47	Cyclopentadiene Ring	6000.	28.00	-3.45	-2.83	-2.14	-1.65	-1.28	-1.04	-
48	Cyclohexane Ring	-360.	18.80	-5.80	-4.10	-2.90	-1.30	1.10	2.20	3.30
49	Cyclohexene Ring	1400.	21.50	-4.28	-3.04	-1.98	-1.43	-.29	.08	.81
50	Cyclohexadiene 1,3 Ring	4800.	24.00	-	-	-	-	-	-	-
51	Cyclohexadiene 1,4 Ring	500.	25.40	-	-	-	-	-	-	-
52	Cycloheptane Ring	6400.	15.90	-9.08	-	-	-	-	-	-
53	Cycloheptene Ring	5400.	15.10	-	-	-	-	-	-	-
54	Cycloheptadiene 1,3 Ring	6600.	19.40	-	-	-	-	-	-	-
55	Cycloheptatriene 1,3,5 Ring	4700.	23.70	-	-	-	-	-	-	-
56	Cyclooctane Ring	9900.	16.50	-10.55	-	-	-	-	-	-
57	Cis-cyclooctene Ring	6000.	15.00	-	-	-	-	-	-	-
58	Trans-cyclooctene Ring	15300.	15.00	-	-	-	-	-	-	-
59	Cyclooctatriene 1,3,5 Ring	8900.	21.10	-	-	-	-	-	-	-
60	Cyclooctatetraene Ring	17100.	27.60	-	-	-	-	-	-	-
61	Cyclononane Ring	12800.	12.20	-	-	-	-	-	-	-
62	Cis-cyclononene Ring	9900.	11.20	-	-	-	-	-	-	-
63	Trans-cyclononene Ring	12800.	11.20	-	-	-	-	-	-	-
64	Cyclodecane Ring	12600.	-	-	-	-	-	-	-	
65	Cyclododecane Ring	4400.	-	-	-	-	-	-	-	
66	Spiropentane Ring	63500.	67.60	-	-	-	-	-	-	
67	Bicyclo-(1,1,0)-butane Ring	67000.	69.20	-	-	-	-	-	-	
68	Bicyclo-(2,1,0)-pentane Ring	55300.	64.70	-	-	-	-	-	-	

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
69	Bicyclo-(3,1,0)-hexane Ring	32700.	60.90	-	-	-	-	-	-	
70	Bicyclo-(4,1,0)-heptane Ring	28900.	55.50	-	-	-	-	-	-	-
71	Bicyclo-(5,1,0)-octane Ring	29600.	50.60	-	-	-	-	-	-	-
72	Bicyclo-(6,1,0)-nonane Ring	31100.	49.20	-	-	-	-	-	-	-
73	Bicycloheptadiene Ring	29700.	-	-	-	-	-	-	-	-
74	Biphenylene Ring	58800.	-	-	-	-	-	-	-	
75	CO-(C)-(CO)	-29200.	15.80	5.99	7.03	7.79	8.39	9.30	9.78	-
76	CO-(C/D)-(O)	-32000.	15.20	5.58	6.16	7.39	7.68	8.79	9.42	-
77	CO-(C/B)-(O)	-36600.	15.10	2.18	2.75	3.98	5.03	6.29	7.06	-
78	CO-(C)-(O)	-35100.	14.78	5.97	6.70	7.45	8.02	8.87	9.36	10.00
79	CO-(H)-(O)	-32100.	34.93	7.03	7.87	8.82	9.68	11.16	12.20	-
80	CO-(C/D)-(H)	-29100.	35.40	5.81	7.22	9.50	11.65	15.08	17.84	-
81	CO-(C/B)/2	-25800.	9.50	5.26	6.77	7.67	8.48	9.62	9.85	-
82	CO-(C)-(C/B)	-30900.	12.30	8.29	8.98	9.93	10.42	10.83	11.00	-
83	CO-(C/B)-(H)	-29100.	35.40	8.01	10.56	11.65	14.21	16.38	17.68	-
84	CO-(C)/2	-31400.	15.01	5.59	6.32	7.09	7.76	8.89	9.61	-
85	CO-(C)-(H)	-29100.	34.93	7.03	7.87	8.82	9.68	11.16	12.20	-
86	CO-(CO)-(H)	-25300.	21.30	6.72	7.83	8.90	9.89	11.43	12.12	-
87	CO-(CO)-(O)	-29300.	17.20	-	-	-	-	-	-	-
88	O-(C/B)-(CO)	-36700.	10.20	2.06	2.70	3.11	3.42	3.88	4.18	-
89	O-(CO)/2	-46500.	8.55	3.19	4.01	4.27	4.58	5.15	5.41	-
90	O-(CO)-(O)	-19000.	8.20	.36	1.50	2.30	2.84	3.65	4.14	-
91	O-(C/D)-(CO)	-45200.	3.80	1.44	2.98	3.98	4.49	4.97	5.20	-
92	O-(C)-(CO)	-43100.	8.39	2.78	3.79	4.38	4.73	4.91	5.03	-
93	O-(CO)-(H)	-58100.	24.52	3.81	4.98	5.80	6.34	7.17	7.75	8.92
94	O-(C)-(O)	-4500.	9.40	3.70	3.70	3.70	3.70	4.20	4.20	4.80
95	O-(O)/2	19000.	9.40	3.70	3.70	3.70	3.70	4.20	4.20	4.80
96	O-(H)-(O)	-16270.	27.85	5.17	5.79	6.28	6.66	7.15	7.51	8.17
97	O-(C/D)/2	-33000.	10.10	2.70	3.19	3.53	3.86	4.40	4.73	-
98	O-(C)-(C/D)	-30500.	9.70	3.04	3.32	3.50	3.70	4.19	4.53	-
99	O-(C/B)/2	-21100.	7.95	1.09	1.22	1.50	1.99	2.85	3.51	
100	O-(C)-(C/B)	-23000.	11.90	.62	.72	1.18	1.78	2.84	3.58	-
101	O-(C/B)-(H)	-37900.	29.10	4.30	4.50	4.80	5.20	6.00	6.60	
102	O-(C)/2	-23200.	8.68	3.40	3.70	3.70	3.80	4.40	4.60	

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
103	O-(C)-(H)	-37880.	29.07	4.33	4.45	4.82	5.23	6.02	6.61	8.04
104	C/D-(CO)-(O)	11600.	-12.60	5.59	7.00	7.48	7.75	8.02	8.13	-
105	C/D-(C)-(CO)	7500.	-11.80	5.48	6.98	7.41	7.64	8.01	8.20	-
106	C/D-(CO)-(H)	5000.	7.97	7.58	8.85	9.27	9.63	10.38	11.04	-
107	C/D-(C/D)-(O)	8900.	-14.60	4.40	5.47	5.93	6.28	6.50	6.62	-
108	C/D-(C)-(O)	10300.	-12.70	4.10	4.61	4.99	5.26	5.80	6.08	-
109	C/D-(H)-(O)	8600.	8.00	4.16	5.03	5.81	6.50	7.65	8.45	9.62
110	C/B-(CO)	3700.	-7.70	2.67	3.14	3.68	4.15	4.96	5.44	-
111	C/B-(O)	-900.	-10.20	3.90	5.30	6.20	6.60	6.90	6.90	-
112	C-(CO)/2-(H)/2	-7600.	11.30	3.83	6.37	7.68	9.03	10.86	12.36	-
113	C-(C)/2-(CO)-(H)	-1700.	-12.00	2.92	4.99	6.50	7.54	8.88	9.77	-
114	C-(C)-(CO)-(H)/2	-5200.	9.60	6.20	7.70	8.70	9.50	11.10	12.20	-
115	C-(C)/3-(CO)	1400.	-33.00	2.32	4.38	5.70	6.49	7.27	7.57	-
116	C-(CO)-(H)/3	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
117	C-(C)/2-(O)/2	-18600.	-35.80	1.59	3.95	6.20	7.39	7.62	8.48	-
118	C-(C)-(H)-(O)/2	-16300.	-13.10	2.22	4.45	6.72	8.07	8.71	9.09	-
119	C-(H)/2-(O)/2	-16100.	7.80	2.83	5.06	7.52	9.12	10.32	11.29	-
120	C-(C/B)-(H)/2-(O)	-8100.	9.70	3.71	6.27	8.28	9.79	11.79	13.20	-
121	C-(C/D)-(H)/2-(O)	-6500.	8.90	4.66	6.97	8.65	9.88	11.54	12.73	-
122	C-(C)/3-(O)	-6600.	-33.56	4.33	6.19	7.25	7.70	8.20	8.24	-
123	C-(C)/2-(H)-(O)	-7200.	-11.00	4.80	6.64	8.10	8.73	9.81	10.40	-
124	C-(C)-(H)/2-(O)	-8100.	9.80	4.99	6.85	8.30	9.43	11.11	12.33	14.60
125	C-(H)/3-(O)	-10080.	30.41	6.19	7.84	9.40	10.79	13.03	14.77	17.58
126	C-(C/T)-(H)/2-(O)	-6500.	.00	-	-	-	-	-	-	-
127	O-(C/D)-(H)	-37900.	34.93	-	-	-	-	-	-	-
128	O-(C/T)-(H)	-37900.	34.93	-	-	-	-	-	-	-
129	C-(C/T)-(CO)-(H)/2	-5400.	10.60	-	-	-	-	-	-	-
130	C-(C/B)-(CO)-(H)/2	-5400.	9.60	-	-	-	-	-	-	-
131	C-(C)-(CO)/2-(H)	-5400.	-10.20	-	-	-	-	-	-	-
132	CO-(C/T)-(H)	-29100.	35.40	-	-	-	-	-	-	-
133	CO-(C/B)-(CO)	-26800.	12.30	-	-	-	-	-	-	-
134	CO-(O)/2	-29900.	5.80	-	-	-	-	-	-	-
135	CO-(C)-(C/D)	-29300.	-	-	-	-	-	-	-	
136	C-(C/D)-(CO)-(H)/2	-3800.	-	-	-	-	-	-	-	
137	Ethylene Oxide Ring	26800.	30.50	-2.00	-2.80	-3.00	-2.60	-2.30	-2.30	

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
138	Propylene Oxide Ring	25200.	27.70	-4.60	-5.00	-4.20	-3.50	-2.60	.20	.00
139	Tetrahydrofuran Ring	5900.	24.20	-	-	-	-	-	-	-
140	Tetrahydropyran Ring	500.	18.80	-	-	-	-	-	-	
141	1,3-Dioxane Ring	200.	15.80	-	-	-	-	-	-	
142	1,4-Dioxane Ring	3300.	15.80	-	-	-	-	-	-	
143	1,3,5-Trioxane Ring	6600.	12.80	-	-	-	-	-	-	-
144	Furan Ring	-5800.	28.40	-	-	-	-	-	-	-
145	Dihydropyran Ring	1200.	20.20	-	-	-	-	-	-	-
146	Cyclopentanone Ring	5200.	24.60	-	-	-	-	-	-	-
147	Cyclohexanone Ring	2200.	15.90	-	-	-	-	-	-	-
148	Succinic Anhydride Ring	4500.	30.20	-	-	-	-	-	-	-
149	Glutaric Anhydride Ring	800.	20.10	-	-	-	-	-	-	-
150	Maleic Anhydride Ring	3600.	27.40	-	-	-	-	-	-	-
151	Dihydrofuran Ring	4700.	22.00	-	-	-	-	-	-	-
152	4,5-Benzodioxole	10300.	22.00	-	-	-	-	-	-	-
153	1,4-Benzodioxane Ring	2000.	15.80	-	-	-	-	-	-	-
154	Dibenzofuran Ring	6500.	28.00	-	-	-	-	-	-	-
155	Xanthene Ring	2300.	22.00	-	-	-	-	-	-	

TABLE 1 (continued

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
156	Dioxolane Ring	6000.	22.00	-	-	-	-	-	-	
157	Cyclobutanone Ring	22600.	27.90	-	-	-	-	-	-	-
158	Cycloheptanone Ring	2300.	17.20	-	-	-	-	-	-	
159	Cyclooctanone Ring	1500.	15.40	-	-	-	-	-	-	-
160	Cyclononanone Ring	4700.	13.90	-	-	-	-	-	-	
161	Cyclodecanone Ring	3600.	11.90	-	-	-	-	-	-	-
162	Cyclohendecane Ring	4400.	9.50	-	-	-	-	-	-	-
163	Cyclododecanone Ring	3000.	6.70	-	-	-	-	-	-	-
164	Cyclopentadecanone Ring	2100.	1.90	-	-	-	-	-	-	-
165	Cycloheptadecanone Ring	1100.	-2.40	-	-	-	-	-	-	-
166	Cis-bicyclo-(3.3.0)-octan-2-one Ring	5400.	54.00	-	-	-	-	-	-	-
167	Trans-bicyclo-(3.3.0)-octan-2-one Ring	11000.	54.00	-	-	-	-	-	-	-
168	Phthalic Anhydride Ring	10300.	27.40	-	-	-	-	-	-	-
169	1,2,4,5-Benzenetetracarboxylic Anhydride Ring	21100.	54.00	-	-	-	-	-	-	-
170	Beta-propiolactone Ring	23900.	27.90	-	-	-	-	-	-	-
171	Malonic Anhydride Ring	22000.	27.90	-	-	-	-	-	-	-
172	C-(H)/3-(N)	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
173	C-(C)-(H)/2-(N)	-6600.	9.80	5.25	6.90	8.28	9.39	11.09	12.34	
174	C-(C)/2-(H)-(N)	-5200.	-11.70	5.56	6.52	7.30	8.09	9.17	9.58	
175	C-(C)/3-(N)	-3200.	-34.10	4.35	6.16	7.31	7.91	8.49	8.50	
176	C-(C)-(H)-(N/I)	10100.	-	-	-	-	-	-	-	

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
177	N-(C)-(H)/2	4800.	29.71	5.72	6.51	7.32	8.07	9.41	10.47	12.28
178	N-(C)/2-(H)	15400.	8.94	4.20	5.21	6.13	6.83	7.90	8.65	9.55
179	N-(C)/3	24400.	-13.46	3.48	4.56	5.43	5.97	6.56	6.67	6.50
180	N-(H)/2-(N)	11400.	29.13	6.10	7.38	8.43	9.27	10.54	11.52	13.19
181	N-(C)-(H)-(N)	20900.	9.61	4.82	5.80	6.50	7.00	7.80	8.30	9.00
182	N-(C)/2-(N)	29200.	13.80	1.56	2.50	3.31	3.87	4.62	4.99	
183	N-(C/B)-(H)-(N)	22100.	8.10	3.28	4.05	4.75	5.31	6.28	6.91	
184	N/I-(H)	16300.	12.30	2.95	4.58	6.45	7.71	9.13	9.92	
185	N/I-(C)	21300.	5.90	2.48	3.34	3.95	4.29	4.59	4.60	
186	N/I-(C/B)	16700.	30.80	1.19	3.20	4.55	5.39	6.17	6.28	
187	N/A-(H)	25100.	26.80	4.38	4.89	5.44	5.94	6.77	7.42	8.44
188	N/A-(C)	34300.	8.50	2.70	4.10	4.92	5.34	5.69	5.71	
189	N-(C/B)-(H)/2	4800.	29.71	5.72	6.51	7.32	8.07	9.41	10.47	12.28
190	N-(C)-(C/B)-(H)	14900.	6.80	3.82	4.89	5.71	6.28	7.19	7.73	
191	N-(C)/2-(C/B)	26200.	-15.50	.62	2.02	3.27	4.13	5.23	5.59	
192	N-(C/B)/2-(H)	16300.	4.30	2.16	3.12	4.13	5.10	6.76	7.88	
193	C/B-(N)	-500.	-9.69	3.95	5.21	5.94	6.32	6.53	6.56	
194	C/B-(NO/2)	400.	26.90	16.20	-	-	-	-	-	
195	N/A-(N)	23000.	8.50	2.12	4.18	5.51	6.77	6.86	7.05	
196	CO-(H)-(N)	-29600.	34.93	7.03	7.87	8.82	9.68	11.16	12.20	
197	CO-(C)-(N)	-32800.	16.20	5.37	6.17	7.07	7.66	9.62	11.19	
198	N-(CO)-(H)/2	-14900.	24.69	4.07	5.74	7.13	8.29	9.96	11.22	
199	N-(C)-(CO)-(H)	-4400.	3.90	.66	1.55	2.46	3.48	4.24	4.53	
200	N-(C)/2-(CO)	6100.	-16.90	3.11	4.58	5.62	6.25	6.79	6.87	
201	N-(C/B)-(CO)-(H)	400.	-2.90	.57	1.51	2.38	3.33	4.04	4.35	
202	N-(CO)/2-(H)	-18500.	7.60	3.59	5.54	6.70	7.39	7.95	8.19	
203	N-(C)-(CO)/2	-5900.	15.20	1.07	3.10	4.31	5.00	5.48	6.47	
204	N-(C/B)-(CO)/2	-500.	-16.70	.98	3.06	4.23	4.85	5.28	5.29	
205	C-(C)-(CN)-(H)/2	22500.	40.20	11.10	13.40	15.50	17.20	19.70	21.30	
206	C-(C)/2-(CN)-(H)	25800.	19.80	11.00	12.70	14.10	15.40	17.30	18.60	
207	C-(C)/3-(CN)	29000.	-2.80	8.65	11.16	12.89	14.05	15.51	16.19	
208	C-(C)/2-(CN)/2	19600.	28.40	14.72	17.79	20.00	21.61	23.78	24.96	
209	C/D-(CN)-(H)	37400.	36.58	9.80	11.70	13.30	14.50	16.30	17.30	
210	C/D-(CN)/2	34100.	15.90	13.60	16.55	18.68	20.25	22.34	23.59	

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
211	C/D-(H)-(NO/2)	7100.	44.40	12.30	15.10	17.40	19.20	21.60	23.20	25.30
212	C/B-(CN)	35800.	20.50	9.80	11.20	12.30	13.10	14.20	14.90	
213	C/T-(CN)	63800.	35.40	10.30	11.30	12.10	12.70	13.60	14.30	15.30
214	C-(C)-(H)/2-(NO/2)	-14400.	48.40	12.59	15.82	18.52	20.66	23.79	25.90	-
215	C-(C)/2-(H)-(NO/2)	-13600.	26.90	11.99	15.21	17.72	19.61	22.18	23.70	
216	C-(C)/3-(NO/2)	-16500.	3.90	9.89	13.34	15.86	17.62	19.81	20.86	-
217	C-(C)-(H)-(NO/2)/2	-9900.	65.90	12.30	15.96	18.71	20.68	23.10	24.33	-
218	O-(C)-(NO)	-5900.	41.90	9.10	10.30	11.20	12.00	13.30	13.90	14.50
219	O-(C)-(NO/2)	-19400.	48.50	9.54	11.54	13.26	15.60	16.39	17.38	-
220	C/B-(NO)	5400.	-	-	-	-	-	-	-	-
221	C-(C)/2-(NO/2)/2	-10200.	-	-	-	-	-	-	-	-
222	C-(C)-(NO/2)/3	-5000.	-	-	-	-	-	-	-	-
223	C/D-(C)-(NO/2)	4400.	-	-	-	-	-	-	-	-
224	Ethyleneimine Ring	27700.	31.60	-	-	-	-	-	-	-
225	Azetidine Ring	26200.	29.30	-	-	-	-	-	-	
226	Pyrrolidine Ring	6800.	26.70	-6.17	-5.58	-4.80	-4.00	-2.87	-2.17	-
227	Piperidine Ring	1000.	23.80	-	-	-	-	-	-	-
228	1,4-Diazabicyclo-(2,2,2)-octane Ring	3400.	-	-	-	-	-	-	-	-

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
229	Succinimide Ring	8500.	-	-	-	-	-			
230	C-(C)-(F)/3	-158400.	42.50	12.70	15.00	16.40	17.90	19.30	20.00	
231	C-(C)-(F)/2-(H)	-102300.	39.10	9.90	12.00	13.70	15.10	16.70	17.80	
232	C-(C)-(F)-(H)/2	-51500.	35.40	8.10	10.00	12.00	13.00	15.20	16.60	
233	C-(C)/2-(F)/2	-97000.	17.80	9.90	11.80	13.50	14.40	16.10	16.60	
234	C-(C)/2-(F)-(H)	-49000.	14.00	7.30	9.04	10.47	11.56	13.10	14.01	
235	C-(C)/3-(F)	-48500.	-7.70	6.80	8.86	10.20	11.16	12.43	12.72	
236	C-(C)-(Cl)-(F)/2	-106300.	40.50	13.70	16.10	17.50	18.60	19.80	20.40	
237	C-(C)-(Cl)/3	-24900.	50.40	16.30	18.00	19.10	19.80	20.60	21.00	
238	C-(C)-(Cl)/2-(H)	-18900.	43.70	12.10	14.00	15.40	16.50	17.90	18.70	
239	C-(C)-(Cl)-(H)/2	-15600.	37.80	8.90	10.70	12.30	13.40	15.30	16.70	
240	C-(C)/2-(Cl)/2	-22200.	22.40	13.02	14.88	15.95	16.48	16.96	17.02	
241	C-(C)/2-(Cl)-(H)	-14800.	17.60	9.00	9.90	10.50	11.20	13.90	14.60	
242	C-(C)/3-(Cl)	-12800.	-5.40	9.30	10.50	11.00	11.30	12.40	12.70	
243	C-(Br)/3-(C)	3900.	55.70	16.70	18.00	18.80	19.40	19.90	20.30	
244	C-(Br)-(C)-(H)/2	-5400.	40.80	9.10	11.00	12.60	13.70	15.50	16.80	
245	C-(Br)-(C)/2-(H)	-3400.	19.10	8.93	10.66	11.96	12.84	14.05	14.72	
246	C-(Br)-(C)/3	-400.	-3.20	9.30	11.00	11.50	12.30	13.30	13.30	
247	C-(C)-(H)/2-(I)	8000.	43.00	9.20	11.00	12.90	13.90	15.80	17.20	
248	C-(C)/2-(H)-(I)	10500.	21.30	9.23	10.91	12.16	13.00	14.17	14.80	
249	C-(C)/3-(I)	13000.	1.00	9.83	11.75	12.92	13.45	13.79	13.60	
250	C-(C)-(H)-(I)/2	26000.	54.60	13.60	15.15	16.63	17.72	19.04	19.49	
251	C-(Br)-(C)-(Cl)-(H)	-10100.	45.70	12.40	14.00	15.60	16.30	17.90	19.00	
252	N-(C)-(F)/2	-7800.	-	6.33	8.26	9.77	10.90	12.16	12.79	
253	C-(C)-(Cl)-(H)-(O)	-21600.	15.40	12.70	13.54	13.97	14.23	14.55	14.78	
254	C-(H)/2-(I)-(O)	3800.	40.70	8.22	10.49	12.23	13.55	15.35	16.57	
255	C/D-(C)-(Cl)	-2100.	15.00	-	-	-	-	-	-	
256	C/D-(F)/2	-77500.	37.30	9.70	11.00	12.00	12.70	13.80	14.50	
257	C/D-(Cl)/2	-1800.	42.10	11.40	12.50	13.30	13.90	14.60	15.00	
258	C/D-(Br)/2	7500.	47.60	12.30	13.20	13.90	14.30	14.90	15.20	
259	C/D-(Cl)-(F)	-43200.	39.80	10.30	11.70	12.60	13.30	14.20	14.70	
260	C/D-(Br)-(F)	-31300.	42.50	10.80	12.00	12.80	13.50	14.30	14.70	

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol-1)	S^o 298K (cal K-1 mol-1)	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
261	C/D-(Br)-(Cl)	6500.	45.10	12.10	12.70	13.50	14.10	14.70	15.00	
262	C/D-(F)-(H)	-37600.	32.80	6.80	8.40	9.50	10.50	11.80	12.70	
263	C/D-(Cl)-(H)	-1200.	35.40	7.90	9.20	10.30	11.20	12.30	13.10	
264	C/D-(Br)-(H)	12700.	38.30	8.10	9.50	10.60	11.40	12.40	13.20	
265	C/D-(H)-(I)	24500.	40.50	8.80	10.00	10.90	11.60	12.60	13.30	
266	C/T-(Cl)	17800.	33.40	7.90	8.40	8.70	9.00	9.40	9.60	
267	C/T-(Br)	23600.	36.10	8.30	8.70	9.00	9.20	9.50	9.70	
268	C/T-(I)	33800.	37.90	8.40	8.80	9.10	9.30	9.60	9.80	
269	C/B-(F)	-42800.	16.10	6.30	7.60	8.50	9.10	9.80	10.20	
270	C/B-(Cl)	-4300.	18.90	7.40	8.40	9.20	9.70	10.20	10.40	
271	C/B-(Br)	8700.	21.60	7.80	8.70	9.40	9.90	10.30	10.50	
272	C/B-(I)	22600.	23.70	8.00	8.90	9.60	9.90	10.30	10.50	
273	C-(C/B)-(F)/3	-162700.	42.80	12.50	15.30	17.20	18.50	20.10	21.00	
274	C-(Br)-(C/B)-(H)/2	-6900.	42.20	7.29	11.10	12.47	13.69	15.59	16.71	
275	C-(C/B)-(H)/2-(I)	8400.	44.50	8.10	10.79	12.83	14.31	16.28	17.63	
276	CO-(C/B)-(Cl)	-52300.	40.00	-	-	-	-	-	-	
277	CO-(Br)-(C/B)	-37800.	-	-	-	-	-	-	-	
278	CO-(C/B)-(I)	-23700.	-	-	-	-	-	-	-	
279	C-(H)/3-(S)	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	
280	C-(C)-(H)/2-(S)	-5590.	9.88	5.38	7.08	8.60	9.97	12.26	14.15	
281	C-(C)/2-(H)-(S)	-2640.	-11.32	4.85	6.51	7.78	8.69	9.90	10.57	
282	C-(C)/3-(S)	-550.	-34.41	4.57	6.27	7.45	8.15	8.72	8.10	
283	C-(C/B)-(H)/2-(S)	-4730.	4.90	9.10	11.71	13.72	15.22	17.34	18.83	
284	C-(C/D)-(H)/2-(S)	-6450.	10.90	5.31	6.83	8.23	9.76	12.18	14.21	
285	C/B-(S)	-1800.	10.20	3.90	5.30	6.20	6.60	6.90	6.90	
286	C/D-(H)-(S)	8560.	8.00	4.16	5.03	5.81	6.50	7.65	8.45	
287	C/D-(C)-(S)	10930.	-12.41	3.50	3.57	3.83	4.09	4.41	5.00	
288	S-(C)-(H)	4620.	32.73	5.86	6.20	6.51	6.78	7.30	7.71	
289	S-(C/B)-(H)	11960.	12.66	5.12	5.26	5.57	6.03	6.99	7.84	
290	S-(C)/2	11340.	13.15	4.99	4.96	5.02	5.07	5.41	5.73	
291	S-(C)-(C/D)	9410.	13.20	4.22	5.08	5.56	5.77	5.87	5.87	
292	S-(C/D)/2	9860.	16.48	4.79	5.58	5.53	6.29	7.94	9.73	
293	S-(C)-(C/B)	19160.	-7.80	3.02	3.39	3.71	4.04	4.62	5.00	
294	S-(C/B)/2	25900.	-27.00	2.00	2.01	2.24	2.74	3.80	4.71	

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
295	S-(C)-(S)	7050.	12.37	5.23	5.42	5.51	5.51	5.38	5.12	
296	S-(C/B)-(S)	14500.	-8.00	2.89	3.39	3.72	4.15	4.78	5.10	
297	S-(S)/2	3010.	13.40	4.70	5.00	5.10	5.20	5.30	5.40	
298	C-(H)/3-(SO)	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	
299	C-(C)-(H)/2-(SO)	7720.	9.40	4.55	6.42	7.95	9.16	10.95	12.22	
300	C-(C)/3-(SO)	3050.	34.50	3.06	4.58	4.84	6.60	7.54	7.96	
301	C-(C/D)-(H)/2-(SO)	-7350.	10.10	4.40	6.36	6.94	9.25	10.97	12.25	
302	C/B-(SO)	2300.	10.40	2.67	3.14	3.68	4.15	4.96	5.44	
303	SO-(C)/2	14410.	18.10	8.88	10.03	10.50	10.79	10.98	11.17	
304	SO-(C/B)/2	12000.	-23.70	5.72	9.09	9.70	11.45	11.46	11.25	
305	C-(H/3)-(SO/2)	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	
306	C-(C)-(H)/2-(SO/2)	-7680.	9.40	4.09	5.97	7.54	8.80	10.65	11.93	
307	C-(C)/2-(H)-(SO/2)	-2620.	-12.00	4.42	6.25	7.56	8.48	9.64	10.30	
308	C-(C)/3-(SO/2)	-610.	-34.50	2.32	4.38	5.70	6.49	7.27	7.46	
309	C-(C/D)-(H)/2-(SO/2)	-7140.	10.50	4.86	6.81	8.35	9.58	11.27	12.54	
310	C-(C/B)-(H)/2-(SO/2)	-5540.	9.60	3.71	6.57	8.28	9.79	11.89	13.20	
311	C/B-(SO/2)	2300.	8.60	2.67	3.14	3.68	4.15	4.96	5.44	
312	C/D-(H)-(SO/2)	12500.	11.90	3.04	4.67	5.93	6.84	7.87	8.67	
313	C/D-(C)-(SO/2)	14500.	-9.60	3.70	6.22	7.96	9.20	10.66	11.34	
314	SO/2-(C/D)-(C/B)	-68600.	-6.30	9.89	11.50	13.35	14.61	15.72	15.92	
315	SO/2-(C/D)/2	-73600.	13.50	11.52	11.97	13.35	14.28	15.38	15.88	
316	SO/2-(C)/2	-69740.	20.90	11.52	11.97	13.35	14.28	15.38	15.88	
317	SO/2-(C)-(C/B)	-72290.	1.40	9.94	11.50	13.45	14.51	15.62	15.92	
318	SO/2-(C/B)/2	-68580.	-17.30	8.36	11.03	13.55	14.94	15.86	15.96	
319	SO/2-(C/B)-(SO/2)	-76250.	-3.20	9.81	11.50	13.52	14.73	15.71	16.03	
320	SO/2-(C)-(C/D)	-71670.	18.10	-	-	-	-	-	-	
321	CO-(C)-(S)	-31560.	15.43	5.59	6.32	7.09	7.76	8.89	9.61	
322	S-(CO)-(H)	-1410.	31.20	7.63	8.09	8.12	8.17	8.50	8.24	
323	C-(F)/3-(S)	-150300.	38.90	9.88	13.01	14.83	16.37	18.17	19.11	
324	CS-(N)/2	-31560.	15.43	5.59	6.32	7.09	7.76	8.89	9.61	
325	N-(CS)-(H)/2	12780.	29.19	6.07	7.28	8.18	8.91	10.09	10.98	
326	S-(N)-(S)	-4900.	-	-	-	-	-			
327	N-(C)/2-(S)	29900.	-	3.82	5.17	6.21	6.94	7.39	9.24	
328	SO-(N)/2	-31560.	-	-		-				

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f° 298K (cal mol-1)	S° 298K (cal K-1 mol-1)	C_p° (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
329	N-(C)/2-(SO)	16000.		4.20	5.88	6.12	6.53	6.83	8.34	
330	SO/2-(N)/2	-31560.	-	-	-	-			-	
331	N-(C)/2-(SO/2)	-20400.	-	6.02	6.35	7.54	8.23	9.03	9.19	
332	C/B-(SO/2N/3), Azidosulfonyl Group	74600.	-	-	-	-		-	-	
333	SO-(C)-(C/B)	-	-3.00	-	-	-			-	
334	C-(H)/3-(SO/4)	-10080.	30.41	-	-	-	-	-	-	
335	SO/4-(C)/2	-143900.	33.10	-	-	-	-		-	
336	C-(C)-(H)/2-(SO/4)	-8700.	9.80	-	-	-	-	-	-	
337	C-(H)/3-(SO/3) Sulfite	-10080.	30.41	-	-	-	-	-	-	
338	SO/3-(C)/2 Sulfite	-94800.	30.30	-	-	-	-	-	-	
339	C-(C)-(H)/2-(SO/3) Sulfite	-8500.	9.80	-	-	-	-	-	-	
340	C-(C)/2-(H)-(SO/4)	-6000.	-11.70	-	-	-	-	-	-	
341	C-(C)/3-(SO/4)	-4000.	-	-	-	-	-	-		
342	C-(C)/2-(H)-(SO/3) Sulfite	-3500.	-11.70	-	-	-	-	-	-	
343	C-(C)/3-(SO/3) Sulfite	-1500.	-34.30	-	-	-	-	-	-	
344	C-(C)/2-(H)-(SO)	-	-11.70	-	-	-	-	-	-	
345	C/B-(HSO/3)	-130900.	29.50	15.63	18.99	20.19	23.32	26.10	27.07	
346	Ethylene Sulfide Ring	17700.	29.47	-2.85	-2.59	-2.66	-3.02	-4.32	-5.82	
347	Thietane Ring	19370.	27.18	-4.59	-4.18	-3.91	-3.91	-4.60	-5.70	
348	Thiolane Ring	1730.	23.56	-4.90	-4.67	-3.68	-3.66	-4.41	-5.57	
349	Thiane (Thiacyclohexane) Ring	-620.	17.46	-6.22	-4.26	-2.24	-.69	.86	1.29	
350	Thiepane (Thiacycloheptane) Ring	3890.	17.30	-	-	-	-	-	-	
351	3-Thiolene Ring	5070.	25.40	-	-	-	-	-		

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
352	2-Thiolene Ring	5070.	25.40	-	-	-	-	-	-	
353	1,2-Dihydrothiophene 1,1-dioxide Ring	5740.	20.50	-	-	-	-	-	-	
354	Thiophene Ring	1730.	23.56	-4.90	-4.67	-3.68	-3.66	-4.41	-5.57	
355	C-(H)/3-(Sn)	-10080.	-	-	-	-	-	-	-	
356	C-(C)-(H)/2-(Sn)	-2180.	-	-	-	-	-	-	-	
357	C-(C)/2-(H)-(Sn)	3380.	-	-	-	-	-	-	-	
358	C-(C)/3-(Sn)	8160.	-	-	-	-	-	-	-	
359	C-(C/B)-(H)/2-(Sn)	-7770.	-	-	-	-	-	-	-	-
360	C/B-(Sn)	5510.	-	-	-	-	-	-	-	
361	C/D-(H)-(Sn)	8770.	-	-	-	-	-	-	-	
362	Sn-(C)/4	36200.	-	-	-	-	-	-	-	-
363	Sn-(C)/3-(Cl)	-9800.	-	-	-	-	-	-	-	
364	Sn-(C)/2-(Cl)/2	-49200.	-	-	-	-	-	-	-	-
365	Sn-(C)-(Cl)/3	-89500.	-	-	-	-	-	-	-	
366	Sn-(Br)-(C)/3	-1800.	-	-	-	-	-	-	-	
367	Sn-(C)/3-(I)	9900.	-	-	-	-	-	-	-	-
368	Sn-(C)/3-(H)	34800.	-	-	-	-	-	-	-	
369	Sn-(C/D)/4	36200.	-	-	-	-	-	-	-	
370	Sn-(C/D)/3-(Cl)	-8200.	-	-	-	-	-	-	-	
371	Sn-(C/D)/2-(Cl)/2	-50700.	-	-	-	-	-	-	-	
372	Sn-(C/D)-(Cl)/3	-82200.	-	-	-	-	-	-	-	
373	Sn-(C)/3-(C/D)	37600.	-	-	-	-	-	-	-	
374	Sn-(C/B)/4	26260.	-	-	-	-	-	-	-	
375	Sn-(C)/3-(C/B)	34930.	-	-	-	-	-	-	-	
376	Sn-(C)/3-(Sn)	26400.	-	-	-	-	-	-		
377	C-(H)/3-(Pb)	-10080.	-	-	-	-	-	-		
378	C-(C)-(H)/2-(Pb)	-1700.	-	-	-	-	-	-		

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f° 298K (cal mol^{-1})	S° 298K (cal K^{-1} mol^{-1})	C_p° (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
379	Pb-(C)/4	72900.								
380	O-(C)-(Cr)	23500.								
381	Cr-(O)/4	64000.								
382	C-(H)/3-(Zn)	10080.								
383	C-(C)-(H)/2-(Zn)	1780.								
384	Zn-(C)/2	33300.								
385	O-(C)-(Tl)	23500.								
386	Tl-(O)/4	157000.	-	-						
387	N-(C)/2-(Tl)	39100.	-	-						
388	Tl-(N)/4	123000.	-	-						
389	O-(C)-(V)	23500.	-	-	-					
390	V-(O)/4	87000.	-	-	-					
391	C-(Cd)-(H)/3	-10080.	-	-	-	-				
392	C-(C)-(Cd)-(H)/2	-300.	-	-	-	-				
393	Cd-(C)/2	46400.	-	-	-	-				
394	C-(Al)-(H)/3	-10080.	-	-	-	-				
395	C-(Al)-(C)-(H)/2	700.		-	-	-				
396	Al-(C)/3	9200.		-	-	-				
397	C-(C)-(Ge)-(H)/2	-7700.	-	-	-	-				
398	Ge-(C)/4	36200.	-	-	-	-				
399	Ge-(C)/3-(Ge)	15600.	-	-	-	-				
400	C-(H)/3-(Hg)	10080.	-	-	-					
401	C-(C)-(H)/2-(Hg)	2680.	-	-	-	-				
402	C-(C)/2-(H)-(Hg)	3620.	-	-	-	-				
403	C/B-(Hg)	1800.	-	-	-	-				
404	Hg-(C)/2	42500.	-	-	-					
405	Hg-(C)-(Cl)	2820.	-	-						
406	Hg-(Br)-(C)	4880.		-						
407	Hg-(C)-(I)	15780.	-							
408	Hg-(C/B)/2	64400.								
409	Hg-(C/B)-(Cl)	9900.		-						
410	Hg-(Br)-(C/B)	18100.								
411	Hg-(C/B)-(I)	27900.								
412	C-(H)/3-(P)	10080.	30.40	.00	.00	.00	.00	.00	.00	.00

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
413	C-(C)-(H)/2-(P)	-2470.	-	-	-	-	-	-	-	
414	C-(H)/3-(PO)	-10080.	30.40	.00	.00	.00	.00	.00	.00	.00
415	C-(C)-(H)/2-(PO)	-3400.	-	-	-	-	-	-	-	-
416	C-(H)/3-(P=N)	-10080.	30.40	.00	.00	.00	.00	.00	.00	.00
417	C-(C)-(H)/2-(N=P)	19400.	-	-	-	-	-	-	-	-
418	C/B-(P)	-1800.	-	-	-	-	-	-	-	
419	C/B-(PO)	2300.	-	-	-	-	-	-	-	-
420	C/B-(P=N)	2300.	-	-	-	-	-	-	-	-
421	P-(C)/3	7000.	-	-	-	-	-	-	-	
422	P-(C)-(Cl)/2	-50300.	-	-	-	-	-	-	-	-
423	P-(C/B)/3	28300.	-	-	-	-	-	-	-	-
424	P-(O)/3	-66800.	-	-	-	-	-	-	-	-
425	P-(N)/3	-66800.	-	-	-	-	-	-	-	-
426	PO-(C)/3	-72800.	-	-	-	-	-	-	-	-
427	PO-(C)-(F)/2	-	46.77	-	-	-	-	-	-	-
428	PO-(C)-(Cl)-(F)	-	50.80	-	-	-	-	-	-	-
429	PO-(C)-(Cl)/2	-123000.	52.97	-	-	-	-	-	-	-
430	PO-(C)-(Cl)-(O)	-112600.	-	-	-	-	-	-	-	-
431	PO-(C)-(O)/2	-99500.	-	-	-	-	-	-	-	-
432	PO-(O)/3	-104600.	-	-	-	-	-	-	-	-
433	PO-(F)-(O)/2	-167700.	-	-	-	-	-	-	-	-
434	PO-(C/B)/3	-52900.	-	-	-	-	-	-	-	-
435	PO-(N)/3	-104600.	-	-	-	-	-	-	-	-
436	O-(C)-(P)	-23500.	-	-	-	-	-	-	-	-
437	O-(H)-(P)	-58700.	-	-	-	-	-	-	-	-
438	O-(C)-(PO)	-40700.	-	-	-	-	-	-	-	-
439	O-(H)-(PO)	-65000.	-	-	-	-	-	-	-	
440	O-(PO)/2	-54500.	-	-	-	-	-	-	-	
441	O-(C)-(P=N)	-40700.	-	-	-	-	-	-	-	
442	N-(C)/2-(P)	32200.	-	-	-	-	-	-	-	
443	N-(C)/2-(PO)	17800.	-	-	-	-	-	-	-	
444	P=N-(C)-(C)/3	500.	-	-	-	-	-	-	-	
445	P=N-(C)-(C/B)/3	-25700.	-	-	-	-	-	-	-	
446	P=N-(C)/2-(P=N)-(P=N)	-15500.	-	-	-	-	-	-		

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
447	P-N-(C/B)/2-(N=P)-(P=N)	-22900.	-	-	-	-	-	-	-	
448	P=N-(Cl)/2-(N=P)-(P=N)	-58200.	-	-	-	-	-	-	-	
449	P=N-(N=P)-(O)/2-(P=N)	-43400.	-	-	-	-	-	-	-	
450	C-(B)-(H)/3	-10080.	-	-	-	-	-	-	-	
451	C-(B)-(C)-(H)/2	-2220.	-	-	-	-	-	-	-	
452	C-(B)-(C)/2-(H)	1100.	-	-	-	-	-	-	-	
453	C-(BO/3)-(H)/3	-10080.	-	-	-	-	-	-	-	
454	C-(BO/3)-(C)-(H)/2	-2200.	-	-	-	-	-	-	-	
455	C/D-(B)-(H)	15600.	-	-	-	-	-	-	-	
456	B-(C)/3	900.	-	-	-	-	-	-	-	
457	B-(C)-(F)/2	-187900.	-	-	-	-	-	-	-	
458	B-(C)/2-(Cl)	-42700.	-	-	-	-	-	-	-	
459	B-(Br)-(C)/2	-26900.	-	-	-	-	-	-	-	
460	B-(C)/2-(I)	-8900.	-	-	-	-	-	-	-	
461	B-(C)/2-(O)	29300.	-	-	-	-	-	-	-	
462	B-(C/D)-(F)/2	-192900.	-	-	-	-	-	-	-	
463	B-(O)/3	24400.	-	-	-	-	-	-	-	
464	B-(Cl)-(O)/2	-19700.	-	-	-	-	-	-	-	
465	B-(Cl)/2-(O)	-61200.	-	-	-	-	-	-	-	
466	B-(H)-(O)/2	19900.	-	-	-	-	-	-	-	
467	B-(N)/3	24400.	-	-	-	-	-	-	-	
468	B-(Cl)-(N)/2	-23800.	-	-	-	-	-	-	-	
469	B-(Cl)/2-(N)	-67900.	-	-	-	-	-	-	-	
470	BO/3-(C)/3	-208700.	-	-	-	-	-	-	-	
471	O-(B)-(H)	-115500.	-	-	-	-	-	-	-	
472	O-(B)-(C)	-69430.	-	-	-	-	-	-	-	
473	N-(B)-(C)/2	-9930.	-	-	-	-	-	-	-	
474	B-(S)/3	24500.	-	-	-	-	-	-	-	
475	S-(B)-(C)	-14500.	-	-	-	-	-	-	-	
476	S-(B)-(C/B)	-7800.	-	-	-	-	-	-	-	
477	C/B-(Pb)	5510.	-	-	-	-	-	-	-	
478	Pb-(C/B)/4	81600.	-	-	-	-	-	-	-	
479	C-(H)/3-(Si)	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
480	Si-(C)/4	-28200.	44.08	27.05	32.24	36.91	40.90	47.45	52.49	60.41

TABLE 1 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
481	Si-(C)-(H)/3	-2000.	30.85	9.47	-	-			-	
482	Si-(C/B)/4	-145300.	-	-	-	-	-	-	-	
483	C/B-(Si)	5510.	-7.69	2.67	3.14	3.68	4.15	4.96	5.44	5.98
484	C-(C)-(H)/2-(Si)	7630.	-	-	-	-	-	-	-	
485	Alkane Gauche Correction	800.	.00	-	-	-	-	-	-	
486	Alkene Gauche Correction - Not With Halogen	500.	.00	-	-	-	-	-	-	
487	Gauche Interaction Through An Ether Oxygen	300.	.00	-	-	-	-	-	-	-
488	Gauche Interaction Between Cl, Br, Or I	1000.	.00	-	-	-	-	-	-	
489	Gauche Interaction Across C-B Bond	800.	.00	-	-	-	-	-	-	
490	Cis Interaction - No t-Butyl Group	1000.	.00	-1.34	-1.09	-.81	-.61	-.39	-.26	-
491	Cis Interaction - One t-Butyl Group	4000.	.00	-1.34	-1.09	-.81	-.61	-.39	-.26	-
492	Cis Interaction - Two T-Butyl Groups	10000.	.00	-1.34	-1.09	-.81	-.61	-.39	-.26	-
493	Cis Interaction Between Two Of Cl, Br And I	-300.	.00	-	-	-	-	-	-	-
494	Cis Interaction Between Alk. And Cl, Br, Or I	-800.	.00	-	-	-	-	-	-	-
495	A Second Cis Interaction	2000.	.00	-	-	-	-	-	-	-
496	Ortho Interaction - Nonpolar/Nonpolar	750.	-1.61	1.12	1.35	1.30	1.17	.88	.66	-.05
497	Ortho Interaction Between F And F	5000.	-1.40	.00	-.20	-.10	.30	.70	.00	.00
498	Ortho Interaction Between Cl And Cl	2200.	-2.30	-.50	1.20	.50	-.60	-.30	.00	.00
499	Ortho Interaction Between Alk. And Br, Cl Or I	600.	.00	-	-	-	-	-	-	-
500	Ortho Interaction On Pyridine Ring	-1500.	.00	-	-	-	-	-	-	-
501	Para Interaction On Pyridine Ring	-1500.	.00	-	-	-	-	-	-	-
502	But-2-ene Structure	0.	1.20	-1.34	-1.09	-.81	-.61	-.39	-.26	.00
503	3-Ene Structure	0.	-.60	-1.34	-1.09	-.81	-.61	-.39	-.26	.00
504	Di-tertiary Ether	7800.	.00	-	-	-	-	-	-	-
505	Symmetrical Phenyl Or P-phenylene Group	-	-	-	-	-	-	-	-	-
506	Ortho Interaction (Alkane Or Alkene) And (NO/2)	4500.	-	-	-	-	-	-	-	
507	Ortho Interaction Between (NH/2) And (NO/2)	-1200.	-	-	-	-	-	-	-	
508	Ortho Interaction - Nonpolar/Polar	340.	-	-	-	-	-	-	-	
509	Ortho Interaction - Polar/Polar	2400.	-	-	-	-	-	-	-	
510	Ether-oxygen Gauche	500.	-	-	-	-	-	-	-	

TABLE 2

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
396	Al-(C)/3	9200.	-	-	-	-	-	-	-	
459	B-(Br)-(C)/2	-26900.	-	-	-	-	-	-	-	
457	B-(C)-(F)/2	-187900.	-	-	-	-	-	-	-	
458	B-(C)/2-(Cl)	-42700.	-	-	-	-	-	-	-	
460	B-(C)/2-(I)	-8900.	-	.00	.00	.00	.00	.00	.00	.00
461	B-(C)/2-(O)	29300.	-	.00	.00	.00	.00	.00	.00	.00
456	B-(C)/3	900.	-	-	-	-	-	-	-	-
462	B-(C/D)-(F)/2	-192900.	-	.00	.00	.00	.00	.00	.00	.00
468	B-(Cl)-(N)/2	-23800.	-	-	-	-	-	-	-	-
464	B-(Cl)-(O)/2	-19700.	-	.00	.00	.00	.00	.00	.00	.00
469	B-(Cl)/2-(N)	-67900.	-	-	-	-	-	-	-	-
465	B-(Cl)/2-(O)	-61200.	-	-	-	-	-	-	-	-
466	B-(H)-(O)/2	19900.	-	.00	.00	.00	.00	.00	.00	.00
467	B-(N)/3	24400.	-	.00	.00	.00	.00	.00	.00	.00
463	B-(O)/3	24400.	-	.00	.00	.00	.00	.00	.00	.00
474	B-(S)/3	24500.	-	-	-	-	-	-	-	-
470	BO/3-(C)/3	-208700.	-	.00	.00	.00	.00	.00	.00	.00
395	C-(Al)-(C)-(H)/2	700.	-	-	-	-	-	-	-	
394	C-(Al)-(H)/3	-10080.	-	-	-	-	-	-	-	
451	C-(B)-(C)-(H)/2	-2220.	-	-	-	-	-	-	-	
452	C-(B)-(C)/2-(H)	1100.	-	-	-	-	-	-	-	
450	C-(B)-(H)/3	-10080.	-	-	-	-	-	-	-	
454	C-(BO/3)-(C)-(H)/2	-2200.	-	.00	.00	.00	.00	.00	.00	.00
453	C-(BO/3)-(H)/3	-10080.	-	.00	.00	.00	.00	.00	.00	.00
251	C-(Br)-(C)-(Cl)-(H)	-10100.	45.70	12.40	14.00	15.60	16.30	17.90	19.00	.00
244	C-(Br)-(C)-(H)/2	-5400.	40.80	9.10	11.00	12.60	13.70	15.50	16.80	.00
245	C-(Br)-(C)/2-(H)	-3400.	19.10	8.93	10.66	11.96	12.84	14.05	14.72	. .
246	C-(Br)-(C)/3	-400.	-3.20	9.30	11.00	11.50	12.30	13.30	13.30	. .
274	C-(Br)-(C/B)-(H)/2	-6900.	42.20	7.29	11.10	12.47	13.69	15.59	16.71	. .
243	C-(Br)/3-(C)	3900.	55.70	16.70	18.00	18.80	19.40	19.90	20.30	.00
22	C-(C)-(C/B)-(H)/2	4860.	9.34	-	-	-	-	-	-	

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
18	C-(C)-(C/D)-(H)/2	-4760.	9.80	-	-	-	-	-	-	
21	C-(C)-(C/T)-(H)/2	-4730.	10.30	4.95	6.56	7.93	9.08	10.86	12.19	14.20
205	C-(C)-(CN)-(H)/2	22500.	40.20	11.10	13.40	15.50	17.20	19.70	21.30	.00
114	C-(C)-(CO)-(H)/2	-5200.	9.60	6.20	7.70	8.70	9.50	11.10	12.20	.00
131	C-(C)-(CO)/2-(H)	-5400.	-10.20	-	-	-	-	-	-	
392	C-(C)-(Cd)-(H)/2	-300.	-	-	-	-	-	-	-	
239	C-(C)-(Cl)-(H)/2	-15600.	37.80	8.90	10.70	12.30	13.40	15.30	16.70	.00
253	C-(C)-(Cl)-(H)-(O)	-21600.	15.40	12.70	13.54	13.97	14.23	14.55	14.78	.00
236	C-(C)-(Cl)-(F)/2	-106300.	40.50	13.70	16.10	17.50	18.60	19.80	20.40	.00
238	C-(C)-(Cl)/2-(H)	-18900.	43.70	12.10	14.00	15.40	16.50	17.90	18.70	.00
237	C-(C)-(Cl)/3	-24900.	50.40	16.30	18.00	19.10	19.80	20.60	21.00	.00
232	C-(C)-(F)-(H)/2	-51500.	35.40	8.10	10.00	12.00	13.00	15.20	16.60	.00
231	C-(C)-(F)/2-(H)	-102300.	39.10	9.90	12.00	13.70	15.10	16.70	17.80	.00
230	C-(C)-(F)/3	-158400.	42.50	12.70	15.00	16.40	17.90	19.30	20.00	.00
397	C-(C)-(Ge)-(H)/2	-7700.	-	.00	.00	.00	.00	.00	.00	.00
250	C-(C)-(H)-(I)/2	26000.	54.60	13.60	15.15	16.63	17.72	19.04	19.49	.00
176	C-(C)-(H)-(N/I)	10100.	-	-	-	-	-	-	-	
217	C-(C)-(H)-(NO/2)/2	-9900.	65.90	12.30	15.96	18.71	20.68	23.10	24.33	.00
118	C-(C)-(H)-(O)/2	-16300.	-13.10	2.22	4.45	6.72	8.07	8.71	9.09	.00
306	C-(C)-(H)/2-(SO/2)	-7680.	9.40	4.09	5.97	7.54	8.80	10.65	11.93	.00
299	C-(C)-(H)/2-(SO)	-7720.	9.40	4.55	6.42	7.95	9.16	10.95	12.22	.00
378	C-(C)-(H)/2-(Pb)	-1700.	-	-	-	-	-	-	-	
415	C-(C)-(H)/2-(PO)	-3400.	-	-	-	-	-	-	-	
280	C-(C)-(H)/2-(S)	-5590.	9.88	5.38	7.08	8.60	9.97	12.26	14.15	.00
339	C-(C)-(H)/2-(SO/3) sulfite	-8500.	9.80	-	-	-	-	-	-	
214	C-(C)-(H)/2-(NO/2)	-14400.	48.40	12.59	15.82	18.52	20.66	23.79	25.90	.00
417	C-(C)-(H)/2-(N-P)	19400.	-	-	-	-	-	-	-	
173	C-(C)-(H)/2-(N)	-6600.	9.80	5.25	6.90	8.28	9.39	11.09	12.34	.00
247	C-(C)-(H)/2-(I)	8000.	43.00	9.20	11.00	12.90	13.90	15.80	17.20	.00
401	C-(C)-(H)/2-(Hg)	-2680.	-	-	-	-	-	-	-	
413	C-(C)-(H)/2-(P)	-2470.	-	-	-	-	-	-	-	
124	C-(C)-(H)/2-(O)	-8100.	9.80	4.99	6.85	8.30	9.43	11.11	12.33	14.60

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
336	C-(C)-(H)/2-(SO/4)	-8700.	9.80	-	-	-	-	-	-	
484	C-(C)-(H)/2-(Si)	7630.	-	-	-	-	-	-	-	
356	C-(C)-(H)/2-(Sn)	-2180.	-	-	-	-	-	-	-	
383	C-(C)-(H)/2-(Zn)	-1780.	-	-	-	-	-	-	-	
1	C-(C)-(H)/3	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
222	C-(C)-(NO/2)/3	-5000.	-	-	-	-	-	-	-	
25	C-(C)/2-(C/B)-(H)	-980.	-12.15	-	-	-	-	-	-	
23	C-(C)/2-(C/D)-(H)	-1480.	-11.69	4.16	5.91	7.34	8.19	9.46	10.19	11.28
24	C-(C)/2-(C/T)-(H)	-1720.	-11.19	-	-	-	-	-	-	
206	C-(C)/2-(CN)-(H)	25800.	19.80	11.00	12.70	14.10	15.40	17.30	18.60	.00
208	C-(C)/2-(CN)/2	19600.	28.40	14.72	17.79	20.00	21.61	23.78	24.96	.00
113	C-(C)/2-(CO)-(H)	-1700.	-12.00	2.92	4.99	6.50	7.54	8.88	9.77	.00
241	C-(C)/2-(Cl)-(H)	-14800.	17.60	-	-	-	-	-	-	
240	C-(C)/2-(Cl)/2	-22200.	22.40	13.02	14.88	15.95	16.48	16.96	17.02	.0
234	C-(C)/2-(F)-(H)	-49000.	14.00	7.30	9.04	10.47	11.56	13.10	14 01	.00
233	C-(C)/2-(F)/2	-97000.	17.80	9.90	11.80	13.50	14.40	16.10	16.60	.00
402	C-(C)/2-(H)-(Hg)	3620.	-	-	-	-	-	-	-	
342	C-(C)/2-(H)-(SO/3) sulfite	-3500.	-11.70	-	-	-	-	-	-	
307	C-(C)/2-(H)-(SO/2)	-2620.	-12.00	4.42	6.25	7.56	8.48	9.64	10.30	.00
344	C-(C)/2-(H)-(SO)	-	-11.70	-	-	-	-	-	-	
281	C-(C)/2-(H)-(S)	-2640.	-11.32	4.85	6.51	7.78	8.69	9.90	10.57	.00
123	C-(C)/2-(H)-(O)	-7200.	-11.00	4.80	6.64	8.10	8.73	9.81	10.40	.00
357	C-(C)/2-(H)-(Sn)	3380.	-	-	-	-	-	-	-	
340	C-(C)/2-(H)-(SO/4)	-6000.	-11.70	-	-	-	-	-	-	
248	C-(C)/2-(H)-(I)	10500.	21.30	9.23	10.91	12.16	13.00	14.17	14.80	.00
215	C-(C)/2-(H)-(NO/2)	-13600.	26.90	11.99	15.21	17.72	19.61	22.18	23.70	.00
174	C-(C)/2-(H)-(N)	-5200.	-11.70	5.56	6.52	7.30	8.09	9.17	9.58	.0
5	C-(C)/2-(H)/2	-4950.	9.42	-	-	-	-	-		
221	C-(C)/2-(NO/2)/2	-10200.	-	-	-	-	-	-	-	
117	C-(C)/2-(O)/2	-18600.	-35.80	1.59	3.95	6.20	7.39	7.62	8.48	.00
27	C-(C)/3-(C/B)	2810.	-35.18	4.37	6.79	8.09	8.78	9.19	8.96	7.68
26	C-(C)/3-(C/D)	1680.	-34.72	3.99	6.04	7.43	8.26	8.92	8.96	8.1

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	150
39	C-(C)/3-(C/T)	460.	-35.00	-	-	-	-	-	-	
207	C-(C)/3-(CN)	29000.	-2.80	8.65	11.16	12.89	14.05	15.51	16.19	
115	C-(C)/3-(CO)	1400.	-33.00	2.32	4.38	5.70	6.49	7.27	7.57	
242	C-(C)/3-(Cl)	-12800.	-5.40	9.30	10.50	11.00	11.30	12.40	12.70	
235	C-(C)/3-(F)	-48500.	-7.70	6.80	8.86	10.20	11.16	12.43	12.72	
6	C-(C)/3-(H)	-1900.	-12.07	-	-	-	-	-	-	
249	C-(C)/3-(I)	13000.	1.00	-	-	-	-	-	-	
175	C-(C)/3-(N)	-3200.	-34.10	-	-	-	-	-	-	
216	C-(C)/3-(NO/2)	-16500.	3.90	-	-	-	-	-	-	
122	C-(C)/3-(O)	-6600.	-33.56	4.33	6.19	7.25	7.70	8.20	8.24	
282	C-(C)/3-(S)	-550.	-34.41	-	-	-	-	-	-	
300	C-(C)/3-(SO)	-3050.	-34.50	3.06	4.58	4.84	6.60	7.54	7.96	
341	C-(C)/3-(SO/4)	-4000.	-	-	-	-	-	-	-	
343	C-(C)/3-(SO/3) sulfite	-1500.	-34.30	-	-	-	-	-	-	
308	C-(C)/3-(SO/2)	-610.	-34.50	-	-	-	-	-	-	
358	C-(C)/3-(Sn)	8160.	-	-	-	-	-	-	-	
7	C-(C)/4	500.	-35.10	-	-	-	-	-	-	
20	C-(C/B)-(C/D)-(H)/2	-4290.	10.20	4.70	6.80	8.40	9.60	11.30	12.60	14.4
130	C-(C/B)-(CO)-(H)/2	-5400.	9.60	-	-	-	-	-	-	
273	C-(C/B)-(F)/3	-162700.	42.80	12.50	15.30	17.20	18.50	20.10	21.00	
283	C-(C/B)-(H)/2-(S)	-4730.	4.90	-	-	-	-	-	-	
120	C-(C/B)-(H)/2-(O)	-8100.	9.70	3.71	6.27	8.28	9.79	11.79	13.20	
275	C-(C/B)-(H)/2-(I)	8400.	44.50	8.10	10.79	12.83	14.31	16.28	17.63	
310	C-(C/B)-(H)/2-(SO/2)	-5540.	9.60	3.71	6.57	8.28	9.79	11.89	13.20	
2	C-(C/B)-(H)/3	-10000.	30.28	6.08	7.99	9.72	11.19	13.49	15.29	
359	C-(C/B)-(H)/2-(Sn)	-7770.	-	.00	.00	.00	.00	.00	.00	
136	C-(C/D)-(CO)-(H)/2	-3800.	-	-	-	-	-	-	-	
301	C-(C/D)-(H)/2-(SO)	-7350.	10.10	-	-	-	-	-	-	
284	C-(C/D)-(H)/2-(S)	-6450.	10.90	5.31	6.83	8.23	9.76	12.18	14.21	
121	C-(C/D)-(H)/2-(O)	-6500.	8.90	-	-	-	-	-	-	
309	C-(C/D)-(H)/2-(SO/2)	-7140.	10.50	4.86	6.81	8.35	9.58	11.27	12.54	
3	C-(C/D)-(H)/3	-10080.	30.41	-	-	-	-	-		

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
19	C-(C/D)/2-(H)/2	-4290.	10.20	4.70	6.80	8.40	9.60	11.30	12.60	14.40
129	C-(C/T)-(CO)-(H)/2	-5400.	10.60	-	-	-	-	-	-	
126	C-(C/T)-(H)/2-(O)	-6500.	.00	.00	.00	.00	.00	.00	.00	.00
4	C-(C/T)-(H)/3	-10(	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
116	C-(CO)-(H)/3	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
112	C-(CO)/2-(H)/2	-7600.	11.30	-	-	-	-	-	-	-
391	C-(Cd)-(H)/3	-10080.	-	-	-	-	-	-	-	-
323	C-(F)/3-(S)	-150300.	38.90	9.88	13.01	14.83	16.37	18.17	19.11	.00
254	C-(H)/2-(I)-(O)	3800.	40.70	8.22	10.49	12.23	13.55	15.35	16.57	.00
119	C-(H)/2-(O)/2	-16100.	7.80	2.83	5.06	7.52	9.12	10.32	11.29	.00
400	C-(H)/3-(Hg)	-10080.	-	-	-	-	-	-	-	-
172	C-(H)/3-(N)	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
125	C-(H)/3-(O)	-10080.	30.41	6.19	7.84	9.40	10.79	13.03	14.77	17.58
412	C-(H)/3-(P)	-10080.	30.40	.00	.00	.00	.00	.00	.00	.00
416	C-(H)/3-(P=N)	-10080.	30.40	.00	.00	.00	.00	.00	.00	.00
414	C-(H)/3-(PO)	-10080.	30.40	-	-	-	-	-	-	-
377	C-(H)/3-(Pb)	-10080.	-	-	-	-	-	-	-	-
279	C-(H)/3-(S)	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	.00
298	C-(H)/3-(SO)	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	.00
337	C-(H)/3-(SO/3) sulfite	-10080.	30.41	-	-	-	-	-	-	-
305	C-(H)/3-(SO/2)	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	.00
334	C-(H)/3-(SO/4)	-10080.	30.41	-	-	-	-	-	-	
479	C-(H)/3-(Si)	-10080.	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
355	C-(H)/3-(Sn)	-10080.	-	-	-	-	-	-	-	-
382	C-(H)/3-(Zn)	-10080.	-	-	-	-	-	-	-	
37	C/A	34200.	6.00	-	-	-	-	-	-	
271	C/B-(Br)	8700.	21.60	7.80	8.70	9.40	9.90	10.30	10.50	.00
33	C/B-(C)	5510.	-7.69	2.67	3.14	3.68	4.15	4.96	5.44	5.98
36	C/B-(C/B)	4960.	-8.64	-	-	-	-	-	-	
34	C/B-(C/D)	5680.	-7.80	-	-	-	-	-	-	
35	C/B-(C/T)	5680.	-7.80	3.59	3.97	4.38	4.72	5.28	5.61	5.75
212	C/B-(CN)	35800.	20.50	9.80	11.20	12.30	13.10	14.20	14.90	.00

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
110	C/B-(CO)	3700.	-7.70	2.67	3.14	3.68	4.15	4.96	5.44	.00
270	C/B-(Cl)	-4300.	18.90	7.40	8.40	9.20	9.70	10.20	10.40	.00
269	C/B-(F)	-42800.	16.10	6.30	7.60	8.50	9.10	9.80	10.20	.00
32	C/B-(H)	3300.	11.53	3.24	4.44	5.46	6.30	7.54	8.41	9.73
345	C/B-(HSO/3)	-130900.	29.50	15.63	18.99	20.19	23.32	26.10	27.07	.00
403	C/B-(Hg)	-1800.	-	-	-	-	-	-	-	
272	C/B-(I)	22600.	23.70	-	-	-	-	-	-	
193	C/B-(N)	-500.	-9.69	3.95	5.21	5.94	6.32	6.53	6.56	.00
220	C/B-(NO)	5400.	-	-	-	-	-	-	-	
194	C/B-(NO/2)	400.	26.90	16.20	.00	.00	.00	.00	.00	.00
111	C/B-(O)	-900.	-10.20	3.90	5.30	6.20	6.60	6.90	6.90	.00
418	C/B-(P)	-1800.	-	-	-	-	-	-	-	
420	C/B-(P=N)	2300.	-	.00	.00	.00	.00	.00	.00	.00
419	C/B-(PO)	2300.	-	.00	.00	.00	.00	.00	.00	.00
477	C/B-(Pb)	5510.	-	-	-	-	-	-	-	
285	C/B-(S)	-1800.	10.20	-	-	-	-	-	-	-
302	C/B-(SO)	2300.	10.40	2.67	3.14	3.68	4.15	4.96	5.44	.00
311	C/B-(SO/2)	2300.	8.60	-	-	-	-	-	-	
332	C/B-(SO/2N/3), azidosulfonyl group	74600.	-	-	-	-	-	-	-	
483	C/B-(Si)	5510.	-7.69	2.67	3.14	3.68	4.15	4.96	5.44	5.98
360	C/B-(Sn)	5510.	-	.00	.00	.00	.00	.00	.00	.00
455	C/D-(B)-(H)	15600.	-	-	-	-	-	-	-	
261	C/D-(Br)-(Cl)	6500.	45.10	12.10	12.70	13.50	14.10	14.70	15.00	.00
260	C/D-(Br)-(F)	-31300.	42.50	10.80	12.00	12.80	13.50	14.30	14.70	.00
264	C/D-(Br)-(H)	12700.	38.30	8.10	9.50	10.60	11.40	12.40	13.20	.00
258	C/D-(Br)/2	7500.	47.60	12.30	13.20	13.90	14.30	14.90	15.20	.00
14	C/D-(C)-(C/B)	8640.	-14.60	-	-	-	-	-	-	
12	C/D-(C)-(C/D)	8880.	-14.60	-	-	-	-	-	-	
105	C/D-(C)-(CO)	7500.	-11.80	5.48	6.98	7.41	7.64	8.01	8.20	.00
255	C/D-(C)-(Cl)	-2100.	15.00	.00	.00	.00	.00	.00	.00	.00
9	C/D-(C)-(H)	8590.	7.97	4.16	5.03	5.81	6.50	7.65	8.45	9.62
223	C/D-(C)-(NO/2)	4400.	-	.00	.00	.00	.00	.00	.00	.00

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
108	C/D-(C)-(O)	10300.	-12.70	4.10	4.61	4.99	5.26	5.80	6.08	.00
287	C/D-(C)-(S)	10930.	-12.41	3.50	3.57	3.83	4.09	4.41	5.00	.00
313	C/D-(C)-(SO/2)	14500.	-9.60	3.70	6.22	7.96	9.20	10.66	11.34	.00
10	C/D-(C)/2	10340.	-12.70	-	-	-	-	-	-	
13	C/D-(C/B)-(H)	6780.	6.38	4.46	5.79	6.75	7.42	8.35	8.99	9.98
16	C/D-(C/B)/2	8000.	-12.70	-	-	-	-	-	-	
11	C/D-(C/D)-(H)	6730.	6.38	4.46	5.79	6.75	7.42	8.35	8.99	9.98
107	C/D-(C/D)-(O)	8900.	-14.60	-	-	-	-	-	-	
17	C/D-(C/D)/2	4600.	-8.80	.00	.00	.00	.00	.00	.00	.00
15	C/D-(C/T)-(H)	6780.	6.38	4.46	5.79	6.75	7.42	8.35	8.99	9.98
209	C/D-(CN)-(H)	37400.	36.58	9.80	11.70	13.30	14.50	16.30	17.30	.00
210	C/D-(CN)/2	34100.	15.90	13.60	16.55	18.68	20.25	22.34	23.59	.00
106	C/D-(CO)-(H)	5000.	7.97	7.58	8.85	9.27	9.63	10.38	11.04	.00
104	C/D-(CO)-(O)	11600.	-12.60	5.59	7.00	7.48	7.75	8.02	8.13	.00
259	C/D-(Cl)-(F)	-43200.	39.80	10.30	11.70	12.60	13.30	14.20	14.70	.00
263	C/D-(Cl)-(H)	-1200.	35.40	7.90	9.20	10.30	11.20	12.30	13.10	.00
257	C/D-(Cl)/2	-1800.	42.10	11.40	12.50	13.30	13.90	14.60	15.00	.00
262	C/D-(F)-(H)	-37600.	32.80	6.80	8.40	9.50	10.50	11.80	12.70	.00
256	C/D-(F)/2	-77500.	37.30	9.70	11.00	12.00	12.70	13.80	14.50	.00
265	C/D-(H)-(I)	24500.	40.50	-	-	-	-	-	-	
211	C/D-(H)-(NO/2)	7100.	44.40	12.30	15.10	17.40	19.20	21.60	23.20	25.30
109	C/D-(H)-(O)	8600.	8.00	-	-	-	-	-	-	
286	C/D-(H)-(S)	8560.	8.00	-	-	-	-	-	-	
312	C/D-(H)-(SO/2)	12500.	11.90	-	-	-	-	-	-	
361	C/D-(H)-(Sn)	8770.	-	.00	.00	.00	.00	.00	.00	.00
8	C/D-(H)/2	6260.	27.61	5.10	6.36	7.51	8.50	10.07	11.27	13.19
267	C/T-(Br)	23600.	36.10	-	-	-	-	-		
29	C/T-(C)	27550.	6.35	-	-	-	-	-	-	
31	C/T-(C/B)	29200.	6.43	2.57	3.54	3.50	4.92	5.34	5.50	5.80
30	C/T-(C/D)	29200.	6.43	2.57	3.54	3.50	4.92	5.34	5.50	5.80
38	C/T-(C/T)	29570.	5.87	.00	.00	.00	.00	.00	.00	.00
213	C/T-(CN)	63800.	35.40	10.30	11.30	12.10	12.70	13.60	14.30	15.40

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
266	C/T-(Cl)	17800.	33.40	7.90	8.40	8.70	9.00	9.40	9.60	.00
28	C/T-(H)	26930.	24.70	5.27	5.99	6.49	6.87	7.47	7.96	8.87
268	C/T-(I)	33800.	37.90	8.40	8.80	9.10	9.30	9.60	9.80	.00
277	CO-(Br)-(C/B)	-37800.		-	-			-	-	
82	CO-(C)-(C/B)	-30900.	12.30	-	-	-	-	-		
135	CO-(C)-(C/D)	-29300.	-	-	-	-			-	
75	CO-(C)-(CO)	-29200.	15.80	5.99	7.03	7.79	8.39	9.30	9.78	.00
85	CO-(C)-(H)	-29100.	34.93	-	-	-	-	-	-	
197	CO-(C)-(N)	-32800.	16.20	5.37	6.17	7.07	7.66	9.62	11.19	.00
78	CO-(C)-(O)	-35100.	14.78	5.97	6.70	7.45	8.02	8.87	9.56	10.00
321	CO-(C)-(S)	-31560.	15.43	5.59	6.32	7.09	7.76	8.89	9.61	.00
84	CO-(C)/2	-31400.	15.01	-	-	-	-	-	-	
133	CO-(C/B)-(CO)	-26800.	12.30	.00	.00	.00	.00	.00	.00	.00
276	CO-(C/B)-(Cl)	-52300.	40.00	-	-	-	-	-	-	
83	CO-(C/B)-(H)	-29100.	35.40	8.01	10.56	11.65	14.21	16.38	17.68	.00
278	CO-(C/B)-(I)	-23700.	-	.00	.00	.00	.00	.00	.00	.00
77	CO-(C/B)-(O)	-36600.	15.10	-	-	-	-	-	-	
81	CO-(C/B)/2	-25800.	9.50	-	-	-	-	-	-	
80	CO-(C/D)-(H)	-29100.	35.40	-	-	-	-	-	-	
76	CO-(C/D)-(O)	-32000.	15.20	-	-	-	-	-	-	
132	CO-(C/T)-(H)	-29100.	35.40	-	-	-	-	-	-	
86	CO-(CO)-(H)	-25300.	21.30	6.72	7.83	8.90	9.89	11.43	12.12	.00
87	CO-(CO)-(O)	-29300.	17.20	-	-	-	-	-	-	
196	CO-(H)-(N)	-29600.	34.93	-	-	-	-	-	-	
79	CO-(H)-(O)	-32100.	34.93	7.03	7.87	8.82	9.68	11.16	12.20	.00
134	CO-(O)/2	-29900.	5.80	-	-	-	-	-	-	
324	CS-(N)/2	-31560.	15.43	5.59	6.32	7.09	7.76	8.89	9.61	
393	Cd-(C)/2	46400.	-	.00	.00	.00	.00	.00	.00	.00
381	Cr-(O)/4	-64000.	-	-	-	-	-			
399	Ge-(C)/3-(Ge)	15600.	-	.00	.00	.00	.00	.00	.00	.00
398	Ge-(C)/4	36200.	-	-	-	-	-			
406	Hg-(Br)-(C)	4880.	-	-	-					

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f° 298K (cal mol^{-1})	S° 298K (cal K^{-1} mol^{-1})	C_p° (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
410	Hg-(Br)-(C/B)	18100.	-	-	-	-				
405	Hg-(C)-(Cl)	-2820.	-	-	-	-	-	-	-	
407	Hg-(C)-(I)	15780.	-	.00	.00	.00	.00	.00	.00	.00
404	Hg-(C)/2	42500.	-	.00	.00	.00	.00	.00	.00	.00
409	Hg-(C/B)-(Cl)	9900.		.00	.00	.00	.00	.00	.00	.00
411	Hg-(C/B)-(I)	27900.	-	.00	.00	.00	.00	.00	.00	.00
408	Hg-(C/B)/2	64400.	-	.00	.00	.00	.00	.00	.00	.00
506	Interaction, ortho (alkane or alkene) and (NO/2)	4500.	-	.00	.00	.00	.00	.00	.00	.00
486	Interaction, gauche, alkene - not with halogen	500.	.00	-	-	-	-		-	
507	Interaction, ortho - between (NH/2) and (NO/2)	-1200.	-	-	-	-	-			
504	Interaction, ether, di-tertiary	7800.	.00	-	-	-	-	-		
492	Interaction, cis - two t-butyl groups	10000.	.00	-	-	-	-	-		
485	Interaction, gauche, alkane	800.	.00	.00	.00	.00	.00	.00	.00	.00
510	Interaction, gauche ether-oxygen	500.	-	-	-	-	-	-		
487	Interaction, gauche - through an ether oxygen	300.	.00	-	-	-	-	-	-	
488	Interaction, gauche - between Cl, Br, or I	1000.	.00	-	-	-	-	-		
489	Interaction, gauche - across C-B bond	800.	.00	-	-	-	-	-		
499	Interaction, ortho - between alk and Br, Cl or I	600.	.00	-	-	-	-	-		
501	Interaction, para - on pyridine ring	-1500.	.00	-	-	-	-	-	-	
509	Interaction, ortho - polar/polar	2400.	-	-	-	-	-	-		
491	Interaction, cis - one t-butyl group	4000.	.00	-1.34	-1.09	-.81	-.61	-.39	-.26	.00
490	Interaction, cis - no t-butyl group	1000.	.00	-1.34	-1.09	-.81	-.61	-.39	-.26	.00
502	Interaction, structure, but-2-ene	0.	1.20	-1.34	-1.09	-.81	-.61	-.39	-.26	.00
503	Interaction, structure, 3-ene	0.	-.60	-	-	-	-	-	-	
505	Interaction, phenyl (sym) or p-phenylene (sym)	-	-	-	-	-	-	-		
498	Interaction, ortho - between Cl and Cl	2200.	-2.30	-.50	1.20	.50	-.60	-.30	.00	
493	Interaction, cis - between two of Cl, Br and I	-300.	.00	-	-	-	-	-	-	
494	Interaction, cis - between alk and Cl, Br, or I	-800.	.00	-	-	-	-	-		
495	Interaction, cis - a second cis Interaction	2000.	.00	-	-	-	-	-		
497	Interaction, ortho - between F and F	5000.	-1.40	-	-	-	-	-		

.00 .00 .00 .00 .00 .00 .00

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
508	Interaction, ortho - nonpolar/polar	340.	-	-	-	-	-	-	-	
496	Interaction, ortho - nonpolar/nonpolar	750.	-1.61	1.12	1.35	1.30	1.17	.88	.66	.00
473	N-(B)-(C)/2	-9930.	-	-	-	-	-	-	-	
190	N-(C)-(C/B)-(H)	14900.	6.80	-	-	-	-	-	-	
199	N-(C)-(CO)-(H)	-4400.	3.90	.66	1.55	2.46	3.48	4.24	4.53	.00
203	N-(C)-(CO)/2	-5900.	15.20	1.07	3.10	4.31	5.00	5.48	6.47	.00
252	N-(C)-(F)/2	-7800.	-	6.33	8.26	9.77	10.90	12.16	12.79	.00
181	N-(C)-(H)-(N)	20900.	9.61	-	-	-	-	-	-	-
177	N-(C)-(H)/2	4800.	29.71	5.72	6.51	7.32	8.07	9.41	10.47	12.28
191	N-(C)/2-(C/B)	26200.	-15.50	.62	2.02	3.27	4.13	5.23	5.59	.00
200	N-(C)/2-(CO)	6100.	-16.90	3.11	4.58	5.62	6.25	6.79	6.87	.00
178	N-(C)/2-(H)	15400.	8.94	4.20	5.21	6.13	6.83	7.90	8.65	9.55
182	N-(C)/2-(N)	29200.	-13.80	-	-	-	-	-	-	-
442	N-(C)/2-(P)	32200.	-	-	-	-	-	-	-	-
443	N-(C)/2-(PO)	17800.	-	-	-	-	-	-	-	-
327	N-(C)/2-(S)	29900.	-	3.82	5.17	6.21	6.94	7.39	9.24	.00
329	N-(C)/2-(SO)	16000.	-	4.20	5.88	6.12	6.53	6.83	8.34	.00
331	N-(C)/2-(SO/2)	-20400.	-	-	-	-	-	-	-	-
387	N-(C)/2-(Ti)	39100.	-	-	-	-	-	-	-	-
179	N-(C)/3	24400.	-13.46	3.48	4.56	5.43	5.97	6.56	6.67	6.50
201	N-(C/B)-(CO)-(H)	400.	-2.90	.57	1.51	2.38	3.33	4.04	4.35	.00
204	N-(C/B)-(CO)/2	-500.	-16.70	.98	3.06	4.23	4.85	5.28	5.29	.00
183	N-(C/B)-(H)-(N)	22100.	8.10	3.28	4.05	4.75	5.31	6.28	6.91	.00
189	N-(C/B)-(H)/2	4800.	29.71	5.72	6.51	7.32	8.07	9.41	10.47	12.28
192	N-(C/B)/2-(H)	16300.	4.30	-	-	-	-	-	-	
198	N-(CO)-(H)/2	-14900.	24.69	4.07	5.74	7.13	8.29	9.96	11.22	.00
202	N-(CO)/2-(H)	-18500.	7.60	-	-	-	-	-	-	
325	N-(CS)-(H)/2	12780.	29.19	6.07	7.28	8.18	8.91	10.09	10.98	.00
180	N-(H)/2-(N)	11400.	29.13	-	-	-	-	-		
188	N/A-(C)	34300.	8.50	2.70	4.10	4.92	5.34	5.69	5.71	.00
187	N/A-(H)	25100.	26.80	-	-	-	-	-		
195	N/A-(N)	23000.	8.50	-	-	-				

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
185	N/I-(C)	21300.	5.90	-	-	-	-	-	-	
186	N/I-(C/B)	16700.	30.80	1.19	3.20	4.55	5.39	6.17	6.28	.00
184	N/I-(H)	16300.	12.30	-	-	-	-	-	-	
472	O-(B)-(C)	-69430.	-	-	-	-	-	-	-	
471	O-(B)-(H)	-115500.	-	.00	.00	.00	.00	.00	.00	.00
100	O-(C)-(C/B)	-23000.	11.90	.62	.72	1.18	1.78	2.84	3.58	.00
98	O-(C)-(C/D)	-30500.	9.70	-	-	-	-	-	-	-
92	O-(C)-(CO)	-43100.	8.39	2.78	3.79	4.38	4.73	4.91	5.03	.00
380	O-(C)-(Cr)	-23500.	-	-	-	-	-	-	-	-
103	O-(C)-(H)	-37880.	29.07	-	-	-	-	-	-	-
218	O-(C)-(NO)	-5900.	41.90	-	-	-	-	-	-	-
219	O-(C)-(NO/2)	-19400.	48.50	9.54	11.54	13.26	15.60	16.39	17.38	.00
94	O-(C)-(O)	-4500.	9.40	3.70	3.70	3.70	3.70	4.20	4.20	4.80
436	O-(C)-(P)	-23500.	-	-	-	-	-	-	-	-
441	O-(C)-(P=N)	-40700.	-	-	-	-	-	-	-	-
438	O-(C)-(PO)	-40700.	-	.00	.00	.00	.00	.00	.00	.00
385	O-(C)-(Ti)	-23500.	-	-	-	-	-	-	-	-
389	O-(C)-(V)	-23500.	-	.00	.00	.00	.00	.00	.00	.00
102	O-(C)/2	-23200.	8.68	-	-	-	-	-	-	-
88	O-(C/B)-(CO)	-36700.	10.20	2.06	2.70	3.11	3.42	3.88	4.18	.00
101	O-(C/B)-(H)	-37900.	29.10	4.30	4.50	4.80	5.20	6.00	6.60	.00
99	O-(C/B)/2	-21100.	7.95	1.09	1.22	1.50	1.99	2.85	3.51	.00
91	O-(C/D)-(CO)	-45200.	3.80	-	-	-	-	-	-	-
127	O-(C/D)-(H)	-37900.	34.93	-	-	-	-	-	-	-
97	O-(C/D)/2	-33000.	10.10	2.70	3.19	3.53	3.86	4.40	4.73	.00
128	O-(C/T)-(H)	-37900.	34.93	-	-	-	-	-	-	
93	O-(CO)-(H)	-58100.	24.52	3.81	4.98	5.80	6.34	7.17	7.75	8.42
90	O-(CO)-(O)	-19000.	8.20	-	-	-	-	-	-	-
89	O-(CO)/2	-46500.	8.55	3.19	4.01	4.27	4.58	5.15	5.41	.00
96	O-(H)-(O)	-16270.	27.85	-	-	-	-	-	-	
437	O-(H)-(P)	-58700.	-	-	-	-	-	-		
439	O-(H)-(PO)	-65000.	-	.00	.00	.00	.00	.00	.00	.00

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
95	O-(O)/2	19000.	9.40	3.70	3.70	3.70	3.70	4.20	4.20	4.80
440	O-(PO)/2	-54500.	-	-	-	-	-	-	-	
422	P-(C)-(Cl)/2	-50300.	-	-	-	-	-	-	-	
421	P-(C)/3	7000.	-	-	-	-	-	-	-	
423	P-(C/B)/3	28300.	-	-	-	-	-	-	-	
425	P-(N)/3	-66800.	-	.00	.00	.00	.00	.00	.00	.00
424	P-(O)/3	-66800.	-	.00	.00	.00	.00	.00	.00	.00
444	P=N-(C)-(C)/3	500.	-	.00	.00	.00	.00	.00	.00	.00
445	P=N-(C)-(C/B)/3	-25700.	-	.00	.00	.00	.00	.00	.00	.00
446	P=N-(C)/2-(P=N)-(P=N)	-15500.	-	.00	.00	.00	.00	.00	.00	.00
447	P=N-(C/B)/2-(N=P)-(P=N)	-22900.	-	-	-	-	-	-	-	-
448	P=N-(Cl)/2-(N=P)-(P=N)	-58200.	-	-	-	-	-	-	-	-
449	P=N-(N=P)-(O)/2-(P=N)	-43400.	-	.00	.00	.00	.00	.00	.00	.00
428	PO-(C)-(Cl)-(F)	-	50.80	-	-	-	-	-	-	
430	PO-(C)-(Cl)-(O)	-112600.	-	.00	.00	.00	.00	.00	.00	.00
429	PO-(C)-(Cl)/2	-123000.	52.97	-	-	-	-	-	-	
427	PO-(C)-(F)/2	-	46.77	.00	.00	.00	.00	.00	.00	.00
431	PO-(C)-(O)/2	-99500.	-	.00	.00	.00	.00	.00	.00	.00
426	PO-(C)/3	-72800.	-	.00	.00	.00	.00	.00	.00	.00
434	PO-(C/B)/3	-52900.	-	-	-	-	-	-	-	-
433	PO-(F)-(O)/2	-167700.	-	-	-	-	-	-	-	
435	PO-(N)/3	-104600.	-	-	-	-	-	-	-	
432	PO-(O)/3	-104600.	-	-	-	-	-	-	-	
379	Pb-(C)/4	72900.	-	-	-	-	-	-	-	
478	Pb-(C/B)/4	81600.	-	-	-	-	-	-	-	
225	Ring, azetidine	26200.	29.30	.00	.00	.00	.00	.00	.00	.00
169	Ring, benzene-(1,2,4,5)-tetracarboxylic anhydrid	21100.	54.00	.00	.00	.00	.00	.00	.00	.00
152	Ring, benzodioxole (4,5)	10300.	22.00	.00	.00	.00	.00	.00	.00	.00
153	Ring, benzodioxane (1,4)	2000.	15.80	-	-	-	-	-	-	
74	Ring, biphenylene	58800.	-	.00	.00	.00	.00	.00	.00	.00
67	Ring, butane, (1,1,0)-bicyclo	67000.	69.20	-	-	-	-	-	-	
157	Ring, cyclobutanone	22600.	27.90	.00	.00	.00	.00	.00	.00	.00

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
43	Ring, cyclobutane	26200.	29.80	-4.61	-3.89	-3.14	-2.64	-1.88	-1.38	.67
44	Ring, cyclobutene	29800.	29.00	-2.53	-2.19	-1.89	-1.68	-1.48	-1.33	1.23
161	Ring, cyclodecanone	3600.	11.90	.00	.00	.00	.00	.00	.00	.00
64	Ring, cyclodecane	12600.	-	-	-	-	-	-	-	
65	Ring, cyclododecane	4400.	-	-	-	-	-	-		
163	Ring, cyclododecanone	3000.	6.70	-	-	-	-	-	-	
53	Ring, cycloheptene	5400.	15.10	-	-	-	-	-	-	
50	Ring, cyclohexa-(1,3)-diene	4800.	24.00	-	-	-	-	-	-	
162	Ring, cyclohendecane	4400.	9.50	-	-	-	-	-	-	
158	Ring, cycloheptanone	2300.	17.20	-	-	-	-	-	-	
52	Ring, cycloheptane	6400.	15.90	-	-	-	-	-	-	
165	Ring, cycloheptadecanone	1100.	-2.40	-	-	-	-	-	-	
55	Ring, cyclohepta-(1,3,5)-triene	4700.	23.70	-	-	-	-	-	-	
54	Ring, cyclohepta-(1,3)-diene	6600.	19.40	-	-	-	-	-	-	
51	Ring, cyclohexa-(1,4)-diene	500.	25.40	.00	.00	.00	.00	.00	.00	.00
48	Ring, cyclohexane	-360.	18.80	-	-	-	-	-	-	
147	Ring, cyclohexanone	2200.	15.90	-	-	-	-	-	-	
49	Ring, cyclohexene	1400.	21.50	-	-	-	-	-	-	
160	Ring, cyclononanone	4700.	13.90	.00	.00	.00	.00	.00	.00	.00
63	Ring, cyclononene (trans)	12800.	11.20	-	-	-	-	-	-	
61	Ring, cyclononane	12800.	12.20	-	-	-	-	-	-	
62	Ring, cyclononene (cis)	9900.	11.20	-	-	-	-	-	-	
59	Ring, cycloocta-(1,3,5)-triene	8900.	21.10	.00	.00	.00	.00	.00	.00	.00
56	Ring, cyclooctane	9900.	16.50	-	-	-	-	-	-	
57	Ring, cyclooctene (cis)	6000.	15.00	-	-	-	-	-	-	
60	Ring, cyclooctatetraene	17100.	27.60	-	-	-	-	-	-	
58	Ring, cyclooctene (trans)	15300.	15.00	.00	.00	.00	.00	.00	.00	.00
159	Ring, cyclooctanone	1500.	15.40	-	-	-	-	-	-	
47	Ring, cyclopentadiene	6000.	28.00	-3.45	-2.83	-2.14	-1.65	-1.28	-1.04	.00
164	Ring, cyclopentadecanone	2100.	1.90	-	-	-	-	-	-	
46	Ring, cyclopentene	5900.	25.80	-5.98	-5.35	-4.89	-4.14	-2.93	-2.26	1.08
40	Ring, cyclopropane	27600.	32.10	-	-	-	-	-		

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
146	Ring, cyclopentanone	5200.	24.60	-	-	-	-	-	-	
45	Ring, cyclopentane	6300.	27.30	-	-	-	-	-	-	
42	Ring, cyclopropene	53700.	33.60	-	-	-	-	-	-	
154	Ring, dibenzofuran	6500.	28.00	.00	.00	.00	.00	.00	.00	.00
151	Ring, dihydrofuran	4700.	22.00	.00	.00	.00	.00	.00	.00	.00
145	Ring, dihydropyran	1200.	20.20	-	-	-	-	-	-	-
142	Ring, dioxane (1,4)	3300.	15.80	-	-	-	-	-	-	-
141	Ring, dioxane (1,3)	200.	15.80	-	-	-	-	-	-	-
156	Ring, dioxolane	6000.	22.00	-	-	-	-	-	-	-
137	Ring, ethylene oxide	26800.	30.50	-	-	-	-	-	-	-
224	Ring, ethyleneimine	27700.	31.60	.00	.00	.00	.00	.00	.00	.00
346	Ring, ethylene sulfide	17700.	29.47	-2.85	-2.59	-2.66	-3.02	-4.32	-5.82	.00
144	Ring, furan	-5800.	28.40	.00	.00	.00	.00	.00	.00	.00
149	Ring, glutaric anhydride	800.	20.10	-	-	-	-	-	-	
73	Ring, heptadiene, bicyclo	29700.	-	.00	.00	.00	.00	.00	.00	.00
70	Ring, heptane, (4,1,0)-bicyclo	28900.	55.50	.00	.00	.00	.00	.00	.00	.00
69	Ring, hexane, (3,1,0)-bicyclo	32700.	60.90	-	-	-	-	-	-	-
150	Ring, maleic anhydride	3600.	27.40	.00	.00	.00	.00	.00	.00	.00
171	Ring, malonic anhydride	22000.	27.90	.00	.00	.00	.00	.00	.00	.00
41	Ring, methylene cyclopropane	40900.	-	-	-	-	-	-	-	
72	Ring, nonane, (6,1,0)-bicyclo	31100.	49.20	.00	.00	.00	.00	.00	.00	.00
166	Ring, octan-2-one, cis-(3,3,0)-bicyclo	5400.	54.00	.00	.00	.00	.00	.00	.00	.00
167	Ring, octan-2-one, trans-3,3,0)-bicyclo	11000.	54.00	.00	.00	.00	.00	.00	.00	.00
71	Ring, octane, (5,1,0)-bicyclo	29600.	50.60	.00	.00	.00	.00	.00	.00	.00
228	Ring, octane, (1,4)-diaza, (2,2,2)-bicyclo	3400.	-	-	-	-	-	-	-	
68	Ring, pentane, (2,1,0)-bicyclo	55300.	64.70	.00	.00	.00	.00	.00	.00	.00
168	Ring, phthalic anhydride	10300.	27.40	-	-	-	-	-	-	
227	Ring, piperidine	1000.	23.80	.00	.00	.00	.00	.00	.00	.00
170	Ring, propiolactone (beta)	23900.	27.90	.00	.00	.00	.00	.00	.00	.00
138	Ring, propylene oxide	25200.	27.70	-	-	-	-	-	-	
226	Ring, pyrrolidine	6800.	26.70	-6.17	-5.58	-4.80	-4.00	-2.87	2.17	.00
66	Ring, spiropentane	63500.	67.60	-	-	-	-	-	-	

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f^o 298K (cal mol^{-1})	S^o 298K (cal K^{-1} mol^{-1})	C_p^o (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
229	Ring, succinimide	8500.	-	-	-	-	-	-	-	
148	Ring, succinic anhydride	4500.	30.20	-	-	-	-	-	-	
140	Ring, tetrahydropyran	500.	18.80	-	-	-	-	-	-	
139	Ring, tetrahydrofuran	5900.	24.20	-	-	-	-	-	-	-
349	Ring, thiane (thiacyclohexane)	-620.	17.46	-	-	-	-	-	-	-
350	Ring, thiepane (thiacycloheptane)	3890.	17.30	.00	.00	.00	.00	.00	.00	.00
347	Ring, thietane	19370.	27.18	-	-	-	-	-	-	-
351	Ring, thiol-3-ene	5070.	25.40	-	-	-	-	-	-	-
352	Ring, thiol-2-ene	5070.	25.40	.00	.00	.00	.00	.00	.00	.00
348	Ring, thiolane	1730.	23.56	-	-	-	-	-	-	-
354	Ring, thiophene	1730.	23.56	-	-	-	-	-	-	-
353	Ring, thiophene, (1,2)-dihydro, (1,1)-dioxide	5740.	20.50	-	-	-	-	-	-	-
143	Ring, trioxane (1,3,5)	6600.	12.80	-	-	-	-	-	-	-
155	Ring, xanthene	2300.	22.00	.00	.00	.00	.00	.00	.00	.00
475	S-(B)-(C)	-14500.	-	.00	.00	.00	.00	.00	.00	.00
476	S-(B)-(C/B)	-7800.	-	.00	.00	.00	.00	.00	.00	.00
293	S-(C)-(C/B)	19160.	-7.80	-	-	-	-	-	-	-
291	S-(C)-(C/D)	9410.	13.20	4.22	5.08	5.56	5.77	5.87	5.87	.00
288	S-(C)-(H)	4620.	32.73	-	-	-	-	-	-	-
295	S-(C)-(S)	7050.	12.37	5.23	5.42	5.51	5.51	5.38	5.12	.00
290	S-(C)/2	11340.	13.15	4.99	4.96	5.02	5.07	5.41	5.73	.00
289	S-(C/B)-(H)	11960.	12.66	-	-	-	-	-	-	
296	S-(C/B)-(S)	14500.	-8.00	2.89	3.39	3.72	4.15	4.78	5.10	.00
294	S-(C/B)/2	25900.	-27.00	2.00	2.01	2.24	2.74	3.80	4.71	.00
292	S-(C/D)/2	9860.	16.48	4.79	5.58	5.53	6.29	7.94	9.73	.00
322	S-(CO)-(H)	-1410	31.20	-	-	-	-	-	-	
326	S-(N)-(S)	-4900.	-	.00	.00	.00	.00	.00	.00	.00
297	S-(S)/2	3010.	13.40	4.70	5.00	5.10	5.20	5.30	5.40	.00
333	SO-(C)-(C/B)	-	-3.00	-	-	-	-	-		
303	SO-(C)/2	-14410.	18.10	-	-					
304	SO-(C/B)/2	-12000.	-23.70	-	-	-				
328	SO-(N)/2	-31560.	-		-	-				

TABLE 2 (continued)

Sequence Number	Group Name	ΔH_f° 298K (cal mol^{-1})	S° 298K (cal K^{-1} mol^{-1})	C_p° (cal K^{-1} mol^{-1}) 300K	400K	500K	600K	800K	1000K	1500K
317	SO/2-(C)-(C/B)	72290.	1.40	-	-					
320	SO/2-(C)-(C/D)	-71670.	18.10	.00	.00	.00	.00	.00	.00	.00
316	SO/2-(C)/2	-69740.	20.90	-	-	-				
314	SO/2-(C/B)-(C/D)	-68600.	-6.30	9.89	11.50	13.35	14.61	15.72	15.92	.00
319	SO/2-(C/B)-(SO/2)	-76250.	-3.20	9.81	11.50	13.52	14.73	15.71	16.03	.00
318	SO/2-(C/B)/2	-68580.	17.30	8.36	11.03	13.55	14.94	15.86	15.96	.00
315	SO/2-(C/D)/2	-73600.	13.50	-	-	-	-			
330	SO/2-(N)/2	-31560.	-	-		-				
338	SO/3-(C)/2 sulfite	-94800.	30.30	-	-	-				
335	SO/4-(C)/2	-143900.	33.10	-	-	-	-			
481	Si-(C)-(H)/3	-2000.	30.85	-	-	-				
480	Si-(C)/4	-28200.	44.08	-	-	-				
482	Si-(C/B)/4	-145300.	-	-	-	-	-			
366	Sn-(Br)-(C)/3	-1800.	-	.00	.00	.00	.00	.00	.00	.00
365	Sn-(C)-(Cl)/3	-89500.	-	-	-	-	-	-	-	
364	Sn-(C)/2-(Cl)/2	-49200.	-	-	-	-	-	-	-	
375	Sn-(C)/3-(C/B)	34930.	-	.00	.00	.00	.00	.00	.00	.00
373	Sn-(C)/3-(C/D)	37600.	-	-	-	-	-	-	-	
363	Sn-(C)/3-(Cl)	-9800.	-	-	-	-	-	-	-	-
368	Sn-(C)/3-(H)	34800.	-	-	-	-	-	-	-	
367	Sn-(C)/3-(I)	9900.	-	-	-	-	-	-		
376	Sn-(C)/3-(Sn)	26400.	-	-	-	-	-	-	-	
362	Sn-(C)/4	36200.	-	.00	.00	.00	.00	.00	.00	.00
374	Sn-(C/B)/4	26260.	-	-	-	-	-	-		
372	Sn-(C/D)-(Cl)/3	-82200.	-	.00	.00	.00	.00	.00	.00	.00
371	Sn-(C/D)/2-(Cl)/2	-50700.	-	.00	.00	.00	.00	.00	.00	.00
370	Sn-(C/D)/3-(Cl)	-8200.	-	.00	.00	.00	.00	.00	.00	.00
369	Sn-(C/D)/4	36200.	-	.00	.00	.00	.00	.00	.00	
388	Ti-(N)/4	-123000.	-	-	-	-	-			
386	Ti-(O)/4	-157000.	-	-	-	-	-			
390	V-(O)/4	-87000.	-	.00	.00	.00	.00	.00	.00	
384	Zn-(C)/2	33300.	-	-	-	-	-			

APPENDIX 1

GROUP ADDITIVITY PROGRAMME
Version 2.2

P.J.Sanders and R.K.Solly.
Materials Research Laboratories, Maribyrnong
Victoria, AUSTRALIA
P.O. Box 50, Ascot Vale, 3032

Extracts group thermodynamic data from a data base and compiles
corresponding data for gas phase compounds by the method of Benson et. al.
Reference:- Chem. Rev.; Vol. 69 Part 3, pp 279-324. June 1969.

If you wish output data to be appended to a disk
file, type in the name of the that file.
A blank name causes this operation to be bypassed.
-- ? **mydata.txt**

The output data can be incorporated into a command file
for input to the CSIRO/NPL "THERMODATA" program "FILER".
To use this option, type in a name for a "FILER" command file.

A blank name causes this operation to be bypassed.
-- ? **myfiler.fil**

"FILER" requires a unique formula and name for the data base
as part of its input.

What is the formula to be for this compound? (EG. C8H9 (G))
A blank field stops the program.
-- ? **c5h12 (g)**

What is the name of the compound. (48 CHARS max.)

##

-- ? **2-methylbutane (g)**

Overall Symmetry Number for the molecule.
-- ? **27**

Number of Optical Isomers for the molecule.
-- ? **1**

Input the group sequence number followed on the same line by
a comma then how many of that group type are required

```
At any time the user may scroll (B)ackwards or (F)orwards
through the data and (D)elete or overtype lines as desired.
A blank field terminates input, after which
a further option to correct errors is presented.

 The required input format is:-
 ? <group sequence number>,<how many required>

  1 -------------- ? 6,1
  2 -------------- ? 5,1
  3 -------------- ? 1,3
  4 -------------- ? 485,1
  5 -------------- ?

Are you (S)atisfied with the above or do you wish to
perform some corrections? -- answer S or a line number
 -- ? s

2-methylbutane (g)                                  Formula = C5H12 (G)
 Symmetry =  27.0, Isomers =  1.0,   Entropy Contribution =   -6.55
        dHf (298K) dS (298K) Cp300  Cp400  Cp500  Cp600  Cp800  Cp1000 Cp1500
          cal/mol  cal/mol/K ---------------------------cal/mol/K------------
 3. Required of Seq.   1   C-(C)-(H)/3
         -10080.0    30.41    6.19   7.84   9.40  10.79  13.02  14.77  17.58
 1. Required of Seq.   5   C-(C)/2-(H)/2
          -4950.0     9.42    5.50   6.95   8.25   9.35  11.07  12.34  14.25
 1. Required of Seq.   6   C-(C)/3-(H)
          -1900.0   -12.07    4.54   6.00   7.17   8.05   9.31  10.05  11.17
 1. Required of Seq. 485   Alkane Gauche Correction
            800.0      .00       -      -      -      -      -      -      -

Press <ENTER> to continue --

          ************************************************************

TOTALS  --  2-methylbutane (g)
          Hf (298K)  S (298K) Cp300  Cp400  Cp500  Cp600  Cp800  Cp1000 Cp1500
           cal/mol  cal/mol/K ---------------------------cal/mol/K
           -36290.0    82.03  28.61  36.47  43.62  49.77  59.44  66.70  78.16
                               *      *      *      *      *      *      *
          dhf (289K) S (298K) Cp300  Cp400  Cp500  Cp600  Cp800  Cp1000 Cp1500
            J/mol    J/mol/K ------------------- ------J/mol/K--------------
           -151837.4 343.22  119.70 152.59 182.51 208.24 248.70 279.07 327.02

List file = mydata.txt
"FILER" batch file = myfiler.fil

 What do you wish do do next with this data?

 (A)ppend the totals to the current output files, go back and
 (R)e-enter all data; just (E)dit sequence numbers or
 (D)iscard this molecule. Answer  A, R, E, or  D  -- a

Creating a new "FILER" command file. "FILER" requires an access
code (usually the surname of a user) and the name of a "THERMODATA"
data base. What will your access code be? -- myname
```

What is the name of the "THERMODATA" data base
---) **cpdben**

Group Additivity data has been appended to files

Continue using the same output filenames or quit? (Y/N/Q) -- **q**
Stop - Program terminated.

APPENDIX 2

GROUP ADDITIVITY PROGRAMME
Version 2.2

P.J. Sanders and R.K. Solly
Materials Research Laboratories, Maribyrnong
Victoria, AUSTRALIA
P.O. Box 50, Ascot Vale, 3032

Extracts group thermodynamic data from a data base and compiles corresponding data for gas phase compounds by the method of Benson et. al. Reference:- Chem. Rev.; Vol. 69 Part 3, pp 279-324. June 1969.

If you wish output data to be appended to a disk
file, type in the name of the that file.
A blank name causes this operation be bypassed.
-- ? **mydata.txt**

The output data can be incorporated into a command file
for input to the CSIRO/NPL "THERMODATA" program "FILER".
To use this option, type in a name for a "FILER" command file.

A blank name causes thi operation be bypassed.
-- ? **myfiler.inp**

"FILER" requires a unique formula and name for the data base
as part of its input.

What is the formula to be for this compound? (EG. C8H9 (G))
A blank field stops the program
-- ? **c11h22 (g)**

What is the name of the compound. (48 CHARS max.)

****

-- ? **(n-hexylcyclopentane)**

Overall Symmetry Number for the molecule.
-- ? **3**

Number of Optical Isomers for the molecule.
-- ? **1**

Input the group sequence number followed on the same line by a comma then how many of that group type are required.

At any time the user amy scroll (B)ackwards or (F)orwards
through the data and (D)elete or overtype lines as desired.
A blank field terminates input, after which
a further option to correct errors is presented.

```
The required input format is:-
 - ? <group sequence number>,<how many required>

  1 --------------- ? 5,9
  2 --------------- ? 6,1
  3 --------------- ? 1,1
  4 --------------- ? 45,1
  5 --------------- ?

Are you (S)atisfied with the above or do you wish to
perform some corrections? -- answer S or a line number
 -- ? s

n-hexylcyclopentane                                  Formula = C11H22 (G)
 Symmetry =    3., Isomers =    1.,  Entropy Contribution =   -2.18
        dHf(298K)  S(298K)  Cp300  Cp400  Cp500  Cp600  Cp800  Cp1000  Cp1500
         cal/mol  cal/mol/K _____________________________cal/mol/K_____________
 1. Required of Seq.  1   C-(C)-(H)/3
         -10080.0   30.41    6.19   7.84   9.40  10.79  13.02  14.77  17.58
 9. Required of Seq.  5   C-(C)/2-(H)/2
          -4950.0    9.42    5.50   6.95   8.25   9.35  11.07  12.34  14.25
 1. Required of Seq.  6   C-(C)/3-(H)
          -1900.0  -12.07    4.54   6.00   7.17   8.05   9.31  10.05  11.17
 1. Required of Seq. 45   Cyclopentane Ring
           6300.0   27.30   -6.50  -5.50  -4.50  -3.80  -2.80  -1.93   -.37

Press <ENTER> to continue --

*******************************************************************************

TOTALS  --  n-hexylcyclopentane
        dHf(298K)   S(298K)  Cp300  Cp400  Cp500  Cp600  Cp800  Cp1000  Cp1500
         cal/mol   cal/mol/K _____________________________cal/mol/K_____________
          -50230.0   128.24  53.73  70.89  86.32  99.19  119.16  133.95 156.63

        dHf(298K)   S(298K)  Cp300  Cp400  Cp500  Cp600  Cp800  Cp1000  Cp1500
          J/mol     J/mol/K _____________________________J/mol/K_____________
         -210162.3   536.54  224.81 296.60 361.16 415.01 498.57  560.45 655.34

List file = mydata.txt
"FILER" batch file = myfiler.inp

 What do you wish to do next with this data?

 (A)ppend the totals to the current output files, go back and
 (R)e-enter all data;  just (E)dit sequence numbers or
 (D)iscard this molecule. Answer A, R, E, or D -- a

Creating a new "FILER" command file.  "FILER" requires an access
code (usually the surname of a user) and the name of a "THERMODATA"
data base. What will your access code be? -- myname

What is the name of the "THERMODATA" data base
 --- ? cpdben
```

Group Additivity data has been appended to files

Continue using the same output filenames or quit? (Y/N/Q) -- **q**
Stop - Program terminated.

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Thermodynamic values from computer summation of group additivity data

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KEYWORDS

Entropy	Database	Computer
Heat capacity	Summation	Group values
Enthalpy	Estimation	

COSATI GROUPS 600 0099F

ABSTRACT

The second order approximation for the estimation of standard enthalpy of formation, entropy of formation and heat capacity of molecules by summation of atomic contributions with nearest neighbour interactions has been incorporated into a Fortran 77 computer programme which currently executes on the IBM PC/XT and VAX 11/780 computers. The data base for the programme also includes group corrections for next-to-nearest neighbor interactions and corrections for ring compounds. The programme prompts for the required input, including the symmetry and optical isomers of the molecule, in an interactive manner and allows re-entry and correction of the data after input from a computer terminal.


DA
FILM
2