

MULTIWELL THERMODYNAMICS DATABASE

J. R. Barker, T. L. Nguyen, J. F. Stanton, C. Aieta, M. Ceotto, F. Gabas, T. J. D. Kumar, C. G. L. Li, L. L. Lohr, A. Maranzana, N. F. Ortiz, J. M. Preses, J. M. Simmie¹, J. A. Sonk, and P. J. Stimac

MultiWell-2017 Software Suite
University of Michigan, Ann Arbor
Michigan, 48109-2143, USA

<http://clasp-research.engin.umich.edu/multiwell/>

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A database of species properties such as zero-point corrected electronic energies, vibrational frequencies, rotational constants, etc which are necessary in the calculation of the thermochemistry of chemical compounds and the kinetics of chemical reactions. Although the input datafiles listed below are formatted specifically towards the **Multiwell** suite of applications this data is just as useful for other purposes.

Units and Standard State

Units

In this document the enthalpy of formation at 0 K, $\Delta_f H(0)$ or $dH_f(0)$, and at 298.15 K, $\Delta_f H(298)$, and the enthalpy function $H(T)-H(0)$, are in kJ/mol whilst entropy and specific heat are in J/K/mol. The units of molecular properties are various but are specified in each datafile.

Standard state

1 bar = 100,000 Pa or 100 kPa ideal gas.

¹ JMS thanks the Irish Centre for High-End Computing, ICHEC, for the provision of computational resources, **ngche041c**.

Contents

Units and Standard State	1
Datafile structure	6
Examples	6
Thermochemistry of buta-1,3-diene	6
Reaction of γ -valerolactone	8
Frequent Data References	10
Formation enthalpy, $\Delta_f H(T)$	11
An example:	11
THERMO.DAT input files	13
Acetone oxide, propanone oxide, Criegee intermediate $(\text{CH}_3)_2\text{C}=\text{O}-\text{O}$	13
Acetonitrile, methyl cyanide CH_3CN	14
Acetylene/ethyne HCCH	14
Adamantane $\text{C}_{10}\text{H}_{16}$	14
Amidogen NH_2	15
Ammonia NH_3	15
Argon	15
Benzene C_6H_6	16
Bromine atom (^2P)	16
Buta-1,3-diene, <i>trans</i> butadiene, $\text{CH}_2=\text{CH}-\text{CH}=\text{CH}_2$	16
t-Butyl radical $(\text{CH}_3)_3\text{C}\cdot$	17
C-60 buckminsterfullerene	18
C-70 fullerene	18
Carbon atom	21
Carbon disulfide CS_2	21
Carbon monoxide $^{12}\text{C}^{16}\text{O}$	21
Carbon monoxide $^{12}\text{C}^{17}\text{O}$	21
Carbon monoxide $^{12}\text{C}^{18}\text{O}$	21
Carbon monoxide $^{13}\text{C}^{16}\text{O}$	22
Carbon dioxide	22
Carbon suboxide or tricarbon dioxide, $\text{O}=\text{C}=\text{C}=\text{O}$	22
Chlorine atom ($^2\text{P}_{3/2}$)	22
Chloroxyl radical $(\text{ClO})\cdot$	23
Chlorine dioxide, or chloryl radical $(\text{O}-\text{Cl}-\text{O})\cdot$	23
Chlorine $^{35}\text{Cl}_2$, $^{37}\text{Cl}_2$, $^{35}\text{Cl}^{37}\text{Cl}$	23
Chlorosyl chloride $\text{Cl}-\text{Cl}=\text{O}$	24
Chlorine peroxide $\text{Cl}-\text{O}-\text{O}-\text{Cl}$	24
Chlorine chlorite $\text{Cl}-\text{O}-\text{Cl}-\text{O}$	25
Chloryl chloride $\text{Cl}-\text{Cl}(\text{O})_2$	26
Chlorine chlorate $\text{Cl}-\text{O}-\text{ClO}_2$ or Cl_2O_3	26
Cyclopropane $(\text{CH}_2)_3$	27
Cubane, tetraprismane C_8H_8	27
Cyanoimidogen, $^3\text{N}-\text{C}\equiv\text{N}$ ($\text{D}_{\infty\text{h}}$)	28
Deuterium atom ($^2\text{S}_{1/2}$)	28
Deuteroxyl radical OD	28

Diacetylene or 1,3-butadiyne HCCCCH.....	28
Diazene or diimide, HN=NH, trans or (E) conformer.....	29
Dideuterium D ₂	29
Ditritium T ₂	29
Diethyl ether, CH ₃ CH ₂ OCH ₂ CH ₃	29
Dinitrogen N ₂	30
Dinitrogen ¹⁴ N ₂	31
Dinitrogen ¹⁵ N ₂	31
Dinitrogen pentoxide O ₂ N-O-NO ₂ or N ₂ O ₅	31
Dihydrogen H ₂	32
Deuterium hydride HD.....	32
Diazenyl, H-N=N.....	32
1,2-Dioxete, dioxirene, cyclo(OOCHCH).....	32
Dioxirane, dioxacyclopropane, cyclo-H ₂ (COO).....	33
Dioxiranylmethyl, cyclo(OOCH)CH ₂ '.....	33
Dioxygen O ₂	34
Dioxygen O ₂ (¹ Δ _g).....	34
Dioxymethyl or methanal oxide CH ₂ =O ^{δ+} -O ^{δ-} 'Crige intermediate'.....	34
Disulfur, diatomic sulfur S=S.....	35
Ethanal oxide CH ₃ CH=O ^{δ+} -O ^{δ-} <i>anti</i> conformer 'C2 Crige intermediate'.....	35
Ethanal oxide CH ₃ CH=O ^{δ+} -O ^{δ-} <i>cis</i> conformer 'C2 Crige intermediate'.....	36
Ethane C ₂ H ₆	37
Ethanol, CH ₃ CH ₂ OH <i>trans</i>	38
Ethene/ethylene CH ₂ =CH ₂	38
Ethylene carbonate, 2-Oxo-1,3-dioxolane.....	39
Ethoxy ethene CH ₂ =CH-O-CH ₂ CH ₃ C=COC <i>cis</i> , COCC <i>trans</i>	39
Ethyl radical C ₂ H ₅	41
Ethylhydroperoxide CH ₃ CH ₂ OOH.....	42
Ethynediol, HO-C≡C-OH.....	43
Ethynol, acetylenol HCCOH.....	43
Ethynyloxy or ketenyl, O=C=C-H / O-C≡C-H.....	44
Fluorine atom ¹⁹ F (² P _{3/2}).....	44
Formaldehyde, methanal HCHO.....	44
Formic acid, HCOOH, syn H-O-C=O.....	45
Formyl, oxomethyl HC'O.....	45
Formylmethylene, oxo-ethylidene HC=CHO' or H'C-CH=O.....	46
Formyloxymethylene, HC:-O-CHO.....	47
Helium He.....	47
Glyoxal or 1,2-ethanedione, HCOCHO <i>trans</i> conformer.....	47
Glyoxal, HCOCHO <i>cis</i> conformer.....	48
Hydrazine, N ₂ H ₄	48
Hydrogen atom H (² S _{1/2}).....	49
Hydroperoxy water radical complex HO ₂ ·H ₂ O.....	49
Hydroperoxyl radical, hydroperoxo HO ₂	50
Hydrogen bromide.....	50
Hydrogen chloride HCl.....	50

Hydrogen iodide HI.....	51
Hydrogen sulfide H ₂ S.....	51
Hydroxyethenone or hydroxyketene, O=C=CH(OH).....	51
Hydroxyformyl radical HOC'=O cis.....	52
Hydroxyformyl radical HOC'=O trans.....	52
Hydroxyl radical OH.....	53
Hydroxymethyl, [*] CH ₂ OH.....	53
Hydroxymethylene, HCOH trans.....	53
Hydroxysulfonyl or "sulfo" H-O-S(O) ₂	54
Hydrogen peroxide HOOH.....	54
Iodine atom I (² P).....	54
Isoformyl, hydroxymethylidene C'OH.....	55
Isoprene, <i>trans</i> 2-methyl-1,3-butadiene, CH ₂ =CH-C(CH ₃)=CH ₂	55
Krypton Kr.....	56
Mercapto radical HS.....	56
Methane.....	56
Methanediol, CH ₂ (OH) ₂	56
Methanimine, methylenimine, CH ₂ =NH.....	57
Methanol CH ₃ OH.....	57
Methoxy ethene, methyl vinyl ether CH ₂ =CHOCH ₃	58
Methyl hydroperoxide, CH ₃ OOH.....	59
Methyl radical C'H ₃	59
Methylthio CH ₃ S.....	59
Methylsulfinyl radical CH ₃ -S=O.....	60
Methylsulfonyl radical CH ₃ -S-O-O <i>syn</i> OOSCH coplanar.....	60
Methyl vinyl ketone, CH ₃ C(O)CH=CH ₂	61
Neopentane (CH ₃) ₄ C.....	61
Nitric acid HONO ₂	62
Nitric oxide NO.....	62
Nitrogen dioxide O-N-O or NO ₂	62
Nitromethane CH ₃ NO ₂	63
Nitroxyl radical NO ₃	63
Oxalic acid (COOH) ₂	64
3-Oxetanyl.....	64
2-Oxiranone (OCH ₂ C)=O.....	65
2-Oxiranylidene.....	65
4-Oxo-1,3-dioxetan-2-yl.....	66
Oxygen atom O.....	66
Ozone O ₃	66
Phosphine PH ₃	67
Peroxynitrous acid HOONO <i>cis/cis</i>	67
Peroxynitrous acid HOONO <i>trans/perp</i>	67
Propene CH ₃ CH=CH ₂	68
n-Propyl radical C ₃ H ₇	68
iso-Propyl radical (CH ₃) ₂ C'H.....	69
Propane C ₃ H ₈	69

n-Propanal oxide <i>syn</i> , CH ₃ CH ₂ CHOO	70
Styrene or ethenylbenzene, C ₆ H ₅ -CH=CH ₂	70
Sulfur atom S.....	71
Sulfur atom ³² S	71
Sulfur atom ³³ S	72
Sulfur atom ³⁴ S	72
Sulfur atom ³⁶ S	72
Sulfur dioxide SO ₂	72
Sulfuric acid H ₂ SO ₄	73
Toluene C ₆ H ₅ CH ₃	74
Trioxidane or dihydrogen trioxide, <i>trans</i> HOOOH.....	75
Trioxidanyl or hydrotrioxy HO-O-O or HO ₃ <i>trans</i>	76
Trioxidanyl deuterated DO-O-O or DO ₃ <i>trans</i>	76
Tritium hydride HD.....	76
Water H ₂ O.....	76
Xenon atom.....	77
Formation enthalpies at 298.15 K.....	77

Datafile structure

For a complete description see the Multiwell manual; here we show data for the methyl radical. In this particular case sufficient information is available in the open literature to build a datafile. Normally this is not the case and then details of the computations used to construct the input file should be given such as level of theory, basis set, scale factors, relaxed potential energy scans, *etc.* See "Toluene" entry for both approaches.

The methyl radical datafile

```
none CH3 149.88 ! Species category2, Name, ΔfH(0)
CH3 ! Empirical Formula
! Frequencies from WebBook (11/2002) comment line
! Moments of inertia from JANAF (1998) comment line
! ΔfH(0) from ATcT v.1.112 (2013) comment line
6 1 2 ! external symmetry, optical isomers3, electronic states
0.0 2 ! electronic energy (cm-1), degeneracy of lowest electronic state
46205. 2 ! electronic energy (cm-1), degeneracy of higher electronic state
6 'HAR' 'GMCM' ! number of ro-vibs, freq. category4, units for rotors5
1 vib 3004.43 0. 1 ! CH str index, DOF type6, anharmonicity, degeneracy
2 vib 606.453 0. 1 ! OPLA ...
3 vib 3160.821 0. 2 ! CH-str ...
4 vib 1402. 0. 2 ! deform ...
5 qro 5.846e-40 1. 1 ! K-rotor index, DOF type, rot. parameter, rot. symm, dim
6 qro 2.923e-40 1. 2 ! 2-D rotor index, DOF type, rot. parameter, rot. symm, dim
```

Examples

The calculation of a reaction rate constant depends essentially on two quantities, (1) the difference in zero-point corrected electronic energies between the transition state, **TS**, and the reactant(s), **A** and **B**, more commonly known as the barrier height, E^\ddagger and (2) the ratio of partition functions, ($Q_{TS}/Q_A Q_B$).

Thus the $\Delta_f H(0\text{ K})$ quoted here are not that critical since validated formation enthalpies for transition states are rarely accessible. However they can be used to check that the computed reaction enthalpy at a particular level of theory matches the reaction enthalpy change:

$$\Delta H_R = | \Delta_f H(\text{products}) - \Delta_f H(\text{reactants}) |$$

The partition functions can be separated into individual contributions due to translational (T), rotational (R), vibrational (V) and electronic components. Of these the most critical are the vibrational terms which are very species dependent as opposed to translational or whole-molecule rotational partition functions. For small systems such as the aminoxyl radical, $\dot{\text{O}}\text{-NH}_2$, the contributions to the entropy S are $T > R >> V$ while for molecules containing many more atoms the vibrational contribution to the entropy, S_v , becomes increasingly important. Calculations based on this are known as rigid rotor harmonic oscillator (RRHO) treatment. In all cases low frequency vibrations contribute heavily to S_v and it is precisely here that hindered internal rotations are a better description of a 'vibrational' mode. Thus, classification and a proper theoretical treatment of these crucially important modes becomes imperative. Many sources typically use the RRHO approximation.

The lack of a comprehensive validated database for entropies and specific heats is seriously hindering progress given the scarcity of reliable experimental data. As the complexity of species increases high-accuracy theoretical methods are less applicable and more computationally affordable treatments have to be used.

Thermochemistry of buta-1,3-diene

The lowest energy conformer whose dihedral C=C-C angle is 180° or *trans* has just one vibrational mode at $\approx 170\text{ cm}^{-1}$ which is more correctly described as a hindered rotor. A potential energy scan reveals this variation, $V(\chi)$, as well as the change in the reduced moment of inertia or rotational constant $B(\chi)$. Fits via MULTIWELL/LAMM code

² **Reac**(tant), **prod**(uct), **none** (useful for checking individual species)

³ Strictly *chiral stereoisomers*

⁴ **HAR**(monic) or **OBS**(erved) \equiv **FUN**(damental); always cm^{-1}

⁵ Allowed categories: **AMUA**, **GMCM**, **MHZ**, **GHZ**

⁶ Allowed categories: **vib**, **rot**, **qro**, **top**, **hra**, **hrb**, **hrc**, **hrd**, **box**, **kro**

result in Fourier series expressions, see

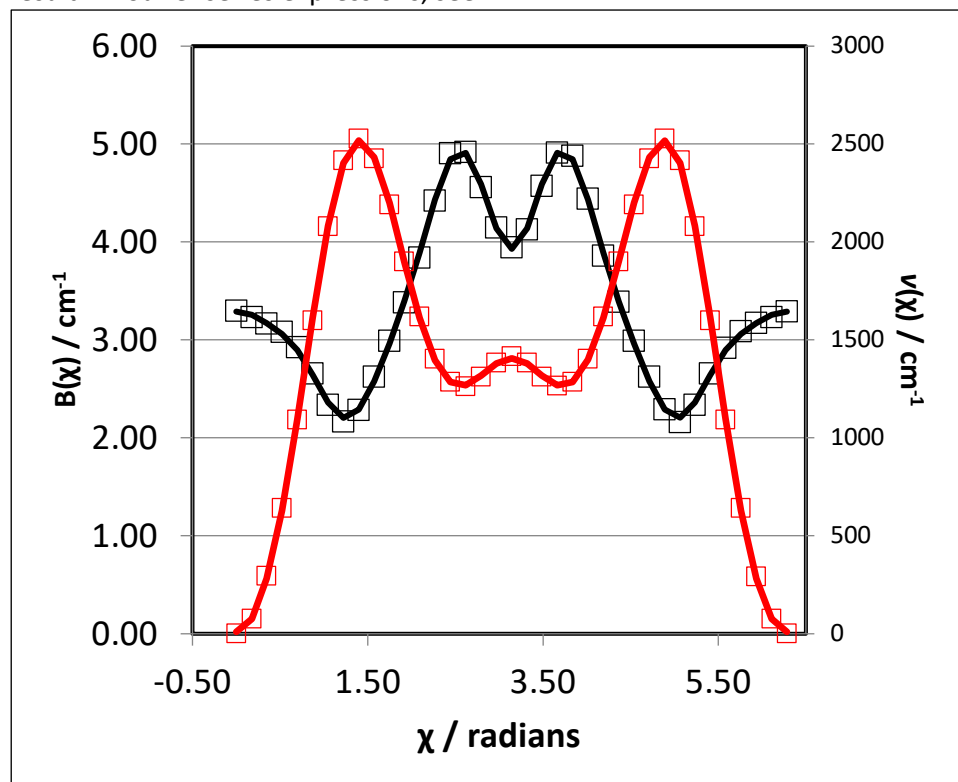


Figure 1.

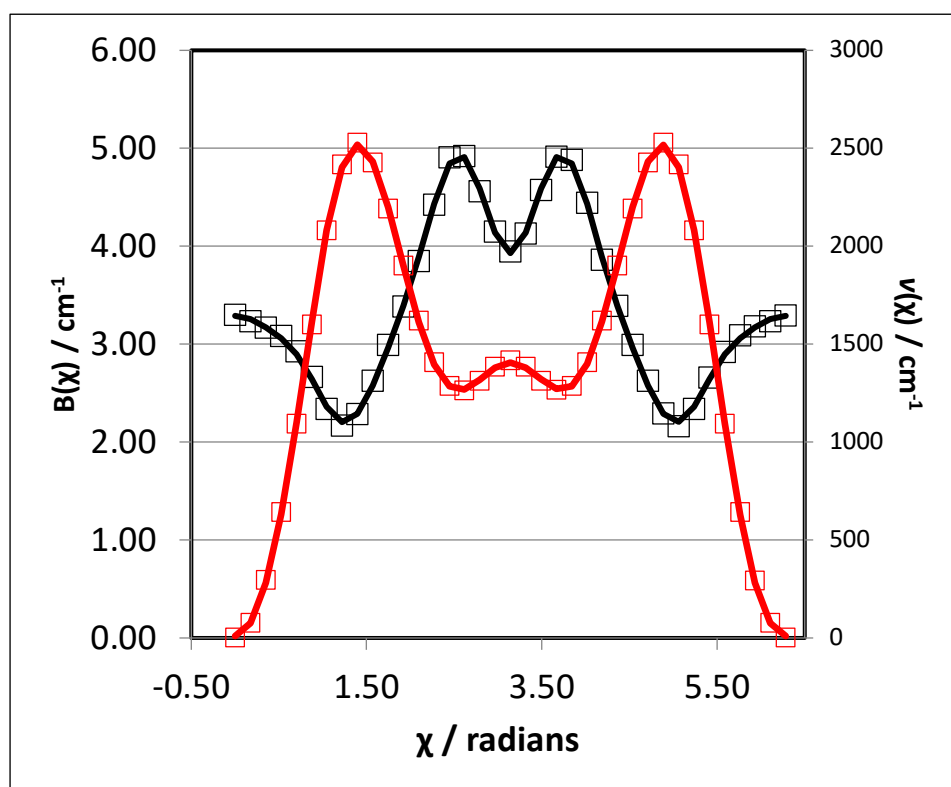


Figure 1: PE scan at B3LYP/cc-pVTZ+d

Wong and Raman [J Comp Chem 2006, 28, 759–766] have shown that the B3LYP functional overestimates the trans gauche barrier; their best results were obtained at CCSD(T)//MP2/cc-pVTZ. Experiment and CCSD(T)/cc-pV5Z theory indicate 11.8 and 12.1 kJ/mol, respectively [Engeln, R.; Consalvo, D.; Reuss, J. Chem Phys 1992, 160, 427; Karpfen, A.; Parasuk, V. Mol Phys 2004, 102, 819] These are computationally expensive methods; tests show that although the barriers for trans to gauche and gauche to gauche' do vary as well as the energy difference between trans and gauche, Table 1, the net effect is quite small, Table 2.

Table 1: barrier variation with different methods, kJ/mol

Scan @ cc-pVTZ+d	Trans to gauche	(Gauche – trans)	Gauche to gauche'
B3LYP	30.3	15.1	17.0
† @ 6-311G**	29.8	14.7	16.7
M06-2X	27.5	12.3	15.2
MN12SX	30.5	13.6	15.8
MP2	27.2	12.2	15.5
QCISD	25.3	12.0	14.9
† Vansteenkiste et al. J. Chem. Phys. 124 , 044314_2006			

Table 2: impact of scan type on thermochemical parameters

Scan @ cc-pVTZ+d	S (298.15 K)	S (2,000 K)	C _p (298.15 K)	C _p (2,000 K)	H(298.15 K)–H(0)
B3LYP	276.9	560.7	76.00	206.9	14.80
M06-2X	277.8	561.1	77.53	206.4	14.95
MN12SX	277.1	560.9	76.65	206.8	14.84
MP2	277.8	561.2	77.51	206.4	14.94
QCISD	278.2	561.3	77.98	206.0	15.00

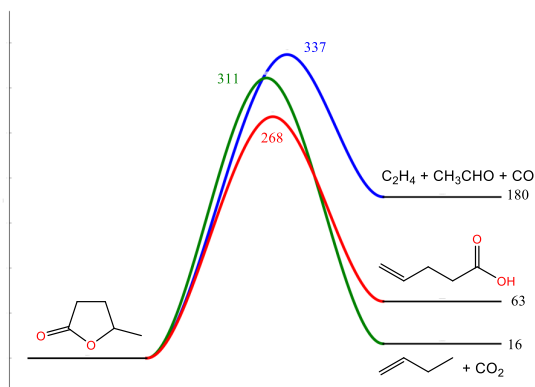
As can be seen some differences are apparent at room temperature but these disappears at higher temperatures. A more detailed analysis on a per mode basis is provided by the `thermo.details` file which shows that the actual impact of the different scan methodologies is quite small, **Error! Reference source not found.**, at least in this case.

Table 3: hindered rotor impact

Scan @ cc-pVTZ+d	S (298.15 K)	C _p (298.15 K)	H(298.15 K)–H(0)
B3LYP	10.54	9.63	1.69
M06-2X	11.41	11.15	1.84
MN12SX	10.74	10.28	1.74
MP2	11.39	11.13	1.84
QCISD	11.78	11.61	1.90

Reaction of γ -valerolactone

Gamma-valerolactone, GVL, can decompose to eliminate CO, ethene and ethanal in a single concerted step



The input file to calculate the high-pressure limiting rate constant is straightforward reflecting the presence of an 'asymmetric' carbon atom in the ring which gives rise to optical isomers in both the reactant and the transition state. The methyl rotors are well-behaved and can be treated simply as 3-fold rotors with a specified barrier in cm^{-1} .

```
KJOU ATM ! Units of energy and concentration; GVL ==> ethene+ethanal+CO
17 ! Number of temperatures to be specified
298.15 300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 1600 1800 2000
2 ! Just two species involved
```

```
react GammaVaLac 0.00 ! HoF 298K -406.5 ± 1.1 kJ -97.16 kcal Pilcher 1990
C5H8O2
! cbs-qb3 "Gamma-valerolactones.log"
! Equatorial methyl group
! Scaling factor: 0.990; scan at B3LYP/CBSB7
```



```

1 2 1 ! no symmetry, optical isomers, only 1 e-state
0.0 1 ! which is the ground state and is a Singlet
41 'HAR' 'GHZ'
1 vib 121.31 0.0 1
2 vib 151.08 0.0 1
3 hrb 230.33 1078. 3 ! Barrier 12.90 kJ
4 vib 297.86 0.0 1
5 vib 450.85 0.0 1
6 vib 509.41 0.0 1
7 vib 528.40 0.0 1
8 vib 602.38 0.0 1
9 vib 657.04 0.0 1
10 vib 797.66 0.0 1
11 vib 819.02 0.0 1
12 vib 892.95 0.0 1
13 vib 944.53 0.0 1
14 vib 961.70 0.0 1
15 vib 997.42 0.0 1
16 vib 1068.45 0.0 1
17 vib 1097.97 0.0 1
18 vib 1117.00 0.0 1
19 vib 1166.90 0.0 1
20 vib 1200.18 0.0 1
21 vib 1227.42 0.0 1
22 vib 1292.92 0.0 1
23 vib 1311.99 0.0 1
24 vib 1355.78 0.0 1
25 vib 1381.96 0.0 1
26 vib 1404.70 0.0 1
27 vib 1454.31 0.0 1
28 vib 1470.03 0.0 1
29 vib 1484.28 0.0 1
30 vib 1487.79 0.0 1
31 vib 1848.98 0.0 1
32 vib 2983.13 0.0 1
33 vib 3003.09 0.0 1
34 vib 3012.06 0.0 1
35 vib 3016.61 0.0 1
36 vib 3068.17 0.0 1
37 vib 3072.28 0.0 1
38 vib 3081.70 0.0 1
39 vib 3090.27 0.0 1
40 gro 5.30477 1 1
41 gro 1.90491 1 2 ! 2.1859404 & 1.6600093

```

```

ctst GVL-TS 337. 537.2 159. ! barrier, imag. freq., reverse barrier kJ/mol
C5H8O2

```

```

! cbs-qb3 "GVL_concerted.log"
! Equatorial methyl group
! Scaling factor: 0.990; scan at B3LYP/CBSB7
1 2 1 ! no symmetry, optical isomers, only 1 e-state
0.0 1 ! which is the ground state and is a Singlet
40 'HAR' 'GHZ'
1 vib 47.91 0.0 1
2 vib 83.20 0.0 1
3 vib 157.39 0.0 1
4 vib 200.95 0.0 1
5 hrb 215.47 872.7 3 ! HR Me 10.44 kJ
6 vib 251.99 0.0 1
7 vib 283.60 0.0 1

```

8	vib	410.67	0.0	1		
9	vib	469.03	0.0	1		
10	vib	505.27	0.0	1		
11	vib	596.64	0.0	1		
12	vib	648.12	0.0	1		
13	vib	841.22	0.0	1		
14	vib	854.86	0.0	1		
15	vib	885.80	0.0	1		
16	vib	936.83	0.0	1		
17	vib	1012.41	0.0	1		
18	vib	1015.17	0.0	1		
19	vib	1060.75	0.0	1		
20	vib	1108.55	0.0	1		
21	vib	1238.15	0.0	1		
22	vib	1263.46	0.0	1		
23	vib	1346.29	0.0	1		
24	vib	1383.94	0.0	1		
25	vib	1450.91	0.0	1		
26	vib	1458.44	0.0	1		
27	vib	1464.15	0.0	1		
28	vib	1502.41	0.0	1		
29	vib	1555.27	0.0	1		
30	vib	2069.83	0.0	1		
31	vib	2987.52	0.0	1		
32	vib	2993.04	0.0	1		
33	vib	3051.31	0.0	1		
34	vib	3084.55	0.0	1		
35	vib	3101.88	0.0	1		
36	vib	3116.70	0.0	1		
37	vib	3174.14	0.0	1		
38	vib	3207.81	0.0	1		
39	qro	3.40112	1	1		
40	qro	1.66003	1	2	! 1.9774039	1.3936004

Note that in order to benefit from the cancellation of systemic errors *both the reactant and the transition state* and the products are all computed at the same level of theory appropriate to the molecules under consideration. Although straightforward there are a number of improvements that could be undertaken such as a proper treatment of the ring flexing vibrational modes which are not amenable to the usual relaxed potential energy scans, for example, a complete scan over 360° is not possible in these cases. Note that remnants of these puckering modes are evident in the transition state, modes #1 and #2, shifted to lower frequencies. In addition more accurate computations of the zero-point corrected electronic energy E^\ddagger could be made.

Frequent Data References

There are no validated comprehensive sources of basic thermochemical parameters such as entropy, specific heat at constant pressure and enthalpy function. The references listed below: **CCCBDB**, **NIST-JANAF**, **NASA/JPL**, **3rd Mill**, **RMG** and **WebBook** are worth consulting as are **Pedley** and the **ATcT** for enthalpies of formation.

CCCBDB [Chemistry Comparison and Benchmark DataBase](#), Release 18 (October 2016) NIST Standard Reference Database 101. *A valuable collection of experimental and calculated molecular parameters at many different levels of theory.*

NIST-JANAF 1998 Chase, M. W., Jr. (1998), [NIST-JANAF Thermochemical Tables](#). Fourth Edition, JPCRD, Monograph No. 9, 1-1951.

NASA/JPL [Data Evaluation \(NASA/JPL-15\)](#): J. B. Burkholder, S. P. Sander, J. Abbatt, J. R. Barker, R. E. Huie, C. E. Kolb, M. J. Kurylo, V. L. Orkin, D. M. Wilmoth, P. H. Wine "Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation No. 18," JPL Publication 15-10, Jet Propulsion Laboratory, Pasadena, 2015

3rd Mill Elke Goos, Alexander Burcat and Branko Ruscic. [Extended Third Millennium Thermodynamic Database](#) for Combustion and Air-Pollution Use with updates from Active Thermochemical Tables. *The requisite thermodata for a very large number of chemical*

species is present in the so-called Table 6 document **hf.doc**. Typically raw data such as vibrational frequencies, symmetry numbers, moments of inertia, etc. computed at specified levels of theory is also provided.

RMG Reaction Mechanism Generator is an automatic chemical reaction mechanism generator that constructs kinetic models composed of elementary chemical reaction steps. *Inter alia* it calculates thermochemical parameters from a species sketch or name.

WebBook [NIST Standard Reference Database Number 69](#)

Pedley Pedley, J. B., Naylor, R. D., Kirby, S. P. "Thermochemical Data of Organic Compounds", 2nd ed., Chapman and Hall, London, 1986.

ATcT Active Thermochemical Tables Enthalpies of formation only

B. Ruscic, R. E. Pinzon, M. L. Morton, G. von Laszewski, S. Bittner, S. G. Nijssure, K. A. Amin, M. Minkoff, A. F. Wagner, Introduction to Active Thermochemical Tables: Several "Key" Enthalpies of Formation Revisited. JPCA 108, 9979-9997 (2004)

B. Ruscic, R. E. Pinzon, G. von Laszewski, D. Kodeboyina, A. Burcat, D. Leahy, D. Montoya, and A. F. Wagner, Active Thermochemical Tables: Thermochemistry for the 21st Century. J. Phys. Conf. Ser. 16, 561-570 (2005) [DOI: 10.1088/1742-6596/16/1/078]

B. Ruscic, Active Thermochemical Tables (ATcT) values based on **ATcT v. 1.118**; available at ATcT.anl.gov

ATcT v.1.122: B. Ruscic, D. Feller, and K. A. Peterson, Active Thermochemical Tables: dissociation energies of several homonuclear first-row diatomics and related thermochemical values, Theor Chem Acc (2014) 133:1415. DOI 10.1007/s00214-013-1415-z

There are occasional references to **W3X-L JMS unpublished** throughout; some of these refer to a work in progress "A Database of Oxygenates: C_xH_yO_z, x=y=1,2 and z=1-8" by Simmie and Würmel which contains validated and cross-referenced data for over 200 neutral, radical and excited states species satisfying those molecular formulas.

Formation enthalpy, $\Delta_f H(T)$

The enthalpy of formation of a species at 0 K, if known, can be input to **THERMO** which then computes the formation at 298.15 K.

none SpeciesName DfH(0) ! Typical entry

This calculation is thus very useful for validation purposes since tables of the enthalpy of formation of many species at 298.15 K are available. Alternatively, if $\Delta_f H(0K)$ is not known, but a value of the enthalpy of formation at 298.15 K, $\Delta_f H(298.15K)$, is known **THERMO** can be run with a trial value for $\Delta_f H(0K)$ to obtain the enthalpy function, which is computed by **THERMO** and shown as $[H(T) - H(0)]$ at 298.15 K in the output.

The enthalpy of formation at $T=298.15$ K follows therefore from:

$$\Delta_f H(298.15K) = \Delta_f H(0K) + [H(T) - H(0)] + \sum n_i [H(T) - H(0)]_i$$

where the terms in the summation refer to the elements, in the species under consideration, in their standard states.

An example:

Oxalic acid has the general formula C₂H₂O₄ and a computed value of $[H(T) - H(0)] = 17.60$ kJ mol⁻¹.

The Table shows the absolute enthalpies of a selection of elements on a per atom basis:

Table 4: NIST-JANAF; standard state 1 bar

Element / standard state	$[H(T) - H(0)] / \text{kJ mol}^{-1}$
Carbon / graphite	-1.051 ₀
Hydrogen / H ₂	-4.233 ₅
Oxygen / O ₂	-4.341 ₅
Nitrogen / N ₂	-4.335 ₀

ATcT lists $\Delta_f H(0K) = -710.8$ kJ thus the calculated 298.15 K formation enthalpy is:

$$\Delta_f H(298.15K) = -710.8 + 17.60 + \{(2 \times -1.051) + (2 \times -4.2335) + (4 \times -4.3415)\} = -721.1$$

ATcT quotes -721.4 kJ mol⁻¹.

THERMO.DAT input files

Acetone oxide, propanone oxide, Criegee intermediate (CH₃)₂C=O-O

none AcetoneOxide 4.2 ! W2X JMS unpub. T1 > 0.036

C3H6O2

! B3LYP/cc-pVTZ+d vib,rots,scans of 2 methyl rotors, scale=0.9681

! An isodesmic calc. gives dHf(0)=0.52 based on W1BD energies

! AcetoneOxide + HCHO = trans EthanalOxide + Acetaldehyde DrH(0K)=13.3

! Calc. S=318.06, Cp=95.55, H(T)-H(0)=18.90

1 1 1 ! One methyl group cis to O--O--C, the other trans

0.0 1 ! Cs symmetry

28 'HAR' 'GHZ'

1 vib 3038.33 0.0 1 !

2 vib 3034.43 0.0 1 !

3 vib 2967.46 0.0 1 !

4 vib 2960.87 0.0 1 !

5 vib 2927.96 0.0 1 !

6 vib 2923.32 0.0 1 !

7 vib 1507.72 0.0 1 !

8 vib 1430.07 0.0 1 !

9 vib 1422.34 0.0 1 !

10 vib 1411.49 0.0 1 !

11 vib 1390.15 0.0 1 !

12 vib 1365.05 0.0 1 !

13 vib 1350.93 0.0 1 !

14 vib 1264.76 0.0 1 !

15 vib 1058.97 0.0 1 !

16 vib 1038.47 0.0 1 !

17 vib 953.27 0.0 1 !

18 vib 907.53 0.0 1 !

19 vib 903.73 0.0 1 !

20 vib 787.29 0.0 1 !

21 vib 581.76 0.0 1 !

22 vib 465.17 0.0 1 !

23 vib 350.76 0.0 1 !

24 vib 300.95 0.0 1 !

25 vib 268.06 0.0 1 !

26 hrb 220.90 660.4 3 ! HR cis methyl group 7.90 kJ

27 hrb 131.01 558.4 3 ! HR trans methyl group 6.68 kJ

28 top 3.6110 8.8507 1 ! 8.8506995 4.3281353 3.0126936

none (CH₃)₂COO -39. ! ± 12 kJ/mol (estimated)

C3H6O2

! dHf(0) for CH₂=C(CH₃)OOH from Sebbar et al. PCCP 2002, 4, 3691D3703

! vib, rots, and torsions: Fang et al. JCP 144, 061102 (2016)

! Calc. S=316.35, Cp=94.63, H(T)-H(0)=18.69

1 1 1

0.0 1

28 'HAR' 'cm-1'

1 vib 3028 0 1 !

2 vib 3023 0 1 !

3 vib 2958 0 1 !

4 vib 2938 0 1 !

5 vib 2932 0 1 !

6 vib 2924 0 1 !

7 vib 1485 0 1 !

8 vib 1449 0 1 !

9 vib 1438 0 1 !

10 vib 1424 0 1 !

11 vib 1395 0 1 !

12 vib 1381 0 1 !

13 vib 1367 0 1 !

14 vib 1285 0 1 !

15 vib 1078 0 1 !

16 vib 1040 0 1 !

```

17 vib 970 0 1 !
18 vib 933 0 1 !
19 vib 925 0 1 !
20 vib 806 0 1 !
21 vib 603 0 1 !
22 vib 469 0 1 !
23 vib 362 0 1 !
24 vib 312 0 1 !
25 vib 268 0 1 !
26 hrb 194 763 3 !
27 hrb 160 520 3 !
28 top 0.121 0.2957 1 !

```

Acetonitrile, methyl cyanide CH₃CN

none Acetonitrile 81.15 ! ex 74.04±0.37 @ 298K An & Mansson JChemThermo 1983,15,287
C2H3N1

! JMS 74.4±1.6 @ 298 K J Phys Chem A 2015, 119, 10511-10526; 81.8±1.9 @ 0 K
! B3LYP/cc-pVTZ+d vibs, rots, anharm
! Lit. S=243.51, Cp=52.34, H(T)-H(0)=12.11 JPC 1967,71,914 cf Dortmund DataBank,
! Calc. 242.93 52.05, 12.03

```

3 1 1 ! C3v
0.0 1 1 ! 1A1
9 'HAR' 'GHZ'
1 vib 3047.86 -17.45 1 ! A1
2 vib 2367.35 -11.30 1 ! A1
3 vib 1414.47 -9.80 1 ! A1
4 vib 928.05 -4.60 1 ! A1
5 vib 3115.41 -31.67 2 ! E
6 vib 1475.43 -2.71 2 ! E
7 vib 1062.69 0.93 2 ! E
8 vib 380.97 -3.55 2 ! E
9 top 9.2787 159.883 1 ! 159.883 2776 9.2786735 9.2786735

```

Acetylene/ethyne HCCH

none Acetylene 228.87 ! ± 0.14 ATcT v.1.118
C2H2

! Bo, harm vibs, and X(ii) from Herman JPCRD, 32, 921-1361 (2003)
! Lit. S=200.9, Cp=44.04 NIST-JANAF;
! calc. 200.5, Cp=43.55

```

2 1 1 ! Dinfh
0.0 1
6 'HAR' 'CM-1'
1 vib 3493.720 -24.81 1
2 vib 2005.301 -7.451 1
3 vib 3411.000 -27.63 1
4 vib 624.702 3.458 2
5 vib 743.264 -2.374 2
6 qro 1.17664632 1. 2 ! 2D rotor Bo JPCRD, 32, 921-1361 (2003)

```

Adamantane C₁₀H₁₆

none Adamantane 188.9 ! estim from 132.3 2.2 @298K Bazyleva JPCB 2011,115, 10064-72
C10H16

! B3LYP/cc-pVTZ+d vibs,rots, scale=0.9681
! Lit. S=322.1, Cp=149.2 calc by Bazyleva
! 342.3, 147.0 calc @ 300K Miranda JMolStruc 2016,1122,299 no -R*ln(sigma)
! Calc. 324.73 151.83, H(T)-H(0)=21.65

```

12 1 1 ! Td external symmetry number, no. of OIs, no. of e-states
0.0 1 ! 1A1
31 'HAR' 'GHZ' Expt Bisticic Spectchim Acta 1995, 51, 1643
1 vib 307.99 0.0 3 ! T1 355
2 vib 395.62 0.0 2 ! E 400
3 vib 430.34 0.0 3 ! T2 444
4 vib 629.36 0.0 3 ! T2 638

```

5	vib	728.68	0.0	1 ! A1	758
6	vib	773.35	0.0	3 ! T2	800
7	vib	870.19	0.0	3 ! T1	
8	vib	877.13	0.0	2 ! E	
9	vib	942.28	0.0	3 ! T2	972
10	vib	1010.11	0.0	3 ! T1	
11	vib	1025.66	0.0	1 ! A1	
12	vib	1084.52	0.0	3 ! T2	1105
13	vib	1094.17	0.0	1 ! A2	1105
14	vib	1097.53	0.0	3 ! T1	
15	vib	1201.24	0.0	2 ! E	1220
16	vib	1268.52	0.0	3 ! T1	
17	vib	1293.32	0.0	3 ! T2	1312
18	vib	1315.44	0.0	3 ! T1	1312
19	vib	1347.85	0.0	3 ! T2	1353
20	vib	1359.28	0.0	2 ! E	1370
21	vib	1438.27	0.0	2 ! E	1436
22	vib	1450.67	0.0	3 ! T2	1450
23	vib	1471.78	0.0	1 ! A1	1472
24	vib	2907.04	0.0	1 ! A1	2913
25	vib	2908.20	0.0	3 ! T2	2944
26	vib	2908.71	0.0	2 ! E	2913
27	vib	2928.48	0.0	3 ! T2	2950
28	vib	2938.88	0.0	3 ! T1	2944
29	vib	2939.53	0.0	1 ! A1	
30	vib	2945.02	0.0	3 ! T2	
31	gro	1.68585	1.0	3 ! 3D rotor	symm=1 1.6858538 1.6858538 1.6858538

Amidogen NH₂

none NH2 188.94 ! ± 0.15 ATcT v1.118
 NH2
 ! vibs: WebBook
 ! rots: Martin-Drumel JPCA 118, 1331-1338 (2014)
 ! 298.15 K Lit. WebBook S= 194.71, Cp=33.66; this work 194.60, 33.58
 2 1 2 ! C2v symm
 0.0 2 ! 2B1
 11122.23 2
 5 'OBS' 'GHZ'
 1 vib 3219.37 0.0 1 ! A1
 2 vib 1497.2 0.0 1 ! A1
 3 vib 3301.11 0.0 1 ! B2
 4 gro 710.302 1.0 1 ! GHZ; K-rotor
 5 gro 308.441 1.0 2 ! GHZ; 2D-rotor

Ammonia NH₃

none NH3 -38.568 ! ± 0.030 ATcT v1.118
 NH3
 ! rotations: Herzberg 1966
 ! vibs: T. Shimanouchi, 1972, Tables of Molecular Vibrational Frequencies Consolidated
 ! Volume I, NSRDS-NBS 39.
 3 1 1 ! C3v
 0.0 1 ! 1A1
 6 'OBS' 'CM-1'
 1 vib 3337 0.0 1
 2 vib 950 0.0 1
 3 vib 3444 0.0 2
 4 vib 1627 0.0 2
 5 gro 6.196 1.0 1 ! K-rotor
 6 gro 9.4443 1.0 2 ! 2D-rotor

Argon

none Ar 0.0 ! By definition

Ar
 ! NIST-JANAF 1998
 !
 !
 1 1 1
 0.0 1
 0 'HAR' 'AMUA'

Benzene C₆H₆

none Benzene 100.71 ! ATcT v.1.118 ± 0.26
 C6H6
 ! vibs: Miani JCP, 112, 248-259 (2000)
 ! rots: Riehn JPCA, 105, 5618-5621 (2001)
 ! 298.15 K Lit. TRC S=269.3, Cp=82.44; this work 264.81, 82.12
 12 1 1 ! D6h
 0.0 1 ! 1A1g
 21 'OBS' 'MHZ'

1	vib	993.071	-0.58	1
2	vib	3073.942	-9.74	1
3	vib	1350	-1.27	1
4	vib	702.24	0	1
5	vib	992.93	0	1
6	vib	608.13	0	2
7	vib	3057.04	-15.17	2
8	vib	1609.518	-1.75	2
9	vib	1177.776	0	2
10	vib	847.1062	0	2
11	vib	673.97465	0	1
12	vib	1013.74	0	1
13	vib	3057	-10.2	1
14	vib	1309.4	-1.47	1
15	vib	1147.6751	1.08	1
16	vib	398.131	0	2
17	vib	967.98	0	2
18	vib	1038.267	-0.62	2
19	vib	1483.9854	4.03	2
20	vib	3047.908	-14.93	2
21	top	5689.10	2844.55	1 ! B2 = 5689.10, B1 = B2/2

Bromine atom (²P)

none Br(2P) 117.914 ! ATcT v.1.118 ± 0.056
 Br
 ! NIST-JANAF pg. 429
 ! 298.15 Lit. S=175.017; Cp=20.786
 !
 1 1 2
 0.0 4 ! 2P3/2
 3685.24 2 ! 2P1/2
 0 'HAR' 'AMUA'

Buta-1,3-diene, *trans* butadiene, CH₂=CH-CH=CH₂

none C=C-C=C 125.4 ! W3X-L JMS unpub. 110.5₄ @ 298.15K; ATcT v1.122 125.05, 110.57 ± 0.42
 C4H6
 ! B3LYP/cc-pVTZ+d vibs, rots, scan, anharmonics
 ! Lit. S=277.7 Cp=78.0 Vansteenkiste et al JChemPhys 124, 044314,2006
 ! @300K S=278.1 Cp=77.86 Wong,Raman J Comp Chem 28 759-766,2001
 ! Calc. 276.76 75.68, H(T)-H(0)=14.75
 2 1 1 ! C2h symm trans conformer
 0.0 1 ! 1Ag
 25 'HAR' 'GHZ'

1	vib	3221.60	-17.55	1 ! Ag
2	vib	3137.86	-12.80	1 ! Ag

3	vib	3125.28	-22.76	1	!	Ag
4	vib	1705.35	-3.00	1	!	Ag
5	vib	1478.94	-2.77	1	!	Ag
6	vib	1318.81	-0.67	1	!	Ag
7	vib	1230.03	-1.87	1	!	Ag
8	vib	901.04	0.65	1	!	Ag
9	vib	519.22	0.83	1	!	Ag
10	vib	1061.42	-2.44	1	!	Au
11	vib	944.55	0.93	1	!	Au
12	vib	543.08	-1.39	1	!	Au
13	hrd	13 10 1	! FREQUENCY REMOVED = 171 cm-1			
Vhrd3	1 0	1456.0061	-339.3676	-874.1588	-389.3532	114.1551 30.3715 12.1788 0.0165
		0.3914	-0.1901	0.1916	0.1728	0.0928
Bhrd1	1 0	3.4022	-0.8948	0.6304	0.4039	-0.317 0.1062 -0.1142 0.0658 0.0071 -0.0001
14	vib	1007.22	-1.69	1	!	Bg
15	vib	945.29	0.18	1	!	Bg
16	vib	784.84	-0.37	1	!	Bg
17	vib	3222.00	-17.24	1	!	Bu
18	vib	3138.31	-20.26	1	!	Bu
19	vib	3135.18	-10.46	1	!	Bu
20	vib	1654.36	-1.10	1	!	Bu
21	vib	1420.07	-1.35	1	!	Bu
22	vib	1324.61	-0.93	1	!	Bu
23	vib	1007.66	0.50	1	!	Bu
24	vib	296.96	2.68	1	!	Bu
25	top	4.23180	42.662	1	!	42.6623908 4.4468851 4.0271209

t-Butyl radical (CH₃)₃C•

none tert-Butyl 73.7 ! W3X-L 73.7 JMS unpub. cf J Phys Chem A 2015, 119, 8922
C4H9

! B3LYP/cc-pVTZ+d freqs, rots, scan Scaling factor: 0.9681

! Non-planar calc. S=320.68, Cp=90.76, H(T)-H(0)=19.54

! Lit. S=315 ± 4 Seetula, Slagle 10.1039/a608224f

3 1 1 ! C3v, 3 fold symmetry, no optical isomers, only 1 e-state

0.0 2 ! ground state doublet 2A"

24		'HAR'	'GHZ'			
1	hrb	128.84	332.7	3	!	methyl rotors barrier 3.98 kJ
2	hrb	128.84	332.7	3	!	methyl rotors barrier 3.98 kJ
3	hrb	129.52	332.7	3	!	methyl rotors barrier 3.98 kJ
4	vib	256.31	0.0	1	!	A1
5	vib	369.01	0.0	2	!	E
6	vib	733.54	0.0	1	!	A1
7	vib	908.21	0.0	2	!	E
8	vib	942.03	0.0	1	!	A2
9	vib	976.08	0.0	2	!	E
10	vib	1061.74	0.0	1	!	A1
11	vib	1253.21	0.0	2	!	E
12	vib	1354.29	0.0	2	!	E
13	vib	1381.17	0.0	1	!	A1
14	vib	1421.95	0.0	1	!	A2
15	vib	1424.27	0.0	2	!	E
16	vib	1441.44	0.0	1	!	A1
17	vib	1444.71	0.0	2	!	E
18	vib	2822.66	0.0	2	!	E
19	vib	2830.58	0.0	1	!	A1
20	vib	2932.39	0.0	2	!	E
21	vib	2935.30	0.0	1	!	A1
22	vib	2972.83	0.0	1	!	A2
23	vib	2977.29	0.0	2	!	E
24	top	8.02107	4.34865	1	!	GHz 8.0210691 8.0210691 4.3486543

C-60 buckminsterfullerene

none C-60 2535. ! 2530 ± 13 kJ/mol @ 298.15 K Diky & Kabo

C60

! Diky & Kabo, Thermodynamic properties of C60 and C70 fullerenes

! Russ Chem Rev, 2000, 69 (2), 95-104

! freqs Schettino et al., J Phys Chem A 2001,105,11192-96; DOI: 10.1021/jp012874t

! Lit. S=543.9, Cp=498.5, H-H(0)=58.44 Russ Chem Rev, 2000, 69 (2), 95-104

! Calc. 543.82 500.93 58.43

60 1 1 ! Ih point group

0.0 1 ! 1Ag

48 'HAR' 'MHZ'

1	vib	496	0.0	1	!	Ag
2	vib	1468	0.0	1	!	Ag
3	vib	264	0.0	5	!	Hg
4	vib	430	0.0	5	!	Hg
5	vib	709	0.0	5	!	Hg
6	vib	773	0.0	5	!	Hg
7	vib	1101	0.0	5	!	Hg
8	vib	1251	0.0	5	!	Hg
9	vib	1425	0.0	5	!	Hg
10	vib	1576	0.0	5	!	Hg
11	vib	525	0.0	3	!	T1u
12	vib	578	0.0	3	!	T1u
13	vib	1182	0.0	3	!	T1u
14	vib	1433	0.0	3	!	T1u
15	vib	560	0.0	3	!	T1g
16	vib	825	0.0	3	!	T1g
17	vib	1260	0.0	3	!	T1g
18	vib	552	0.0	3	!	T2g
19	vib	713	0.0	3	!	T2g
20	vib	796	0.0	3	!	T2g
21	vib	1345	0.0	3	!	T2g
22	vib	485	0.0	4	!	Gg
23	vib	567	0.0	4	!	Gg
24	vib	751	0.0	4	!	Gg
25	vib	1078	0.0	4	!	Gg
26	vib	1315	0.0	4	!	Gg
27	vib	1497	0.0	4	!	Gg
28	vib	956	0.0	1	!	Au
29	vib	341	0.0	3	!	T2u
30	vib	706	0.0	3	!	T2u
31	vib	963	0.0	3	!	T2u
32	vib	1166	0.0	3	!	T2u
33	vib	1540	0.0	3	!	T2u
34	vib	354	0.0	4	!	Gu
35	vib	741	0.0	4	!	Gu
36	vib	756	0.0	4	!	Gu
37	vib	972	0.0	4	!	Gu
38	vib	1307	0.0	4	!	Gu
39	vib	1428	0.0	4	!	Gu
40	vib	403	0.0	5	!	Hu
41	vib	533	0.0	5	!	Hu
42	vib	665	0.0	5	!	Hu
43	vib	738	0.0	5	!	Hu
44	vib	1215	0.0	5	!	Hu
45	vib	1341	0.0	5	!	Hu
46	vib	1566	0.0	5	!	Hu
47	rot	83.3717	1	1	!	K-rotor
48	rot	83.3717	1	2	!	J-rotor
! 47	qro	83.3717	1	3	!	3D quantized; yields same result

C-70 fullerene

none C70 2759. ! 2755 ± 23 kJ/mol @ 298.15 K Diky & Kabo

C70

! Diky & Kabo, Thermodynamic properties of C60 and C70 fullerenes
! Russ Chem Rev, 2000, 69 (2), 95-104
! theor. freqs scaled by 0.98 Sun, Kertesz, J PhysChem A, 106, 6381-86
! Note that a 2% change in scale factor changes S(vib) by 6.9 J/K/mol
! Rots: Christides et al. Phys.Rev. B49 (1994) 2897
! Lit. S=613.9 , Cp=585.1 , H-H(0)=68.127 @ 298.15 K
! Calc. 618.88, 589.87, 69.14

10	1	1	!	D5h
0.0	1	!		
124	'HAR'	'MHZ'		
1	vib	318.0	0.0	1 ! A2"
2	vib	458.8	0.0	1 ! A2"
3	vib	563.9	0.0	1 ! A2"
4	vib	703.8	0.0	1 ! A2"
5	vib	895.8	0.0	1 ! A2"
6	vib	1142.9	0.0	1 ! A2"
7	vib	1205.6	0.0	1 ! A2"
8	vib	1320.8	0.0	1 ! A2"
9	vib	1462.4	0.0	1 ! A2"
10	vib	1567.6	0.0	1 ! A2"
11	vib	325.7	0.0	2 ! E1'
12	vib	358.2	0.0	2 ! E1'
13	vib	414.5	0.0	2 ! E1'
14	vib	507.2	0.0	2 ! E1'
15	vib	533.1	0.0	2 ! E1'
16	vib	573.1	0.0	2 ! E1'
17	vib	639.5	0.0	2 ! E1'
18	vib	665.5	0.0	2 ! E1'
19	vib	729.3	0.0	2 ! E1'
20	vib	751.3	0.0	2 ! E1'
21	vib	827.7	0.0	2 ! E1'
22	vib	905.0	0.0	2 ! E1'
23	vib	1087.2	0.0	2 ! E1'
24	vib	1176.9	0.0	2 ! E1'
25	vib	1254.6	0.0	2 ! E1'
26	vib	1290.3	0.0	2 ! E1'
27	vib	1318.2	0.0	2 ! E1'
28	vib	1415.1	0.0	2 ! E1'
29	vib	1431.1	0.0	2 ! E1'
30	vib	1489.1	0.0	2 ! E1'
31	vib	1569.2	0.0	2 ! E1'
32	vib	253.3	0.0	1 ! A1'
33	vib	393.4	0.0	1 ! A1'
34	vib	448.3	0.0	1 ! A1'
35	vib	564.7	0.0	1 ! A1'
36	vib	701.4	0.0	1 ! A1'
37	vib	708.8	0.0	1 ! A1'
38	vib	1060.9	0.0	1 ! A1'
39	vib	1185.1	0.0	1 ! A1'
40	vib	1229.0	0.0	1 ! A1'
41	vib	1449.7	0.0	1 ! A1'
42	vib	1471.5	0.0	1 ! A1'
43	vib	1574.0	0.0	1 ! A1'
44	vib	219.6	0.0	2 ! E2'
45	vib	298.9	0.0	2 ! E2'
46	vib	426.1	0.0	2 ! E2'
47	vib	502.4	0.0	2 ! E2'
48	vib	533.5	0.0	2 ! E2'
49	vib	665.2	0.0	2 ! E2'
50	vib	688.5	0.0	2 ! E2'
51	vib	722.1	0.0	2 ! E2'
52	vib	734.7	0.0	2 ! E2'
53	vib	741.1	0.0	2 ! E2'
54	vib	750.2	0.0	2 ! E2'
55	vib	766.5	0.0	2 ! E2'
56	vib	945.0	0.0	2 ! E2'

57	vib	1059.0	0.0	2	!	E2'
58	vib	1186.7	0.0	2	!	E2'
59	vib	1256.9	0.0	2	!	E2'
60	vib	1328.9	0.0	2	!	E2'
61	vib	1349.1	0.0	2	!	E2'
62	vib	1372.9	0.0	2	!	E2'
63	vib	1501.0	0.0	2	!	E2'
64	vib	1523.0	0.0	2	!	E2'
65	vib	1573.2	0.0	2	!	E2'
66	vib	245.3	0.0	2	!	E1"
67	vib	408.3	0.0	2	!	E1"
68	vib	478.6	0.0	2	!	E1"
69	vib	514.9	0.0	2	!	E1"
70	vib	546.0	0.0	2	!	E1"
71	vib	674.5	0.0	2	!	E1"
72	vib	713.5	0.0	2	!	E1"
73	vib	734.7	0.0	2	!	E1"
74	vib	740.2	0.0	2	!	E1"
75	vib	794.3	0.0	2	!	E1"
76	vib	1054.4	0.0	2	!	E1"
77	vib	1168.7	0.0	2	!	E1"
78	vib	1225.5	0.0	2	!	E1"
79	vib	1296.3	0.0	2	!	E1"
80	vib	1312.8	0.0	2	!	E1"
81	vib	1366.2	0.0	2	!	E1"
82	vib	1432.1	0.0	2	!	E1"
83	vib	1515.5	0.0	2	!	E1"
84	vib	1573.7	0.0	2	!	E1"
85	vib	485.2	0.0	1	!	A2'
86	vib	545.8	0.0	1	!	A2'
87	vib	628.8	0.0	1	!	A2'
88	vib	723.3	0.0	1	!	A2'
89	vib	744.6	0.0	1	!	A2'
90	vib	935.9	0.0	1	!	A2'
91	vib	1215.1	0.0	1	!	A2'
92	vib	1338.2	0.0	1	!	A2'
93	vib	1450.0	0.0	1	!	A2'
94	vib	336.3	0.0	1	!	A1"
95	vib	529.3	0.0	1	!	A1"
96	vib	612.0	0.0	1	!	A1"
97	vib	733.6	0.0	1	!	A1"
98	vib	779.3	0.0	1	!	A1"
99	vib	891.8	0.0	1	!	A1"
100	vib	1240.4	0.0	1	!	A1"
101	vib	1347.3	0.0	1	!	A1"
102	vib	1557.8	0.0	1	!	A1"
103	vib	304.4	0.0	2	!	E2"
104	vib	382.6	0.0	2	!	E2"
105	vib	406.9	0.0	2	!	E2"
106	vib	514.7	0.0	2	!	E2"
107	vib	555.4	0.0	2	!	E2"
108	vib	632.9	0.0	2	!	E2"
109	vib	700.5	0.0	2	!	E2"
110	vib	717.1	0.0	2	!	E2"
111	vib	727.6	0.0	2	!	E2"
112	vib	781.3	0.0	2	!	E2"
113	vib	920.0	0.0	2	!	E2"
114	vib	1074.5	0.0	2	!	E2"
115	vib	1155.6	0.0	2	!	E2"
116	vib	1257.6	0.0	2	!	E2"
117	vib	1315.7	0.0	2	!	E2"
118	vib	1327.3	0.0	2	!	E2"
119	vib	1398.5	0.0	2	!	E2"
120	vib	1454.7	0.0	2	!	E2"
121	vib	1516.5	0.0	2	!	E2"
122	vib	1572.7	0.0	2	!	E2"

123 gro 67.68 1 1 ! K-rotor ; Christides Phys.Rev. B49(1994) 2897
 124 gro 58.28 1 2 ! J-rotor ; ditto

Carbon atom

none C-atom 711.401 ! ± 0.050 ATcT v1.122 716.886 at 298.15 K

C
 ! NIST-JANAF pg 551
 !
 ! S=157.99, Cp=20.84, HT)-H(0)=6.54
 1 1 6 ! Six e-levels
 0.0 1 ! energy & quantum weights
 16.40 3 !
 43.40 5 !
 10192.63 5 !
 21648.01 1 !
 33735.20 5 !
 0 'HAR' 'GHZ'

Carbon disulfide CS2

none CS2 115.91 ! ± 1.0; Burkholder et al., JPL Publication 15-10, 2015;

CS2
 ! vibs, rots, e-states Herzberg, Electronic spectra and electronic structure of
 ! polyatomic molecules, Van Nostrand, New York, 1966
 !

2 1 2
 0.0 1
 26187 3
 4 OBS CM-1
 1 vib 657.98 0.0 1
 2 vib 1535.35 0.0 1
 3 vib 396.7 0.0 2
 4 gro 0.1091 1 2

Carbon monoxide ¹²C¹⁶O

none C(12)O(16) -113.802 ! ATcT v1.118 ± 0.026

[C12][O16]
 ! Guelachvilli, JMS 1983, 98, 64-79
 ! NIST-JANAF pg. 641
 !

1 1 1
 0.0 1
 2 'HAR' 'AMUA'
 1 vib 2169.81 -13.288 1
 2 gro 8.72867 1 2

Carbon monoxide ¹²C¹⁷O

none CO(17) -113.81

C[O17]
 ! Guelachvilli, JMS 1983, 98, 64-79 (dHf from NIST-JANAF)
 !

1 1 1
 0.0 1
 2 'HAR' 'AMUA'
 1 vib 2142.165 -12.951 1
 2 gro 8.95545 1 2

Carbon monoxide ¹²C¹⁸O

none CO(18) -113.81

C[O18]

! Guelachvilli, JMS 1983, 98, 64-79 (dHf from NIST-JANAF)

!
!
1 1 1
0.0 1
2 'HAR' 'AMUA'
1 vib 2117.398 -12.654 1
2 gro 9.16615 1 2

Carbon monoxide $^{13}\text{C}^{16}\text{O}$

none C(13)O -113.81
[C13][O16]
! Guelachvilli, JMS 1983, 98, 64-79 (dHf from NIST-JANAF)

!
!
1 1 1
0.0 1
2 'HAR' 'AMUA'
1 vib 2121.439 -12.702 1
2 gro 9.13121 1 2

Carbon dioxide

none CO2 -393.108 ! ± 0.015 ATcT v1.118
CO2
!
! Anharmonicities from Herzberg, Infrared and Raman Spectra
! vibs, rots: NIST-JANAF pg. 643

2 1 1
0.0 1
4 'OBS' 'CM-1'
1 vib 1384.86 -0.3 1
2 vib 667.30 -1.3 2
3 vib 2349.3 -12.5 1
4 gro 0.391514 1. 2

Carbon suboxide or tricarbon dioxide, $\text{O}=\text{C}=\text{C}=\text{O}$

none $\text{O}=\text{C}=\text{C}=\text{O}$ -96.2 ! ± 1.2 ATcT v1.122;
C3O2
! Tricarbon dioxide, carbon suboxide
! MP2/cc-pVTZ vibs, rots, scaling factor: none
! Miller, F. A. et al Spectrochim. Acta 1965, 21 (10), 1709-&
! Lit. S=276.07, Cp=66.99, NIST-JANAF pg 690
! calc. 276.31 67.48, H(T)-H(0)=15.08

2 1 1 ! Dinfh symmetry, no optical isomers
0.0 1 ! Singlet
8 'HAR' 'GHZ'
1 vib 62.97 0.0 2 ! Pi u agrees expt Miller 62 \pm 3
2 vib 541.95 0.0 2 ! Pi u
3 vib 578.63 0.0 2 ! Pi g
4 vib 769.87 0.0 1 ! Sigma g
5 vib 1607.60 0.0 1 ! Sigma u
6 vib 2234.75 0.0 1 ! Sigma g
7 vib 2455.00 0.0 1 ! Sigma u
8 gro 2.19125 1 2 ! 0.000000 2.1912489 2.1912489

Chlorine atom ($^2\text{P}_{3/2}$)

none Cl(2P) 119.621 ! ± 0.0021 ATcT v.1.118

Cl
!
!
!
1 1 2

0.0 4
882.36 2
0 'HAR' 'AMUA'

Chloroxyl radical (ClO)•

none ClO 101.116 ! ± 0.035 ATcT v.1.118
ClO
! vib, rot, electronic parameters from NIST-JANAF pg. 795
!
!
1 1 4 ! C₁∞v
0.0 2 ! 2PI3/2
320.31 2
31650. 2
32169. 2
2 'HAR' 'CM-1'
1 vib 853.72446 -5.579573 1
2 qro 0.6205058 1 2 ! Bo = 0.62347334 - 0.005935/2

Chlorine dioxide, or chloryl radical (O-Cl-O)•

none OClO 101.5 ! ± 0.7 Karton JPCA 2009, 113, 4802
ClO2 ! 99.8 W3X-L JMS unpub.
! C2v symm 2B1
! B3LYP/cc-pVTZ+d Anharmonic unscaled
! Lit. NIST-JANAF S(298K) = 256.8, Cp=41.95; this work 256.88, 42.06
2 1 2
0.0 2
21013.9 2
5 'HAR' 'GHZ'
1 vib 1100.13 -5.16 1 ! B2
2 vib 948.69 -3.59 1 ! A1
3 vib 447.71 -0.27 1 ! A1
4 qro 51.3451 1 1 !
5 qro 9.03912 1 2 ! 9.8697276 8.2784208

none OClO 100.6 ! Delmdahl JCP 114 8339 (2001) ??
ClO2 !
! Rotational constants from Esposito et al. JPCA, 1999 103, 1748-1757
! vibrations from NIST-JANAF pg. 797 C2v
! Lit. NIST-JANAF S(298K) = 256.8, Cp=41.95; this work 256.72, 41.95
2 1 2
0.0 2
21013.9 2
5 'OBS' 'CM-1'
1 vib 945.580 0.0 1 ! sym. stretch
2 vib 447.675 0.0 1 ! bend
3 vib 1110.1054 0.0 1 ! asym. stretch
4 qro 1.737 1 1 ! cm-1
5 qro 0.304 1 2 ! cm-1; 0.332 & 0.278

Chlorine ³⁵Cl₂, ³⁷Cl₂, ³⁵Cl³⁷Cl

none ³⁵Cl³⁵Cl 0.0 ! By definition
[Cl35]2
! electronic states: Cl2 (natural abundance) from NIST-JANAF 1998
! B3LYP/cc-pVTZ+d freqs, rots, anharmonic
! 57.4% in Cl2; NIST-JANAF lit. S=223.1, Cp=33.95; calc. 222.96, 34.02
2 1 2
0.0 1
17832.8 6
2 'OBS' 'GHZ'
1 vib 536.12 -2.303 1
2 qro 7.132913 1.0 2 !

none 37Cl37Cl 0.0 ! By definition
 [Cl37]2
 ! electronic states: Cl2 (natural abundance) from NIST-JANAF 1998
 ! B3LYP/cc-pVTZ+d freqs, rots, anharmonic
 ! 5.9% abundant in Cl2; lit. NIST-JANAF S=223.1, Cp=33.95; calc. 224.25, 34.16
 2 1 2
 0.0 1
 17832.8 6
 2 'OBS' 'GHZ'
 1 vib 521.63 -2.179 1
 2 qro 6.7475637 1.0 2 !

none 35Cl37Cl 0.0 ! By definition
 [Cl35][Cl37]
 ! electronic states: Cl2 (natural abundance) from NIST-JANAF 1998
 ! B3LYP/cc-pVTZ+d freqs, rots, anharmonic
 ! 36.7% abundant in Cl2; NIST-JANAF lit. S=223.1, Cp=33.95; calc. 229.37, 34.09
 1 1 2
 0.0 1
 17832.8 6
 2 'OBS' 'GHZ'
 1 vib 528.97 -2.241 1
 2 qro 6.9402383 1.0 2 !

Chlorosyl chloride Cl-Cl=O

none ClClO 125.0 ! W3X-L JMS unpub. Indirect 154.? Xu, Lin JPCA 2010, 114, 11477
 Cl2O
 ! NIST-JANAF pg. 842 dHf(0)=91 ± 30
 ! B3LYP/cc-pVTZ+d anharmonic unscaled
 ! 298.15 K NIST-JANAF pg. 842 S=278.8, Cp=48.84; this work 276.93, 48.58
 1 1 1 ! Cs symm
 0.0 1 ! 1A'
 4 'HAR' 'GHZ'
 1 vib 249.4 -0.150 1 ! 240.2 Observed Ar matrix Johnsson JPC 1995, 99, 3965
 2 vib 402.8 -1.74 1 ! 374.2
 3 vib 986.3 -7.22 1 ! 961.9
 4 top 3.7654 31.9939 1 ! GHZ 31.9939350 3.9935201 3.5503600

none ClClO 92.5
 Cl2O
 ! enthalpy:JPL-06-2
 ! vibs: WebBook (11/2007); rotational moments:[HyperChem PM3]
 ! this work S=277.48 Cp=45.04
 1 1 1 !
 0.0 2 !
 5 'OBS' 'AMUA'
 1 vib 754. 0.0 1
 2 vib 648. 0.0 1
 3 vib 543. 0.0 1
 4 qro 19.22 1. 1 ! symm top: A-B = 1/17.0137 - 1/147.9 = 1/19.22
 5 qro 147.9 1. 2 ! B: 2-D Adiabatic Rotor

Chlorine peroxide Cl-O-O-Cl

none ClOOC1 133.3 ! 128.8 W3X-L JMS unpub.; 137.7 Matus JPCA Letts 2008, 112, 9623
 Cl2O2
 ! B3LYP/cc-pVTZ+d freqs, rots., scan, anharmonics
 ! Replaced 4 vib 125.18 0.267 1 by HR treatment
 ! 298.15 K Lit. S=302.1 PCCP 2010, 12, 11596; Calc. S=301.16, Cp=66.23
 2 1 1 ! C2 symm
 0.0 1 ! 1A
 7 'OBS' 'GHZ'
 1 vib 813.17 -8.38 1 ! A
 2 vib 531.90 -4.80 1 ! A

3 vib 315.36 -1.70 1 ! A
4 hrd 13 10 1
Vhrd3 1 0.0077 1602.530 36.190 -1369.689 -86.352 -161.749 -24.433 3.429 -380.722 -
262.773 295.485 -64.428 47.642 2.203
Bhrd1 1 0.0077 1.842 9.979E-02 -7.260E-01 -7.036E-02 -7.821E-02 -5.281E-02 -7.172E-03 -
2.619E-05 3.325E-03 1.381E-03
5 vib 622.69 -3.74 1 ! B
6 vib 433.55 -0.508 1 ! B
7 top 2.1319 13.3076 1 ! 13.3075867 2.2539426 2.0164721

none ClOOC1 133.3 ! ± 1 dHf(0) from NASA/JPL-15
Cl2O2

! vibs: Observed freq. [Jacobs et al. 1994]
! anharmonicities: calculated using B3LYP [Maranzana 2007, unpublished]
! rots: from NIST/JANAF [Birk et al 1989; Chase et al. 1998]
! unsymm hindered rotor (B3LYP very tight convergence) from D. Thogluva 5/17/2009
! note: optical isomers are handled by the hindered rotor parameterization
! This Work: S=301.33 , Cp=66.46
! 11/2016 revised dHf(0) (JRB)

2 1 1
0.0 1
7 'OBS' 'GHZ'
1 vib 754. -9.329 1 ! obs frequency & calculated anharmonicity
2 vib 648. -3.061 1 ! obs frequency & calculated anharmonicity
3 vib 543. -3.889 1 ! obs frequency & calculated anharmonicity
4 vib 419. 0.069 1 ! obs frequency & calculated anharmonicity
5 vib 321. -1.695 1 ! obs frequency & calculated anharmonicity
6 hrd 8 8 1 ! Dhillip Thogluva 5/17/2009
Vhrd2 1 -0.0033172 1581.3 231.05 1345.9 480.4 -107.26 -55.538 -3.0586 0.067678
Ihrd1 1 0.00007 11.831 -4.9066 -3.1732 -0.46872 1.0715 0.74663 -0.19779 -0.42143
7 top 2.258 13.086 1 ! GHz [Birk et al 1989; isotopic average]

Chlorine chlorite Cl-O-Cl-O

none ClOClO 164.2 ! Matus JPCA Letts 2008, 112, 9623; W3X-L 164.2 JMS unpub.
Cl2O2 ! [Cl-O-O-Cl - Cl-O-Cl-O] diff. in v good agreement

! B3LYP/cc-pVTZ+d freqs, rots, scan, anharmonics; replaced #6 vib 109.34 -1.58 1
! Cl symm
! 298.15 K Calc. S=312.53 Cp=69.77 H(T)-H(0)=15.54
1 1 1 ! optical isomers are handled by the HR
0.0 1 ! 1A

7 'OBS' 'GHZ'
1 vib 999.73 -7.54 1
2 vib 602.01 -5.12 1
3 vib 418.54 -4.31 1
4 vib 343.51 -1.02 1
5 vib 250.36 -1.05 1
6 hrd 13 10 1
Vhrd3 1 2.027 874.692 -338.939 203.0 -30.608 109.470 35.743 10.971 -249.591 637.560
93.650 -77.464 0.568 7.117
Bhrd1 1 2.027 1.558 1.33E-01 1.53E-03 -1.64E-02 -4.17E-03 -2.83E-02 3.88E-04 -1.73E-02
-4.27E-04 2.62E-02
7 top 2.31965 14.8331 1 ! 14.8331447 2.4207235 2.2228049

none ClOClO 166.5 ± 5 ! dHf(0): NASA/JPL-15
Cl2O2

! vibs: CCSD(T)//CBS from Matus et al., JPCA, 2008, 112, 9623-9627
! in good agreement with experiments (Jacobs et al., JACS 116, 1106 (1994))
! anharmonicity: B3LYP/cc-pVTZ+d computed by Simmie (11/2016)
! external rots: geometry from Matus et al. 2008
! hindered internal rotor: B3LYP/cc-pVTZ+d relaxed scan by J. M. Simmie (11/2016)
! (replaced #6 vib 103.9 -1.58 1 [Matus vib and Simmie anharmonicity])
! excited electronic states: Matus et al. (2008)
! This Work: S=311.25 , Cp=68.91 //
! 11/2016 revised anharmonicities, rots, hindered rotor, excited states, and dHf(0)

```

1 1 1 ! optical isomers handled by hindered rotor
0.0 1
7 'HAR' 'GHZ'
1 vib 1003.8 -7.54 1
2 vib 647.4 -5.12 1
3 vib 483.0 -4.31 1
4 vib 351.5 -1.02 1
5 vib 251.5 -1.05 1
6 hrd 13 10 1
Vhrd3 1 2.027 874.692 -338.939 203.000 -30.608 109.470 35.743 10.971 -249.591
637.560 93.650 -77.464 0.568 7.117
Bhrd1 1 2.027 1.558 1.334E-01 1.531E-03 -1.644E-02 -4.168E-03 -2.834E-02 3.876E-
04 -1.728E-02 -4.274E-04 2.624E-02
7 top 2.5419 13.1036 1 ! 13.1036 2.6962 2.3965 GHz (Matus 2008)

```

Chloryl chloride Cl-Cl(O)₂

```

none ChlorylChloride 113.5 ! W3X-L, 119.4 W2X JMS unpub.
Cl2O2
! B3LYP/cc-pVTZ+d freqs, rots; scale=0.9681
!
! 298.15 K Calc. S=295.45 Cp=61.33 H(T)-H(0)=13.92
1 1 1 ! Cs symm
0.0 1 ! 1A1
7 'HAR' 'GHZ'
1 vib 236.91 0.0 1 ! A"
2 vib 259.18 0.0 1 ! A'
3 vib 430.51 0.0 1 ! A'
4 vib 509.81 0.0 1 ! A'
5 vib 1032.63 0.0 1 ! A'
6 vib 1200.42 0.0 1 ! A"
7 top 3.05539 9.42025 1 ! 9.4202539 3.4518381 2.7044706

```

```

none ClClO2 113.5 ! W3X-L, 119.4 W2X JMS unpub. 118.7± 5 NASA/JPL-15
Cl2O2
! vibs: observed freq. Muller et al. JCP, 1999, 110, 24, 11865. doi:10.1063/1.479179
! Rots: microwave Cl(35) isotopomer [Muller et al. 1999]
! This Work: S=293.84 , Cp=60.60 //
! 11/2016 revised vibs, rots, dHf(0) (JRB)
1 1 1
0.0 1
7 'OBS' 'MHZ'
1 vib 1062.84 0.0 1
2 vib 527.73 0.0 1
3 vib 443.51 0.0 1
4 vib 274.08 0.0 1
5 vib 1240.70 0.0 1
6 vib 253.16 0.0 1
7 top 3162.8 9450.93 1 ! MHZ

```

Chlorine chlorate Cl-O-ClO₂ or Cl₂O₃

```

none Cl2O3 145.36 !
Cl2O3
! dHf(0) adjusted to fit 3rd law Do = 56.3 kJ/mol
! vibs Zhu & Lin [JCP 118, 8645 (2003)]
! consistent Richard & Vaida, JCP, 1991, 94, 153.
! HR Thogluva B3LYP/6-311+G(3DF); external rots Friedl, JMS 170, 383-396 (1985)
! S=349.3 ± 8.0 and HoF(298)=138.3 ± 2.4 PCCP 2003, 5, 5409
1 1 2
0.0 1
37450. 3
11 'HAR' 'MHZ'
1 hrd 7 8 1
Vhrd2 1 -3.1416 236.74 -281.84 217.34 -80.528 82.475 9.3318 -3.5737
Ihrd1 1 -3.1416 16.833 0.92708 2.4859 0.63008 0.1878 -0.029472 -0.27384 -0.14777

```

2	vib	185	0.0	1
3	vib	257	0.0	1
4	vib	368	0.0	1
5	vib	434	0.0	1
6	vib	1231	0.0	1
7	vib	1061	0.0	1
8	vib	764	0.0	1
9	vib	540	0.0	1
10	gro	8597.1	1	1
11	gro	1920.9	1	2

Cyclopropane (CH₂)₃

none Cyclopropane 70.80 ! ±0.46 ATcT v1.122 53.65 @ 298KC3H6
! Stein & Rabinovitch, JCP 2438 (1973)
! Symmetry D3h; Dorofeeva JPhyChemRefData, 1986, 15, 437-464
! Lit. S=237.4 Ruehrwein 1946, Cp=55.6 Dorofeeva
! Calc S=235.57, 55.83, H(T)-H(0)=11.426 1 1
0.0 1

	'OBS'	'AMUA'			
1	vib	3060.3	-80.35	6	! 3221+2*(-80.35)=3060.3
2	vib	1453.8	-12.11	3	! 1478+2*(-12.11)=1453.8
3	vib	1101.7	-8.15	7	! 1118+2*(-8.15)=1101.7
4	vib	864.1	-7.43	3	! 879+2*(-7.43)=864.1
5	vib	738.9	-5.55	2	! 750+2*(-5.55)=738.9
6	gro	25.4	1.0	1	
7	gro	25.4	1.0	2	

none Cyclopropane 70.80 ! ±0.46 ATcT v1.122 53.65 @ 298K
C3H6

! B3LYP/cc-pVTZ+d freqs, rots, scaled=0.9681
! Lit. S=237.4 Ruehrwein 1946, Cp=55.6 Dorofeeva JPCRD 1986, 15, 437
! 237.63 56.40, H(T)-H(0)=11.49

6 1 1 ! D3h symm
0.0 1 ! 1A1'

	'HAR'	'GHZ'			
1	vib	720.21	0.0	2	! E''
2	vib	835.66	0.0	1	! A2''
3	vib	853.99	0.0	2	! E'
4	vib	1022.31	0.0	2	! E'
5	vib	1061.59	0.0	1	! A2'
6	vib	1118.18	0.0	1	! A1''
7	vib	1174.21	0.0	1	! A1'
8	vib	1176.08	0.0	2	! E''
9	vib	1430.70	0.0	2	! E''
10	vib	1472.55	0.0	1	! A1'
11	vib	3027.79	0.0	2	! E'
12	vib	3034.66	0.0	1	! A1'
13	vib	3098.00	0.0	2	! E''
14	vib	3118.68	0.0	1	! A2''
15	top	20.2499	12.649	1	! 20.2498788 20.2498788 12.6488952

Cubane, tetraprismane C₈H₈

none Cubane 630.6 ! JMS est 603.3@298K cf 603.4±4 Agapito, JPCA 2015,119,2998-3007
C8H8

! B3LYP/cc-pVTZ+d vibs,rots, scale=0.9681
! dHf(298.15K) 597.1 ± 5.0 Kybett et al JACS, 1966, 88, 3, 626-626.
! Lit. CCCBDB lists S=300 but omits -R*ln(sigma)
! Lit. S=272.0, Cp=100.2, Karpushenkava et al. J Mol Struc THEOCHEM 913 (2009) 43-49
! Calc. 272.65, 101.30, H(T)-H(0)=14.94

24 1 1 ! Oh external symmetry number, OIs, e-states
0.0 1 ! 1Alg; Exptal IR Boudon et al. JPCA 2016, 120, 4418-4428
19 'HAR' 'GHZ' ! IR active u, Raman active g
1 vib 602.84 0.0 2 ! Eu
2 vib 659.33 0.0 3 ! T2g

3	vib	808.38	0.0	3	!	T2u =F2u 819
4	vib	811.43	0.0	3	!	T2g
5	vib	836.14	0.0	3	!	T1u =Flu IR 852
6	vib	882.61	0.0	2	!	Eg
7	vib	984.33	0.0	1	!	A1g
8	vib	1018.76	0.0	1	!	A2u
9	vib	1032.20	0.0	3	!	T2u
10	vib	1076.62	0.0	2	!	Eg
11	vib	1129.29	0.0	3	!	T1g
12	vib	1146.93	0.0	2	!	Eu
13	vib	1181.39	0.0	3	!	T2g
14	vib	1226.98	0.0	3	!	T1u =Flu IR 1235
15	vib	2991.41	0.0	1	!	A2u
16	vib	3000.66	0.0	3	!	T2g
17	vib	3008.04	0.0	3	!	T1u =Flu IR 2991
18	vib	3025.66	0.0	1	!	A1g
19	gro	3.3676	1.0	3	!	3D rotor symmetry=1 3.3675957 3.3675957 3.3675957

Cyanoimidogen, $^3\text{N}-\text{C}\equiv\text{N}$ ($D_{\infty h}$)

none NCN-triplet 454.5 ! W3X-L, 450.39 ± 0.68 ATcT v1.122
C1N2
! B3LYP/cc-pVTZ+d freqs, rots anharm
! Lit. S=226.21 NIST-JANAF,
! 225.8, Cp=41.9 @ 300K Canneau Comput Theor Chem 967 2011 67-74
! Calc. 225.41 41.53, H(T)-H(0)=10.12
2 1 1 ! Dinfh
0.0 3 ! 3Sgg
5 'HAR' 'GHZ'
1 vib 1273.97 -3.023 1 ! P1lu
2 vib 1560.71 4.083 1 ! Sgg
3 vib 448.57 -0.967 1 ! Sgu
4 vib 448.57 -0.967 1 ! Sgu
5 gro 12.0360 1 2 ! 0.0000000 12.0360028 12.0360028

Deuterium atom ($^2\text{S}_{1/2}$)

none D 219.804 ! ATcT v.1.122 221.717 at 298.15 K
D
! NIST-JANAF pg 1029
! S=123.350, Cp=20.786
! S=123.24, Cp=20.79, HT)-H(0)=6.20
1 1 1 !
0.0 2 ! 2S1/2
0 'HAR' 'AMUA'

Deuteroxyl radical OD

none OD 34.741 !
OD
! NIST-JANAF pg. 1038
! OD-OH dhf(0) difference NIST-JANAF combined with OH dhf(0)
! OH dhf(0) from Ruscic, JPCA, 2006, 110 (21), 6592-6601
1 1 4
0.0 2
139.7 2
35474. 2
68769. 2
2 'HAR' 'AMUA'
1 vib 2720.9 -44.2 1
2 gro 1.6822 1.0 2 !

Diacetylene or 1,3-butadiyne HCCCCH

none diacetylene 458.63 ! ATcT v1.118 ± 0.87

C4H2

! vibs. Simmonett, JCP, 130, 044301 (2009) TableIV
! rots. Thorwirth, JMolSpectr. 251 (2008) 220D223
! Maranzana JPCA 2015 S=251.0, Dorofeeva ThermActa 1991 Cp=73.7;
! Calc. 249.9, 73.51
2 1 1
0.0 1
10 'HAR' 'MHz'
1 vib 3463.3 -64.25 1
2 vib 2243.0 -23.55 1
3 vib 894.4 -13.75 1
4 vib 3464.5 -65.65 1
5 vib 2064.0 -19.10 1
6 vib 636.3 -2.60 2
7 vib 484.5 +2.10 2
8 vib 639.6 -3.65 2
9 vib 221.4 -0.25 2
10 qro 4389.3019 1.0 2 ! 2-D rotor

Diazene or diimide, HN=NH, trans or (E) conformer

none HNNH 208.8 ! W3X-L JMS JPhysChemA 2016,120,7370-7384 trans or (E)-diazene/diimide
N2H2
! B3LYP/cc-pVTZ+d vibs, rots, anharmonic; no HR, barrier > 50 kcal
! Gaussian-16 S=217.98, Cp=34.88
! Calc. 217.97 34.88, H(T)-H(0)=9.98
2 1 1 ! C2h symmetry
0.0 1 ! 1Ag
7 'OBS' 'GHZ'
1 vib 2983.11 -47.71 1 ! Gaussian: E(anharm) vibs + Xjj
2 vib 1618.71 -7.33 1 !
3 vib 1557.00 -2.84 1 !
4 vib 1316.02 -6.04 1 !
5 vib 3069.12 -46.13 1 !
6 vib 1325.82 -5.60 1 !
7 top 37.38 304.064 1 ! 304.0639076 39.7434349 35.1491741

Dideuterium D₂

none D2 0.00
D2
! WebBook March 6, 2009
!
!
2 1 1
0.0 1
2 'HAR' 'CM-1'
1 vib 3115.50 -61.82 1
2 qro 29.9043 1.0 2 !Ia

Ditritium T₂

none T2 0.00
T2
! WebBook March 6, 2009
!
!
2 1 1
0.0 1
2 'HAR' 'CM-1'
1 vib 2546.47 -41.23 1
2 qro 20.04065 1.0 2 ! Ia

Diethyl ether, CH₃CH₂OCH₂CH₃

none CH3CH2OCH2CH3 0.00 ! -252.7 ± 2.0 at 298.15 K Pedley 1986
C4H10O

```

! Diethyl ether DEE CCOC, COCC trans/trans conformer
! MN12SX/6-311++G(d,p) vibs, rots; scans scaling factor: 0.97554
! Lit. S=342.2 Counsell JF JACS 1971 313-316; Cp=119.46 ±0.15
! calc. 343.24 122.84, H(T)-H(0)=23.46
2 1 1 ! C2v symmetry, no optical isomers
0.0 1 ! Singlet
40 'HAR' 'GHZ'
1 hrd 13 10 1 !FREQUENCY REMOVED = 100.4 cm-1 , Max % Error V(x) = 2.3%, B(x) = 8.2%
Vhrd3 1 -0.0008 847.7209 -589.2633 221.2907 -485.7751 15.4159 -25.4792 16.0879 0.0288 -
0.2263 -0.153 0.0597 -0.0456 -0.0725
Bhrd1 1 -0.0008 1.8392 -0.4918 0.3937 -0.0334 -0.4111 0.4609 -0.234 0 -0.0528 0.1058
2 hrd 13 10 1 !FREQUENCY REMOVED = 114.9 cm-1 , Max % Error V(x) = 2.3%, B(x) = 8.2%
Vhrd3 1 -0.0008 847.7209 -589.2633 221.2907 -485.7751 15.4159 -25.4792 16.0879 0.0288 -
0.2263 -0.153 0.0597 -0.0456 -0.0725
Bhrd1 1 -0.0008 1.8392 -0.4918 0.3937 -0.0334 -0.4111 0.4609 -0.234 0 -0.0528 0.1058
3 vib 189.51 0.0 1 ! A1 rocking
4 hrb 247.00 1074.2 3 ! A2 Me HRs 12.85 kJ
5 hrb 253.25 1074.2 3 ! B1 Me HRs 12.85 kJ
6 vib 422.92 0.0 1 ! B2
7 vib 438.98 0.0 1 ! A1
8 vib 787.73 0.0 1 ! A2
9 vib 801.42 0.0 1 ! B1
10 vib 849.18 0.0 1 ! A1
11 vib 937.08 0.0 1 ! B2
12 vib 1064.95 0.0 1 ! A2
13 vib 1079.52 0.0 1 ! B2
14 vib 1139.09 0.0 1 ! A2
15 vib 1167.61 0.0 1 ! B1
16 vib 1168.56 0.0 1 ! A1
17 vib 1176.23 0.0 1 ! B2
18 vib 1268.68 0.0 1 ! A2
19 vib 1276.94 0.0 1 ! B1
20 vib 1343.87 0.0 1 ! B2
21 vib 1358.51 0.0 1 ! A1
22 vib 1377.96 0.0 1 ! B2
23 vib 1420.23 0.0 1 ! A1
24 vib 1439.77 0.0 1 ! A2
25 vib 1439.93 0.0 1 ! B1
26 vib 1453.51 0.0 1 ! B2
27 vib 1456.86 0.0 1 ! A1
28 vib 1474.70 0.0 1 ! B2
29 vib 1494.55 0.0 1 ! A1
30 vib 2883.60 0.0 1 ! B2
31 vib 2893.70 0.0 1 ! A1
32 vib 2929.75 0.0 1 ! B1
33 vib 2931.55 0.0 1 ! A2
34 vib 2968.24 0.0 1 ! B2
35 vib 2968.63 0.0 1 ! A1
36 vib 3069.44 0.0 1 ! B2
37 vib 3069.62 0.0 1 ! A1
38 vib 3069.67 0.0 1 ! A2
39 vib 3069.82 0.0 1 ! B1
40 top 2.19314 18.1229 1 ! 18.1228537 2.2665683 2.1220978

```

Dinitrogen N₂

```

none N2 0.0 ! By definition
N2
! NIST-JANAF 1998
!
!
2 1 4
0.0 1
49754.78 3
59306.81 6
59380. 6

```

```

2 'HAR' 'AMUA'
1 vib 2358.583 -14.33594 1
2 qro 8.43642 1.0 2

```

Dinitrogen ¹⁴N₂

none 14N2 0.0 ! By definition

[N14]2

1. electronic states same as "N2" in NIST-JANAF 1998
2. vibs from Gilson, JRS 9, 361-368 (1980)
3. rots from Bendtsen, JRS 2, 133-145 (1974)

```

2 1 4
0.0 1
49754.78 3
59306.81 6
59380. 6

```

```

2 'HAR' 'AMUA'
1 vib 2358.5665 -14.31921 1
2 qro 8.47298 1.0 2

```

Dinitrogen ¹⁵N₂

none 15N2 0.0 ! By definition

[N15]2

- ! electronic states same as "N2" in NIST-JANAF 1998
! vibs from Gilson, JRS 9, 361-368 (1980)
! rots from Bendtsen, JRS 2, 133-145 (1974)

```

2 1 4
0.0 1
49754.78 3
59306.81 6
59380. 6

```

```

2 'HAR' 'AMUA'
1 vib 2278.9107 -13.39285 1
2 qro 9.07458 1.0 2

```

Dinitrogen pentoxide⁷ O₂N-O-NO₂ or N₂O₅

none N2O5 24.33 ! ± 0.35 ATcT v.1.118

N2O5

- ! vibs & rots: CCSD(T)/avdz from Halpern & Glendening, JCP 127,164307 (2007)
! optical isomers: 2 for structure #1 (Alecú & Marshall, JPCA 2014, 118, 11405-11416)
! This Work: S=343.12 , Cp=93.50 // NIST-JANAF: 346.548, 96.303
! Note: S=353.45 , Cp=86.53 from multi-conformer method (Alecú & Marshall 2014)
! 11/2016 revised dHf(0) (JRB)

```

2 2 1 ! C2 symm, 2 optical isomers
0.0 1

```

```

16 'HAR' 'AMUA'
1 vib 1782. 0.0 1
2 vib 1356. 0.0 1
3 vib 856. 0.0 1
4 vib 799. 0.0 1
5 vib 651. 0.0 1
6 vib 376. 0.0 1
7 vib 233. 0.0 1
8 hra 78. 28.3 2 ! reduced Ir (JANAF 1998); freq. (Halpern & Glendening)
9 vib 1742. 0.0 1
10 vib 1264. 0.0 1
11 vib 738. 0.0 1
12 vib 715. 0.0 1
13 vib 572. 0.0 1
14 vib 367. 0.0 1
15 hra 51. 28.3 2 ! reduced Ir (JANAF 1998); freq. (Halpern & Glendening)
16 top 273.2 77.69 1 ! AMUA Halpern & Glendening, JCP 127,164307 (2007)

```

⁷ Needs more work.

Dihydrogen H₂

none H2 0.00 ! By definition
H2
! WebBook March 6, 2009
! Lit. S=130.68 NIST-JANAF
!
2 1 1
0.0 1
2 'HAR' 'CM-1'
1 vib 4401.213 -121.336 1
2 qro 59.3219 1.0 2 !Ia Bo = Be-alphae/2

Deuterium hydride HD

none HD 0.328 ! ± 0.000 ATcT v.1.118
HD
! vib & rot: WebBook September 13, 2016
! dHf(0)
!
1 1 1
0.0 1
2 'HAR' 'CM-1'
1 vib 3813.15 -91.65 1
2 qro 44.662 1.0 2 ! Be = 45.655 cm-1, alpha(e) = 1.986 cm-1

Diazenyl, H-N=N

none Diazenyl 252.25 ! ±0.48 ATcT v1.122
N2H
! B3LYP/cc-pVTZ+d vibs, rots, scaled=0.9681
! Lit. S=224.22, Cp=34.57, JPCA 2016, 120, 7192-7197
! Calc. 224.33 34.57, H(T)-H(0)=9.98
1 1 1 ! Cs
0.0 2 ! 2A'
4 'HAR' 'GHZ'
1 vib 1089.38 0.0 1 ! A'
2 vib 1816.14 0.0 1 ! A'
3 vib 2685.70 0.0 1 ! A'
4 top 45.3437 665.114 1 ! 665.1136201 46.9157265 43.8244418

none Diazenyl 252.25 ! ±0.48 ATcT v1.122
N2H
! B3LYP/cc-pVTZ+d vibs, rots, anharmonics unscaled
! Lit. S=224.22, Cp=34.57, JPCA 2016, 120, 7192-7197
! Calc. 224.31 34.50, H(T)-H(0)=9.98
1 1 1 ! Cs
0.0 2 ! 2A'
4 'HAR' 'GHZ'
1 vib 1125.3 -8.25 1 ! A'
2 vib 1876.0 -10.66 1 ! A'
3 vib 2774.2 -188.8 1 ! A'
4 top 45.3437 665.114 1 ! 665.1136201 46.9157265 43.8244418

1,2-Dioxete, dioxirene, cyclo(OOCHCH)

none Dioxete 140.7 ! ±1.7 Isodesmic JMS unpub.
C2H2O2
! Dioxete + Cyclopropane = Dioxirane + Cyclobutene
; DrH= -25.29±1.22 at 0 K CBS-QB3, -APNO, G3, G4, W1BD
! B3LYP/cc-pVTZ+d freqs, rots, anharm, unscaled O---CH
! Lit. S=256.7 Cp=53.60 | | PM3 JPCA, 1997, 101, 2471-2477
! Calc. 254.90 53.42, H(T)-H(0)=11.47 O---CH
2 1 1 ! C2v symm
0.0 1 ! 1A1
13 'HAR' 'GHZ'

1	vib	3319.21	-25.60	1
2	vib	1648.82	-7.21	1
3	vib	1221.86	-3.13	1
4	vib	1071.71	-0.89	1
5	vib	878.06	-3.33	1
6	vib	707.26	4.19	1
7	vib	601.19	-0.76	1
8	vib	691.47	0.22	1
9	vib	3283.72	-26.09	1
10	vib	1253.07	-2.64	1
11	vib	1005.56	-1.54	1
12	vib	893.16	0.18	1
13	top	15.9674	7.9810	1 ! 16.3926831 15.5531940 7.9809542

Dioxirane, dioxacyclopropane, cyclo-H2 (COO)

none dioxirane 8.8 ! W3X-L JMS unpub. 1.1 at 298K; ATcT (0K) 9.41, 298K 1.74±0.54
C1H2O2

! B3LYP/cc-pVTZ+d vibs, rots, unscaled, anharmonic

! NIST WEBBOOK Cp=43.9±3.0 at 1 bar Dorofeeva, Thermochim. Acta 1992, 194,9-46

! calc. S=246.30, Cp=42.00, H(T)-H(0)=10.46

2 1 1 ! C2v, Sopt, Nele

0.0 2 ! 1A1

10		'HAR'	'GHZ'	
1	vib	3052.409	-29.10	1 ! A1
2	vib	1548.394	-0.098	1 ! A1
3	vib	1310.824	-3.69	1 ! A1
4	vib	822.932	-3.00	1 ! A1
5	vib	1026.372	-1.19	1 ! A2
6	vib	3145.584	-34.39	1 ! B1
7	vib	1179.977	-1.13	1 ! B1
8	vib	1259.376	-4.33	1 ! B2
9	vib	896.314	-1.71	1 ! B"
10	top	27.226	14.981	1 ! 28.85822 25.68609 14.98119

Dioxiranylmethyl, cyclo(OOCH)CH2'

none Dioxiranylmethyl 196.7 ! JMS unpub. W3X-L 187.1 at 298K cf
C2H3O2

! B3LYP/cc-pVTZ+d vibs, rots, scale=0.9681

! Lit.

! calc S=283.20, Cp=69.05, H(T)-H(0)=14.01

1 1 1 ! Cs symm

0.0 2 ! 2A" ground state

16		'HAR'	'GHZ'	
1	vib	246.20	0.0	1 ! A"
2	vib	382.36	0.0	1 ! A"
3	vib	436.99	0.0	1 ! A'
4	vib	604.51	0.0	1 ! A"
5	vib	754.64	0.0	1 ! A"
6	vib	763.55	0.0	1 ! A'
7	vib	929.86	0.0	1 ! A'
8	vib	1107.76	0.0	1 ! A"
9	vib	1115.85	0.0	1 ! A'
10	vib	1201.05	0.0	1 ! A'
11	vib	1361.68	0.0	1 ! A'
12	vib	1419.72	0.0	1 ! A'
13	vib	3017.35	0.0	1 ! A'
14	vib	3061.82	0.0	1 ! A'
15	vib	3172.85	0.0	1 ! A'
16	top	7.1918	19.8608	1 ! 19.8608 7.7153037 6.7037475

none Dioxiranylmethyl 196.7 ! JMS unpub. W3X-L 187.1 at 298K cf
C2H3O2

! B3LYP/cc-pVTZ+d vibs, rots, anharmonics

! Lit.

```

! calc S=282.65, Cp=68.45, H(T)-H(0)=13.90
1 1 1 ! Cs symm
0.0 2 ! 2A" ground state
16 'HAR' 'GHZ'
1 vib 3278.38 -32.30 1 ! A'
2 vib 3163.47 -27.98 1 ! A'
3 vib 3117.11 -65.05 1 ! A'
4 vib 1466.52 -7.80 1 ! A'
5 vib 1407.10 -7.58 1 ! A'
6 vib 1241.57 -4.32 1 ! A'
7 vib 1152.48 -4.21 1 ! A'
8 vib 960.63 -1.12 1 ! A'
9 vib 789.20 -1.78 1 ! A'
10 vib 451.45 0.94 1 ! A'
11 vib 1144.43 -4.20 1 ! A"
12 vib 780.30 0.33 1 ! A"
13 vib 624.73 13.85 1 ! A"
14 vib 394.38 -0.05 1 ! A"
15 vib 256.82 -6.47 1 ! A"
16 top 7.1918 19.8608 1 ! 19.8608 7.7153037 6.7037475

```

Dioxygen O₂

```

none O2 0.0 ! By definition for the ground state
O2
! NIST-JANAF 1998 and Ruscic et al. JPCA 2002, 106, 2727-2747
! Lit. CODATA S=205.152 Cp=29.38; this work 204.97, 29.36
!
2 1 4
0.0 3
7882.39 2
13120.9 1
32664.1 1
2 'HAR' 'AMUA'
1 vib 1580.1932 -11.98 1
2 qro 11.6612 1.0 2

```

Dioxygen O₂ (¹Δ_g)

```

none O2delta 94.410 ! ATcT v1.118
O2
! NIST WebBook [http://WebBook.nist.gov/ accessed March 5, 2013]
! Lit. CODATA S=205.152; this work 201.73, Cp=29.46
!
2 1 1
0.0 2
2 'HAR' 'cm-1'
1 vib 1483.5 -12.9 1
2 qro 1.4264 1.0 2

```

Dioxymethyl or methanal oxide CH₂=O^{δ+}-O^{δ-} 'Crige intermediate'

```

MethanalOxide 113.6 ! ± 1.2 ATcT v.1.118; W2X 115.7, W3X-L 110.8 JMS unpub.
CH2O2
! T1 > 0.04
! B3LYP/cc-pVTZ+d vibs,rots,anharmonics; scan of HCOO v diff, barrier > 50 kJ
! Lit. S= Cp= ; calc. 248.91, 47.75
1 1 1 ! External symmetry, optical isomers, elec. states
0.0 1 ! 1A1
10 'OBS' 'GHZ'
1 vib 3124.09 -32.867 1 ! A'
2 vib 3018.83 -29.053 1 ! A'
3 vib 1490.75 -5.647 1 ! A'
4 vib 1369.83 -3.571 1 ! A'
5 vib 1220.73 -0.439 1 ! A'

```

```

6 vib 909.03 -8.382 1 ! A'
7 vib 521.55 -0.411 1 ! A'
8 vib 920.31 1.100 1 ! A" HRD C--O "Lanczos difficulty"
9 vib 659.42 -3.184 1 ! A"
10 top 11.567 81.325 1 ! 81.3249651 12.4187061 10.7735363

```

none Methanal_oxide 113.6 !± 1.2 ATcT v.1.118

CH2O2

```

! CH2O0; formaldehyde oxide; dioxymethyl; Criegee Intermediate;
! dHf(0) reasonably consistent with [Lehman et al. JCP 139,141103 (2013)].
! vibs: Lanczos fit from Yu et al. JCP 143,084311 (2015)
! rots: Daly et al. JMS 297, 16-20 (2014).
! This Work: S=249.33 , Cp=48.09 //

```

```

1 1 1
0.0 1
10 'HAR' 'MHZ'
1 vib 3177.0 -19.2 1 ! a-CH str
2 vib 3092.0 -50.5 1 ! s-CH str
3 vib 1544.3 -6.3 1 ! CH2 scissor / CO str
4 vib 1364.5 -6.8 1 ! CO str / CH2 scissor
5 vib 1300.6 -11.0 1 ! CH2 rock
6 vib 959.5 -14.4 1 ! OO str
7 vib 522.5 -0.1 1 ! COO deform
8 vib 886.1 -5.5 1 ! CH2 Wag
9 vib 637.8 -7.8 1 ! CH2 twist
10 top 11560.435 77748.949 1 ! MHZ; K-rotornone

```

Disulfur, diatomic sulfur S=S

none S2 128.30

S2

```

! CODATA Key Value
! gas phase Sulfur dimer
! NIST-JANAF 1998

```

```

2 1 4
0.0 3
4700 2
8500 1
21855 6
2 'HAR' 'CM-1'
1 vib 724.67 -2.836 1
2 qro 0.2946 1 2

```

Ethanal oxide CH₃CH=O^{δ+}-O^{δ-} anti conformer 'C2 Criegee intermediate'

none anti-CH₃CHOO 63.5 ! 65.4 W3-F12 Karton CPL 2015,621,193; W2X 67.9, W3X-L 63.5
C2H4O2

```

! B3LYP/cc-pVTZ+d vibs,rots,scan,anharmonic; trans (anti) <=> cis (syn) scan fails
! C--C--O--O 180 degrees or E-conformer
! Calc. S=287.79, Cp=70.49

```

```

1 1 1 !
0.0 1 ! Cs symm
19 'OBS' 'GHZ'
1 vib 3001.272 -46.06 1 ! A'
2 vib 2984.102 -37.65 1 ! A'
3 vib 2907.628 -21.69 1 ! A'
4 vib 1527.241 -7.69 1 ! A'
5 vib 1415.453 -6.38 1 ! A'
6 vib 1381.681 -1.35 1 ! A'
7 vib 1314.059 -1.84 1 ! A'
8 vib 1129.655 -2.85 1 ! A'
9 vib 954.533 -4.37 1 ! A'
10 vib 884.036 -1.32 1 ! A'
11 vib 551.380 -0.48 1 ! A'
12 vib 325.300 0.02 1 ! A'
13 vib 2916.319 -32.22 1 ! A"

```

```

14 vib 1424.387 -6.94 1 ! A"
15 vib 1020.666 -1.63 1 ! A"
16 vib 848.035 -0.46 1 ! A"
17 vib 251.726 -1.05 1 ! A"
18 hrb 151.656 452.2 3 ! A" methyl rotor barrier 5.41 kJ
19 top 4.2984 49.915 1 ! 49.9147175 4.4286437 4.1719642

```

none anti-ethanal_oxide 60.6

C2H4O2

```

! anti-CH3CHOO; anti-acetaldehyd oxide; Criegee intermediate;
! dHf(0): W3-F12 theory [Kettner et al., CPL 621 (2015) 193-198]
! vibs: experimental, or MULTIMODE, or NEVPT2(8,8) [Lin et al., 2015, Nat. Comm.,
! DOI: 10.1038/ncomms8012]
! rots and tors: microwave [Nakajima et al., JMS 310 (2015) 109-112;
! http://dx.doi.org/10.1016/j.jms.2014.11.004]
! This Work: S=288.85 , Cp=70.38 //
! 11/2016 new entry (JRB)

```

```

1 1 1
0.0 1
19 'OBS' 'GHZ'
1 vib 3097.0 0 1 ! NEVPT2(8,8)
2 vib 3021.0 0 1 ! NEVPT2(8,8)
3 vib 2917.0 0 1 ! NEVPT2(8,8)
4 vib 1479.0 0 1 ! experiment
5 vib 1427.0 0 1 ! MULTIIMODE
6 vib 1390.0 0 1 ! MULTIIMODE
7 vib 1279.4 0 1 ! experiment
8 vib 1136.0 0 1 ! MULTIIMODE
9 vib 883.7 0 1 ! experiment
10 vib 851.8 0 1 ! experiment
11 vib 565.0 0 1 ! MULTIIMODE
12 vib 330.0 0 1 ! MULTIIMODE
13 vib 2895.0 0 1 ! NEVPT2(8,8)
14 vib 1446.0 0 1 ! MULTIIMODE
15 vib 1034.0 0 1 ! MULTIIMODE
16 vib 840.0 0 1 ! MULTIIMODE
17 vib 255.0 0 1 ! MULTIIMODE
18 hrc 158.20 399.1 3 ! GHZ
19 top 4.2986 48.8550 1 ! GHZ

```

Ethanal oxide $\text{CH}_3\text{CH}=\text{O}^{\delta+}-\text{O}^{\delta-}$ cis conformer 'C2 Criegee intermediate'

none cis-CH3CHOO 49.1 ! W3X-L JMS unpub. 51.3 W3-F12 Kettner CPL 621,2015,193D198
C2H4O2

```

! B3LYP/cc-pVTZ+d vibs,rots,scan,anharmonic; cis (syn) <=> trans (anti) scan fails
! cis C-C-O-O = 0 degrees or Z-conformer

```

```

! Calc. 283.82 69.82
1 1 1 !
0.0 1 ! Cs symm
19 'OBS' 'GHZ'
1 vib 3065.39 -54.09 1 ! A'
2 vib 3002.90 -43.84 1 ! A'
3 vib 2894.93 -21.68 1 ! A'
4 vib 1511.76 -9.47 1 ! A'
5 vib 1419.68 -6.20 1 ! A'
6 vib 1364.69 -6.08 1 ! A'
7 vib 1318.87 -3.07 1 ! A'
8 vib 1086.47 -2.24 1 ! A'
9 vib 967.88 -1.42 1 ! A'
10 vib 888.31 -6.95 1 ! A'
11 vib 671.66 0.44 1 ! A'
12 vib 284.82 0.27 1 ! A'
13 vib 2899.95 -32.38 1 ! A"
14 vib 1388.11 -6.33 1 ! A"
15 vib 1018.90 -1.65 1 ! A"
16 vib 736.88 0.04 1 ! A"

```

```

17 vib      454.88      -0.67      1 ! A"
18 hrb      174.31      589.3      3 ! A" methyl rotor barrier 7.05 kJ=589.3/cm
19 top       6.0827      17.857     1 ! 17.8573979      7.0779507      5.2274616

```

```

none syn-ethanal_oxide 46.6
C2H4O2

```

```

! syn-CH3CHOO; syn-acetaldehyd oxide; syn-dioxyethyl; Criegee intermediate;
! dHf(0): W3-F12 theory and scaled vibs [Kettner et al., CPL 621 (2015) 193-198]
! vibs: experimental, MULTIMODE, or NEVPT2(8,8) [Lin et al., 2015, Nat. Comm.,
! DOI: 10.1038/ncomms8012]
! rots and torsion [Nakajima & Endo, JCP, 140, 011101 (2014);
! doi: 10.1063/1.4861494]
! This Work: S=283.38 , Cp=70.90 //
! 11/2016 new entry (JRB)

```

```

1 1 1
0.0 1
19 'OBS' 'GHZ'
1 vib 3103.0 0 1 ! MULIIMODE
2 vib 3048.0 0 1 ! MULIIMODE
3 vib 2853.0 0 1 ! NEVPT2(8,8)
4 vib 1476.8 0 1 ! experiment
5 vib 1431.0 0 1 ! MULIIMODE
6 vib 1371.0 0 1 ! MULIIMODE
7 vib 1280.8 0 1 ! experiment
8 vib 1090.6 0 1 ! experiment
9 vib 956.0 0 1 ! experiment
10 vib 871.2 0 1 ! experiment
11 vib 676.0 0 1 ! MULIIMODE
12 vib 314.0 0 1 ! MULIIMODE
13 vib 2976.0 0 1 ! MULIIMODE
14 vib 1408.0 0 1 ! MULIIMODE
15 vib 1008.0 0 1 ! MULIIMODE
16 vib 723.0 0 1 ! MULIIMODE
17 vib 449.0 0 1 ! MULIIMODE
18 hrc 158.02 837.1 3 ! GHZ
19 top 6.1076 17.5865 1 ! GHZ

```

Ethane C₂H₆

```

none Ethane -68.12 ! ± 0.15 ATcT
C2H6

```

```

! Frequencies from Shimanouchi (1972) and Stein & Rabinovitch, JCP 2438 (1973)
! Moments Golden 3/26/2002; torsion Waage & Rabinovitch, IJCK, 3, 105 (1971)
!

```

```

6 1 1
0.0 1
14 'HAR' 'AMUA'
1 vib 2953.7 0. 1 ! CH3 s-str
2 vib 1388.4 0. 1 ! CH3 s-deform
3 vib 994.8 0. 1 ! CC str
4 hrd 1. 1. 3 ! torsion
Vhrd1 3 0. 1024.
Bhrd1 1 0. 10.705
5 vib 2895.8 0. 1 ! CH3 s-str
6 vib 1379.2 0. 1 ! s-deform
7 vib 2968.7 0. 2 ! CH3 d-str
8 vib 1468.1 0. 2 ! CH3 d-deform
9 vib 1190. 0. 2 ! CH3 rock
10 vib 2985.4 0. 2 ! CH3 d-str
11 vib 1469. 0. 2 ! CH3 d-deform
12 vib 821.6 0. 2 ! CH3 rock
13 gro 7.037 1. 1 ! K-rotor
14 gro 25.3 1. 2 ! 2-D rotor

```

Ethanol, CH₃CH₂OH *trans*

none Ethanol -216.89 ! ±0.21 ATcT v1.122 -234.61 @ 298K

C2H6O1

! mn12sx/6-311++G(d,p) vibs, rots, scan, anharmonic, unscaled

! Lit. S=281.6 Cp=65.6 TRC

! calc 281.33 65.38, H(T)-H(0)=14.68

1 1 1 !

0.0 1 !

22 'HAR' 'GHZ'

1 vib 3932.779 -61.91 1

2 vib 3146.914 -27.38 1

3 vib 3144.436 -22.84 1

4 vib 3041.378 -12.49 1

5 vib 3025.670 -25.79 1

6 vib 2979.762 -20.31 1

7 vib 1523.624 0.33 1

8 vib 1490.727 -1.39 1

9 vib 1472.410 -1.73 1

10 vib 1461.686 -2.13 1

11 vib 1391.102 -5.43 1

12 vib 1302.656 -2.81 1

13 vib 1277.572 -4.91 1

14 vib 1178.152 -1.21 1

15 vib 1138.165 -6.35 1

16 vib 1052.969 -2.47 1

17 vib 919.020 -0.38 1

18 vib 808.678 5.41 1

19 vib 417.829 1.21 1

20 hrd 13 10 1 !FREQUENCY REMOVED = 294 cm-1 HR OH rotor

Vhrd3 1 -0.0001 257.9682 -59.0842 -8.417 -209.3956 17.4086 -0.4172 1.9372 0.1279 0.0439

-0.0252 -0.0875 0.0788 0.1045

Bhrd1 1 -0.0001 23.4005 -1.1164 0.2737 -0.0038 0.0154 0.0343 -0.137 -0.0049 -0.0027

0.0081

21 hrb 240.03 1145.2 3 ! HR Me rotor 13.7 kJ

22 top 8.8488 35.2720 1 ! 35.2720120 9.4879061 8.2527809

Ethene/ethylene CH₂=CH₂

none Ethylene 61.05 ! ± 0.14 ATcT v1.118, 60.8 W3X-L Chan & Radom

C2H4

! B3LYP/cc-pVTZ+d vibs, rots, scale=0.9681

! NIST-JANAF pg 676

! Lit. S=219.3, Cp=42.89; this work 219.08, 42.96

4 1 1 ! D2h symm

0.0 1 ! 1Ag

13 'HAR' 'GHZ'

1 vib 809.42 0.0 1 ! B2u

2 vib 947.87 0.0 1 ! B3u

3 vib 952.30 0.0 1 ! B2g

4 vib 1033.15 0.0 1 ! Au

5 vib 1206.80 0.0 1 ! B3g

6 vib 1338.03 0.0 1 ! Ag

7 vib 1431.71 0.0 1 ! Blu

8 vib 1638.77 0.0 1 ! Ag

9 vib 3025.86 0.0 1 ! Blu

10 vib 3039.19 0.0 1 ! Ag

11 vib 3092.80 0.0 1 ! B3g

12 vib 3120.34 0.0 1 ! B2u

13 top 27.67 147.898 1 ! 147.8979364 30.3815147 25.2040451

none Ethylene 61.05

C2H4

! dHf(0) from ATcT v.1.118 (2015)

! NIST-JANAF 1998

! This Work: S=219.22 , Cp=42.88 // NIST-JANAF 1998 S=219.330 , Cp=42.886

```

4      1      1
0.0    1
13    'HAR'  'GMCM'
1     vib    3026.4  0.0    1
2     vib    1622.9  0.0    1
3     vib    1342.2  0.0    1
4     vib    1023.0  0.0    1
5     vib    3102.5  0.0    1
6     vib    1222.0  0.0    1
7     vib    949.3   0.0    1
8     vib    943.0   0.0    1
9     vib    3105.5  0.0    1
10    vib     826.0  0.0    1
11    vib    2988.7  0.0    1
12    vib    1443.5  0.0    1
13    top     3.0751e-39  5.763e-40    1    ! GMCM

```

Ethylene carbonate, 2-Oxo-1,3-dioxolane

```

none    EthyleneCarbonate  -491.92  ! Estimated from 298K value
C3H4O3
! B3LYP/cc-pVTZ+d freqs, rots scale=0.9681
! 1,3-Dioxolan-2-one, 2-Oxo-1,3-dioxolane non-planar ring
! -510.7 ± 0.9 kJ/mol @ 298K Verevkin J Chem Thermo 2008
! Lit. S=301.6, Cp=78.7 JChemEngData DOI:10.1021/acs.jced.7b00578
! Calc. S=298.17, Cp=79.56, H(T)-H(0)=15.5
2     1     1  ! C2 symm
0.0   1     1  ! 1A
25    'HAR'  'GHZ'
1     vib    137.95   0.0    1 ! A ring-puckering mode
2     vib    182.25   0.0    1 ! B ring-puckering mode
3     vib    506.38   0.0    1 ! B
4     vib    680.07   0.0    1 ! B
5     vib    699.38   0.0    1 ! A
6     vib    749.05   0.0    1 ! B
7     vib    857.15   0.0    1 ! B
8     vib    862.75   0.0    1 ! A
9     vib    936.00   0.0    1 ! A
10    vib    1022.79  0.0    1 ! B
11    vib    1059.92  0.0    1 ! A
12    vib    1092.50  0.0    1 ! B
13    vib    1121.85  0.0    1 ! A
14    vib    1201.28  0.0    1 ! B
15    vib    1210.08  0.0    1 ! A
16    vib    1344.44  0.0    1 ! A
17    vib    1364.63  0.0    1 ! B
18    vib    1476.82  0.0    1 ! B
19    vib    1484.98  0.0    1 ! A
20    vib    1841.65  0.0    1 ! A
21    vib    2953.57  0.0    1 ! A
22    vib    2957.05  0.0    1 ! B
23    vib    3013.10  0.0    1 ! A
24    vib    3026.16  0.0    1 ! B
25    top     3.2220  8.0649 1 !      3.8366213      2.7057802

```

Ethoxy ethene CH₂=CH-O-CH₂CH₃ C=COC cis, COCC trans

```

none    CH2CHOC2CH5      -120.0  ! W2X John Simmie unpub. 2016
C4H8O1
! dHf(298K)-143.9; Pedley =-140.8±0.9
! G4: B3LYP/GTbas3 vibs, rots, HRS scale=0.9854; cg <=SCAN_2=> ct <=SCAN_1=> tt
! Cs symmetry; relaxed PE scans; aka ethyl vinyl ether; S=327.8, Cp=114.0, H(T)=20.57
1     1     1
0.0   1
35    'HAR'  'GHZ'
1     hrd   13    10    1    ! 1     vib    103.5     0.0    1    ! SCAN_2 C-C--O-CHCH2

```

Vhrd3 1 0.000 1265.699 -1195.294 542.418 -620.305 -55.512 23.690 56.819 -2.789 6.846
-10.588 12.659 -14.112 17.104
Bhrd1 1 0.000 1.560 -0.502 0.007 0.750 -0.181 -0.025 -0.174 0.043 0.036 0.000
2 hrd 13 10 1 ! 2 vib 208.6 0.0 1 ! SCAN_1 C-O--CH=CH2
Vhrd3 1 0.000 1191.623 -34.666 -874.813 -311.147 5.187 6.291 17.556 -0.035 -0.223
0.117 -0.579 0.036 -0.428
Bhrd1 1 0.000 2.456 0.895 0.803 0.884 0.542 0.045 -0.385 -0.220 -0.011 0.000
3 vib 225.3 0.0 1
4 hrb 273.0 1028.2 3 ! SCAN_3 O-C--C-H Barrier 12.30 kJ
5 vib 381.5 0.0 1
6 vib 599.8 0.0 1
7 vib 711.3 0.0 1
8 vib 812.3 0.0 1
9 vib 824.9 0.0 1
10 vib 850.7 0.0 1
11 vib 973.5 0.0 1
12 vib 992.5 0.0 1
13 vib 1044.2 0.0 1
14 vib 1119.3 0.0 1
15 vib 1169.9 0.0 1
16 vib 1224.7 0.0 1
17 vib 1278.0 0.0 1
18 vib 1339.8 0.0 1
19 vib 1378.5 0.0 1
20 vib 1402.6 0.0 1
21 vib 1430.8 0.0 1
22 vib 1463.0 0.0 1
23 vib 1478.4 0.0 1
24 vib 1502.0 0.0 1
25 vib 1673.3 0.0 1
26 vib 2952.5 0.0 1
27 vib 2987.1 0.0 1
28 vib 3002.2 0.0 1
29 vib 3075.8 0.0 1
30 vib 3079.0 0.0 1
31 vib 3127.4 0.0 1
32 vib 3140.8 0.0 1
33 vib 3217.8 0.0 1
34 qro 16.60328 1 1 !
35 qro 2.62347 1 2 ! 2.7927131 2.4644801

none CH2CHOC2CH5 -120.0 ! W2X Simmie unpub. 2016
C4H8O1

! dHf(298K)-143.9; cf Pedley =-140.8±0.9
! G4 composite: B3LYP/GTBas3 vibs, rots, anharmonics cg <=SCAN_2=> ct <=SCAN_1=> tt
! Cs symmetry; relaxed PE scans; aka ethyl vinyl ether; S=327.8, Cp=114.0, H(T)=20.57
1 1 1 !
0.0 1 !

		'OBS'	'GHZ'		
35					
1	vib	3114.78	-32.86	1	!
2	vib	3044.44	-20.52	1	!
3	vib	3002.26	-28.59	1	!
4	vib	2985.05	-31.08	1	!
5	vib	2969.13	-17.55	1	!
6	vib	2849.78	-31.78	1	!
7	vib	1670.06	-3.19	1	!
8	vib	1484.18	-0.33	1	!
9	vib	1463.77	-1.38	1	!
10	vib	1404.58	-3.76	1	!
11	vib	1390.29	-5.40	1	!
12	vib	1371.42	-3.99	1	!
13	vib	1331.66	-2.21	1	!
14	vib	1210.17	-3.47	1	!
15	vib	1116.03	-1.73	1	!
16	vib	1036.39	-3.21	1	!
17	vib	966.66	-0.72	1	!


```

18 vib      848.11      -0.67  1  !
19 vib      600.63       0.52  1  !
20 vib      375.55      -6.96  1  !
21 vib      227.66      -0.83  1  !
22 vib     2983.91     -31.61  1  !
23 vib     2885.16     -36.56  1  !
24 vib     1454.99     -1.17  1  !
25 vib     1265.48     -3.19  1  !
26 vib     1163.04     -1.32  1  !
27 vib      981.51     -3.22  1  !
28 vib      828.96       0.71  1  !
29 vib      812.60     -0.15  1  !
30 vib      706.89     -0.46  1  !
31 hrb      273.0      1028.2  3  ! Methyl Barrier 12.30 kJ
32 hrd  13  10  1  ! 2  vib  208.6      0.0  1  ! SCAN_1 C-O--CH=CH2
Vhrd3  1  0.0 1191.623 -34.666 -874.813 -311.147 5.187 6.291 17.556 -0.035 -0.223 0.117
-0.579 0.036 -0.428
Bhrd1  1  0.0 2.456 0.895 0.803 0.884 0.542 0.045 -0.385 -0.220 -0.011 0.000
33 hrd  13  10  1  ! 33  vib  103.77      -1.52  ! SCAN_2 C-C--O-CHCH2
Vhrd3  1  0.0 1265.699 -1195.294 542.418 -620.305 -55.512 23.690 56.819 -2.789 6.846
-10.588 12.659 -14.112 17.104
Bhrd1  1  0.0 1.560 -0.502 0.007 0.750 -0.181 -0.025 -0.174 0.043 0.036 0.000
34 qro  16.60328  1  1  !
35 qro   2.62347  1  2  ! 2.7927131      2.4644801

```

Ethyl radical C₂H₅

```

none Ethyl 131.04 ! ± 0.32 ATcT v1.118; 130.1 W3X-L
C2H5
! B3LYP/cc-pVTZ+d vib, rots, scan; scale=0.9681
! Lit. 3rd Mill S=242.96, Cp=50.67; RMG S=247.36, Cp=51.25 (300K)
! Lit. Gurvich 4th ed. 1989 S=250.52, Cp=46.60; calc. 247.86, 51.70, 12.34
1 1 1 ! Cs symm
0.0 2 ! 2A'
16 'HAR' 'GHZ'
1 hrd 13 10 6 !FREQUENCY REMOVED = 105 cm-1 A"
Vhrd3 1 -0.4703 9.6827 -0.2438 0.0655 -2.2267 -0.0352 -0.0278 9.7646 0.136 0.0795 -
0.0306 -0.4965 -0.0695 -0.1117
Bhrd1 1 -0.4703 16.0447 -0.1608 0.5063 -5.6166 -0.0943 0.0673 -1.4538 0.0006 0.0119 -
0.3826
2 vib 471.96 0.0 1 ! A'
3 vib 787.70 0.0 1 ! A"
4 vib 951.06 0.0 1 ! A'
5 vib 1028.04 0.0 1 ! A'
6 vib 1157.73 0.0 1 ! A"
7 vib 1357.42 0.0 1 ! A'
8 vib 1420.72 0.0 1 ! A'
9 vib 1434.27 0.0 1 ! A"
10 vib 1435.06 0.0 1 ! A'
11 vib 2849.14 0.0 1 ! A'
12 vib 2938.01 0.0 1 ! A'
13 vib 2979.19 0.0 1 ! A"
14 vib 3042.33 0.0 1 ! A'
15 vib 3136.92 0.0 1 ! A"
16 top 21.9865 104.2619 1 ! 104.2619428 22.8392497 21.1656797

```

```

none Ethyl AnHarmonic 131.04 ! ± 0.32 ATcT v1.118; 130.1 W3X-L
C2H5
! B3LYP/cc-pVTZ+d vib, rots, anharm, scan; unscaled
! Lit. 3rd Mill S=242.96, Cp=50.67; RMG S=247.36, Cp=51.25 (300K)
! Lit. Gurvich 4th ed. 1989 S=250.52, Cp=46.60; calc. 246.54, 50.13, 12.08
1 1 1 ! Cs symm
0.0 2 ! 2A'
16 'HAR' 'GHZ'
1 vib 3027.593 -27.02 1 ! A'
2 vib 2873.065 -27.45 1 ! A'

```

3	vib	2770.758	-66.09	1	!	A'
4	vib	1451.825	-1.49	1	!	A'
5	vib	1433.962	-5.35	1	!	A'
6	vib	1369.204	-9.34	1	!	A'
7	vib	1039.559	-5.69	1	!	A'
8	vib	955.572	-2.03	1	!	A'
9	vib	538.674	28.60	1	!	A'
10	vib	3103.126	-31.58	1	!	A"
11	vib	2939.202	-32.31	1	!	A"
12	vib	1404.379	-2.85	1	!	A"
13	vib	1172.040	-1.76	1	!	A"
14	vib	818.798	3.70	1	!	A"

15 hrd 13 10 6 ! FREQUENCY REMOVED = 105 cm-1 A"
Vhrd3 1 -0.4703 9.6827 -0.2438 0.0655 -2.2267 -0.0352 -0.0278 9.7646 0.136 0.0795 -
0.0306 -0.4965 -0.0695 -0.1117
Bhrd1 1 -0.4703 16.0447 -0.1608 0.5063 -5.6166 -0.0943 0.0673 -1.4538 0.0006 0.0119 -
0.3826
16 top 21.9865 104.2619 1 ! 104.2619428 22.8392497 21.1656797

none Ethyl 131.04

C2H5

! dHf(0) from ATcT v.1.118 (2015)

! vibs & rots: Pacansky 1982, JACS 104,415; Chettur 1987, JPC 91,3483;

! Sears 1996, JCP 104,781; Sears 1999, JCP, 111,9213; Davis 2000, JCP 112,1823;

! Häber 2006, JCP 124,054316; Golden 2012, JPCA 116,5847;

! This Work: S=246.61, Cp=50.05 // 3rd Mill S=242.96 , Cp=50.67

1 1 1

0.0 2

16 'OBS' 'CM-1'

1	vib	3037	0	1	!	CH2 s-stretch [Davis 2000]
2	vib	2876	0	1	!	CH3 s-stretch [Häber 2006]
3	vib	2854	0	1	!	2-CH stretch [Häber 2006]
4	vib	1440	0	1	!	CH2 deform. [Pacansky 1982]
5	vib	1366	0	1	!	[Pacansky 1982]
6	vib	1175	0	1	!	H deform. [Pacansky 1982]
7	vib	1138	0	1	!	CC stretch [Pacansky 1982]
8	vib	528	0	1	!	CCH2 umbrella [Sears 1996]
9	vib	3129	0	1	!	CH2 a-stretch [Davis 2000]
10	vib	3000	0	1	!	CH3 a-stretch [Häber 2006]
11	vib	1440	0	1	!	CH3 deform. [Pacansky 1982]
12	vib	1025	0	1	!	[Chettur 1987]
13	vib	1383	0	1	!	[Chettur 1987]
14	vib	836	0	1	!	[Golden 2012]
15	hrc	15.45	16.6 6	!	CM-1;	[Sears 1999]
16	top	0.7293	3.658	1	!	CM-1; K-rotor [Golden 2012]

Ethylhydroperoxide CH₃CH₂OOH

none EthylHydroperoxide -142.59 ! ±0.79 JMS unpub, DfH(298)=-161.13

C2H6O2

! MN12SX/6-311++G(d,p) vibs, rots; scans scaling factor: 0.97554

! Isodesmic: EtOOH + MeOH = MeOOH + EtOH at W1BD & G4 key values from ATcT 1.122

! DfH(298) -161.1 ± 4 Goldsmith/Magoon/Green JPCA 2012,116,9033

! Lit.S=317.8 Burke/Simmie/Curran JPCRD 2015,44,013101

! Calc. 317.33, Cp=83.15, H(T)-H(0)=17.64

1 1 1 ! No symmetry, no optical isomers HR interconverts

0.0 1 ! Singlet

25 'HAR' 'GHZ'

1 hrd 13 10 1 !FREQUENCY REMOVED = 127 cm-1 , CC--OO rotor

Vhrd3 1 -0.0454 718.6652 -353.7672 258.7424 -662.3183 -4.0959 41.6874 11.8328 -23.9762
37.5166 -68.5387 25.7244 35.0929 18.0904

Bhrd1 1 -0.0454 2.0933 -0.8163 0.3554 -0.1223 0.1814 0.1813 0.2024 -0.0002 0.057 0.0377

2 hrd 13 10 1 !FREQUENCY REMOVED = 147 cm-1 CO--OH rotor

Vhrd3 1 -0.316 653.8846 -834.2318 199.2664 13.689 -17.6878 5.471 -0.4611 -532.9226
428.1869 -100.8705 21.0742 -1.1574 0.1426
Bhrd1 1 -0.316 21.2782 -0.4448 -0.0203 -0.0247 0.2623 -0.2678 0.1712 -0.1133 -0.0294
0.0451
3 hrb 234.16 998.1 3 ! Me rotor 11.94 kJ
4 vib 289.81 0.0 1
5 vib 475.73 0.0 1
6 vib 797.78 0.0 1
7 vib 865.44 0.0 1
8 vib 982.24 0.0 1
9 vib 1062.90 0.0 1
10 vib 1143.77 0.0 1
11 vib 1155.82 0.0 1
12 vib 1249.80 0.0 1
13 vib 1343.31 0.0 1
14 vib 1362.83 0.0 1
15 vib 1396.55 0.0 1
16 vib 1439.03 0.0 1
17 vib 1456.17 0.0 1
18 vib 1487.10 0.0 1
19 vib 2935.20 0.0 1
20 vib 2971.21 0.0 1
21 vib 2990.08 0.0 1
22 vib 3071.41 0.0 1
23 vib 3074.96 0.0 1
24 vib 3794.91 0.0 1
25 top 4.0810 31.475 1 ! GHZ 31.4754209 4.2262142 3.9407624

Ethynediol, HO-C≡C-OH

none EthyneDiol -19.40 ! JMS unpub -22.9 @ 298K
C2H2O2
! -21.3±3.8 at 298K JPCA 2012,116,9033-9057
! HOCCHO + HCCH = 2 HCCOH DrH= -19.64±1.01 at 0 K CBS-QB3, -APNO, G3, G4, W1BD
! B3LYP/cc-pVTZ+d freqs, rots, anharmonics unscaled
! Lit. S=282.0 Cp=72.4, JPCA 2012,116,9033-9057
! Calc. 276.05 73.43, H(T)-H(0)=15.74
2 1 1 ! C2 symm
0.0 1 ! 1A
13 'HAR' 'GHZ'
1 vib 3759.08 -45.71 1 ! A
2 vib 2457.37 -9.51 1 ! A
3 vib 1270.68 -4.92 1 ! A
4 vib 813.02 -1.46 1 ! A
5 vib 382.18 2.28 1 ! A
6 vib 323.28 -11.15 1 ! A
7 vib 242.37 -0.84 1 ! A
8 vib 3758.14 -45.02 1 ! B
9 vib 1382.72 -1.36 1 ! B
10 vib 1230.02 -4.47 1 ! B
11 vib 375.10 3.59 1 ! B
12 vib 240.21 -0.54 1 ! B
13 top 3.6838 336.33 1 ! 336.3335657 3.6849249 3.6827403

Ethynol, acetylenol HCCOH

none ethynol 95.0 ! W3X-L
C2H2O
! B3LYP/cc-pVTZ+d vibs, rots, anharmonic
!
! Lit. S=247.3 ± 2.9, Cp=56.1 ± 2.5 SmallDB
! calc. S=247.49, Cp=56.08, H(T)-H(0)=12.42
1 1 1 ! CS
0.0 1 ! 1A
10 'HAR' 'GHZ'
1 vib 3765.16 -90.69 1 ! A'

2 vib 3489.29 -51.91 1 ! A'
3 vib 2282.82 -7.64 1 ! A'
4 vib 1256.46 -12.74 1 ! A'
5 vib 1084.47 -9.79 1 ! A'
6 vib 649.94 -2.34 1 ! A'
7 vib 401.58 -0.36 1 ! A'
8 vib 545.81 -2.07 1 ! A"
9 vib 440.53 0.27 1 ! A"
10 top 9.7114 678.4582 1 ! 678.4581995 9.7811434 9.6421354

Ethynyloxy or ketyl, $O=C=\dot{C}-H / \dot{O}-C\equiv C-H$

none Ethynyloxy 175.6 ! W3X-L JMS unpub. Ketyl; DfH(298)=175.4
C2H1O1
!Linear H-C-C-O isomer 1d Sattelmeyer paper); v similar geom OCC=170, HCC=137
!DfH(298K)=175.6 Sebbar PCCP 2002, 4, 3691 or 169.0 Scott, Radom JPC 1996, 100, 16502
! B3LYP/cc-pVTZ+d vibs, rots, scaling factor: 0.9681
! Good agreement vibs Sattelmeyer et al CPL 2004, 383, 266-269
! calc. S=230.59, Cp=45.65, H(T)-H(0)=10.50
1 1 1 ! Cs symmetry, no optical isomers
0.0 2 ! doublet 2A"
7 'HAR' 'GHZ'
1 vib 461.4 0.0 1 ! A'
2 vib 487.5 0.0 1 ! A"
3 vib 548.6 0.0 1 ! A'
4 vib 1224.3 0.0 1 ! A'
5 vib 2016.7 0.0 1 ! A'
6 vib 3235.6 0.0 1 ! A'
7 qro 10.830 1 2 ! 2-D rotor 10.8309927 10.8309918

Fluorine atom ^{19}F ($^2P_{3/2}$)

none F 77.287
F
! NIST-JANAF 1998
! gas phase atomic Fluorine
! dhf(0) from ATcT v.1.112 (2013)
1 1 2
0.0 4
404.1 2
0 'HAR' 'AMUA'

Formaldehyde, methanal HCHO

none Methanal -105.32 ! ± 0.11 ATcT v.1.118
H2CO
! B3LYP/cc-pVTZ+d freqs, rots scale=0.9681
!
! Lit. NIST-JANAF 1998 S=218.95, Cp=35.402; Calc. S=218.02, Cp=35.43, H(T)-H(0)=10.02
2 1 1 ! C2v symm
0.0 1 !
7 'HAR' 'GHZ'
1 vib 1164.56 0.00 1 ! B1
2 vib 1227.89 0.00 1 ! B2
3 vib 1487.72 0.00 1 ! A1
4 vib 1767.05 0.00 1 ! A1
5 vib 2785.94 0.00 1 ! A1
6 vib 2837.83 0.00 1 ! B2
7 top 36.722 285.528 1 ! 285.5278467 39.1593401 34.4364746

none Methanal -105.32 ! ± 0. AtcT v1.118
CH2O
! B3LYP/cc-pVTZ+d vibs, rots, anharmonics; unscaled
!
! Lit. NIST-JANAF S=218.95, Cp=35.402; calc. 218.50, 35.32, H(T)-H(0)=10.01
2 1 1 ! C2v symm

0.0 1 ! 1A1
 7 'OBS' 'GHZ'
 1 vib 2720.241 -33.18 1 ! A1
 2 vib 1797.145 -9.45 1 ! A1
 3 vib 1503.197 0.92 1 ! A1
 4 vib 1183.712 -2.87 1 ! B1
 5 vib 2678.188 -39.02 1 ! B2
 6 vib 1247.192 -2.08 1 ! B2
 7 top 36.7134 285.424 1 ! 285.4235287 39.1504730 34.4280999

none Formaldehyde -105.32 ! ± 0.11 ATcT v.1.118

H2CO

! Vib: Shimanouchi, Tables of Molecular Vibrational Frequencies, NBS, 1972, 1-160.

! rots: JMS 74, 327-329 (1979)

!
 2 1 1
 0.0 1
 7 'OBS' 'MHZ'
 1 vib 2782.5 0 1
 2 vib 1746.1 0 1
 3 vib 1500.1 0 1
 4 vib 2843.1 0 1
 5 vib 1249.1 0 1
 6 vib 1167.3 0 1
 7 top 36338.8 281970.6 1 ! 281970.58, 38836.04, 34002.20

Formic acid, HCOOH, syn H-O-C=O

none FormicAcid -371.12 ! ± 0.22 ATcTv1.122 cis H-O-C=O aka syn

C1H2O2

! B3LYP/cc-pVTZ+d vib, rots, scale=0.9681

! Scan OC--OH barrier ca 4,600/cm, anti HOCO at +1,500/cm. Anharm. VPT2 problem

! Lit. S=248.70 ± 0.42, JPCRD 1986, 15, 13691436;

! Lit. Cp=45.68 ± 0.07 Millikan RC, J Chem Phys, 1957, 27, 1305-1308

! calc S=248.82, Cp=45.85, H(T)-H(0)=10.90; DfH(298)=-378.45 exact agree ATcT

1 1 1 ! CS symm

0.0 1 ! 1A' ground state

10 'HAR' 'GHZ'
 1 vib 609.98 0.0 1 !
 2 hrd 13 10 1 !FREQUENCY REMOVED=662 cm-1, Max % Error V(x)=0.4%, B(x)=16.1%
 Vhrd3 1 0 2634.8902 -708.6507 -1911.8564 -41.0282 36.2573 -5.7748 -3.8375 0.0362 0.0589
 0.0011 -0.2915 -0.0155 0.0014
 Bhrd1 1 0 24.9501 2.1166 0.2084 -0.1451 -0.3156 1.0448 0.121 0.5144 -0.6295 0.5616
 3 vib 1022.09 0.0 1 !
 4 vib 1088.90 0.0 1 !
 5 vib 1264.34 0.0 1 !
 6 vib 1360.76 0.0 1 !
 7 vib 1767.74 0.0 1 !
 8 vib 2945.89 0.0 1 !
 9 vib 3602.09 0.0 1 !
 10 top 11.2268 78.1466 1 ! 78.1466452 12.0621512 10.4492764

Formyl, oxomethyl HC*O

none formyl 41.426 ! ATcT v1.122 @ 298K 41.803 ± 0.099

C1H1O1

! B3LYP/cc-pVTZ+d vib, rots, anharmonics

! Lit. S=224.28, Cp=34.68, H(T)-H(0)=10.00 3rd Millennium

! calc. 224.33 34.55, 9.98, HoF(298)=41.48

1 1 1 ! Cs symmetry, no optical isomers

0.0 2 ! 2A'

4 'HAR' 'GHZ'
 1 vib 2637.38 -115.21 1 ! A'
 2 vib 1936.11 -11.68 1 ! A'
 3 vib 1108.05 -9.32 1 ! A'
 4 top 43.689 716.05 1 ! 716.0560393 45.0426383 42.3769665

Formylmethylene, oxo-ethylidene HC=CHO[•] or H[•]C-CH=O

none FormylCH2 255.6 ! W3X-L 252.0 @ 298K cf 163.2±3.8 @ 298K JPCA2012,116,9033
C2H2O

! H-C-C-H trans; triplet see JPCA 2013, 117, 2152-2159.
! B3LYP/cc-pVTZ+d vib, rots, scan scale=0.9681
! Lit. S=262.8±3.3, Cp=54.8±3.3 JPCA 2012, 116, 9033; IJChemKin 2016,48, 724-738
! calc 259.63 49.42, H(T)-H(0)=11.44

1 1 1 ! Cs symm
0.0 3 ! 3A" ground state
10 'HAR' 'GHZ'
1 vib 423.22 0.0 1 ! A'
2 vib 615.46 0.0 1 ! A" HR barrier >> hi
3 vib 892.49 0.0 1 ! A'
4 vib 934.88 0.0 1 ! A"
5 vib 1109.14 0.0 1 ! A'
6 vib 1356.71 0.0 1 ! A'
7 vib 1466.99 0.0 1 ! A'
8 vib 2897.78 0.0 1 ! A'
9 vib 3093.81 0.0 1 ! A'
10 top 12.0585 65.8707 1 ! 65.8707224 13.2126993 11.0052148

none FormylCH2 255.6 ! W3X-L 252.0 @ 298K cf 163.2±3.8 @ 298K JPCA2012,116,9033
C2H2O

! H-C-C-H trans; triplet see JPCA 2013, 117, 2152-2159.
! singlet at 270.6 kJ/mol W3XL JMS unpub.
! B3LYP/cc-pVTZ+d vib, rots, anharmonics unscaled
! Lit. S=262.8±3.3, Cp=54.8±3.3 JPCA 2012, 116, 9033
! calc 259.37 49.07, H(T)-H(0)=11.39

1 1 1 ! Cs symm
0.0 3 ! 3A" ground state
10 'HAR' 'GHZ'
1 vib 3195.76 -65.95 1 ! A'
2 vib 2993.26 -70.77 1 ! A'
3 vib 1515.33 -17.02 1 ! A'
4 vib 1401.42 1.02 1 ! A'
5 vib 1145.69 -7.47 1 ! A'
6 vib 921.90 -13.63 1 ! A'
7 vib 437.17 -0.51 1 ! A'
8 vib 965.69 -2.10 1 ! A"
9 vib 635.74 -9.64 1 ! A"
10 top 12.0585 65.8707 1 ! 65.8707224 13.2126993 11.0052148

none Formylmethylene-cis 0.0 !
C2H2O

! H-C-C-H cis; triplet see JPCA 2013, 117, 2152-2159.
! B3LYP/cc-pVTZ+d vib, rots, anharmonics unscaled
! Lit.
! calc S=259.85, Cp=50.75, H(T)-H(0)=11.65

1 1 1 ! Cs symm
0.0 3 ! 3A" ground state
10 'HAR' 'GHZ'
1 vib 3203.58 -63.86 1 ! A'
2 vib 2834.70 -80.36 1 ! A'
3 vib 1538.69 -20.68 1 ! A'
4 vib 1381.41 0.45 1 ! A'
5 vib 1117.15 -9.08 1 ! A'
6 vib 869.74 -10.35 1 ! A'
7 vib 443.76 0.33 1 ! A'
8 vib 946.85 -2.65 1 ! A"
9 vib 491.11 -5.52 1 ! A" HR barrier >>
10 top 10.9873 96.658 1 ! 96.6579553 11.629594 10.3806005

Formyloxymethylene, HC:-O-CHO

none HCOCHO-singlet-trans 0.00 ! more stable than trans/triplet
 C2H2O2
 ! B3LYP/cc-pVTZ+d freqs, rots, scan anharmonics; OCOC trans
 ! Lit. S=277.8, Cp=61.0, JMS(Theochem) 2003, 626,187-194
 ! Calc. 276.18 62.79, H(T)-H(0)=13.73
 1 1 1 ! C1 symm no OI
 0.0 1 ! 1A
 13 'HAR' 'GHZ'
 1 vib 3038.23 -62.25 1
 2 vib 2897.62 -67.26 1
 3 vib 1902.57 -10.62 1
 4 vib 1405.59 -0.89 1
 5 vib 1332.54 -5.09 1
 6 vib 1283.12 -6.44 1
 7 vib 1055.29 -2.66 1
 8 vib 903.16 -11.10 1
 9 hrd 13 10 1 !FREQUENCY REMOVED = 680 cm-1 scan OH
 Vhrd3 1 0 1449.3251 -905.8557 -498.0036 -119.3118 96.8758 -13.1212 -9.9087 0.1744 -
 0.0001 -0.2063 0.0005 0.1971 0
 Bhrd1 1 0 4.6348 -1.8219 0.521 0.0879 0.0743 0.0497 -0.0663 0.0279 -0.0224 -0.0002
 10 vib 618.72 -2.17 1
 11 vib 407.43 -0.91 1
 12 hrd 13 10 1 !FREQUENCY REMOVED = 145 cm-1 S scan OCOC
 Vhrd3 1 -0.0001 4068.5987 -342.4632 -2833.7279 -327.909 -20.6604 64.3508 26.4605 -
 0.4447 -160.55 -343.8773 -323.0788 -138.0722 -18.0598
 Bhrd1 1 -0.0001 8.5954 -1.1476 2.6615 -0.3154 -2.6097 0.4814 -0.0002 0.0542 0.9781
 0.5334
 13 top 5.1148 62.340 1 ! 62.3395476 5.328935 4.9092781

Helium He

none He 0.0 ! By definition
 He
 ! NIST-JANAF 1998
 !
 !
 1 1 1
 0.0 1
 0 'HAR' 'AMUA'

Glyoxal or 1,2-ethanedione, HCOCHO *trans* conformer

none Glyoxal-trans -208.8 ! W3X-L, -214.47@298K; -206.99±0.52 ATcT v1.122 & -212.63
 C2H2O2
 ! B3LYP/cc-pVTZ+d freqs, rots, scan, anharmonics
 ! Lit. S=272.5, Cp=60.41, H(T)-H(0)=13.68 Table 6 **hf.doc**
 ! <http://garfield.chem.elte.hu/Burcat/burcat.html>
 ! Calc. 271.61 59.78 13.58
 2 1 1 ! C2h symm
 0.0 1 ! 1Ag
 13 'HAR' 'GHZ'
 1 vib 2935.67 -33.07 1 !
 2 vib 1804.00 -5.30 1 !
 3 vib 1380.45 -6.12 1 !
 4 vib 1065.03 -5.75 1 !
 5 vib 552.54 1.17 1 !
 6 vib 815.98 -2.26 1 !
 7 hrd 13 10 1 !FREQUENCY REMOVED = 130 cm-1
 Vhrd3 1 0 1396.1184 -763.8387 -631.3009 -31.1474 35.0883 -3.6693 -1.2503 66.8273
 111.3157 8.3468 -12.7697 1.7135 0.7182
 Bhrd1 1 0 4.3718 -1.2305 -0.2087 -0.1339 0.1707 0.0009 -0.0221 -0.002 -0.0026 0.0026
 8 vib 1081.79 -1.47 1 !
 9 vib 2930.74 -33.17 1 !

10 vib 1802.20 -5.56 1 !
 11 vib 1337.55 -4.45 1 !
 12 vib 337.13 1.37 1 !
 13 top 4.6011 56.246 1 ! 56.2428597 4.7934 4.41670

Glyoxal, HCOCHO *cis* conformer

none Glyoxal-*cis* -191.3 ! W3X-L, -196.7 @ 298K; less stable than trans C2H2O2

! B3LYP/cc-pVTZ+d freqs, rots, scan scale=0.9681
 ! Lit.

! Calc. S=277.16, Cp=60.23, H(T)-H(0)=13.92

2 1 1 ! C2v symm

0.0 1 ! 1A1

13		'HAR'	'GHZ'						
1	vib	92.64	0.0	1	!	A2	HR		
2	vib	272.46	0.0	1	!	A1			
3	vib	711.45	0.0	1	!	B1			
4	vib	787.27	0.0	1	!	A1			
5	vib	798.52	0.0	1	!	B2			
6	vib	1049.88	0.0	1	!	A2			
7	vib	1348.35	0.0	1	!	B2			
8	vib	1349.92	0.0	1	!	A1			
9	vib	1739.88	0.0	1	!	A1			
10	vib	1782.24	0.0	1	!	B2			
11	vib	2772.14	0.0	1	!	B2			
12	vib	2806.83	0.0	1	!	A1			
13	top	5.5669	26.974	1	!	26.9738709	6.1709490	5.0220331	

none Glyoxal-*cis* -191.3 ! W3X-L, -196.7 @ 298K; less stable than trans C2H2O2

! B3LYP/cc-pVTZ+d freqs, rots, scan, anharmonics
 ! Lit.

! Calc. S=273.45, Cp=59.95, H(T)-H(0)=13.64

2 1 1 ! C2v symm

0.0 1 ! 1A1

13		'HAR'	'GHZ'								
1	vib	2899.40	-32.15	1	!	A1					
2	vib	1796.71	-5.80	1	!	A1					
3	vib	1394.63	0.19	1	!	A1					
4	vib	813.18	-10.35	1	!	A1					
5	vib	281.16	0.67	1	!	A1					
6	vib	1084.77	-1.55	1	!	A2					
7	hrd	13 10 1	!	FREQUENCY REMOVED = 96 cm-1							
Vhrd3	1 0	1389.916	783.0	-631.602	14.7185	50.9883	6.1756	-5.409	-0.0024	0.0205	0 0.0508
		0.004	-0.0052								
Bhrd1	1 0	4.3441	1.1682	0.5235	0.2189	-0.0623	-0.0997	0.004	0.0144	-0.011	-0.0002 !
8	vib	735.48	2.43	1	!	B1					
9	vib	2863.59	-34.33	1	!	B2					
10	vib	1840.50	-5.13	1	!	B2					
11	vib	1393.06	0.63	1	!	B2					
12	vib	824.72	-0.29	1	!	B2					
13	top	5.5669	26.974	1	!	26.9738709	6.1709490	5.0220331			

Hydrazine, N₂H₄

none Hydrazine 112.1 ! W3X-L Chan, Radom J Chem Theo Comput 2015, 11, 2109-2119. N2H4

! Freqs, rots, scan B3LYP/cc-pVTZ+d scale=0.9970 appropriate for entropy

! G-09 HR treatment S=231.71+Rln2=237.47, Cp=47.53

! Calc. S=237.51 (238.66 Chase 1998, 3rdM 238.45 Cp=48.3 H298-H0=11.37 (11.53) kJ

2 1 1 ! C2 symmetry, no optical isomers, one e-state

0.0 1 ! Singlet

13 'OBS' 'GHZ' ! B3LYP/cc-pVTZ+d anharmonic analysis

1 hrd 19 10 1 ! 1 vib 432.69 0.0 1 ! Vibrational mode replaced

Vhrd3 1 0.000 994.753 16.229 -976.137 -51.232 -17.148 40.386 -3.198 -2.310 1.730 -
3.073 -682.412 -119.445 288.439 42.496 -20.777 5.061 -9.293 3.498 0.000
Bhrd1 1 0.000 19.909 2.107 4.563 0.968 1.898 -1.038 0.426 -0.438 0.055 0.041
2 vib 3550.836 -28.51700 1
3 vib 3454.903 -27.06180 1
4 vib 1687.074 -3.93518 1
5 vib 1331.867 -5.58504 1
6 vib 1112.390 -3.45875 1
7 vib 809.705 -4.57684 1
8 vib 3557.639 -33.61660 1
9 vib 3444.246 -33.79820 1
10 vib 1675.160 -1.76153 1
11 vib 1300.346 -5.77467 1
12 vib 998.949 -15.52310 1
13 top 24.27506 144.9490 1 ! 144.9490355 24.2932501 24.2568934

Hydrogen atom H ($^2S_{1/2}$)

none H-atom 216.034 ! ATcT v1.122 217.998 at 298.15 K
H
! NIST-JANAF pg 1261
!
! S=114.61, Cp=20.79, HT)-H(0)=6.20
1 1 1 ! $2S_{1/2}$ ground state
0.0 2
0 'HAR' 'AMUA'

Hydroperoxy water radical complex HO₂··H₂O

Very sensitive to low frequency modes

none HO2.H2O -252.7 ! W3X-L JMS unpub.; -259.57 NASA-JPL
H3O3
! B3LYP/cc-pVTZ+d freqs, rots, scale=0.9681
! G-09 "no hindered rotor corr. needed"; Hydrogen-donor structure cf PCCP, 2010,12,3904
! calc. S=303.05, Cp=73.10, H(T)-H(0)=16.24
1 2 1 ! C1 symm, optical isomers
0.0 2 ! 2A
13 'HAR' 'GHZ'
1 vib 142.00 0.0 1 !
2 vib 226.60 0.0 1 ! O-H---OH2 rotor
3 vib 268.42 0.0 1 !
4 vib 304.00 0.0 1 !
5 vib 518.46 0.0 1 !
6 vib 694.44 0.0 1 !
7 vib 1151.26 0.0 1 !
8 vib 1518.20 0.0 1 !
9 vib 1584.26 0.0 1 !
10 vib 3189.98 0.0 1 !
11 vib 3615.19 0.0 1 !
12 vib 3746.89 0.0 1 !
13 top 5.60951 31.9490 1 ! 31.9490372 6.0830075 5.1728673

none HO2.H2O -252.7 ! W3X-L JMS unpub.; -259.57 NASA-JPL
H3O3
! B3LYP/cc-pVTZ+d freqs, rots, anharm; unscaled
! G-09 "no hindered rotor corr. needed"; Hydrogen-donor structure cf PCCP, 2010,12
! calc. S=311.10, Cp=69.86, H(T)-H(0)=16.69
1 2 1 ! C1 symm, optical isomers
0.0 2 ! 2A
13 'OBS' 'GHZ'
1 vib 3699.640 -66.72 1 !
2 vib 3573.909 -76.59 1 !
3 vib 3153.972 -130.67 1 !
4 vib 1588.837 -18.84 1 !
5 vib 1507.343 -7.61 1 !

6	vib	1165.249	-7.05	1	!			
7	vib	619.998	-43.38	1	!			
8	vib	422.623	-44.39	1	!			
9	vib	268.039	-6.83	1	!			
10	vib	247.137	-6.32	1	!			
11	vib	163.541	-17.37	1	!			
12	vib	86.704	-14.31	1	!			
13	top	5.60951	31.9490	1	!	31.9490372	6.0830075	5.1728673

none HO2.H2O -259.57 ! NASA-JPL

HO2H2O

! harm vibs, rots: B3LYP/6-311++G(3df,3dp) Aliosio & Francisco, JPCA 102,1899-1902 (1998)

! v10 treated as Morse oscil., based on Do = 35.9 kJ/mol + 1127 cm-1 (del zpe)

! This Work: S=314.48, Cp=75.05 // H(T)-H(0)=17.27

!

1 2 1 ! Optical isomer

0.0 2 ! Doublet

13 'HAR' MHZ

1	vib	3871.	0.0	1				
2	vib	3752.	0.0	1				
3	vib	3306.	0.0	1				
4	vib	1625.	0.0	1				
5	vib	1556.	0.0	1				
6	vib	1183.	0.0	1				
7	vib	679.	0.0	1				
8	vib	465.	0.0	1				
9	vib	293.	0.0	1				
10	vib	255.	-3.94	1	!	Morse oscil.: Do = 35.9 kJ/mol + 1127 cm-1 (del zpe)		
11	vib	103.	0.0	1				
12	vib	98.	0.0	1				
13	top	5226.7	32810.0	1	!	MHZ : Suma et al., Science 311, 1278 (2006)		

Hydroperoxyl radical, hydroperoxo HO₂

none HO2 15.16 ! ATcT v.1.118

HO2

! vibs: gas phase values from WebBook (11/2016)

! rots: Charo & De Luca, JMS 94, 426-436 (1982); doi:10.1016/0022-2852(82)90018-2

! Calc. S=229.10, Cp=34.89 // NIST-JANAF 1998 S= 229.106 , Cp=34.905

1 1 2

0.0 2

7029.764 2

4 'OBS' 'MHZ'

1	vib	3436.2	0.0	1				
2	vib	1391.8	0.0	1				
3	vib	1097.6	0.0	1				
4	top	32579.60	610273.22	1	!	MHZ	610273.223	33517.816 31667.654

Hydrogen bromide

none HBr -27.97 ! ± 0.15 ATcT v1.118

HBr

! 298.15 K Lit. NIST-JANAF pg 438 S= 198.699; Cp=29.14

! This work S=198.6 & Cp=29.11

!

1 1 1

0.0 1

2 'HAR' 'CM-1'

1 vib 2649.1816 -45.2245 1 ! data from NIST-JANAF pg 438

2 gro 8.34954 1.0 2 ! Bo = Be - alpha/2

Hydrogen chloride HCl

none HCl -91.989 ! ATcT v1.118 ± 0.0062

HCl

!

! 298.15 K Lit. NIST-JANAF pg 762 S=186.9; Cp=29.14

! This work S=198.6 & Cp=29.11

1 1 1

0.0 1

2 'HAR' 'CM-1'

1 vib 2990.95 -52.82 1

2 qro 10.4394 1 2 ! Bo = 10.593 - 0.3072/2

Hydrogen iodide HI

none HI 28.643 ! ± 0.036 ATcT v1.118

HI

! NIST-JANAF 1998

!

!

1 1 1

0.0 1

2 'HAR' 'CM-1'

1 vib 2309.06 -39.73 1

2 qro 6.42625 1.0 2 ! Bo = Be - alpha/2

Hydrogen sulfide H₂S

none H2S -17.68

H2S

! dHf(0): CODATA Key Value, NASA/JPL-15

! vibs from NIST-JANAF 1998

! rots from Cook et al., J. Mol. Struct. 28 (1975) 237-246

2 1 1

0.0 1

4 'OBS' 'CM-1'

1 vib 2614.6 0.0 1

2 vib 1182.7 0.0 1

3 vib 2626.5 0.0 1

4 top 9.669 4.7268 1 ! cm-1 10.34657 9.03572 4.72680

Hydroxyethenone or hydroxyketene, O=C=CH(OH)

none Hydroxyethenone -145.14 ! ±1.43 at 0K from isodesmic JMS unpub.

C2H2O2

! O=C=CH(OH) + CH₄ => O=C=CH₂ + CH₃OH DHr=-23.59±1.42 at CBS-QB3, -APNO, G3, G4, W1BD

! Calc. DfH(298K)=-150.2 cf DfH(298K)=-151.5±3.8 JPCA 2012, 116, 9033-90

! B3LYP/cc-pVTZ+d freqs, rots, scan, anharmonics

! Lit. S=278.7±4.2, Cp=66.5±4.2 JPhysChemA 2012, 116, 9033-9057

! Calc. 285.56 66.03, H(T)-H(0)=14.25

1 1 1 ! C1 symm HR negates OI

0.0 1 ! 1A

13 'HAR' 'GHZ'

1 vib 3771.22 -92.34 1

2 vib 3172.66 -60.76 1

3 vib 2205.40 -11.21 1

4 vib 1430.01 -9.91 1

5 vib 1269.51 -7.91 1

6 vib 1177.12 -3.11 1

7 vib 1032.15 -3.16 1

8 vib 689.61 -2.87 1

9 vib 583.64 -2.54 1

10 vib 515.39 0.88 1

11 hrd 13 10 1 !FREQUENCY REMOVED = 272 cm-1

Vhrd3 1 -0.8371 447.3647 -62.4622 422.6033 118.8655 24.952 10.8591 5.4763 1.2071 -

17.428 -7.1283 -2.0335 -0.9045 -0.5189

Bhrd1 1 -0.8371 22.4022 -3.6347 0.7074 -1.3126 0.1995 -0.5101 -0.5204 -0.196 -0.1713 -

0.0931

12 vib 218.59 0.77 1

13 top 4.50575 49.0872 1 ! 49.0871839 4.6863929 4.3320693

Hydroxyformyl radical HOC*=O cis

none cis-HOCO -176.7 ! W3X-L JMS unpub.; -174.03 ± 0.51 ATcT v1.118
 CHO2
 ! B3LYP/cc-pVTZ+d vib, rots, scan; scale=0.9681
 !
 ! calc. S=254.10, Cp=48.47, H(T)-H(0)=11.41
 1 1 1 ! Cs symm
 0.0 2 ! 2A'
 7 'HAR' 'GHZ'
 1 hrd 13 10 1 !FREQUENCY REMOVED = 575.42 cm-1
 Vhrd3 1 0 1814.2881 297.1931 -1548.9496 -11.8987 22.0806 0.837 -1.2877 -0.0625 -0.2638
 -0.1224 -0.3469 -0.0617 -0.2117
 Bhrd1 1 0 27.7136 3.1006 -0.0005 0.1459 0.3664 0.1434 0.0425 0.0387 0.0344 0.0233
 2 vib 580.56 0.0 1 ! A'
 3 vib 1039.40 0.0 1 ! A'
 4 vib 1257.44 0.0 1 ! A'
 5 vib 1807.41 0.0 1 ! A'
 6 vib 3457.57 0.0 1 ! A'
 7 top 11.3333 142.6963 1 ! 142.6962955 11.7923258 10.8922016

none cis-HOCO -174.03

HCO2
 ! dHf(0) = -174.03 ± 0.51 kJ/mol [ATcT v.1.118 (2015)]
 ! Vib from Fortenberry et al. JCP 135, 214303 (2011);
 ! Francisco et al.,Accounts Chem. Res. 43, 1519-1526 (2010)
 ! rot constants from Oyama et al., JCP 134, 174303 (2011)
 ! This Work: S=252.09 , Cp=44.61 //
 1 1 1
 0.0 2
 7 'OBS' 'MHZ'
 1 vib 3452.3 -99.114 1 ! OH str [Fortenberry (2011)]
 2 vib 1824.1 -13.319 1 ! C=O str [Fortenberry (2011)]
 3 vib 1280.2 -7.365 1 ! HOC bend [[Fortenberry (2011)]
 4 vib 1042.4 -7.551 1 ! C-O str [Fortenberry (2011)]
 5 vib 601.2 0.674 1 ! C-O str [Fortenberry (2011)]
 6 vib 540.2 -3.142 1 ! C-O str [Fortenberry (2011)]
 7 top 11275.651 142944.929 1 ! MHz [Oyama (2011)]

Hydroxyformyl radical HOC*=O trans

none trans-HOCO -183.2 ! W3X-L JMS unpub.; -180.95 ± 0.48 ATcT v1.118
 HCO2
 ! B3LYP/cc-pVTZ+d vib, rots, scan; scale=0.9681
 !
 ! Calc. S=253.49, Cp=48.37, H(T)-H(0)=11.38
 1 1 1 ! C1 symm
 0.0 2 ! 2A'
 7 'HAR' 'GHZ'
 1 hrd 13 10 1 !FREQUENCY REMOVED = 528 cm-1
 Vhrd3 1 0 1814.0516 -296.8639 -1548.8894 11.8508 21.8468 -0.8451 -1.1507 -0.0005 -
 0.0003 -0.0001 0.0016 0.0004 0.0001
 Bhrd1 1 0 27.681 -3.0767 -0.0017 -0.1299 0.3341 -0.1255 0.0179 -0.022 0.0081 -0.0024
 2 vib 602.26 0.0 1
 3 vib 1049.76 0.0 1
 4 vib 1203.01 0.0 1
 5 vib 1841.90 0.0 1
 6 vib 3672.64 0.0 1
 7 top 11.1081 166.6079742 1 ! 11.4845954 10.7439922

none trans-HOCO -180.95

HCO2
 ! dHf(0) = -180.95 ± 0.48 kJ/mol [ATcT v.1.118 (2015)]
 ! Vib from Fortenberry et al. JCP 135, 134301 (2011);
 ! rot constants from Oyama et al., JCP 134, 174303 (2011)

! Calc. S=251.88, Cp=45.09, H(T)-H(0)=11.02
 1 1 1
 0.0 2
 7 'OBS' 'MHZ'
 1 vib 3635.702 -85.526 1 ! OH str [Fortenberry (2011)]
 2 vib 1852.567 -13.089 1 ! C=O str [Fortenberry (2011)]
 3 vib 1211.2 -11.488 1 ! HOC bend [Fortenberry (2011)]
 4 vib 1050.4 -8.733 1 ! C-O str [Fortenberry (2011)]
 5 vib 615. -0.131 1 ! C-O str [Fortenberry (2011)]
 6 vib 508.1 -13.768 1 ! C-O str [Fortenberry (2011)]
 7 top 11053.673 167768.064 1 ! MHZ [Oyama (2011)]

Hydroxyl radical OH

none OH 37.250 ! ± 0.027 ATcT v.1.122
 OH
 ! NIST-JANAF pg. 1298 small revisions Bernath & Colin, JMS 257, 20-23 (2009)
 ! Lit. S=183.708, Cp=29.986, H(T)-H(0)=9.172 NIST-JANAF
 ! Calc. 183.55 29.94 9.16
 1 1 5 !
 0.0 2 ! X ²Π_i
 139.05 2 !
 32403. 2 ! A ²Σ⁺
 68372. 2 ! B ²Σ⁺
 89420. 2 ! C ²Σ⁺
 2 'HAR' 'CM-1'
 1 vib 3735.21 -82.81 1
 2 gro 18.535 1.0 2 ! Bernath & Colin, JMS 257, 20-23 (2009)

Hydroxymethyl, [•]CH₂OH

none Hydroxymethyl -11.3 ! W3X-L; -10.25 ±0.33 ATcT v1.122
 C1H3O1
 ! B3LYP/cc-pVTZ+d freqs, rots, scan scale=0.9681
 ! Lit. S=244.2, Cp=47.40, H(T)-H(0)=11.78 Table 16 JPC 1996,100,19874-90
 ! Calc. 243.48 48.32 12.04
 1 1 1 ! Cs symm HR negates OI
 0.0 1 ! 2A
 10 'HAR' 'GHZ'
 1 hrd 13 10 1 !FREQUENCY REMOVED = 410 cm-1
 Vhrd3 1 0.0355 607.5028 -146.3011 -513.5804 67.8269 -28.5375 23.1727 15.2773 -66.5952 -
 549.9467 175.2901 204.0288 -24.5705 -25.2244
 Bhrd1 1 0.0355 28.0868 5.6249 7.8951 -2.8856 4.833 0.0411 0.4438 8.7419 1.7124 2.1389
 2 vib 535.48 0.0 1
 3 vib 1022.05 0.0 1
 4 vib 1166.34 0.0 1
 5 vib 1319.56 0.0 1
 6 vib 1437.25 0.0 1
 7 vib 3024.44 0.0 1
 8 vib 3160.55 0.0 1
 9 vib 3705.21 0.0 1
 10 top 27.9717 193.927 1 ! 193.9273742 29.9256877 26.1452454

Hydroxymethylene, HCOH trans

none Hydroxymethylene 112.40 ! ± 0.33 ATcT v1.122; JMS W2X 112.6 W3X-L 111.6
 C1H2O1
 ! Trans HCOH singlet; rotn barrier to cis is >120 kJ/mol
 ! B3LYP/cc-pVTZ+d vibs, rots, anharm unscaled
 ! Lit. S=225.212, Cp=36.066, DfH(0K)=108.16 Third Millennium Table 6 July 2016
 ! calc. 225.06, Cp=36.29, H(T)-H(0)=10.07
 1 1 1 ! Cs symm
 0.0 1 ! 1A'
 7 'HAR' 'GHZ'
 1 vib 3697.23 -98.32 1 ! A'
 2 vib 2832.66 -66.66 1 ! A'

```

3  vib      1508.06    -0.65    1 ! A'
4  vib      1326.11   -10.83    1 ! A'
5  vib      1216.89    -6.11    1 ! A'
6  vib      1092.62    -9.55    1 ! A"
7  top        34.4469  290.308  1 ! 290.3080832   36.5510924   32.4637592

```

Hydroxysulfonyl or "sulfo" H-O-S(O)₂

```

none  HOSO2    -367.5  ! ± 4.4 Nagy JPCA 2011, 115, 7823-7833
HSO3
! Rotation constants from Nagy et al., JPCA, 115, 7823-7833 (2011)
! S(298) = 294.1 ± 1.5 Nagy
! harmonic vibs and diagonal anharmonicities from Nagy et al.(2011)
! HR: V(angle) from Fig. 1c in Nagy et al.(2011);
! B(hr) from geom of Klopper, JCP 129, 114308 (2008)
1  1  1
0.0  2
10  'HAR'  'GHZ'
1  hrd    5      1      1
Vhrd2  1  1.0437  652.02 -60.763  675.26 -33.391  24.988 ! cm-1 from Fig. 1c Nagy 2011
Bhrd1  1  0.0    19.72 ! cm-1 from geom of Klopper, JCP 129, 114308 (2008)
2  vib    432    -1.3    1      ! Nagy et al., JPCA, 115, 7823-7833 (2011)
3  vib    435    -0.1    1      ! ...
4  vib    539    -0.4    1      ! ...
5  vib    794    -5.7    1      ! ...
6  vib   1122    -4.1    1      ! ...
7  vib   1136    -7.9    1      ! ...
8  vib   1347    -6.0    1      ! ...
9  vib   3783   -82.4    1      ! ...
10 top    9.208  4.898    1      ! ...

```

Hydrogen peroxide HOOH

```

none  HydrogenPeroxide  -129.472 ! +/-0.064 ATcT v1.122
H2O2
! B3LYP/cc-pVTZ+d freqs, rots, scan anharm unscaled
! Lit. S=232.991, Cp=43.116 NIST-JANAF
! Calc. 234.20    41.79  H(T)-H(0)=11.13
2  1  1 ! C2 symm
0.0  1 ! 1A
7  'OBS'  'GHZ'
1  vib    3579.33  -44.72  1 !
2  vib    1399.38  -11.62  1 !
3  vib     929.00   -5.38  1 !
4  hrd  13 10 1 !FREQUENCY REMOVED = 369 cm-1 H--O--O--H rotor
Vhrd3  1 -1.1514  816.5625 -1076.2935  634.1939 -48.1113  0.987  0.406 -0.2407 -31.7294
37.5683 -4.2149  0.0495  0.1161 -0.0959
Bhrd1  1 -1.1514  40.8599 -1.6583  0.355 -0.1055  0.127 -0.0521  0.0094 -0.0026 -0.0148
0.0011
5  vib    3581.48  -43.97  1 !
6  vib    1272.27  -11.23  1 !
7  top     25.9901  303.243  1 ! 303.2430735   26.4293221   25.5582772

```

Iodine atom I (²P)

```

none  I(2P)    107.157      ! ± 0.0021  ATcT v1.118
I
! NIST-JANAF 1998
!
!
1  1  2
0.0  4
7603.15  2
0  'HAR'  'AMUA'

```

Isoformyl, hydroxymethylidene C'OH

none isoformyl 216.6 ! W3X-L; 3rd Millennium: 217.7 & 298K 218.1±0.83
 C1H1O1
 ! B3LYP/cc-pVTZ+d vib, rots, anharmonics
 ! Lit. S=225.03, Cp=34.97, H(T)-H(0)=10.00 3rd Millennium
 ! calc. 225.03 34.90 10.00, HoF(298)=217.0
 1 1 1 ! Cs symmetry, no optical isomers
 0.0 2 ! 2A'
 4 'HAR' 'GHZ'
 1 vib 3262.999 -240.76 1 ! A'
 2 vib 1388.631 -13.70 1 ! A'
 3 vib 1133.104 -11.48 1 ! A'
 4 top 40.868 701.943 1 ! 701.9425226 42.0757922 39.6963182

Isoprene, trans 2-methyl-1,3-butadiene, CH₂=CH-C(CH₃)=CH₂

none Isoprene 96.3 ! 75.7±1.0 @ 298K Fraser & Prosen J Res NBS 1955 54 143-148
 C5H8
 ! B3LYP/cc-pVTZ+d freqs, rots, scans 0.9681
 ! Trans C=C-C=C totally dominant >97%
 ! DeltaH(0K) = 11.8 kJ/mol trans to cis (gauche) Franke & Douberly
 DOI:10.1021/acs.jpca.7b10260
 ! Lit. S=314.76, Cp=102.69 Messerly JChemEngData, 1970, 15, 227-232; NIST WebBook
 ! Calc. 315.31, 104.55, H(T)-H(0)=18.70
 1 1 1 ! Cs symm
 0.0 1 ! 1A'
 34 'HAR' 'GHZ'
 1 hrd 13 10 1 !FREQUENCY REMOVED = 157 cm-1 CCCC HR
 Vhrd3 1 0 1304.8146 -251.228 -728.8122 -426.1963 75.1911 15.6268 16.0371 -0.0615 -
 0.1091 -0.1259 -0.109 -0.061 0.0003
 Bhrd1 1 0 1.9687 -0.0083 0.4952 0.3967 -0.0716 0.0563 -0.0405 0.0284 0.0077 -0.0001
 2 hrb 195.56 815.0 3 ! Me HR 9.75 kJ/mol barrier
 3 vib 271.16 0.0 1 !
 4 vib 399.19 0.0 1 !
 5 vib 415.14 0.0 1 !
 6 vib 521.44 0.0 1 !
 7 vib 626.67 0.0 1 !
 8 vib 764.80 0.0 1 !
 9 vib 767.06 0.0 1 !
 10 vib 900.59 0.0 1 !
 11 vib 911.62 0.0 1 !
 12 vib 931.65 0.0 1 !
 13 vib 982.40 0.0 1 !
 14 vib 999.65 0.0 1 !
 15 vib 1038.19 0.0 1 !
 16 vib 1057.88 0.0 1 !
 17 vib 1288.10 0.0 1 !
 18 vib 1290.20 0.0 1 !
 19 vib 1368.40 0.0 1 !
 20 vib 1387.54 0.0 1 !
 21 vib 1416.80 0.0 1 !
 22 vib 1435.74 0.0 1 !
 23 vib 1455.83 0.0 1 !
 24 vib 1607.29 0.0 1 !
 25 vib 1643.81 0.0 1 !
 26 vib 2927.75 0.0 1 !
 27 vib 2970.77 0.0 1 !
 28 vib 3010.36 0.0 1 !
 29 vib 3031.70 0.0 1 !
 30 vib 3037.13 0.0 1 !
 31 vib 3046.59 0.0 1 !
 32 vib 3114.66 0.0 1 !
 33 vib 3121.80 0.0 1 !
 34 top 3.4620 8.5752 1 ! 8.5751909 4.1867755 2.8627349

Krypton Kr

```
none Kr 0.0 ! By definition
Kr
! NIST-JANAF 1998
!
!
1 1 1
0.0 1
0 'HAR' 'AMUA'
```

Mercapto radical HS

```
none HS 142.47
HS
! dHf(0) NASA/JPL-15
! all other NIST-JANAF 1998
!
!
1 1 4
0.0 2
377.01 2
30663 2
59622 2
2 'HAR' 'CM-1'
1 vib 2689.6 -45.5 1
2 qro 9.601 1 2
```

Methane

```
none CH4 -66.550 ! ± 0.057 ATcT v1.122
CH4
! Frequencies from WebBook (accessed 7/19/2011) [Shimanouchi 1972]
! Moments of Inertia from JANAF (1998)
! Lit. S=186.25, Cp=35.69 NIST WebBook
! Calc. 186.25 35.64, H(T)-H(0)=10.00
12 1 1
0.0 1
6 'HAR' 'GMCM'
1 vib 2917. 0. 1 ! Sym str
2 vib 1534. 0. 2 ! Deg deform
3 vib 3019. 0. 3 ! Deg str
4 vib 1306. 0. 3 ! Deg deform
5 qro 0.5313e-39 1. 1 ! K-rotor
6 qro 0.5313e-39 1. 2 ! 2-D rotor
```

```
none CH4 -66.550 ! ± 0.057 ATcT v1.122
CH4
! B3LYP/cc-pVTZ+d vibs, rots, scale=0.9681
! Lit. S=186.25, Cp=35.69 NIST WebBook
! Calc. 186.21 35.73, H(T)-H(0)=10.01
12 1 1 ! Td symmetry 3x4
0.0 1 ! 1A1
5 'HAR' 'GHZ'
1 vib 1299.16 0. 3 ! T2
2 vib 1509.69 0. 2 ! E
3 vib 2932.26 0. 1 ! A1
4 vib 3031.33 0. 3 ! T2
5 qro 158.765 1.0 3 ! 3D rotor symm=1 158.7652659 158.7652659 158.7652659
```

Methanediol, CH₂(OH)₂

```
none MethaneDiol -381.5 ! -379.05 ± 0.95 ATcT v1.122; JMS W2X -381.2, W3X-L -381.5
C1H4O2
! B3LYP/cc-pVTZ+d vibs, rots, anharmonic
! CH2(OH)2 conrot., gauche
! calc. S=259.89, Cp=69.07, H(T)-H(0)=13.46
```



```

2      1      1 ! C2 symm
0.0    1      ! 1A
16      'HAR'    'GHZ'
1  vib  3797.297  -41.41  1 !
2  vib  3022.229  -30.72  1 !
3  vib  1530.776  -0.90  1 !
4  vib  1393.918  -3.12  1 !
5  vib  1207.063  -1.57  1 !
6  vib  1032.312  -2.97  1 !
7  vib   558.539  -2.38  1 !
8 hrd 13 10 1 !FREQUENCY REMOVED = 370 cm-1
Vhrd3 1 0.0274 928.9131 -380.2696 -373.8221 -184.4011 2.8509 4.2038 3.6188 67.5621 -
114.8033 3.957 13.5932 2.7808 -0.4243
Bhrd1 1 0.0274 21.2704 0.7659 1.43 0.3808 0.5134 -0.0508 -0.4423 -0.0119 0.2165 -0.0609
9  vib  3796.627  -41.26  1 !
10 vib  3066.334  -36.09  1 !
11 vib  1447.648   0.44  1 !
12 vib  1373.676  -4.35  1 !
13 vib  1057.302  -5.28  1 !
14 vib  1010.776   0.57  1 !
15 hrd 13 10 1 !FREQUENCY REMOVED = 373 cm-1
Vhrd3 1 0.0274 928.9131 -380.2696 -373.8221 -184.4011 2.8509 4.2038 3.6188 67.5621 -
114.8033 3.957 13.5932 2.7808 -0.4243
Bhrd1 1 0.0274 21.2704 0.7659 1.43 0.3808 0.5134 -0.0508 -0.4423 -0.0119 0.2165 -0.0609
16 top    9.5600   41.990 1 ! 41.9900763   10.1518076   9.0026865

```

Methanimine, methylenimine, CH₂=NH

```

none  Methanimine  96.53 ! ± 0.63 ATcT v1.122; JMS W2X 97.3 W3X-L 96.9
C1H3N1
! Methylenimine, azomethine CH2=NH
! B3LYP/cc-pVTZ+d vibs, rots, anharmonic unscaled
! Lit. S=226.98, Cp=38.00 (300K), DfH(0K)=96.99 Bugler JPCA, 2016, 120, 7192-7197
! calc. 227.03, Cp=37.64, H(T)-H(0)=10.14
1      1      1 ! Cs symm
0.0    1      ! 1A'
10      'HAR'    'GHZ'
1  vib  3424.84  -76.06  1 ! A'
2  vib  3104.28  -49.26  1 ! A'
3  vib  3011.01  -47.16  1 ! A'
4  vib  1712.68  -6.50  1 ! A'
5  vib  1492.70  -1.16  1 ! A'
6  vib  1372.56  -5.75  1 ! A'
7  vib  1074.54   2.55  1 ! A'
8  vib  1169.36  -4.95  1 ! A''
9  vib  1101.41  -1.24  1 ! A''
10 top    32.3498 199.024 1 ! 199.0234589   35.0855246   29.8273153

```

Methanol CH₃OH

```

none  Methanol  -189.84 ! ± 0.17 ATcT v1.118
CH4O
! B3LYP/cc-pVTZ+d vibs, rots, scan scale=0.9681
! Lit. Chao et al JPCRD 1986, 15, 1369
! S=239.81±0.09, Cp=44.04±0.03, H(T)-H(0)=11.435±0.013
! calc. S=240.13, Cp=44.47, H(T)-H(0)=11.49
1      1      1 ! Cs symm
0.0    1      ! 1A'
13      'HAR'    'GHZ'
1  hrb   291.05  372.8   3 ! HR OH rotor barrier 4.46 kJ/mol
2  vib  1012.82   0.0   1 !
3  vib  1048.16   0.0   1 !
4  vib  1133.54   0.0   1 !
5  vib  1331.47   0.0   1 !
6  vib  1434.79   0.0   1 !
7  vib  1448.16   0.0   1 !

```

8	vib	1463.20	0.0	1	!			
9	vib	2889.39	0.0	1	!			
10	vib	2930.43	0.0	1	!			
11	vib	3002.43	0.0	1	!			
12	vib	3707.47	0.0	1	!			
13	top	24.3268	128.7399	1	!	128.7398867	24.7601735	23.9009964

none Methanol -189.94

CH3OH

! dHf(298) = -200.72 kJ/mol: ATcT v.1.118

! vibs: Serrallach et al., JMS 52 (1974) 94.

! rots: Herbst et al., JMS 108 (1984) 42

! Hindered rotor: Munoz-Caro et al, CPL 273 (1997) 135

! This Work: S=248.90, Cp=44.03 // 3rd Millennium (2011): 239.81 , 44.039

! (S=238.73 if torsion is treated as 295 cm-1 harmonic vib)

! 11/2016 new entry (JRB)

1 1 1

0.0 1

13 'OBS' 'MHZ'

1 vib 3682.4 0. 1

2 vib 3004.3 0. 1

3 vib 2861.9 0. 1

4 vib 1474.6 0. 1

5 vib 1457.7 0. 1

6 vib 1343.9 0. 1

7 vib 1079.3 0. 1

8 vib 1035.5 0. 1

9 vib 2960.8 0. 1

10 vib 1473.4 0. 1

11 vib 1159.3 0. 1

12 hrd 3 3 3

Vhrd2 3 0. 189.54 188.97 -0.57

Bhrd1 3 0. 27.3043 0.1117 -0.0011

13 top 24220.4 127630.8 1

Methoxy ethene, methyl vinyl ether CH₂=CHOCH₃

none Methoxyethene -90.7 ! W3X-L J. Simmie unpub. 298.15 K -108.6, cis C=C-O-C
C3H6O

! G4; B3LYP/GTbas3 freqs, rots, scans, anharm. scale=0.9854

! WebBook Cp=79.5, JPC 2009,113,8683 S=282.8, Cp=84.2;

! Calc. S=291.5 Cp=86.33 H(T)-H(0)=16.22

! Cs symm

1 1 1 !

0.0 1 ! 1-A'

26 'OBS' 'GHZ'

1 vib 3123.09 -31.57 1 !

2 vib 3044.68 -24.72 1 !

3 vib 3004.62 -21.46 1 !

4 vib 2998.77 -51.55 1 !

5 vib 2948.14 -24.80 1 !

6 vib 1686.71 -3.18 1 !

7 vib 1461.48 -1.12 1 !

8 vib 1485.58 -0.88 1 !

9 vib 1394.93 -2.76 1 !

10 vib 1337.31 -2.51 1 !

11 vib 1213.83 -3.67 1 !

12 vib 1194.70 -1.56 1 !

13 vib 1011.52 -2.23 1 !

14 vib 891.52 -1.20 1 !

15 vib 592.33 0.52 1 !

16 vib 306.87 -0.20 1 !

17 vib 2894.69 -36.25 1 !

18 vib 1455.10 -4.10 1 !

19 vib 1157.17 -1.93 1 !

20 vib 981.90 -2.95 1 !

21 vib 825.36 3.92 1 !
 22 vib 713.07 -0.11 1 !
 23 hrd 13 10 1 ! replaces vib 255.14 A" C--C--O--C SCAN_1 cis <==> trans
 Vhrd3 1 0.00 1248.671 -50.886 -899.227 -322.687 2.996 5.110 16.659 -0.287 -0.817 -0.195
 -0.316 -0.776 0.211
 Bhrd1 1 0.00 3.046 1.246 0.797 0.762 0.404 0.111 -0.196 -0.118 -0.012 0.000
 24 hrb 236.31 1178.7 3 ! A" methyl barrier 14.1 kJ
 25 qro 18.5096 1 1 ! cf. Daly et al J Mol Spectr 2014, 306, 11-18
 26 qro 5.5581 1 2 ! GHZ 6.3430330 4.8702715

Methyl hydroperoxide, CH₃OOH

none CH3OOH -114.90 ! ±0.74 ATcT 1.122; -115.7 W3X-L JMS JPCA 2016,120,7370-7384
 C1H4O2
 ! MN12SX/6-311++G(d,p) vib, rots, anharmonic, scan, unscaled
 ! HRs confirmed by Freq=HinderedRotor
 ! Gaussian-16 S=271.9, Cp=60.56 unscaled harmonic; 261.26 & 53.56 anharmonic
 ! Gaussian-16 275.1, 60.59 scaled 0.9755 & HR treatment
 ! Lit. 277.3, 60.79 (300K) Wang, Bozzelli JCED 2016,61,1836
 ! Calc. 274.90 60.03, H(T)-H(0)=13.87; lit. Cp=63±3 WebBook
 1 1 1 ! C1 HR interconverts OIs
 0.0 1 1 ! 1A
 16 'HAR' 'GHZ'
 1 vib 3891.84 -77.69 1 ! E(harm) Xjj
 2 vib 3144.13 -32.07 1 !
 3 vib 3103.78 -23.13 1 !
 4 vib 3007.52 -12.46 1 !
 5 vib 1507.03 -1.03 1 !
 6 vib 1454.05 -6.75 1 !
 7 vib 1450.27 -0.57 1 !
 8 vib 1415.42 -17.81 1 !
 9 vib 1213.45 -3.29 1 !
 10 vib 1179.07 -1.47 1 !
 11 vib 1104.73 -6.92 1 !
 12 vib 928.43 -4.47 1 !
 13 vib 452.97 -0.01 1 !
 14 hrb 256.90 1071.7 3 ! HR Me rotor 12.82 kJ SCAN_1
 15 hrd 13 10 1 !FREQUENCY REMOVED = 137.4 cm-1 ! 15 vib 137.35 1 ! HR HO--OC SCAN_2
 Vhrd3 1 -1.2192 708.1927 -1074.2203 484.6517 -104.5947 28.6774 -7.2339 0.6944 3.7558 -
 3.4924 0.9983 -0.2648 0.1083 0.0152
 Bhrd1 1 -1.2192 21.7483 -1.3107 0.2288 0.0319 -0.1067 0.0236 0.0024 0.0134 -0.0288
 0.0363
 16 top 9.9552 44.262 1 ! 44.2616786 10.6954370 9.2662002

Methyl radical C•H₃

none CH3 149.788 ! ± 0.080 ATcT v1.122
 CH3
 ! Frequencies from WebBook (11/2002)
 ! Moments of Inertia from NIST-JANAF (1998)
 ! HoF(298) from ATcT v.1.118 146.427
 6 1 2
 0.0 2
 46205. 2
 6 'HAR' 'GMCM'
 1 vib 3004.43 0. 1 ! CH str
 2 vib 606.453 0. 1 ! OPLA
 3 vib 3160.821 0. 2 ! CH-str
 4 vib 1402. 0. 2 ! deform
 5 qro 0.5846e-39 1. 1 ! K-rotor
 6 qro 0.2923e-39 1. 2 ! 2-D rotor

Methylthio CH₃S

none CH3S 131.93
 CH3S

! NIST CCC Database (accessed 5/28/2015)
! B3LYP/aug-cc-pVTZ vibrations and rotations
! HoF(298) = 124.7 kJ/mol from NASA/JPL-15

```
3 1 1
0.0 2
10 'HAR' 'cm-1'
1 vib 543 0 1
2 vib 707 0 1
3 vib 864 0 1
4 vib 1330 0 1
5 vib 1369 0 1
6 vib 1471 0 1
7 vib 3015 0 1
8 vib 3083 0 1
9 vib 3103 0 1
10 top 0.444 5.309 1 ! cm-1
```

Methylsulfinyl radical CH₃-S=O

none CH3SO -61.27

CH3SO

! Methylsulfinyl freqs (except torsion): Turnipseed, JPC, 1993, 97, 5926D5934
! torsion and geometry from Estep & Schaefer, PCCP, 2016, 18, 22293! HoF(298 K) = -70.3:
! Burkholder, JPL Publication 15-10, 2015;

```
1 1 1
0.0 2
13 OBS GHz
1 vib 2995 0 1 ! Turnipseed 1993
2 vib 2919 0 1 ! ...
3 vib 1417 0 1 ! ...
4 vib 1288 0 1 ! ...
5 vib 1068 0 1 ! ...
6 vib 926 0 1 ! ...
7 vib 669 0 1 ! ...
8 vib 340 0 1 ! ...
9 vib 2995 0 1 ! ...
10 vib 1405 0 1 ! ...
11 vib 868 0 1 ! ...
12 hrb 128 343 3 ! freq & barrier from Estep & Schaefer 2016
13 top 7.5656 27.4570 1 ! geom Estep; rot constants from MOMINERT
```

Methylsulfonyl radical CH₃-S-O-O syn OOSCH coplanar

none syn-CH3SOO 92.44

CH3SO2

! L.K. Chu and Y.P. Lee, JCP, 133, 184303 (2010); doi: 10.1063/1.3495765
! B3LYP/aug-cc-pVTZ: vibrations and rotations
! from 3rd Law analysis of Turnipseed's Keq [JPC 1992, 96,7502-7505] and CH3S dhf(0)
[NASA/JPL-15]

```
1 1 1
0.0 2
16 'HAR' 'cm-1'
1 vib 93 0 1
2 vib 141 0 1
3 vib 240 0 1
4 vib 387 0 1
5 vib 561 0 1
6 vib 710 0 1
7 vib 955 0 1
8 vib 974 0 1
9 vib 1155 0 1
10 vib 1339 0 1
11 vib 1435 0 1
12 vib 1469 0 1
13 vib 3042 0 1
```

14 vib 3122 0 1
 15 vib 3144 0 1
 16 top 0.1422 0.35 1 ! cm-1

Methyl vinyl ketone, CH₃C(O)CH=CH₂

none MethylVinylKetone -96.78 ! ± 3.38 average methods QB3/APNO/G3/G4/W1BD
 C4H6O1

! 2-butenone, 3-oxobutene CH₂=CH-C(=O)-CH₃ O-C-C=C trans or antiperiplanar
 ! dhf(298K)=-111.1 ± 3.4 cf. -115. ± 11 Guthrie 1978 Can J Chem 56, 962

! B3LYP/cc-pVTZ+d vibs, rots, HRs, scans, anharmonics unscaled

! Lit. S=301, 316.5, 320.34; Cp=79.23, 92.2 see WebBook

! Calc 321.97 88.49, H(T)-H(0)=18.02

1 1 1 ! C1 symm

0.0 1 !

28 'HAR' 'GHZ'

1	vib	3224.21	-29.23	1
2	vib	3165.50	-50.23	1
3	vib	3143.53	-16.72	1
4	vib	3142.72	-17.38	1
5	vib	3092.68	-31.12	1
6	vib	3037.33	-20.14	1
7	vib	1753.06	-9.10	1
8	vib	1684.38	-3.39	1
9	vib	1480.00	-3.49	1
10	vib	1474.04	-6.18	1
11	vib	1448.49	-2.95	1
12	vib	1388.82	-9.36	1
13	vib	1311.36	-1.98	1
14	vib	1269.81	-3.42	1
15	vib	1075.11	-0.45	1
16	vib	1051.51	-1.09	1
17	vib	1046.96	-2.72	1
18	vib	996.61	-0.18	1
19	vib	945.26	-0.44	1
20	vib	759.26	-2.00	1
21	vib	700.58	-1.20	1
22	vib	538.64	-0.28	1
23	vib	491.84	0.43	1
24	vib	432.55	0.45	1
25	vib	278.25	-0.01	1

26 hrb 127.35 285.9 3 ! HRs Methyl barrier 3.42 kJ/mol

27 hrd 13 10 1 !FREQUENCY REMOVED = 116 cm-1 , Max % Error V(x) = 19.6%, B(x) = 7%
 Vhrd3 1 0.0018 899.4526 -7.1595 -973.5517 -0.5213 105.8096 -5.5386 -18.4864 -0.0134 -
 3.4659 0.014 0.7532 -0.0536 -0.1973

Bhrd1 1 0.0018 1.8903 0.1603 0.5065 0.0803 0.0208 0.084 0.1041 -0.0001 0.0109 -0.0262

28 top 3.5509 8.9713 1 ! 8.9712981 4.2762227 2.9485767

Neopentane (CH₃)₄C

none neopentane -134.64 ! ±0.41 ATcT v1.122
 C5H12

! B3LYP/cc-pV(T+d)Z; NIST CCDB

!

! HoF(298.15) = -167.5 ± 0.63 kJ/mol WebBook

12 1 1

0.0 1

22 'HAR' 'CM-1'

1	vib	3025.74	0.00	1	! A1
2	vib	1440.461	0.00	1	! A1
3	vib	728.5354	0.00	1	! A1
4	hra	244.7031	5.32924	3	! CH3 internal rotor; singly degenerate A2
5	vib	3078.364	0.00	2	! E
6	vib	1496.501	0.00	2	! E
7	vib	1096.322	0.00	2	! E
8	vib	336.4633	0.00	2	! E

9	vib	3077.497	0.00	3	!	T1
10	vib	1489.42	0.00	3	!	T1
11	vib	968.9296	0.00	3	!	T1
12	hra	310.3035	5.32924	3	!	CH3 rotor; triply degenerate T1
13	hra	310.3035	5.32924	3	!	CH3 rotor; triply degenerate T1
14	hra	310.3035	5.32924	3	!	CH3 rotor; triply degenerate T1
15	vib	3083.212	0.00	3	!	T2
16	vib	3016.537	0.00	3	!	T2
17	vib	1523.829	0.00	3	!	T2
18	vib	1402.379	0.00	3	!	T2
19	vib	1276.677	0.00	3	!	T2
20	vib	931.0572	0.00	3	!	T2
21	vib	424.3655	0.00	3	!	T2
22	gro	0.1492	1.00	3	!	3D spherical rotor

Nitric acid HONO₂

```

none      HONO2      -124.45    ! ± 0.18  ATcT v.1.118
HNO3
! NIST / JANAF 2003, Dorofeeva et al. JPCRD 32 (2003) 879
! dhf(0)
!
1      1      1
0.0    1
11 'OBS'   'CM-1'
1  vib    3550.00    0.    1
2  vib    1709.57    0.    1
3  vib    1325.74    0.    1
4  vib    1303.52    0.    1
5  vib     879.11    0.    1
6  vib     646.83    0.    1
7  vib     580.30    0.    1
8  vib     763.15    0.    1
9  hrd     2      1      2
Vhrd2    2      0.    1134.4    -1369.2
Bhrd1    2      0.    21.064
10 gro    0.2088327  1.  1    ! K-rotor
11 gro    0.4185286  1.  2    ! 2-D adiabatic rotor

```

Nitric oxide NO

```

none      NO      90.586    ! ± 0.064  ATcT v1.118
NO
! NIST-JANAF 1998 Part II, p1603
! dhf(0) from ATcT v.1.118a (2014)
!
1      1      2 ! e-states and quantum states
0.0    2
121.1  2
2 'HAR'   'AMUA'
1  vib    1903.6    -13.97  1
2  gro     9.8918    1.0    2

```

Nitrogen dioxide O-N-O or NO₂

```

none      NO2      36.826    ! ± 0.064  ATcT v1.118
NO2
! NIST-JANAF 1998
! dhf(0) from ATcT v.1.112 (2013)
!
2      1      1
0.0    2
5 'HAR'   'AMUA'
1  vib    1357.8    0    1
2  vib     756.8    0    1

```

```

3   vib    1665.5    0    1
4   qro    2.1066    1    1    !Ia
5   qro    39.955    1    2    !Ib & Ic

```

Nitromethane CH₃NO₂

```

none MeNO2allvb -61.4 ! W3X-L Chan/Radom JCTC 2015, 11, 2109
C1H3N1O2          ! 298 K = -74.2
! Freqs etc APFD/6-311+G(2d,p) scale=0.989
! Problematic low freq "vibration" gives S(298 K)=296.8
! Lit. S(298 K) = 275.8 ± 1.4 Ervin et al. JPCA 2015, 119, 7169
1 1 1 ! Cs symmetry, optical isomers, one e-state
0.0 1 ! Singlet
17 'HAR' 'GHZ'
1  vib    13.66    0.0    1    ! Low freq vib
2  vib    486.29    0.0    1
3  vib    621.61    0.0    1
4  vib    674.25    0.0    1
5  vib    944.84    0.0    1
6  vib   1102.04    0.0    1
7  vib   1124.91    0.0    1
8  vib   1390.24    0.0    1
9  vib   1437.98    0.0    1
10 vib   1441.68    0.0    1
11 vib   1460.14    0.0    1
12 vib   1640.35    0.0    1
13 vib   3056.85    0.0    1
14 vib   3151.04    0.0    1
15 vib   3181.89    0.0    1
16 qro    5.9547    1    1    ! 5.9546882
17 qro   11.5093    1    2    ! 12.3841598      10.6960760

```

```

none Nitromethane -61.4 ! dHf(298)=-74.7±0.6 McCullough JACS 1954, 76, 4791
C1H3N1O2          !          =-71.5±0.4 Verevkin JCT 2014, 73, 163
! dHf(0) W3X-L Chan/Radom JCTC 2015, 11, 2109 Freqs APFD/6-311+G(2d,p) scale=0.989
! Scan of N--N bond 72 x 5 degrees << 1 kJ Free rotor
! S=274.9 Lit. S=275.8 ± 1.4 Ervin JPCA 2015, 119, 7169; 3rd Mill. 273.7
1 1 1 ! Cs symmetry, no optical isomers, one e-state
0.0 1 ! Singlet
17 'HAR' 'GHZ'
1  rot    169.15    6    1    ! I(red.) ex MOMINERT
2  vib    486.29    0.0    1
3  vib    621.61    0.0    1
4  vib    674.25    0.0    1
5  vib    944.84    0.0    1
6  vib   1102.04    0.0    1
7  vib   1124.91    0.0    1
8  vib   1390.24    0.0    1
9  vib   1437.98    0.0    1
10 vib   1441.68    0.0    1
11 vib   1460.14    0.0    1
12 vib   1640.35    0.0    1
13 vib   3056.85    0.0    1
14 vib   3151.04    0.0    1
15 vib   3181.89    0.0    1
16 qro    5.9547    1    1    ! 5.9546882
17 qro   11.5093    1    2    ! 12.3841598      10.6960760

```

Nitroxyl radical NO₃

```

none NO3      79.35    ! ± 0.19 ATcT v1.118
NO3
! NIST-JANAF 1998: 78.95 ; NASA/JPL 10-6: 79.9 ± 1.1
! vibs: Stanton, JCP 126, 134309 (2007); Stanton, MP 107,1059 (2009)
! Friedl, JPC 91, 2721 (1987); Fujimori, JMS 283, 10 (2013)
! rots: Fujimori et al. JMS 283, 10-17 (2013)

```

```

6      1      1
0.0    2
6 'OBS' 'CM-1'
1  vib  1051.2  0.0  1  ! Stanton, JCP 126, 134309 (2007)
2  vib   762.3  0.0  1  ! Friedl, Fujimori
3  vib  1067.   0.0  2  ! Stanton, MP 107, 1059-1075 (2009)
4  vib   365.5  0.0  2  ! Fujimori J. Mol. Spectrosc 283, 10-17 (2013)
5  gro   0.2286  1.0  1  ! ...
6  gro   0.4585  1.0  2  !

```

Oxalic acid (COOH)₂

```

none OxalicAcid -725.5 ! -710.8 ± 2.1 ATcT v1.122 different conformer ?
C2H2O4
! HOCO/HOCO trans/trans or HOCC cis/cis < c/t < tt
! B3LYP/cc-pVTZ+d vibs, rots; scans, anharmonics
! Lit. S=320.64 Cp=86.18 H(T)-H(0)=17.32 Dorofeeva JPCRD 2001,30,475; neglects OH rotor
! calc. 310.50, 91.20, H(T)-H(0)=17.60 Dorofeeva uncertainty: Cp ± 5-7, S ± 5-10
2 1 1 ! C2h symmetry, no optical isomers
0.0 1 ! Singlet
19
19 'HAR' 'GHZ'
1  vib  3635.194 -50.65 1 ! Ag
2  vib  1832.194 -4.79 1 ! Ag
3  vib  1439.580 -5.09 1 ! Ag
4  vib  1224.581 -2.34 1 ! Ag
5  vib   824.444 -1.45 1 ! Ag
6  vib   563.337 -0.40 1 ! Ag
7  vib   405.286 -0.16 1 ! Ag
8  hrd 13 10 1 !FREQUENCY REMOVED = 710 cm-1 Au HR OH rotor
Vhrd3 1 0 2756.6359 -410.516 -2315.1199 -64.5241 31.9745 3.6391 -2.0895 0.0028 0.025 -
0.0008 -0.0024 -0.0028 -0.0005
Bhrd1 1 0 15.6572 -6.6767 1.717 -2.4698 -1.5938 -0.7427 -0.1247 0.2087 0.3306 0.087 !
9  vib   465.276 0.59 1 ! Au
10 hrd 13 10 1 !FREQUENCY REMOVED = 125 cm-1 , Au HR C--C
Vhrd3 1 0 3780.0372 -2664.8385 -828.0946 -410.9745 187.04 -121.1646 79.118 -8.8302
17.3912 -25.4255 32.6858 -38.9531 44.038
Bhrd1 1 0 0.8202 0.1094 0.1779 0.1191 -0.0527 0.0663 -0.0049 -0.0148 0.0343 -0.0313 !
11 vib   838.449 -0.61 1 ! Bg
12 hrd 13 10 1 !FREQUENCY REMOVED = 708 cm-1 Bg HR OH rotor
Vhrd3 1 0 2756.6359 -410.516 -2315.1199 -64.5241 31.9745 3.6391 -2.0895 0.0028 0.025 -
0.0008 -0.0024 -0.0028 -0.0005
Bhrd1 1 0 15.6572 -6.6767 1.717 -2.4698 -1.5938 -0.7427 -0.1247 0.2087 0.3306 0.087 !
13 vib  3638.493 -49.95 1 ! Bu
14 vib  1855.568 -4.79 1 ! Bu
15 vib  1336.717 -6.10 1 ! Bu
16 vib  1206.204 -2.61 1 ! Bu
17 vib   675.553 0.20 1 ! Bu
18 vib   261.673 1.60 1 ! Bu
19 top    2.9744 5.8130 1 ! 5.8129930 3.8311805 2.3092311

```

3-Oxetanyl

```

none 3-Oxetanyl -113.0 ! Multiple composite -127.4 @ 298.15K
C3H5O1
! B3LYP/cc-pVTZ+d freqs, rots, scale=0.9681
! Lit. S=277.0, Cp(300 K)=66.3 JPCA 2014, Vol.118(17), p.3147-31677
Lit. 279.5 ± 4.2, 67.8 ± 5.8 SmallDataBase
! Calc. 286.72 68.43, H(T)-H(0)=14.2
1 1 1 ! Cs symm OI
0.0 2 ! 2A1
22
22 'HAR' 'GHZ'
1  vib  141.00 0.0 1 ! A'
2  vib  222.98 0.0 1 ! A'
3  vib  825.63 0.0 1 ! A'
4  vib  838.52 0.0 1 ! A''
5  vib  878.33 0.0 1 ! A'

```


6	vib	898.51	0.0	1 ! A"			
7	vib	964.43	0.0	1 ! A"			
8	vib	966.04	0.0	1 ! A'			
9	vib	1045.42	0.0	1 ! A'			
10	vib	1072.13	0.0	1 ! A'			
11	vib	1076.02	0.0	1 ! A"			
12	vib	1225.40	0.0	1 ! A"			
13	vib	1247.89	0.0	1 ! A"			
14	vib	1311.96	0.0	1 ! A'			
15	vib	1433.00	0.0	1 ! A"			
16	vib	1457.74	0.0	1 ! A'			
17	vib	2858.27	0.0	1 ! A"			
18	vib	2869.31	0.0	1 ! A'			
19	vib	2881.83	0.0	1 ! A'			
20	vib	2883.24	0.0	1 ! A"			
21	vib	3129.38	0.0	1 ! A'			
22	top	12.8917	7.0163	1 ! 13.3070	12.4893	7.0163	

2-Oxiranone (OCH₂C)=O

none 2-Oxiranone -165.1 ! ±2.2 JMS unpub -172.5 @ 298K
C2H2O2

! cf. -171.5±3.8 @ 298K JPCA 2012,116,9033-9057

! Oxiranone + CH₄ = Oxirane + H₂C=O DrH=86.36±2.21 at 0K CBS-QB3, -APNO, G3, G4, W1BD

! B3LYP/cc-pVTZ+d freqs, rots, anharmonic, unscaled

! Lit. S=264.0±2.9 Cp=54.8±3.8, JPCA 2012,116,9033-9057

! Calc. 263.99, 54.05, H(T)-H(0)=11.74

1 1 1 ! Cs symm

0.0 1 ! 1A'

13		'HAR'	'GHZ'				
1	vib	3116.66	-28.05	1 ! A'			
2	vib	2007.23	-9.79	1 ! A'			
3	vib	1483.43	0.11	1 ! A'			
4	vib	1193.53	-5.12	1 ! A'			
5	vib	1120.03	-2.06	1 ! A'			
6	vib	945.17	-5.00	1 ! A'			
7	vib	717.39	-2.99	1 ! A'			
8	vib	535.48	-0.48	1 ! A'			
9	vib	3214.98	-33.28	1 ! A"			
10	vib	1062.06	-1.67	1 ! A"			
11	vib	999.66	-1.13	1 ! A"			
12	vib	494.01	0.56	1 ! A"			
13	top	7.2030	25.1291	1 ! 25.1291410	8.1100511	6.3974757	

2-Oxiranylidene

none 2-oxiranylidene 213.6 ! W3X-L unpub. H2C

C2H2O1 | \

! B3LYP/cc-pVTZ+d freqs, rots, anhrms | C:

! Lit. S=274.9 , Cp=59.83 @ 300 K SmallDB | /

! Calc. 244.46 43.68, H(T)-H(0)=10.61 O

1 1 1 ! CS symm

0.0 1 ! 1A'

10		'HAR'	'GHZ'				
1	vib	3130.94	-29.80	1 ! A'			
2	vib	1528.00	-1.69	1 ! A'			
3	vib	1418.43	-2.99	1 ! A'			
4	vib	1096.11	-8.82	1 ! A'			
5	vib	836.12	-6.25	1 ! A'			
6	vib	827.17	-1.48	1 ! A'			
7	vib	3240.83	-35.42	1 ! A"			
8	vib	1117.94	-1.30	1 ! A"			
9	vib	884.79	-2.38	1 ! A"			
10	top	19.8222	38.7711	1 ! 38.7711356	23.8834192	16.4515325	

4-Oxo-1,3-dioxetan-2-yl

```

none 13Dioxentan2yl4one -229.1 ! W3X-L JMS, -227.0 ± 4.3 Isodesmic
C2H1O3
! B3LYP/cc-pVTZ+d vib, rots, anharm O--CH
! Lit. | |
! calc S=281.99, Cp=60.51, H(T)-H(0)=12.59 O=C--O
1 1 1 ! Cs symm
0.0 2 ! 2A' ground state
13 'HAR' 'GHZ'
1 vib 3149.11 -66.57 1 ! A'
2 vib 1993.30 -10.75 1 ! A'
3 vib 1148.76 -3.37 1 ! A'
4 vib 1032.73 -1.21 1 ! A'
5 vib 942.61 -27.50 1 ! A'
6 vib 804.02 -1.44 1 ! A'
7 vib 745.83 -0.86 1 ! A'
8 vib 313.45 -1.05 1 ! A'
9 vib 1294.63 -5.67 1 ! A"
10 vib 1060.45 -1.45 1 ! A"
11 vib 812.88 -6.47 1 ! A"
12 vib 524.47 0.50 1 ! A"
13 top 5.1414 15.2068 1 ! 15.2067912 6.0583389 4.3633175

```

Oxygen atom O

```

none O-atom 246.844 ! ± 0.0021 ATcT v.1.122 249.229 at 298.15 K
O
! NIST-JANAF pg 1717
!
! S=160.95, Cp= 21.91, HT)-H(0)=6.72
1 1 5 ! 5 e-states
0.0 5 ! 3P2
158.265 3 ! 3P1
226.997 1 ! 3P0
15867.86 5 ! 1D2
33792.58 1 ! 1S0
0 'HAR' 'AMUA'

```

Ozone O₃

```

none O3 144.396 ! ± 0.039 ATcT v1.122
O3
! HoF(298) 141.733 v1.122
! Rot and vib parameters from Barbe, J. Mol. Struct. 616 (2002) 55D65
! diagonal anharmonicities from Barbe
2 1 1
0.0 1
5 'HAR' 'CM-1'
1 vib 1133.013 -5.197 1
2 vib 714.967 -1.137 1
3 vib 1087.277 -9.994 1
4 qro 3.55256 1.0 1
5 qro 0.42315 1.0 2

none Ozone 144.396 ! ± 0.039 ATcT v1.122; W3X-L 149.7 JMS unpub
O3
! B3LYP/cc-pVTZ+d vib, rots scale=0.9681
! Lit. S=238.932, Cp=39.328, H(T)-H(0)=10.351 NIST-JANAF
! Calc. 238.06 38.37 10.28
2 1 1 ! C2v
0.0 1 ! 1A1
4 'HAR' 'GHZ'
1 vib 721.92 0.0 1 ! A1
2 vib 1154.67 0.0 1 ! B2

```

3 vib 1211.33 0.0 1 ! A1
4 top 12.8577 113.683 1 ! 113.6832666 13.6053131 12.1511014

Phosphine PH₃

none PH3 13.39
PH3
! vibs: Sousa-Silva et al., JMS 288, 28-37 (2013)
! rots: Herzberg 1966
! HoF(298) = 5.47 kJ/mol [NIST WebBook, accessed 9/12/2016]
3 1 1
0.0 1
5 'HAR' 'CM-1'
1 vib 2321.12 0.0 1
2 vib 992.13 -11.7 1
3 vib 2326.86 0.0 2
4 vib 1118.31 -9.79 2
5 top 4.45236 3.930 1 ! cm-1 Herzberg 1966

Peroxynitrous acid HOONO *cis/cis*

none cc-HOONO -6.14 ! ± 0.37 ATcT v1.118
HNO3
! vibs: Bean et al. JPCA 107, 6974 (2003), Zhang et al. JCP 124, 084305 (2006)
! rot consts: Fry et al. JCP 124, 084304 (2006)
! HOON internal rotor McCoy et al., JCP 122, 104311 (2006)
! HoF(298) -14.58
1 1 1
0.0 1
11 'OBS' 'AMUA'
1 vib 3306. 0.0 1 ! gas phase: Bean JPCA 107, 6974 (2003)
2 vib 1600.6 0.0 1 ! matrix isolation: Zhang JCP 124, 084305 (2006)
3 vib 1392.0 0.0 1 ! ...
4 vib 922.8 0.0 1 ! ...
5 vib 789.7 0.0 1 ! ...
6 vib 617.0 0.0 1 ! ...
7 vib 376.0 0.0 1 ! calculated: Zhang
8 vib 462.0 0.0 1 ! ...
9 hrd 9 6 1 ! calculated Vhr and geometries for Ihr: JCP 122, 104311 (2006)
Vhrd3 1 0.0 738.69 -399.11 -39.667 -159.55 -98.182 -23.539 -11.01 -4.6407 -1.6787
Ihrd1 1 0.0 0.87658 -0.026743 0.017256 -0.00093998 -0.0078867 -0.023668
10 qro 23.61 1 1 ! K-rotor: Fry et al. JCP 124, 084304 (2006)
11 qro 74.49 1 2 ! 2-D adiabatic rotor:

Peroxynitrous acid HOONO *trans/perp*

none tp-HOONO 7.56 ! ± 0.42 ATcT v1.118
HNO3
! HoF(298) 0.48
! fundamental vibs, diagonal anharmonicities CCSD(T)/ANO Konen JCP 122, 094320 (2005)
! internal rotor treated as in Golden, Barker, and Lohr, JPCA, 2003, 107, 11057-11071
1 2 1
0.0 1
11 'OBS' 'AMUA'
1 vib 3582.8 -88.4 1
2 vib 1700.9 -15.2 1
3 vib 1366.7 -10.3 1
4 vib 952.6 -4.7 1
5 vib 792.0 -3.8 1
6 vib 483.1 -2.9 1
7 vib 352.3 -1.8 1
8 vib 269.7 -16.7 1
9 hra 205.5 0.913 2 ! 2-fold HR; alternative: 9 vib 205.5 -0.2 1
10 qro 9.32 1 1
11 qro 105.4 1 2

Propene CH₃CH=CH₂

none Propene 35.26

C₃H₆

! vibs: Vibrational Spectra of Polyatomic Molecules Wiley, New York 1974
 ! rots: Herzberg, G., Electronic spectra and electronic structure of polyatomics
 ! HRs geom & barrier: NIST CCCBC Data Base (accessed 5/17/2016)

```

1      1      1
0.0    1
22      'OBS'      'CM-1'
1      vib      3090      0      1
2      vib      3013      0      1
3      vib      2991      0      1
4      vib      2954      0      1
5      vib      2871      0      1
6      vib      1650      0      1
7      vib      1470      0      1
8      vib      1420      0      1
9      vib      1378      0      1
10     vib      1297      0      1
11     vib      1171      0      1
12     vib      963      0      1
13     vib      920      0      1
14     vib      428      0      1
15     vib      2954      0      1
16     vib      1443      0      1
17     vib      1045      0      1
18     vib      991      0      1
19     vib      912      0      1
20     vib      578      0      1
21     hrc      6.17759  693.8      3 ! Bred = 6.17759 cm-1; Barrier = 8.3 kJ/mol
22     top      0.29020  1.53700  1 ! 1.53700 0.31039 0.27132
    
```

n-Propyl radical C₃H₇

none n-propyl 118.28 ! ATcT v.1.118

C₃H₇

! CCDB
 ! B3LYP/aug-cc-pVTZ vibs and rots, SCALED; NOTE: torsions cf Burcat's thermo tables
 !

```

1      1      1
0.0    2
25     'HAR'      'CM-1'
1      vib      3128      0      1      !
2      vib      3033      0      1      !
3      vib      2989      0      1      !
4      vib      2983      0      1      !
5      vib      2927      0      1      !
6      vib      2902      0      1      !
7      vib      2825      0      1      !
8      vib      1455      0      1      !
9      vib      1450      0      1      !
10     vib      1420      0      1      !
11     vib      1417      0      1      !
12     vib      1365      0      1      !
13     vib      1320      0      1      !
14     vib      1228      0      1      !
15     vib      1134      0      1      !
16     vib      1047      0      1      !
17     vib      1018      0      1      !
18     vib      895      0      1      !
19     vib      849      0      1      !
20     vib      733      0      1      !
21     vib      478      0      1      !
22     hra      362      10.1375  2 ! CH2 torsion? B = 10.1375 cm-1  symm=2
23     hra      235      5.90      3 ! CH3 torsion? B = 5.90 cm-1  symm=3
    
```

24 vib 93 0 1 !
 25 top 0.278 1.108 1 ! 1.108 sqrt(0.299 x 0.259)=0.278

iso-Propyl radical (CH₃)₂C•H

none i-propyl 105.75 ! ATcT v.1.118

C3H7

! CCDB

! B3LYP/aug-cc-pVTZ vibs and rots, SCALED; NOTE: torsions cf Burcat's thermo tables

!
 2 1 1
 0.0 2
 25 'HAR' 'cm-1'
 1 vib 3067 0 1 !
 2 vib 2983 0 1 !
 3 vib 2906 0 1 !
 4 vib 2843 0 1 !
 5 vib 1442 0 1 !
 6 vib 1429 0 1 !
 7 vib 1367 0 1 !
 8 vib 1143 0 1 !
 9 vib 993 0 1 !
 10 vib 857 0 1 !
 11 vib 372 0 1 !
 12 vib 335 0 1 !
 13 hra 100 5.93 3 ! CH3 torsion? B= 5.93 cm-1
 14 vib 2985 0 1 !
 15 vib 2905 0 1 !
 16 vib 2840 0 1 !
 17 vib 1428 0 1 !
 18 vib 1419 0 1 !
 19 vib 1364 0 1 !
 20 vib 1326 0 1 !
 21 vib 1108 0 1 !
 22 vib 919 0 1 !
 23 vib 911 0 1 !
 24 hra 105 5.93 3 ! CH3 torsion? B= 5.93 cm-1
 25 top 0.264 1.254 1 ! cm-1 1.254 0.279 0.249

Propane C₃H₈

none Propane -82.75 ! ATcT v1.122, -105.03 at 298K

C3H8

! Thermo data JPCRD 2, 427 (1973)

! rots: JCP 33, 1514 (1960)

! HoF(298) = -104.63 kJ/mol:

2 1 1
 0.0 1
 28 'OBS' 'MHZ'
 1 vib 2977 0 1
 2 vib 2962 0 1
 3 vib 2887 0 1
 4 vib 1476 0 1
 5 vib 1462 0 1
 6 vib 1392 0 1
 7 vib 1158 0 1
 8 vib 869 0 1
 9 vib 369 0 1
 10 vib 2967 0 1
 11 vib 1451 0 1
 12 vib 1278 0 1
 13 vib 940 0 1
 14 hrb 241 1150.7 3 ! 3-fold HR
 15 vib 2968 0 1
 16 vib 2887 0 1
 17 vib 1464 0 1

```

18  vib    1378    0    1
19  vib    1338    0    1
20  vib    1054    0    1
21  vib     922    0    1
22  vib    2973    0    1
23  vib    2968    0    1
24  vib    1472    0    1
25  vib    1192    0    1
26  vib     748    0    1
27  hrb     241  1150.7  3 ! 3-fold HR
28  top    7937.195  29207.36  1 ! 29207.36, (8446.07, 7458.98)

```

n-Propanal oxide *syn*, CH₃CH₂CHOO

none syn-CH₃CH₂CHOO -5.62

C₃H₆O₂

! syn-propanal oxide; Criegee Intermediate

! vibs and torsions: Fang et al. JCP 145, 044312 (2016)

! dhf(0): Fang et al. JCP 145, 044312 (2016) Sebbar et al. PCCP 2003, 5, 300D307

! rots: estimated structure created by replacing H with CH₃ and setting C-C

1 1 1

0.0 1

28 'HAR' 'cm-1'

1 vib 3099 0 1

2 vib 3008 0 1

3 vib 2989 0 1

4 vib 2974 0 1

5 vib 2884 0 1

6 vib 2897 0 1

7 vib 1488 0 1

8 vib 1475 0 1

9 vib 1465 0 1

10 vib 1401 0 1

11 vib 1399 0 1

12 vib 1316 0 1

13 vib 1286 0 1

14 vib 1216 0 1

15 vib 1124 0 1

16 vib 1068 0 1

17 vib 1035 0 1

18 vib 945 0 1

19 vib 908 0 1

20 vib 799 0 1

21 vib 698 0 1

22 vib 691 0 1

23 vib 451 0 1

24 vib 363 0 1

25 vib 224 0 1

26 hrc 5.97 784 3 ! Methyl rotor, Table III in Fang et al. 2016

27 hrd 13 1 1 ! Ethyl rotor, Table III in Fang et al. 2016

Vhrd3 1 0.0 785.0 -668.0 405.0 -506.0 -66.0 66.0 -13.0 -13.0 12.0 0.0 -2.0 2.0 -1.0

Bhrd1 1 0.0 1.27

28 top 0.230 0.119 1 ! estimated: Ba = 0.2685, Bb = 0.1972, Bc = 0.1189 cm-1

Styrene or ethenylbenzene, C₆H₅-CH=CH₂

none PhCHCH₂ 168.39 ! 298.15 K: 146.9± 1 Prossen & Rossini 1945

C₈H₈

! B3LYP/cc-pVTZ+d freqs, rots, scan; scale=0.9681

! JMS isodesmic 168.39 => 146.5 at 298.15K ;

! PhCH=CH₂ + CH₄ = PhH + CH₃CH=CH₂ at 0 K from CBS-QB3, CBS-APNO G3, G4, W1BD

! Lit. S=345.1 Pitzer 1946, Cp=120.19 TRC 1997;

! calc. 343.6, 120.39, H(T)-H(0)=20.43

1 1 1 ! Cs symm

0.0 1 ! 1A'

44 'HAR' 'CM-1'

```

1      hrd 13  10  2  !  replaced      22.68      0.00      1  !  A"
Vhrd3 1 0.000 576.630 1.072 -715.238 -4.425 142.118 3.135 -2.079 1.849 0.629 -0.442 -
0.308 -1.110 0.529
Bhrd1 1 0.000 1.551 -0.092 0.213 0.011 -0.195 0.014 -0.008 0.016 0.002 0.000
 2     vib      199.01      0.00      1  !  A"
 3     vib      228.86      0.00      1  !  A'
 4     vib      401.73      0.00      1  !  A"
 5     vib      435.31      0.00      1  !  A'
 6     vib      435.72      0.00      1  !  A"
 7     vib      544.29      0.00      1  !  A'
 8     vib      616.57      0.00      1  !  A'
 9     vib      639.58      0.00      1  !  A"
10     vib      691.86      0.00      1  !  A"
11     vib      764.31      0.00      1  !  A'
12     vib      778.78      0.00      1  !  A"
13     vib      829.26      0.00      1  !  A"
14     vib      907.64      0.00      1  !  A"
15     vib      908.53      0.00      1  !  A"
16     vib      954.77      0.00      1  !  A"
17     vib      973.82      0.00      1  !  A"
18     vib      987.12      0.00      1  !  A'
19     vib     1000.69      0.00      1  !  A"
20     vib     1011.17      0.00      1  !  A'
21     vib     1025.56      0.00      1  !  A'
22     vib     1078.91      0.00      1  !  A'
23     vib     1147.13      0.00      1  !  A'
24     vib     1169.02      0.00      1  !  A'
25     vib     1189.69      0.00      1  !  A'
26     vib     1279.07      0.00      1  !  A'
27     vib     1305.22      0.00      1  !  A'
28     vib     1325.29      0.00      1  !  A'
29     vib     1410.92      0.00      1  !  A'
30     vib     1441.58      0.00      1  !  A'
31     vib     1485.42      0.00      1  !  A'
32     vib     1567.65      0.00      1  !  A'
33     vib     1592.28      0.00      1  !  A'
34     vib     1637.77      0.00      1  !  A'
35     vib     3030.27      0.00      1  !  A'
36     vib     3045.70      0.00      1  !  A'
37     vib     3058.43      0.00      1  !  A'
38     vib     3064.80      0.00      1  !  A'
39     vib     3074.07      0.00      1  !  A'
40     vib     3082.32      0.00      1  !  A'
41     vib     3090.31      0.00      1  !  A'
42     vib     3121.36      0.00      1  !  A'
43     qro      0.1743309      1      1  !
44     qro      0.0453102      1      2  !  0.0515794  0.0398029

```

Sulfur atom S

```

none  S  274.92
S
! CODATA Key Value
! gas phase atomic Sulfur
!
1      1      5
0.0    5
396.09 3
573.65 1
9238.58 5
22179.99 1
0  'HAR'  'AMUA'

```

Sulfur atom ³²S

```

none  32S  274.92
[S32]

```

```
! CODATA Key Value
! gas phase atomic Sulfur
!
1 1 5
0.0 5
396.09 3
573.65 1
9238.58 5
22179.99 1
0 'HAR' 'AMUA'
```

Sulfur atom ³³S

```
none 33S 274.92
[S33]
! CODATA Key Value
! gas phase atomic Sulfur
!
1 1 5
0.0 5
396.09 3
573.65 1
9238.58 5
22179.99 1
0 'HAR' 'AMUA'
```

Sulfur atom ³⁴S

```
none 34S 274.92
[S34]
! CODATA Key Value
! gas phase atomic Sulfur
!
1 1 5
0.0 5
396.09 3
573.65 1
9238.58 5
22179.99 1
0 'HAR' 'AMUA'
```

Sulfur atom ³⁶S

```
none 36S 274.92
[S36]
! CODATA Key Value
! gas phase atomic Sulfur
!
1 1 5
0.0 5
396.09 3
573.65 1
9238.58 5
22179.99 1
0 'HAR' 'AMUA'
```

Sulfur dioxide SO₂

```
none SO2 -294.30
SO2
! CODATA Key Value
!
!
2 1 1
0.0 1
5 'HAR' 'AMUA'
1 vib 517.69 0 1
```


2	vib	1151.38	0	1
3	vib	1361.76	0	1
4	qro	8.3105	1	1
5	qro	53.023	1	2

Sulfuric acid H₂SO₄

none SulfuricAcid -719.5 ! W3X-L JMS unpub. -720.8±2 Dorofeeva et al. JPCRD 32,2003 879 H2SO4

! B3LYP/cc-pVTZ+d freqs, rots, scan, anharm unscaled
 ! cf MP2/6-311G(2d,p) Demaison JPCA 2007, 111, 2602; Partanen JCTC, 2016, 12, 5511
 ! Lit. S=298.78, Cp=83.76 NIST-JANAF 1998 Calc. 312.90, 92.67 7 18.77

2 1 1 ! C2 symm lowest conformer

0.0 1 ! 1A

16		'OBS'	'GHZ'		
1	vib	3587.18	-42.1	1	!
2	vib	1201.27	-3.70	1	!
3	vib	1109.89	-5.63	1	!
4	vib	798.70	-2.13	1	!
5	vib	536.71	-0.17	1	!
6	vib	427.00	-1.46	1	!
7	vib	342.25	-1.67	1	!

8 hrd 13 10 1

Vhrd3 1 -0.073 571.157 -182.799 -363.891 -31.579 24.400 -2.605 -0.832 -291.564 59.644
 127.045 1.916 -1.909 0.390

Bhrd1 1 -0.073 16.7995 2.5178 0.0835 2.2885 -2.7007 0.6784 0.0808 0.3519 0.1194 0.0461

9	vib	3582.70	-42.0	1	!
10	vib	1444.29	-4.61	1	!
11	vib	1132.37	-4.91	1	!
12	vib	851.58	-2.35	1	!
13	vib	544.26	-0.25	1	!
14	vib	486.87	-0.08	1	!

15 hrd 13 10 1

Vhrd3 1 -0.073 571.157 -182.799 -363.891 -31.579 24.400 -2.605 -0.832 -291.564 59.644
 127.045 1.916 -1.909 0.390

Bhrd1 1 -0.073 16.7995 2.5178 0.0835 2.2885 -2.7007 0.6784 0.0808 0.3519 0.1194 0.0461

16	top	5.0840	4.8867	1	!	5.0840592	4.9772848	4.7976813
----	-----	--------	--------	---	---	-----------	-----------	-----------

none H2SO4 -720.8 ! ±2 Dorofeeva et al. JPCRD 32,2003 879 via CBS-QB3

H2SO4

! Sulfuric acid

! Dorofeeva et al. JPCRD 32 (2003) 879 S=311.3, Cp=90.24

! This Work: S=311.15 , Cp=90.21, HT-H0=18.38 // 3rd Millennium: 311.333, 90.235

2 1 1

0.0 1

16	'OBS'	'CM-1'		
1	vib	3563.	0.	1
2	vib	1216.	0.	1
3	vib	1136.	0.	1
4	vib	831.	0.	1
5	vib	548.	0.	1
6	vib	420.	0.	1
7	vib	355.	0.	1
8	hrd	9	1	1

Vhrd3 1 0. 534.8 -153.3 -342. -60.4 23.1 -283.4 -1.8 106.3 9.0

Bhrd1 1 0. 21.

9	vib	3567.	0.	1
10	vib	1452.	0.	1
11	vib	1157.	0.	1
12	vib	882.	0.	1
13	vib	558.	0.	1
14	vib	475.	0.	1
15	hrd	9	1	1

Vhrd3 1 0. 534.8 -153.3 -342. -60.4 23.1 -283.4 -1.8 106.3 9.0

Bhrd1 1 0. 21.
16 top 0.1698546 0.1628133 1 ! cm-1

Toluene C₆H₅CH₃

none Toluene 73.69

C7H8

! vib: H. F. Hamerka and J. O. Jensen, J. Mol. Struct. (Theochem) 331, 203-214 (1995)
! rots & hind. rotor: Lovas et al., JPCRD, 18, 1245-1524 (1989)
! HoF(298): 50.41 ATcT v.1.118; calc. S=318.2, Cp=102.5

1 1 1
0.0 1

40		'OBS'	'MHZ'		
1	hrc	160948.	4.879	6	! C-CHs tors B=160948 MHz, V=4.879 cm-1
2	vib	225	0	1	! C-CHs wag
3	vib	354	0	1	! C-CHs wag
4	vib	409	0	1	! C-C bend
5	vib	466	0	1	! CC bend
6	vib	522	0	1	! C-C bend
7	vib	637	0	1	! CCHs bend
8	vib	698	0	1	! C-C bend
9	vib	733	0	1	! C-H bend
10	vib	779	0	1	! C-C bend
11	vib	836	0	1	! C-H bend
12	vib	904	0	1	! C-H bend
13	vib	966	0	1	! CH bend
14	vib	985	0	1	! C-C bend
15	vib	1011	0	1	! C-C bend
16	vib	1030	0	1	! C-C bend
17	vib	1032	0	1	! C-H bend
18	vib	1078	0	1	! C-CHs bend
19	vib	1090	0	1	! C-H bend
20	vib	1153	0	1	! CH bend
21	vib	1197	0	1	! C-H bend
22	vib	1214	0	1	! CCHs stretch
23	vib	1258	0	1	! CH bend
24	vib	1376	0	1	! C-H bend
25	vib	1455	0	1	! C-H3 bend
26	vib	1465	0	1	! CC stretch
27	vib	1506	0	1	! C-C stretch
28	vib	1513	0	1	! C-H3 bend
29	vib	1527	0	1	! CH3 bend
30	vib	1587	0	1	! C-C stretch
31	vib	1601	0	1	! C-C stretch
32	vib	2901	0	1	! CHa sym str
33	vib	2954	0	1	! CHs asym str
34	vib	2974	0	1	! C-Hs asym str
35	vib	3038	0	1	! C-H stretch
36	vib	3044	0	1	! C-H stretch
37	vib	3055	0	1	! CH stretch
38	vib	3066	0	1	! CH stretch
39	vib	3080	0	1	! C-H stretch
40	top	2077.16	5729.32	1	! B2 = 2077.16 B1 = 5729.32

none C₆H₅CH₃ 73.69 ! ex ATcT v1.118

C7H8 !

! Toluene.log at B3LYP/cc-pVTZ+d SCALE: 0.9886

! 6-fold symmetry for rotn Ph--CH3 bond v low barrier << 1 kJ

! S=319.7, Cp=102.0; Lit. 3rd Mllnm S=320.2, Cp=103.3 WebBook 103.7 ±1.4

1 1 1 ! external symmetry, optical isomers, electronic level degeneracies

0.0 1 ! state, multiplicity

41 'HAR' 'CM-1'

1	qro	5.587	6	1	! I(red) ex MOMINERT = 167.49 GHz
2	vib	208.31	0.0	1	
3	vib	341.12	0.0	1	

4	vib	413.84	0.0	1
5	vib	474.78	0.0	1
6	vib	526.09	0.0	1
7	vib	634.21	0.0	1
8	vib	711.63	0.0	1
9	vib	742.69	0.0	1
10	vib	794.78	0.0	1
11	vib	853.17	0.0	1
12	vib	910.57	0.0	1
13	vib	976.35	0.0	1
14	vib	994.36	0.0	1
15	vib	997.82	0.0	1
16	vib	1015.35	0.0	1
17	vib	1046.53	0.0	1
18	vib	1058.61	0.0	1
19	vib	1105.48	0.0	1
20	vib	1174.67	0.0	1
21	vib	1197.50	0.0	1
22	vib	1221.86	0.0	1
23	vib	1318.68	0.0	1
24	vib	1353.11	0.0	1
25	vib	1405.78	0.0	1
26	vib	1462.59	0.0	1
27	vib	1479.96	0.0	1
28	vib	1494.76	0.0	1
29	vib	1523.62	0.0	1
30	vib	1615.24	0.0	1
31	vib	1636.49	0.0	1
32	vib	2999.90	0.0	1
33	vib	3051.44	0.0	1
34	vib	3077.98	0.0	1
35	vib	3130.92	0.0	1
36	vib	3132.59	0.0	1
37	vib	3145.28	0.0	1
38	vib	3153.50	0.0	1
39	vib	3165.99	0.0	1
40	qro	0.186176	1	1
41	qro	0.070327	1	2 ! 0.0843110 0.0586617

Trioxidane or dihydrogen trioxide, *trans* HOOOH

none HOOOH -82.15 ! W3X-L -82.1 JMS unpub. -81.43 ± 0.70 ATcT v1.122 *trans* HOOOH
H2O3
! B3LYP/cc-pVTZ+d vib, rots, anharmonic, hindered rotors full treatment
! Trioxidane, dihydrogen trioxide DfH(298)=-90.55 cf ATcT -90.27
!
! Calc. S=257.31, Cp=63.70, H(T)-H(0)=13.09
2 1 1 ! C2 symmetry, no optical isomers, 1 electronic state
0.0 1 ! Singlet A1
10 'HAR' 'GHZ'
1 vib 3513.248 -46.50 1 ! A
2 vib 1355.744 -5.84 1 ! A
3 vib 923.125 -2.62 1 ! A
4 vib 509.944 -1.55 1 ! A
5 hrd 13 10 1 !FREQUENCY REMOVED = 331.227 -7.27 1 ! A
Vhrd3 1 0.0139 1248.9512 -417.582 -797.2321 -33.4842 0.6116 -0.1118 -0.7991 -128.8603 -
44.4319 75.7364 -12.2189 -2.3415 -0.2748
Bhrd1 1 0.0139 20.448 0.9645 -0.669 0.6445 -0.2297 -0.0323 0.0716 -0.0483 0.0124 0.0142
6 vib 3508.970 -46.25 1 ! B
7 vib 1361.538 -5.63 1 ! B
8 vib 792.226 -3.09 1 ! B
9 hrd 13 10 1 !FREQUENCY REMOVED = 370.955 -13.93 1 ! B
Vhrd3 1 0.0139 1248.9512 -417.582 -797.2321 -33.4842 0.6116 -0.1118 -0.7991 -128.8603 -
44.4319 75.7364 -12.2189 -2.3415 -0.2748
Bhrd1 1 0.0139 20.448 0.9645 -0.669 0.6445 -0.2297 -0.0323 0.0716 -0.0483 0.0124 0.0142
10 top 10.0091 52.1387 1 ! 52.1386904 10.6620578 9.3961685

Trioxidanyl or hydrotrioxy HO-O-O or HO₃ *trans*

none trans-HO3 25.32 ! ± 0.13 ATcT v1.118
 HO3
 ! rotations from Suma et al., Science, 308, 1885-1886 (2005)
 ! Vibs 1, 3-6 from Derro et al., JCP 128, 244313 (2008)
 ! vib 2 from Fabian et al., Theor Chem Acc (2005) 114: 182D188
 ! Here, Do = 11.9, cf Do = 12.3±0.3 kJ/mol from Le Pickard , Science 328, 1258 (2010)
 1 1 1
 0.0 2
 8 'OBS' 'MHZ'
 1 vib 3569.3 0.0 1 ! Derro et al., JCP 128, 244313 (2008)
 2 vib 1341. 0.0 1 ! Fabian et al., Theor Chem Acc (2005) 114: 182D188
 3 vib 997.9 0.0 1 ! Derro
 4 vib 481.9 0.0 1 ! ...
 5 vib 243.7 0.0 1 ! ...
 6 vib 128.7 0.0 1 ! ...
 7 qro 70778.165 1.0 1 ! Suma et al., Science, 308, 1885-1886 (2005)
 8 qro 9368.554 1.0 2 ! ...

Trioxidanyl deuterated DO-O-O or DO₃ *trans*

none trans-DO3 17.84 ! dHf(0) from HO3, with zpe corrections
 DO3
 ! rotations from Suma et al., Science, 308, 1885-1886 (2005)
 ! Vibs 1, 3-6 from Derro, JCP 128, 244313 (2008); vib 2 estimated, based on HO3
 ! dHf(0) (DO3) = dHf(0) (HO3) + zpe(DO3) - zpe(HO3)
 1 1 1
 0.0 2
 8 'OBS' 'MHZ'
 1 vib 2635.1 0.0 1 ! Derro JCP 128, 244313 (2008)
 2 vib 1300. 0.0 1 ! estimated
 3 vib 783.9 0.0 1 ! Derro
 4 vib 463.0 0.0 1 ! ...
 5 vib 245.3 0.0 1 ! ...
 6 vib 102.2 0.0 1 ! ...
 7 qro 67857.371 1.0 1 ! Suma, Science, 308, 1885-1886 (2005)
 8 qro 8873.992 1.0 2 ! ...

Tritium hydride HD

none HT 0.328
 HT
 ! vib & rot: WebBook September 13, 2016
 ! dHf(0): assumed to be similar to HD
 !
 1 1 1
 0.0 1
 2 'HAR' 'CM-1'
 1 vib 3597.05 -81.678 1
 2 qro 39.763 1.0 2 ! Be = 40.595 cm-1; alpha(e) = 1.664 cm-1

Water H₂O

none H2O -238.928 ! ± 0.026 ATcT v1.118
 H2O
 ! NIST-JANAF 1998
 !
 !
 2 1 1
 0.0 1
 5 'OBS' 'CM-1'
 1 vib 3651.1 0.0 1
 2 vib 1594.7 0.0 1
 3 vib 3755.9 0.0 1
 4 qro 27.8847 1.0 1 ! K-rotor

```
5   gro   11.6051  1.0    2    ! 2-D rotor
```

Xenon atom

```
none  Xe   0.0  ! By definition
```

```
Xe
```

```
! NIST-JANAF 1998
```

```
!
```

```
!
```

```
1     1     1
```

```
0.0   1
```

```
0  'HAR'  'AMUA'
```

Formation enthalpies at 298.15 K

Note that **THERMO** can compute the formation enthalpy at 298.15 K from the supplied formation enthalpy at 0 K and the enthalpy function $H(298.15\text{ K}) - H(0\text{ K})$ for the molecular species together with a similar set of terms for the constituent elements:

$$\Delta_f H(298.15\text{ K}) = \Delta_f H(0\text{ K}) + \{H(298.15\text{ K}) - H(0\text{ K})\} - \sum n_i \{H(298.15\text{ K}) - H(0\text{ K})\}_i$$

where $\{H(298.15\text{ K}) - H(0\text{ K})\}_i$ is the enthalpy shift for an element in its standard state. This necessitates an inbuilt table⁸ of these quantities, for example⁹:

Element	$\{H(298.15\text{ K}) - H(0\text{ K})\}_i$
C (graphite)	1.046
(1/2) H ₂ (gas)	4.226
(1/2) O ₂ (gas)	4.351
(1/2) N ₂ (gas)	4.351
(1/2) Cl ₂ (gas)	4.591

So for propane, C₃H₈, for which $\Delta_f H(0\text{ K}) = -82.75$ and $H(298.15\text{ K}) - H(0\text{ K}) = 14.94$ the calculated $\Delta_f H(298.15\text{ K}) = -82.75 + 14.94 - \{(3 \times 1.046) + (8 \times 4.226)\} = -104.76$ kJ/mol.

Of course this computed shift is reliant on the best possible calculated enthalpy shift for the molecular species itself.

⁸ In **SUBROUTINE ELEMENT** of **element.f**

⁹ Sourced from NIST-JANAF