SUPPORTING INFORMATION

Effect of temperature on the gas-phase reaction of CH_3CN with OH radicals: Experimental (T=11.7-177.5 K) and computational (T=10-400 K) kinetic study

Daniel González,[1,2] André Canosa,[3] Emilio Martínez-Núñez,[4] Antonio Fernández-Ramos,[4,5,*] Bernabé Ballesteros,[1,2] Marcelino Agúndez,[6] José Cernicharo [6] and Elena Jiménez[1,2,*]

[1] Departamento de Química Física, Facultad de Ciencias y Tecnologías Químicas, Universidad de Castilla-La Mancha (UCLM), Avda. Camilo José Cela 1B, 13071 Ciudad Real, Spain.
[2] Instituto de Investigación en Combustión y Contaminación Atmosférica, UCLM, Camino de Moledores s/n, 13071 Ciudad Real, Spain.
[3] Institut de Physique de Rennes-CNRS – UMR 6251, Université de Rennes, F-35000 Rennes, France.
[4] Departamento de Química Física, Facultade de Química, Campus Vida, Universidade de Santiago de Compostela, Avda. das Ciencias s/n, 15782, Santiago de Compostela, Spain.
[5] Centro Singular de Investigación en Química Biológica y Materiales Moleculares (CIQUS), Campus Vida, Universidade de Santiago de Compostela, C/ Jenaro de la Fuente s/n, 15782, Santiago de Compostela, Spain.
[6] Molecular Astrophysics Group, Instituto de Física Fundamental (IFF-CSIC); Consejo Superior de Investigaciones Científicas, C/Serrano 123, 28006, Madrid, Spain.

*** Correspondence:** Elena.Jimenez@uclm.es; qf.ramos@usc.es

Kinetic analysis

As discussed in our previous works,[1,2] the initial increase of I_{LIF} is due to the population of the OH($X^2\Pi$,v''=0) from rotational relaxation within the electronic ground state. As shown in Fig. S1.A, the timescale for which rotational relaxation is produced lies on the order of a few tens of microseconds. After the collisional relaxation is complete, the OH loss results from a typical *pseudo*-first order scenario and the temporal evolution of I_{LIF} follows a single exponential behaviour, as shown by the integrated rate equation ES1 in terms of the LIF intensities:

$$\boldsymbol{I_{LIF}(t) = I_{LIF}(t_0)\ exp^{-k'(t-t_0)}} \qquad \text{(ES1)}$$

where t_0 is the reaction time from which the analysis of the decays was started.

In Figure S1.A, we present an example of the I_{LIF} vs. reaction time profiles recorded at 36.2 K in the absence of CH_3CN (black circles) together with the value of k'_0 derived from the regression analysis. When CH_3CN is present ([CH_3CN]=1.46×10^{13} cm^{-3} (red squares) and [CH_3CN]=1.39×10^{14} cm^{-3} (blue triangles)) the OH-decay is faster, as shown by the values of k' derived from the regression analysis (Figure S1.B). In Figure S1, the difference $I_{LIF,exp}$- $I_{LIF,fit}$ (residual) is also depicted, showing the goodness of the fit.

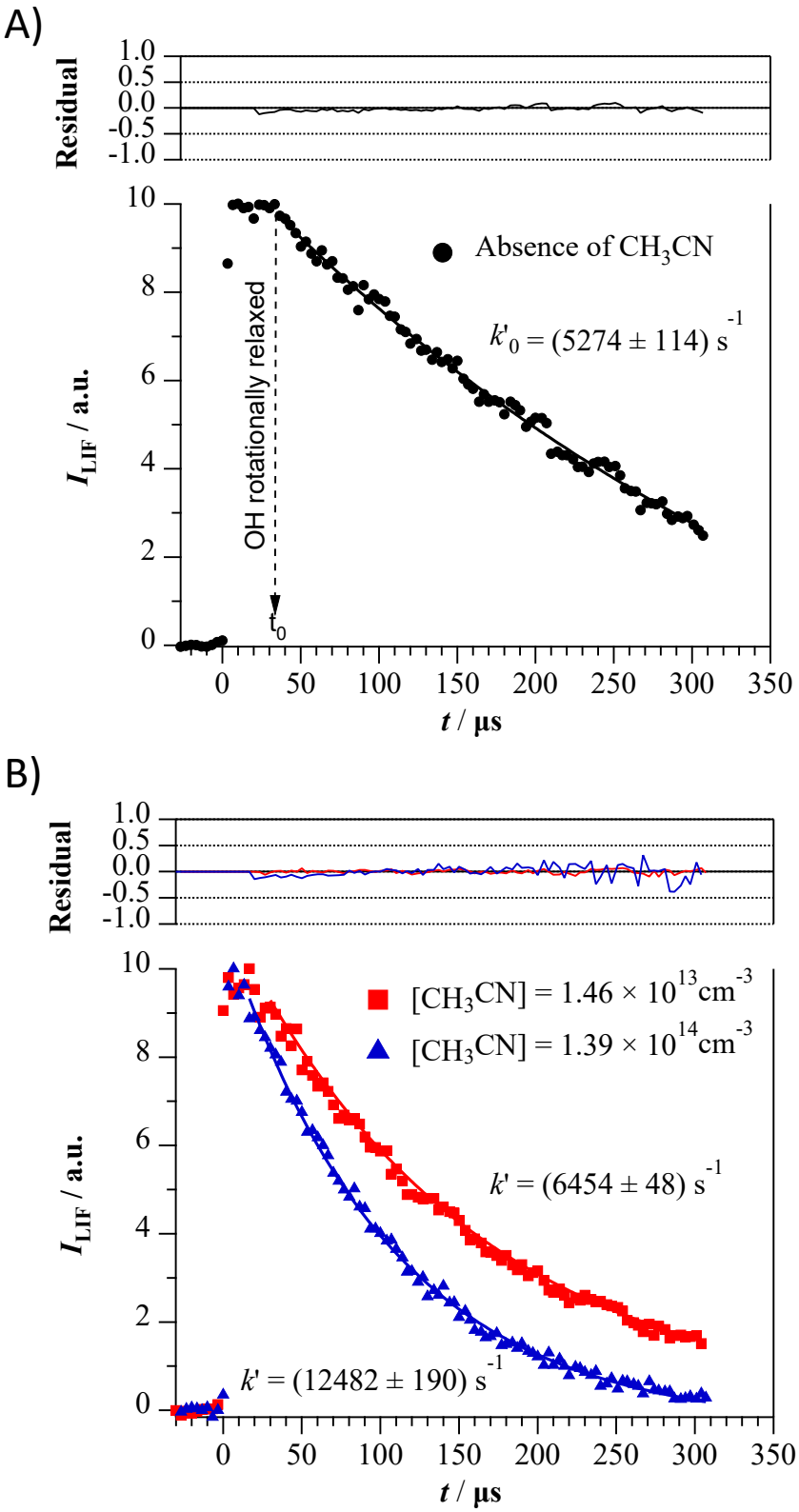

Figure S1. Examples of the I_{LIF} recorded as a function of the reaction time at 36.2 K A) in the absence (black circles) and B) in the presence (red squares and blue triangles) of CH_3CN together with the corresponding values of k'_0 and k' derived from the regression analysis.

Determination of [CH_3CN] in the jet

Gaseous CH_3CN was introduced in the system from diluted gas mixtures or pure liquid samples (≥99.9%, Sigma-Aldrich).

Method 1: Flow rate measurements

Diluted mixtures of CH_3CN in Ar, N_2, or He were prepared in a 20-L or 50-L storage bulb by introducing a controlled partial pressure of pure CH_3CN. The dilution factor (*f*) of these mixtures ranged from 0.4% to 5.5%. [CH_3CN] was calculated from the mass flow rate of the CH_3CN/buffer gas mixture, considering the mixing ratio *f*, the total gas jet density and the total mass flow through the system, as explained for other reactants.[3–5] All gases were introduced through a calibrated mass flow controller (Sierra Instruments, Inc., model: SmartTrak 100).

Method 2: Vapor pressure measurements

In some experiments carried out at 36.2 K, pure CH_3CN was introduced into the *reservoir* by bubbling a small flow of helium (F_{He/CH_3CN}) through the liquid acetonitrile contained in a glass bubbler similar to that described in Sleiman *et al*.[6] This bubbler was immersed in a water bath at a constant temperature (22.3º C). The temperature of the water was accurately measured with a CRISON portable thermometer. In these experiments, [CH_3CN] was calculated from the partial flow rate of pure CH_3CN, F_{CH_3CN}, introduced in the *reservoir*, which was determined from the measured total pressure in the bubbler (P_T) and the vapor pressure of CH_3CN, P_{v,CH_3CN}, at that temperature according to equation ES2. P_T (175-180 mbar) was precisely measured over the bubbler with a 1000-Torr full scale capacitance manometer (Leybold Oerlikon, CERAVAC). As room temperature in the laboratory was slightly higher than that of the water bath, the condensation of gaseous CH_3CN in the Teflon tubes from the bubbler to the reservoir is unlikely to occur.

$$F_{CH_3CN} = P_{v,CH_3CN} \times \frac{F_{buffer/CH_3CN}}{P_T - P_{v,CH_3CN}} \quad \text{(ES2)}$$

P_{v,CH_3CN} (103.96 mbar at 22.3 ºC) was calculated using Antoine's law obtained by Dojcansky and Heinrich.[7] For this method, [CH_3CN] in the jet was calculated considering the proportion of CH_3CN in the total mass flow and the gas density.

$$[CH_3CN] = n \times \frac{F_{CH_3CN}}{F_{Total}} \quad \text{(ES3)}$$

In separate experiments carried out at 36.2 K, a diluted mixture (method 1), prepared as described above, was used as well to compare both methods. As it can be seen in Figure S2, both procedures provide similar [CH_3CN] and, therefore, similar *k'* values.

As we confirmed that [CH_3CN] from flow measurements (ES2) is well-determined, for the rest of the experiments we used the method 1 using diluted mixtures of acetonitrile.

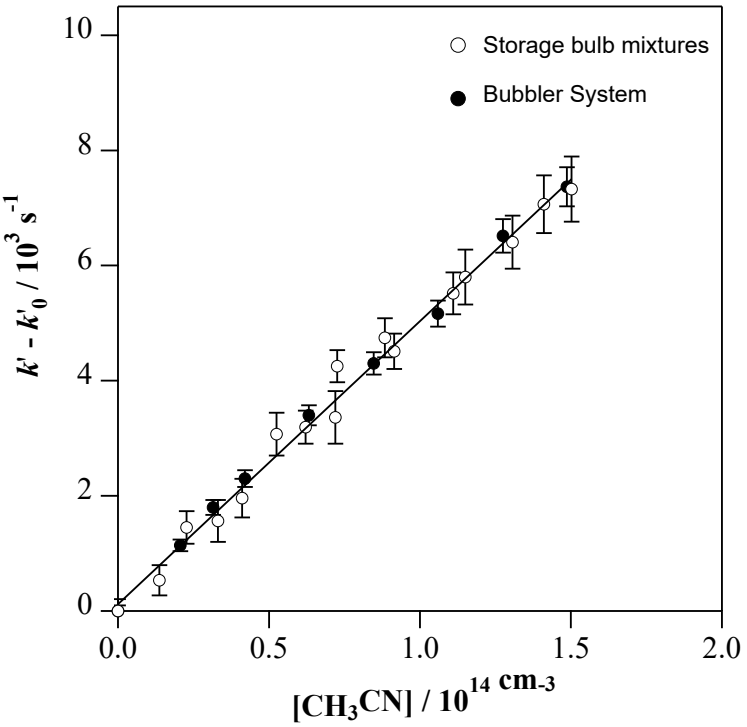

Figure S2. Example of k'-k'$_0$ versus [CH_3CN] plot using the two different methods described to obtain [CH_3CN] in the jet at 36.2 K.

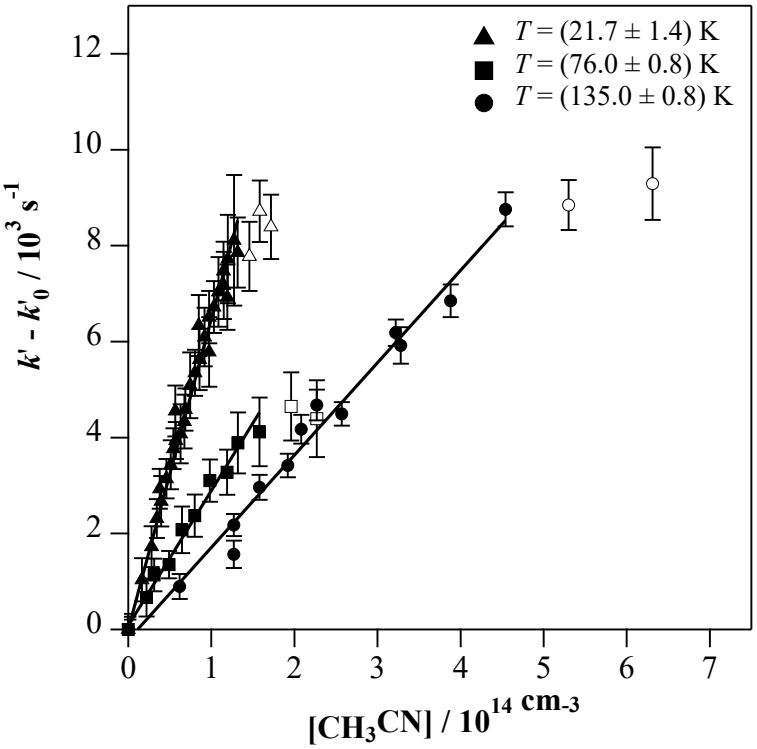

Figure S3. Example of the downward curvature observed at 21.7, 76.0, and 135.0 K. Empty symbols denote the acetonitrile concentrations for which dimerization starts affecting the kinetic results.

REFERENCES

1 E. Jiménez, B. Ballesteros, A. Canosa, T. M. Townsend, F. J. Maigler, V. Napal, B. R. Rowe and J. Albaladejo, *Rev. Sci. Instrum.*, 2015, **86**, 45108.

2 A. J. Ocaña, S. Blázquez, B. Ballesteros, A. Canosa, M. Antiñolo, J. Albaladejo and E. Jiménez, *Phys. Chem. Chem. Phys.*, 2018, **20**, 5865–5873.

3 S. Blázquez, D. González, A. García-Sáez, M. Antiñolo, A. Bergeat, F. Caralp, R. Mereau, A. Canosa, B. Ballesteros, J. Albaladejo and E. Jiménez, *ACS Earth Sp. Chem.*, 2019, **3**, 1873–1883.

4 S. Blázquez, D. González, E. M. Neeman, B. Ballesteros, M. Agúndez, A. Canosa, J. Albaladejo, J. Cernicharo and E. Jiménez, *Phys. Chem. Chem. Phys.*, 2020, **22**, 20562–20572.

5 D. González, A. Lema-Saavedra, S. Espinosa, E. Martínez-Núñez, A. Fernández-Ramos, A. Canosa, B. Ballesteros and E. Jiménez, *Phys. Chem. Chem. Phys.*, 2022, **24**, 23593–23601.

6 C. Sleiman, S. González, S. J. Klippenstein, D. Talbi, G. El Dib and A. Canosa, *Phys. Chem. Chem. Phys.*, 2016, **18**, 15118–15132.

7 J. Dojcansky and J. Heinrich, *Chem. Zvesti*, 1974, **28**, 157–159.

Electronic structure data: M08-HX/MG3S

CH_3CN information

```
-------------------------
 Analysis of STRUC: CH3CN
-------------------------

    Number of conformers: 1

       V0 = electronic energy
       V1 = electronic energy + zero-point energy (ZPE)

       ZPE is calculated using scaled frequencies
       Frequency scale factor: 0.97300

       min(V0) = -132.75766660 hartree
       min(V1) = -132.71334082 hartree

       Relative energies (in kcal/mol):
       ------------------------------------------------------------------------
        name | V0-min(V0) | V1-min(V1) |   ZPE   | mass (amu) | weight |  PGS
       ------------------------------------------------------------------------
          001 |     0.000  |     0.000  |   27.81 |     41.03  |    1   |  C3v
       ------------------------------------------------------------------------
       weight: equals 2 if the structure has a conformational enantiomer,
               equals 1 otherwise
       PGS   : point group of symmetry

    ------------------
    Conformation: 001
    ------------------
     | Molecular formula     : C(2)H(3)N
     | Number of atoms       : 6
     | Number of electrons   : 22
     | Vibrational DOFs      : 12
     | Charge                : 0
     | Multiplicity          : 1
     | Electronic energy (V0): -132.75766660 hartree
     | Total mass [root]     : 41.0265 amu
     | Total mass            : 41.0265 amu
     | Point group symmetry  : C3v
     | Rotational sym num    : 3
     | Cartesian coordinates (Angstrom):
     |    N    +0.00000000   +0.00000000   -1.31409210  [ 14.003 amu]
     |    C    +0.00000000   +0.00000000   -0.17054440  [ 12.000 amu]
     |    C    +0.00000000   +0.00000000   +1.28604781  [ 12.000 amu]
     |    H    -0.04402010   +1.02475150   +1.65878098  [  1.008 amu]
     |    H    -0.86545079   -0.55049827   +1.65878098  [  1.008 amu]
     |    H    +0.90947088   -0.47425323   +1.65878098  [  1.008 amu]
     | Moments and product of inertia (au):
     |         +2.071E+04  +3.534E+05  +3.534E+05  [ 2.586E+15]
     | Vibrational frequencies [1/cm] (scaled by 0.973):
     |     378.89    378.90    918.94   1029.81   1029.82   1363.50
     |    1428.17   1428.17   2374.39   2987.89   3069.14   3069.14
     | Vibrational zero-point energies [kcal/mol]:
     |       0.54      0.54      1.31      1.47      1.47      1.95
     |       2.04      2.04      3.39      4.27      4.39      4.39
     | Vibrational zero-point energy:    +0.04432578 hartree  =
     |                                       +27.81 kcal/mol =
     |                                        +1.21 eV       =
     |                                     +9728.38 cm^-1
     | V0 + zero-point energy (V1)  :  -132.71334082 hartree
     |
```

Partition functions (pfns):

T (K)	Qtr (au)	Qtr (cm^-3)	Qrot	Qvib [V0]	Qvib [V1]	Qel
10.00	2.314E-01	1.562E+24	1.514E+01	1.318E-608	1.000E+00	1.000E+00
20.00	6.546E-01	4.417E+24	4.283E+01	1.148E-304	1.000E+00	1.000E+00
30.00	1.202E+00	8.115E+24	7.869E+01	2.362E-203	1.000E+00	1.000E+00
40.00	1.851E+00	1.249E+25	1.212E+02	1.071E-152	1.000E+00	1.000E+00
50.00	2.587E+00	1.746E+25	1.693E+02	2.654E-122	1.000E+00	1.000E+00
60.00	3.401E+00	2.295E+25	2.226E+02	4.861E-102	1.000E+00	1.000E+00
70.00	4.286E+00	2.892E+25	2.805E+02	1.447E-87	1.001E+00	1.000E+00
80.00	5.236E+00	3.534E+25	3.427E+02	1.037E-76	1.002E+00	1.000E+00
90.00	6.248E+00	4.217E+25	4.089E+02	2.883E-68	1.005E+00	1.000E+00
100.00	7.318E+00	4.939E+25	4.789E+02	1.643E-61	1.009E+00	1.000E+00
110.00	8.443E+00	5.698E+25	5.525E+02	5.550E-56	1.014E+00	1.000E+00
120.00	9.620E+00	6.492E+25	6.295E+02	2.252E-51	1.022E+00	1.000E+00
130.00	1.085E+01	7.320E+25	7.098E+02	1.792E-47	1.031E+00	1.000E+00
140.00	1.212E+01	8.181E+25	7.933E+02	3.962E-44	1.042E+00	1.000E+00
150.00	1.344E+01	9.073E+25	8.798E+02	3.148E-41	1.055E+00	1.000E+00
160.00	1.481E+01	9.995E+25	9.692E+02	1.089E-38	1.070E+00	1.000E+00
170.00	1.622E+01	1.095E+26	1.061E+03	1.899E-36	1.087E+00	1.000E+00
180.00	1.767E+01	1.193E+26	1.156E+03	1.873E-34	1.106E+00	1.000E+00
190.00	1.917E+01	1.293E+26	1.254E+03	1.142E-32	1.126E+00	1.000E+00
200.00	2.070E+01	1.397E+26	1.355E+03	4.634E-31	1.148E+00	1.000E+00
210.00	2.227E+01	1.503E+26	1.457E+03	1.325E-29	1.172E+00	1.000E+00
220.00	2.388E+01	1.612E+26	1.563E+03	2.802E-28	1.198E+00	1.000E+00
230.00	2.553E+01	1.723E+26	1.670E+03	4.556E-27	1.225E+00	1.000E+00
240.00	2.721E+01	1.836E+26	1.781E+03	5.890E-26	1.254E+00	1.000E+00
250.00	2.893E+01	1.952E+26	1.893E+03	6.221E-25	1.285E+00	1.000E+00
260.00	3.068E+01	2.070E+26	2.008E+03	5.496E-24	1.318E+00	1.000E+00
270.00	3.247E+01	2.191E+26	2.125E+03	4.142E-23	1.353E+00	1.000E+00
280.00	3.429E+01	2.314E+26	2.244E+03	2.710E-22	1.390E+00	1.000E+00
300.00	3.803E+01	2.566E+26	2.488E+03	8.025E-21	1.469E+00	1.000E+00
320.00	4.189E+01	2.827E+26	2.741E+03	1.571E-19	1.558E+00	1.000E+00
340.00	4.588E+01	3.096E+26	3.002E+03	2.187E-18	1.655E+00	1.000E+00
360.00	4.999E+01	3.373E+26	3.271E+03	2.293E-17	1.762E+00	1.000E+00
400.00	5.855E+01	3.951E+26	3.831E+03	1.277E-15	2.010E+00	1.000E+00

Qtr : translational pfn per volume unit
Qrot: rotational pfn (rigid-rotor); includes rotational symmetry number
Qvib: vibrational pfn (harmonic-oscillator) relative to V0 and to V1
Qel : electronic pfn

T (K)	Qtot [V0]	Qtot [V1]	Qtot [V0]	Qtot [V1]
10.00	4.618E-608	3.505E+00	3.116E-583	2.365E+25
20.00	3.218E-303	2.804E+01	2.172E-278	1.892E+26
30.00	2.235E-201	9.462E+01	1.508E-176	6.386E+26
40.00	2.403E-150	2.243E+02	1.622E-125	1.514E+27
50.00	1.163E-119	4.381E+02	7.847E-95	2.956E+27
60.00	3.680E-99	7.572E+02	2.483E-74	5.110E+27
70.00	1.739E-84	1.203E+03	1.173E-59	8.119E+27
80.00	1.861E-73	1.798E+03	1.256E-48	1.214E+28
90.00	7.365E-65	2.567E+03	4.970E-40	1.732E+28
100.00	5.759E-58	3.535E+03	3.886E-33	2.385E+28
110.00	2.589E-52	4.731E+03	1.747E-27	3.193E+28
120.00	1.364E-47	6.187E+03	9.204E-23	4.175E+28
130.00	1.379E-43	7.938E+03	9.309E-19	5.357E+28
140.00	3.810E-40	1.002E+04	2.571E-15	6.763E+28
150.00	3.723E-37	1.248E+04	2.513E-12	8.423E+28
160.00	1.563E-34	1.536E+04	1.055E-09	1.037E+29
170.00	3.270E-32	1.872E+04	2.207E-07	1.263E+29
180.00	3.828E-30	2.260E+04	2.583E-05	1.525E+29

```
|     190.00 |  2.746E-28 |  2.707E+04 |  1.853E-03 |  1.827E+29
|     200.00 |  1.299E-26 |  3.219E+04 |  8.768E-02 |  2.172E+29
|     210.00 |  4.301E-25 |  3.804E+04 |  2.902E+00 |  2.567E+29
|     220.00 |  1.046E-23 |  4.470E+04 |  7.056E+01 |  3.016E+29
|     230.00 |  1.943E-22 |  5.224E+04 |  1.311E+03 |  3.525E+29
|     240.00 |  2.853E-21 |  6.077E+04 |  1.926E+04 |  4.101E+29
|     250.00 |  3.406E-20 |  7.039E+04 |  2.299E+05 |  4.750E+29
|     260.00 |  3.385E-19 |  8.120E+04 |  2.284E+06 |  5.480E+29
|     270.00 |  2.857E-18 |  9.334E+04 |  1.928E+07 |  6.299E+29
|     280.00 |  2.085E-17 |  1.069E+05 |  1.407E+08 |  7.216E+29
|     300.00 |  7.594E-16 |  1.390E+05 |  5.125E+09 |  9.383E+29
|     320.00 |  1.804E-14 |  1.789E+05 |  1.217E+11 |  1.207E+30
|     340.00 |  3.013E-13 |  2.279E+05 |  2.033E+12 |  1.538E+30
|     360.00 |  3.750E-12 |  2.881E+05 |  2.531E+13 |  1.944E+30
|     400.00 |  2.864E-10 |  4.507E+05 |  1.932E+15 |  3.042E+30
| ------------------------------------------------------------------
|            |          in au          |        in cm^-3
| ------------------------------------------------------------------
|   Qtot: total pfn per unit volume
|         * [V0] --> from the bottom of the potential (V0)
|         * [V1] --> from the zero-point energy (V1)
|         * includes rotational symmetry number
|
|
| Gibbs free energy (hartree):
| ------------------------------------------
|   T (K)  |   v = 1 cm^3   |   v = kbT/p0
| ------------------------------------------
|    10.00 |  -132.71519105 |  -132.71366997
|    20.00 |  -132.71717298 |  -132.71417473
|    30.00 |  -132.71920462 |  -132.71474576
|    40.00 |  -132.72126854 |  -132.71535984
|    50.00 |  -132.72335647 |  -132.71600593
|    60.00 |  -132.72546357 |  -132.71667756
|    70.00 |  -132.72758667 |  -132.71737050
|    80.00 |  -132.72972363 |  -132.71808184
|    90.00 |  -132.73187290 |  -132.71880945
|   100.00 |  -132.73403335 |  -132.71955178
|   110.00 |  -132.73620414 |  -132.72030761
|   120.00 |  -132.73838459 |  -132.72107598
|   130.00 |  -132.74057415 |  -132.72185612
|   140.00 |  -132.74277238 |  -132.72264735
|   150.00 |  -132.74497889 |  -132.72344913
|   160.00 |  -132.74719333 |  -132.72426096
|   170.00 |  -132.74941541 |  -132.72508240
|   180.00 |  -132.75164487 |  -132.72591309
|   190.00 |  -132.75388146 |  -132.72675267
|   200.00 |  -132.75612498 |  -132.72760085
|   210.00 |  -132.75837524 |  -132.72845734
|   220.00 |  -132.76063206 |  -132.72932191
|   230.00 |  -132.76289529 |  -132.73019433
|   240.00 |  -132.76516478 |  -132.73107439
|   250.00 |  -132.76744042 |  -132.73196192
|   260.00 |  -132.76972209 |  -132.73285673
|   270.00 |  -132.77200967 |  -132.73375869
|   280.00 |  -132.77430309 |  -132.73466765
|   300.00 |  -132.77890706 |  -132.73650607
|   320.00 |  -132.78353337 |  -132.73837105
|   340.00 |  -132.78818150 |  -132.74026181
|   360.00 |  -132.79285097 |  -132.74217763
|   400.00 |  -132.80225230 |  -132.74608205
| ------------------------------------------
|   v : volume per molecule
|   p0: 1bar
```

OH information

```
----------------------
 Analysis of STRUC: OH
----------------------

    Number of conformers: 1

       V0 = electronic energy
       V1 = electronic energy + zero-point energy (ZPE)

       ZPE is calculated using scaled frequencies
       Frequency scale factor: 0.97300

       min(V0) = -75.72715520 hartree
       min(V1) = -75.71873895 hartree

       Relative energies (in kcal/mol):
       ------------------------------------------------------------------------
        name | V0-min(V0) | V1-min(V1) |   ZPE   | mass (amu) | weight |  PGS
       ------------------------------------------------------------------------
          001 |     0.000  |     0.000  |    5.28 |     17.00  |    1   | Cinfv
       ------------------------------------------------------------------------
       weight: equals 2 if the structure has a conformational enantiomer,
               equals 1 otherwise
       PGS   : point group of symmetry

    ------------------
    Conformation: 001
    ------------------
     | Molecular formula     : HO
     | Number of atoms       : 2
     | Number of electrons   : 9
     | Vibrational DOFs      : 1
     | Charge                : 0
     | Multiplicity          : 2
     | Electronic energy (V0): -75.72715520 hartree
     | Total mass [root]     : 17.0027 amu
     | Total mass            : 17.0027 amu
     | Point group symmetry  : Cinfv
     | Rotational sym num    : 1
     | Cartesian coordinates (Angstrom):
     |    O    -0.05750407   +0.00000000   +0.00000000  [ 15.995 amu]
     |    H    +0.91263116   +0.00000000   +0.00000000  [  1.008 amu]
     | Moments and product of inertia (au):
     |         +5.809E+03
     | Vibrational frequencies [1/cm] (scaled by 0.973):
     |    3694.31
     | Vibrational zero-point energies [kcal/mol]:
     |       5.28
     | Vibrational zero-point energy:    +0.00841625 hartree  =
     |                                         +5.28 kcal/mol =
     |                                         +0.23 eV       =
     |                                      +1847.15 cm^-1
     | V0 + zero-point energy (V1)  :   -75.71873895 hartree
     |
     | Partition functions (pfns):
     | ------------------------------------------------------------------------------------
     |    T (K)   |  Qtr (au)  | Qtr (cm^-3) |    Qrot    |  Qvib [V0] |  Qvib [V1] |     Qel
     | ------------------------------------------------------------------------------------
     |      10.00 |  6.174E-02 |   4.167E+23 |  3.679E-01 | 3.804E-116 |  1.000E+00 |  2.000E+00
     |      20.00 |  1.746E-01 |   1.178E+24 |  7.358E-01 |  1.950E-58 |  1.000E+00 |  2.000E+00
     |      30.00 |  3.208E-01 |   2.165E+24 |  1.104E+00 |  3.363E-39 |  1.000E+00 |  2.002E+00
     |      40.00 |  4.939E-01 |   3.333E+24 |  1.472E+00 |  1.397E-29 |  1.000E+00 |  2.013E+00
```

50.00	6.903E-01	4.658E+24	1.839E+00	8.242E-24	1.000E+00	2.036E+00
60.00	9.074E-01	6.124E+24	2.207E+00	5.799E-20	1.000E+00	2.070E+00
70.00	1.143E+00	7.717E+24	2.575E+00	3.247E-17	1.000E+00	2.113E+00
80.00	1.397E+00	9.428E+24	2.943E+00	3.737E-15	1.000E+00	2.161E+00
90.00	1.667E+00	1.125E+25	3.311E+00	1.498E-13	1.000E+00	2.213E+00
100.00	1.952E+00	1.318E+25	3.679E+00	2.871E-12	1.000E+00	2.267E+00
110.00	2.253E+00	1.520E+25	4.047E+00	3.216E-11	1.000E+00	2.320E+00
120.00	2.567E+00	1.732E+25	4.415E+00	2.408E-10	1.000E+00	2.373E+00
130.00	2.894E+00	1.953E+25	4.783E+00	1.323E-09	1.000E+00	2.425E+00
140.00	3.234E+00	2.183E+25	5.151E+00	5.698E-09	1.000E+00	2.474E+00
150.00	3.587E+00	2.421E+25	5.518E+00	2.020E-08	1.000E+00	2.522E+00
160.00	3.952E+00	2.667E+25	5.886E+00	6.113E-08	1.000E+00	2.568E+00
170.00	4.328E+00	2.920E+25	6.254E+00	1.624E-07	1.000E+00	2.612E+00
180.00	4.715E+00	3.182E+25	6.622E+00	3.871E-07	1.000E+00	2.653E+00
190.00	5.113E+00	3.451E+25	6.990E+00	8.419E-07	1.000E+00	2.693E+00
200.00	5.522E+00	3.727E+25	7.358E+00	1.694E-06	1.000E+00	2.731E+00
210.00	5.942E+00	4.010E+25	7.726E+00	3.190E-06	1.000E+00	2.766E+00
220.00	6.371E+00	4.299E+25	8.094E+00	5.671E-06	1.000E+00	2.801E+00
230.00	6.810E+00	4.596E+25	8.462E+00	9.588E-06	1.000E+00	2.833E+00
240.00	7.259E+00	4.899E+25	8.829E+00	1.552E-05	1.000E+00	2.864E+00
250.00	7.718E+00	5.208E+25	9.197E+00	2.417E-05	1.000E+00	2.894E+00
260.00	8.185E+00	5.524E+25	9.565E+00	3.637E-05	1.000E+00	2.922E+00
270.00	8.662E+00	5.846E+25	9.933E+00	5.311E-05	1.000E+00	2.948E+00
280.00	9.148E+00	6.173E+25	1.030E+01	7.549E-05	1.000E+00	2.974E+00
300.00	1.015E+01	6.846E+25	1.104E+01	1.421E-04	1.000E+00	3.022E+00
320.00	1.118E+01	7.542E+25	1.177E+01	2.472E-04	1.000E+00	3.066E+00
340.00	1.224E+01	8.260E+25	1.251E+01	4.030E-04	1.000E+00	3.106E+00
360.00	1.334E+01	9.000E+25	1.324E+01	6.221E-04	1.000E+00	3.143E+00
400.00	1.562E+01	1.054E+26	1.472E+01	1.302E-03	1.000E+00	3.209E+00

Qtr : translational pfn per volume unit
Qrot: rotational pfn (rigid-rotor); includes rotational symmetry number
Qvib: vibrational pfn (harmonic-oscillator) relative to V0 and to V1
Qel : electronic pfn

T (K)	Qtot [V0]	Qtot [V1]	Qtot [V0]	Qtot [V1]
10.00	1.728E-117	4.543E-02	1.166E-92	3.066E+23
20.00	5.012E-59	2.570E-01	3.382E-34	1.734E+24
30.00	2.384E-39	7.090E-01	1.609E-14	4.785E+24
40.00	2.043E-29	1.463E+00	1.379E-04	9.874E+24
50.00	2.130E-23	2.585E+00	1.438E+02	1.744E+25
60.00	2.404E-19	4.146E+00	1.622E+06	2.798E+25
70.00	2.020E-16	6.221E+00	1.363E+09	4.198E+25
80.00	3.321E-14	8.887E+00	2.241E+11	5.997E+25
90.00	1.830E-12	1.222E+01	1.235E+13	8.244E+25
100.00	4.675E-11	1.628E+01	3.155E+14	1.099E+26
110.00	6.802E-10	2.115E+01	4.590E+15	1.427E+26
120.00	6.476E-09	2.689E+01	4.370E+16	1.815E+26
130.00	4.440E-08	3.356E+01	2.996E+17	2.265E+26
140.00	2.349E-07	4.122E+01	1.585E+18	2.782E+26
150.00	1.008E-06	4.992E+01	6.805E+18	3.369E+26
160.00	3.651E-06	5.973E+01	2.464E+19	4.031E+26
170.00	1.148E-05	7.069E+01	7.747E+19	4.770E+26
180.00	3.207E-05	8.284E+01	2.164E+20	5.590E+26
190.00	8.103E-05	9.625E+01	5.468E+20	6.495E+26
200.00	1.880E-04	1.109E+02	1.269E+21	7.487E+26
210.00	4.051E-04	1.270E+02	2.734E+21	8.570E+26
220.00	8.189E-04	1.444E+02	5.526E+21	9.746E+26
230.00	1.565E-03	1.633E+02	1.056E+22	1.102E+27
240.00	2.849E-03	1.836E+02	1.922E+22	1.239E+27
250.00	4.964E-03	2.054E+02	3.350E+22	1.386E+27
260.00	8.320E-03	2.288E+02	5.615E+22	1.544E+27

```
|     270.00 |  1.347E-02 |  2.537E+02 |  9.093E+22 |  1.712E+27
|     280.00 |  2.116E-02 |  2.803E+02 |  1.428E+23 |  1.891E+27
|     300.00 |  4.809E-02 |  3.384E+02 |  3.245E+23 |  2.283E+27
|     320.00 |  9.974E-02 |  4.034E+02 |  6.730E+23 |  2.722E+27
|     340.00 |  1.916E-01 |  4.756E+02 |  1.293E+24 |  3.209E+27
|     360.00 |  3.454E-01 |  5.551E+02 |  2.331E+24 |  3.746E+27
|     400.00 |  9.601E-01 |  7.375E+02 |  6.479E+24 |  4.977E+27
| ------------------------------------------------------------
|            |          in au          |        in cm^-3
| ------------------------------------------------------------
|   Qtot: total pfn per unit volume
|         * [V0] --> from the bottom of the potential (V0)
|         * [V1] --> from the zero-point energy (V1)
|         * includes rotational symmetry number
|
|
| Gibbs free energy (hartree):
| -----------------------------------------
|   T (K)  |   v = 1 cm^3   |   v = kbT/p0
| -----------------------------------------
|    10.00 |   -75.72045155 |   -75.71893048
|    20.00 |   -75.72227392 |   -75.71927566
|    30.00 |   -75.72413781 |   -75.71967896
|    40.00 |   -75.72602920 |   -75.72012051
|    50.00 |   -75.72794187 |   -75.72059133
|    60.00 |   -75.72987221 |   -75.72108621
|    70.00 |   -75.73181773 |   -75.72160156
|    80.00 |   -75.73377648 |   -75.72213469
|    90.00 |   -75.73574688 |   -75.72268343
|   100.00 |   -75.73772763 |   -75.72324605
|   110.00 |   -75.73971764 |   -75.72382111
|   120.00 |   -75.74171601 |   -75.72440741
|   130.00 |   -75.74372198 |   -75.72500394
|   140.00 |   -75.74573489 |   -75.72560986
|   150.00 |   -75.74775418 |   -75.72622443
|   160.00 |   -75.74977939 |   -75.72684702
|   170.00 |   -75.75181008 |   -75.72747708
|   180.00 |   -75.75384591 |   -75.72811413
|   190.00 |   -75.75588655 |   -75.72875776
|   200.00 |   -75.75793171 |   -75.72940758
|   210.00 |   -75.75998115 |   -75.73006326
|   220.00 |   -75.76203464 |   -75.73072450
|   230.00 |   -75.76409198 |   -75.73139102
|   240.00 |   -75.76615298 |   -75.73206259
|   250.00 |   -75.76821747 |   -75.73273897
|   260.00 |   -75.77028531 |   -75.73341996
|   270.00 |   -75.77235635 |   -75.73410537
|   280.00 |   -75.77443047 |   -75.73479503
|   300.00 |   -75.77858746 |   -75.73618647
|   320.00 |   -75.78275545 |   -75.73759313
|   340.00 |   -75.78693370 |   -75.73901401
|   360.00 |   -75.79112157 |   -75.74044823
|   400.00 |   -75.79952398 |   -75.74335373
| -----------------------------------------
|   v : volume per molecule
|   p0: 1bar
|
```

Pre-reactive complex information

```
-------------------------
 Analysis of STRUC: CPLX
-------------------------

    Number of conformers: 1

       V0 = electronic energy
       V1 = electronic energy + zero-point energy (ZPE)

       ZPE is calculated using scaled frequencies
       Frequency scale factor: 0.97300

       min(V0) = -208.49102788 hartree
       min(V1) = -208.43672518 hartree

       Relative energies (in kcal/mol):
       ------------------------------------------------------------------------
        name | V0-min(V0) | V1-min(V1) |   ZPE   | mass (amu) | weight |  PGS
       ------------------------------------------------------------------------
          001 |     0.000  |     0.000  |   34.08 |     58.03  |    1   |   C1
       ------------------------------------------------------------------------
       weight: equals 2 if the structure has a conformational enantiomer,
               equals 1 otherwise
       PGS   : point group of symmetry

    ------------------
    Conformation: 001
    ------------------
     | Molecular formula     : C(2)H(4)NO
     | Number of atoms       : 8
     | Number of electrons   : 31
     | Vibrational DOFs      : 18
     | Charge                : 0
     | Multiplicity          : 2
     | Electronic energy (V0): -208.49102788 hartree
     | Total mass [root]     : 58.0293 amu
     | Total mass            : 58.0293 amu
     | Point group symmetry  : C1
     | Rotational sym num    : 1
     | Cartesian coordinates (Angstrom):
     |    N    +0.35085956   -0.71184246   -1.22480033  [ 14.003 amu]
     |    C    +0.47391305   -0.62854964   -0.08955590  [ 12.000 amu]
     |    C    +0.61315739   -0.49976156   +1.35414996  [ 12.000 amu]
     |    H    +0.98446988   +0.49826613   +1.59351144  [  1.008 amu]
     |    H    -0.36248218   -0.63142916   +1.82525524  [  1.008 amu]
     |    H    +1.30763428   -1.25063531   +1.73401219  [  1.008 amu]
     |    O    -1.17037030   +1.47575688   -0.13275420  [ 15.995 amu]
     |    H    -1.17352703   +1.28766629   -1.08537870  [  1.008 amu]
     | Moments and product of inertia (au):
     |         +3.512E+05  +5.844E+05  +9.150E+05  [ 1.878E+17]
     | Vibrational frequencies [1/cm] (scaled by 0.973):
     |      22.57     82.74    121.70    158.69    319.18    381.57
     |     386.94    915.93   1029.51   1030.29   1360.48   1419.56
     |    1424.61   2360.89   2988.50   3070.79   3074.09   3688.07
     | Vibrational zero-point energies [kcal/mol]:
     |       0.03      0.12      0.17      0.23      0.46      0.55
     |       0.55      1.31      1.47      1.47      1.94      2.03
     |       2.04      3.38      4.27      4.39      4.39      5.27
     | Vibrational zero-point energy:    +0.05430270 hartree  =
     |                                       +34.08 kcal/mol =
     |                                        +1.48 eV       =
     |                                    +11918.06 cm^-1
     | V0 + zero-point energy (V1)  :  -208.43672518 hartree
```

|
| Partition functions (pfns):

T (K)	Qtr (au)	Qtr (cm^-3)	Qrot	Qvib [V0]	Qvib [V1]	Qel
10.00	3.893E-01	2.627E+24	3.872E+02	2.062E-745	1.040E+00	2.000E+00
20.00	1.101E+00	7.430E+24	1.095E+03	5.561E-373	1.249E+00	2.000E+00
30.00	2.023E+00	1.365E+25	2.012E+03	9.019E-249	1.547E+00	2.000E+00
40.00	3.114E+00	2.102E+25	3.098E+03	1.285E-186	1.926E+00	2.000E+00
50.00	4.352E+00	2.937E+25	4.329E+03	2.757E-149	2.404E+00	2.000E+00
60.00	5.721E+00	3.861E+25	5.691E+03	2.292E-124	3.002E+00	2.000E+00
70.00	7.210E+00	4.865E+25	7.171E+03	1.538E-106	3.742E+00	2.000E+00
80.00	8.809E+00	5.944E+25	8.762E+03	3.800E-93	4.652E+00	2.000E+00
90.00	1.051E+01	7.093E+25	1.045E+04	1.037E-82	5.762E+00	2.000E+00
100.00	1.231E+01	8.308E+25	1.224E+04	2.408E-74	7.112E+00	2.000E+00
110.00	1.420E+01	9.584E+25	1.413E+04	1.744E-67	8.743E+00	2.000E+00
120.00	1.618E+01	1.092E+26	1.610E+04	9.357E-62	1.071E+01	2.000E+00
130.00	1.825E+01	1.231E+26	1.815E+04	6.780E-57	1.306E+01	2.000E+00
140.00	2.039E+01	1.376E+26	2.028E+04	1.018E-52	1.588E+01	2.000E+00
150.00	2.262E+01	1.526E+26	2.249E+04	4.337E-49	1.923E+01	2.000E+00
160.00	2.491E+01	1.681E+26	2.478E+04	6.633E-46	2.321E+01	2.000E+00
170.00	2.729E+01	1.841E+26	2.714E+04	4.362E-43	2.791E+01	2.000E+00
180.00	2.973E+01	2.006E+26	2.957E+04	1.419E-40	3.345E+01	2.000E+00
190.00	3.224E+01	2.176E+26	3.207E+04	2.551E-38	3.996E+01	2.000E+00
200.00	3.482E+01	2.350E+26	3.463E+04	2.769E-36	4.758E+01	2.000E+00
210.00	3.746E+01	2.528E+26	3.726E+04	1.950E-34	5.649E+01	2.000E+00
220.00	4.017E+01	2.711E+26	3.996E+04	9.442E-33	6.687E+01	2.000E+00
230.00	4.294E+01	2.898E+26	4.271E+04	3.302E-31	7.892E+01	2.000E+00
240.00	4.577E+01	3.089E+26	4.553E+04	8.684E-30	9.290E+01	2.000E+00
250.00	4.866E+01	3.284E+26	4.840E+04	1.776E-28	1.091E+02	2.000E+00
260.00	5.161E+01	3.483E+26	5.133E+04	2.910E-27	1.277E+02	2.000E+00
270.00	5.462E+01	3.686E+26	5.432E+04	3.910E-26	1.492E+02	2.000E+00
280.00	5.768E+01	3.892E+26	5.737E+04	4.403E-25	1.739E+02	2.000E+00
300.00	6.397E+01	4.317E+26	6.362E+04	3.524E-23	2.347E+02	2.000E+00
320.00	7.047E+01	4.756E+26	7.009E+04	1.679E-21	3.141E+02	2.000E+00
340.00	7.718E+01	5.208E+26	7.677E+04	5.216E-20	4.172E+02	2.000E+00
360.00	8.409E+01	5.674E+26	8.364E+04	1.134E-18	5.503E+02	2.000E+00
400.00	9.848E+01	6.646E+26	9.796E+04	2.267E-16	9.396E+02	2.000E+00

|
| Qtr : translational pfn per volume unit
| Qrot: rotational pfn (rigid-rotor); includes rotational symmetry number
| Qvib: vibrational pfn (harmonic-oscillator) relative to V0 and to V1
| Qel : electronic pfn
|

T (K)	Qtot [V0]	Qtot [V1]	Qtot [V0]	Qtot [V1]
10.00	6.217E-743	3.137E+02	4.196E-718	2.117E+27
20.00	1.341E-369	3.013E+03	9.051E-345	2.033E+28
30.00	7.341E-245	1.259E+04	4.954E-220	8.497E+28
40.00	2.480E-182	3.716E+04	1.673E-157	2.508E+29
50.00	1.039E-144	9.060E+04	7.010E-120	6.114E+29
60.00	1.492E-119	1.955E+05	1.007E-94	1.319E+30
70.00	1.590E-101	3.869E+05	1.073E-76	2.611E+30
80.00	5.865E-88	7.180E+05	3.958E-63	4.845E+30
90.00	2.279E-77	1.266E+06	1.538E-52	8.546E+30
100.00	7.260E-69	2.144E+06	4.899E-44	1.447E+31
110.00	6.996E-62	3.508E+06	4.721E-37	2.368E+31
120.00	4.875E-56	5.578E+06	3.290E-31	3.764E+31
130.00	4.491E-51	8.653E+06	3.031E-26	5.839E+31
140.00	8.422E-47	1.314E+07	5.683E-22	8.865E+31
150.00	4.412E-43	1.957E+07	2.978E-18	1.320E+32
160.00	8.191E-40	2.866E+07	5.527E-15	1.934E+32
170.00	6.461E-37	4.134E+07	4.360E-12	2.790E+32

```
|     180.00 |  2.495E-34 |  5.881E+07 |  1.684E-09 |  3.969E+32
|     190.00 |  5.275E-32 |  8.263E+07 |  3.560E-07 |  5.576E+32
|     200.00 |  6.678E-30 |  1.148E+08 |  4.507E-05 |  7.744E+32
|     210.00 |  5.443E-28 |  1.577E+08 |  3.673E-03 |  1.064E+33
|     220.00 |  3.031E-26 |  2.146E+08 |  2.045E-01 |  1.448E+33
|     230.00 |  1.211E-24 |  2.895E+08 |  8.174E+00 |  1.954E+33
|     240.00 |  3.619E-23 |  3.872E+08 |  2.442E+02 |  2.613E+33
|     250.00 |  8.368E-22 |  5.137E+08 |  5.647E+03 |  3.467E+33
|     260.00 |  1.542E-20 |  6.767E+08 |  1.040E+05 |  4.567E+33
|     270.00 |  2.320E-19 |  8.853E+08 |  1.566E+06 |  5.974E+33
|     280.00 |  2.914E-18 |  1.151E+09 |  1.966E+07 |  7.766E+33
|     300.00 |  2.868E-16 |  1.910E+09 |  1.936E+09 |  1.289E+34
|     320.00 |  1.659E-14 |  3.103E+09 |  1.119E+11 |  2.094E+34
|     340.00 |  6.180E-13 |  4.943E+09 |  4.171E+12 |  3.336E+34
|     360.00 |  1.594E-11 |  7.741E+09 |  1.076E+14 |  5.224E+34
|     400.00 |  4.373E-09 |  1.813E+10 |  2.951E+16 |  1.223E+35
| ------------------------------------------------------------------
|            |          in au          |        in cm^-3
| ------------------------------------------------------------------
|   Qtot: total pfn per unit volume
|         * [V0] --> from the bottom of the potential (V0)
|         * [V1] --> from the zero-point energy (V1)
|         * includes rotational symmetry number
|
| Gibbs free energy (hartree):
| ------------------------------------------
|   T (K)  |   v = 1 cm^3   |   v = kbT/p0
| ------------------------------------------
|    10.00 |  -208.43871774 |  -208.43719666
|    20.00 |  -208.44085357 |  -208.43785532
|    30.00 |  -208.44305363 |  -208.43859478
|    40.00 |  -208.44530021 |  -208.43939151
|    50.00 |  -208.44758506 |  -208.44023452
|    60.00 |  -208.44990314 |  -208.44111714
|    70.00 |  -208.45225085 |  -208.44203468
|    80.00 |  -208.45462543 |  -208.44298363
|    90.00 |  -208.45702471 |  -208.44396126
|   100.00 |  -208.45944694 |  -208.44496536
|   110.00 |  -208.46189067 |  -208.44599414
|   120.00 |  -208.46435466 |  -208.44704606
|   130.00 |  -208.46683785 |  -208.44811982
|   140.00 |  -208.46933930 |  -208.44921427
|   150.00 |  -208.47185817 |  -208.45032841
|   160.00 |  -208.47439370 |  -208.45146132
|   170.00 |  -208.47694520 |  -208.45261219
|   180.00 |  -208.47951205 |  -208.45378027
|   190.00 |  -208.48209369 |  -208.45496489
|   200.00 |  -208.48468957 |  -208.45616544
|   210.00 |  -208.48729924 |  -208.45738134
|   220.00 |  -208.48992223 |  -208.45861209
|   230.00 |  -208.49255816 |  -208.45985720
|   240.00 |  -208.49520664 |  -208.46111625
|   250.00 |  -208.49786732 |  -208.46238881
|   260.00 |  -208.50053988 |  -208.46367453
|   270.00 |  -208.50322403 |  -208.46497305
|   280.00 |  -208.50591949 |  -208.46628405
|   300.00 |  -208.51134331 |  -208.46894232
|   320.00 |  -208.51680945 |  -208.47164713
|   340.00 |  -208.52231627 |  -208.47439658
|   360.00 |  -208.52786228 |  -208.47718894
|   400.00 |  -208.53906666 |  -208.48289642
| ------------------------------------------
|   v : volume per molecule
|   p0: 1bar
```

TS1a information

```
 ----------------------
   Analysis of STRUC: TS1a
  ----------------------

      Number of conformers: 1

         V0 = electronic energy
         V1 = electronic energy + zero-point energy (ZPE)

         ZPE is calculated using scaled frequencies
         Frequency scale factor: 0.97300

         min(V0) = -208.47578120 hartree
         min(V1) = -208.42555963 hartree

         Relative energies (in kcal/mol):
         ------------------------------------------------------------------------------------------
          name | V0-min(V0) | V1-min(V1) |   ZPE   | mass (amu) | weight |  PGS  | imag.freq.
         ------------------------------------------------------------------------------------------
           001 |     0.000  |     0.000  |   31.51 |     58.03  |    1   |   Cs  |  -1293.51
         ------------------------------------------------------------------------------------------
         weight: equals 2 if the structure has a conformational enantiomer,
                 equals 1 otherwise
         PGS   : point group of symmetry

      ------------------
      Conformation: 001
      ------------------
       | Molecular formula     : C(2)H(4)NO
       | Number of atoms       : 8
       | Number of electrons   : 31
       | Vibrational DOFs      : 18
       | Charge                : 0
       | Multiplicity          : 2
       | Electronic energy (V0): -208.47578120 hartree
       | Total mass [root]     : 58.0293 amu
       | Total mass            : 58.0293 amu
       | Point group symmetry  : Cs
       | Rotational sym num    : 1
       | Cartesian coordinates (Angstrom):
       |    N    +0.50652583   -0.56621703   -1.81284331  [ 14.003 amu]
       |    C    +0.50658384   -0.56628324   -0.66727861  [ 12.000 amu]
       |    C    +0.47690970   -0.53311375   +0.77324865  [ 12.000 amu]
       |    H    -0.28876253   +0.32279144   +1.11853867  [  1.008 amu]
       |    H    +0.08754837   -1.45584679   +1.20280946  [  1.008 amu]
       |    H    +1.43714414   -0.24853140   +1.20281088  [  1.008 amu]
       |    O    -1.17417062   +1.31254347   +1.26464367  [ 15.995 amu]
       |    H    -1.34912985   +1.50812248   +0.33153978  [  1.008 amu]
       | Moments and product of inertia (au):
       |         +2.063E+05  +8.966E+05  +1.081E+06  [ 2.000E+17]
       | Vibrational frequencies [1/cm] (scaled by 0.973):
       |   -1293.51     80.41    144.22    289.88    380.38    382.84
       |     719.20    806.41    949.94   1011.66   1109.68   1223.42
       |    1377.63   1397.75   2348.22   3024.20   3100.84   3698.03
       | Vibrational zero-point energies [kcal/mol]:
       |       0.00      0.11      0.21      0.41      0.54      0.55
       |       1.03      1.15      1.36      1.45      1.59      1.75
       |       1.97      2.00      3.36      4.32      4.43      5.29
       | Vibrational zero-point energy:    +0.05022157 hartree  =
       |                                       +31.51 kcal/mol =
       |                                        +1.37 eV       =
       |                                    +11022.36 cm^-1
       | V0 + zero-point energy (V1)  :  -208.42555963 hartree
```

|
| Partition functions (pfns):

T (K)	Qtr (au)	Qtr (cm^-3)	Qrot	Qvib [V0]	Qvib [V1]	Qel
10.00	3.893E-01	2.627E+24	3.996E+02	1.842E-689	1.000E+00	2.000E+00
20.00	1.101E+00	7.430E+24	1.130E+03	4.306E-345	1.003E+00	2.000E+00
30.00	2.023E+00	1.365E+25	2.076E+03	2.701E-230	1.023E+00	2.000E+00
40.00	3.114E+00	2.102E+25	3.196E+03	6.975E-173	1.065E+00	2.000E+00
50.00	4.352E+00	2.937E+25	4.467E+03	2.020E-138	1.128E+00	2.000E+00
60.00	5.721E+00	3.861E+25	5.872E+03	1.966E-115	1.210E+00	2.000E+00
70.00	7.210E+00	4.865E+25	7.400E+03	5.323E-99	1.309E+00	2.000E+00
80.00	8.809E+00	5.944E+25	9.041E+03	1.153E-86	1.424E+00	2.000E+00
90.00	1.051E+01	7.093E+25	1.079E+04	4.638E-77	1.557E+00	2.000E+00
100.00	1.231E+01	8.308E+25	1.264E+04	2.286E-69	1.708E+00	2.000E+00
110.00	1.420E+01	9.584E+25	1.458E+04	4.589E-63	1.879E+00	2.000E+00
120.00	1.618E+01	1.092E+26	1.661E+04	8.348E-58	2.071E+00	2.000E+00
130.00	1.825E+01	1.231E+26	1.873E+04	2.396E-53	2.286E+00	2.000E+00
140.00	2.039E+01	1.376E+26	2.093E+04	1.611E-49	2.526E+00	2.000E+00
150.00	2.262E+01	1.526E+26	2.321E+04	3.392E-46	2.793E+00	2.000E+00
160.00	2.491E+01	1.681E+26	2.557E+04	2.781E-43	3.091E+00	2.000E+00
170.00	2.729E+01	1.841E+26	2.801E+04	1.048E-40	3.422E+00	2.000E+00
180.00	2.973E+01	2.006E+26	3.051E+04	2.068E-38	3.790E+00	2.000E+00
190.00	3.224E+01	2.176E+26	3.309E+04	2.365E-36	4.198E+00	2.000E+00
200.00	3.482E+01	2.350E+26	3.574E+04	1.701E-34	4.650E+00	2.000E+00
210.00	3.746E+01	2.528E+26	3.845E+04	8.221E-33	5.150E+00	2.000E+00
220.00	4.017E+01	2.711E+26	4.123E+04	2.819E-31	5.704E+00	2.000E+00
230.00	4.294E+01	2.898E+26	4.407E+04	7.170E-30	6.317E+00	2.000E+00
240.00	4.577E+01	3.089E+26	4.698E+04	1.404E-28	6.994E+00	2.000E+00
250.00	4.866E+01	3.284E+26	4.994E+04	2.185E-27	7.743E+00	2.000E+00
260.00	5.161E+01	3.483E+26	5.297E+04	2.775E-26	8.571E+00	2.000E+00
270.00	5.462E+01	3.686E+26	5.606E+04	2.940E-25	9.485E+00	2.000E+00
280.00	5.768E+01	3.892E+26	5.920E+04	2.650E-24	1.049E+01	2.000E+00
300.00	6.397E+01	4.317E+26	6.565E+04	1.415E-22	1.284E+01	2.000E+00
320.00	7.047E+01	4.756E+26	7.233E+04	4.706E-21	1.569E+01	2.000E+00
340.00	7.718E+01	5.208E+26	7.921E+04	1.060E-19	1.915E+01	2.000E+00
360.00	8.409E+01	5.674E+26	8.630E+04	1.726E-18	2.336E+01	2.000E+00
400.00	9.848E+01	6.646E+26	1.011E+05	2.095E-16	3.464E+01	2.000E+00

|
| Qtr : translational pfn per volume unit
| Qrot: rotational pfn (rigid-rotor); includes rotational symmetry number
| Qvib: vibrational pfn (harmonic-oscillator) relative to V0 and to V1
| Qel : electronic pfn
|

T (K)	Qtot [V0]	Qtot [V1]	Qtot [V0]	Qtot [V1]
10.00	5.732E-687	3.111E+02	3.868E-662	2.099E+27
20.00	1.072E-341	2.496E+03	7.231E-317	1.685E+28
30.00	2.269E-226	8.589E+03	1.531E-201	5.796E+28
40.00	1.389E-168	2.120E+04	9.372E-144	1.430E+29
50.00	7.854E-134	4.386E+04	5.300E-109	2.960E+29
60.00	1.321E-110	8.128E+04	8.914E-86	5.485E+29
70.00	5.680E-94	1.396E+05	3.833E-69	9.423E+29
80.00	1.836E-81	2.269E+05	1.239E-56	1.531E+30
90.00	1.052E-71	3.532E+05	7.098E-47	2.383E+30
100.00	7.113E-64	5.315E+05	4.800E-39	3.587E+30
110.00	1.900E-57	7.780E+05	1.282E-32	5.250E+30
120.00	4.488E-52	1.113E+06	3.028E-27	7.512E+30
130.00	1.637E-47	1.562E+06	1.105E-22	1.054E+31
140.00	1.375E-43	2.156E+06	9.279E-19	1.455E+31
150.00	3.561E-40	2.933E+06	2.403E-15	1.979E+31
160.00	3.544E-37	3.939E+06	2.391E-12	2.658E+31
170.00	1.602E-34	5.230E+06	1.081E-09	3.530E+31

```
|     180.00 |  3.752E-32 |  6.876E+06 |  2.532E-07 |  4.640E+31
|     190.00 |  5.046E-30 |  8.957E+06 |  3.405E-05 |  6.044E+31
|     200.00 |  4.233E-28 |  1.157E+07 |  2.857E-03 |  7.809E+31
|     210.00 |  2.368E-26 |  1.484E+07 |  1.598E-01 |  1.001E+32
|     220.00 |  9.337E-25 |  1.889E+07 |  6.301E+00 |  1.275E+32
|     230.00 |  2.714E-23 |  2.391E+07 |  1.831E+02 |  1.613E+32
|     240.00 |  6.039E-22 |  3.008E+07 |  4.076E+03 |  2.030E+32
|     250.00 |  1.062E-20 |  3.764E+07 |  7.169E+04 |  2.540E+32
|     260.00 |  1.517E-19 |  4.686E+07 |  1.024E+06 |  3.162E+32
|     270.00 |  1.800E-18 |  5.808E+07 |  1.215E+07 |  3.919E+32
|     280.00 |  1.810E-17 |  7.166E+07 |  1.221E+08 |  4.836E+32
|     300.00 |  1.188E-15 |  1.078E+08 |  8.018E+09 |  7.276E+32
|     320.00 |  4.797E-14 |  1.599E+08 |  3.237E+11 |  1.079E+33
|     340.00 |  1.296E-12 |  2.342E+08 |  8.747E+12 |  1.580E+33
|     360.00 |  2.505E-11 |  3.391E+08 |  1.690E+14 |  2.288E+33
|     400.00 |  4.172E-09 |  6.897E+08 |  2.815E+16 |  4.655E+33
| ------------------------------------------------------------
|            |          in au          |        in cm^-3
| ------------------------------------------------------------
|   Qtot: total pfn per unit volume
|         * [V0] --> from the bottom of the potential (V0)
|         * [V1] --> from the zero-point energy (V1)
|         * includes rotational symmetry number
|
| Gibbs free energy (hartree):
| ------------------------------------------
|   T (K)  |   v = 1 cm^3   |   v = kbT/p0
| ------------------------------------------
|    10.00 |  -208.42755192 |  -208.42603084
|    20.00 |  -208.42967611 |  -208.42667786
|    30.00 |  -208.43185174 |  -208.42739289
|    40.00 |  -208.43406354 |  -208.42815484
|    50.00 |  -208.43630464 |  -208.42895410
|    60.00 |  -208.43857087 |  -208.42978486
|    70.00 |  -208.44085936 |  -208.43064319
|    80.00 |  -208.44316801 |  -208.43152621
|    90.00 |  -208.44549520 |  -208.43243175
|   100.00 |  -208.44783969 |  -208.43335811
|   110.00 |  -208.45020045 |  -208.43430392
|   120.00 |  -208.45257664 |  -208.43526804
|   130.00 |  -208.45496754 |  -208.43624951
|   140.00 |  -208.45737253 |  -208.43724750
|   150.00 |  -208.45979103 |  -208.43826128
|   160.00 |  -208.46222257 |  -208.43929020
|   170.00 |  -208.46466671 |  -208.44033370
|   180.00 |  -208.46712303 |  -208.44139126
|   190.00 |  -208.46959120 |  -208.44246241
|   200.00 |  -208.47207087 |  -208.44354674
|   210.00 |  -208.47456177 |  -208.44464387
|   220.00 |  -208.47706361 |  -208.44575347
|   230.00 |  -208.47957616 |  -208.44687520
|   240.00 |  -208.48209919 |  -208.44800880
|   250.00 |  -208.48463249 |  -208.44915399
|   260.00 |  -208.48717588 |  -208.45031053
|   270.00 |  -208.48972918 |  -208.45147820
|   280.00 |  -208.49229222 |  -208.45265679
|   300.00 |  -208.49744694 |  -208.45504595
|   320.00 |  -208.50263890 |  -208.45747658
|   340.00 |  -208.50786710 |  -208.45994741
|   360.00 |  -208.51313061 |  -208.46245728
|   400.00 |  -208.52376025 |  -208.46759001
| ------------------------------------------
|   v : volume per molecule
|   p0: 1bar
```

TS1b information

```
-------------------------
  Analysis of STRUC: TS1b
 -------------------------

    Number of conformers: 1

       V0 = electronic energy
       V1 = electronic energy + zero-point energy (ZPE)

       ZPE is calculated using scaled frequencies
       Frequency scale factor: 0.97300

       min(V0) = -208.48294650 hartree
       min(V1) = -208.42748030 hartree

       Relative energies (in kcal/mol):
       ------------------------------------------------------------------------------------
        name | V0-min(V0) | V1-min(V1) |   ZPE   | mass (amu) | weight |  PGS  | imag.freq.
       ------------------------------------------------------------------------------------
          001 |     0.000  |     0.000  |   34.81 |     58.03  |    1   |   Cs  |   -691.53
       ------------------------------------------------------------------------------------
       weight: equals 2 if the structure has a conformational enantiomer,
               equals 1 otherwise
       PGS   : point group of symmetry

    ------------------
    Conformation: 001
    ------------------
     | Molecular formula     : C(2)H(4)NO
     | Number of atoms       : 8
     | Number of electrons   : 31
     | Vibrational DOFs      : 18
     | Charge                : 0
     | Multiplicity          : 2
     | Electronic energy (V0): -208.48294650 hartree
     | Total mass [root]     : 58.0293 amu
     | Total mass            : 58.0293 amu
     | Point group symmetry  : Cs
     | Rotational sym num    : 1
     | Cartesian coordinates (Angstrom):
     |    C    -0.46676007   -0.00000000   -1.42882242  [ 12.000 amu]
     |    C    -0.46676007   -0.00000000   +0.03611256  [ 12.000 amu]
     |    O    +1.44299322   -0.00000000   +0.31040506  [ 15.995 amu]
     |    N    -0.85791855   +0.00000000   +1.13294357  [ 14.003 amu]
     |    H    +0.06252529   -0.88513636   -1.78395679  [  1.008 amu]
     |    H    -1.49399153   +0.00000000   -1.79399951  [  1.008 amu]
     |    H    +0.06252529   +0.88513636   -1.78395679  [  1.008 amu]
     |    H    +1.50307965   +0.00000000   +1.27680839  [  1.008 amu]
     | Moments and product of inertia (au):
     |         +3.260E+05  +4.022E+05  +7.076E+05  [ 9.278E+16]
     | Vibrational frequencies [1/cm] (scaled by 0.973):
     |    -691.53    140.85    221.22    262.84    369.52    403.23
     |     814.53    896.96   1002.59   1032.77   1354.03   1417.01
     |    1426.41   2135.87   2993.69   3078.33   3087.16   3709.84
     | Vibrational zero-point energies [kcal/mol]:
     |       0.00      0.20      0.32      0.38      0.53      0.58
     |       1.16      1.28      1.43      1.48      1.94      2.03
     |       2.04      3.05      4.28      4.40      4.41      5.30
     | Vibrational zero-point energy:    +0.05546620 hartree  =
     |                                       +34.81 kcal/mol =
     |                                        +1.51 eV       =
     |                                     +12173.42 cm^-1
     | V0 + zero-point energy (V1)  :  -208.42748030 hartree
```

Partition functions (pfns):

T (K)	Qtr (au)	Qtr (cm^-3)	Qrot	Qvib [V0]	Qvib [V1]	Qel
10.00	3.893E-01	2.627E+24	2.721E+02	2.192E-761	1.000E+00	2.000E+00
20.00	1.101E+00	7.430E+24	7.697E+02	4.683E-381	1.000E+00	2.000E+00
30.00	2.023E+00	1.365E+25	1.414E+03	2.802E-254	1.001E+00	2.000E+00
40.00	3.114E+00	2.102E+25	2.177E+03	6.889E-191	1.007E+00	2.000E+00
50.00	4.352E+00	2.937E+25	3.043E+03	7.530E-153	1.020E+00	2.000E+00
60.00	5.721E+00	3.861E+25	4.000E+03	1.744E-127	1.043E+00	2.000E+00
70.00	7.210E+00	4.865E+25	5.040E+03	2.323E-109	1.076E+00	2.000E+00
80.00	8.809E+00	5.944E+25	6.158E+03	9.257E-96	1.119E+00	2.000E+00
90.00	1.051E+01	7.093E+25	7.348E+03	3.563E-85	1.174E+00	2.000E+00
100.00	1.231E+01	8.308E+25	8.606E+03	1.065E-76	1.239E+00	2.000E+00
110.00	1.420E+01	9.584E+25	9.928E+03	9.306E-70	1.317E+00	2.000E+00
120.00	1.618E+01	1.092E+26	1.131E+04	5.753E-64	1.407E+00	2.000E+00
130.00	1.825E+01	1.231E+26	1.276E+04	4.639E-59	1.509E+00	2.000E+00
140.00	2.039E+01	1.376E+26	1.426E+04	7.550E-55	1.625E+00	2.000E+00
150.00	2.262E+01	1.526E+26	1.581E+04	3.417E-51	1.755E+00	2.000E+00
160.00	2.491E+01	1.681E+26	1.742E+04	5.464E-48	1.900E+00	2.000E+00
170.00	2.729E+01	1.841E+26	1.907E+04	3.711E-45	2.062E+00	2.000E+00
180.00	2.973E+01	2.006E+26	2.078E+04	1.235E-42	2.241E+00	2.000E+00
190.00	3.224E+01	2.176E+26	2.254E+04	2.252E-40	2.439E+00	2.000E+00
200.00	3.482E+01	2.350E+26	2.434E+04	2.464E-38	2.658E+00	2.000E+00
210.00	3.746E+01	2.528E+26	2.619E+04	1.739E-36	2.899E+00	2.000E+00
220.00	4.017E+01	2.711E+26	2.808E+04	8.410E-35	3.164E+00	2.000E+00
230.00	4.294E+01	2.898E+26	3.002E+04	2.927E-33	3.455E+00	2.000E+00
240.00	4.577E+01	3.089E+26	3.200E+04	7.635E-32	3.775E+00	2.000E+00
250.00	4.866E+01	3.284E+26	3.402E+04	1.546E-30	4.127E+00	2.000E+00
260.00	5.161E+01	3.483E+26	3.608E+04	2.501E-29	4.511E+00	2.000E+00
270.00	5.462E+01	3.686E+26	3.818E+04	3.316E-28	4.933E+00	2.000E+00
280.00	5.768E+01	3.892E+26	4.032E+04	3.678E-27	5.395E+00	2.000E+00
300.00	6.397E+01	4.317E+26	4.472E+04	2.848E-25	6.454E+00	2.000E+00
320.00	7.047E+01	4.756E+26	4.926E+04	1.309E-23	7.721E+00	2.000E+00
340.00	7.718E+01	5.208E+26	5.395E+04	3.919E-22	9.235E+00	2.000E+00
360.00	8.409E+01	5.674E+26	5.878E+04	8.196E-21	1.104E+01	2.000E+00
400.00	9.848E+01	6.646E+26	6.885E+04	1.517E-18	1.576E+01	2.000E+00

Qtr : translational pfn per volume unit
Qrot: rotational pfn (rigid-rotor); includes rotational symmetry number
Qvib: vibrational pfn (harmonic-oscillator) relative to V0 and to V1
Qel : electronic pfn

T (K)	Qtot [V0]	Qtot [V1]	Qtot [V0]	Qtot [V1]
10.00	4.645E-759	2.119E+02	3.135E-734	1.430E+27
20.00	7.937E-378	1.695E+03	5.356E-353	1.144E+28
30.00	1.603E-250	5.728E+03	1.082E-225	3.865E+28
40.00	9.342E-187	1.365E+04	6.304E-162	9.213E+28
50.00	1.994E-148	2.701E+04	1.346E-123	1.823E+29
60.00	7.983E-123	4.772E+04	5.387E-98	3.220E+29
70.00	1.688E-104	7.816E+04	1.139E-79	5.275E+29
80.00	1.004E-90	1.214E+05	6.777E-66	8.193E+29
90.00	5.504E-80	1.813E+05	3.714E-55	1.223E+30
100.00	2.256E-71	2.626E+05	1.523E-46	1.772E+30
110.00	2.624E-64	3.714E+05	1.771E-39	2.506E+30
120.00	2.106E-58	5.150E+05	1.421E-33	3.475E+30
130.00	2.159E-53	7.024E+05	1.457E-28	4.740E+30
140.00	4.390E-49	9.446E+05	2.962E-24	6.374E+30
150.00	2.443E-45	1.255E+06	1.649E-20	8.468E+30
160.00	4.742E-42	1.649E+06	3.200E-17	1.113E+31
170.00	3.864E-39	2.146E+06	2.607E-14	1.448E+31

```
|     180.00 |  1.526E-36 |  2.769E+06 |  1.030E-11 |  1.869E+31
|     190.00 |  3.272E-34 |  3.545E+06 |  2.208E-09 |  2.392E+31
|     200.00 |  4.176E-32 |  4.505E+06 |  2.818E-07 |  3.040E+31
|     210.00 |  3.413E-30 |  5.688E+06 |  2.303E-05 |  3.838E+31
|     220.00 |  1.897E-28 |  7.138E+06 |  1.280E-03 |  4.817E+31
|     230.00 |  7.545E-27 |  8.908E+06 |  5.091E-02 |  6.011E+31
|     240.00 |  2.236E-25 |  1.106E+07 |  1.509E+00 |  7.463E+31
|     250.00 |  5.118E-24 |  1.366E+07 |  3.454E+01 |  9.219E+31
|     260.00 |  9.316E-23 |  1.680E+07 |  6.287E+02 |  1.134E+32
|     270.00 |  1.383E-21 |  2.057E+07 |  9.332E+03 |  1.388E+32
|     280.00 |  1.711E-20 |  2.509E+07 |  1.154E+05 |  1.693E+32
|     300.00 |  1.629E-18 |  3.692E+07 |  1.100E+07 |  2.492E+32
|     320.00 |  9.092E-17 |  5.361E+07 |  6.135E+08 |  3.618E+32
|     340.00 |  3.263E-15 |  7.691E+07 |  2.202E+10 |  5.190E+32
|     360.00 |  8.102E-14 |  1.092E+08 |  5.468E+11 |  7.366E+32
|     400.00 |  2.057E-11 |  2.136E+08 |  1.388E+14 |  1.442E+33
| ------------------------------------------------------------
|            |          in au          |        in cm^-3
| ------------------------------------------------------------
|   Qtot: total pfn per unit volume
|         * [V0] --> from the bottom of the potential (V0)
|         * [V1] --> from the zero-point energy (V1)
|         * includes rotational symmetry number
|
| Gibbs free energy (hartree):
| ------------------------------------------
|   T (K)  |   v = 1 cm^3   |   v = kbT/p0
| ------------------------------------------
|    10.00 |  -208.42946043 |  -208.42793935
|    20.00 |  -208.43157226 |  -208.42857401
|    30.00 |  -208.43373391 |  -208.42927506
|    40.00 |  -208.43592848 |  -208.43001978
|    50.00 |  -208.43814858 |  -208.43079804
|    60.00 |  -208.44039034 |  -208.43160433
|    70.00 |  -208.44265141 |  -208.43243525
|    80.00 |  -208.44493027 |  -208.43328848
|    90.00 |  -208.44722579 |  -208.43416234
|   100.00 |  -208.44953711 |  -208.43505553
|   110.00 |  -208.45186351 |  -208.43596698
|   120.00 |  -208.45420438 |  -208.43689577
|   130.00 |  -208.45655915 |  -208.43784112
|   140.00 |  -208.45892732 |  -208.43880230
|   150.00 |  -208.46130843 |  -208.43977868
|   160.00 |  -208.46370205 |  -208.44076968
|   170.00 |  -208.46610777 |  -208.44177477
|   180.00 |  -208.46852524 |  -208.44279346
|   190.00 |  -208.47095411 |  -208.44382532
|   200.00 |  -208.47339407 |  -208.44486993
|   210.00 |  -208.47584482 |  -208.44592693
|   220.00 |  -208.47830612 |  -208.44699597
|   230.00 |  -208.48077770 |  -208.44807674
|   240.00 |  -208.48325933 |  -208.44916894
|   250.00 |  -208.48575082 |  -208.45027232
|   260.00 |  -208.48825196 |  -208.45138661
|   270.00 |  -208.49076256 |  -208.45251158
|   280.00 |  -208.49328247 |  -208.45364703
|   300.00 |  -208.49834955 |  -208.45594855
|   320.00 |  -208.50345201 |  -208.45828969
|   340.00 |  -208.50858883 |  -208.46066914
|   360.00 |  -208.51375905 |  -208.46308572
|   400.00 |  -208.52419631 |  -208.46802607
| ------------------------------------------
|   v : volume per molecule
|   p0: 1bar
```

$CH_3C(OH)N$ information

```
--------------------------
 Analysis of STRUC: CH3C(OH)N
--------------------------

    Number of conformers: 1

       V0 = electronic energy
       V1 = electronic energy + zero-point energy (ZPE)

       ZPE is calculated using scaled frequencies
       Frequency scale factor: 0.97300

       min(V0) = -208.53099790 hartree
       min(V1) = -208.47176626 hartree

       Relative energies (in kcal/mol):
       ------------------------------------------------------------------------
        name | V0-min(V0) | V1-min(V1) |   ZPE   | mass (amu) | weight |  PGS
       ------------------------------------------------------------------------
          001 |     0.000  |     0.000  |   37.17 |     58.03  |    1   |   Cs
       ------------------------------------------------------------------------
       weight: equals 2 if the structure has a conformational enantiomer,
               equals 1 otherwise
       PGS   : point group of symmetry

    ------------------
    Conformation: 001
    ------------------
     | Molecular formula     : C(2)H(4)NO
     | Number of atoms       : 8
     | Number of electrons   : 31
     | Vibrational DOFs      : 18
     | Charge                : 0
     | Multiplicity          : 2
     | Electronic energy (V0): -208.53099790 hartree
     | Total mass [root]     : 58.0293 amu
     | Total mass            : 58.0293 amu
     | Point group symmetry  : Cs
     | Rotational sym num    : 1
     | Cartesian coordinates (Angstrom):
     |    N    -0.00912958   -0.00000006   -1.38236074  [ 14.003 amu]
     |    C    -0.00912958   -0.00000006   -0.13073032  [ 12.000 amu]
     |    O    +1.12906676   -0.00000006   +0.60735532  [ 15.995 amu]
     |    C    -1.25317533   -0.00000006   +0.70207476  [ 12.000 amu]
     |    H    -1.25752679   +0.88592765   +1.34172901  [  1.008 amu]
     |    H    -2.13593156   +0.00000094   +0.06444604  [  1.008 amu]
     |    H    -1.25753173   -0.88592257   +1.34173475  [  1.008 amu]
     |    H    +1.88878430   -0.00000302   +0.01702177  [  1.008 amu]
     | Moments and product of inertia (au):
     |         +2.804E+05  +3.458E+05  +6.056E+05  [ 5.872E+16]
     | Vibrational frequencies [1/cm] (scaled by 0.973):
     |     163.66    368.66    465.11    467.58    554.94    769.00
     |     974.39   1021.08   1166.00   1287.79   1354.90   1419.05
     |    1424.64   1699.00   2971.03   3053.46   3086.90   3752.48
     | Vibrational zero-point energies [kcal/mol]:
     |       0.23      0.53      0.66      0.67      0.79      1.10
     |       1.39      1.46      1.67      1.84      1.94      2.03
     |       2.04      2.43      4.25      4.37      4.41      5.36
     | Vibrational zero-point energy:    +0.05923164 hartree  =
     |                                       +37.17 kcal/mol =
     |                                        +1.61 eV       =
     |                                     +12999.84 cm^-1
     | V0 + zero-point energy (V1)  :  -208.47176626 hartree
```

|
| Partition functions (pfns):
| ---
| T (K) | Qtr (au) | Qtr (cm^-3) | Qrot | Qvib [V0] | Qvib [V1] | Qel
| ---
| 10.00 | 3.893E-01 | 2.627E+24 | 2.165E+02 | 5.035E-813 | 1.000E+00 | 2.000E+00
| 20.00 | 1.101E+00 | 7.430E+24 | 6.123E+02 | 7.096E-407 | 1.000E+00 | 2.000E+00
| 30.00 | 2.023E+00 | 1.365E+25 | 1.125E+03 | 1.715E-271 | 1.000E+00 | 2.000E+00
| 40.00 | 3.114E+00 | 2.102E+25 | 1.732E+03 | 8.447E-204 | 1.003E+00 | 2.000E+00
| 50.00 | 4.352E+00 | 2.937E+25 | 2.420E+03 | 3.502E-163 | 1.009E+00 | 2.000E+00
| 60.00 | 5.721E+00 | 3.861E+25 | 3.182E+03 | 4.224E-136 | 1.020E+00 | 2.000E+00
| 70.00 | 7.210E+00 | 4.865E+25 | 4.009E+03 | 9.397E-117 | 1.037E+00 | 2.000E+00
| 80.00 | 8.809E+00 | 5.944E+25 | 4.899E+03 | 3.069E-102 | 1.058E+00 | 2.000E+00
| 90.00 | 1.051E+01 | 7.093E+25 | 5.845E+03 | 6.017E-91 | 1.083E+00 | 2.000E+00
| 100.00 | 1.231E+01 | 8.308E+25 | 6.846E+03 | 6.560E-82 | 1.114E+00 | 2.000E+00
| 110.00 | 1.420E+01 | 9.584E+25 | 7.898E+03 | 1.640E-74 | 1.148E+00 | 2.000E+00
| 120.00 | 1.618E+01 | 1.092E+26 | 8.999E+03 | 2.418E-68 | 1.188E+00 | 2.000E+00
| 130.00 | 1.825E+01 | 1.231E+26 | 1.015E+04 | 4.041E-63 | 1.233E+00 | 2.000E+00
| 140.00 | 2.039E+01 | 1.376E+26 | 1.134E+04 | 1.222E-58 | 1.283E+00 | 2.000E+00
| 150.00 | 2.262E+01 | 1.526E+26 | 1.258E+04 | 9.406E-55 | 1.338E+00 | 2.000E+00
| 160.00 | 2.491E+01 | 1.681E+26 | 1.386E+04 | 2.385E-51 | 1.400E+00 | 2.000E+00
| 170.00 | 2.729E+01 | 1.841E+26 | 1.517E+04 | 2.423E-48 | 1.467E+00 | 2.000E+00
| 180.00 | 2.973E+01 | 2.006E+26 | 1.653E+04 | 1.149E-45 | 1.541E+00 | 2.000E+00
| 190.00 | 3.224E+01 | 2.176E+26 | 1.793E+04 | 2.869E-43 | 1.623E+00 | 2.000E+00
| 200.00 | 3.482E+01 | 2.350E+26 | 1.936E+04 | 4.153E-41 | 1.711E+00 | 2.000E+00
| 210.00 | 3.746E+01 | 2.528E+26 | 2.083E+04 | 3.769E-39 | 1.808E+00 | 2.000E+00
| 220.00 | 4.017E+01 | 2.711E+26 | 2.234E+04 | 2.286E-37 | 1.913E+00 | 2.000E+00
| 230.00 | 4.294E+01 | 2.898E+26 | 2.388E+04 | 9.761E-36 | 2.027E+00 | 2.000E+00
| 240.00 | 4.577E+01 | 3.089E+26 | 2.545E+04 | 3.068E-34 | 2.151E+00 | 2.000E+00
| 250.00 | 4.866E+01 | 3.284E+26 | 2.706E+04 | 7.363E-33 | 2.285E+00 | 2.000E+00
| 260.00 | 5.161E+01 | 3.483E+26 | 2.870E+04 | 1.392E-31 | 2.431E+00 | 2.000E+00
| 270.00 | 5.462E+01 | 3.686E+26 | 3.037E+04 | 2.129E-30 | 2.589E+00 | 2.000E+00
| 280.00 | 5.768E+01 | 3.892E+26 | 3.208E+04 | 2.694E-29 | 2.761E+00 | 2.000E+00
| 300.00 | 6.397E+01 | 4.317E+26 | 3.557E+04 | 2.639E-27 | 3.148E+00 | 2.000E+00
| 320.00 | 7.047E+01 | 4.756E+26 | 3.919E+04 | 1.486E-25 | 3.601E+00 | 2.000E+00
| 340.00 | 7.718E+01 | 5.208E+26 | 4.292E+04 | 5.310E-24 | 4.132E+00 | 2.000E+00
| 360.00 | 8.409E+01 | 5.674E+26 | 4.676E+04 | 1.298E-22 | 4.754E+00 | 2.000E+00
| 400.00 | 9.848E+01 | 6.646E+26 | 5.477E+04 | 3.122E-20 | 6.337E+00 | 2.000E+00
| ---
| Qtr : translational pfn per volume unit
| Qrot: rotational pfn (rigid-rotor); includes rotational symmetry number
| Qvib: vibrational pfn (harmonic-oscillator) relative to V0 and to V1
| Qel : electronic pfn
|
| ---
| T (K) | Qtot [V0] | Qtot [V1] | Qtot [V0] | Qtot [V1]
| ---
| 10.00 | 8.487E-811 | 1.686E+02 | 5.727E-786 | 1.137E+27
| 20.00 | 9.568E-404 | 1.348E+03 | 6.457E-379 | 9.100E+27
| 30.00 | 7.803E-268 | 4.553E+03 | 5.266E-243 | 3.072E+28
| 40.00 | 9.112E-200 | 1.082E+04 | 6.149E-175 | 7.300E+28
| 50.00 | 7.379E-159 | 2.126E+04 | 4.980E-134 | 1.435E+29
| 60.00 | 1.538E-131 | 3.715E+04 | 1.038E-106 | 2.507E+29
| 70.00 | 5.433E-112 | 5.993E+04 | 3.666E-87 | 4.044E+29
| 80.00 | 2.649E-97 | 9.127E+04 | 1.788E-72 | 6.159E+29
| 90.00 | 7.394E-86 | 1.331E+05 | 4.989E-61 | 8.982E+29
| 100.00 | 1.106E-76 | 1.877E+05 | 7.462E-52 | 1.267E+30
| 110.00 | 3.679E-69 | 2.577E+05 | 2.483E-44 | 1.739E+30
| 120.00 | 7.042E-63 | 3.461E+05 | 4.752E-38 | 2.335E+30
| 130.00 | 1.496E-57 | 4.566E+05 | 1.010E-32 | 3.081E+30
| 140.00 | 5.650E-53 | 5.934E+05 | 3.813E-28 | 4.004E+30
| 150.00 | 5.351E-49 | 7.614E+05 | 3.611E-24 | 5.138E+30
| 160.00 | 1.646E-45 | 9.664E+05 | 1.111E-20 | 6.522E+30
| 170.00 | 2.006E-42 | 1.215E+06 | 1.354E-17 | 8.200E+30

```
|     180.00 |  1.129E-39 |  1.515E+06 |  7.621E-15 |  1.023E+31
|     190.00 |  3.316E-37 |  1.876E+06 |  2.238E-12 |  1.266E+31
|     200.00 |  5.600E-35 |  2.307E+06 |  3.779E-10 |  1.557E+31
|     210.00 |  5.884E-33 |  2.822E+06 |  3.970E-08 |  1.904E+31
|     220.00 |  4.102E-31 |  3.433E+06 |  2.768E-06 |  2.317E+31
|     230.00 |  2.002E-29 |  4.157E+06 |  1.351E-04 |  2.805E+31
|     240.00 |  7.149E-28 |  5.012E+06 |  4.824E-03 |  3.382E+31
|     250.00 |  1.939E-26 |  6.019E+06 |  1.309E-01 |  4.062E+31
|     260.00 |  4.124E-25 |  7.203E+06 |  2.783E+00 |  4.861E+31
|     270.00 |  7.062E-24 |  8.591E+06 |  4.766E+01 |  5.798E+31
|     280.00 |  9.968E-23 |  1.022E+07 |  6.727E+02 |  6.894E+31
|     300.00 |  1.201E-20 |  1.432E+07 |  8.104E+04 |  9.667E+31
|     320.00 |  8.209E-19 |  1.989E+07 |  5.540E+06 |  1.342E+32
|     340.00 |  3.518E-17 |  2.738E+07 |  2.374E+08 |  1.847E+32
|     360.00 |  1.021E-15 |  3.739E+07 |  6.888E+09 |  2.523E+32
|     400.00 |  3.368E-13 |  6.836E+07 |  2.273E+12 |  4.613E+32
| ------------------------------------------------------------
|            |          in au          |        in cm^-3
| ------------------------------------------------------------
|   Qtot: total pfn per unit volume
|         * [V0] --> from the bottom of the potential (V0)
|         * [V1] --> from the zero-point energy (V1)
|         * includes rotational symmetry number
|         |
| Gibbs free energy (hartree):
| ------------------------------------------
|   T (K)  |   v = 1 cm^3   |   v = kbT/p0
| ------------------------------------------
|    10.00 |  -208.47373914 |  -208.47221807
|    20.00 |  -208.47584373 |  -208.47284548
|    30.00 |  -208.47799806 |  -208.47353921
|    40.00 |  -208.48018496 |  -208.47427626
|    50.00 |  -208.48239663 |  -208.47504609
|    60.00 |  -208.48462873 |  -208.47584272
|    70.00 |  -208.48687848 |  -208.47666231
|    80.00 |  -208.48914394 |  -208.47750215
|    90.00 |  -208.49142370 |  -208.47836025
|   100.00 |  -208.49371668 |  -208.47923511
|   110.00 |  -208.49602209 |  -208.48012556
|   120.00 |  -208.49833930 |  -208.48103069
|   130.00 |  -208.50066779 |  -208.48194976
|   140.00 |  -208.50300717 |  -208.48288215
|   150.00 |  -208.50535711 |  -208.48382735
|   160.00 |  -208.50771731 |  -208.48478494
|   170.00 |  -208.51008753 |  -208.48575452
|   180.00 |  -208.51246755 |  -208.48673577
|   190.00 |  -208.51485718 |  -208.48772839
|   200.00 |  -208.51725624 |  -208.48873210
|   210.00 |  -208.51966457 |  -208.48974667
|   220.00 |  -208.52208202 |  -208.49077188
|   230.00 |  -208.52450847 |  -208.49180751
|   240.00 |  -208.52694378 |  -208.49285339
|   250.00 |  -208.52938784 |  -208.49390934
|   260.00 |  -208.53184055 |  -208.49497520
|   270.00 |  -208.53430181 |  -208.49605083
|   280.00 |  -208.53677151 |  -208.49713607
|   300.00 |  -208.54173592 |  -208.49933493
|   320.00 |  -208.54673313 |  -208.50157081
|   340.00 |  -208.55176256 |  -208.50384286
|   360.00 |  -208.55682364 |  -208.50615031
|   400.00 |  -208.56703877 |  -208.51086853
| ------------------------------------------
|   v : volume per molecule
|   p0: 1bar
```

CH_2CN information

```
-------------------------
  Analysis of STRUC: CH2CN
 -------------------------

    Number of conformers: 1

       V0 = electronic energy
       V1 = electronic energy + zero-point energy (ZPE)

       ZPE is calculated using scaled frequencies
       Frequency scale factor: 0.97300

       min(V0) = -132.09059340 hartree
       min(V1) = -132.06010267 hartree

       Relative energies (in kcal/mol):
       ------------------------------------------------------------------------
        name | V0-min(V0) | V1-min(V1) |   ZPE   | mass (amu) | weight |  PGS
       ------------------------------------------------------------------------
          001 |     0.000  |     0.000  |   19.13 |     40.02  |    1   |  C2v
       ------------------------------------------------------------------------
       weight: equals 2 if the structure has a conformational enantiomer,
               equals 1 otherwise
       PGS   : point group of symmetry

    ------------------
    Conformation: 001
    ------------------
     | Molecular formula     : C(2)H(2)N
     | Number of atoms       : 5
     | Number of electrons   : 21
     | Vibrational DOFs      : 9
     | Charge                : 0
     | Multiplicity          : 2
     | Electronic energy (V0): -132.09059340 hartree
     | Total mass [root]     : 40.0187 amu
     | Total mass            : 40.0187 amu
     | Point group symmetry  : C2v
     | Rotational sym num    : 2
     | Cartesian coordinates (Angstrom):
     |    N    +0.09818799   -0.17006658   -1.24904303  [ 14.003 amu]
     |    C    +0.00844726   -0.01463109   -0.10743434  [ 12.000 amu]
     |    C    -0.09933212   +0.17204827   +1.26356165  [ 12.000 amu]
     |    H    +0.67055160   +0.71289283   +1.79441332  [  1.008 amu]
     |    H    -0.95265910   -0.22426830   +1.79441332  [  1.008 amu]
     | Moments and product of inertia (au):
     |         +1.152E+04  +3.177E+05  +3.293E+05  [ 1.206E+15]
     | Vibrational frequencies [1/cm] (scaled by 0.973):
     |     376.43    427.65    648.58   1008.35   1022.71   1402.05
     |    2177.69   3106.57   3213.85
     | Vibrational zero-point energies [kcal/mol]:
     |       0.54      0.61      0.93      1.44      1.46      2.00
     |       3.11      4.44      4.59
     | Vibrational zero-point energy:    +0.03049073 hartree  =
     |                                        +19.13 kcal/mol =
     |                                         +0.83 eV       =
     |                                       +6691.94 cm^-1
     | V0 + zero-point energy (V1)  :  -132.06010267 hartree
     |
     | Partition functions (pfns):
     | ------------------------------------------------------------------------------------------
     |    T (K)   |  Qtr (au)  | Qtr (cm^-3) |    Qrot    |  Qvib [V0] |  Qvib [V1] |     Qel
     | ------------------------------------------------------------------------------------------
```

10.00	2.229E-01	1.505E+24	1.551E+01	7.121E-419	1.000E+00	2.000E+00
20.00	6.306E-01	4.255E+24	4.387E+01	8.439E-210	1.000E+00	2.000E+00
30.00	1.158E+00	7.818E+24	8.060E+01	4.145E-140	1.000E+00	2.000E+00
40.00	1.784E+00	1.204E+25	1.241E+02	2.905E-105	1.000E+00	2.000E+00
50.00	2.493E+00	1.682E+25	1.734E+02	2.347E-84	1.000E+00	2.000E+00
60.00	3.277E+00	2.211E+25	2.280E+02	2.036E-70	1.000E+00	2.000E+00
70.00	4.129E+00	2.786E+25	2.873E+02	1.840E-60	1.001E+00	2.000E+00
80.00	5.045E+00	3.404E+25	3.510E+02	5.398E-53	1.002E+00	2.000E+00
90.00	6.020E+00	4.062E+25	4.188E+02	3.473E-47	1.004E+00	2.000E+00
100.00	7.050E+00	4.758E+25	4.905E+02	1.542E-42	1.007E+00	2.000E+00
110.00	8.134E+00	5.489E+25	5.659E+02	9.806E-39	1.011E+00	2.000E+00
120.00	9.268E+00	6.254E+25	6.448E+02	1.452E-35	1.018E+00	2.000E+00
130.00	1.045E+01	7.052E+25	7.270E+02	7.011E-33	1.026E+00	2.000E+00
140.00	1.168E+01	7.881E+25	8.125E+02	1.404E-30	1.035E+00	2.000E+00
150.00	1.295E+01	8.740E+25	9.011E+02	1.392E-28	1.047E+00	2.000E+00
160.00	1.427E+01	9.629E+25	9.927E+02	7.789E-27	1.061E+00	2.000E+00
170.00	1.563E+01	1.055E+26	1.087E+03	2.724E-25	1.077E+00	2.000E+00
180.00	1.703E+01	1.149E+26	1.185E+03	6.438E-24	1.094E+00	2.000E+00
190.00	1.846E+01	1.246E+26	1.285E+03	1.094E-22	1.114E+00	2.000E+00
200.00	1.994E+01	1.346E+26	1.387E+03	1.405E-21	1.135E+00	2.000E+00
210.00	2.145E+01	1.448E+26	1.493E+03	1.420E-20	1.159E+00	2.000E+00
220.00	2.301E+01	1.552E+26	1.601E+03	1.166E-19	1.184E+00	2.000E+00
230.00	2.459E+01	1.660E+26	1.711E+03	8.001E-19	1.212E+00	2.000E+00
240.00	2.621E+01	1.769E+26	1.824E+03	4.689E-18	1.241E+00	2.000E+00
250.00	2.787E+01	1.881E+26	1.939E+03	2.393E-17	1.273E+00	2.000E+00
260.00	2.956E+01	1.995E+26	2.056E+03	1.080E-16	1.306E+00	2.000E+00
270.00	3.128E+01	2.111E+26	2.176E+03	4.373E-16	1.342E+00	2.000E+00
280.00	3.303E+01	2.229E+26	2.298E+03	1.607E-15	1.380E+00	2.000E+00
300.00	3.663E+01	2.472E+26	2.549E+03	1.685E-14	1.462E+00	2.000E+00
320.00	4.036E+01	2.723E+26	2.808E+03	1.330E-13	1.553E+00	2.000E+00
340.00	4.420E+01	2.983E+26	3.075E+03	8.315E-13	1.653E+00	2.000E+00
360.00	4.816E+01	3.250E+26	3.350E+03	4.278E-12	1.764E+00	2.000E+00
400.00	5.640E+01	3.806E+26	3.924E+03	7.098E-11	2.018E+00	2.000E+00

Qtr : translational pfn per volume unit
Qrot: rotational pfn (rigid-rotor); includes rotational symmetry number
Qvib: vibrational pfn (harmonic-oscillator) relative to V0 and to V1
Qel : electronic pfn

T (K)	Qtot [V0]	Qtot [V1]	Qtot [V0]	Qtot [V1]
10.00	4.925E-418	6.916E+00	3.324E-393	4.667E+25
20.00	4.669E-208	5.533E+01	3.151E-183	3.734E+26
30.00	7.740E-138	1.867E+02	5.223E-113	1.260E+27
40.00	1.286E-102	4.426E+02	8.677E-78	2.987E+27
50.00	2.029E-81	8.646E+02	1.369E-56	5.834E+27
60.00	3.042E-67	1.494E+03	2.053E-42	1.008E+28
70.00	4.366E-57	2.374E+03	2.946E-32	1.602E+28
80.00	1.912E-49	3.547E+03	1.290E-24	2.394E+28
90.00	1.751E-43	5.060E+03	1.182E-18	3.415E+28
100.00	1.067E-38	6.963E+03	7.198E-14	4.699E+28
110.00	9.027E-35	9.310E+03	6.091E-10	6.282E+28
120.00	1.735E-31	1.216E+04	1.171E-06	8.207E+28
130.00	1.065E-28	1.558E+04	7.189E-04	1.052E+29
140.00	2.665E-26	1.965E+04	1.799E-01	1.326E+29
150.00	3.249E-24	2.445E+04	2.192E+01	1.650E+29
160.00	2.207E-22	3.006E+04	1.489E+03	2.028E+29
170.00	9.256E-21	3.659E+04	6.246E+04	2.469E+29
180.00	2.597E-19	4.414E+04	1.752E+06	2.979E+29
190.00	5.191E-18	5.284E+04	3.503E+07	3.566E+29
200.00	7.776E-17	6.283E+04	5.248E+08	4.240E+29
210.00	9.095E-16	7.424E+04	6.138E+09	5.010E+29
220.00	8.589E-15	8.723E+04	5.796E+10	5.887E+29

```
|     230.00 |  6.733E-14 |  1.020E+05 |  4.544E+11 |  6.882E+29
|     240.00 |  4.483E-13 |  1.187E+05 |  3.025E+12 |  8.009E+29
|     250.00 |  2.586E-12 |  1.376E+05 |  1.745E+13 |  9.282E+29
|     260.00 |  1.313E-11 |  1.588E+05 |  8.860E+13 |  1.072E+30
|     270.00 |  5.953E-11 |  1.827E+05 |  4.017E+14 |  1.233E+30
|     280.00 |  2.439E-10 |  2.095E+05 |  1.646E+15 |  1.414E+30
|     300.00 |  3.146E-09 |  2.729E+05 |  2.123E+16 |  1.842E+30
|     320.00 |  3.015E-08 |  3.519E+05 |  2.035E+17 |  2.375E+30
|     340.00 |  2.260E-07 |  4.494E+05 |  1.525E+18 |  3.033E+30
|     360.00 |  1.380E-06 |  5.691E+05 |  9.315E+18 |  3.841E+30
|     400.00 |  3.142E-05 |  8.931E+05 |  2.120E+20 |  6.027E+30
| ------------------------------------------------------------
|            |          in au          |        in cm^-3
| ------------------------------------------------------------
|   Qtot: total pfn per unit volume
|         * [V0] --> from the bottom of the potential (V0)
|         * [V1] --> from the zero-point energy (V1)
|         * includes rotational symmetry number
|
|
| Gibbs free energy (hartree):
| ------------------------------------------
|   T (K)  |   v = 1 cm^3   |   v = kbT/p0
| ------------------------------------------
|    10.00 |  -132.06197442 |  -132.06045335
|    20.00 |  -132.06397788 |  -132.06097963
|    30.00 |  -132.06603105 |  -132.06157219
|    40.00 |  -132.06811650 |  -132.06220780
|    50.00 |  -132.07022596 |  -132.06287542
|    60.00 |  -132.07235457 |  -132.06356856
|    70.00 |  -132.07449916 |  -132.06428299
|    80.00 |  -132.07665755 |  -132.06501576
|    90.00 |  -132.07882817 |  -132.06576472
|   100.00 |  -132.08100987 |  -132.06652829
|   110.00 |  -132.08320178 |  -132.06730525
|   120.00 |  -132.08540324 |  -132.06809464
|   130.00 |  -132.08761371 |  -132.06889568
|   140.00 |  -132.08983277 |  -132.06970774
|   150.00 |  -132.09206005 |  -132.07053030
|   160.00 |  -132.09429525 |  -132.07136288
|   170.00 |  -132.09653810 |  -132.07220510
|   180.00 |  -132.09878837 |  -132.07305660
|   190.00 |  -132.10104585 |  -132.07391706
|   200.00 |  -132.10331036 |  -132.07478622
|   210.00 |  -132.10558171 |  -132.07566381
|   220.00 |  -132.10785975 |  -132.07654961
|   230.00 |  -132.11014435 |  -132.07744339
|   240.00 |  -132.11243536 |  -132.07834497
|   250.00 |  -132.11473267 |  -132.07925416
|   260.00 |  -132.11703615 |  -132.08017079
|   270.00 |  -132.11934569 |  -132.08109471
|   280.00 |  -132.12166119 |  -132.08202576
|   300.00 |  -132.12630969 |  -132.08390870
|   320.00 |  -132.13098091 |  -132.08581859
|   340.00 |  -132.13567419 |  -132.08775449
|   360.00 |  -132.14038889 |  -132.08971556
|   400.00 |  -132.14988033 |  -132.09371009
| ------------------------------------------
|   v : volume per molecule
|   p0: 1bar
```

H_2O information

```
------------------------
  Analysis of STRUC: H2O
 ------------------------

     Number of conformers: 1

        V0 = electronic energy
        V1 = electronic energy + zero-point energy (ZPE)

        ZPE is calculated using scaled frequencies
        Frequency scale factor: 0.97300

        min(V0) = -76.42802340 hartree
        min(V1) = -76.40689392 hartree

        Relative energies (in kcal/mol):
        ------------------------------------------------------------------------
         name | V0-min(V0) | V1-min(V1) |   ZPE   | mass (amu) | weight |  PGS
        ------------------------------------------------------------------------
          001 |     0.000  |     0.000  |   13.26 |     18.01  |    1   |  C2v
        ------------------------------------------------------------------------
        weight: equals 2 if the structure has a conformational enantiomer,
                equals 1 otherwise
        PGS   : point group of symmetry

     ------------------
     Conformation: 001
     ------------------
      | Molecular formula     : H(2)O
      | Number of atoms       : 3
      | Number of electrons   : 10
      | Vibrational DOFs      : 3
      | Charge                : 0
      | Multiplicity          : 1
      | Electronic energy (V0): -76.42802340 hartree
      | Total mass [root]     : 18.0106 amu
      | Total mass            : 18.0106 amu
      | Point group symmetry  : C2v
      | Rotational sym num    : 2
      | Cartesian coordinates (Angstrom):
      |    O    -0.05149210   +0.00000000   -0.03890814  [ 15.995 amu]
      |    H    -0.05149210   +0.00000000   +0.91765982  [  1.008 amu]
      |    H    +0.86870891   +0.00000000   -0.30015964  [  1.008 amu]
      | Moments and product of inertia (au):
      |         +3.875E+03  +7.643E+03  +1.152E+04  [ 3.411E+11]
      | Vibrational frequencies [1/cm] (scaled by 0.973):
      |    1590.53   3793.63   3890.61
      | Vibrational zero-point energies [kcal/mol]:
      |       2.27      5.42      5.56
      | Vibrational zero-point energy:    +0.02112948 hartree  =
      |                                        +13.26 kcal/mol =
      |                                         +0.57 eV       =
      |                                     +4637.39 cm^-1
      | V0 + zero-point energy (V1)  :   -76.40689392 hartree
      |
      | Partition functions (pfns):
      | ------------------------------------------------------------------------------------------
      |    T (K)   |  Qtr (au)  | Qtr (cm^-3) |    Qrot    |  Qvib [V0] |  Qvib [V1] |     Qel
      | ------------------------------------------------------------------------------------------
      |      10.00 |  6.731E-02 |   4.542E+23 |  2.609E-01 | 1.706E-290 |  1.000E+00 |  1.000E+00
      |      20.00 |  1.904E-01 |   1.285E+24 |  7.379E-01 | 1.306E-145 |  1.000E+00 |  1.000E+00
      |      30.00 |  3.498E-01 |   2.360E+24 |  1.356E+00 |  2.574E-97 |  1.000E+00 |  1.000E+00
      |      40.00 |  5.385E-01 |   3.634E+24 |  2.087E+00 |  3.614E-73 |  1.000E+00 |  1.000E+00
```

50.00	7.526E-01	5.079E+24	2.917E+00	1.113E-58	1.000E+00	1.000E+00
60.00	9.893E-01	6.676E+24	3.834E+00	5.074E-49	1.000E+00	1.000E+00
70.00	1.247E+00	8.413E+24	4.832E+00	4.023E-42	1.000E+00	1.000E+00
80.00	1.523E+00	1.028E+25	5.904E+00	6.012E-37	1.000E+00	1.000E+00
90.00	1.817E+00	1.226E+25	7.044E+00	6.361E-33	1.000E+00	1.000E+00
100.00	2.129E+00	1.436E+25	8.250E+00	1.055E-29	1.000E+00	1.000E+00
110.00	2.456E+00	1.657E+25	9.518E+00	4.544E-27	1.000E+00	1.000E+00
120.00	2.798E+00	1.888E+25	1.085E+01	7.123E-25	1.000E+00	1.000E+00
130.00	3.155E+00	2.129E+25	1.223E+01	5.130E-23	1.000E+00	1.000E+00
140.00	3.526E+00	2.379E+25	1.367E+01	2.006E-21	1.000E+00	1.000E+00
150.00	3.910E+00	2.639E+25	1.516E+01	4.810E-20	1.000E+00	1.000E+00
160.00	4.308E+00	2.907E+25	1.670E+01	7.753E-19	1.000E+00	1.000E+00
170.00	4.718E+00	3.184E+25	1.829E+01	9.012E-18	1.000E+00	1.000E+00
180.00	5.140E+00	3.469E+25	1.992E+01	7.976E-17	1.000E+00	1.000E+00
190.00	5.575E+00	3.762E+25	2.161E+01	5.611E-16	1.000E+00	1.000E+00
200.00	6.021E+00	4.063E+25	2.334E+01	3.248E-15	1.000E+00	1.000E+00
210.00	6.478E+00	4.371E+25	2.511E+01	1.590E-14	1.000E+00	1.000E+00
220.00	6.946E+00	4.687E+25	2.692E+01	6.741E-14	1.000E+00	1.000E+00
230.00	7.425E+00	5.011E+25	2.878E+01	2.520E-13	1.000E+00	1.000E+00
240.00	7.914E+00	5.341E+25	3.068E+01	8.440E-13	1.000E+00	1.000E+00
250.00	8.414E+00	5.678E+25	3.261E+01	2.566E-12	1.000E+00	1.000E+00
260.00	8.924E+00	6.022E+25	3.459E+01	7.164E-12	1.000E+00	1.000E+00
270.00	9.444E+00	6.373E+25	3.660E+01	1.853E-11	1.000E+00	1.000E+00
280.00	9.973E+00	6.730E+25	3.866E+01	4.480E-11	1.000E+00	1.000E+00
300.00	1.106E+01	7.464E+25	4.287E+01	2.194E-10	1.000E+00	1.000E+00
320.00	1.218E+01	8.223E+25	4.723E+01	8.812E-10	1.001E+00	1.000E+00
340.00	1.334E+01	9.006E+25	5.172E+01	3.006E-09	1.001E+00	1.000E+00
360.00	1.454E+01	9.812E+25	5.635E+01	8.946E-09	1.002E+00	1.000E+00
400.00	1.703E+01	1.149E+26	6.600E+01	5.718E-08	1.003E+00	1.000E+00

Qtr : translational pfn per volume unit
Qrot: rotational pfn (rigid-rotor); includes rotational symmetry number
Qvib: vibrational pfn (harmonic-oscillator) relative to V0 and to V1
Qel : electronic pfn

T (K)	Qtot [V0]	Qtot [V1]	Qtot [V0]	Qtot [V1]
10.00	2.996E-292	1.756E-02	2.022E-267	1.185E+23
20.00	1.835E-146	1.405E-01	1.238E-121	9.481E+23
30.00	1.221E-97	4.742E-01	8.237E-73	3.200E+24
40.00	4.062E-73	1.124E+00	2.741E-48	7.585E+24
50.00	2.443E-58	2.195E+00	1.648E-33	1.481E+25
60.00	1.925E-48	3.793E+00	1.299E-23	2.560E+25
70.00	2.423E-41	6.024E+00	1.635E-16	4.065E+25
80.00	5.405E-36	8.992E+00	3.648E-11	6.068E+25
90.00	8.144E-32	1.280E+01	5.496E-07	8.640E+25
100.00	1.853E-28	1.756E+01	1.250E-03	1.185E+26
110.00	1.062E-25	2.337E+01	7.168E-01	1.577E+26
120.00	2.162E-23	3.035E+01	1.459E+02	2.048E+26
130.00	1.979E-21	3.858E+01	1.336E+04	2.604E+26
140.00	9.666E-20	4.819E+01	6.523E+05	3.252E+26
150.00	2.851E-18	5.927E+01	1.924E+07	4.000E+26
160.00	5.577E-17	7.193E+01	3.764E+08	4.854E+26
170.00	7.776E-16	8.628E+01	5.247E+09	5.823E+26
180.00	8.169E-15	1.024E+02	5.513E+10	6.912E+26
190.00	6.759E-14	1.205E+02	4.561E+11	8.129E+26
200.00	4.563E-13	1.405E+02	3.079E+12	9.481E+26
210.00	2.587E-12	1.626E+02	1.746E+13	1.098E+27
220.00	1.261E-11	1.870E+02	8.507E+13	1.262E+27
230.00	5.385E-11	2.137E+02	3.634E+14	1.442E+27
240.00	2.049E-10	2.428E+02	1.383E+15	1.638E+27
250.00	7.042E-10	2.744E+02	4.752E+15	1.852E+27
260.00	2.211E-09	3.087E+02	1.492E+16	2.083E+27

```
|     270.00 |  6.406E-09 |  3.457E+02 |  4.323E+16 |  2.333E+27
|     280.00 |  1.727E-08 |  3.856E+02 |  1.165E+17 |  2.602E+27
|     300.00 |  1.040E-07 |  4.744E+02 |  7.021E+17 |  3.201E+27
|     320.00 |  5.071E-07 |  5.759E+02 |  3.422E+18 |  3.887E+27
|     340.00 |  2.075E-06 |  6.911E+02 |  1.400E+19 |  4.664E+27
|     360.00 |  7.330E-06 |  8.208E+02 |  4.947E+19 |  5.539E+27
|     400.00 |  6.427E-05 |  1.128E+03 |  4.337E+20 |  7.610E+27
| ------------------------------------------------------------
|            |          in au          |        in cm^-3
| ------------------------------------------------------------
|   Qtot: total pfn per unit volume
|         * [V0] --> from the bottom of the potential (V0)
|         * [V1] --> from the zero-point energy (V1)
|         * includes rotational symmetry number
|
| Gibbs free energy (hartree):
| ------------------------------------------
|   T (K)  |   v = 1 cm^3   |   v = kbT/p0
| ------------------------------------------
|    10.00 |   -76.40857642 |   -76.40705535
|    20.00 |   -76.41039063 |   -76.40739238
|    30.00 |   -76.41225456 |   -76.40779570
|    40.00 |   -76.41415076 |   -76.40824206
|    50.00 |   -76.41607097 |   -76.40872043
|    60.00 |   -76.41801031 |   -76.40922430
|    70.00 |   -76.41996556 |   -76.40974939
|    80.00 |   -76.42193442 |   -76.41029263
|    90.00 |   -76.42391520 |   -76.41085175
|   100.00 |   -76.42590655 |   -76.41142497
|   110.00 |   -76.42790741 |   -76.41201088
|   120.00 |   -76.42991693 |   -76.41260832
|   130.00 |   -76.43193437 |   -76.41321633
|   140.00 |   -76.43395913 |   -76.41383410
|   150.00 |   -76.43599068 |   -76.41446092
|   160.00 |   -76.43802856 |   -76.41509619
|   170.00 |   -76.44007239 |   -76.41573938
|   180.00 |   -76.44212181 |   -76.41639003
|   190.00 |   -76.44417652 |   -76.41704773
|   200.00 |   -76.44623622 |   -76.41771209
|   210.00 |   -76.44830068 |   -76.41838279
|   220.00 |   -76.45036967 |   -76.41905953
|   230.00 |   -76.45244299 |   -76.41974203
|   240.00 |   -76.45452044 |   -76.42043005
|   250.00 |   -76.45660187 |   -76.42112336
|   260.00 |   -76.45868710 |   -76.42182175
|   270.00 |   -76.46077600 |   -76.42252502
|   280.00 |   -76.46286844 |   -76.42323301
|   300.00 |   -76.46706346 |   -76.42466247
|   320.00 |   -76.47127127 |   -76.42610895
|   340.00 |   -76.47549112 |   -76.42757143
|   360.00 |   -76.47972236 |   -76.42904903
|   400.00 |   -76.48821676 |   -76.43204652
| ------------------------------------------
|   v : volume per molecule
|   p0: 1bar
```

Torsional potential and anharmonic/harmonic ratios

All internal rotations were fitted to Fourier series of the type:

$$V(x) = V_0 \sum_{i}^{n_{max}} a_i \cos(ix) \tag{ES.4}$$

Table S1: Parameters for the C...OH rotation in TS1a. V_0 = +237.09361, Reduced moment of inertia = 0.785 amu Å^2

i	a_i
1	-198.77693
2	-29.77956
3	-5.32847
4	-1.84741
5	-1.18707
6	-0.35570

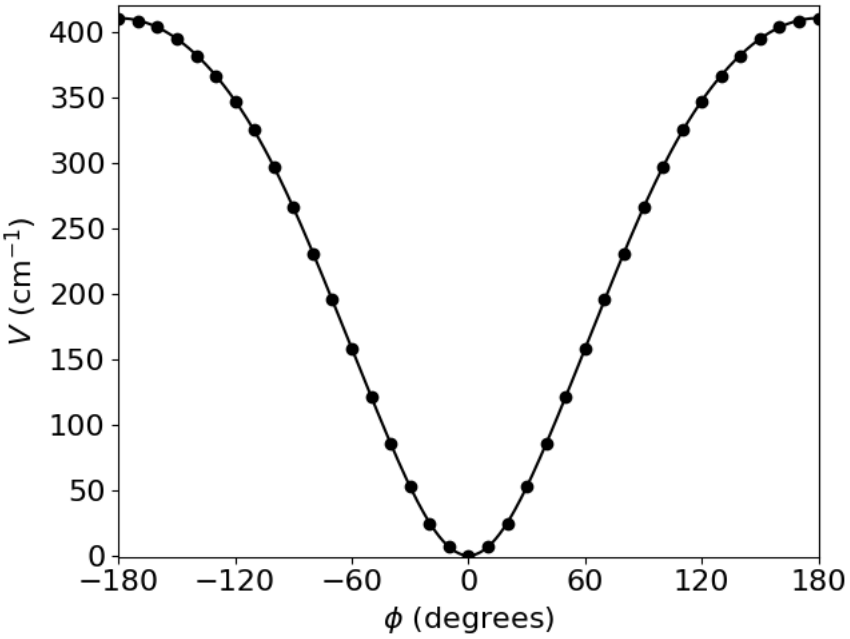

Figure S4: Fitted (solid curve) versus calculated (dots) torsional potential.

Table S2: Parameters for the C...OH rotation in TS1b. V_0 = +1601.78885, Reduced moment of inertia = 0.785 amu Å^2

i	a_i
1	-1755.78852
2	+181.52297
3	-32.62399
4	+18.89707
5	-14.68224
6	-5.57603

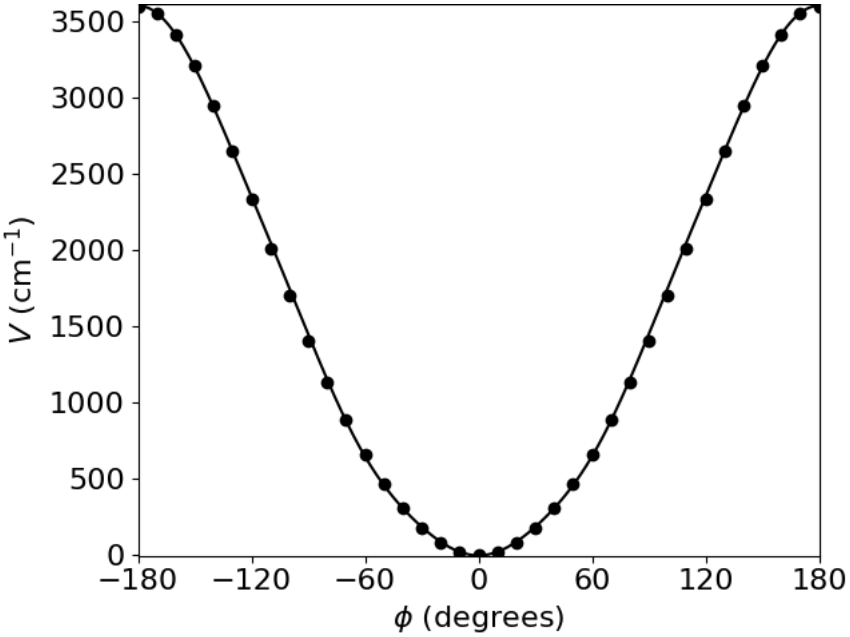

Figure S5: Fitted (solid curve) versus calculated (dots) torsional potential.

Table S3: Parameters for the CH3 rotation in TS1b. V_0 = +167.0566, Reduced moment of inertia = 3.019 amu Å^2

i	a_i
3	-190.08196
6	+26.85520

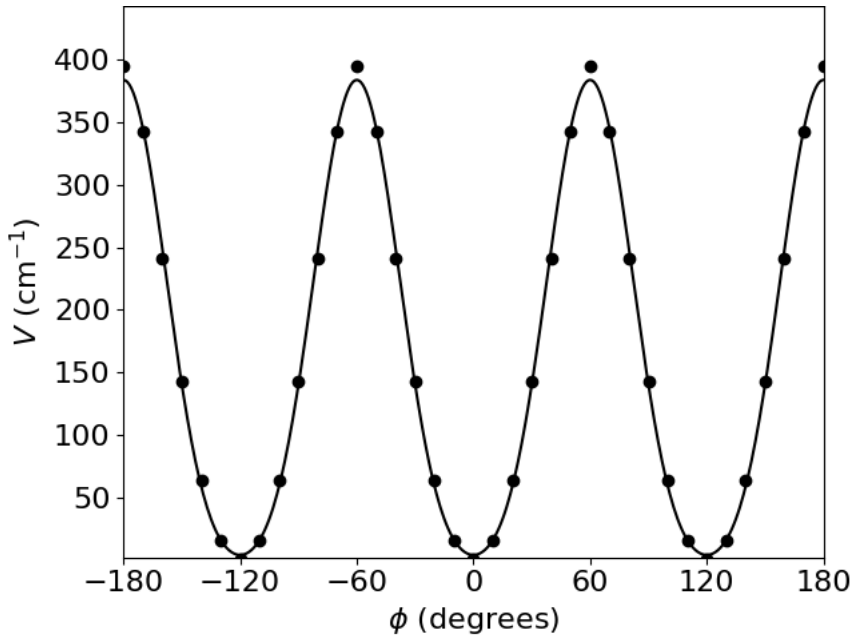

Figure S6: Fitted (solid curve) versus calculated (dots) torsional potential.

Table S4: Ratios between the anharmonic and harmonic 1D partition functions for TS1a (OH internal rotation) and TS1b (OH and CH_3 internal rotations), respectively.

T(K)	TS1a	TS1b
10	4.735	3.347
20	2.177	1.830
30	1.686	1.504
40	1.496	1.376
50	1.404	1.316
60	1.357	1.285
70	1.332	1.269
80	1.322	1.260
90	1.320	1.256
100	1.325	1.254
110	1.333	1.254
120	1.344	1.255
130	1.358	1.257
140	1.372	1.258
150	1.387	1.260
160	1.403	1.262
170	1.419	1.263
180	1.434	1.265
190	1.449	1.266
200	1.464	1.267
210	1.478	1.268
220	1.492	1.268
230	1.505	1.268
240	1.517	1.268
250	1.528	1.268
260	1.539	1.267
270	1.549	1.267
280	1.559	1.266
300	1.576	1.263
320	1.590	1.260
340	1.602	1.256
360	1.612	1.251
400	1.627	1.241

Thermal rate coefficients and branching ratios

Table S5: Variational, Γ^{CVT}, tunneling effects, $\kappa_{\mathrm{LPL}}^{\mathrm{CVT/SCT}}$, $\kappa_{\mathrm{HPL}}^{\mathrm{CVT/SCT}}$, harmonic-oscillator, $k^{\mathrm{TST,HO}}$, and anharmonic, $k^{\mathrm{TST,Anh}}$, TST rate constans, and CVT/SCT rate coefficients in the low-pressure, $k_{\mathrm{LPL}}^{\mathrm{CVT/SCT}}$, and high-pressure, $k_{\mathrm{HPL}}^{\mathrm{CVT/SCT}}$, regimes, for the hydrogen abstraction from the methyl group. Rate coefficients in $\mathrm{cm^3 molecule^{-1} s^{-1}}$.

T(K)	Γ^{CVT}	$\kappa_{\mathrm{LPL}}^{\mathrm{CVT/SCT}}$	$\kappa_{\mathrm{HPL}}^{\mathrm{CVT/SCT}}$	$k^{\mathrm{TST,HO}}$	$k^{\mathrm{TST,Anh}}$	$k_{\mathrm{LPL}}^{\mathrm{CVT/SCT}}$	$k_{\mathrm{HPL}}^{\mathrm{CVT/SCT}}$
10	1.844e-25⋆	5.369e+86	5.568e+107	2.311e-100	1.094e-99	1.083e-37	1.123e-16
20	4.364e-13	2.515e+40	1.071e+49	4.188e-56	9.116e-56	1.000e-27	4.261e-19
30	5.905e-09	9.805e+24	3.319e+29	1.856e-41	3.129e-41	1.812e-24	6.132e-20
40	6.943e-07	2.131e+17	7.421e+19	3.529e-34	5.278e-34	7.808e-23	2.719e-20
50	1.219e-05	5.895e+12	1.674e+14	7.822e-30	1.098e-29	7.891e-22	2.241e-20
60	8.262e-05	5.884e+09	3.989e+10	6.001e-27	8.141e-27	3.956e-21	2.682e-20
70	3.246e-04	4.604e+07	1.435e+08	6.788e-25	9.045e-25	1.351e-20	4.211e-20
80	9.070e-04	1.317e+06	2.610e+06	2.332e-23	3.083e-23	3.680e-20	7.294e-20
90	2.019e-03	8.782e+04	1.365e+05	3.634e-22	4.798e-22	8.502e-20	1.321e-19
100	3.831e-03	1.129e+04	1.476e+04	3.261e-21	4.320e-21	1.867e-19	2.440e-19
110	6.475e-03	2.279e+03	2.682e+03	1.963e-20	2.617e-20	3.858e-19	4.540e-19
120	1.003e-02	6.472e+02	7.141e+02	8.768e-20	1.179e-19	7.642e-19	8.432e-19
130	1.453e-02	2.385e+02	2.532e+02	3.116e-19	4.230e-19	1.464e-18	1.554e-18
140	1.998e-02	1.075e+02	1.114e+02	9.256e-19	1.270e-18	2.724e-18	2.822e-18
150	2.632e-02	5.653e+01	5.782e+01	2.384e-18	3.307e-18	4.912e-18	5.024e-18
160	3.352e-02	3.355e+01	3.402e+01	5.469e-18	7.672e-18	8.612e-18	8.732e-18
170	4.149e-02	2.186e+01	2.206e+01	1.141e-17	1.619e-17	1.465e-17	1.478e-17
180	5.016e-02	1.533e+01	1.542e+01	2.199e-17	3.153e-17	2.419e-17	2.433e-17
190	5.944e-02	1.139e+01	1.144e+01	3.968e-17	5.750e-17	3.883e-17	3.900e-17
200	6.925e-02	8.865e+00	8.889e+00	6.766e-17	9.905e-17	6.063e-17	6.079e-17
210	7.950e-02	7.160e+00	7.174e+00	1.100e-16	1.626e-16	9.218e-17	9.236e-17
220	9.013e-02	5.961e+00	5.969e+00	1.714e-16	2.557e-16	1.367e-16	1.369e-16
230	1.010e-01	5.086e+00	5.091e+00	2.578e-16	3.879e-16	1.981e-16	1.983e-16
240	1.122e-01	4.430e+00	4.433e+00	3.757e-16	5.698e-16	2.814e-16	2.816e-16
250	1.235e-01	3.925e+00	3.927e+00	5.326e-16	8.140e-16	3.918e-16	3.920e-16
260	1.349e-01	3.527e+00	3.529e+00	7.368e-16	1.134e-15	5.354e-16	5.358e-16
270	1.464e-01	3.209e+00	3.210e+00	9.974e-16	1.545e-15	7.200e-16	7.203e-16
280	1.579e-01	2.950e+00	2.950e+00	1.324e-15	2.064e-15	9.530e-16	9.530e-16
300	1.807e-01	2.556e+00	2.557e+00	2.220e-15	3.498e-15	1.600e-15	1.601e-15
320	2.031e-01	2.276e+00	2.276e+00	3.517e-15	5.592e-15	2.559e-15	2.559e-15
340	2.250e-01	2.068e+00	2.068e+00	5.318e-15	8.520e-15	3.921e-15	3.921e-15
360	2.460e-01	1.909e+00	1.909e+00	7.735e-15	1.247e-14	5.789e-15	5.789e-15
400	2.854e-01	1.686e+00	1.686e+00	1.490e-14	2.424e-14	1.152e-14	1.152e-14

⋆ 1.844e-25 means 1.844×10^{-25}

Table S6: Same as Table S5 but for the OH addition, being TS1b the transition state.

T(K)	Γ^{CVT}	$\kappa_{\mathrm{LPL}}^{\mathrm{CVT/SCT}}$	$\kappa_{\mathrm{HPL}}^{\mathrm{CVT/SCT}}$	$k^{\mathrm{TST,HO}}$	$k^{\mathrm{TST,Anh}}$	$k_{\mathrm{LPL}}^{\mathrm{CVT/SCT}}$	$k_{\mathrm{HPL}}^{\mathrm{CVT/SCT}}$
10	2.291e-01	7.587e+59	1.060e+133	3.443e-74	1.152e-73	2.003e-14	2.799e+59
20	4.773e-01	6.703e+27	3.107e+58	4.206e-43	7.699e-43	2.463e-15	1.142e+16
30	6.095e-01	1.424e+17	4.999e+33	7.455e-33	1.121e-32	9.733e-16	3.417e+01
40	6.883e-01	6.909e+11	2.460e+21	8.742e-28	1.203e-27	5.721e-16	2.037e-06
50	7.395e-01	4.720e+08	1.674e+14	8.930e-25	1.175e-24	4.102e-16	1.455e-10
60	7.745e-01	3.863e+06	7.077e+09	8.648e-23	1.111e-22	3.325e-16	6.092e-13
70	7.989e-01	1.319e+05	1.190e+07	2.201e-21	2.793e-21	2.943e-16	2.655e-14
80	8.163e-01	1.110e+04	1.600e+05	2.448e-20	3.085e-20	2.796e-16	4.030e-15
90	8.290e-01	1.721e+03	8.002e+03	1.575e-19	1.978e-19	2.822e-16	1.312e-15
100	8.379e-01	4.132e+02	9.644e+02	6.937e-19	8.702e-19	3.013e-16	7.032e-16
110	8.441e-01	1.371e+02	2.131e+02	2.324e-18	2.915e-18	3.374e-16	5.244e-16
120	8.485e-01	5.812e+01	7.179e+01	6.355e-18	7.977e-18	3.934e-16	4.859e-16
130	8.515e-01	2.926e+01	3.242e+01	1.488e-17	1.870e-17	4.658e-16	5.162e-16
140	8.534e-01	1.733e+01	1.794e+01	3.086e-17	3.883e-17	5.742e-16	5.944e-16
150	8.542e-01	1.143e+01	1.144e+01	5.816e-17	7.328e-17	7.155e-16	7.161e-16
160	8.547e-01	8.070e+00	8.070e+00	1.014e-16	1.279e-16	8.824e-16	8.824e-16
170	8.545e-01	6.120e+00	6.120e+00	1.659e-16	2.096e-16	1.096e-15	1.096e-15
180	8.540e-01	4.896e+00	4.896e+00	2.574e-16	3.255e-16	1.361e-15	1.361e-15
190	8.534e-01	4.079e+00	4.079e+00	3.822e-16	4.838e-16	1.684e-15	1.684e-15
200	8.523e-01	3.504e+00	3.504e+00	5.466e-16	6.925e-16	2.068e-15	2.068e-15
210	8.512e-01	3.084e+00	3.084e+00	7.571e-16	9.597e-16	2.519e-15	2.519e-15
220	8.500e-01	2.767e+00	2.767e+00	1.020e-15	1.293e-15	3.042e-15	3.042e-15
230	8.486e-01	2.521e+00	2.521e+00	1.342e-15	1.702e-15	3.641e-15	3.641e-15
240	8.473e-01	2.325e+00	2.325e+00	1.729e-15	2.193e-15	4.320e-15	4.320e-15
250	8.457e-01	2.168e+00	2.168e+00	2.187e-15	2.773e-15	5.084e-15	5.084e-15
260	8.443e-01	2.038e+00	2.038e+00	2.722e-15	3.450e-15	5.936e-15	5.936e-15
270	8.428e-01	1.930e+00	1.930e+00	3.340e-15	4.231e-15	6.882e-15	6.882e-15
280	8.413e-01	1.839e+00	1.839e+00	4.046e-15	5.121e-15	7.923e-15	7.923e-15
300	8.383e-01	1.695e+00	1.695e+00	5.741e-15	7.251e-15	1.030e-14	1.030e-14
320	8.349e-01	1.587e+00	1.587e+00	7.846e-15	9.883e-15	1.310e-14	1.310e-14
340	8.315e-01	1.503e+00	1.503e+00	1.040e-14	1.306e-14	1.632e-14	1.632e-14
360	8.281e-01	1.436e+00	1.436e+00	1.342e-14	1.679e-14	1.997e-14	1.997e-14
400	8.217e-01	1.339e+00	1.339e+00	2.103e-14	2.609e-14	2.871e-14	2.871e-14

Table S7: Rate coefficients (in $cm^3molecule^{-1}s^{-1}$) of association, k_a, CVT/SCT, $k_i^{CVT/SCT}$, and CCUS, k_i^{CCUS}, for R1a ($i = 1a$) and R1b ($i = 1b$) in the low-pressure limit. The global rate coefficient k^{CCUS} is also given.

T(K)	k_a	$k_{1a}^{CVT/SCT}$	k_{1a}^{CCUS}	$k_{1b}^{CVT/SCT}$	k_{1b}^{CCUS}	k^{CCUS}
10	1.275e-09	1.083e-37	1.083e-37	2.003e-14	2.003e-14	2.003e-14
20	1.135e-09	1.000e-27	1.000e-27	2.463e-15	2.463e-15	2.463e-15
30	1.061e-09	1.812e-24	1.812e-24	9.733e-16	9.733e-16	9.733e-16
40	1.012e-09	7.808e-23	7.808e-23	5.721e-16	5.721e-16	5.721e-16
50	9.747e-10	7.891e-22	7.891e-22	4.102e-16	4.102e-16	4.102e-16
60	9.455e-10	3.956e-21	3.956e-21	3.325e-16	3.325e-16	3.325e-16
70	9.215e-10	1.351e-20	1.351e-20	2.943e-16	2.943e-16	2.943e-16
80	9.012e-10	3.680e-20	3.680e-20	2.796e-16	2.796e-16	2.796e-16
90	8.837e-10	8.502e-20	8.502e-20	2.822e-16	2.822e-16	2.823e-16
100	8.683e-10	1.867e-19	1.867e-19	3.013e-16	3.013e-16	3.015e-16
110	8.547e-10	3.858e-19	3.858e-19	3.374e-16	3.374e-16	3.378e-16
120	8.423e-10	7.642e-19	7.642e-19	3.934e-16	3.934e-16	3.941e-16
130	8.312e-10	1.464e-18	1.464e-18	4.658e-16	4.658e-16	4.673e-16
140	8.210e-10	2.724e-18	2.724e-18	5.742e-16	5.742e-16	5.769e-16
150	8.116e-10	4.912e-18	4.912e-18	7.155e-16	7.155e-16	7.204e-16
160	8.029e-10	8.612e-18	8.612e-18	8.824e-16	8.824e-16	8.910e-16
170	7.948e-10	1.465e-17	1.465e-17	1.096e-15	1.096e-15	1.111e-15
180	7.873e-10	2.419e-17	2.419e-17	1.361e-15	1.361e-15	1.385e-15
190	7.802e-10	3.883e-17	3.883e-17	1.684e-15	1.684e-15	1.723e-15
200	7.736e-10	6.063e-17	6.063e-17	2.068e-15	2.068e-15	2.129e-15
210	7.673e-10	9.218e-17	9.218e-17	2.519e-15	2.519e-15	2.611e-15
220	7.614e-10	1.367e-16	1.367e-16	3.042e-15	3.042e-15	3.179e-15
230	7.558e-10	1.981e-16	1.981e-16	3.641e-15	3.641e-15	3.839e-15
240	7.504e-10	2.814e-16	2.814e-16	4.320e-15	4.320e-15	4.601e-15
250	7.454e-10	3.918e-16	3.918e-16	5.084e-15	5.084e-15	5.476e-15
260	7.405e-10	5.354e-16	5.354e-16	5.936e-15	5.936e-15	6.471e-15
270	7.359e-10	7.200e-16	7.200e-16	6.882e-15	6.882e-15	7.602e-15
280	7.314e-10	9.530e-16	9.530e-16	7.923e-15	7.923e-15	8.875e-15
300	7.231e-10	1.600e-15	1.600e-15	1.030e-14	1.030e-14	1.190e-14
320	7.153e-10	2.559e-15	2.559e-15	1.310e-14	1.309e-14	1.565e-14
340	7.081e-10	3.921e-15	3.921e-15	1.632e-14	1.632e-14	2.024e-14
360	7.014e-10	5.789e-15	5.789e-15	1.997e-14	1.997e-14	2.575e-14
400	6.892e-10	1.152e-14	1.152e-14	2.871e-14	2.871e-14	4.022e-14

Table S8: Same as Table S7 but for the high-pressure limit.

T(K)	k_{a}	$k_{1\mathrm{a}}^{\mathrm{CVT/SCT}}$	k_{1a}^{CCUS}	$k_{1\mathrm{b}}^{\mathrm{CVT/SCT}}$	k_{1b}^{CCUS}	k^{CCUS}
10	1.275e-09	1.123e-16	1.123e-16	2.799e+59	1.275e-09	1.275e-09
20	1.135e-09	4.261e-19	4.261e-19	1.142e+16	1.135e-09	1.135e-09
30	1.061e-09	6.132e-20	6.132e-20	3.417e+01	1.061e-09	1.061e-09
40	1.012e-09	2.719e-20	2.719e-20	2.037e-06	1.011e-09	1.011e-09
50	9.747e-10	2.241e-20	2.241e-20	1.455e-10	1.266e-10	1.266e-10
60	9.455e-10	2.682e-20	2.682e-20	6.092e-13	6.088e-13	6.088e-13
70	9.215e-10	4.211e-20	4.211e-20	2.655e-14	2.655e-14	2.655e-14
80	9.012e-10	7.294e-20	7.294e-20	4.030e-15	4.030e-15	4.030e-15
90	8.837e-10	1.321e-19	1.321e-19	1.312e-15	1.312e-15	1.312e-15
100	8.683e-10	2.440e-19	2.440e-19	7.032e-16	7.032e-16	7.034e-16
110	8.547e-10	4.540e-19	4.540e-19	5.244e-16	5.244e-16	5.248e-16
120	8.423e-10	8.432e-19	8.432e-19	4.859e-16	4.859e-16	4.867e-16
130	8.312e-10	1.554e-18	1.554e-18	5.162e-16	5.162e-16	5.177e-16
140	8.210e-10	2.822e-18	2.822e-18	5.944e-16	5.944e-16	5.972e-16
150	8.116e-10	5.024e-18	5.024e-18	7.161e-16	7.161e-16	7.211e-16
160	8.029e-10	8.732e-18	8.732e-18	8.824e-16	8.824e-16	8.911e-16
170	7.948e-10	1.478e-17	1.478e-17	1.096e-15	1.096e-15	1.111e-15
180	7.873e-10	2.433e-17	2.433e-17	1.361e-15	1.361e-15	1.385e-15
190	7.802e-10	3.900e-17	3.900e-17	1.684e-15	1.684e-15	1.723e-15
200	7.736e-10	6.079e-17	6.079e-17	2.068e-15	2.068e-15	2.129e-15
210	7.673e-10	9.236e-17	9.236e-17	2.519e-15	2.519e-15	2.612e-15
220	7.614e-10	1.369e-16	1.369e-16	3.042e-15	3.042e-15	3.179e-15
230	7.558e-10	1.983e-16	1.983e-16	3.641e-15	3.641e-15	3.840e-15
240	7.504e-10	2.816e-16	2.816e-16	4.320e-15	4.320e-15	4.601e-15
250	7.454e-10	3.920e-16	3.920e-16	5.084e-15	5.084e-15	5.476e-15
260	7.405e-10	5.358e-16	5.358e-16	5.936e-15	5.936e-15	6.472e-15
270	7.359e-10	7.203e-16	7.203e-16	6.882e-15	6.882e-15	7.602e-15
280	7.314e-10	9.530e-16	9.530e-16	7.923e-15	7.923e-15	8.875e-15
300	7.231e-10	1.601e-15	1.601e-15	1.030e-14	1.030e-14	1.190e-14
320	7.153e-10	2.559e-15	2.559e-15	1.310e-14	1.309e-14	1.565e-14
340	7.081e-10	3.921e-15	3.921e-15	1.632e-14	1.632e-14	2.024e-14
360	7.014e-10	5.789e-15	5.789e-15	1.997e-14	1.997e-14	2.575e-14
400	6.892e-10	1.152e-14	1.152e-14	2.871e-14	2.871e-14	4.022e-14

Table S9: Branching ratios in percentage in the low-pressure (LP) and high-pressure (HP) limits.

T(K)	$\left(\frac{k_{1a}^{CCUS}}{k^{CCUS}}\right)_{LPL}$	$\left(\frac{k_{1b}^{CCUS}}{k^{CCUS}}\right)_{LPL}$	$\left(\frac{k_{1a}^{CCUS}}{k^{CCUS}}\right)_{HPL}$	$\left(\frac{k_{1b}^{CCUS}}{k^{CCUS}}\right)_{HPL}$
10	0	100	0	100
20	0	100	0	100
30	0	100	0	100
40	0	100	0	100
50	0	100	0	100
60	0	100	0	100
70	0	100	0	100
80	0	100	0	100
90	0	100	0	100
100	0	100	0	100
110	0	100	0	100
120	0	100	0	100
130	0	100	0	100
140	0	100	0	100
150	1	99	1	99
160	1	99	1	99
170	1	99	1	99
180	2	98	2	98
190	2	98	2	98
200	3	97	3	97
210	4	96	4	96
220	4	96	4	96
230	5	95	5	95
240	6	94	6	94
250	7	93	7	93
260	8	92	8	92
270	9	91	9	91
280	11	89	11	89
300	13	87	13	87
320	16	84	16	84
340	19	81	19	81
360	22	78	22	78
400	29	71	29	71