Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Info – Contents

Supplementary Info 1 – Additional Tables and Figures

Table S1: Rotational and vibrational partition functions, as a function of temperature, for important stationary points on the $2H_4SiO_4 \rightarrow H_6Si_2O_7 + H_2O$ potential energy surface. Two four explicit waters are associated with each stationary point.

Hydrolysis; HF/6-31+G(d)

T/ K	Q(rot - P)	Q(rot - TS)	Q(rot - TS)/ Q(rot - P)	Q(vib - P)	Q(vib - TS)	Q(vib - TS)/ Q(vib - P)
300	4.137E+06	3.796E+06	9.177E-01	2.983E+11	9.460E+09	3.171E-02
500	8.901E+06	8.168E+06	9.177E-01	9.957E+17	1.112E+16	1.117E-02
800	1.801E+07	1.653E+07	9.177E-01	7.002E+25	3.394E+23	4.848E-03

Hydrolysis; B3LYP/6-31+G(d)

T/ K	Q(rot - P)	Q(rot - TS)	Q(rot - TS)/ Q(rot - P)	Q(vib - P)	Q(vib - TS)	Q(vib - TS)/ Q(vib - P)
300	4.072E+06	3.689E+06	9.060E-01	3.721E+10	8.392E+08	2.255E-02
500	8.761E+06	7.937E+06	9.060E-01	7.718E+16	6.960E+14	9.018E-03
800	1.773E+07	1.606E+07	9.060E-01	4.064E+24	1.846E+22	4.543E-03

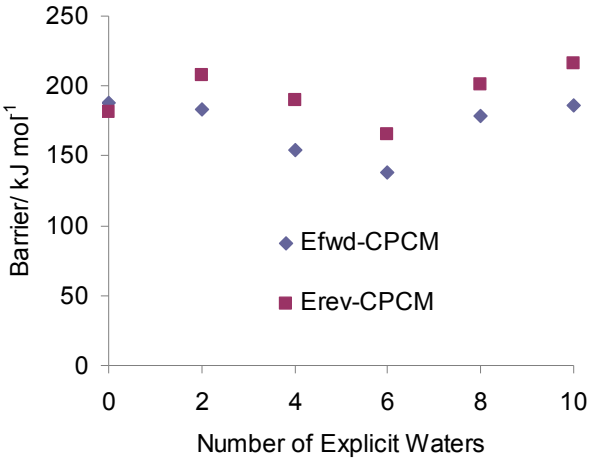

Figure S1: The changes in the reaction barrier of the unimolecular H_4SiO_4 dimerization system, reaction (a), as a function of the number of explicit waters. The barriers are computed at the HF/6-31+G(d) level of theory and are inclusive of CPCM implicit solvation corrections.

Table S2: Pertinent rate parameters computed with conventional and variational transition state theory for reaction (a). Data for the hydrolysis reaction is given here. The reaction coordinate was followed *via* IRCmax calculations performed at both the HF/6-31+G(d) and DFT/B3LYP/6-31+G(d) levels of theory.

No. water	$E(s_{min})$/ kJ mol^{-1}	$E(s = 0)$/ kJ mol^{-1}	$A(s_{min})$/ s^{-1}	$A(s =0)$/ s^{-1}	$k(s_{min})$/ s^{-1}	$k(s = 0)$/ s^{-1}
			HF/6-31+G(d)			
			Hydrolysis			
0	185.0	184.9	1.09×10^{10}	1.07×10^{10}	6.60E-23	6.74E-23
2	196.2	196.1	3.07×10^{11}	3.21×10^{11}	2.04E-23	2.28E-23
4	192.5	192.5	1.82×10^{11}	1.83×10^{11}	5.33E-23	5.43E-23
6	171.9	171.9	3.36×10^{11}	3.38×10^{11}	3.97E-19	4.03E-19
			DFT/B3LYP/6-31+G(d)			
			Hydrolysis			
0	126.3	126.2	4.55×10^{9}	4.57×10^{9}	4.81×10^{-13}	4.92×10^{-13}
2	148.7	148.7	3.40×10^{11}	3.37×10^{11}	4.24×10^{-15}	4.40×10^{-15}
4	139.3	139.3	1.29×10^{11}	1.28×10^{11}	6.94×10^{-14}	7.00×10^{-14}
6	111.8	111.5	1.01×10^{12}	9.47×10^{11}	3.41×10^{-8}	3.61×10^{-8}

Supplementary Info II – Iterative fitting procedure for the derivation of acid/base kinetic parameters

The following is a script, in the Python programming language, for the derivation of the kinetic parameters for proton loss from H_2O, H_4SiO_4, and $H_6Si_2O_7$.

```
##From Henley, 1984:
##
##H4SiO4 <=> H3SiO4- + H+
##T/ K    273     298     400     500     573
##pK1     10.28   9.82    8.97    8.89    9.22
##
##Assuming equilibrium constants take on a similar non-Arrhenius form as
##rate constants do, i.e. AT^nexp(-Ea/RT), one finds:
##ln K(Ti) = lnA + nlnTi - Ea/R * 1/Ti
##
##To use the five data points provided, iterative solution for A, n and Ea may
##be possible using (ignore 273 - not interested in around 0 C:
##    n = [lnK(T3)-lnK(T2) - Ea/T(1/T2 - 1/T3)]/[ln(T3)-ln(T2)]        (1)
##    lnA = lnK(T4) - nlnT4 + Ea/R * 1/T4                              (2)
##    E = R*T5 * [lnA - lnK(T5) + ln(T4)]                              (3)
##
##Following the following steps:
##    (a) Guess Ea
##    (b) Use (1) to find n
##    (c) Use (2) to find A
##    (d) Use (3) to find Ea_2
##    (e) If |Ea - Ea_2| < tol, print A, n, and Ea;
##        Otherwise, use Ea_2 in place of Ea in step (a) and repeat.
##

##  Enter guess of Ea/ J mol-1 below:
E = 300
##  Enter tolerance, in J mol-1
tol = 1e-7
##  Enter max number of iteration cycles:
k = 5000

import math

##expt data
T1 = 273.0
pK_T1 = 10.28
T2 = 298.0
pK_T2 = 9.82
T3 = 400.0
pK_T3 = 8.97
```

```
T4 = 500.0
pK_T4 = 8.89
T5 = 573.0
pK_T5 = 9.22

R = 8.314472e-3                         # kJ K-1 mol-1

lnK_1 = math.log(pow(10, - pK_T1))
lnK_2 = math.log(pow(10, - pK_T2))  # skip this temp?
lnK_3 = math.log(pow(10, - pK_T3))
lnK_4 = math.log(pow(10, - pK_T4))
lnK_5 = math.log(pow(10, - pK_T5))


for _ in range(k):
    n = (lnK_3-lnK_2 - E/R * (1/T2 - 1/T3))/(math.log(T3)-math.log(T2))
    A = math.exp(lnK_4 - n * math.log(T4) + E/R * (1/T4))
    E_2 = R * T5 * (math.log(A) - lnK_5 + n*math.log(T5))
    deltaE = abs(E - E_2)
    print "A  = ", A
    print "n  = ", n
    print "Ea = ", E_2
    if deltaE < tol:
        print ' '
        print '****************************'
        print 'KINETIC PARAMETERS: '
        print "K(T) = AT^nexp(-Ea/RT)"
        print "A  = ", A, " L-mol-s"
        print "n  = ", n
        print "Ea = ", E_2, "kJ mol-1"
        print '****************************'
        break

    else:
        E = E_2
        print "Not converged yet"
```

Supplementary Info III – Structural parameters of pertinent stationary points used in the derivation of the kinetic model.

$H_3SiO_4^-$ (no explicit solvation)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
94.98006 -590.2988786 0.048943

Rotational constant/ cm^{-1}
0.135779933463 0.135765590207 0.133381607619
Rotational symmetry number
1.0

Non-imaginary Vibrational Frequencies/ cm^{-1}
[150.31535572 151.34400845 161.83904647 331.39298843
331.40688914 383.40945498 431.94379303 432.02024695
757.49848216 870.21936065 870.30971528 982.07839496
982.08534531 1019.96478715 1208.52100324 4139.43760282
4139.46540424 4140.25079451]

Ground State Electronic Degeneracy and Irreducible Representation
2 (E)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.013041	0.059637	-0.048506
2	8	0	-0.303129	-0.754870	1.229654
3	8	0	-0.754394	1.551879	-0.134078
4	1	0	-1.052122	1.797810	0.729769
5	8	0	-0.416722	-0.698290	-1.485070
6	1	0	-1.036207	-1.388846	-1.298736
7	8	0	1.638655	0.429075	-0.258019
8	1	0	2.159761	-0.142507	0.287045

$H_3SiO_4^-$ (Tetrahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
167.02232 -894.4970702 0.157418

Rotational constant/ cm^{-1}
0.0346142797228 0.0223271127121 0.0197116366416
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[8.96595963 16.6044012 27.58596416 33.42426345
60.89207155 62.51150457 75.07079841 112.09534642
146.95138327 148.26500061 188.22259898 202.1997655
222.92572799 236.87509309 242.15041352 313.79468627
344.08433903 351.45171671 376.9178222 389.49101674
399.54123196 413.55315026 428.72577806 446.98436406
456.77741609 461.18394199 521.79799929 558.76694445
674.4208733 789.08785155 815.34629765 866.66077822
893.78801887 913.58958397 914.44447779 971.62505908
1108.31076609 1109.68693664 1191.17291391 1872.7526542

```
  1874.01066869  1874.53889577  1892.98514139  3702.03778009
  3729.39438249  3870.53526789  4028.59332053  4064.61006688
  4068.38411035  4102.64241656  4114.77773866  4133.70355887
  4136.21263749  4137.38029735]

Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0       -0.177732   -0.233008    0.122582
      2          8           0       -1.383273   -0.898603    1.060157
      3          1           0       -1.080683   -1.139958    1.929341
      4          8           0       -0.899679    1.086974   -0.592779
      5          1           0       -0.350452    1.863526   -0.567810
      6          8           0        1.134304    0.101077    0.907626
      7          8           0        0.097136   -1.324596   -1.108151
      8          1           0       -0.669244   -1.559593   -1.611838
      9          1           0        1.606596    1.807387    0.553562
     10          8           0        1.701839    2.668657    0.120401
     11          1           0        2.389160    2.541464   -0.518809
     12          1           0       -3.296664   -0.375682    0.218511
     13          8           0       -3.711078    0.132090   -0.472342
     14          1           0       -3.023642    0.744843   -0.714979
     15          1           0        2.564030   -1.780875   -0.938455
     16          8           0        3.188145   -1.418623   -0.321685
     17          1           0        2.635187   -0.840552    0.212445
     18          8           0        0.769859   -1.170751    3.312539
     19          1           0        1.299421   -1.950198    3.216940
     20          1           0        1.019953   -0.610135    2.563067
 ---------------------------------------------------------------------
```

H_4SiO_4 (no explicit solvation)

```
Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u.  Energy a.u.  ZPE a.u.
95.98789      -590.8664147 0.060759

Rotational constant/ cm-1
0.137108519254   0.131740138706   0.12813130876
Rotational symmetry number
1.0

Vibrational Frequencies/ cm-1

[   65.78512239   271.12644894   278.73013873   306.67057106
   369.57129559   370.98916827   382.45725617   394.02264905
   405.70619799   795.99650571   915.07696022   927.51114764
   958.5166871    969.23413651   977.69967049  1016.35060188
  1071.05685632  4008.51374118  4009.66750032  4027.75232742
  4147.87533537]

Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0        0.081717    0.044517    0.145100
```

2	8	0	-0.301038	-0.786756	1.497397
3	1	0	-1.230575	-0.935487	1.637051
4	8	0	-0.578716	1.537650	0.121014
5	1	0	-1.529312	1.565302	0.156501
6	8	0	-0.168678	-0.803941	-1.237103
7	1	0	-1.073197	-1.026986	-1.430925
8	8	0	1.712798	0.253047	0.168040
9	1	0	2.145933	-0.137351	-0.577075

H_4SiO_4 (Tetrahydrate)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
168.03015	-895.033739	0.170188

Rotational constant/ cm^{-1}

0.0400166838086	0.0199965003789	0.0157949270358

Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

[20.90667175	25.74411974	30.95688696	46.29632332
80.51292739	113.36726162	138.38854431	148.91138375
158.30826546	184.39990302	185.40770468	192.16345101
197.35536716	209.40033463	223.91267859	237.88984511
265.98318528	279.94645109	310.88943734	323.97695825
362.94065567	389.77598135	401.1398139	417.43144907
445.42748425	459.69656574	548.70977888	576.1914877
642.24767398	685.40938661	694.26414054	731.58755387
811.25253779	856.50630767	943.53171891	961.03271608
989.82804223	1055.88422851	1128.37644473	1162.98226875
1206.15093174	1820.23576199	1823.23831591	1834.44229027
1851.95023779	3887.82775437	3939.865072	3953.97429529
3976.40309507	3982.13713902	4012.85771387	4025.56991554
4126.37093297	4149.52952017	4151.58682563	4159.97590569
4162.95760854]			

Ground State Electronic Degeneracy and Irreducible Representation

1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.542811	0.126488	-0.037786
2	8	0	-0.735359	-0.321910	1.497656
3	1	0	-0.004135	-0.618770	2.042465
4	8	0	0.840644	0.990792	-0.179738
5	1	0	1.245585	0.973119	-1.046714
6	8	0	-0.446519	-1.057171	-1.158983
7	1	0	-1.273262	-1.424836	-1.466431
8	8	0	-1.899243	0.981722	-0.421511
9	1	0	-2.233212	1.557077	0.253792
10	1	0	1.060500	-0.586049	-2.556210
11	8	0	1.691376	0.104607	-2.744680
12	1	0	1.542432	0.382978	-3.638087
13	1	0	-3.184026	-0.304551	-1.556186
14	8	0	-3.187551	-1.179511	-1.934435
15	1	0	-3.942964	-1.632696	-1.585207
16	1	0	2.217812	1.288200	1.182656
17	8	0	2.859418	1.230382	1.890009
18	1	0	3.710821	1.165232	1.478990

19	8	0	1.498568	-0.931985	3.115135
20	1	0	1.382250	-0.868091	4.053304
21	1	0	2.106873	-0.237857	2.859017

2 - $H_3SiO_4^-$/H_4SiO_4 H-bonded dimer (no explicit solvation)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
190.96795 -1181.290346 0.11447

Rotational constant/ cm^{-1}
0.0673862849478 0.0158462959065 0.0157508965753
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[22.07433161 47.85320313 69.96228652 89.08966706
98.27803809 115.91109203 121.77719275 137.87421794
157.80783981 162.08925929 304.89127985 322.11426276
328.68929982 350.35356041 381.74831982 398.6585367
412.58705073 419.87102414 431.44336738 459.85642393
623.3496552 748.84528857 778.66926745 801.86955679
829.43466988 869.72588535 887.89411672 931.0002265
951.70533792 958.61399208 963.16647546 973.64066241
995.78449758 1041.28848028 1127.15318202 1151.54198228
1181.76908184 1303.29606176 3846.13951728 3878.83399332
3983.94423166 4140.45930519 4147.0273919 4147.75022895
4150.75973323]
Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Cartesian Coordinates
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.003179	-0.082905	0.013426
2	14	0	2.052899	0.023282	-0.008382
3	8	0	1.589652	-0.605382	1.431473
4	1	0	0.691070	-0.937935	1.340825
5	8	0	1.521589	1.545333	-0.246758
6	1	0	0.572719	1.647176	-0.300639
7	8	0	1.595146	-1.004984	-1.196957
8	1	0	0.691674	-1.286760	-1.023986
9	8	0	3.692705	0.154076	-0.013817
10	1	0	4.144699	-0.652904	0.183723
11	8	0	-3.076848	-0.407534	-1.216399
12	1	0	-2.792792	-1.133530	-1.752480
13	8	0	-0.825688	-1.086058	0.162394
14	8	0	-1.421397	1.463270	-0.296920
15	1	0	-2.080973	2.134727	-0.392358
16	8	0	-2.996892	0.085757	1.341762
17	1	0	-2.548612	-0.091876	2.156075

2 - $H_3SiO_4^-$/H_4SiO_4 H-bonded dimer (Octahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
335.05247 -1789.584477 0.335384

Rotational constant/ cm^{-1}
0.00994821557519 0.00534036116412 0.00450978656708

Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}

[15.91631593	18.43234491	26.80752425	29.81007817
36.52412236	39.29036417	41.71603852	49.93135967
50.52909031	60.18313521	60.92682333	69.53136443
95.35193809	99.3275419	108.73137397	116.63392908
139.56315452	141.87067281	148.54301486	158.91294646
164.11181298	167.0657144	173.38358828	174.53039707
177.3244403	180.19493746	188.55621609	195.86104056
203.48558142	212.66700209	218.08828001	230.5433185
236.95849737	250.43523823	259.3942475	299.33099481
319.51482951	329.1063212	340.03228131	351.61852526
367.23597587	390.18605237	399.25626735	411.03017092
420.93442865	429.38606191	436.45457427	445.23287428
450.73060611	457.23613961	477.5798325	492.41189285
497.63856079	502.15629238	510.03104607	544.93573541
582.16879412	649.95561912	657.99718136	669.31931177
678.70924314	713.52357785	728.16797857	735.27819307
769.46699571	804.12147223	812.21863732	843.84970884
856.66616586	864.22120316	872.69368749	910.4827747
921.70760013	952.28916785	966.39144078	978.40165647
984.05229615	1003.15187526	1006.07797526	1099.45601216
1114.93445565	1152.21616684	1187.78114004	1217.15334576
1225.25051085	1349.5089808	1857.62867889	1859.41492046
1861.82669409	1869.59024208	1876.10272594	1883.21294043
1886.88967891	1907.62954212	3549.02568613	3701.8779219
3766.48843407	3866.66391943	3885.86080354	3899.30279262
3917.14435725	3922.46833017	3932.73400643	3970.50919293
3980.30224495	3984.79912548	4017.06267943	4025.97303621
4045.53828919	4089.64525028	4090.24298092	4128.92171374
4139.84767384	4142.24554676	4144.40015722	4145.4844128
4147.50696648]			

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.982070	0.115574	0.544762
2	14	0	2.186651	-1.013558	-0.180381
3	8	0	1.612587	0.504869	-0.038321
4	1	0	0.769793	0.573301	0.446802
5	8	0	1.018399	-1.999797	-0.782769
6	1	0	0.105310	-1.703244	-0.776630
7	8	0	2.713917	-1.629045	1.245634
8	1	0	2.110558	-1.552800	1.986962
9	8	0	3.461119	-0.977996	-1.187933
10	1	0	4.056389	-1.719625	-1.116779
11	8	0	-3.236210	-0.567979	1.404128
12	1	0	-3.618412	-0.012235	2.068412
13	8	0	-0.688578	0.487586	1.354111
14	8	0	-1.648966	-1.042148	-0.593449
15	1	0	-2.409974	-1.462794	-0.986781
16	8	0	-2.685775	1.420456	-0.197663
17	1	0	-2.142905	2.204529	-0.308429
18	8	0	-4.965227	0.960723	-1.806028
19	1	0	-4.243122	1.233499	-1.233597
20	1	0	-4.690159	1.181752	-2.685085
21	8	0	4.490235	-3.556565	-0.162968
22	1	0	3.776096	-4.114374	-0.464325

23	1	0	4.165498	-3.154265	0.636770
24	8	0	0.074948	2.991942	2.240335
25	1	0	-0.250582	2.109367	2.017261
26	1	0	1.015836	2.946295	2.134023
27	8	0	1.473428	2.796314	-1.722497
28	1	0	1.645015	2.024307	-1.179766
29	1	0	1.509916	2.492270	-2.618842
30	8	0	-4.458635	-1.832700	-1.016126
31	1	0	-4.796543	-1.011364	-1.367277
32	1	0	-4.409841	-1.696393	-0.075049
33	8	0	-0.996526	3.721053	-0.401249
34	1	0	-0.233068	3.514613	-0.936966
35	1	0	-0.677089	3.725385	0.499047
36	8	0	1.871078	-4.724553	-0.910754
37	1	0	1.484396	-3.851460	-0.997857
38	1	0	1.419664	-5.126293	-0.180989
39	8	0	0.676756	-1.044736	3.177132
40	1	0	0.909135	-0.440780	3.868673
41	1	0	0.092137	-0.549881	2.583144

TS3 - $H_3SiO_4^-$-H_4SiO_4 Si-O bond formation TS (no explicit solvation)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
190.96795	-1181.282711	0.115723

Rotational constant/ cm^{-1}

0.0644028876804	0.017530127459	0.0173169800022

Rotational symmetry number

1.0

Imaginary Frequency/ cm^{-1}

-136.9256

Non-imaginary Vibrational Frequencies/ cm^{-1}

[24.94482876	48.17986988	85.78824782	130.57634382	
179.88912178	182.29394506	200.13550968	211.25607976	
280.90560026	313.106601	328.87695944	342.36760102	
360.00760532	370.46789155	403.67669395	418.27939254	
439.59613532	450.80706003	463.99883629	634.15050889	
686.20172723	738.63521516	770.64855628	797.10161236	
827.71793187	893.6073096	907.51497256	932.80036878	
986.91584294	990.36321967	1012.17343774	1016.89272967	
1065.01004634	1091.94962736	1104.80778652	1163.95531864	
1243.55079899	4027.9469374	4035.44637184	4044.62779252	
4131.46554414	4149.82838549	4151.91349238	4155.92384796]	

Ground State Electronic Degeneracy and Irreducible Representation

1) (A)

Cartesian Coordinates

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.000000	0.000000	0.000000
2	14	0	0.000000	0.000000	3.694351
3	8	0	1.637504	0.000000	3.658692
4	1	0	1.889252	-0.210699	2.763979
5	8	0	-0.742804	-1.449092	3.492160
6	1	0	-0.565081	-1.737197	2.600582
7	8	0	-0.737170	1.342397	3.047917
8	1	0	-1.154261	1.845408	3.734093
9	8	0	-0.348392	0.313397	5.306446

10	1	0	-0.304327	-0.447869	5.865365
11	8	0	-0.911506	1.381047	0.136665
12	1	0	-0.960338	1.636272	1.053753
13	8	0	0.483994	-0.519798	1.401850
14	8	0	-0.980140	-1.014907	-0.883651
15	1	0	-1.871787	-0.701987	-0.922250
16	8	0	1.288917	0.278317	-1.016412
17	1	0	2.106837	0.273778	-0.541615

TS3 - $H_3SiO_4^-$-H_4SiO_4 Si-O bond formation TS (Octahydrate)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
335.05247	-1789.553895	0.334457

Rotational constant/ cm^{-1}

0.00951458225143	0.00653985765045	0.00539806775259

Rotational symmetry number

1.0

Imaginary Frequency/ cm^{-1}

-157.8598

Non-imaginary Vibrational Frequencies/ cm^{-1}

[15.64525203	22.18553731	29.15674468	32.11064611
36.13490241	40.86809505	45.51788341	49.68809719
53.3926371	58.65405682	60.8364687	74.86228772
83.54328274	96.97137111	101.23193952	111.47676471
119.83804334	126.81620107	128.71364834	133.30783385
143.20514122	148.584717	160.33081915	168.56004101
181.99507974	187.47891086	198.54387809	206.88430565
229.54941755	234.12275199	238.75863965	270.51481759
279.96730216	284.13751594	293.07567414	301.26319386
309.79128104	320.6129858	329.27312975	346.92703476
359.79909463	364.7338476	376.3756944	387.98973978
416.1386828	425.36180561	438.09485836	441.47968187
450.16762725	451.68280492	462.81727572	476.73883939
497.0477805	500.09203656	524.65459573	552.08070169
613.26468821	625.40001031	637.89675094	666.33760892
675.92215026	687.45974172	723.38613344	737.19649141
761.55053989	765.53309405	776.13933776	791.55522804
808.97977128	823.01254065	847.97127013	884.91936423
896.40135284	917.48873385	963.39583722	968.55995195
993.9843553	1048.28053872	1087.39714398	1102.65317606
1107.58097868	1145.15460484	1173.03248397	1196.21192223
1229.54583105	1840.17633422	1844.65236367	1857.34371428
1865.77449647	1871.98116465	1882.24684091	1885.90967868
1890.28840315	3834.28915979	3884.7209451	3889.53754202
3966.26947558	3968.82025634	3980.11458533	3996.50352549
4000.3192711	4007.96466303	4019.54395663	4031.65842766
4040.48538016	4055.82481652	4061.19744194	4071.69943031
4083.53588709	4112.8316389	4117.89149829	4133.54370068
4141.36285151	4142.55136244	4143.25334843	4151.32966245]

Ground State Electronic Degeneracy and Irreducible Representation

1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.219704	0.539129	0.254031
2	14	0	1.438885	-0.327347	0.255494
3	8	0	0.648427	-1.788635	0.205575

4	1	0	-0.241328	-1.638035	0.511309
5	8	0	1.630730	0.431465	1.698561
6	1	0	0.796150	0.810496	1.953007
7	8	0	1.255901	0.667247	-1.037485
8	1	0	2.059023	0.788630	-1.540462
9	8	0	3.008024	-0.895484	0.003341
10	1	0	3.146318	-1.815972	0.202272
11	8	0	-2.902844	1.921836	0.793394
12	1	0	-2.362486	2.707020	0.812497
13	8	0	-0.771468	0.237551	0.829951
14	8	0	-3.262099	-0.695464	0.696492
15	1	0	-3.187827	-0.959514	1.606677
16	8	0	-2.305495	0.572598	-1.394902
17	1	0	-1.866095	-0.140262	-1.853989
18	1	0	-4.314557	-2.436135	-1.796099
19	8	0	-3.684385	-2.772068	-1.173061
20	1	0	-3.623270	-2.101825	-0.487490
21	1	0	1.740331	-3.405880	0.332733
22	8	0	2.581577	-3.859477	0.310004
23	1	0	2.628549	-4.284232	-0.535506
24	1	0	-0.214613	3.868276	1.012174
25	8	0	-0.966993	4.142139	0.505478
26	1	0	-0.791144	3.847756	-0.391299
27	1	0	0.127059	2.154381	-1.691954
28	8	0	-0.521081	2.801939	-1.962666
29	1	0	-1.317945	2.283728	-2.043228
30	1	0	4.067115	0.073289	-1.595627
31	8	0	4.070163	0.944146	-1.979451
32	1	0	4.366934	1.501332	-1.266389
33	1	0	3.880877	1.762369	1.541346
34	8	0	4.565374	1.362611	1.019342
35	1	0	4.238579	0.477826	0.874886
36	8	0	-1.450546	-1.080145	3.235161
37	1	0	-1.111241	-0.564207	2.497539
38	1	0	-0.718935	-1.577777	3.572888
39	8	0	-1.153246	-1.964324	-2.379894
40	1	0	-0.426196	-2.051942	-1.774128
41	1	0	-1.889227	-2.445439	-2.006033

---

3 – $H_7Si_2O_8^-$ (no explicit solvation)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
190.96795	-1181.300898	0.118957

Rotational constant/ cm^{-1}

0.0626993758462	0.0212333560439	0.0209858514853

Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

[44.40582641	120.88059678	127.61549204	153.51946997
199.96175078	211.62444865	235.46417076	300.38744897
318.37497107	338.62830933	370.88491293	377.0290279
419.16903815	437.58748235	439.74904316	482.06281232
487.1713242	540.61261379	593.88709484	602.609792
612.16653191	629.79958585	656.10668445	681.85775454
722.01691325	840.22857321	864.83283452	883.10532123
924.77270726	954.22831726	1028.49287433	1035.70734417
1074.69884302	1084.03317153	1103.20920457	1141.20680246
1179.82993243	1214.99178495	4001.59813666	4012.53104712
4150.95434321	4152.31661304	4153.39391827	4154.49207457
4158.04370664]			

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.515386	-0.109339	0.511446
2	14	0	1.385448	-0.662389	-0.304102
3	8	0	1.034935	0.753688	-1.174689
4	1	0	1.847975	1.156734	-1.442367
5	8	0	1.574616	-2.160394	-1.055044
6	1	0	0.738983	-2.602020	-1.094006
7	8	0	1.525543	-0.467960	1.375680
8	1	0	2.430078	-0.293526	1.591267
9	8	0	3.120302	-0.371854	-0.503828
10	1	0	3.534375	-1.109077	-0.926405
11	8	0	-3.001599	-0.821733	0.422754
12	1	0	-3.499300	-0.542048	-0.331297
13	8	0	-0.335026	-0.977916	-0.125898
14	8	0	-1.679105	1.294652	-0.340018
15	1	0	-0.870464	1.470264	-0.817051
16	8	0	-1.221967	0.134268	2.105466
17	1	0	-0.298849	-0.030831	2.284365

3 – $H_7Si_2O_8^-$ (Octahydrate)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
335.05247	-1789.572058	0.335061

Rotational constant/ cm^{-1}

0.00850655155574	0.00727670073675	0.00545343939239

Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}

[10.76610191	17.2090822	28.32270193	30.86653233
36.72568269	40.70823685	47.49873496	48.83320337
56.64540385	64.08923545	70.80327964	73.00654258
90.37548298	94.83066137	111.26130366	117.27336186
125.15506591	127.26102387	132.00811722	139.2642892
157.02244955	159.99025169	163.25691915	167.76770039
178.77706477	185.27564791	193.73423153	213.91806623
222.24459308	228.73622586	235.74218501	258.92162328
268.45751212	282.42772829	286.85510525	298.85142022
309.65922427	320.73809222	332.71355612	361.7590951
368.89711102	373.99172219	394.33541509	403.89910536
417.55655549	418.52265501	426.03599017	428.100246
447.7419529	455.95032369	474.40351967	478.47642846
487.96366481	496.70721304	501.09983822	532.04977483
544.49786297	563.04141358	578.90212666	614.39759628
645.13207185	654.10498183	671.79363862	680.39817972
688.44669231	698.29534719	711.85549233	749.67933132
767.27068312	793.73763991	803.96856439	829.78913805
857.76432216	879.22702242	886.36503834	904.59582291
966.09257546	1002.51939284	1044.31188527	1090.01047795
1110.38197227	1134.44410578	1154.94070651	1161.47404144
1192.22241771	1221.84483627	1838.16073089	1845.75747033
1856.08569979	1857.01704753	1863.2723682	1876.81166228
1889.08599151	1898.04500078	3841.32987072	3923.71244395

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  3945.61996701  3957.518977    3960.87599909  3977.68891098
  3979.39869863  4018.77246708  4021.37190034  4033.15970462
  4044.54438824  4055.79701509  4078.24666595  4097.07518116
  4114.76383795  4123.84100328  4127.41348642  4134.65575768
  4137.44980092  4140.35504985  4141.91192966  4145.94313632
  4151.9899463 ]

Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0       -1.354043   -1.019057   -0.524329
      2         14           0        0.948281    0.988588    0.138459
      3          8           0        0.722936    2.407163   -0.901991
      4          1           0        0.177993    2.209144   -1.649738
      5          8           0        2.327566    0.536282   -0.753804
      6          1           0        2.501555    1.198219   -1.409497
      7          8           0        1.197030   -0.393863    1.209660
      8          1           0        1.379920   -0.088628    2.087384
      9          8           0        1.055696    1.989159    1.480078
     10          1           0        0.951420    2.914821    1.295364
     11          8           0       -0.931875   -1.862655   -1.864004
     12          1           0       -0.002519   -2.094062   -1.957289
     13          8           0       -0.516867    0.363486   -0.425453
     14          8           0       -2.950338   -0.687214   -0.707955
     15          1           0       -3.311005   -0.844152   -1.577084
     16          8           0       -1.180658   -1.862111    0.858029
     17          1           0       -0.392799   -1.582926    1.322973
     18          1           0       -3.207187   -2.496401    1.772857
     19          8           0       -4.130977   -2.368933    1.588391
     20          1           0       -4.119570   -1.783890    0.839753
     21          1           0        0.059923    4.078975   -0.203953
     22          8           0       -0.257036    4.711087    0.439481
     23          1           0       -1.119305    4.398915    0.687697
     24          1           0        2.108451   -1.251405   -1.689463
     25          8           0        1.867447   -2.147368   -1.915018
     26          1           0        2.218345   -2.658875   -1.187869
     27          1           0        3.784241   -2.205335    0.704363
     28          8           0        2.951796   -2.666702    0.731105
     29          1           0        2.319884   -1.987982    0.968541
     30          8           0       -2.569785    2.355835    0.586945
     31          1           0       -3.354137    1.825446    0.521049
     32          1           0       -1.892968    1.828143    0.171092
     33          8           0        4.762710   -0.290139    0.518629
     34          1           0        4.828393    0.199853    1.326730
     35          1           0        3.963667    0.021181    0.090245
     36          8           0       -3.203746   -1.521318   -3.520890
     37          1           0       -2.366778   -1.873373   -3.219442
     38          1           0       -2.995058   -0.881786   -4.187732
     39          8           0       -1.289257    2.208050    3.401090
     40          1           0       -0.435402    2.079345    3.001381
     41          1           0       -1.881739    2.289782    2.661630
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TS4 – H_2O-loss TS from $H_7Si_2O_8^-$ (No explicit solvation)

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Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u.  Energy a.u.  ZPE a.u.
190.96795 -1181.232324 0.111649
```

Rotational constant/ cm^{-1}
0.0619114974533 0.019811038742 0.0194281071607
Rotational symmetry number
1.0

Imaginary Frequency/ cm^{-1}
-1690.1961
Non-imaginary Vibrational Frequencies/ cm^{-1}
[24.59036059 48.11036631 130.60414525 147.43790821
  176.29578757 182.93337784 219.01962775 249.0729684
  265.94148314 298.98347699 314.39241691 339.22603998
  348.18504925 362.19001719 378.13413455 413.73385952
  425.18804671 478.55983274 506.9242368 625.12894641
  648.60725 716.46357856 728.75875886 814.58175846
  841.61169412 858.0909889 923.89696236 942.73242794
  948.76533721 999.23187431 1025.38606507 1027.40861875
  1048.9199715 1073.65628958 1133.23474379 1285.0305254
  1599.74960906 1992.09027188 3743.54530792 4132.02157265
  4143.15604344 4146.05434202 4147.05519332 4153.72058502]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.770135	-0.017800	-0.036446
2	14	0	1.284380	0.200716	0.077967
3	8	0	1.118410	-1.048134	-0.934891
4	1	0	2.309509	-1.167461	-0.825447
5	8	0	1.611282	-0.111941	1.684330
6	1	0	0.860086	0.083871	2.225515
7	8	0	1.866240	1.660268	-0.449542
8	1	0	1.174196	2.304446	-0.460210
9	8	0	3.255426	-0.636948	-0.304685
10	1	0	3.536465	-1.098215	0.473553
11	8	0	-2.480856	-0.674105	1.299056
12	1	0	-2.472785	-1.620346	1.298715
13	8	0	-0.362546	0.691331	0.280099
14	8	0	-1.584170	-1.206906	-1.135224
15	1	0	-0.643566	-1.369128	-1.297442
16	8	0	-2.841402	1.131671	-0.532088
17	1	0	-2.456818	1.819521	-1.055384

TS4 – H_2O-loss TS from $H_7Si_2O_8^-$ (Octahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
335.05247 -1789.556807 0.334604

Rotational constant/ cm^{-1}
0.00799252928504 0.00749285027044 0.00494141850627
Rotational symmetry number
1.0

Imaginary Frequency/ cm^{-1}
-194.4714
Non-imaginary Vibrational Frequencies/ cm^{-1}
[18.49489812 24.52780739 27.82227627 34.71007937
  42.90454945 46.41447938 50.9600124 57.54199981
  61.13533402 73.24980505 78.8726433 94.55959747
  98.77151339 104.33874879 115.22995711 122.3888241

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   128.24102411   142.10698493   146.74287258   151.5594695
   156.22315857   161.53323079   170.01961583   175.69805693
   183.17664031   196.68813296   205.74444722   225.76842372
   240.94105153   249.06601804   262.40375178   275.9360955
   282.2192176    282.72659361   304.93993234   323.98390861
   341.93667893   348.0182407    356.03895187   363.36462741
   363.47583311   375.06902742   384.02108634   402.98860868
   408.54194336   413.46974598   426.57116761   432.08280016
   448.37443533   471.43571753   477.46167644   517.68338836
   528.27573136   545.88793423   547.75062971   563.03446322
   564.41758412   604.78525352   615.72511434   635.42242409
   646.2371785    672.56512817   705.78783128   762.19692302
   769.60600284   789.4770715    792.71593754   816.84062426
   821.89353329   862.18474877   881.19397325   900.46731127
   911.59483171   950.54462842   982.36335956   992.72634081
  1013.68861541  1066.43486938  1091.40749957  1136.37630483
  1150.93035093  1153.46028062  1165.42879417  1189.43532484
  1227.84299375  1845.40995251  1860.40187105  1864.56513448
  1867.74839766  1877.99322285  1887.94613307  1888.25194875
  1909.78415257  3435.60282165  3774.02957066  3904.24449595
  3910.00634133  3928.09116842  3934.00592163  3935.31953897
  3941.95017889  3965.60919173  3984.61841622  4005.02466232
  4051.07772317  4057.79176735  4064.67957045  4084.79390158
  4089.08922177  4095.26808853  4108.425113    4126.04426623
  4133.69660851  4137.15788595  4147.33320758  4151.31576174]

Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0        0.249831    2.015340    0.206527
      2         14           0        0.405913   -1.008368   -0.459193
      3          8           0       -1.240278   -1.893488    1.171739
      4          1           0       -1.211300   -1.643319    2.086256
      5          8           0        1.278324   -1.901702    0.624176
      6          1           0        0.609840   -2.302635    1.184366
      7          8           0        1.627979   -0.519428   -1.526496
      8          1           0        1.562278   -0.952952   -2.366932
      9          8           0       -0.558360   -1.799383   -1.493293
     10          1           0       -1.206773   -2.428531   -1.174570
     11          8           0        0.910763    2.331567    1.655178
     12          1           0        1.649192    1.777753    1.910716
     13          8           0       -0.095739    0.429913    0.096445
     14          8           0       -1.100035    2.912947    0.056297
     15          1           0       -1.708242    2.883323    0.794316
     16          8           0        1.214200    2.407033   -1.059470
     17          1           0        1.561386    1.647075   -1.515777
     18          1           0        0.348650    4.095643   -2.264041
     19          8           0       -0.431668    4.625077   -2.384487
     20          1           0       -0.991913    4.339283   -1.671299
     21          1           0       -2.111924   -3.269182    0.377757
     22          8           0       -2.433228   -3.727566   -0.408608
     23          1           0       -3.324928   -3.419238   -0.537441
     24          1           0        2.416184   -0.496843    1.845477
     25          8           0        2.924764    0.292902    1.999929
     26          1           0        3.609035    0.261010    1.333762
     27          1           0        4.518747   -1.381408   -0.282349
     28          8           0        4.403229   -0.447833   -0.435071
     29          1           0        3.577560   -0.385883   -0.908440
     30          8           0       -3.150682   -0.153267    0.438775
     31          1           0       -2.716175    0.359124   -0.232785
```

32	1	0	-2.467843	-0.801958	0.715995
33	8	0	3.727621	-3.285918	0.091868
34	1	0	3.561568	-3.983211	-0.527093
35	1	0	2.874139	-2.904504	0.301486
36	8	0	-2.780267	2.085054	2.234465
37	1	0	-2.142256	1.833975	2.889646
38	1	0	-3.035594	1.279201	1.782525
39	8	0	-4.935975	-2.046502	-0.800176
40	1	0	-4.919562	-1.802737	-1.715380
41	1	0	-4.456343	-1.356218	-0.338835

5 –$H_5Si_2O_7^-$ (No explicit waters)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
172.95738 -1105.251025 0.088143

Rotational constant/ cm^{-1}
0.0707863037702 0.0258989170435 0.0250519978058
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[26.60596392 44.16951429 149.5230151 178.040327 190.446713
222.91182728 234.11580164 262.61921283 268.47836319
319.48007773 361.30732194 371.07257255 376.6467583
397.23371366 422.46350704 465.38195719 513.37416745
701.74272392 812.87892117 872.65893571 889.22858513
902.72617707 940.73767568 961.36633318 977.69967049
999.60024319 1018.77627622 1044.66635345 1084.93671785
1184.82723861 1301.23180594 3636.05109737 4130.69405459
4139.75731921 4140.54965983 4146.16554772]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.448567	0.023892	-0.060603
2	14	0	-1.507298	-0.063587	-0.066952
3	8	0	-1.422887	-0.834717	1.279669
4	8	0	-2.452633	-0.795642	-1.228013
5	1	0	-2.635859	-1.692246	-0.986845
6	8	0	-2.073592	1.504125	0.048416
7	1	0	-2.587985	1.618867	0.834481
8	8	0	2.581548	-0.710105	-1.001092
9	1	0	2.664231	-1.637103	-0.830314
10	8	0	-0.001964	0.140213	-0.762239
11	8	0	1.327761	-0.849187	1.307749
12	1	0	0.397008	-0.981510	1.558803
13	8	0	2.020799	1.550372	0.163641
14	1	0	1.345887	2.211385	0.093914

5 –$H_5Si_2O_7^-$ (Nonahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
335.05247 -1789.591912 0.336998

Rotational constant/ cm^{-1}
0.009183686669 0.00698783423031 0.00582002633302
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}

[24.36794919	30.33830525	33.6397245	41.80639315
42.97405301	48.59689126	52.25972903	58.4663972
60.19008557	79.89434568	85.62838963	91.04966754
104.38045093	110.44811198	119.08740486	125.19676805
135.55974929	141.54400607	148.01478778	150.61422104
164.1396144	171.05521892	174.14117712	178.17238377
181.72401584	182.93337784	191.85068497	202.76274437
211.2352287	214.87026504	221.63991208	225.17069308
247.06431543	254.29963634	261.56970903	279.36262116
292.17907818	305.30135087	348.03214141	353.68973144
362.21086826	382.7700222	389.57442102	397.37272079
404.4481835	430.83173602	441.37542653	458.16748735
476.55117977	487.28948025	496.06778026	501.22494464
518.71899145	520.64424014	545.61687033	550.04424729
557.0571568	594.22071194	607.42638891	611.13787918
676.81179587	680.88470466	692.17903365	717.49918165
736.25819331	756.25436838	817.80672378	838.0044592
848.65240505	858.27864852	867.89099129	880.90900864
902.69142529	914.9518538	940.83498067	954.74264362
978.4920111	986.429318	1002.79740709	1079.61969528
1113.94750505	1139.62212123	1182.84638706	1210.88412438
1248.61065838	1850.81037936	1858.8032891	1864.32187201
1869.93080954	1878.25733639	1883.21294043	1888.40485659
1895.51507108	1920.52245305	3719.76118866	3750.93353667
3809.96986309	3851.06036954	3879.00775222	3936.86946843
3949.09514516	3950.42266322	3975.20763379	3980.65671313
3983.31174923	4025.87573122	4036.23871246	4049.33318373
4056.00552578	4078.44822628	4089.07532106	4095.74071275
4118.69773962	4137.31079379	4142.8919299	4145.56781708
4147.70157646]			

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.626345	-0.728237	-0.844878
2	14	0	0.656149	0.479176	0.823532
3	8	0	2.465297	1.942622	-2.147341
4	1	0	2.753760	1.332842	-2.812540
5	8	0	2.044995	0.391003	0.115828
6	1	0	2.389174	1.423204	-1.334752
7	8	0	0.366041	-0.739507	1.920820
8	1	0	-0.214462	-0.476546	2.634591
9	8	0	0.395588	1.889985	1.664078
10	1	0	1.023064	2.574571	1.479341
11	8	0	-0.957127	-1.454980	-2.149301
12	1	0	-0.041836	-1.733604	-2.033912
13	8	0	-0.607726	0.383286	-0.245974
14	8	0	-3.043576	-0.067797	-1.275073
15	1	0	-3.051152	0.516872	-2.038079
16	8	0	-1.984819	-1.801761	0.347110
17	1	0	-1.293837	-1.890171	0.996169
18	1	0	-3.565743	-0.880042	1.417969
19	8	0	-3.978405	-0.070014	1.704615
20	1	0	-4.095820	0.412012	0.893587

21	1	0	0.571561	2.601117	-2.367287
22	8	0	-0.360966	2.726451	-2.195803
23	1	0	-0.537539	2.162348	-1.449848
24	1	0	1.948352	-1.139395	-1.026579
25	8	0	1.704727	-1.979441	-1.425822
26	1	0	1.878834	-2.616244	-0.736695
27	1	0	3.112701	-2.468957	1.354365
28	8	0	2.309735	-2.985347	1.328107
29	1	0	1.646161	-2.403451	1.687568
30	8	0	-1.674361	0.699952	3.413492
31	1	0	-2.492035	0.569817	2.935958
32	1	0	-1.254655	1.462952	3.029293
33	8	0	4.272648	-0.798243	1.215108
34	1	0	4.475645	-0.325194	2.009645
35	1	0	3.546298	-0.313854	0.796569
36	8	0	-2.659741	1.575947	-3.549171
37	1	0	-2.356827	0.918160	-4.170656
38	1	0	-1.891718	2.089358	-3.299766
39	8	0	-1.822877	-0.931563	-4.827538
40	1	0	-1.448817	-1.180382	-3.980980
41	1	0	-2.576210	-1.492921	-4.949163

$2H_4SiO_4$ Hydrogen-bonded Dimer (No explicit waters)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
191.97577	-1181.831466	0.126335

Rotational constant/ cm^{-1}

0.0683863101052	0.0132625084251	0.0131017305312

Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

[23.4435518	40.79164113	43.66908864	92.09917134
110.87208371	142.85762341	204.04160992	213.29253416
235.10275223	236.40941922	300.02603044	300.81837106
317.97185041	319.27156704	374.20718324	380.66406424
385.57796615	385.81427826	397.00435191	409.04236902
437.20521275	440.90975266	640.87150343	731.47634817
813.00402758	813.17083613	890.00702504	894.97652979
908.10575285	908.14745498	963.09002154	974.39130089
982.69697667	985.92194199	1003.0337192	1006.3907413
1063.49486866	1091.1155846	1091.59515919	1122.03076943
3974.79756276	3993.28551052	4123.97306005	4124.34837929
4138.67306363	4138.95107788	4142.85717812	4143.37845484]

Ground State Electronic Degeneracy and Irreducible Representation

1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.364228	1.207015	-1.412520
2	8	0	1.401274	1.161699	0.233742
3	1	0	2.258361	1.122012	0.637730
4	8	0	2.660262	0.335098	-1.877855
5	1	0	3.039407	0.510071	-2.727633
6	8	0	-0.086011	0.669287	-1.875197
7	1	0	-0.507034	-0.047472	-1.404403
8	8	0	-0.860606	0.289395	1.774056

9	8	0	1.548804	2.698496	-2.042510
10	1	0	-0.090920	0.653042	1.340486
11	14	0	-1.373141	-1.197988	1.411568
12	8	0	-0.578552	-2.443337	2.100201
13	1	0	-0.848532	-2.728845	2.961645
14	8	0	-1.156123	-1.410009	-0.207553
15	1	0	-1.089912	-2.305419	-0.512897
16	8	0	-2.925565	-1.304158	1.895488
17	1	0	-3.432713	-0.505426	1.937630
18	1	0	0.768260	3.203880	-2.222196

$2H_4SiO_4$ Hydrogen-bonded Dimer (Dihydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
227.9969 -1333.893707 0.180038

Rotational constant/ cm^{-1}
0.0243091505658 0.0138265653101 0.0101593616475
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[24.08993494 38.74823638 58.19533331 63.32469626
73.05519508 87.17831908 98.9452723 111.21265117
132.41123789 146.79152507 158.1275562 166.04401203
170.978765 176.55990111 188.9037339 206.95380921
219.80501801 249.2953798 280.94035204 302.54205942
321.39142571 333.63795351 346.4266091 355.44122123
389.01839252 395.53087637 403.82265144 414.39414337
424.16634433 438.48407831 548.24410501 577.25489221
621.59816541 675.05335572 783.20089976 810.41154468
814.94317699 828.05154897 878.14276683 888.12347848
893.25284143 942.32235691 976.10108854 977.85952868
989.47357406 1018.99173727 1034.33117363 1056.33600167
1077.01331167 1112.25856847 1127.27828844 1235.26597428
1813.20200141 1827.48498361 3913.88464014 3958.29046655
3977.31359174 3990.28990696 3998.36622098 4027.02254001
4121.23461967 4141.36980187 4146.24895199 4149.68937836
4157.63363561 4163.52753776]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.336450	-1.887146	-1.079319
2	8	0	0.451343	-1.833519	0.548585
3	1	0	1.306095	-1.929199	0.966518
4	8	0	-1.280939	-2.000859	-1.372123
5	1	0	-1.767848	-2.628027	-0.853683
6	8	0	0.888013	-0.577521	-1.849719
7	1	0	0.560392	0.275276	-1.568343
8	8	0	0.404940	0.778822	1.794068
9	8	0	1.168640	-3.172634	-1.629240
10	1	0	0.184118	-0.092400	1.468503
11	14	0	-0.319194	2.022747	1.012667
12	8	0	-1.796491	2.397471	1.577430

13	1	0	-1.873447	3.005297	2.298683
14	8	0	-0.489210	1.576401	-0.546234
15	1	0	-1.359502	1.490433	-0.939273
16	8	0	0.633599	3.327047	1.222400
17	1	0	1.573586	3.217929	1.212450
18	1	0	1.629676	-3.087386	-2.451993
19	1	0	-2.900541	0.675765	-2.828940
20	8	0	-2.681030	0.506434	-1.922905
21	1	0	-2.335874	-0.383177	-1.878697
22	1	0	2.194693	-0.274063	2.353629
23	8	0	2.648639	-1.096628	2.193337
24	1	0	2.967029	-1.408974	3.029493

$2H_4SiO_4$ Hydrogen-bonded Dimer (Tetrahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
264.01803 -1485.956124 0.235128

Rotational constant/ cm^{-1}
0.0236983947074 0.0076132669088 0.00681037813166
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[16.14567769 20.92752282 25.54950976 46.8245504
  50.32752997 58.84171644 83.75874378 91.64044783
  97.7359103 100.58555639 116.56442552 139.09053029
  150.3501075 154.77748446 162.10316001 176.01082296
  181.2861434 184.74047048 189.25125172 193.24075623
  198.85664412 229.88998501 268.58956889 286.36858031
  287.77950264 293.51354659 310.78518199 316.44972238
  336.25128748 351.38221315 370.25938086 383.5971146
  397.85229537 410.64790132 412.80251178 419.70421558
  426.47386262 441.38237689 521.57558789 544.67857223
  588.07659697 617.86582408 623.96128655 665.94143861
  670.57037591 680.15491725 760.2925254 808.15267888
  814.28289314 831.90899672 937.79767496 947.52122343
  955.45853032 961.38718425 982.49541633 1007.12747906
  1038.73074916 1056.01628528 1077.05501381 1091.14338603
  1120.1263718 1141.19290175 1158.40198395 1167.94482315
  1798.76611138 1817.31661234 1819.68668384 1827.73519644
  3900.25499144 3968.66039815 3970.25202974 3985.02153688
  3988.06579294 4002.00820768 4026.97388751 4028.53076733
  4035.84254215 4048.14467281 4075.59858019 4126.96171326
  4153.22710972 4156.34086934 4162.90895605 4164.7299494]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.096092	0.061263	0.706468
2	8	0	-1.477324	1.018523	-0.464271
3	1	0	-1.088408	1.855713	-0.226554
4	8	0	-2.586022	-1.304541	-0.045748
5	1	0	-3.436600	-1.242062	-0.478124
6	8	0	-1.039575	-0.268612	1.885073
7	1	0	-0.185592	-0.610996	1.623126

8	8	0	1.176202	0.589129	-1.697157
9	8	0	-3.376981	0.815176	1.410239
10	1	0	0.238511	0.434034	-1.629449
11	14	0	2.098243	-0.127243	-0.545809
12	8	0	3.379043	-0.832882	-1.225199
13	1	0	4.224422	-0.733238	-0.794193
14	8	0	1.166517	-1.161434	0.313342
15	1	0	0.821260	-1.956158	-0.097828
16	8	0	2.632539	1.017677	0.506478
17	1	0	2.080307	1.782058	0.630658
18	1	0	-3.409075	0.798179	2.357603
19	1	0	-0.587231	-4.054665	-0.469642
20	8	0	-0.485919	-3.154821	-0.748269
21	1	0	-1.307887	-2.703670	-0.560572
22	1	0	0.901031	2.602673	-1.191842
23	8	0	0.594306	3.074624	-0.420304
24	1	0	0.665775	4.002242	-0.603421
25	1	0	4.641595	0.658141	0.927334
26	8	0	5.365838	0.096573	0.664818
27	1	0	5.672257	-0.345602	1.444760
28	1	0	-5.035083	0.367846	0.033147
29	8	0	-5.154041	-0.223791	-0.703605
30	1	0	-5.397564	0.307077	-1.450119

$2H_4SiO_4$ Hydrogen-bonded Dimer (Hexahydrate)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
300.03916	-1638.027312	0.290222

Rotational constant/ cm^{-1}

0.0140774055096	0.00565958200323	0.00510286352834

Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

[15.65220239	20.85801926	25.8622758	27.89873019
31.37390834	43.62043614	51.37008342	59.75916347
62.79646918	68.51661241	75.63377727	90.38938369
103.60896138	111.17094903	123.87620035	127.39308064
139.94542412	155.29181083	165.61308994	166.70429588
179.13153294	187.17309518	194.0886997	202.27621942
211.22132798	218.08132965	222.95352942	239.49537742
244.10346364	276.17935797	287.70999907	294.38234112
305.80177653	323.65724186	343.50745946	354.93384522
363.14221601	378.40519844	383.22179536	395.92009632
399.73584193	402.14066521	415.77726427	425.64677022
427.16889825	449.02081846	457.70181348	538.52055655
561.98495942	574.87787036	597.13986159	617.27504379
657.14923789	688.18952913	715.86584792	754.05110544
755.99025484	810.55750216	814.70686487	832.70133734
855.31084638	876.11326279	895.62291293	944.01824385
951.628884	975.01683295	985.7620838	1001.6505983
1036.29812446	1047.85656699	1138.4336103	1153.45333027
1173.06723575	1194.25192175	1208.79206713	1279.2408786
1814.64767552	1831.05746675	1835.03307055	1843.49165417
1850.03888981	1856.90584183	3836.04759993	3856.19668285
3894.54874891	3924.76889811	3938.66266036	3946.73897438
3954.80138769	3974.96437131	3984.84082762	3989.57402026
4012.29473501	4017.77856613	4116.11915743	4118.00965434
4145.67207242	4145.77632776	4149.89788905	4153.25491114
4155.39562089	4160.85165058]		

Ground State Electronic Degeneracy and Irreducible Representation

1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.850339	0.220353	-0.152132
2	8	0	0.901984	0.642330	1.132374
3	1	0	1.157111	1.430892	1.593731
4	8	0	1.761936	-1.390653	-0.300225
5	1	0	2.089349	-1.926620	0.427730
6	8	0	1.347577	0.926268	-1.529354
7	1	0	0.439757	0.756126	-1.784528
8	8	0	-1.976639	0.520658	0.703714
9	8	0	3.355544	0.779914	0.155732
10	1	0	-1.045954	0.542302	0.920739
11	14	0	-2.418315	-0.338590	-0.627187
12	8	0	-2.527123	-1.936223	-0.374443
13	1	0	-3.215570	-2.245192	0.218179
14	8	0	-1.265723	-0.142060	-1.770887
15	1	0	-0.957664	-0.964181	-2.165390
16	8	0	-3.879597	0.244661	-1.047979
17	1	0	-4.061691	1.160745	-0.895076
18	1	0	3.778909	1.257808	-0.559286
19	1	0	-0.820164	-3.063529	-1.617237
20	8	0	-0.170115	-2.666530	-2.187177
21	1	0	0.582586	-2.474896	-1.633491
22	1	0	-5.455348	-2.253894	1.139164
23	8	0	-4.593046	-2.365819	1.516956
24	1	0	-4.460603	-1.626503	2.109780
25	1	0	4.468243	0.008916	1.595800
26	8	0	4.789412	-0.552074	2.299981
27	1	0	5.732965	-0.589484	2.220670
28	8	0	3.840630	2.145783	-2.274451
29	1	0	2.930165	1.942013	-2.472796
30	1	0	4.348212	1.955430	-3.051812
31	8	0	-3.856146	0.054562	2.873608
32	1	0	-3.177985	0.346303	2.265985
33	1	0	-3.520110	0.175997	3.751001
34	8	0	2.910121	-2.656016	1.926738
35	1	0	3.627581	-2.078040	2.187839
36	1	0	2.408556	-2.846241	2.707953

$2H_4SiO_4$ Hydrogen-bonded Dimer (Octahydrate)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
336.06029	-1790.098466	0.346008

Rotational constant/ cm^{-1}

0.0103308135924	0.00564257023437	0.00453813951517

Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

[18.04312496	23.9370271	29.6780214	35.16880288
36.64922877	45.59433733	49.65334541	57.56285088
62.81732025	72.64512406	75.35576301	80.0820053
86.67789343	104.29009629	111.40726115	116.9814469
125.86400225	135.02457186	141.5857082	146.24939728
151.37180988	159.35081891	162.30472034	162.49237996
178.06812843	186.12359138	189.38330849	190.83593295

```
   197.81409068   201.9773541    207.63494413   215.23863393
   217.33764153   242.08090996   252.29793372   295.5152492
   298.62205847   300.76276821   314.67043117   327.7232003
   338.82986967   342.19384212   358.01980341   364.16391838
   389.15739964   393.93924478   416.27768993   419.16208779
   424.22889754   427.98208994   433.77868709   444.13471798
   494.20508477   507.87643562   519.00395605   538.05488268
   558.07885918   574.98907606   581.932482     592.44142073
   609.85206326   629.36866376   656.79476972   659.84597614
   681.3225771    708.75563342   719.25067144   773.1437342
   801.67494681   813.83111998   820.75367486   827.59282546
   851.09198011   934.72561748   940.03568969   962.05441845
   976.60151419   987.96534674  1004.15272657  1006.91896838
  1031.3286197   1129.2243882   1148.42822266  1170.55815712
  1179.1348968   1192.61858802  1255.44980898  1296.49166294
  1768.98383463  1813.62597315  1821.21576223  1824.80214608
  1836.23548219  1841.16328481  1876.65875444  1882.52485516
  3819.47100015  3831.4395137   3849.6980997   3880.42562491
  3901.91612659  3951.38181239  3958.04720408  3961.86990004
  3970.31458295  3977.03557749  3987.45416159  3991.14480078
  4009.12537253  4014.30338798  4031.85303764  4085.23177403
  4089.561846    4108.74482939  4129.75575649  4136.0527793
  4152.57377623  4158.13406127  4160.11491281  4164.91760902]

Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0       -2.624479   -0.174126    0.198460
      2          8           0       -1.889600   -0.322216    1.644019
      3          1           0       -1.311885   -1.066393    1.809874
      4          8           0       -2.878629    1.413635   -0.042142
      5          1           0       -3.762919    1.672473   -0.300337
      6          8           0       -1.714525   -0.877229   -0.962547
      7          1           0       -0.815269   -0.549630   -1.048672
      8          8           0        1.947147   -0.169374    1.469441
      9          8           0       -4.099603   -0.898425    0.139957
     10          1           0        1.475469    0.531379    1.931869
     11         14           0        2.187874    0.043229   -0.138893
     12          8           0        3.220778    1.272101   -0.448718
     13          1           0        4.148358    1.040764   -0.478681
     14          8           0        0.762843    0.417132   -0.854506
     15          1           0        0.417573    1.296290   -0.679523
     16          8           0        2.801613   -1.327898   -0.746097
     17          1           0        2.288012   -2.138534   -0.670401
     18          1           0       -4.138101   -1.844114    0.092579
     19          1           0        0.192601    3.532514   -0.609887
     20          8           0       -0.280911    2.896209   -0.077037
     21          1           0       -1.205443    2.899185   -0.303996
     22          1           0        0.902581   -1.618885    2.086707
     23          8           0        0.188907   -2.246829    2.225343
     24          1           0        0.272268   -2.571844    3.112584
     25          1           0        4.876861   -1.028319   -0.953907
     26          8           0        5.535919   -0.353634   -0.809460
     27          1           0        6.177236   -0.715815   -0.213318
     28          1           0       -5.630475    0.508982   -0.368299
     29          8           0       -5.669912    1.430062   -0.608544
     30          1           0       -6.360523    1.825855   -0.094200
     31          8           0        1.090525   -3.503771   -0.308018
     32          1           0        0.360533   -3.666839   -0.902540
     33          1           0        0.706607   -3.387082    0.555543
```

34	8	0	-1.372016	-3.571284	-1.863181
35	1	0	-1.600348	-2.656689	-1.706083
36	1	0	-1.446455	-3.722622	-2.795696
37	8	0	0.139002	1.687830	2.553279
38	1	0	0.056047	2.375506	1.898545
39	1	0	-0.658201	1.172305	2.463921
40	8	0	2.055270	3.838278	-1.340396
41	1	0	2.456419	4.174481	-2.129945
42	1	0	2.559541	3.068620	-1.079984

$2H_4SiO_4$ Hydrogen-bonded Dimer (Decahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
372.08142 -1942.164814 0.401496

Rotational constant/ cm^{-1}
0.00722633255837 0.00563222974742 0.00425094082921
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}

[21.01787745	27.72497128	34.32085941	42.76554232
45.01745776	48.26327415	53.83745991	58.34824115
59.5645535	60.9963269	67.84937821	71.58171954
76.59987679	83.59888559	90.17392265	92.00881671
109.37080675	115.23690747	116.78683692	125.79449869
129.48513789	138.24258682	144.5604607	148.52216379
149.83578113	154.02684598	160.07365597	162.79819564
166.94755835	174.39138994	184.14273984	187.25649946
193.92189115	207.80870304	209.69919995	221.22984106
221.84842277	227.7909774	251.54034488	253.3196361
261.77821972	279.86999717	294.17383043	302.63241405
312.18220361	322.83014946	349.60987229	351.34746136
355.03810056	363.01015924	370.00916803	389.15739964
400.83399823	413.37244099	416.4097467	424.97953602
438.37287261	444.94790967	459.14053724	463.37330422
471.93614318	507.27870497	512.69998289	549.3909138
565.05006655	574.34269292	588.16000125	589.23035612
601.66454354	619.12383857	629.81348656	653.70186117
660.01278469	663.62696996	673.51732698	711.44542131
716.1230111	724.53294223	741.85323013	789.17820618
798.71409503	816.57651072	822.0672922	879.706597
926.73270773	941.66902342	954.74264362	960.57399256
977.70662084	984.87938855	1012.92407622	1021.22280164
1044.02692067	1091.77586845	1129.34254426	1144.36226422
1172.90737755	1190.14426118	1245.12157952	1327.71266344
1814.60597339	1818.65108075	1821.18101045	1825.08711069
1835.92271616	1837.92441878	1858.73378554	1870.21577415
1888.48131051	1895.29265968	3747.59041529	3763.18006447
3794.2690082	3899.1637855	3913.59272518	3931.94861617
3959.98635349	3966.82550409	3969.45273877	3972.99742048
3986.46721099	3989.17089959	3999.35317157	4003.28707324
4012.44764285	4016.61090627	4021.26764499	4043.37672838
4082.59063863	4085.9198593	4113.31816384	4119.78894556
4131.72270732	4136.28909141	4147.70157646	4149.82838549
4160.49718241	4164.7299494]		

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	14	0	2.652390	0.993254	0.404538
2	8	0	2.469685	1.874128	1.741571
3	1	0	1.602987	2.083997	2.087338
4	8	0	2.608587	-0.606320	0.745595
5	1	0	3.065392	-1.175230	0.132488
6	8	0	1.525339	1.328507	-0.732594
7	1	0	0.785655	0.728084	-0.829815
8	8	0	-1.526942	0.051554	1.598008
9	8	0	4.120857	1.356655	-0.237477
10	1	0	-0.976456	-0.681202	1.899464
11	14	0	-2.031906	-0.024930	0.043103
12	8	0	-3.154587	-1.175283	-0.227374
13	1	0	-4.066299	-0.914695	-0.102341
14	8	0	-0.734562	-0.414826	-0.901939
15	1	0	-0.379224	-1.302229	-0.761141
16	8	0	-2.649117	1.403177	-0.393462
17	1	0	-2.225324	2.235627	-0.150266
18	1	0	4.595636	2.073792	0.161195
19	1	0	-0.661281	-3.460790	-1.047800
20	8	0	0.105996	-3.071529	-0.625051
21	1	0	0.807094	-3.096359	-1.277786
22	1	0	-0.736785	1.563838	2.436007
23	8	0	-0.212977	2.327470	2.688666
24	1	0	-0.341606	2.458777	3.619246
25	1	0	-4.773751	1.213687	-0.339536
26	8	0	-5.425536	0.535227	-0.184564
27	1	0	-6.073997	0.894324	0.405487
28	1	0	4.589295	-0.282073	-1.470857
29	8	0	4.271624	-1.163740	-1.652589
30	1	0	5.032347	-1.715348	-1.782911
31	8	0	-1.391356	3.734205	0.362548
32	1	0	-0.722204	4.011816	-0.261079
33	1	0	-0.946476	3.588589	1.191792
34	8	0	0.830772	4.026260	-1.435701
35	1	0	1.152613	3.130627	-1.348499
36	1	0	0.955948	4.289836	-2.336707
37	8	0	0.332917	-1.977098	2.076677
38	1	0	0.227442	-2.636573	1.395430
39	1	0	1.169868	-1.564692	1.879971
40	8	0	-2.317375	-3.366713	-2.083813
41	1	0	-2.042514	-2.883434	-2.855407
42	1	0	-2.809988	-2.750307	-1.548286
43	8	0	1.864276	-2.515502	-2.791882
44	1	0	2.595848	-1.929900	-2.625435
45	1	0	1.235169	-2.051076	-3.336347
46	8	0	-0.677208	-1.174560	-3.691391
47	1	0	-0.791501	-0.687415	-2.877564
48	1	0	-0.973928	-0.616054	-4.397646

$2H_4SiO_4$ Hydrogen-bonded Dimer (12 explicit waters)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
408.10255 -2094.229835 0.456489

Rotational constant/ cm^{-1}
0.006356063834 0.00415153872884 0.00334564787484
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}

```
[   14.727805      20.44099788    25.22979337    31.81873115
    34.20270336    37.96979647    43.92625182    47.53348674
    51.71065088    56.12412713    56.68015563    60.37774519
    63.85292334    68.26639959    69.3784566     76.15505399
    86.78214877    88.90200744    95.31718631   108.11974262
   121.86059702   125.53038515   126.88570463   132.09847185
   132.30698254   138.1035797    147.62556783   148.23719918
   149.71067472   160.18486167   164.55663578   167.31592723
   170.74245289   172.71635408   179.7431643    190.27295409
   194.3111111    204.66019164   213.75820803   216.78161302
   225.11509023   227.54076458   230.29310567   231.16885057
   247.22417362   257.48984988   260.03368028   269.3193563
   283.62318957   306.87908175   310.27085563   325.31837702
   332.43554187   338.81596895   343.5491616    366.87455734
   367.74335188   374.07512647   391.33286116   402.84960155
   406.95031177   419.25244242   424.04123792   428.26010419
   440.48578092   446.72025053   452.78791158   460.87812631
   471.40791611   472.63117882   476.95430043   513.37416745
   546.98609052   573.36269268   579.20099198   593.37971883
   603.74965043   611.94412051   613.89022027   621.09773976
   627.1028476    648.15547684   655.43249988   674.79619254
   686.41023792   703.86258259   710.50017286   726.95861658
   738.00968309   762.78770331   777.96728147   808.84771451
   817.38275205   821.35835585   882.54234237   896.76277136
   920.74845096   963.12477332   974.37044982   977.95683367
   986.93669401  1001.55329331  1014.43925389  1047.34919098
  1104.41161621  1131.25389224  1148.14325805  1171.0863842
  1173.51205855  1180.30255666  1270.3027204   1341.67592925
  1810.17859642  1820.65973372  1822.71008883  1824.32257149
  1837.79236201  1838.48044728  1840.09292994  1844.22144158
  1860.06825395  1863.43917676  1893.31875849  1897.12060339
  3735.53849746  3762.72134096  3815.41894243  3868.62391991
  3907.44165985  3910.06889453  3934.16577983  3951.13854992
  3955.89259363  3962.71089316  3962.79429743  3975.15898129
  3987.06494163  3988.66352358  3992.80593594  3996.63558226
  4000.31232074  4009.49374142  4012.899416    4019.91232551
  4036.48197493  4067.35545762  4104.84567951  4109.43291467
  4118.30851966  4134.20398452  4145.53306529  4147.44441328
  4147.87533537  4149.18895271  4159.22526721  4163.60399168]
Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0        2.690144   -0.292510   -0.405169
      2          8           0        2.736999   -1.858167   -0.848834
      3          1           0        1.938449   -2.384193   -0.797447
      4          8           0        2.116239    0.618408   -1.640660
      5          1           0        2.412783    1.524491   -1.651455
      6          8           0        1.748426   -0.070956    0.909424
      7          1           0        0.863818    0.278675    0.798441
      8          8           0       -1.752356   -1.223688   -0.907020
      9          8           0        4.207198    0.175564   -0.032613
     10          1           0       -1.386786   -0.730863   -1.654671
     11         14           0       -2.138862   -0.274801    0.397305
     12          8           0       -3.506536    0.563735    0.144040
     13          1           0       -4.321378    0.060726    0.063273
     14          8           0       -0.937618    0.844957    0.561150
     15          1           0       -0.900608    1.508656   -0.139362
     16          8           0       -2.269540   -1.189697    1.704907
     17          1           0       -1.623482   -1.857302    1.956299
     18          1           0        4.899687   -0.479107   -0.119471
```

19	1	0	-1.796034	3.249129	-1.101738
20	8	0	-0.983689	2.839630	-1.405031
21	1	0	-0.274581	3.400403	-1.085729
22	1	0	-0.491705	-2.677290	-0.753109
23	8	0	0.248243	-3.275436	-0.635091
24	1	0	0.047527	-4.063872	-1.123128
25	1	0	-5.797799	-1.790520	0.626950
26	8	0	-5.608207	-1.285392	-0.152786
27	1	0	-5.266984	-1.898503	-0.802957
28	1	0	4.195207	2.228378	-0.228354
29	8	0	3.643442	2.933949	-0.560805
30	1	0	4.217600	3.599945	-0.916397
31	8	0	-0.309095	-3.060038	2.302203
32	1	0	0.397692	-2.678685	2.820173
33	1	0	0.079074	-3.353731	1.485221
34	8	0	1.833015	-1.494497	3.411754
35	1	0	1.951941	-0.926879	2.652743
36	1	0	2.675566	-1.586409	3.834749
37	8	0	-0.563369	0.352201	-2.855125
38	1	0	-0.827108	1.254904	-2.688521
39	1	0	0.373312	0.340739	-2.673664
40	8	0	-3.227627	3.526997	0.197913
41	1	0	-2.762909	3.692612	1.010990
42	1	0	-3.560044	2.635073	0.259181
43	8	0	1.009548	4.124915	0.149747
44	1	0	1.882762	3.746102	0.161838
45	1	0	0.614166	3.979653	1.004705
46	8	0	-0.850993	3.161557	2.302485
47	1	0	-0.882070	2.260752	1.987157
48	1	0	-0.840627	3.124398	3.249944
49	8	0	-4.003611	-2.740277	-2.032658
50	1	0	-3.210298	-2.288763	-1.752417
51	1	0	-4.112061	-2.558464	-2.956874
52	8	0	5.578129	-2.259531	-0.535551
53	1	0	4.716795	-2.575176	-0.795925
54	1	0	6.201349	-2.566382	-1.179948

$2H_4SiO_4$ Dimerization/H_2O-loss transition state (No explicit waters)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
191.97577	-1181.744121	0.12348

Rotational constant/ cm^{-1}

0.0547585489959	0.0222393853551	0.0211673103531

Rotational symmmetry number

1.0

Imaginary Frequency/ cm^{-1}

-1498.6943

Non-imaginary Vibrational Frequencies/ cm^{-1}

[34.94639148	47.31107534	116.50882267	130.15237209
166.16911844	214.39764081	245.41708098	261.63226223
302.74361975	309.27000432	324.9708592	339.18433784
364.22647159	371.0169697	386.42590962	425.22974884
443.56478876	455.58890517	471.10210043	484.09231636
505.79132873	570.27673449	593.91489627	686.5561954
798.44998149	826.23055562	857.60446396	886.1009248
908.06405071	925.34263647	962.8745605	983.20435268
1020.93783703	1023.3774121	1048.74621259	1052.45770286
1087.60565467	1105.81558818	1360.19862879	2168.22620126
4098.31929494	4108.64057405	4133.93292063	4139.79207099
4142.35675246	4145.95703703	4166.828957]	

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.026241	-0.055436	-1.715825
2	14	0	-0.066505	0.019231	1.428317
3	8	0	1.879868	0.131292	1.613375
4	1	0	1.633870	0.016426	0.340115
5	8	0	-0.177901	-1.293253	2.409042
6	1	0	0.474180	-1.419416	3.080961
7	8	0	-1.585772	-0.117620	0.708826
8	1	0	-2.317422	-0.165719	1.308973
9	8	0	-0.202723	1.517322	2.066720
10	1	0	0.593926	1.878206	2.429221
11	8	0	-0.834133	1.338869	-1.893448
12	1	0	-1.512027	1.538995	-1.259557
13	8	0	0.648357	-0.092917	-0.174436
14	8	0	-0.902755	-1.401089	-1.882559
15	1	0	-1.497299	-1.594835	-1.167403
16	8	0	1.203556	-0.062951	-2.764648
17	1	0	1.307370	0.678995	-3.343841
18	1	0	2.387858	-0.583003	1.973657

$2H_4SiO_4$ Dimerization/H_2O-loss transition state (Dihydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
227.9969 -1333.818601 0.1783

Rotational constant/ cm^{-1}
0.0235793123255 0.0193944171871 0.0139923466654
Rotational symmmetry number
1.0

Imaginary Frequency/ cm^{-1}
-1651.8617
Non-imaginary Vibrational Frequencies/ cm^{-1}
[25.0977366 35.80823566 44.8993017 47.58213924
  77.50342311 90.16002193 121.60343384 128.26882553
  146.30500013 175.35748947 183.67011561 204.57678736
  220.18033726 245.92445699 254.41779239 291.97751784
  330.52419389 332.06022263 358.54803049 360.44547776
  372.49044523 405.56024051 415.18648399 427.3843593
  453.03117405 476.1480591 510.69132992 533.2313354
  551.91389314 563.81985348 575.70496276 590.04354781
  626.3244077 644.10341911 668.34626189 718.51393367
  814.18558815 836.21126727 896.33879963 921.69369941
  963.9866175 990.46052465 1006.44634415 1017.60861637
  1047.02252423 1050.08763136 1075.94990716 1093.52735824
  1114.46183142 1143.59077468 1386.82544378 1813.06994464
  1815.04384583 2092.23100547 3951.75018127 3984.97288439
  4032.6384279 4045.96226093 4123.28497478 4123.99391112
  4124.51518784 4125.52993986 4138.94412752 4156.06285509
  4171.03392256]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.175417	0.155722	-1.647555
2	14	0	-0.157386	0.113819	1.535652
3	8	0	1.684474	0.140919	1.684597
4	1	0	1.488086	0.295646	0.411931
5	8	0	-0.198357	-1.450832	2.096700
6	1	0	0.631342	-1.731717	2.460066
7	8	0	-1.767450	0.148128	0.998422
8	1	0	-2.236938	-0.675502	0.990082
9	8	0	-0.245300	1.440043	2.500106
10	1	0	-1.123045	1.780453	2.604877
11	8	0	-1.464082	1.125773	-1.699496
12	1	0	-1.979397	1.134419	-0.897928
13	8	0	0.474244	0.287897	-0.113825
14	8	0	-0.440556	-1.398765	-1.997653
15	1	0	-0.947068	-1.956269	-1.409298
16	8	0	0.963925	0.681977	-2.691203
17	1	0	1.227773	0.067692	-3.363753
18	1	0	2.048567	0.908027	2.108692
19	1	0	3.662397	2.412897	-1.080192
20	8	0	3.074873	1.691424	-0.903077
21	1	0	2.523538	1.583224	-1.671589
22	1	0	-1.176853	-2.697277	0.918104
23	8	0	-1.751550	-2.816367	0.162781
24	1	0	-2.100948	-3.696748	0.196838

$2H_4SiO_4$ Dimerization/H_2O-loss transition state (Tetrahydrate)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
264.01803	-1485.865859	0.233246

Rotational constant/ cm^{-1}

0.0173543391809	0.0115036249511	0.00989851452501

Rotational symmmetry number

1.0

Imaginary Frequency/ cm^{-1}

-1694.983

Non-imaginary Vibrational Frequencies/ cm^{-1}

[19.48184871	35.52327105	38.92199528	43.70384042	
60.30824162	86.98370911	88.20002146	104.90172765	
119.86584476	131.59109584	135.21918183	151.05904384	
171.62514814	175.85791512	180.04897997	183.75351988	
199.61423296	210.44983843	216.36459165	225.98388477	
237.35466767	270.95269003	284.61709052	303.626315	
320.24461692	343.01398416	371.55214713	381.47030557	
397.97740179	408.57669515	423.07513839	443.80110088	
457.6670617	461.23954484	479.85259901	509.42636507	
545.32495537	560.4767321	566.49574066	585.90808581	
602.52638772	628.47901815	638.0774602	659.92243005	
691.36584196	720.05691277	726.47904199	784.10444608	
818.08473804	836.08616086	906.20135522	924.23057946	
1000.3300306	1010.97797645	1016.51046007	1045.20153088	
1046.66805606	1082.75430597	1132.10878607	1159.25687778	
1180.7890816	1188.77504099	1419.64502623	1809.10824155	
1819.03335035	1821.68838646	1842.59505821	2034.40404104	

```
  3878.45172372  3936.59145418  3941.00493043  3956.86564351
  4017.24338869  4018.8002685   4023.82537611  4101.64156525
  4122.4856838   4128.51859307  4143.61476696  4149.33491019
  4158.69704013  4162.5822893   4165.80725462]

Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0        1.242499   -0.208958    0.421901
      2         14           0       -1.826811    0.338814   -0.495996
      3          8           0       -1.584364    2.159349   -0.563675
      4          1           0       -0.406353    1.728442   -0.232370
      5          8           0       -2.908767    0.520566    0.755086
      6          1           0       -3.156622    1.425636    0.890295
      7          8           0       -1.707970   -1.352179   -0.358597
      8          1           0       -1.905682   -1.708612    0.498888
      9          8           0       -2.223307    0.346561   -2.089880
     10          1           0       -2.389089   -0.508199   -2.462209
     11          8           0        1.847051   -1.072290   -0.811304
     12          1           0        1.363567   -1.830716   -1.146318
     13          8           0       -0.138054    0.627807   -0.017787
     14          8           0        0.875152   -1.147364    1.681383
     15          1           0        0.017800   -1.136115    2.097556
     16          8           0        2.342931    0.937876    0.765158
     17          1           0        3.231921    0.773931    0.448500
     18          1           0       -1.609102    2.546407   -1.430056
     19          1           0        1.085486    4.101307    0.319214
     20          8           0        1.223985    3.379028   -0.277500
     21          1           0        1.818172    2.771860    0.154132
     22          1           0       -2.432172   -0.562399    2.323131
     23          8           0       -1.862712   -1.261891    2.641817
     24          1           0       -2.192782   -1.555587    3.480328
     25          1           0        3.892342   -0.616214   -1.098984
     26          8           0        4.555558   -0.058852   -0.700034
     27          1           0        5.282132   -0.616652   -0.457728
     28          1           0       -0.664887   -2.621633   -1.305890
     29          8           0        0.081900   -3.068858   -1.706696
     30          1           0        0.078949   -3.961774   -1.389682
 ---------------------------------------------------------------------
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$2H_4SiO_4$ Dimerization/H_2O-loss transition state (Hexahydrate)

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Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u.  Energy a.u.  ZPE a.u.
300.03916 -1637.964027 0.288365

Rotational constant/ cm-1
0.0104442253847   0.00841148578861   0.00697182315374
Rotational symmetry number
1.0

Imaginary Frequency/ cm-1
-1600.5568
Non-imaginary Vibrational Frequencies/ cm-1
[   12.23262709    22.6651119     29.21234753    32.93773851
    40.57618008    45.68469197    51.14767202    60.32909269
    73.44441503    92.07136992   114.28470866   119.83109298
   137.67960796   141.07833219   154.23535667   157.98159872
   169.51919018   174.36358852   181.25139161   193.58827405
   195.58997666   208.78870328   211.4576401    216.46189663
```

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   231.55807052   236.83339095   239.45367528   249.962614
   267.01183801   279.33481973   319.79284376   330.65625066
   335.59100363   345.02263713   361.26561981   385.40420724
   400.77839538   402.68974336   424.08294005   426.63372082
   440.27031988   455.65840873   479.31047122   516.5157285
   527.17062471   565.20992474   567.94141477   579.50680765
   580.95943212   600.85135185   606.56454473   635.29036732
   667.47746735   693.31889208   701.36740468   727.68840399
   778.1688418    796.3648746    809.18133162   819.21764611
   838.37977844   910.37851936   929.60320488   956.84860158
  1002.19967645  1045.48649549  1051.6723126   1076.5476378
  1092.27629411  1130.4337502   1140.94963928  1151.70879083
  1189.5048284   1210.47405336  1372.59111408  1815.00909405
  1816.08639928  1838.02867412  1847.05718695  1855.96754373
  1871.32783116  2162.31839841  3830.86958449  3870.05569331
  3920.2859183   3930.30833208  3935.43074468  3952.22975585
  3972.78890979  3986.44635992  4016.89587088  4021.30239677
  4073.4509201   4122.41618024  4125.78710304  4127.69150067
  4142.91973133  4147.99349142  4150.2245558   4161.38682802
  4163.84725415]

Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0       -0.920531    1.085364    0.275132
      2         14           0        1.687546   -0.912176    0.094471
      3          8           0        1.552568   -0.974226   -1.736721
      4          1           0        0.630240   -0.150134   -1.394077
      5          8           0        1.325019   -2.520332    0.219115
      6          1           0        1.339358   -2.974641   -0.612901
      7          8           0        1.549615   -0.591755    1.759983
      8          1           0        1.055886   -1.233663    2.253080
      9          8           0        3.224492   -0.302864   -0.022020
     10          1           0        3.606518   -0.122820    0.826914
     11          8           0       -0.356183    2.542580    0.713081
     12          1           0        0.223720    2.569206    1.478734
     13          8           0        0.321504    0.144438   -0.343740
     14          8           0       -1.587014    0.305303    1.505846
     15          1           0       -1.536499   -0.652134    1.577603
     16          8           0       -1.931510    1.317018   -0.982285
     17          1           0       -2.021008    2.217607   -1.297367
     18          1           0        2.284110   -0.655576   -2.264376
     19          1           0       -3.538630   -0.930093   -2.749406
     20          8           0       -3.726276   -0.815185   -1.827513
     21          1           0       -3.214707   -0.060344   -1.540110
     22          1           0       -0.559138   -2.799541    1.091486
     23          8           0       -1.330725   -2.469660    1.541679
     24          1           0       -2.093449   -2.803668    1.068017
     25          1           0       -1.087661    4.050572   -0.545347
     26          8           0       -1.641823    4.113055   -1.319202
     27          1           0       -2.251212    4.824124   -1.174203
     28          1           0        1.525645    1.116043    2.624236
     29          8           0        1.389952    2.036023    2.856701
     30          1           0        1.025195    2.045524    3.731667
     31          8           0        4.041065    0.042302   -2.733474
     32          1           0        4.171971    0.091498   -1.790056
     33          1           0        4.267950    0.887727   -3.095838
     34          8           0       -3.578635   -3.096103   -0.098755
     35          1           0       -4.441292   -3.294125    0.239429
     36          1           0       -3.679517   -2.351766   -0.693552
```

$2H_4SiO_4$ Dimerization/H_2O-loss transition state (Octahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
336.06029 -1789.983043 0.343441

Rotational constant/ cm^{-1}
0.00824036740778 0.00718763912333 0.00649616075398
Rotational symmmetry number
1.0

Imaginary Frequency/ cm^{-1}
-1485.835
Non-imaginary Vibrational Frequencies/ cm^{-1}

[18.84936629	27.64156701	35.85688816	41.60483282
50.8001542	60.3916459	62.72696562	73.71547893
77.66328131	82.41037466	88.464135	96.13732835
113.16570129	115.78598562	126.85095285	129.06116615
131.91081223	140.84202008	148.19549705	151.47606522
154.94429302	163.09706096	165.62699065	176.52514933
191.73947927	193.79678474	198.63423272	205.04246123
210.25522846	217.33069117	226.53296291	230.2097014
240.82984582	246.15381875	251.17892636	262.52190784
292.3667378	312.76603354	332.76915897	336.32079104
348.85923381	353.12675258	381.498107	383.50675997
399.31882055	418.99527924	433.18790681	441.47273152
456.86777072	462.04578617	473.72933511	489.9862185
494.60125508	523.5772905	560.72694493	571.33318864
581.77262381	586.84638391	595.29801717	612.59050365
622.55731458	628.99334452	644.92356116	676.65888803
712.08485409	725.24882893	762.94061115	775.29834465
798.96430785	809.73736012	831.08885468	858.60531527
898.15979298	921.50603979	950.60718163	992.69158903
1017.51131138	1037.9940114	1041.72635273	1090.64991073
1121.5581452	1138.80892954	1199.24922793	1228.85774577
1250.25094247	1269.6493869	1402.14402907	1810.7068235
1813.9039874	1814.68937766	1818.15760546	1822.50157814
1833.80980785	1839.45349716	1878.02102428	2145.24137297
3750.96133809	3815.57185027	3906.24619857	3948.60862022
3965.90805705	3969.7655048	3975.49954875	3978.38394661
3985.38295541	3994.47402145	3999.38792336	4007.08196778
4021.01743216	4025.22239773	4092.07787498	4093.89886834
4143.90668192	4145.49136316	4152.74753513	4155.77094013
4160.60838811	4161.65094156	4167.19037553]	

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.810730	-0.752397	-1.004127
2	14	0	-0.288877	1.063112	1.564964
3	8	0	-2.009245	0.999600	0.719798
4	1	0	-1.258827	0.202810	0.048147
5	8	0	-0.232563	2.690449	1.349640
6	1	0	-1.011108	3.105384	1.005822
7	8	0	1.352105	0.934523	1.992989
8	1	0	1.861177	1.679386	1.678217
9	8	0	-0.935747	0.342085	2.892740
10	1	0	-0.327953	0.184434	3.612713

11	8	0	1.588370	-2.022599	-0.373777
12	1	0	2.278736	-1.865102	0.279109
13	8	0	-0.154957	0.010361	0.135200
14	8	0	1.874340	0.353289	-1.539536
15	1	0	1.556656	1.255244	-1.678280
16	8	0	-0.219268	-1.259819	-2.135721
17	1	0	-0.329646	-2.202244	-2.250017
18	1	0	-2.720671	0.598643	1.218413
19	1	0	1.403168	3.237803	-0.718328
20	8	0	1.027139	2.974864	-1.553267
21	1	0	0.085896	3.114908	-1.477491
22	1	0	0.771830	-3.816337	-1.143690
23	8	0	0.090200	-4.070475	-1.759821
24	1	0	0.411808	-4.814327	-2.250368
25	1	0	2.791952	-0.455723	1.848317
26	8	0	3.419350	-1.067318	1.468228
27	1	0	4.036354	-0.535578	0.975071
28	8	0	-3.677334	-0.336065	2.641128
29	1	0	-2.825953	-0.284784	3.070695
30	1	0	-4.316767	0.023965	3.240012
31	8	0	-1.929317	3.143940	-1.126148
32	1	0	-2.582045	3.393705	-1.766147
33	1	0	-2.247750	2.363001	-0.674494
34	8	0	4.504251	0.794387	-0.624198
35	1	0	3.700425	0.562517	-1.094658
36	1	0	5.221981	0.725084	-1.239748
37	8	0	1.237292	0.248890	4.777696
38	1	0	1.660025	0.596108	3.996329
39	1	0	1.354078	0.886183	5.468990
40	8	0	3.099074	2.913038	0.725567
41	1	0	3.768203	2.387407	0.289616
42	1	0	3.531200	3.663336	1.111277

$2H_4SiO_4$ Dimerization/H_2O-loss transition state (Decahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
372.08142 -1941.990765 0.398503

Rotational constant/ cm^{-1}
0.00760926413966 0.00591108933101 0.00549646916068
Rotational symmetry number
1.0

Imaginary Frequency/ cm^{-1}
-1655.4711
Non-imaginary Vibrational Frequencies/ cm^{-1}

[23.42965109	34.04284516	37.49717224	40.97235039
49.42398366	51.91916157	53.42738888	57.93121977
60.57235516	61.84427037	71.79718059	74.39661384
86.94895732	94.69165424	99.79321577	100.50215211
112.04669393	119.73378799	128.24797446	142.23209134
147.47961035	149.61336973	157.21010917	161.14401084
166.31507592	167.94840965	171.4235878	181.00117879
187.49976193	195.68033129	197.70983533	209.40033463
222.02913203	226.22019688	232.72573038	234.35211375
243.11651305	247.00871258	254.65410451	269.95878908
284.02631023	289.09311998	304.0085846	317.25596371
334.33298914	349.35270911	361.86335045	377.66846068
379.53810652	389.2755557	399.20761485	406.1023683
411.83641225	432.13145265	446.81755551	449.93826549
477.4686268	486.66394819	490.24338168	495.64380853
501.41955461	518.09345938	523.87615582	553.87389362

```
   577.77616893   587.79163236   596.46567703   603.01986302
   612.52100008   615.15518512   630.82128822   640.73249631
   649.71235665   667.52611985   680.28697402   692.13038115
   710.52102392   736.27209402   740.08783963   758.88160307
   786.94019145   806.35948696   824.80573258   850.93212191
   904.23440439   923.9386645    944.19200276   961.31768069
  1007.08577693  1038.98096199  1044.57599881  1058.96323636
  1091.80366988  1108.87374495  1174.83262625  1190.70028968
  1216.16639517  1237.85150683  1372.36175232  1806.26554582
  1811.46441234  1816.89959097  1817.19845629  1828.81945202
  1849.87208126  1850.9632872   1875.19917962  1887.66811882
  1907.60174069  2124.94633258  3721.33891954  3750.82928132
  3898.79541661  3901.79797054  3947.8649321   3967.29117796
  3969.27897986  3977.88352096  3987.32905517  3988.33685684
  4000.98650531  4012.5032457   4018.55005568  4050.26453148
  4077.63503459  4079.9078011   4086.80255455  4089.55489565
  4110.89248949  4123.67419473  4127.03121682  4140.38285128
  4150.81533608  4152.14980449  4153.26881186  4153.88739357
  4158.23136626]
Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0        1.046464   -0.471047   -0.853496
      2         14           0       -0.377923    1.238159    1.486356
      3          8           0       -2.020428    1.207718    0.665544
      4          1           0       -1.269209    0.541981   -0.150725
      5          8           0       -0.339262    2.887397    1.390623
      6          1           0       -1.164319    3.268209    1.120115
      7          8           0        1.255640    1.093431    1.940645
      8          1           0        1.834568    1.780305    1.641065
      9          8           0       -0.963044    0.350892    2.756210
     10          1           0       -0.310502    0.064527    3.388189
     11          8           0        1.467806   -1.806246   -0.049770
     12          1           0        2.074193   -1.816247    0.703459
     13          8           0       -0.149031    0.358850   -0.040007
     14          8           0        2.280869    0.552564   -1.079276
     15          1           0        2.046630    1.482099   -1.203480
     16          8           0        0.401118   -0.966724   -2.268264
     17          1           0       -0.003097   -1.831312   -2.247712
     18          1           0       -2.722963    0.694953    1.051034
     19          1           0       -2.971773   -0.248092   -2.000912
     20          8           0       -2.901217    0.510959   -2.574889
     21          1           0       -2.543998    0.199144   -3.398130
     22          1           0        0.925144    3.411670   -0.398111
     23          8           0        1.291682    3.135778   -1.231353
     24          1           0        0.546230    3.101901   -1.835862
     25          1           0        0.302148   -3.352430   -0.613052
     26          8           0       -0.422479   -3.567484   -1.198927
     27          1           0       -0.336568   -4.480353   -1.440465
     28          1           0        2.737501   -1.592775    2.890575
     29          8           0        3.186423   -1.835276    2.085482
     30          1           0        3.776411   -1.113984    1.875938
     31          8           0       -3.345488   -1.024579    2.111635
     32          1           0       -2.567616   -0.745226    2.594640
     33          1           0       -4.054297   -1.117874    2.733839
     34          8           0       -1.007940    2.728246   -2.853461
     35          1           0       -0.811294    2.258850   -3.658146
     36          1           0       -1.736843    2.237089   -2.479098
     37          8           0       -2.729562   -1.760500   -0.679036
     38          1           0       -3.041589   -1.723649    0.220520
```

39	1	0	-2.143105	-2.507149	-0.744884
40	8	0	4.447935	0.472975	0.868497
41	1	0	3.841900	0.519665	0.130754
42	1	0	5.320544	0.589542	0.517792
43	8	0	1.638040	-0.392323	4.191548
44	1	0	1.751580	0.291592	3.528826
45	1	0	1.977735	-0.063175	5.012586
46	8	0	-0.620040	0.366257	-4.614611
47	1	0	-0.205745	0.135312	-5.434811
48	1	0	-0.140005	-0.073804	-3.915261

$2H_4SiO_4$ Dimerization/H_2O-loss transition state (12 explicit waters)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
408.10255 -2094.150809 0.44981

Rotational constant/ cm^{-1}
0.00627100498973 0.00467390010192 0.00412418647303
Rotational symmetry number
1.0

Imaginary Frequency/ cm^{-1}
-1639.9745
Non-imaginary Vibrational Frequencies/ cm^{-1}

[19.21078482	22.65816154	28.53121262	30.24100027
33.32000811	37.74738507	38.73433566	45.15646489
54.80355943	56.89561668	60.27348984	62.31689459
64.24214329	68.03008747	80.29746634	85.29477252
88.43633357	92.64129913	96.07477515	107.48030984
109.30130319	118.26031246	122.42357588	125.53038515
127.22627209	133.32868492	137.8325158	144.13648897
149.4118094	157.22400988	159.2882657	171.9170631
174.71110633	184.09408734	193.97054364	196.75763652
202.88785078	204.05551064	212.29863321	213.20912989
218.49835103	224.43395531	235.37381613	238.34856863
238.91849784	250.44218859	257.11453064	267.79027792
284.79084943	296.37014303	308.05369197	325.09596562
333.28348534	338.16958582	343.62561551	350.49256754
359.86164783	372.39314024	381.05328419	387.94108729
392.84803884	396.81669229	406.9781132	419.04393174
425.47301131	438.24081584	441.81329898	446.44223627
462.81727572	478.63628666	485.50323868	493.26678667
494.85841827	517.1829627	537.95062733	546.03389171
555.6740359	565.8215561	578.93687844	585.15049697
587.54141954	618.40795187	631.80823882	655.21008848
662.68867186	676.42952627	689.69775645	733.7143629
751.11805508	766.32543466	775.27054322	791.22856129
800.70189693	823.90218626	844.62814875	864.52006848
885.51014451	900.37000628	918.18376948	992.8236458
1013.09088477	1024.3157102	1045.64635368	1071.07770739
1084.58224968	1091.42140028	1133.73516944	1173.92907993
1207.00582556	1222.27575836	1412.56261316	1812.53476721
1815.87093823	1819.42952066	1827.22782043	1829.16696984
1841.94867507	1843.67931379	1845.3473993	1871.38343401
1881.58655706	1885.7150687	1889.55166538	2093.19015464
3830.53596738	3848.66944697	3912.77258313	3914.89244181
3937.36294373	3940.74776725	3976.14593189	3986.43940957
3988.06579294	3994.14735471	4002.5781369	4008.91686184
4013.28863596	4029.7123279	4031.35261198	4033.71573313
4045.53133884	4048.10297067	4050.07687186	4086.33688068
4109.0784465	4124.91830851	4126.73930186	4139.30554605
4141.35590116	4148.36186031	4149.63377551	4150.12030045

4155.027252 4157.08455747 4164.63264441]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.565652	-0.008774	1.406167
2	14	0	-0.551112	0.940851	-1.502083
3	8	0	-2.210533	0.120498	-1.201774
4	1	0	-1.551341	-0.082793	-0.114822
5	8	0	-0.301249	-0.018033	-2.831741
6	1	0	-1.077561	-0.445879	-3.166087
7	8	0	1.082043	1.408058	-1.407895
8	1	0	1.520895	1.434350	-2.247652
9	8	0	-1.280924	2.395305	-1.559738
10	1	0	-0.716290	3.164159	-1.505816
11	8	0	0.806626	1.427588	2.118772
12	1	0	1.367019	2.080164	1.687644
13	8	0	-0.459262	0.174476	0.098236
14	8	0	1.924294	-0.699336	0.862962
15	1	0	1.892426	-1.069498	-0.023777
16	8	0	-0.169178	-0.971469	2.486522
17	1	0	-0.699896	-0.535891	3.147968
18	1	0	-2.933504	0.732079	-1.085447
19	1	0	-2.666054	-2.081058	1.270081
20	8	0	-2.042231	-2.791823	1.136361
21	1	0	-1.338273	-2.577561	1.740900
22	1	0	1.165861	-1.338863	-2.264265
23	8	0	1.670731	-1.916096	-1.695218
24	1	0	1.084768	-2.651149	-1.506105
25	1	0	-0.815908	1.726005	3.426031
26	8	0	-1.559314	1.238913	3.776370
27	1	0	-1.693491	1.532009	4.668339
28	1	0	2.051629	2.483459	-0.283791
29	8	0	2.393922	3.025131	0.430432
30	1	0	3.303617	2.748860	0.517550
31	8	0	-5.073942	0.523198	-0.386035
32	1	0	-5.881623	0.962537	-0.615717
33	1	0	-5.103417	-0.355618	-0.765530
34	8	0	-0.477804	-3.715905	-1.088266
35	1	0	-0.393113	-4.654337	-0.983548
36	1	0	-1.058227	-3.415760	-0.387272
37	8	0	-3.296114	-0.203752	1.770301
38	1	0	-3.999362	0.207075	1.274036
39	1	0	-3.011911	0.409174	2.440379
40	8	0	4.419273	0.936259	0.366158
41	1	0	3.736332	0.370051	0.710953
42	1	0	4.848855	0.406241	-0.296363
43	8	0	4.538076	-1.629736	-1.392578
44	1	0	5.113735	-2.118712	-1.965476
45	1	0	3.643108	-1.808556	-1.678626
46	8	0	0.483101	4.678120	-1.048378
47	1	0	1.208931	4.456223	-0.470074
48	1	0	0.241032	5.575634	-0.866023
49	8	0	-4.220959	-1.938861	-1.494240
50	1	0	-3.366418	-1.513637	-1.494526
51	1	0	-4.097749	-2.798650	-1.113519
52	8	0	3.949111	-3.127510	1.217298
53	1	0	4.319096	-2.676771	0.466010
54	1	0	3.297930	-2.532551	1.566989

$H_6Si_2O_7$ (Monohydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
191.97577 -1181.831107 0.124797

Rotational constant/ cm^{-1}
0.0365519535518 0.0236740445285 0.0184547671309
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}

[18.67560738	29.65021998	35.47461856	45.2815713
64.54795897	105.34655045	167.75379968	192.52486953
195.83323913	215.61395317	236.13835532	265.44105749
275.92914514	290.55964516	328.18887417	337.62745803
345.8705806	371.1281754	378.25924096	388.09399513
423.49911012	450.63330112	457.56280635	473.40961872
540.16779099	699.60201418	841.81325445	890.98007492
893.55170675	913.39497399	927.53199871	936.3450505
955.67399137	987.30506289	1010.50535223	1016.69116933
1046.36224038	1066.38621689	1151.73659226	1825.49718171
4067.16084765	4100.57816074	4102.21844483	4123.74369829
4136.768666	4139.88242562	4141.30029831	4171.37449002]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.098372	0.213247	-1.599526
2	14	0	0.128482	0.328915	1.386034
3	8	0	1.748698	0.533214	1.323841
4	1	0	2.220974	0.789896	2.103556
5	8	0	-0.247406	-0.730092	2.563302
6	1	0	-1.036715	-0.568908	3.063562
7	8	0	-0.692687	1.698223	1.693450
8	1	0	-0.876279	2.278740	0.964566
9	8	0	-0.756633	-0.601202	-2.709503
10	1	0	-0.361135	-1.356442	-3.122439
11	8	0	-0.241115	-0.256888	-0.080275
12	8	0	1.675626	-0.024711	-1.920804
13	1	0	2.293110	0.081213	-1.207169
14	8	0	-0.346856	1.786390	-1.616370
15	1	0	-0.351668	2.261298	-2.435707
16	1	0	-0.912752	-2.685357	1.595755
17	8	0	-1.468444	-3.135301	0.971128
18	1	0	-1.520955	-2.547767	0.228620

$H_6Si_2O_7$ (Trihydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
227.9969 -1333.906616 0.1811

Rotational constant/ cm^{-1}
0.0191659257819 0.017211240184 0.0130466924555
Rotational symmmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[19.79461474 31.56156796 38.34511571 51.72455159
  53.05902 69.03093878 86.06626207 138.5484025
  150.89223529 164.75124576 172.49394267 187.97933651
  193.21990516 198.46742417 236.77083775 248.73240094
  257.4550981 263.0848867 275.17850666 285.20787081
  292.95056773 327.30617892 361.21001696 368.01441577
  371.55909749 386.80122886 409.97371676 423.56861369
  438.92195076 451.04337214 463.60961634 473.46522157
  618.22724261 638.4110773 660.41590535 689.33633792
  776.82047268 845.53169507 886.1009248 892.54390509
  906.62532695 955.40292747 958.28732534 973.58505956
  993.24066717 1022.61982326 1040.14862185 1050.66451093
  1122.13502477 1172.99773218 1218.05689208 1811.74937695
  1839.83576676 1852.96498981 3850.05951823 3925.39443018
  3954.04379885 3974.70025778 4006.62324427 4101.87092701
  4126.22497549 4143.9414337 4144.434909 4146.19334914
  4150.37051328 4153.53987575]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.689761	0.235220	-1.650070
2	14	0	-0.633143	0.228789	1.500316
3	8	0	3.135457	0.405650	1.532738
4	1	0	3.270156	0.551886	0.594703
5	8	0	0.613682	-0.736469	1.928990
6	1	0	1.505801	-0.384579	1.859404
7	8	0	-1.997986	-0.579864	1.867416
8	1	0	-2.013658	-1.511442	1.684158
9	8	0	-0.641958	1.660726	2.267384
10	1	0	-0.963523	1.690415	3.157268
11	8	0	-1.911757	1.036201	-2.370333
12	1	0	-2.772004	0.641103	-2.376985
13	8	0	-0.529706	0.553972	-0.080897
14	8	0	-0.893559	-1.357988	-1.870837
15	1	0	-0.739736	-1.962703	-1.148945
16	8	0	0.660750	0.810665	-2.394528
17	1	0	0.508200	1.275965	-3.206675
18	1	0	3.321288	1.229132	1.963791
19	1	0	3.815747	0.211059	-1.820124
20	8	0	3.314569	0.797610	-1.269890
21	1	0	2.440634	0.854187	-1.654677
22	1	0	0.190958	-2.496865	1.100740
23	8	0	-0.468044	-2.931834	0.560223
24	1	0	-0.294788	-3.863642	0.581776

$H_6Si_2O_7$ (Pentahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
264.01803 -1485.969843 0.23569

Rotational constant/ cm^{-1}
0.0162435707439 0.0113425134931 0.00903324926206
Rotational symmmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[17.16738006 29.41390787 31.21405015 42.61958484
  53.26753069 54.03902024 68.32895279 81.6875376
  87.43548226 107.09108988 121.13775997 130.81265594
  144.24074431 152.0042923 172.93876548 181.00812914
  200.45522607 211.03366836 222.20984129 229.63282182
  235.08885152 249.7402026 257.05197743 266.16389454
  273.25325797 294.23638364 315.83114067 327.1185193
  333.92291812 350.33270935 354.34306493 364.80335116
  371.74675711 390.95059157 402.58548801 422.03258494
  430.12279968 441.74379541 452.53769875 457.63230992
  506.33345652 585.65092262 604.72965067 632.54497659
  660.81902602 671.0638512 693.35364386 708.33166169
  797.24756985 844.60729768 876.13411386 916.09171224
  956.11881417 969.96392392 982.58577097 1000.98336409
  1046.46649573 1055.65486676 1085.73600883 1132.15743856
  1144.5568742 1157.69999797 1201.75830656 1797.31348691
  1803.9788786 1842.32399431 1848.26654895 1850.75477651
  3836.4020681 3910.33300807 3961.71004185 3972.44139198
  3974.67940671 4025.28495093 4035.53672648 4044.38453005
  4053.49644716 4058.86907258 4131.50029592 4142.80852562
  4145.58171779 4146.4227109 4152.3235634 4161.9776083]
Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.455543	-0.905395	-0.465747
2	14	0	-1.339818	0.505576	0.029031
3	8	0	0.737118	3.696245	0.216121
4	1	0	1.596980	3.353516	-0.037464
5	8	0	-1.030831	1.717889	1.065222
6	1	0	-0.478317	2.451272	0.777824
7	8	0	-2.132041	-0.668825	0.887738
8	1	0	-1.814969	-0.784225	1.779133
9	8	0	-2.300797	0.964181	-1.187214
10	1	0	-2.873001	0.310338	-1.575923
11	8	0	1.293021	-2.374494	-1.124377
12	1	0	0.457528	-2.828514	-1.022289
13	8	0	0.043295	-0.110839	-0.529999
14	8	0	1.998269	-0.877171	1.063510
15	1	0	1.384489	-0.707443	1.770995
16	8	0	2.594144	-0.132935	-1.364698
17	1	0	2.784225	-0.522007	-2.207991
18	1	0	0.504794	4.355259	-0.424078
19	1	0	3.885750	2.455152	0.153996
20	8	0	3.224510	2.540021	-0.519908
21	1	0	3.092634	1.661674	-0.875103
22	1	0	-0.316674	0.786427	2.737955
23	8	0	-0.140018	-0.112576	3.011391
24	1	0	0.038830	-0.104573	3.942706
25	1	0	-2.046973	-3.242518	-1.304706
26	8	0	-1.416744	-3.241349	-0.594463
27	1	0	-1.711652	-2.549225	-0.011258
28	1	0	-4.927545	-1.516480	-1.364311
29	8	0	-3.998219	-1.438449	-1.193378

30	1	0	-3.892477	-1.296489	-0.257492

$H_6Si_2O_7$ (Heptahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
300.03916 -1638.030316 0.289124

Rotational constant/ cm^{-1}
0.0128268737167 0.00738210699083 0.00703353251135
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}

[22.26199123	25.89007722	29.99078744	34.06369623	
43.34937225	48.28412522	52.27362974	61.67746181	
69.64952049	76.22455755	82.16016183	90.72995115	
92.68995163	106.81307563	119.66428443	129.74925142	
131.73705333	146.84017757	148.48046166	152.73407971	
163.79904694	170.32543151	184.12883912	190.97494008	
216.28118737	219.49225198	227.90913346	236.32601494	
250.21282683	253.06942327	272.62077555	277.63893279	
289.68390026	310.31255776	331.39993878	334.84036515	
350.65242573	356.49767538	363.70519487	375.79186448	
391.31896045	403.42648113	405.62279372	417.16038518	
425.69542272	435.61358116	444.47528544	455.15103272	
459.57840968	507.54281851	549.89828981	579.32609839	
594.42922263	620.88922907	637.04880747	657.94852887	
663.27945215	697.59336121	735.60485981	783.72217649	
816.79197176	846.87311384	890.34064214	911.17085997	
956.31342415	983.39896265	1001.12932158	1010.45669973	
1043.58209786	1050.91472376	1100.22750171	1132.21999177	
1157.24822481	1168.84141912	1204.41334266	1797.80001185	
1809.42795794	1812.09689476	1838.08427697	1846.96683232	
1851.30385465	1892.60287179	3834.34476264	3902.34009833	
3955.69103329	3963.92025515	3966.72124874	3977.44564851	
4016.05487777	4025.77842623	4032.28395973	4043.32807589	
4053.19758184	4059.18183861	4061.315598	4069.94099017	
4143.4479584	4144.35150472	4149.89788905	4151.89959167	
4162.30427505	4168.98356745]			

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.542880	-1.399539	0.250373
2	14	0	-1.447670	1.015573	-0.285615
3	8	0	1.729636	2.973736	-0.886117
4	1	0	2.422817	2.314853	-0.802429
5	8	0	-0.685128	2.302605	0.347761
6	1	0	0.124350	2.611289	-0.071245
7	8	0	-2.712596	0.656712	0.721009
8	1	0	-2.525490	0.772454	1.648060
9	8	0	-2.049933	1.318669	-1.754434
10	1	0	-2.814716	0.825415	-2.033494
11	8	0	-0.169940	-2.842085	0.119223
12	1	0	-1.124600	-2.875652	0.164231
13	8	0	-0.452224	-0.254694	-0.320012
14	8	0	0.985165	-0.987867	1.775380
15	1	0	0.406384	-0.407607	2.263382

16	8	0	1.967530	-1.410507	-0.535879
17	1	0	2.062900	-1.702818	-1.436646
18	1	0	1.739757	3.269040	-1.786682
19	1	0	4.063110	0.916675	0.263409
20	8	0	3.641371	0.866664	-0.590292
21	1	0	3.072053	0.101601	-0.508300
22	1	0	-0.500812	1.845364	2.332399
23	8	0	-0.747944	1.125226	2.911227
24	1	0	-0.603327	1.410217	3.804284
25	1	0	-3.556780	-2.412992	-0.479068
26	8	0	-3.029947	-2.377091	0.310092
27	1	0	-3.045653	-1.461378	0.568799
28	1	0	-5.453607	0.081347	-1.679652
29	8	0	-4.586395	-0.116373	-1.351372
30	1	0	-4.494825	0.320352	-0.509864
31	8	0	3.389905	-0.981705	-2.992473
32	1	0	4.016318	-1.359187	-3.594714
33	1	0	3.845492	-0.301417	-2.505855
34	8	0	3.712596	0.029314	2.236194
35	1	0	4.270853	-0.618182	2.644551
36	1	0	2.855380	-0.381176	2.133982

$H_6Si_2O_7$ (Nonahydrate)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
336.06029 -1790.10514 0.34619

Rotational constant/ cm^{-1}
0.00873270801229 0.00685040582308 0.00608754473737
Rotational symmmetry number
1.0

Vibrational Frequencies/ cm^{-1}

[18.71730952	28.63546796	36.35036345	38.32426464
47.9852599	51.48128912	52.93391359	61.67051146
63.42200125	74.77888344	78.18455803	80.06115423
91.69605068	101.48910271	114.43761649	114.76428324
118.12130533	133.78740844	139.74386379	148.50131272
150.85053315	165.49493388	167.35067901	174.0647232
180.00032748	188.47976217	195.22160778	204.66019164
212.78515815	216.21168381	222.34189806	223.02998334
231.37736126	236.75693703	244.90275462	263.33509953
271.66857673	281.64233802	302.99383258	325.40178129
333.37383997	344.64731789	350.3883122	354.03724925
373.40094191	380.97683028	382.9924336	398.96435238
404.75399918	417.87627188	427.91953673	434.557127
455.4568484	461.90677904	478.89344984	499.55685912
511.74083372	545.0330404	573.25148698	582.57886514
585.79688011	618.99873215	627.91603929	645.25717826
661.7920759	687.58484813	697.83662368	700.71407118
736.65436362	776.6258627	789.44231972	818.51566013
846.97736918	896.92957991	910.77468967	945.51257046
952.69228852	995.70804366	1003.8608116	1029.4520235
1088.33544208	1095.68891905	1146.73928608	1151.72269155
1166.42269512	1207.24213768	1212.52440847	1793.34483346
1807.05788644	1831.05746675	1835.68640405	1837.07647531
1839.66200785	1847.96768363	1893.42301384	1907.62259176
3755.77098465	3859.08108071	3909.74222779	3929.99556605
3951.03429457	3966.54053948	3973.04607298	3974.52649887
3980.76791883	3990.21345304	4004.65629343	4028.68367516
4037.14920914	4043.34892696	4050.13247471	4055.76226331
4072.06779919	4101.21759352	4145.88058311	4149.70327907

4150.12030045 4152.40001732 4155.20101091 4166.37023348]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.349269	-1.646646	0.685408
2	14	0	1.468466	0.614690	-0.613810
3	8	0	-1.489778	1.755338	-2.362156
4	1	0	-2.157836	1.196592	-1.963115
5	8	0	1.016292	0.641938	-2.169925
6	1	0	0.147773	1.011422	-2.376713
7	8	0	3.009400	0.019751	-0.550506
8	1	0	3.157587	-0.728689	-1.121415
9	8	0	1.502614	2.113955	0.034959
10	1	0	2.224889	2.302950	0.631169
11	8	0	0.433013	-2.399012	1.881580
12	1	0	1.326398	-2.134077	2.092334
13	8	0	0.506598	-0.329083	0.258439
14	8	0	-0.565920	-2.574956	-0.649468
15	1	0	0.181543	-2.649992	-1.236569
16	8	0	-1.863293	-1.251891	1.111302
17	1	0	-2.017786	-0.784055	1.935645
18	1	0	-1.476667	2.556939	-1.848370
19	1	0	-3.657636	-0.588852	-1.493265
20	8	0	-3.380480	0.121049	-0.918595
21	1	0	-2.918369	-0.329950	-0.212294
22	1	0	1.418622	-1.258634	-2.823944
23	8	0	1.780339	-2.056372	-2.441215
24	1	0	2.008653	-2.639247	-3.153768
25	1	0	3.264272	-0.713503	2.880138
26	8	0	3.120117	-1.349682	2.191392
27	1	0	3.236960	-0.877400	1.373452
28	1	0	4.781693	2.489060	1.532411
29	8	0	4.056180	1.911362	1.335435
30	1	0	4.312538	1.368088	0.596832
31	8	0	-3.332814	2.343774	1.096797
32	1	0	-2.594000	2.837180	0.750662
33	1	0	-3.644899	1.794389	0.383511
34	8	0	-3.157915	-2.565992	-2.031131
35	1	0	-3.682565	-3.311429	-1.772790
36	1	0	-2.319497	-2.657978	-1.581250
37	8	0	-0.959779	3.666170	-0.156703
38	1	0	-0.113636	3.252303	0.014442
39	1	0	-0.820134	4.603791	-0.141529
40	8	0	-2.487135	0.559110	3.135518
41	1	0	-3.131000	0.451295	3.822112
42	1	0	-2.811799	1.246799	2.549341

$H_6Si_2O_7$ (11 explicit waters)

Parameters from the HF/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
372.08142 -1942.174981 0.401885

Rotational constant/ cm^{-1}
0.00690177469374 0.00563990172161 0.00527198052461
Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

```
[   11.32908077    22.90837437    33.8134834     37.04539908
    39.70043519    42.44582593    45.08696132    51.34923235
    53.06597036    59.97462452    64.11703688    75.15420268
    78.49037371    86.25392169    88.83945424    96.25548441
   112.24825426   123.50783147   128.08811627   132.52939394
   133.77350772   143.79592151   148.46656094   151.0659942
   160.15010988   164.87635217   167.88585645   173.89791465
   180.72316454   186.19309494   187.4719605    200.14246004
   207.45423487   212.81295958   220.89622395   232.62842539
   234.61622729   240.78814369   246.40403158   251.53339453
   255.30048764   267.31765369   272.25240666   278.93169907
   302.21539267   324.95000813   344.73072217   347.47611291
   359.26391719   367.2151248    373.52604832   376.12548158
   382.52675973   391.88193931   399.40222483   406.60279396
   424.80577711   440.47188021   445.30237784   456.04762868
   469.48266741   475.25146314   491.20948121   496.491752
   526.83005725   534.5519031    538.33289693   564.68169766
   580.78567321   596.11120886   606.26567941   634.42852314
   638.73079369   654.49420178   682.44158447   694.98697759
   711.27166241   722.33662964   743.42401065   757.58883679
   788.48317055   804.79565679   839.87410504   849.39609317
   867.76588488   904.9641918    934.55185857   942.95483934
   962.40193627   992.4413762   1002.59584676  1026.33826388
  1041.22592708  1116.89445612  1141.89488774  1162.39148847
  1188.05915429  1207.56185407  1207.9858258   1810.56781638
  1814.44611519  1828.27732423  1832.39193516  1839.52300072
  1850.07364159  1855.26555775  1858.9631473   1871.77960432
  1888.85662975  1903.67478938  3781.16758658  3794.02574573
  3870.59087074  3915.8793924   3926.41613255  3941.62351214
  3944.57046321  3962.27997107  3970.07827084  3988.39245969
  3991.23515541  3991.90238962  3994.1960072   3999.4921787
  4014.20608299  4020.54480794  4055.92212151  4065.7360246
  4090.47234268  4099.18113912  4099.52865694  4104.85262987
  4124.87660637  4147.8058318   4148.7927824   4151.2740596
  4155.22186198  4156.59803253]
```

Ground State Electronic Degeneracy and Irreducible Representation

1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.019789	-1.597277	0.438385
2	14	0	1.449452	0.878573	-0.891915
3	8	0	-1.638411	1.377169	-2.625332
4	1	0	-2.222319	0.863898	-2.066871
5	8	0	1.035641	0.679424	-2.447204
6	1	0	0.117752	0.883373	-2.665763
7	8	0	3.068243	0.683911	-0.692933
8	1	0	3.415305	-0.196139	-0.770634
9	8	0	1.128469	2.412853	-0.416982
10	1	0	1.698336	2.766640	0.261620
11	8	0	1.028215	-2.528907	1.232937
12	1	0	1.578487	-2.167870	1.929470
13	8	0	0.674148	-0.181257	0.040886
14	8	0	-0.586171	-2.384468	-0.865121
15	1	0	0.046132	-2.561556	-1.560253
16	8	0	-1.374056	-1.245911	1.300829
17	1	0	-1.323806	-0.534121	1.941169
18	1	0	-1.739271	2.280785	-2.343109
19	1	0	-3.740843	-0.707176	-1.006670

20	8	0	-3.281468	0.042791	-0.628299
21	1	0	-2.678069	-0.365430	-0.012883
22	1	0	1.369679	-1.205901	-3.024073
23	8	0	1.509893	-2.124267	-2.801198
24	1	0	1.752992	-2.580086	-3.595787
25	1	0	2.200487	-0.426757	3.470100
26	8	0	2.533445	-1.307948	3.283895
27	1	0	2.686242	-1.731552	4.117467
28	1	0	3.949550	3.196492	1.745301
29	8	0	3.256809	2.598554	1.495454
30	1	0	3.646250	1.921351	0.945966
31	8	0	-2.928964	2.448114	1.004223
32	1	0	-2.486048	3.040485	0.401812
33	1	0	-3.348366	1.784969	0.460752
34	8	0	-3.628029	-2.725086	-1.245370
35	1	0	-3.818704	-3.109787	-0.393879
36	1	0	-2.682597	-2.794651	-1.336163
37	8	0	-1.287552	3.837038	-1.008231
38	1	0	-0.419656	3.480939	-0.815382
39	1	0	-1.177349	4.748397	-1.244626
40	8	0	-1.392212	1.112649	2.911470
41	1	0	-1.898773	1.109293	3.713970
42	1	0	-1.885827	1.655988	2.284735
43	8	0	-3.396193	-3.367901	1.624590
44	1	0	-3.011401	-4.164745	1.963690
45	1	0	-2.718649	-2.697615	1.665762
46	8	0	1.498581	1.295789	3.551988
47	1	0	2.004619	1.827205	2.945605
48	1	0	0.581659	1.359677	3.294867

$H_6Si_2O_7$ (13 explicit waters)

Parameters from the HF/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
408.10255	-2094.247019	0.458053

Rotational constant/ cm^{-1}

0.0057933412054	0.00492107109646	0.00440371318481

Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

[29.28880145	32.97249029	36.86468982	41.27816607
44.48228033	48.06171382	50.14682071	52.0095162
58.50114898	60.26653948	68.36370458	76.44696895
79.88739532	82.53548107	87.76909937	91.2790293
95.37278916	97.74981102	101.83662052	116.97449654
122.44442695	127.70584667	128.69279727	133.37038706
142.60741058	145.01918422	150.98954028	156.1397543
158.00244979	162.85379849	164.13266404	166.04401203
168.19167212	181.50160444	182.64146287	189.58486882
195.80543771	206.51593677	212.33338499	215.44019426
231.73877978	236.95849737	243.40842801	252.986019
258.7270133	268.85368243	272.23850595	276.88829431
289.33638245	296.44659694	323.14986585	325.58944091
353.86349035	358.90249866	361.00845662	370.43313977
383.32605071	387.30860487	388.85853432	399.98605476
409.51499325	412.50364646	430.36606215	436.30861679
437.05925527	455.06762844	459.272594	466.20904959
475.9256477	484.82210377	491.16082871	502.76097338
505.86778265	524.33487934	530.62495179	547.2919062
555.23616345	562.71474683	578.53375777	610.56099961

```
   629.13235164   637.70214096   649.93476805   653.50030083
   680.9264068    696.68981489   702.51421347   724.80400612
   769.87011638   774.24189049   785.1191981    795.50998077
   825.58417249   830.26871263   847.22063165   853.85822192
   876.25922028   915.04220843   946.47171963   966.82236288
   978.46420968   997.14676742  1002.22052752  1021.23670235
  1114.17686681  1149.0746058   1161.11957327  1181.3937626
  1194.32142532  1225.8482415   1243.56469971  1814.76583158
  1825.08711069  1826.35902589  1829.29902661  1843.08158315
  1848.28044966  1855.64087699  1859.43577153  1862.3827226
  1871.57804398  1874.27478223  1885.97918224  1902.67393807
  3782.16148753  3791.280355    3800.53822959  3876.0051983
  3882.53853323  3895.24378454  3923.33712471  3940.12223518
  3952.07684802  3969.05656846  3974.85316561  3986.32820387
  3987.16919698  3993.53572335  3995.18990815  4003.96820816
  4017.5770058   4019.09913383  4019.48140342  4060.36339918
  4064.75602437  4089.03361892  4092.02922249  4102.39915409
  4114.12440517  4118.96880351  4123.92440755  4140.42455341
  4145.79022848  4147.34710829  4148.59122207  4157.55023134]
Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0       -1.068193   -0.510360   -0.053956
      2         14           0        1.933492   -0.395983   -1.010587
      3          8           0        0.871893    2.910990   -1.918600
      4          1           0        0.084035    3.040656   -1.391120
      5          8           0        1.665691    0.304712   -2.455073
      6          1           0        1.385503    1.227594   -2.415098
      7          8           0        2.509337   -1.909284   -1.175023
      8          1           0        1.876368   -2.561398   -1.486570
      9          8           0        3.057198    0.456217   -0.176142
     10          1           0        3.568715   -0.049982    0.450596
     11          8           0       -1.532731   -2.061433    0.178521
     12          1           0       -1.178978   -2.517284    0.950557
     13          8           0        0.540864   -0.433870   -0.181649
     14          8           0       -1.829069    0.037167   -1.380425
     15          1           0       -1.569465   -0.305120   -2.233470
     16          8           0       -1.534060    0.475259    1.161420
     17          1           0       -0.939880    0.584515    1.907194
     18          1           0        1.576790    3.339336   -1.442611
     19          1           0       -2.137727    3.421331   -0.378075
     20          8           0       -1.293227    3.249199    0.037674
     21          1           0       -1.416971    2.383708    0.417880
     22          1           0        0.302992   -0.527757   -3.579018
     23          8           0       -0.513147   -0.998382   -3.756965
     24          1           0       -0.750807   -0.825716   -4.658943
     25          1           0        0.360802   -2.713420    2.754626
     26          8           0       -0.364067   -3.235179    2.398878
     27          1           0       -0.824080   -3.617506    3.133877
     28          1           0        4.756503   -2.298566    1.553368
     29          8           0        3.954064   -1.864690    1.293481
     30          1           0        3.633599   -2.298223    0.503512
     31          8           0        0.884781    3.548546    1.986717
     32          1           0        1.662505    3.600418    1.436731
     33          1           0        0.145475    3.767136    1.424255
     34          8           0       -3.797698    2.396370   -1.085481
     35          1           0       -4.315987    2.028523   -0.372225
     36          1           0       -3.315941    1.652549   -1.431297
     37          8           0        3.063874    3.318871    0.022266
     38          1           0        3.196433    2.371460   -0.026849
```

39	1	0	3.915440	3.730302	-0.043559
40	8	0	0.328942	1.106589	3.206153
41	1	0	-0.005154	1.297068	4.073843
42	1	0	0.611617	1.951394	2.834418
43	8	0	-4.580294	0.752415	1.218170
44	1	0	-4.795258	-0.157212	1.028258
45	1	0	-3.666895	0.736651	1.480709
46	8	0	1.698631	-1.528047	3.237205
47	1	0	2.469769	-1.607718	2.683467
48	1	0	1.414701	-0.617850	3.204171
49	8	0	0.226958	-3.318366	-2.065245
50	1	0	-0.433128	-3.274138	-1.380935
51	1	0	-0.124977	-2.832818	-2.805543
52	8	0	-4.492614	-2.141683	0.526184
53	1	0	-4.960363	-2.519825	-0.205903
54	1	0	-3.562422	-2.242520	0.340850

$2H_4SiO_4$ Hydrogen-bonded Dimer (No explicit waters)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
191.97577	-1186.0108544	0.117334

Rotational constant/ cm^{-1}

0.066962992111	0.0133305555005	0.0131751146321

Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

[20.52440216	42.23036488	44.6768903	97.72895995	
120.33151864	155.34741368	198.35621847	210.31083131	
225.14289165	232.95509214	288.06446725	289.0583682	
304.02248531	308.65837297	355.573278	358.57583192	
363.9067552	366.32547919	372.92136732	384.92463265	
400.55598398	403.55158754	679.19576808	736.93237787	
752.60543133	756.79649618	827.46771904	831.29041501	
850.49424947	850.64020695	900.70362339	913.62433575	
928.025474	930.29129016	952.84519635	956.8625023	
1009.57400448	1036.43018123	1049.73316319	1084.76295894	
3509.49900985	3541.17178351	3802.12986118	3802.41482579	
3811.88121107	3812.21482817	3815.96802058	3816.25993554]	

Ground State Electronic Degeneracy and Irreducible Representation

1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.322431	1.106544	-1.505280
2	8	0	1.384636	1.177251	0.166584
3	1	0	2.274600	1.175806	0.549928
4	8	0	2.649966	0.208676	-1.907135
5	1	0	3.009024	0.344018	-2.795467
6	8	0	-0.152448	0.531598	-1.902283
7	1	0	-0.568283	-0.157009	-1.337300
8	8	0	-0.728817	0.391045	1.800131
9	8	0	1.501933	2.563588	-2.262591
10	1	0	0.038420	0.711763	1.275922
11	14	0	-1.332463	-1.096044	1.504120

12	8	0	-0.554416	-2.402689	2.150127
13	1	0	-0.805095	-2.651562	3.051014
14	8	0	-1.222042	-1.347405	-0.147734
15	1	0	-1.224620	-2.274938	-0.428212
16	8	0	-2.871290	-1.129938	2.103769
17	1	0	-3.327315	-0.277068	2.144369
18	1	0	0.683544	3.044995	-2.450957

$2H_4SiO_4$ Hydrogen-bonded Dimer (Dihydrate)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
227.9969	-1338.8905445	0.168407

Rotational constant/ cm^{-1}

0.0255533446408	0.0139930137936	0.0105983319967

Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

[21.789367	41.5283789	65.97278201	67.97448462	
82.25051646	93.23207942	108.93988466	122.52783123	
140.49450227	154.52727164	176.55990111	181.48075337	
196.91054436	209.55324247	233.49721993	239.12005817	
259.97807743	279.06375584	300.53340645	310.32645848	
324.12291573	334.42334377	349.48476588	364.64349297	
374.81186424	388.36505902	391.59002435	393.70293266	
403.88520464	430.30350894	628.27745782	662.22299799	
703.39690872	741.6516698	751.84089213	760.19522041	
819.70417106	832.22176275	836.77424613	868.82233903	
876.33567419	916.63384003	926.33653742	936.10178803	
950.29441559	974.20364127	980.43811087	1014.8840767	
1043.60294893	1085.69430669	1149.35262005	1224.06199993	
1681.15218205	1691.20239726	3315.09059375	3455.8909117	
3484.60283358	3530.70454692	3547.82327449	3596.07264793	
3791.30120606	3815.91936808	3816.55185051	3821.7854688	
3824.11383816	3825.37185265]			

Ground State Electronic Degeneracy and Irreducible Representation

1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.514540	-1.853418	-1.023363
2	8	0	0.400883	-1.821766	0.626882
3	1	0	1.232705	-1.784080	1.156195
4	8	0	-1.070473	-2.098986	-1.518663
5	1	0	-1.538154	-2.816218	-1.064033
6	8	0	1.037799	-0.478659	-1.734353
7	1	0	0.591221	0.355892	-1.459827
8	8	0	0.072156	0.708964	1.806205
9	8	0	1.514310	-3.086444	-1.464890
10	1	0	-0.125696	-0.166623	1.405733
11	14	0	-0.431809	2.014878	0.900966
12	8	0	-1.909133	2.593588	1.337180
13	1	0	-1.990085	3.015607	2.203344

14	8	0	-0.535257	1.556052	-0.681086
15	1	0	-1.406330	1.252889	-1.050960
16	8	0	0.680118	3.209008	1.139186
17	1	0	1.612569	2.952111	1.153481
18	1	0	2.024830	-2.957137	-2.276805
19	1	0	-2.864597	0.451817	-2.700894
20	8	0	-2.602208	0.231420	-1.794877
21	1	0	-2.151736	-0.642426	-1.833877
22	1	0	1.709582	-0.123261	2.445898
23	8	0	2.317881	-0.885845	2.346529
24	1	0	2.498848	-1.217667	3.238388

$2H_4SiO_4$ Hydrogen-bonded Dimer (Tetrahydrate)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
264.01803 -1491.7695253 0.220581

Rotational constant/ cm^{-1}
0.0258568879675 0.00764161985689 0.00677868954262
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[13.60184728 18.02922424 29.1219929 54.53249554
57.56980124 69.62171907 94.21903001 103.96342955
116.00839702 122.6112355 136.67875666 157.73833625
177.02557498 184.58756264 188.52841466 197.78628925
212.10402323 223.433104 228.89608406 250.8383589
264.28729834 272.71113018 284.49198411 302.97298151
304.32830099 311.64702617 326.0690155 330.23227892
351.47951813 369.56434523 378.24534025 389.64392458
393.16775523 400.13201224 402.98860868 414.90846974
430.79698424 482.99416006 580.49375825 643.49873812
649.67065451 698.46215574 704.93988782 715.46967761
730.26003582 743.39620923 751.48642396 760.59834107
837.85155136 877.00985876 878.12886612 898.22234619
907.97369608 931.19483648 948.37611725 968.5043491
995.33967478 1026.60237742 1070.81359385 1081.23217794
1119.43828653 1134.97233286 1161.72425426 1177.46681129
1658.84848868 1680.86721744 1683.61260818 1701.85034312
3315.39640943 3469.93758178 3482.80269129 3508.59546353
3524.35192126 3526.90270202 3592.57661871 3605.79619639
3626.12598857 3630.92868478 3684.61323685 3802.30362009
3817.00362366 3821.74376666 3823.53000823 3825.39965408]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.542838	-1.720052	-1.208781
2	8	0	0.537444	-1.740320	0.447624
3	1	0	1.338993	-1.424101	0.914049
4	8	0	-1.005632	-2.114042	-1.644930
5	1	0	-1.128904	-3.061051	-1.890466
6	8	0	1.037654	-0.292962	-1.835778
7	1	0	0.556371	0.496459	-1.492111

8	8	0	-0.590908	0.403613	1.976481
9	8	0	1.573947	-2.894732	-1.806224
10	1	0	-0.616570	-0.416212	1.442174
11	14	0	-0.457041	1.799771	1.070485
12	8	0	-1.462051	2.954819	1.628866
13	1	0	-1.029242	3.789652	1.915003
14	8	0	-0.695705	1.422967	-0.523497
15	1	0	-1.570718	1.052224	-0.813276
16	8	0	1.107491	2.370506	1.209581
17	1	0	1.780613	1.694093	1.411767
18	1	0	2.230778	-2.569712	-2.440167
19	1	0	-3.272790	0.232228	-2.200717
20	8	0	-2.813896	-0.017589	-1.385222
21	1	0	-2.327941	-0.852608	-1.576103
22	1	0	1.157936	-0.037678	2.602765
23	8	0	2.066455	-0.194404	2.257419
24	1	0	2.630286	-0.425742	3.010975
25	1	0	1.047831	4.193643	1.858102
26	8	0	0.461971	4.901953	2.197599
27	1	0	0.599942	5.671403	1.625703
28	1	0	0.423971	-4.471690	-2.231726
29	8	0	-0.513546	-4.735345	-2.327914
30	1	0	-0.647527	-5.502658	-1.751875

$2H_4SiO_4$ Hydrogen-bonded Dimer (Hexahydrate)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
300.03916 1644.65987879 0.271941

Rotational constant/ cm^{-1}
0.0145263827818 0.0058837370752 0.00531467672879
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[19.77376368 20.94837389 27.38440383 30.9985891
36.36426417 47.64469244 60.79476656 67.55746324
73.40271289 80.53377846 91.32768179 113.65222623
122.52783123 127.10811603 146.52741153 154.06159776
180.0767814 191.07919542 199.23891372 209.12927074
215.99622276 221.3827489 227.25579997 241.6291368
255.11282802 260.32559525 267.61651901 276.45042187
287.36943162 296.12688055 318.15951003 326.60419293
330.83000956 347.33710578 357.4498742 376.8691697
379.58675902 395.3988196 400.3127215 404.36477923
407.54109206 422.59556381 429.19145193 437.44847522
444.66989542 483.5918907 486.76125317 612.74341148
638.91150296 667.33150987 679.89775406 701.37435503
720.73804769 745.59947218 749.380466 769.95352065
801.45948577 841.6464459 852.16928534 863.42886254
875.32787253 894.17028846 906.60447588 921.52689086
943.70547782 948.02859944 951.39952224 967.71895884
990.19641112 1013.13953726 1133.2486445 1163.21858087
1183.97929514 1194.01560964 1220.30880752 1327.90032306
1688.2067937 1701.96154882 1707.98055737 1721.66580893
1724.07758257 1728.88722913 3164.77523804 3235.14064523
3315.91768615 3375.55869357 3387.62451211 3418.58139907
3442.90764613 3496.33503501 3527.77844692 3534.70795215
3598.49832228 3603.94740162 3723.95920387 3784.15623979
3812.38858708 3816.62830442 3817.51099967 3819.3041916
3819.70731227 3823.04348329]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.840823	-0.149317	-0.281194
2	8	0	0.868179	0.704254	-1.354064
3	1	0	1.190401	0.697689	-2.268892
4	8	0	1.528972	0.463800	1.205747
5	1	0	1.822539	1.400855	1.383027
6	8	0	1.515330	-1.764007	-0.321630
7	1	0	0.579169	-2.007463	-0.102419
8	8	0	-1.840486	-0.109468	-1.344612
9	8	0	3.411264	0.028336	-0.782007
10	1	0	-0.916512	0.227891	-1.340208
11	14	0	-2.323959	-0.972554	0.003958
12	8	0	-2.726215	-0.034153	1.289019
13	1	0	-3.487680	0.590933	1.161423
14	8	0	-1.060632	-1.913736	0.523791
15	1	0	-0.829370	-1.725088	1.480816
16	8	0	-3.644289	-1.825081	-0.497530
17	1	0	-3.645615	-2.118913	-1.419201
18	1	0	3.888518	-0.831196	-0.903246
19	1	0	-1.206495	-0.264788	2.831980
20	8	0	-0.417137	-0.835810	2.885819
21	1	0	0.317262	-0.300182	2.518926
22	1	0	-5.615806	1.263562	0.618839
23	8	0	-4.738501	1.674800	0.604134
24	1	0	-4.520160	1.818183	-0.349194
25	1	0	4.328560	1.594753	-0.498277
26	8	0	4.583608	2.505897	-0.226170
27	1	0	5.491309	2.451982	0.107588
28	8	0	4.057844	-2.614876	-1.027166
29	1	0	3.124283	-2.760245	-0.764212
30	1	0	4.602374	-3.137515	-0.419869
31	8	0	-3.806478	1.784003	-1.992857
32	1	0	-3.052849	1.155301	-1.901437
33	1	0	-3.437603	2.610800	-2.336576
34	8	0	2.525331	2.949572	1.525932
35	1	0	3.320780	2.940576	0.936546
36	1	0	1.982240	3.701564	1.246887

$2H_4SiO_4$ Dimerization/H_2O-loss transition state (No explicit waters)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
191.97577 -1185.9574879 0.115663

Rotational constant/ cm^{-1}
0.0553105975735 0.0227137134984 0.0211506321483
Rotational symmetry number
1.0

Imaginary Frequency/ cm^{-1}
-1020.0138

Non-imaginary Vibrational Frequencies/ cm^{-1}

[53.92781454	74.43831598	112.067545	143.1286873
199.12075766	211.11707264	236.85424202	289.25992853
298.23283851	305.97553543	317.55482903	330.16972572
359.18051292	373.48434618	393.65428017	406.08846759
432.93769398	455.86691942	467.77287976	526.79530547
541.59261403	590.67603023	597.05645731	629.81348656
764.00401566	776.0698342	792.96615037	836.635239
852.9060231	896.83922528	906.24305736	929.21398493
952.36562177	954.554984	994.29712133	1019.2419501
1038.03571353	1082.19827747	1338.65947462	1947.47593479
3643.75904251	3685.14841428	3781.43865047	3785.17794216
3811.40163649	3817.27468756	3817.67085787]	

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.060306	0.040708	-1.702575
2	14	0	-0.051637	0.026145	1.412025
3	8	0	1.906582	0.069622	1.500810
4	1	0	1.587528	0.417629	0.278383
5	8	0	-0.002989	-1.646249	1.408559
6	1	0	0.863262	-2.000745	1.662814
7	8	0	-1.644762	0.276049	0.882845
8	1	0	-2.301024	0.274479	1.594294
9	8	0	-0.215212	0.861964	2.847163
10	1	0	0.501336	0.771006	3.490364
11	8	0	-1.517931	0.763837	-1.882637
12	1	0	-2.003599	0.785086	-1.033486
13	8	0	0.553497	0.594932	-0.191177
14	8	0	-0.016176	-1.594322	-1.629975
15	1	0	-0.179066	-1.977835	-0.748152
16	8	0	0.944574	0.510611	-2.906745
17	1	0	0.687821	1.313088	-3.382762
18	1	0	2.350293	0.789796	1.975490

$2H_4SiO_4$ Dimerization/H_2O-loss transition state (Dihydrate)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
227.9969	-1338.8424987	0.166146

Rotational constant/ cm^{-1}

0.0239485677788	0.0191002136551	0.0140690664073

Rotational symmetry number
1.0

Imaginary Frequency/ cm^{-1}
-1150.0902
Non-imaginary Vibrational Frequencies/ cm^{-1}

[30.79007841	51.98866513	53.94866561	68.91278272
87.51193618	111.0805944	129.01251366	137.64485618
149.91918541	183.58671133	196.91749472	219.58955697
231.82913442	252.36743728	272.64857697	288.32163043
311.93894114	332.0810737	332.92206681	357.4498742

```
   375.86831839   384.49371056   396.99045119   438.692589
   454.15018141   474.23671112   499.95302943   527.53204324
   533.35644182   547.7853815    583.39900718   605.14667205
   630.43206827   654.70966283   687.30683388   745.89138714
   765.14387409   797.04600951   836.69779221   849.06942643
   914.05525784   932.01497852   942.55866903   955.70874315
   972.90392464  1003.20747811  1033.21911662  1053.46550452
  1063.41841474  1107.52537583  1264.13775436  1682.06267873
  1687.33799916  1941.06075592  3462.57715446  3531.00341224
  3594.59222204  3644.30812066  3741.73821528  3775.98957113
  3789.68177305  3791.51666711  3802.25496759  3823.33539825
  3831.50206691]

Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          14              0       -0.117390    0.102948   -1.664947
    2          14              0       -0.175419    0.215867    1.550353
    3           8              0        1.649639   -0.092391    1.772180
    4           1              0        1.537231    0.070145    0.445082
    5           8              0       -0.510854   -1.345612    2.114268
    6           1              0        0.288076   -1.760603    2.476877
    7           8              0       -1.763931    0.531789    0.967332
    8           1              0       -2.336626   -0.247159    0.866593
    9           8              0       -0.055794    1.569925    2.511024
   10           1              0       -0.896801    2.047176    2.578287
   11           8              0       -1.311122    1.216376   -1.736066
   12           1              0       -1.749845    1.307951   -0.863655
   13           8              0        0.537332    0.239025   -0.103416
   14           8              0       -0.531525   -1.448410   -1.974970
   15           1              0       -1.161442   -1.880286   -1.354911
   16           8              0        1.104400    0.483864   -2.715236
   17           1              0        1.309100   -0.211881   -3.358101
   18           1              0        2.124694    0.635993    2.202725
   19           1              0        3.936405    1.709819   -1.085724
   20           8              0        3.339189    0.957741   -0.963530
   21           1              0        2.709621    0.985311   -1.709678
   22           1              0       -1.548539   -2.288358    0.948530
   23           8              0       -2.136628   -2.325553    0.157177
   24           1              0       -2.678186   -3.125544    0.228184
 ---------------------------------------------------------------------
```

$2H_4SiO_4$ Dimerization/H_2O-loss transition state (Tetrahydrate)

```
Parameters from the DFT/B3LYP/6-31+G(d) level of theory
Mass/ a.m.u.  Energy a.u.   ZPE a.u.
264.01803     -1491.72627671 0.217741

Rotational constant/ cm-1
0.0177692929153   0.0116283779227   0.010129674443
Rotational symmetry number
1.0

Imaginary Frequency/ cm-1
-1254.4512
Non-imaginary Vibrational Frequencies/ cm-1
```

```
[   30.18539741    37.94199505    48.32582736    50.64724636
    67.1195908     98.5630027    107.36215378   117.28726258
   136.84556521   144.52570892   152.37266118   159.93464884
   190.7803301    206.80785173   214.73125792   219.48530162
   225.27494842   246.30672659   251.90871377   268.10999431
   274.23325821   292.23468103   299.72021476   330.51029317
   335.500649     345.80107704   366.21427349   373.53994903
   381.01853241   413.60180275   422.19244314   438.48407831
   464.79117691   484.31472776   502.62891661   515.50097648
   528.83175986   544.15034515   557.02240502   600.14936587
   622.4113571    664.10654455   675.36612175   682.30257734
   725.13067287   760.33422753   766.50614393   811.7599138
   819.59296535   847.65155374   857.66006681   860.73907466
   936.99143363   945.87398898   955.99370776   968.06647665
   972.89697428  1056.46110809  1075.37302758  1139.76112835
  1203.44724314  1212.46880562  1314.3749297   1678.37203953
  1686.28849536  1692.52296496  1717.38438945  1783.87149782
  3293.73214884  3405.90394918  3420.72905917  3459.71360766
  3571.63519518  3590.88768213  3595.65562655  3699.11863045
  3778.61680582  3788.65312031  3798.84929301  3815.98887164
  3823.057384    3827.83922914  3828.0199384 ]

Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0        1.285280   -0.205151    0.490203
      2         14           0       -1.805703    0.333675   -0.519313
      3          8           0       -1.583614    2.168307   -0.594002
      4          1           0       -0.344592    1.756293   -0.267645
      5          8           0       -2.869276    0.520220    0.789022
      6          1           0       -3.070856    1.458851    0.929908
      7          8           0       -1.704983   -1.385301   -0.372048
      8          1           0       -1.877127   -1.728829    0.523141
      9          8           0       -2.245961    0.329786   -2.125445
     10          1           0       -2.426912   -0.557180   -2.470532
     11          8           0        1.909311   -1.181928   -0.677579
     12          1           0        1.347815   -1.913870   -1.047609
     13          8           0       -0.091584    0.623664   -0.068283
     14          8           0        0.875424   -1.001638    1.853428
     15          1           0       -0.055375   -1.062464    2.153941
     16          8           0        2.426335    0.952653    0.760718
     17          1           0        3.282789    0.778144    0.296776
     18          1           0       -1.614579    2.536897   -1.491285
     19          1           0        1.063577    4.002397    0.412868
     20          8           0        1.180220    3.263574   -0.201595
     21          1           0        1.813604    2.648005    0.222720
     22          1           0       -2.397358   -0.539048    2.184422
     23          8           0       -1.846917   -1.296107    2.497804
     24          1           0       -2.205994   -1.607039    3.341844
     25          1           0        3.729280   -0.662721   -1.092783
     26          8           0        4.423679   -0.012648   -0.852742
     27          1           0        5.172641   -0.523398   -0.511511
     28          1           0       -0.654885   -2.496797   -1.234597
     29          8           0        0.116694   -2.955662   -1.653123
     30          1           0        0.099836   -3.873392   -1.344015
 ---------------------------------------------------------------------
```

$2H_4SiO_4$ Dimerization/H_2O-loss transition state (Hexahydrate)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
300.03916 1644.61408252 0.269463

Rotational constant/ cm^{-1}
0.0107237520965 0.00857593288754 0.00706922386953
Rotational symmetry number
1.0

Imaginary Frequency/ cm^{-1}
-1070.6839
Non-imaginary Vibrational Frequencies/ cm^{-1}

[19.32199052	25.22284302	31.79788008	40.08965514
45.97660693	53.2814314	61.46200077	71.10909531
81.68058725	97.95137135	126.9691089	134.51719585
144.14343932	161.09535834	170.89536073	180.96642701
194.6933807	196.7298351	211.47849117	215.50969782
220.7780679	234.37991518	250.63679857	260.31864489
274.69198172	281.52418197	285.79865109	295.57085205
300.58205894	317.83979364	326.20107227	334.15923023
348.36575851	361.2030666	370.66945188	390.01924382
404.69144597	408.4724398	415.3115904	418.6686125
446.57429304	459.62011182	492.14082895	529.61715013
549.55772235	555.13190811	565.65474755	592.42056966
630.7448343	645.5212918	652.86086805	669.05519823
718.45833082	754.79479356	759.73649689	773.68586199
797.10856272	809.20913304	816.58346108	857.65311646
868.21765804	886.46929368	917.26632245	935.01753244
959.5661909	1003.7496059	1011.73556529	1016.61471541
1065.94139408	1079.75175205	1144.31361173	1152.34822361
1211.05788329	1222.56072297	1268.62073417	1686.22594215
1690.40310629	1704.53318065	1725.68311487	1731.01403816
1751.1909225	2030.96361468	3126.57607981	3298.60434861
3383.09983016	3400.64947982	3438.54282237	3450.17771882
3468.8533262	3528.16766687	3592.47236337	3602.87009639
3647.79024916	3772.88971222	3785.935531	3792.54531984
3811.38773577	3812.6874524	3816.48234694	3821.54220633
3825.19114339]			

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.941187	1.103518	0.364570
2	14	0	1.668339	-0.946388	0.126231
3	8	0	1.491181	-1.075804	-1.697691
4	1	0	0.586094	-0.149954	-1.369673
5	8	0	1.179757	-2.539319	0.350688
6	1	0	1.148068	-3.015594	-0.494507
7	8	0	1.610585	-0.542544	1.808655
8	1	0	1.040373	-1.122361	2.335954
9	8	0	3.269038	-0.442647	-0.031273
10	1	0	3.672381	-0.270860	0.833846
11	8	0	-0.382853	2.574688	0.843306
12	1	0	0.299187	2.551186	1.567080

13	8	0	0.338271	0.196838	-0.312843
14	8	0	-1.577683	0.258184	1.587444
15	1	0	-1.589327	-0.744096	1.563215
16	8	0	-1.964953	1.377275	-0.904729
17	1	0	-2.049258	2.331303	-1.155397
18	1	0	2.259785	-0.793186	-2.248125
19	1	0	-3.424839	-0.696117	-2.825707
20	8	0	-3.677210	-0.603562	-1.894904
21	1	0	-3.129786	0.135225	-1.542056
22	1	0	-0.639694	-2.680720	1.080180
23	8	0	-1.500147	-2.402131	1.451756
24	1	0	-2.191116	-2.681765	0.800590
25	1	0	-1.115441	3.961910	-0.290815
26	8	0	-1.694345	4.094384	-1.071736
27	1	0	-2.384605	4.718580	-0.802721
28	1	0	1.624655	1.110897	2.487185
29	8	0	1.530994	2.072565	2.700503
30	1	0	1.256248	2.119311	3.628566
31	8	0	3.940036	-0.255734	-2.698406
32	1	0	4.085997	-0.173526	-1.732577
33	1	0	4.114200	0.615937	-3.082902
34	8	0	-3.404603	-2.940441	-0.457562
35	1	0	-4.279122	-3.210130	-0.140463
36	1	0	-3.543637	-2.109231	-0.976562

$H_6Si_2O_7$ (Monohydrate)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
191.97577 -1186.00613785 0.11625

Rotational constant/ cm^{-1}
0.0374315620709 0.0231480139504 0.0185101387707
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[15.38113849 26.89092853 40.61093187 50.92526062
  77.0446996 123.32017185 179.70841252 182.80132107
  210.01891634 215.27338571 230.80048168 265.46885891
  272.30800951 280.42602567 307.68532308 322.32972381
  331.34433593 358.63838512 363.05186138 376.0420773
  399.36747305 413.60180275 457.13188426 477.93430067
  562.83985324 662.85548041 772.72671282 830.58147867
  833.8689972 865.68077799 872.05425471 897.72887089
  910.87199465 927.95597044 945.57512366 954.58278543
  991.0096028 1011.21428857 1052.70096533 1701.90594597
  3708.20969649 3731.99381575 3752.89353715 3798.39751985
  3813.24348091 3815.07142461 3817.43454576 3818.55355312]

Ground State Electronic Degeneracy and Irreducible Representation
1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.630114	0.098374	-0.040110
2	14	0	1.248488	-0.564876	-0.013719

3	8	0	0.997204	-1.284524	1.458325
4	1	0	1.664471	-1.904012	1.786345
5	8	0	2.688101	0.241285	0.012852
6	1	0	3.169395	0.273066	-0.827903
7	8	0	1.285111	-1.606624	-1.287931
8	1	0	0.406727	-1.845413	-1.632924
9	8	0	-2.612507	1.315394	-0.534161
10	1	0	-2.955447	1.906045	0.151762
11	8	0	-0.025273	0.473898	-0.131767
12	8	0	-2.038137	-0.284893	1.510388
13	1	0	-1.334453	-0.714944	2.025026
14	8	0	-1.757576	-1.164436	-1.112741
15	1	0	-2.641625	-1.506594	-1.307953
16	1	0	2.306187	2.305654	0.280614
17	8	0	1.859248	3.141723	0.062696
18	1	0	0.965573	2.858707	-0.186725

$H_6Si_2O_7$ (Trihydrate)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
227.9969	-1338.9020385	0.169054

Rotational constant/ cm^{-1}

0.0195435203377	0.0173306561301	0.0132344890411

Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

[25.07688553	34.98809362	44.71859244	57.81306371
61.58710718	79.59548036	100.72456351	140.18868659
170.22117616	175.99692225	191.50316716	206.0016104
213.14657668	229.81353109	242.2338178	253.23623182
259.41509857	270.11169692	291.56744682	300.71411571
319.37582238	338.36419579	349.70717728	359.97285353
377.63370889	387.1765481	402.03640987	414.08137734
429.91428899	461.87897762	497.40919903	508.41856341
602.54723879	676.23491629	723.51819021	777.63366437
783.72217649	829.70573377	839.97141003	868.14120412
900.85653122	912.59568302	919.25412435	929.84646735
963.40278758	994.71414271	1010.39414653	1031.41202398
1101.56197012	1124.61630197	1165.88751769	1679.79686257
1705.56183338	1729.89503079	3233.71582218	3389.75132114
3436.01984303	3514.41986211	3529.18241889	3732.44558891
3809.82390561	3813.53539587	3815.72475811	3820.83326999
3821.98007878	3822.9461783]		

Ground State Electronic Degeneracy and Irreducible Representation

1) (A)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.212143	0.377415	-1.725493
2	14	0	-0.816010	0.537245	1.356588
3	8	0	2.649757	-0.758664	1.993615
4	1	0	3.010697	-0.634903	1.078217
5	8	0	-0.041258	-0.806259	1.943786

6	1	0	0.954769	-0.787178	1.996237
7	8	0	-2.428392	0.196012	1.403741
8	1	0	-2.659835	-0.721923	1.179625
9	8	0	-0.524273	1.917055	2.203220
10	1	0	-0.985448	2.004788	3.049007
11	8	0	-0.896816	1.449080	-2.777667
12	1	0	-1.836391	1.326460	-2.972459
13	8	0	-0.276589	0.843391	-0.163128
14	8	0	-0.880710	-1.102747	-1.935401
15	1	0	-1.101195	-1.656945	-1.154196
16	8	0	1.406804	0.419619	-2.146118
17	1	0	1.582903	0.829357	-3.006023
18	1	0	3.041254	-0.056528	2.534278
19	1	0	3.853641	-1.249923	-0.990240
20	8	0	3.533122	-0.437151	-0.571792
21	1	0	2.804691	-0.105086	-1.146053
22	1	0	-0.842436	-2.198916	1.089227
23	8	0	-1.520531	-2.483618	0.428823
24	1	0	-1.597426	-3.448182	0.474418

$H_6Si_2O_7$ (Pentahydrate)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory

Mass/ a.m.u.	Energy a.u.	ZPE a.u.
264.01803	-1491.78213665	0.220518

Rotational constant/ cm^{-1}

0.01658047048	0.0115860152826	0.00894285339226

Rotational symmetry number

1.0

Vibrational Frequencies/ cm^{-1}

[20.09348007	27.55121238	39.63093163	45.90015301
50.77930313	60.15533378	75.13335161	90.08356802
119.16385878	133.7457063	145.13734027	152.60202294
158.70443577	186.56146383	199.78799187	206.64799354
213.35508737	222.36274913	228.36090662	234.4563691
247.31452825	255.0850266	270.06304443	272.31495987
294.15992972	307.2057485	327.15327108	329.1549737
337.19653594	349.88788654	354.59327776	379.05853194
392.72988278	404.32307709	415.57570394	425.39655739
434.557127	455.88082013	515.79289144	574.19673544
600.00340838	615.07178084	659.90157899	681.2113714
695.84882177	719.43833106	742.43706006	774.797919
820.92743376	853.03807987	881.06191648	902.60802101
907.02844762	929.86731842	966.69725646	1004.27783298
1016.51046007	1049.00337578	1074.82394943	1107.69218438
1120.29318035	1131.67091362	1174.56156235	1665.10380935
1680.58225284	1703.87984716	1710.84410417	1734.30850704
3200.88928937	3362.38776838	3450.18466917	3470.02793641
3534.51334217	3561.81434172	3574.79065694	3595.96839258
3623.15123608	3642.695638	3808.09326689	3815.00192105
3815.79426167	3817.84461678	3819.10958162	3828.43695978]

Ground State Electronic Degeneracy and Irreducible Representation

1) (A)

Input orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	14	0	1.643141	-0.884748	-0.421129
2	14	0	-1.270764	0.272951	-0.330779
3	8	0	0.577429	3.465024	0.200271
4	1	0	1.480683	3.140652	-0.056491
5	8	0	-1.138785	1.487805	0.785775
6	1	0	-0.539324	2.253174	0.553020
7	8	0	-2.007467	-0.991527	0.519042
8	1	0	-1.697079	-1.038415	1.447793
9	8	0	-2.193497	0.584196	-1.638558
10	1	0	-3.155549	0.443845	-1.504743
11	8	0	1.643526	-2.447054	-0.903574
12	1	0	0.784458	-2.923736	-0.822371
13	8	0	0.208947	-0.181016	-0.841894
14	8	0	1.975163	-0.591760	1.158889
15	1	0	1.236981	-0.553735	1.799447
16	8	0	2.889141	-0.121848	-1.223021
17	1	0	3.149444	-0.525070	-2.063683
18	1	0	0.322904	4.115357	-0.470956
19	1	0	3.645181	2.535083	0.320395
20	8	0	3.077078	2.565784	-0.464461
21	1	0	3.071357	1.644780	-0.811279
22	1	0	-0.630348	0.654100	2.343742
23	8	0	-0.397941	-0.221764	2.737942
24	1	0	-0.381597	-0.125469	3.702078
25	1	0	-1.413080	-3.804720	-1.288263
26	8	0	-0.941353	-3.456814	-0.516615
27	1	0	-1.451720	-2.675721	-0.213855
28	1	0	-5.277116	0.013946	-0.097259
29	8	0	-4.575270	-0.433879	-0.592284
30	1	0	-3.963487	-0.815378	0.068041

$H_6Si_2O_7$ (Heptahydrate)

Parameters from the DFT/B3LYP/6-31+G(d) level of theory
Mass/ a.m.u. Energy a.u. ZPE a.u.
300.03916 -1644.65860266 0.271498

Rotational constant/ cm^{-1}
0.0132174772722 0.00766296795899 0.00706755604906
Rotational symmetry number
1.0

Vibrational Frequencies/ cm^{-1}
[28.82312758 30.92213518 31.81873115 38.85944208
  42.6890884 53.03816893 57.35434019 74.68852881
  77.43391955 85.8716521 105.19364261 118.1421564
  142.60741058 145.71421985 151.30230631 154.00599491
  163.6461391 174.63465242 188.02798901 195.9027427
  203.55508498 207.77395126 213.00756955 230.35565888
  238.09140544 248.51693989 249.58729476 258.44899905
  270.82063326 272.30105916 287.18872235 305.82262759
  310.25000456 324.53993711 333.35993926 343.85497727
  356.01115044 369.43228846 384.40335593 389.9427899
  401.57768635 419.12038565 427.66237355 438.89414933
  459.09188474 479.48423013 502.55941305 521.04041045
  582.43290766 600.66369223 613.41759605 641.9418583
  661.59746592 686.41718827 699.89392914 734.97237739
  756.19181518 765.72770402 780.25394869 835.25906846

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   840.65254495   864.77723167   885.21822955   909.10660415
   938.41625667   967.57300136   976.92818094   993.22676646
  1045.84096366  1073.32267247  1100.97118984  1107.84509222
  1122.03771979  1151.49332979  1180.28170559  1667.83529938
  1679.824664    1682.58395545  1702.49672625  1704.13701034
  1728.86637806  1787.32582491  3182.40829197  3336.46988974
  3443.12310717  3465.64921194  3485.18666351  3515.6778766
  3558.41561749  3563.85079612  3582.70711276  3592.81293082
  3617.57009997  3627.32840021  3644.95450379  3656.214081
  3811.54064361  3815.15482889  3817.64305644  3818.06007782
  3828.33965479  3833.71923057]

Ground State Electronic Degeneracy and Irreducible Representation
1 ) (A)

Input orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         14           0        0.710076   -1.541301    0.164474
      2         14           0       -1.434352    0.649410   -0.514511
      3          8           0        1.541065    2.834733   -0.767706
      4          1           0        2.261912    2.151958   -0.707543
      5          8           0       -0.802937    1.986608    0.227451
      6          1           0        0.052891    2.344804   -0.147506
      7          8           0       -2.660955    0.134246    0.530332
      8          1           0       -2.423368    0.267998    1.471581
      9          8           0       -2.105017    0.876432   -1.982535
     10          1           0       -3.040593    1.172832   -1.966360
     11          8           0        0.039011   -3.027178    0.202087
     12          1           0       -0.943889   -3.054804    0.274456
     13          8           0       -0.289825   -0.506197   -0.642609
     14          8           0        1.081374   -0.912804    1.662004
     15          1           0        0.376582   -0.426903    2.141148
     16          8           0        2.200874   -1.571611   -0.535707
     17          1           0        2.337900   -1.686468   -1.497584
     18          1           0        1.535152    3.143793   -1.685823
     19          1           0        3.822876    0.977507    0.376870
     20          8           0        3.467417    0.891496   -0.535201
     21          1           0        2.978317    0.037602   -0.470617
     22          1           0       -0.727913    1.551115    2.016968
     23          8           0       -0.920312    0.834038    2.669778
     24          1           0       -0.862826    1.214340    3.559444
     25          1           0       -3.273596   -3.106487   -0.295061
     26          8           0       -2.738810   -2.739347    0.424904
     27          1           0       -2.875255   -1.768455    0.399308
     28          1           0       -5.184167    2.084567   -0.863770
     29          8           0       -4.723434    1.263305   -1.090705
     30          1           0       -4.353616    0.908122   -0.258501
     31          8           0        3.410858   -0.814844   -2.900303
     32          1           0        4.126121   -1.236091   -3.399063
     33          1           0        3.825350   -0.111252   -2.363776
     34          8           0        3.543941    0.381068    2.212811
     35          1           0        4.174567   -0.206001    2.655136
     36          1           0        2.719938   -0.145317    2.099610
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