TP001216Q

Supplementary Information

SUPPLEMENTARY MATERIAL

Each of the items in this supplement contains:
a) structure in cartesian coordinates (angstrom)
b) internal energy (electronic plus nuclear) in hartree
c) moments of inertia in amu bohr^2
d) unscaled frequencies (cm^{-1}), with torsional modes labelled as e.g. 119.5(t)

calculated at the HF/6-31G* level using the GAMESS program.

H_2O
structure (x y z / angstrom):

O1	8.0	0.0000000000	0.0000000000	0.0278097061
H2	1.0	-0.7540664690	0.0000000000	-0.5455991877
H2	1.0	0.7540664690	0.0000000000	-0.5455991877

energy (hartree): -76.0107465159
moments of inertia (amu bohr^2): 2.10182 4.09291 6.19473
harmonic zero point energy:
0.022977 hartree/molecule 5042.854400 cm^{-1}/molecule
14.418259 kcal/mol 60.325994 kJ/mol
translations and rotations: 0.04 0.04 0.04 2.21 2.64 2.98
vibrations:
1826.56 4070.45 4188.70

CH_3OH
structure (x y z / angstrom):

C1	6.0	-0.0260060861	0.0000004835	0.0016789373
H2	1.0	0.9984972429	-0.0000000376	-0.3434173703
H3	1.0	-0.5212986597	0.8835501658	-0.3939896143
H4	1.0	-0.5212987083	-0.8835504939	-0.3939896226
O5	8.0	0.0092417216	-0.0000002049	1.4007970521
H6	1.0	-0.8748516878	0.0000000871	1.7382250967

energy (hartree): -115.0354183218
moments of inertia (amu bohr^2): 13.76936 70.98812 73.51906
harmonic zero point energy:
0.055338 hartree/molecule 12145.265823 cm^{-1}/molecule
34.725092 kcal/mol 145.289786 kJ/mol
translations and rotations: 1.71 1.21 0.02 5.10 5.38 7.46
vibrations:
348.27(t) 1164.39 1188.59 1289.64 1507.71
1637.60 1651.70 1663.48 3185.10 3231.15
3305.42 4117.49

CH_3CH_2OH

structure (x y z / angstrom):

O1	8.0	0.0317025991	0.0000094145	0.0669223416
C2	6.0	1.4349770731	0.0000009015	0.0077241457
C3	6.0	1.9646513225	-0.0000007240	1.4277855939
H4	1.0	-0.3240133288	-0.0000063872	-0.8103075745
H5	1.0	1.7958746095	0.8777209377	-0.5254615450
H6	1.0	1.7958707870	-0.8777234750	-0.5254622440
H7	1.0	3.0503037398	0.0000016599	1.4314120011
H8	1.0	1.6164086585	-0.8785722014	1.9591831875
H9	1.0	1.6164037144	0.8785698742	1.9591869634

energy (hartree): -154.0757448420
moments of inertia (amu bohr^2): 50.36324 190.32796 218.48845
harmonic zero point energy:
0.086023 hartree/molecule 18879.915956 cm^{-1}/molecule
53.980443 kcal/mol 225.854172 kJ/mol
translations and rotations: 2.20 0.67 0.03 4.90 5.07 7.46
vibrations:

270.17(t)	316.86(t)	447.58	886.75	977.99
1132.94	1217.54	1298.74	1395.58	1423.96
1549.52	1613.45	1628.73	1645.84	1685.96
3175.36	3200.25	3212.23	3276.74	3289.03
4114.62				

CH_3CN

structure (x y z / angstrom):

C1	6.0	-0.4690383773	0.0000047052	0.0052460400
H2	1.0	-1.5440274429	-0.0000008055	-0.1188067137
H3	1.0	-0.0577853229	0.8815536849	-0.4688059842
H4	1.0	-0.0577838024	-0.8815546680	-0.4687973428
C5	6.0	-0.1325710132	0.0000002713	1.4339935159
N6	7.0	0.1275440760	-0.0000033460	2.5385040118

energy (hartree): -131.9275338618
moments of inertia (amu bohr^2): 11.18770 194.06127 194.06128
harmonic zero point energy:
0.048900 hartree/molecule 10732.410179 cm^{-1}/molecule
30.685531 kcal/mol 128.388263 kJ/mol
translations and rotations: 5.45 2.06 0.86 0.14 1.13 3.54
vibrations:

425.21	425.25	973.14	1174.38	1174.38
1563.28	1617.37	1617.38	2622.86	3236.61
3317.47	3317.50			

$(CH_3)_2CO$

structure (x y z / angstrom):

C1	6.0	-0.0059519482	0.0000127645	-0.0095509631
C2	6.0	1.5077612941	-0.0000017533	0.0113578804
C3	6.0	2.1675618218	-0.0000048518	1.3738786361
O4	8.0	2.1478559910	-0.0000061255	-0.9942975361
H5	1.0	-0.3575890861	-0.0000029931	-1.0317905561
H6	1.0	-0.3909481885	-0.8744201534	0.5072464851
H7	1.0	-0.3909776361	0.8744254784	0.5072493552
H8	1.0	3.2425431209	0.0000017555	1.2596582780
H9	1.0	1.8623643585	0.8744185399	1.9414674923
H10	1.0	1.8623685178	-0.8744226613	1.9414711791

energy (hartree): -191.9622363585
moments of inertia (amu bohr^2): 173.97769 211.68567 363.64856
harmonic zero point energy:
0.089914 hartree/molecule 19733.765130 cm^{-1}/molecule
56.421722 kcal/mol 236.068487 kJ/mol
translations and rotations: 4.28 3.09 0.02 1.14 3.22 4.14
vibrations:

51.32(t)	143.56(t)	400.70	531.18	574.88
846.30	980.22	983.30	1190.62	1239.30
1351.95	1546.08	1554.48	1607.52	1610.47
1613.88	1632.37	2021.75	3203.90	3211.60
3258.60	3267.16	3322.58	3323.80	

NO_3^-
structure (x y z / angstrom):

N1	7.0	0.0000000000	0.0000000000	0.0000000000
O3	8.0	1.2259200000	0.0000000000	0.0000000000
O4	8.0	-0.6129600000	1.0616778630	0.0000000000
O5	8.0	-0.6129600000	-1.0616778630	0.0000000000

energy (hartree): -278.9129744992
moments of inertia (amu bohr^2): 128.76416 128.76416 257.52832
harmonic zero point energy:
0.016246 hartree/molecule 3565.632748 cm^{-1}/molecule
10.194666 kcal/mol 42.654482 kJ/mol
translations and rotations: 4.43 0.02 0.03 2.62 6.15 6.39
vibrations:

796.58	796.60	984.40	1243.75	1654.93
1655.01				

ClH_2O
structure (x y z / angstrom):

O1	8.0	0.0975387034	-0.0079159677	0.0000000000
H2	1.0	-0.8600257809	-0.0824550913	0.0000000000
H3	1.0	0.2036212200	0.9334207234	0.0000000000

CL4 17.0 -3.0686105533 0.7928221716 0.0000000000
energy (hartree): -535.5594749635
moments of inertia (amu bohr^2): 3.41290 439.71031 443.12321
harmonic zero point energy:
0.025232 hartree/molecule 5537.680829 cm^{-1}/molecule
15.833040 kcal/mol 66.245439 kJ/mol
translations and rotations: 0.98 0.87 0.10 0.77 1.03 12.48
vibrations:
167.73 273.28 707.44 1884.60 3910.29
4132.02

$H^+(H_2O)_3$
structure (x y z / angstrom):

O1	8.0	0.0266330237	-0.4836838986	-0.0572214138
O2	8.0	2.4381684766	0.3620611275	-0.1878027799
O3	8.0	-1.2299215931	-0.2794461724	2.1625605645
H4	1.0	0.9639069063	-0.1271104657	-0.0843664467
H5	1.0	-0.4474243632	-0.3739191056	0.8200176625
H6	1.0	-0.5008186863	-0.1866882512	-0.7992044452
H7	1.0	3.1718976032	-0.2213787300	-0.3516879764
H8	1.0	2.7867957787	1.2397351449	-0.0741927746
H9	1.0	-1.4780821954	0.4940305343	2.6574387632
H10	1.0	-1.5206988685	-1.0416315279	2.6525970973

energy (hartree): -228.4038749905
moments of inertia (amu bohr^2): 91.54723 671.45834 746.46708
harmonic zero point energy:
0.089390 hartree/molecule 19618.897643 cm^{-1}/molecule
56.093299 kcal/mol 234.694365 kJ/mol
translations and rotations: 2.35 0.92 0.12 0.04 0.74 4.15
vibrations:
57.84(t) 64.83 107.24(t) 197.27 248.67
303.65 339.77 368.54 392.86 497.46
512.78 993.23 1261.43 1809.66 1812.77
1839.80 1845.39 3051.66 3140.80 4010.52
4044.85 4046.67 4144.70 4145.40

H^+CH_3OH
structure (x y z / angstrom):

C1	6.0	-0.0036428218	-0.0014393216	-0.0442785521
H2	1.0	1.0385099476	0.0204797626	-0.3058252737
H3	1.0	-0.5063934171	0.9125255355	-0.3028894529
H4	1.0	-0.5145353355	-0.8851203981	-0.3833538096
O5	8.0	-0.0104019761	-0.0181174441	1.4666169127
H6	1.0	-0.8688198686	0.0765548589	1.8909729164

H7	1.0	0.5019290887	-0.7149425413	1.8883682187

energy (hartree): -115.3389926840
moments of inertia (amu bohr^2): 16.78586 84.96923 88.65420
harmonic zero point energy:
0.068593 hartree/molecule 15054.523992 cm^{-1}/molecule
43.043087 kcal/mol 180.092277 kJ/mol
translations and rotations: 2.47 0.61 0.07 2.23 3.72 6.01
vibrations:

242.45(t)	708.15	823.10	987.69	1262.32
1382.33	1593.14	1609.25	1613.20	1848.83
3297.91	3436.10	3442.32	3886.87	3975.39

$H^+CH_3CH_2OH$
structure (x y z / angstrom):

O1	8.0	0.0065498696	0.0326731567	0.0064632027
C2	6.0	1.5515284967	-0.0406913849	-0.0011307628
C3	6.0	2.0025399176	0.0062440944	1.4329124091
H4	1.0	-0.4297908214	-0.0537312883	-0.8459230089
H5	1.0	1.8671425790	0.7914105310	-0.6072444385
H6	1.0	1.7215077322	-0.9840081071	-0.4893245150
H7	1.0	1.7526701292	0.9491836561	1.9055297152
H8	1.0	3.0833737712	-0.0840488538	1.4351241442
H9	1.0	1.5903641260	-0.8154274834	2.0032108571
H10	1.0	-0.3777284664	0.7584868022	0.5061871803

energy (hartree): -154.3871612948
moments of inertia (amu bohr^2): 57.94881 211.18625 243.40397
harmonic zero point energy:
0.098870 hartree/molecule 21699.387033 cm^{-1}/molecule
62.041723 kcal/mol 259.582569 kJ/mol
translations and rotations: 3.11 0.54 0.47 1.31 3.52 6.85
vibrations:

205.48(t)	271.72(t)	396.32	674.84	713.72
880.40	986.30	1028.57	1233.87	1305.51
1394.46	1526.68	1567.99	1615.68	1633.04
1643.17	1837.84	3226.71	3299.54	3322.98
3329.66	3414.65	3898.17	3991.47	

H^+CH_3CN
structure (x y z / angstrom):

C1	6.0	-0.4649123961	0.0000039354	0.0222837257
H2	1.0	-1.5354408854	-0.0000003648	-0.1424684182
H3	1.0	-0.0170762602	0.8894995636	-0.4036388446
H4	1.0	-0.0170743235	-0.8895003670	-0.4036279067
C5	6.0	-0.2165268486	0.0000014508	1.4663228365

N6	7.0	-0.0260286709	-0.0000026762	2.5737552611
H7	1.0	0.1433975017	-0.0000015404	3.5587068733

energy (hartree): -132.2367532555
moments of inertia (amu bohr^2): 11.39031 210.12157 210.12160
harmonic zero point energy:
0.060654 hartree/molecule 13311.915024 cm^{-1}/molecule
38.060713 kcal/mol 159.246024 kJ/mol
translations and rotations: 2.65 1.63 0.91 3.20 4.54 5.43
vibrations:

429.85	429.86	721.59	721.59	900.89
1164.67	1164.68	1540.66	1572.33	1572.33
2599.74	3224.90	3328.57	3328.60	3923.58

$H^+(CH_3)_2CO$
structure (x y z / angstrom):

C1	6.0	-0.0183959083	0.0608524568	-0.0058039223
C2	6.0	1.4640558912	0.0133365682	-0.0104059273
C3	6.0	2.2576362306	-0.0042382499	1.2386393543
O4	8.0	2.1197764161	-0.0147431163	-1.0817624275
H5	1.0	-0.4303010097	0.3604552331	-0.9606437667
H6	1.0	-0.3707285384	-0.9411535102	0.2357945659
H7	1.0	-0.3672283210	0.7214943513	0.7784408631
H8	1.0	1.7437065191	-0.5615991223	2.0110721388
H9	1.0	3.2503828317	-0.3920289005	1.0629569676
H10	1.0	2.3367317272	1.0291945573	1.5755028467
H11	1.0	1.6073004432	0.0239331820	-1.8918861960

energy (hartree): -192.2878392403
moments of inertia (amu bohr^2): 181.74564 216.55579 376.29358
harmonic zero point energy:
0.103344 hartree/molecule 22681.468228 cm^{-1}/molecule
64.849637 kcal/mol 271.330881 kJ/mol
translations and rotations: 1.54 0.82 0.22 2.12 3.88 4.85
vibrations:

87.88(t)	130.89(t)	407.83	507.33	543.52
778.14(t)	855.68	1013.92	1037.63	1180.80
1210.71	1254.12	1509.04	1537.50	1554.67
1565.20	1583.99	1607.13	1619.78	1765.70
3195.82	3202.20	3285.10	3292.80	3329.74
3354.00	3951.83			

HNO_3
structure (x y z / angstrom):

N1	7.0	-0.0258321136	0.0126501816	0.0000000000
O2	8.0	1.3079031987	0.0006496563	0.0000000000

O3	8.0	-0.5378773721	1.0845413353	0.0000000000
O4	8.0	-0.5268300630	-1.0473392868	0.0000000000
H5	1.0	1.5686246967	0.9196609018	0.0000000000

energy (hartree): -279.4442641451
moments of inertia (amu bohr^2): 131.33675 138.88524 270.22199
harmonic zero point energy:
0.030033 hartree/molecule 6591.410641 cm^{-1}/molecule
18.845808 kcal/mol 78.850859 kJ/mol
translations and rotations: 4.08 1.22 0.90 0.02 3.64 6.15
vibrations:
549.99(t) 684.82 783.11 908.76 1138.00
1505.48 1608.06 1979.25 4025.35

$H^+(H_2O)_4$
structure (x y z / angstrom):

O1	8.0	0.0670711982	0.4154742923	-0.0046673658
O2	8.0	2.6479266590	-0.0248651573	0.0761347074
O3	8.0	-1.1726554323	-0.1480525984	2.2330811290
H4	1.0	1.0359301095	0.2349234440	0.0555247389
H5	1.0	-0.4199237309	0.1825187927	0.8220336066
H6	1.0	-0.3459027799	0.0323317487	-0.8155516859
H7	1.0	3.2799212680	0.6516991872	-0.1402384218
H8	1.0	3.1206486800	-0.7160241651	0.5257445713
H9	1.0	-1.6358913109	-0.9420987202	2.4743509661
H10	1.0	-1.4433168510	0.5300701663	2.8420753069
O11	8.0	-1.1022295797	-0.5597077876	-2.1361969629
H12	1.0	-1.6269483617	-0.0172699843	-2.7144627867
H13	1.0	-0.9147406072	-1.3663059559	-2.6026165029

energy (hartree): -304.4488481819
moments of inertia (amu bohr^2): 689.58202 690.47263 1317.30607
harmonic zero point energy:
0.116330 hartree/molecule 25531.486496 cm^{-1}/molecule
72.998256 kcal/mol 305.424704 kJ/mol
translations and rotations: 2.42 0.64 0.18 0.29 0.96 2.35
vibrations:
58.11 58.22 63.95 94.30(t) 95.47(t)
107.54(t) 223.15 261.28 270.98 271.52
323.69 323.83 377.07 377.47 428.64
645.77 887.18 887.75 1275.84 1819.57
1819.62 1826.38 1874.68 1875.01 3381.17
3381.48 3427.58 4053.22 4053.25 4054.60
4154.64 4154.71 4155.31

$H^+(CH_3OH)_2$

structure (x y z / angstrom):

C1	6.0	0.0866559695	-0.1871584300	0.0902198484
H2	1.0	1.1618535853	-0.1241671228	0.0827818195
H3	1.0	-0.3487144477	0.1243352363	-0.8426804630
H4	1.0	-0.2590394061	-1.1647078295	0.3750977017
O5	8.0	-0.4388643729	0.7251852020	1.1187450122
H6	1.0	-0.2956415575	0.4434924776	2.1011245856
H7	1.0	-0.2497685413	1.6513422424	0.9702788959
O8	8.0	-0.1649950977	-0.0386620772	3.4574198113
H9	1.0	0.6617034882	-0.0349163713	3.9261968233
C10	6.0	-1.2666252119	-0.3003026351	4.3407916356
H11	1.0	-2.1562096626	-0.3178224025	3.7318501586
H12	1.0	-1.1289617102	-1.2604519664	4.8145109158
H13	1.0	-1.3407757663	0.4838336760	5.0796499603

energy (hartree): -230.4211559230

moments of inertia (amu bohr^2): 94.50210 761.97983 774.05667

harmonic zero point energy:

0.125479 hartree/molecule 27539.464393 cm^{-1}/molecule

78.739359 kcal/mol 329.445478 kJ/mol

translations and rotations: 2.40 1.33 0.95 1.41 1.68 2.76

vibrations:

54.62(t)	68.41(t)	109.88(t)	131.54	154.80
326.54	361.69	515.27	963.72	1043.86
1079.12	1148.95	1270.76	1282.92	1316.77
1424.33	1526.85	1600.28	1624.52	1628.16
1631.73	1638.33	1652.82	1840.07	2496.13
3258.39	3289.63	3351.85	3364.90	3408.45
3422.37	4004.63	4086.63		

$H^+(CH_3CH_2OH)_2$

structure (x y z / angstrom):

O1	8.0	0.2117019994	0.5173068795	0.2806803593
C2	6.0	1.6269803094	0.0892200767	0.0484318738
C3	6.0	2.4337750399	0.4815819760	1.2607536516
H4	1.0	-0.3500218924	0.4709228111	-0.4925680636
H5	1.0	1.9150999391	0.6218493536	-0.8419652205
H6	1.0	1.6009782234	-0.9732195911	-0.1324933432
H7	1.0	3.4639615029	0.1917836304	1.0895605421
H8	1.0	2.0849270177	-0.0279802830	2.1503932596
H9	1.0	2.4004123330	1.5516559904	1.4190879881
O10	8.0	-0.9070255789	-0.3850339495	2.3480249020
C11	6.0	-1.6290226363	-1.6085295735	2.5914487280
C12	6.0	-1.2629578118	-2.6080511822	1.5169982219
H13	1.0	-1.0891554770	0.2551689424	3.0268534732
H14	1.0	-2.6881056176	-1.3891270082	2.5819553127

H15	1.0	-1.3508655345	-1.9699938682	3.5714201016
H16	1.0	-1.7864769251	-3.5400613386	1.6919058900
H17	1.0	-0.1984858449	-2.8163946061	1.5264671704
H18	1.0	-1.5510494597	-2.2512284010	0.5327082033
H19	1.0	-0.2539702569	0.1266998003	1.0982785273

energy (hartree): -308.5070656720
moments of inertia (amu bohr^2): 355.62496 1357.82523 1404.13153
harmonic zero point energy:
0.186963 hartree/molecule 41033.541572 cm^{-1}/molecule
117.320900 kcal/mol 490.870647 kJ/mol
translations and rotations: 1.07 0.47 0.21 1.72 2.70 5.78
vibrations:

26.34(t)	48.07	71.63(t)	90.97	126.15
260.19(t)	284.01(t)	302.17	395.30	419.33
445.13	531.51	834.09	882.58	884.56
939.07	1041.80	1063.48	1113.64	1148.65
1224.02	1254.85	1291.68	1350.21	1418.57
1425.50	1452.39	1532.41	1552.91	1576.56
1599.23	1622.26	1630.85	1640.64	1643.39
1653.86	1674.15	1860.59	2743.83	3210.59
3232.55	3261.59	3271.29	3302.95	3305.44
3312.27	3319.92	3320.22	3386.66	4006.14
4080.88				

$H^+(CH_3CN)_2$
structure (x y z / angstrom):

C1	6.0	-0.4092847286	0.0000031087	-0.2717548620
H2	1.0	-1.4504536758	-0.0000019272	-0.5652779117
H3	1.0	0.0776759765	0.8840050846	-0.6611031571
H4	1.0	0.0776811872	-0.8839976834	-0.6611094245
C5	6.0	-0.3174228612	-0.0000051441	1.1932746532
N6	7.0	-0.2465727511	-0.0000072928	2.3235423870
H7	1.0	-0.1440113957	0.0000207240	3.9657945532
N8	7.0	-0.0786768603	0.0000035479	5.0158138316
C9	6.0	-0.0090610517	-0.0000032455	6.1370392514
C10	6.0	0.0817354150	-0.0000071636	7.6001587223
H11	1.0	1.1262356282	0.0000050518	7.8837416190
H12	1.0	-0.4082297297	0.8876127627	7.9789336399
H13	1.0	-0.4082128730	-0.8876278199	7.9789466978

energy (hartree): -264.2073085708
moments of inertia (amu bohr^2): 22.59215 2450.79265 2450.79270
harmonic zero point energy:
0.110877 hartree/molecule 24334.706839 cm^{-1}/molecule
69.576488 kcal/mol 291.108026 kJ/mol
translations and rotations: 4.09 3.32 1.69 0.29 0.77 5.30

vibrations:

10.00(t)	55.89	55.98	139.43	139.49
191.44	444.59	444.60	461.60	461.61
918.61	962.21	1154.38	1154.39	1171.52
1171.56	1173.03	1173.07	1547.72	1557.64
1583.68	1583.69	1601.71	1601.72	2432.58
2631.14	3037.25	3234.54	3240.78	3332.34
3332.35	3334.42	3334.43		

$H^+[(CH_3)_2CO]_2$

structure (x y z / angstrom):

C1	6.0	-0.0021488339	-0.0279285692	0.2263911412
C2	6.0	1.4666143850	0.0415514896	0.0172965504
C3	6.0	2.3984093270	0.1783364449	1.1694473400
O4	8.0	1.8717397131	-0.0189628035	-1.1565286598
H5	1.0	-0.5328891533	0.1936516951	-0.6875743541
H6	1.0	-0.2370532265	-1.0445533078	0.5359886777
H7	1.0	-0.3067596648	0.6343172484	1.0268475401
H8	1.0	2.0609396932	-0.4407155088	1.9915798535
H9	1.0	3.4178447152	-0.0556396382	0.9025573663
H10	1.0	2.3455071362	1.2129339217	1.5031523012
O11	8.0	4.4184194856	-0.0075155862	-1.3963563023
C12	6.0	5.2140477058	-0.0149210146	-2.3113770265
C13	6.0	4.7705831929	0.0163749894	-3.7466707131
C14	6.0	6.6878154332	-0.0537405867	-2.0310661855
H15	1.0	5.3138579216	-0.7178902543	-4.3302825674
H16	1.0	3.7073061061	-0.1597419707	-3.8343095970
H17	1.0	5.0039696583	0.9925761692	-4.1627035155
H18	1.0	6.8782375519	0.1232681991	-0.9827061776
H19	1.0	7.0698070432	-1.0335151421	-2.3045521697
H20	1.0	7.2128731972	0.6758915117	-2.6372298845
H21	1.0	2.8636422978	-0.0049526584	-1.3013838613

energy (hartree): -384.2958215197

moments of inertia (amu $bohr^2$): 412.38082 2507.56194 2873.11459

harmonic zero point energy:

0.194658 hartree/molecule 42722.472259 cm^{-1}/molecule

122.149800 kcal/mol 511.074765 kJ/mol

translations and rotations: 2.33 1.30 0.52 1.71 3.03 4.01

vibrations:

29.71(t)	51.93	54.52	87.39(t)	90.90(t)
109.04(t)	120.53(t)	135.82	151.63	212.65
412.23	416.67	521.51	535.32	567.77
616.02	850.23	860.65	962.23	979.14
1007.29	1036.91	1190.77	1197.25	1221.77
1237.00	1241.69	1352.73	1387.93	1541.00

1547.43	1553.48	1562.01	1573.45	1584.20
1593.73	1598.02	1602.85	1609.60	1620.93
1623.55	1652.07	1821.42	1924.36	3018.71
3206.59	3212.53	3214.13	3220.47	3280.77
3287.50	3289.24	3293.66	3325.16	3339.69
3352.32	3356.87			

$NO_3^-HNO_3$

structure (x y z / angstrom):

N1	7.0	-0.1979796588	0.2349990648	-0.0871045431
O2	8.0	0.6825597935	0.6976364719	0.6095844077
O3	8.0	-1.1024879618	0.9140234130	-0.5133094881
O4	8.0	-0.1693955151	-0.9835019081	-0.3681111694
N5	7.0	2.7727269136	-2.5052007617	0.0512533203
O6	8.0	1.6848127437	-2.3327375652	0.7398593336
H7	1.0	1.0520439696	-1.7111426590	0.2523636794
O8	8.0	2.8668221099	-1.9730785822	-1.0090863755
O9	8.0	3.5927950764	-3.2060009642	0.5565487654

energy (hartree): -558.4049238506

moments of inertia (amu bohr^2): 273.31059 2139.80678 2156.42855

harmonic zero point energy:

0.047013 hartree/molecule 10318.169421 cm^{-1}/molecule

29.501156 kcal/mol 123.432838 kJ/mol

translations and rotations: 5.69 2.34 0.84 0.53 2.47 3.36

vibrations:

33.13(t)	50.85(t)	57.25(t)	125.11	150.02
227.11	739.04	792.90	797.83	809.15
932.95	972.49	1152.70	1191.24	1245.18
1541.20	1636.12	1647.04	1736.28	1909.96
2888.79				

$H^+(CH_3OH)_3$

structure (x y z / angstrom):

O1	8.0	-0.7036108310	0.0274276788	-0.4472157879
O2	8.0	0.8814622377	1.4291599311	-1.9054379188
O3	8.0	0.1805352881	-2.0420656996	0.7930785336
H4	1.0	0.5409600345	-2.8161527129	0.3786755614
H5	1.0	-0.0478177356	0.5302091187	-1.0022102716
H6	1.0	1.3407983726	1.1126156674	-2.6733326708
C7	6.0	-1.9862768392	-0.2128858748	-1.0927635854
C8	6.0	1.2984572399	2.7553060438	-1.5800202417
C9	6.0	0.3174678423	-2.1200406186	2.2120966980
H10	1.0	-2.3502538529	0.7472176280	-1.4138493858
H11	1.0	-1.8492317983	-0.8841440415	-1.9250292256

H12	1.0	-2.6300043094	-0.6377889219	-0.3427843244
H13	1.0	2.3538528894	2.7708037819	-1.3463061040
H14	1.0	1.0860079506	3.4244575100	-2.4017624646
H15	1.0	0.7323279838	3.0587562101	-0.7132514418
H16	1.0	-0.2132187699	-2.9822092760	2.5905128590
H17	1.0	1.3618229675	-2.1715968071	2.4866333835
H18	1.0	-0.1188702248	-1.2214321916	2.6195122859
H19	1.0	-0.3110109950	-0.7676374262	0.0051841405

energy (hartree): -345.4934450687
moments of inertia (amu bohr^2): 514.31930 1788.65686 2142.94600
harmonic zero point energy:
0.183779 hartree/molecule 40334.929242 cm^{-1}/molecule
115.323465 kcal/mol 482.513379 kJ/mol
translations and rotations: 1.22 0.39 0.19 0.82 2.56 3.22
vibrations:

28.59(t)	36.75(t)	62.40(t)	65.53	75.72
88.42	101.72(t)	127.10	135.51	156.62
289.93	328.43	351.35	371.79	935.19
1022.39	1103.77	1105.68	1130.05	1170.77
1218.00	1246.14	1285.02	1285.27	1305.49
1476.00	1514.67	1517.72	1607.25	1630.13
1631.29	1633.32	1640.05	1642.00	1642.38
1655.92	1656.11	1865.81	3159.33	3210.39
3249.85	3250.25	3288.81	3331.81	3332.02
3350.94	3351.16	3393.89	3412.53	4098.96
4099.61				

$NO_3^-(HNO_3)_2$
structure (x y z / angstrom):

N1	7.0	0.1865528783	0.0458292211	-0.0316907431
O2	8.0	1.2749837938	0.4784039555	-0.3015867256
O3	8.0	-0.8256984359	0.7238192841	-0.2055050902
O4	8.0	0.0586596919	-1.0923778847	0.4359713509
N5	7.0	2.8610876092	-3.0463576125	0.0839394601
O6	8.0	2.3216422589	-2.3078988560	1.0174957192
H7	1.0	1.5268501801	-1.8456109039	0.6517046181
O8	8.0	2.3336345693	-3.0788355307	-0.9804139977
O9	8.0	3.8442763234	-3.6291309715	0.4060450081
H10	1.0	-2.2207436390	-0.0460659729	0.2809102374
O11	8.0	-3.0670412073	-0.3084429333	0.7214336428
N12	7.0	-3.8835608418	-0.8043875037	-0.1698563803
O13	8.0	-3.5183051044	-0.8538134739	-1.2999285050
O14	8.0	-4.9358393523	-1.1587931882	0.2506873942

energy (hartree): -837.8857584438
moments of inertia (amu bohr^2): 1077.42558 6130.43276 6671.93111

harmonic zero point energy:
0.078783 hartree/molecule 17290.943805 cm^{-1}/molecule
49.437339 kcal/mol 206.845825 kJ/mol
translations and rotations: 5.14 2.48 0.64 0.31 1.01 2.15
vibrations:

14.12(t)	21.11(t)	30.44	44.24	50.59
60.98	91.80	112.17	133.83	146.97
202.69	229.46	728.71	730.30	791.62
793.59	802.03	809.65	926.94	927.55
968.07	1018.32	1028.95	1180.90	1181.42
1252.07	1535.62	1573.95	1628.14	1638.60
1642.48	1739.96	1929.43	1934.13	3317.76
3363.32				

$H^+(H_2O)_2$
structure (x y z / angstrom):

O1	8.0	-0.0694441865	-0.0575457034	0.0404846505
O2	8.0	2.3627134256	0.1347609391	-0.2375174601
H3	1.0	0.9725023390	0.0466511598	-0.0533915965
H4	1.0	-0.5755428608	0.7319718261	-0.1684987739
H5	1.0	-0.3635702711	-0.4591222345	0.8622974292
H6	1.0	2.8361165832	-0.3571360476	-0.9033048777
H7	1.0	2.9820571726	0.6685970809	0.2522101095

energy (hartree): -152.3524873342
moments of inertia (amu $bohr^2$): 9.60184 219.22878 219.73888
harmonic zero point energy:
0.061876 hartree/molecule 13580.250380 cm^{-1}/molecule
38.827923 kcal/mol 162.456031 kJ/mol
translations and rotations: 1.21 0.53 0.09 1.50 2.06 3.31
vibrations:

61.22	205.70(t)	350.48	447.81	456.88
618.75	1328.29	1712.08	1795.60	1832.00
2280.70	3919.13	4009.30	4022.26	4120.31