Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Decomposition of Nitrous Oxide in Hydrated Cobalt(I) Clusters: A Theoretical Insight into Mechanistic Roles of Ligand-binding Modes

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Supporting Information

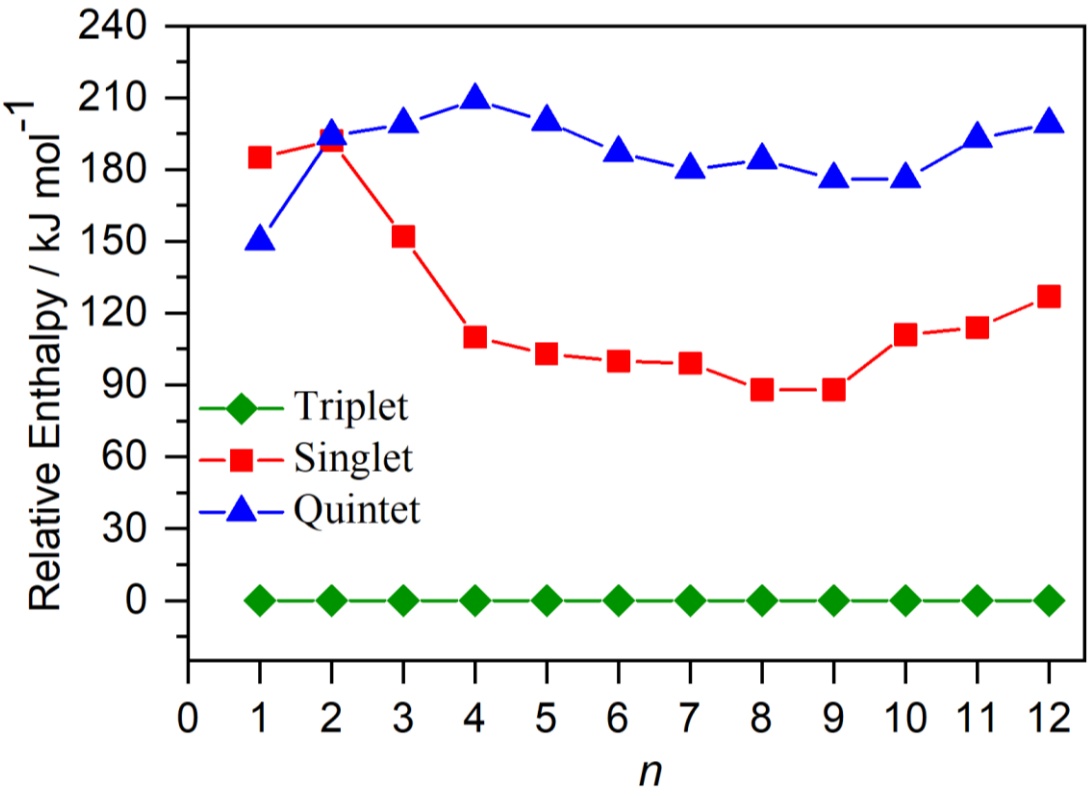


Figure S1: Relative enthalpies at 0 K of the lowest-energy structures of $[Co(H_2O)_n]^+$, n = 1 – 12, at their singlet, triplet and quintet electronic states.

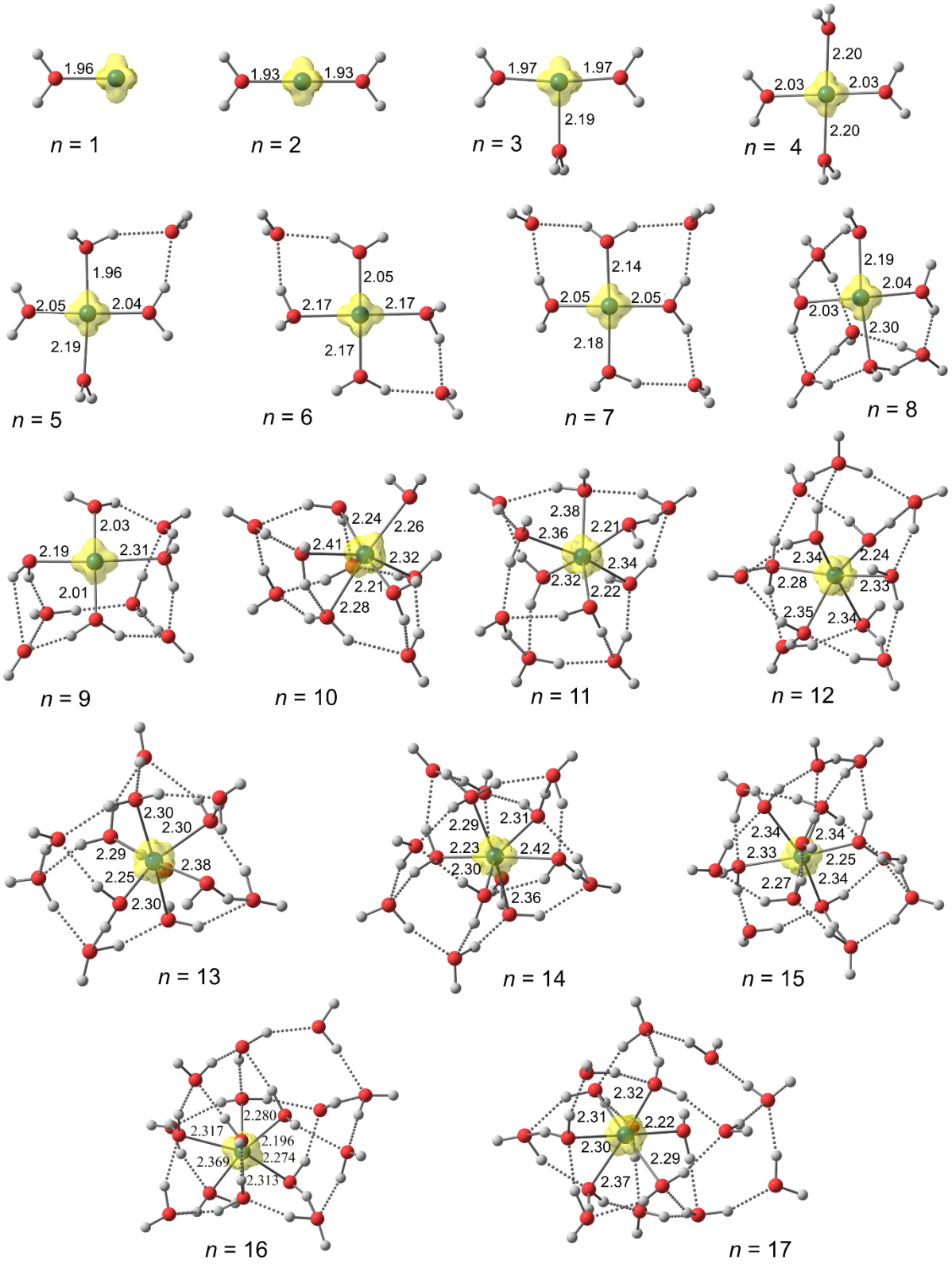


Figure S2: Lowest-lying geometries of $[Co(H_2O)_n]^+$, $n = 1 - 17$, at their ground triplet state. Bond lengths are displaced in Å.

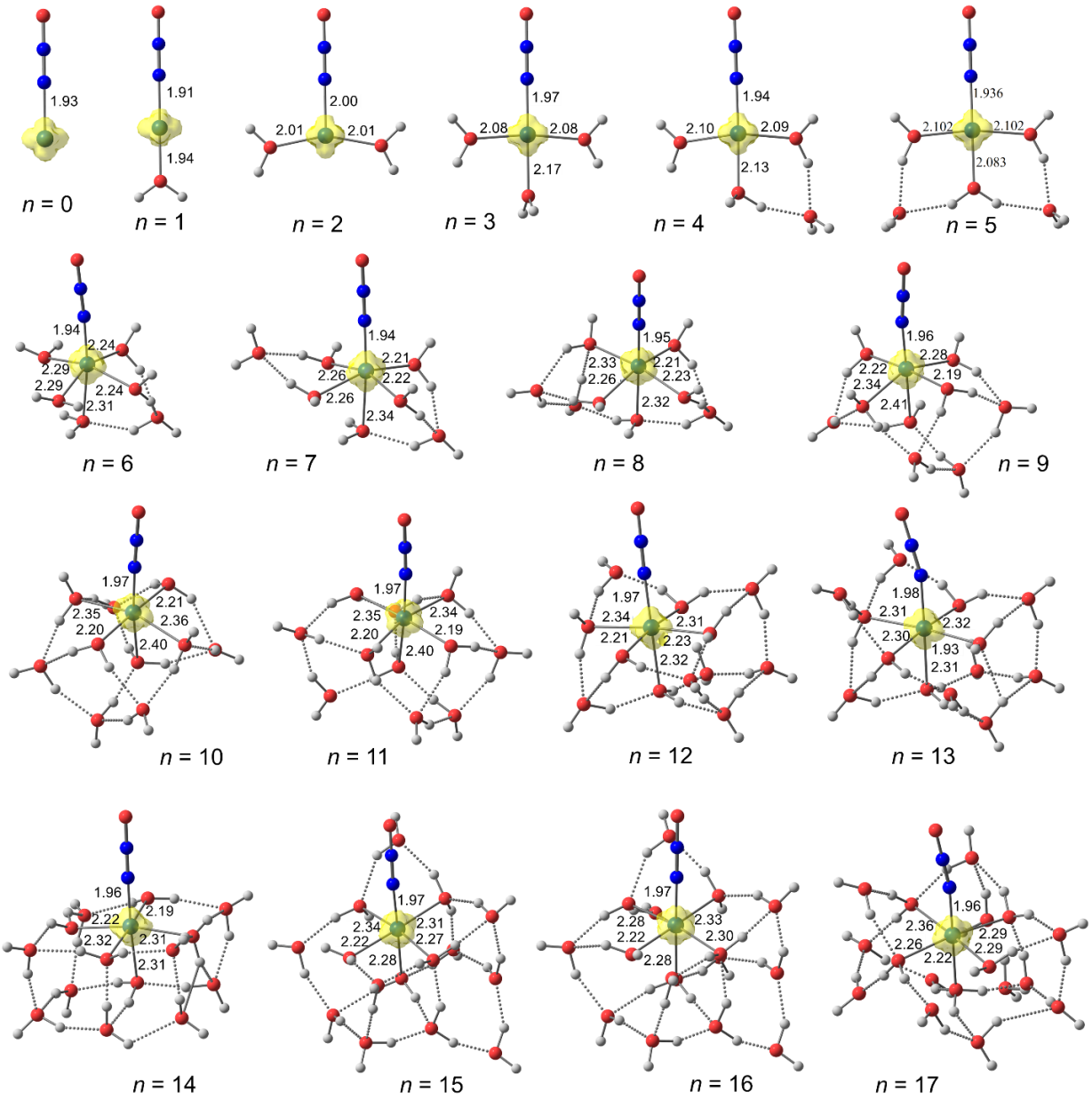


Figure S3: Lowest-lying geometries of N end-on coordination mode of $[Co(N_2O)(H_2O)_n]^+$ (η^1–NL), n = 1 – 17, at the ground triplet electronic state. Bond lengths are displaced in Å.

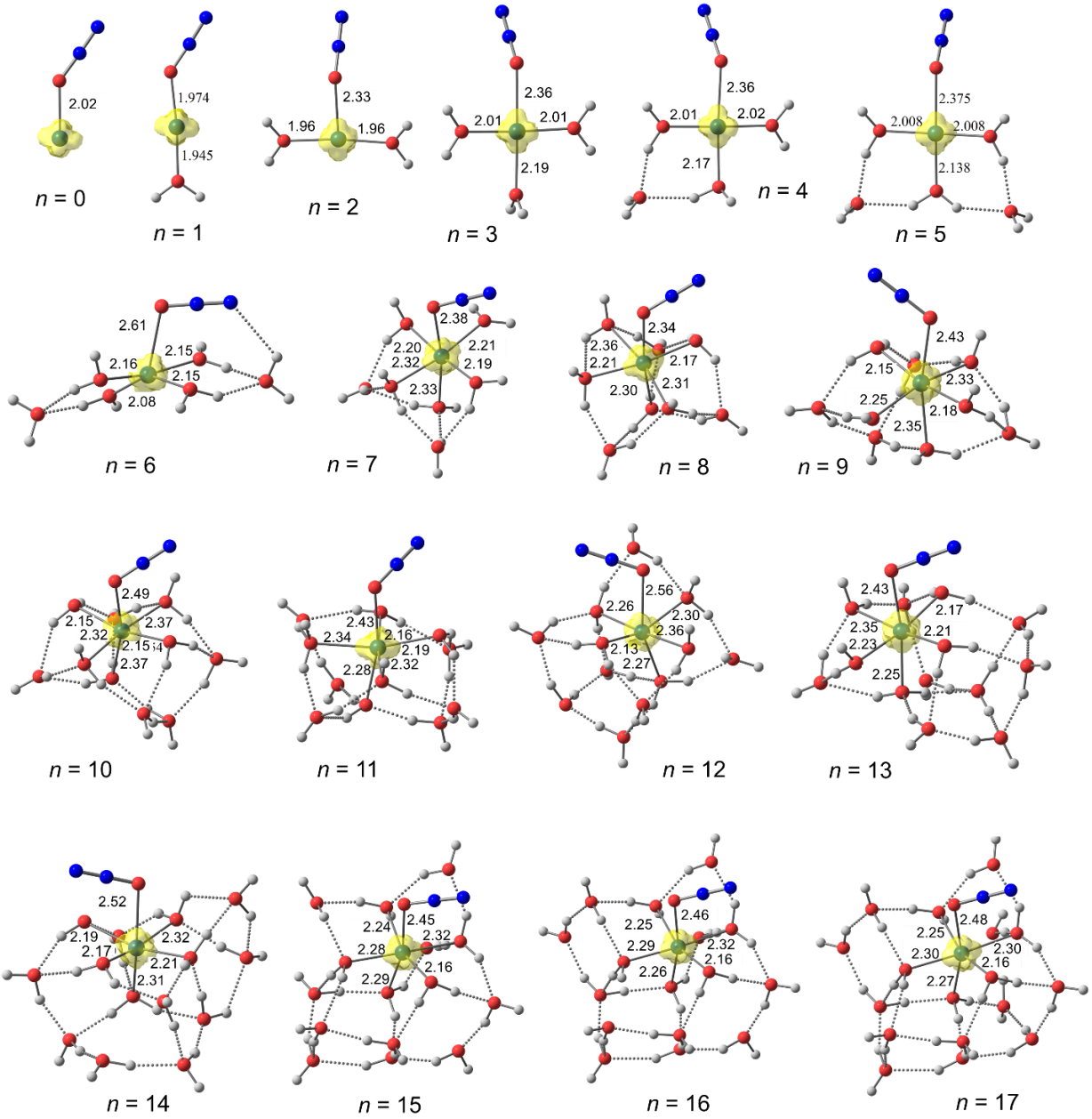


Figure S4: Lowest-lying geometries of O end-on coordination mode of $[Co(N_2O)(H_2O)_n]^+$ (η^1–OL), n = 1 – 17, at the ground triplet electronic state. Bond lengths are displaced in Å.

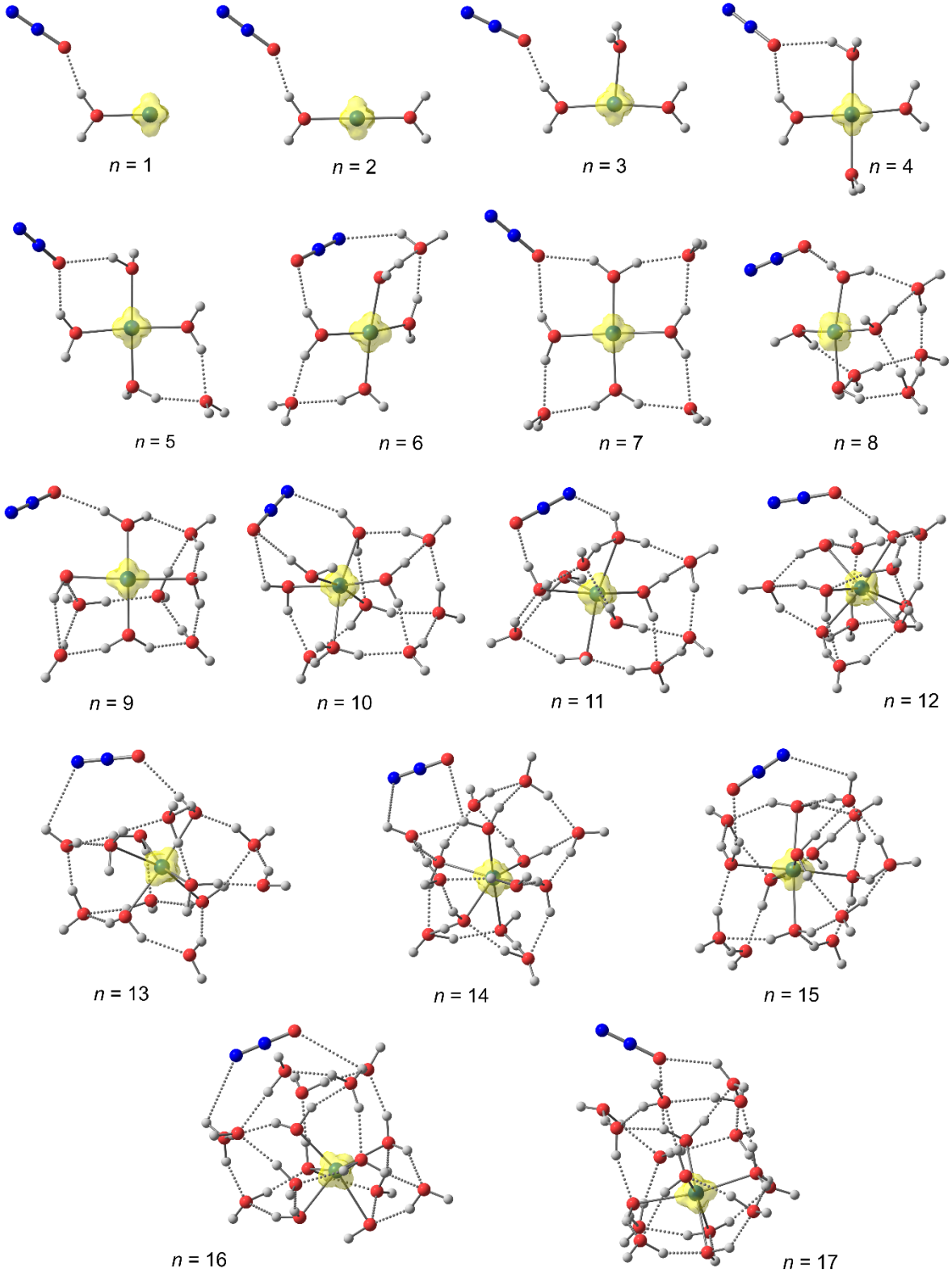


Figure S5: Lowest-lying geometries of surface-solvated mode of $[Co(N_2O)(H_2O)_n]^+$, n = 1 – 17, at the ground triplet electronic state.

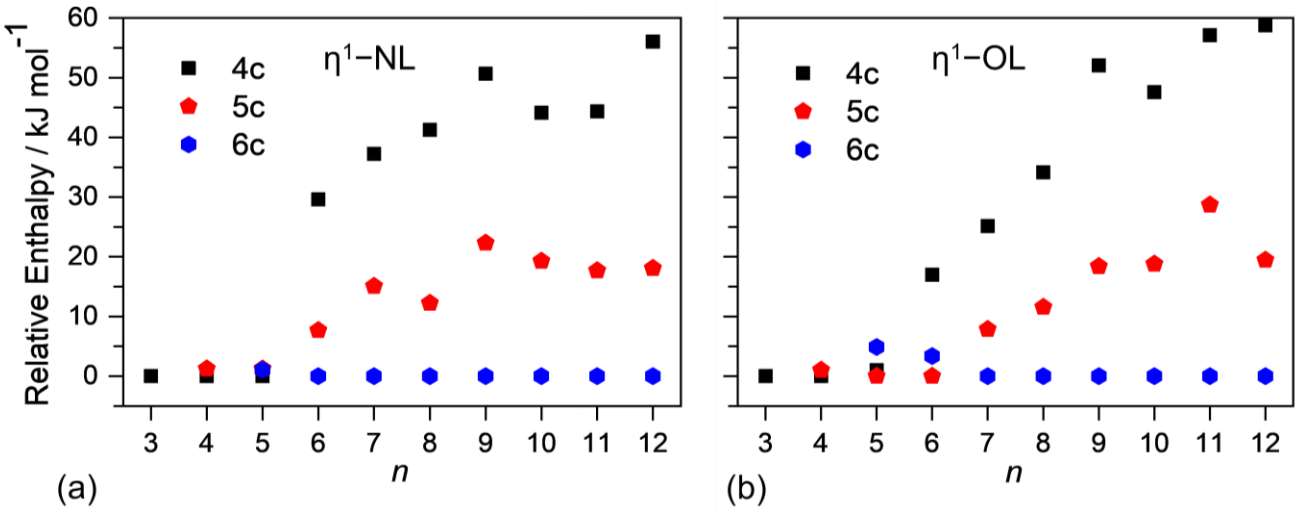


Figure S6: Relative enthalpies at 0 K ($\Delta H_0°$ / kJ mol^{-1}) of lowest-lying conformers of (a) η^1–NL and (b) η^1–OL coordination modes of $[Co(N_2O)(H_2O)_n]^+$ (n = 3 – 12) with tetra-, penta-, and hexa-coordinate cores (4c, 5c, and 6c, respectively).

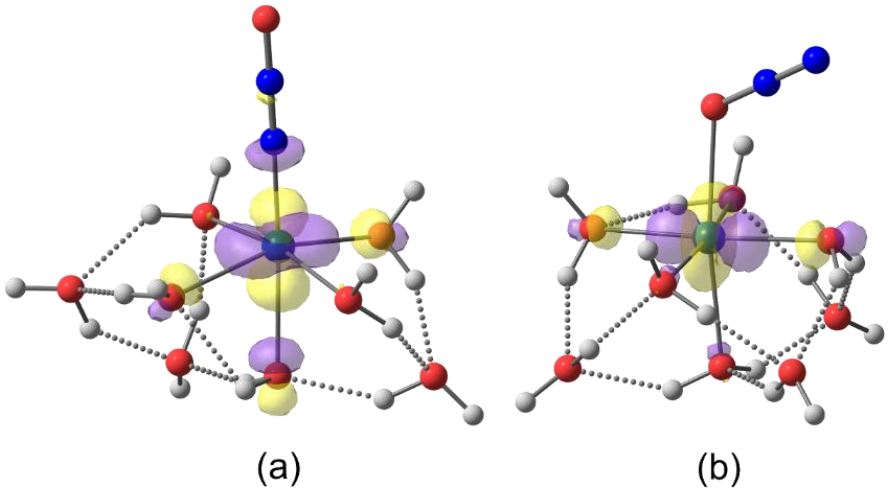


Figure S7: The singly occupied molecular orbital (SOMO) of (a) η^1–NL and (b) η^1–OL of $[Co^+(N_2O)(H_2O)_8]$.

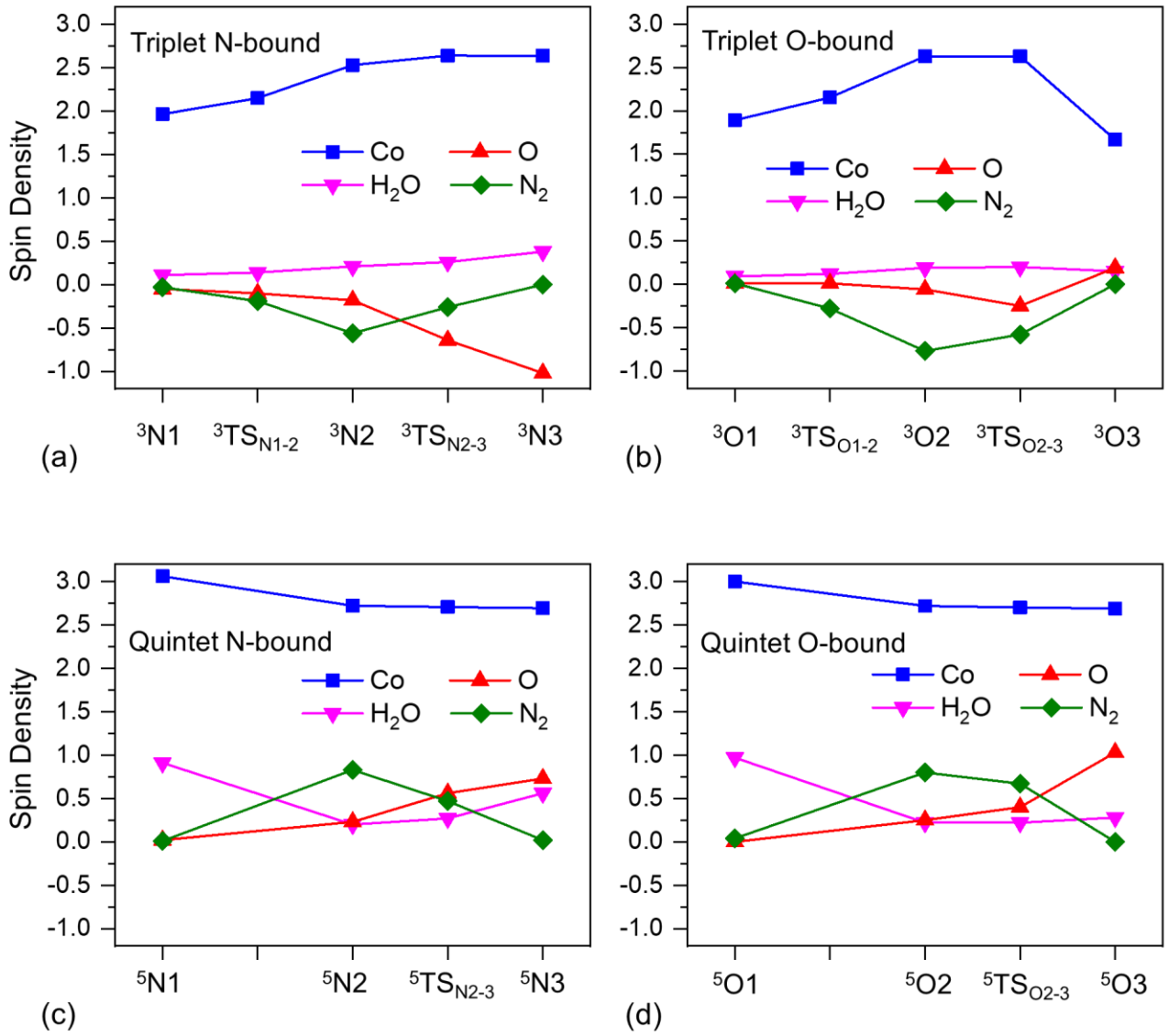


Figure S8: NBO spin density population analysis of Co, the N_2 moiety of N_2O, the O moiety of N_2O and the sum of all H_2O molecules along the reaction pathways (electron transfer and N–O bond dissociation) in $[Co(N_2O)(H_2O)_8]^+$ as shown in Figure 7 for triplet state of (a) N-bound & (b) O-bound and quintet state of (c) N-bound & (d) O-bound coordination.

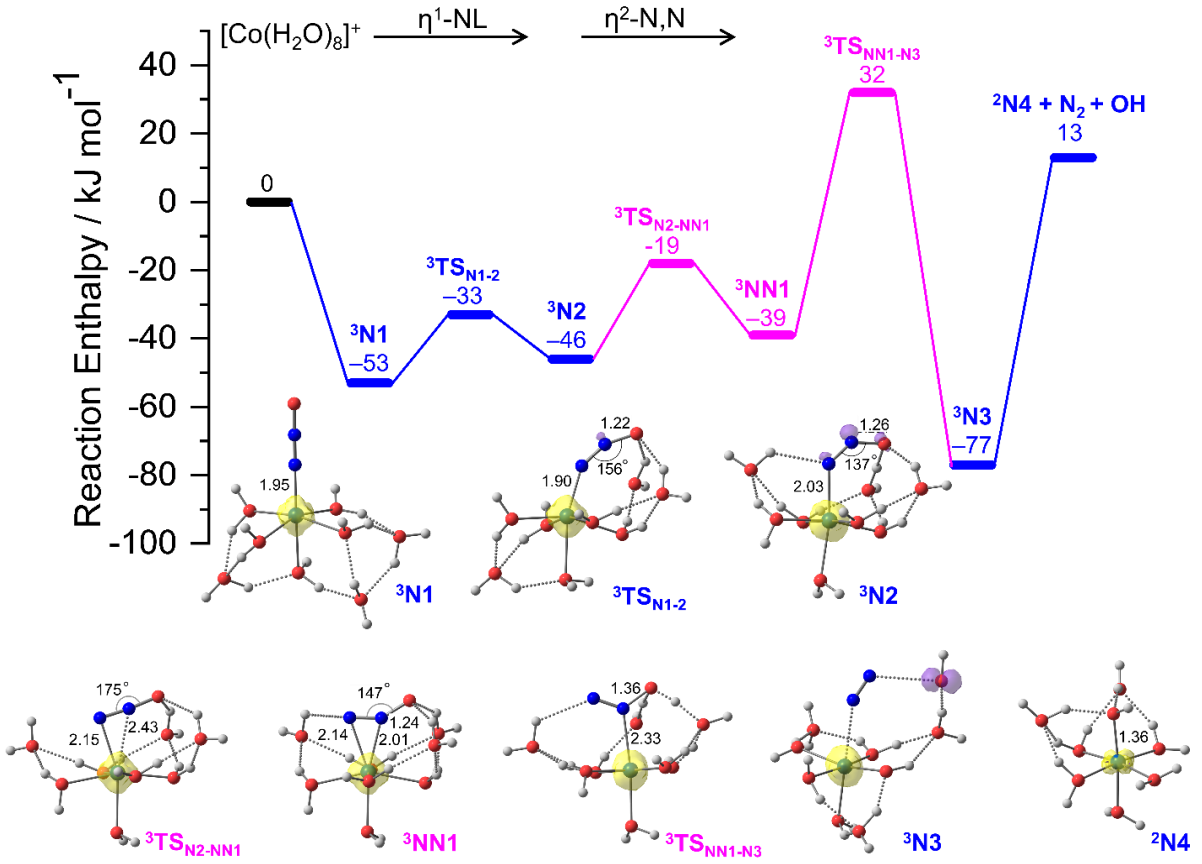
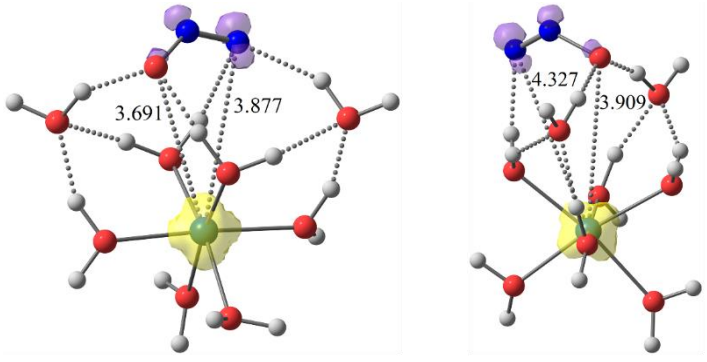


Figure S9: Potential energy surfaces of the reaction between $[Co(H_2O)_8]^+$ and N_2O, resulting in $[CoOH(H_2O)_7]^+$, N_2 and OH (Reaction 2), through the N-bound mode involving the η^2–N,N species (pink). Optimized geometries (bond lengths in Å and angles in °) with spin density distribution (an isovalue of 0.06 au) and their relative enthalpies (in kJ mol^{-1}) along the reaction pathways were evaluated at the M06/6-311++G** level of theory.



ΔH^o = 18 kJ mol^{-1} ΔH^o = 55 kJ mol^{-1}

Figure S10: Transition structures for the reduction of N_2O solvated on the cluster surface of $[Co(N_2O)_8]^+$ with different distances from the metal core.

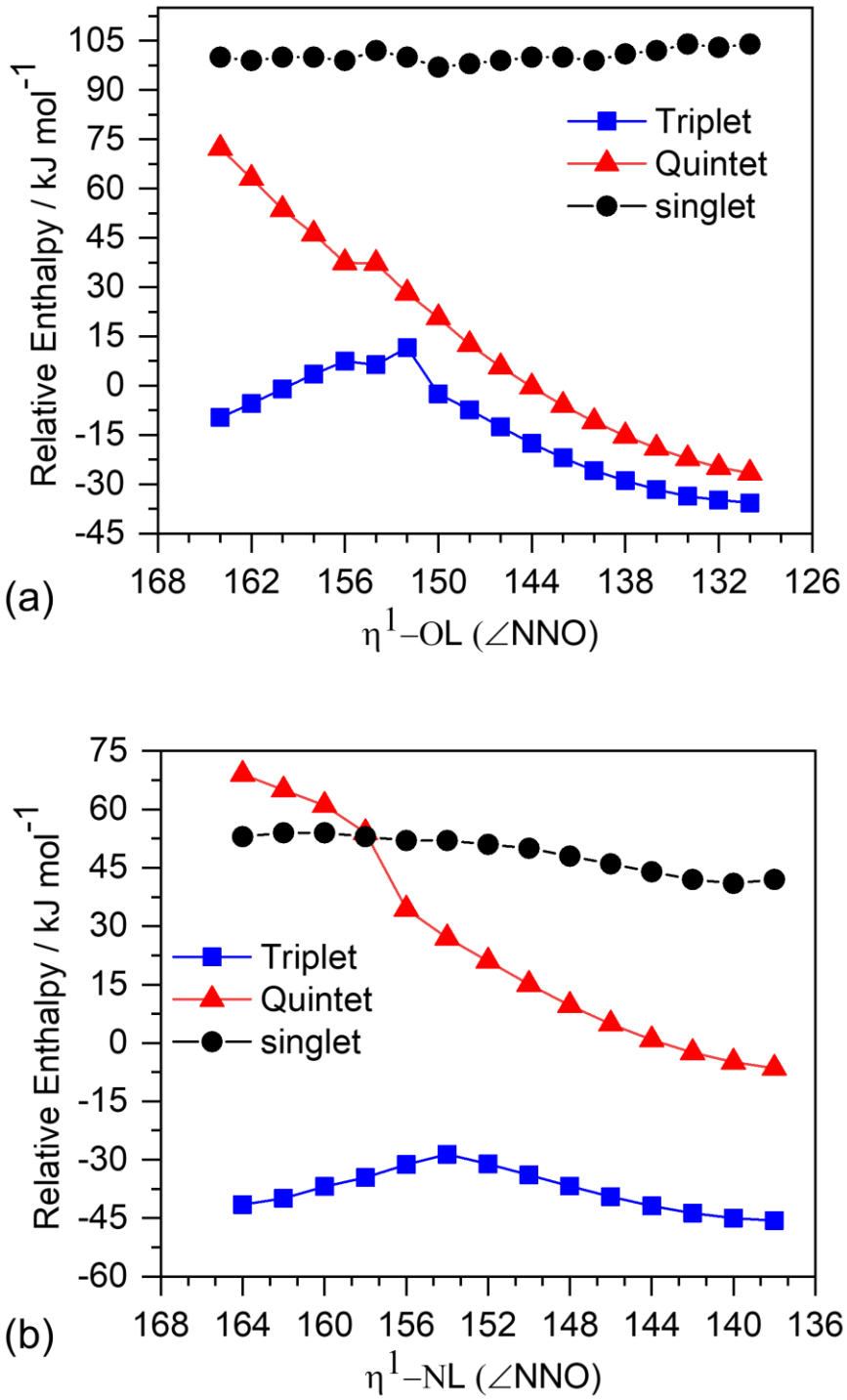


Figure S11: Potential energy surface scans of the singlet, triplet, and quintet electronic states for (a) η^1–OL and (b) η^1–NL with respect to their ∠NNO angles. The electron-transfer process on the triplet surface is preferred.

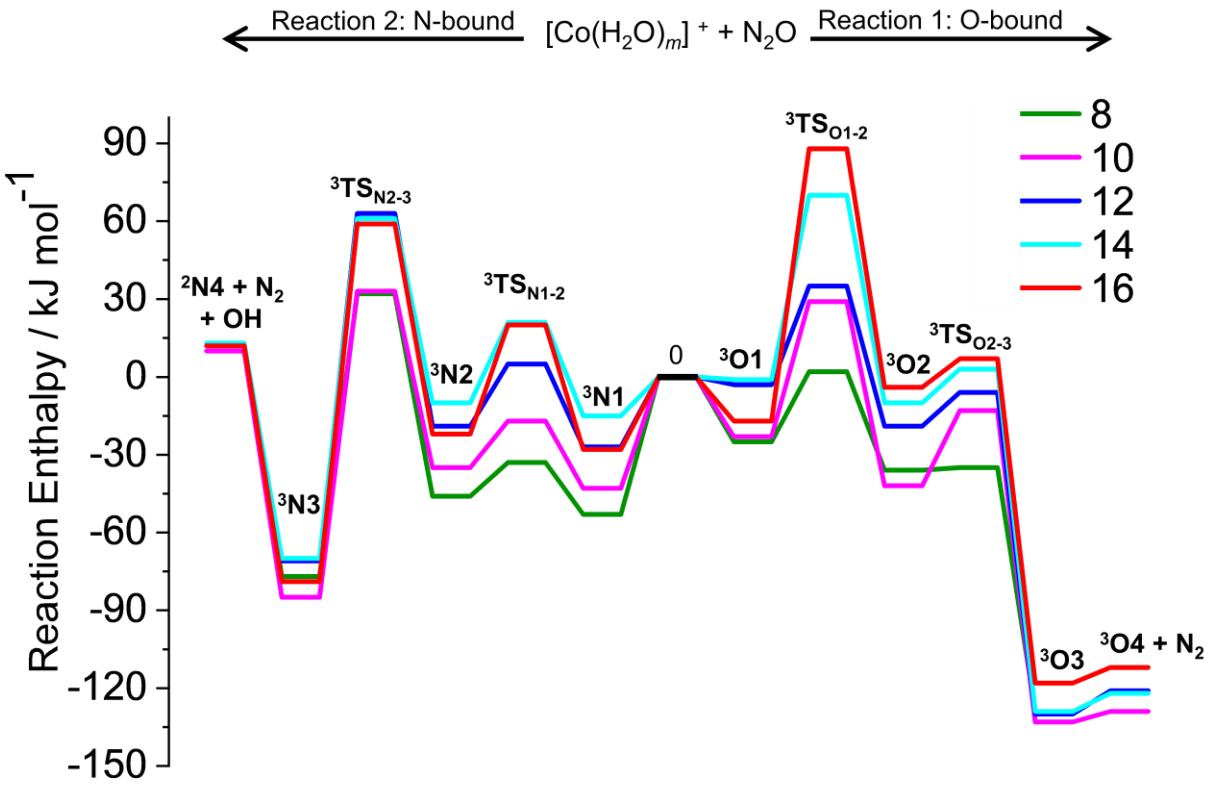


Figure S12: Potential energy surfaces of the reactions between $[Co(H_2O)_n]^+$ (n = 8, 10, 12, 14 and 16) and N_2O through (a) the O-bound mode resulting in $[CoO(H_2O)_{n-x}]^+$, N_2, and xH_2O (Reaction 1) and (b) the N-bound mode resulting in $[CoOH(H_2O)_{n-x}]^+$, N_2, OH, and xH_2O (Reaction 2) at the triplet electronic state. Their relative enthalpies (in kJ mol^{-1}) along the reaction pathways were evaluated at the M06/6-311++G** level of theory.

Table S1: Cartesian coordinates, harmonic vibration analyses (frequency in cm^{-1}, IR intensity in km mol^{-1}) and energies (E, E_{zpc}, H_{298}, G_{298} in a.u.) of the optimized geometries discussed in main text.

$[Co(H_2O)_1]^+$

Co	0.000000	0.000000	0.560847
O	0.000000	0.000000	-1.400202
H	0.000000	0.779014	-1.970625
H	0.000000	-0.779014	-1.970625

335.1, 320.2; 408.6, 6.4; 612.3, 87.6; 1646.9, 90.1; 3812.2, 162.1; 3899.3, 293.4;

-1458.796903940 -1458.772494 -1458.767883 - 1458.797437

$[Co(H_2O)_2]^+$

Co	0.000000	-0.000002	0.000000
O	1.931818	0.000010	0.000030
O	-1.931818	-0.000004	-0.000034
H	2.497005	0.781166	-0.000092
H	2.496951	-0.781221	-0.000092
H	-2.497009	-0.781157	0.000104
H	-2.496947	0.781229	0.000104

104.7, 21.2; 137.7, 16.5; 187.7, 0.0; 284.5, 0.0; 309.7, 542.9; 382.1, 0.0; 503.4, 11.1; 590.6, 0.0; 637.6, 114.4; 1641.0, 0.0; 1641.8, 202.4; 3827.5, 321.8; 3830.8, 0.0; 3917.7, 0.0; 3919.1, 562.8;

-1535.284435830 -1535.234508 -1535.227052 - 1535.264117

$[Co(H_2O)_3]^+$

Co	-0.000001	0.355539	0.000001
O	-1.966194	0.491750	0.000000
O	1.966191	0.491758	0.000001
O	0.000004	-1.834078	-0.000004
H	0.000016	-2.406305	0.773995
H	0.000012	-2.406306	-0.774002
H	-2.546991	-0.276280	-0.000002
H	-2.511250	1.285077	0.000002
H	2.546991	-0.276271	-0.000008
H	2.511244	1.285086	0.000010

18.1, 18.9; 96.7, 21.6; 124.3, 15.6; 155.9, 0.0; 194.7, 28.3; 257.8, 0.0; 265.8, 2.4; 278.3, 430.0; 282.8, 249.9; 306.9, 0.0; 344.6, 0.2; 443.5, 99.8; 449.9, 25.3; 547.1, 4.3; 588.5, 126.0; 1619.8, 94.5; 1625.6, 199.4; 1626.4, 0.5; 3843.5, 218.3; 3844.8, 71.0; 3846.0, 1.8; 3942.1, 2.2; 3943.2, 472.7; 3951.1, 189.8;

-1611.737251520 -1611.662989 -1611.652167 - 1611.698933

$[Co(H_2O)_4]^+$

Co	0.000064	0.000010	-0.000031
O	-0.796543	-1.868541	-0.000128
O	2.095968	-0.670597	0.000164
O	0.796334	1.868611	-0.000422
O	-2.095967	0.670462	0.000075
H	-1.749505	-2.003418	0.000255
H	-0.367276	-2.728473	0.000983
H	-2.558088	1.010693	-0.772327
H	-2.557536	1.010223	0.773013
H	0.367144	2.728584	0.000536
H	1.749305	2.003468	-0.000062
H	2.557670	-1.010134	0.773121
H	2.558223	-1.010703	-0.772211

54.3, 0.1; 73.3, 0.0; 94.7, 6.5; 109.6, 12.9; 133.1, 12.0; 179.2, 0.0; 188.7, 0.0; 194.3, 5.1; 238.2, 357.9; 239.6, 0.6; 276.6, 12.8; 310.1, 0.0; 316.0, 0.0; 326.7, 416.0; 341.2, 0.0; 375.5, 94.0; 392.6, 138.8; 432.3, 0.0; 449.8, 113.3; 500.2, 0.0; 538.7, 142.9; 1610.3, 228.3; 1612.5, 0.0; 1613.5, 152.7; 1613.5, 17.4; 3845.8, 114.1; 3846.5, 0.0; 3851.0, 129.2; 3852.1, 0.1; 3954.0, 0.0; 3954.6, 348.9; 3959.5, 0.4; 3960.6, 374.9;

-1688.186144830 -1688.087185 -1688.073269 - 1688.125959

$[Co(H_2O)_5]^+$

Co	-0.510708	0.012923	0.073750
O	-1.809683	1.553236	-0.276917
H	-2.747635	1.459076	-0.466480
O	-2.208601	-1.372082	-0.024624
H	-2.641128	-1.763003	0.740230
O	0.878722	-1.474856	0.118906
H	1.820737	-1.273776	-0.018997
O	1.058755	1.494762	0.302270
H	1.110764	2.001091	1.117918
H	-1.528102	2.428578	-0.559021
H	1.952555	1.157559	0.126870
H	-2.515995	-1.852001	-0.799085
H	0.734900	-2.418131	0.013444
O	3.312284	-0.166603	-0.281209
H	4.064760	-0.255656	0.313479
H	3.686449	-0.108317	-1.167018

34.9, 11.4; 47.7, 16.2; 58.8, 0.7; 90.8, 2.8; 112.3, 10.7; 124.5, 2.7; 159.6, 21.8; 171.9, 12.8; 199.5, 11.4; 221.8, 13.4; 230.0, 132.2; 243.2, 171.4; 254.6, 47.2; 282.1, 137.3; 286.9, 27.3; 298.0, 19.4; 319.1, 4.3; 331.9, 14.3; 351.5, 73.3; 383.1, 47.1; 425.7, 75.2; 454.4, 108.2; 494.6, 55.8; 540.4, 54.9; 593.8, 313.2; 695.5, 154.0; 708.5, 99.6; 1602.7, 196.7; 1603.8, 35.9; 1611.5, 94.1; 1625.0, 96.3; 1646.8, 20.2; 3674.9, 290.0; 3725.7, 643.8; 3845.9, 38.6; 3852.6, 51.0; 3853.3, 52.3; 3923.3, 179.5; 3937.5, 160.5; 3946.8, 172.1; 3962.6, 183.2; 3962.9, 177.3;

-1764.630738930 -1764.505689 -1764.489286 - 1764.548482

$[Co(H_2O)_6]^+$

Co	0.000033	0.000003	-0.255645
O	-1.393740	-1.480115	0.012076
H	-2.293621	-1.255260	0.302078
O	-1.554432	1.509171	-0.336210
H	-1.694708	1.993400	-1.154631
O	1.393744	1.480116	0.012439
H	2.293545	1.255255	0.302685
O	1.554526	-1.509171	-0.335823
H	1.694989	-1.993425	-1.154196
H	-1.154447	-2.342666	0.360994
H	2.423454	-1.181021	-0.052221
H	-2.423424	1.181024	-0.052802
H	1.154369	2.342676	0.361280
O	3.741934	0.074883	0.618888
H	4.548498	0.221512	0.113490
H	4.027509	-0.081326	1.525278
O	-3.742105	-0.074888	0.617885
H	-4.027964	0.081285	1.524191
H	-4.548509	-0.221505	0.112230

28.4, 11.1; 48.5, 1.6; 69.1, 0.0; 73.7, 4.2; 93.3, 0.0; 114.0, 3.6; 128.7, 0.4; 153.9, 3.0; 173.4, 5.5; 216.9, 0.0; 223.9, 4.8; 224.4, 23.7; 243.5, 16.6; 249.3, 40.2; 258.6, 3.5; 260.4, 45.8; 302.1, 13.6; 323.3, 43.2; 323.7, 51.8; 324.8, 29.7; 342.6, 146.4; 365.7, 39.9; 381.0, 47.2; 444.4, 3.5; 448.1, 305.7; 528.8, 127.6; 531.2, 95.8; 562.5, 1.4; 592.3, 314.6; 687.7, 107.5; 688.3, 381.2; 713.4, 71.7; 717.7, 15.0; 1597.1, 167.5; 1598.3, 80.4; 1620.1, 207.2; 1620.2, 10.1; 1640.0, 4.4; 1641.4, 21.9; 3692.9, 9.8; 3695.5, 345.7; 3726.2, 1264.2; 3731.5, 116.6; 3848.0, 61.0; 3848.0, 10.1; 3924.8, 203.5; 3925.1, 192.0; 3931.3, 0.9; 3932.2, 317.4; 3950.2, 52.6; 3950.4, 289.7;

-1841.074794780 -1840.922816 -1840.904465 - 1840.967973

$[Co(H_2O)_7]^+$

Co	0.006021	-0.407060	0.190738
O	1.439645	1.054382	0.175839
H	2.346262	0.868755	-0.109954
O	1.526354	-1.965679	0.264727

H	2.403388	-1.621137	0.030442
O	-1.417161	-1.860688	-0.088383
H	-2.337017	-1.621182	-0.290835
O	-1.531077	1.080513	0.276804
H	-1.301118	1.988076	0.032807
H	1.207040	1.981282	0.011049
H	-2.406736	0.864932	-0.072556
H	1.629448	-2.433187	1.098264
H	-1.222598	-2.727887	-0.451503
O	-3.836315	-0.484407	-0.405322
H	-4.374569	-0.464481	-1.202769
H	-4.456641	-0.554755	0.327764
O	3.775701	-0.369524	-0.533109
H	4.593721	-0.316982	-0.028382
H	4.043337	-0.472796	-1.452075
O	0.005884	3.470273	-0.062206
H	-0.005254	4.014426	0.732047
H	0.013922	4.086596	-0.801026

23.8, 3.2; 35.2, 11.2; 49.6, 14.8; 66.5, 1.1; 78.0, 4.0; 92.0, 2.2; 95.0, 1.2; 118.7, 2.4; 131.8, 0.8; 147.6, 1.2; 172.1, 2.6; 199.0, 12.7; 203.5, 0.6; 204.3, 11.7; 218.5, 20.2; 224.9, 5.0; 234.8, 18.1; 243.9, 63.5; 253.6, 12.7; 262.4, 2.3; 271.8, 8.1; 297.8, 40.7; 316.7, 38.6; 330.7, 0.9; 352.6, 52.8; 380.6, 52.7; 412.1, 92.0; 433.8, 255.4; 438.3, 132.0; 514.8, 53.3; 541.2, 87.3; 580.8, 131.1; 598.9, 63.9; 616.6, 238.3; 642.9, 524.5; 668.7, 201.8; 697.7, 79.5; 720.2, 78.6; 759.5, 30.8; 1575.1, 46.5; 1588.8, 189.2; 1598.2, 93.2; 1614.9, 75.7; 1622.4, 73.3; 1631.2, 46.1; 1638.5, 12.0; 3697.6, 410.4; 3705.6, 24.0; 3725.2, 349.5; 3746.7, 199.1; 3802.6, 976.0; 3834.1, 641.4; 3853.3, 15.8; 3855.1, 8.9; 3864.3, 115.1; 3925.0, 156.4; 3939.9, 183.1; 3956.9, 128.8; 3957.9, 138.9; 3959.4, 213.9;

-1917.515325380 -1917.338258 -1917.316821 -1917.388006

$[Co(H_2O)_8]^+$

Co	-0.639804	-0.635424	-0.609322
O	-2.647768	-0.283325	0.202404
H	-2.596825	0.587929	0.632785
O	2.137589	1.550416	-1.082183
H	2.865295	2.011658	-1.508528
O	1.543674	-1.118166	-1.163269
H	1.667208	-1.827118	-1.803222
O	-0.586865	1.231087	-1.413567
H	0.300299	1.606461	-1.543257
O	1.865327	-1.296931	1.561500
H	2.556762	-1.569238	2.171457
O	-0.573229	-2.201746	0.700606
H	-1.361931	-2.285364	1.246337
H	2.209232	0.603019	-1.306665
H	-1.067656	1.845126	-0.833853
H	1.885580	-1.432565	-0.303289
H	1.672517	-0.354150	1.739620
H	0.206358	-2.166830	1.281691
H	-3.457336	-0.304776	-0.315456
O	1.241079	1.471111	1.557674
H	1.632618	1.647980	0.676751
H	1.705566	2.046195	2.174483
O	-1.533935	2.136810	1.040301
H	-1.854435	2.911940	1.509489
H	-0.655509	1.922120	1.405617

57.9, 0.2; 64.0, 0.1; 76.7, 0.6; 93.2, 2.7; 99.7, 1.0; 110.6, 2.3; 130.0, 4.1; 138.4, 2.1; 162.5, 2.7; 164.7, 1.9; 185.8, 2.7; 191.6, 4.4; 205.7, 7.7; 215.0, 7.1; 245.2, 12.6; 248.8, 2.5; 259.9, 0.4; 266.8, 20.5; 273.3, 17.7; 325.2, 22.1; 331.7, 24.2; 344.6, 24.4; 356.0, 7.8; 367.4, 23.8; 388.7, 34.4; 395.1, 8.8; 404.8, 21.4; 424.5, 201.0; 442.6, 31.8; 464.2, 30.1; 476.4, 107.1; 488.6, 119.5; 521.9, 63.5; 540.5, 262.1; 570.1, 29.6; 593.2, 328.4; 616.8, 118.1; 661.2, 19.1; 679.6, 754.0; 696.5, 70.1; 753.6, 107.0; 783.4, 53.0; 808.0, 136.2; 839.1, 35.0; 917.1, 106.8; 1591.1, 173.4; 1600.9, 54.3; 1609.6, 26.7; 1611.7, 103.1; 1624.8, 135.5; 1634.9, 105.7; 1636.6, 12.7; 1673.0, 33.8; 3545.3, 131.1; 3597.9, 431.8; 3616.3, 607.9; 3648.0, 104.3; 3666.6, 528.1; 3686.6, 4.2; 3700.8, 451.9; 3714.3, 495.7; 3765.0, 687.7; 3898.6, 172.4; 3902.2, 110.4; 3903.7, 219.3; 3924.2, 189.0; 3925.2, 166.9; 3928.8, 172.9; 3931.6, 96.9;

-1993.961028530 -1993.754358 -1993.733064 -1993.801126

$[Co(H_2O)_9]^+$

Co	0.030743	-0.822680	-0.676820
O	1.039123	-2.192732	0.437428
H	1.776633	-1.864778	0.978220
O	0.835888	1.565630	1.797932
H	1.081063	2.108156	2.554449
O	2.022374	0.085116	-1.405399
H	1.836836	1.042317	-1.479883
H	1.539672	0.887947	1.715605
H	2.327089	-0.224509	-2.264518
H	0.519894	-2.828768	0.938727
O	-1.755989	-1.732086	0.199084
H	-2.554678	-1.667303	-0.336207
H	-1.917779	-1.137684	0.953463
O	-0.961072	0.712772	-1.522374
H	-0.518160	1.575477	-1.493775
H	-1.896642	0.828124	-1.256839
O	-3.386954	0.697008	-0.313606
H	-3.117861	0.862799	0.604564
H	-4.240026	1.114648	-0.452674
O	-1.822474	0.455262	1.990509
H	-2.054052	0.465412	2.923325
H	-0.923285	0.830871	1.925383
O	0.993243	2.548362	-0.839997
H	1.229745	3.467940	-0.987555
H	0.920846	2.410343	0.124966
O	2.851726	-0.291881	1.173006
H	2.874154	-0.157524	0.204776
H	3.759567	-0.280707	1.489432

45.7, 1.2; 51.4, 0.5; 62.1, 1.1; 67.1, 2.1; 77.7, 4.0; 93.4, 0.1; 105.3, 2.3; 110.4, 5.1; 122.2, 0.4; 135.6, 4.0; 158.8, 2.0; 169.5, 8.4; 179.1, 2.3; 188.8, 1.3; 208.2, 7.0; 224.3, 14.1; 234.5, 2.0; 246.4, 27.1; 254.1, 4.1; 266.0, 16.3; 275.7, 21.9; 292.3, 33.1; 294.6, 4.7; 324.1, 86.2; 337.2, 6.1; 348.8, 34.2; 359.2, 6.4; 364.3, 51.6; 374.5, 9.2; 391.9, 48.0; 408.4, 47.3; 413.6, 118.5; 436.5, 76.8; 450.1, 107.5; 469.2, 56.9; 474.9, 247.8; 501.9, 57.5; 506.1, 24.5; 554.2, 161.7; 568.1, 170.0; 608.9, 11.3; 615.7, 195.2; 667.5, 178.8; 687.3, 240.2; 720.1, 320.5; 734.8, 248.1; 782.5, 108.0; 785.6, 82.7; 817.3, 52.6; 904.0, 72.3; 914.1, 128.5; 1584.1, 210.2; 1588.6, 120.3; 1593.4, 15.2; 1613.6, 65.8; 1616.5, 35.7; 1627.0, 232.3; 1638.6, 21.9; 1650.1, 43.4; 1652.4, 15.5; 3538.2, 126.8; 3564.6, 365.7; 3592.5, 848.9; 3612.0, 673.8; 3634.2, 298.6; 3655.5, 316.4; 3692.9, 302.7; 3717.0, 363.1; 3738.4, 303.8; 3759.2, 605.3; 3891.6, 165.2; 3901.5, 88.1; 3903.3, 179.6; 3914.9, 224.3; 3925.8, 124.1; 928.1, 200.8; 3934.2, 93.4; 3953.3, 189.0;

-2070.402566170 -2070.170637 -2070.146471 -2070.221393

$[Co(H_2O)_{10}]^+$

Co	0.537993	-0.546460	0.258962
O	1.302836	1.513045	1.014652
H	0.476124	2.010499	1.164457
O	-2.932482	-1.301575	-0.392019
H	-3.716625	-1.852626	-0.459610
O	-0.475868	-2.201884	-1.170331
H	-0.019228	-3.031356	-1.335685
O	-1.249220	-0.330496	1.594433
H	-2.026844	-0.732284	1.172582
O	-0.027131	0.382990	-1.740583
H	0.710322	0.967662	-1.983682
O	2.368290	-1.008311	-0.882490
H	2.709704	-0.172704	-1.247634
H	-2.179613	-1.814882	-0.752695
H	-1.459310	0.610448	1.715834
H	-0.175413	-1.567749	-1.843764
H	-0.842813	0.910905	-1.730256
H	3.114960	-1.464585	-0.488666
H	1.672846	1.303103	1.878994
O	-2.560804	1.350486	-1.096517
H	-2.857111	0.437456	-0.896632
H	-3.228360	1.741598	-1.666736
O	-1.332744	2.422803	1.153956
H	-1.720918	3.208708	1.547347

H	-1.817087	2.244586	0.323269
O	1.190485	-1.148946	2.341630
H	1.647957	-1.927571	2.668279
H	0.286376	-1.185240	2.684985
O	2.427083	1.673058	-1.489097
H	2.989593	2.362006	-1.850347
H	2.226085	1.897089	-0.561086

51.7, 0.9; 62.3, 0.6; 74.9, 0.9; 78.2, 0.3; 83.4, 5.6; 89.1, 1.8; 96.9, 3.1; 102.7, 2.8; 118.0, 3.4; 122.0, 3.1; 134.4, 4.2; 150.2, 7.4; 158.3, 3.3; 169.0, 1.7; 185.2, 6.4; 196.3, 10.5; 209.2, 4.4; 222.8, 11.1; 237.5, 2.4; 239.5, 21.1; 247.4, 8.9; 256.2, 22.1; 269.1, 7.0; 277.1, 7.2; 277.7, 25.9; 286.9, 24.9; 292.7, 24.7; 306.1, 77.0; 325.6, 75.7; 339.4, 33.8; 347.5, 5.4; 360.4, 55.5; 372.0, 69.0; 374.0, 37.0; 397.5, 90.2; 411.3, 62.3; 419.8, 16.3; 438.3, 95.6; 447.8, 134.0; 461.4, 50.8; 488.1, 86.0; 502.8, 139.3; 530.9, 16.5; 542.0, 104.5; 562.0, 63.5; 601.6, 213.0; 618.3, 147.3; 649.5, 194.8; 685.3, 714.7; 700.2, 57.2; 714.7, 227.6; 769.6, 28.2; 779.4, 21.0; 795.8, 192.1; 820.3, 231.9; 846.8, 41.8; 873.7, 92.6; 1578.2, 66.7; 1581.6, 95.8; 1584.4, 138.7; 1610.8, 75.6; 1617.3, 143.7; 1620.6, 155.7; 1632.2, 41.1; 1646.1, 19.8; 1656.7, 16.3; 1672.1, 13.5; 3532.3, 399.7; 3583.3, 535.4; 3603.1, 204.4; 3629.5, 549.6; 3654.6, 74.6; 3668.8, 32.4; 3697.1, 373.5; 3703.9, 905.1; 719.1, 13.3; 3764.6, 581.5; 3767.7, 975.6; 3783.9, 100.5; 3894.2, 160.7; 3927.3, 116.9; 3930.1, 157.7; 3933.7, 185.1; 3935.0, 131.7; 3944.4, 82.5; 3945.5, 262.2; 3948.0, 131.9;

-2146.847952950 -2146.590664 -2146.563770 -2146.643520

$[Co(H_2O)_{11}]^+$

Co	-0.357470	-0.022685	0.285249
O	0.347526	-2.100689	1.141018
H	1.308348	-1.911644	1.173691
O	1.675707	2.773156	-0.454291
H	1.904615	3.699021	-0.568335
O	-0.799503	1.834444	-1.073909
H	-1.749162	2.001106	-0.929921
O	1.113333	0.985977	1.612647
H	1.461633	1.773253	1.164233
O	0.522865	-0.545598	-1.682233
H	0.351429	-1.478134	-1.890371
O	-2.337414	-1.099444	-0.478515
H	-2.004954	-1.849725	-1.003520
H	0.743305	2.661835	-0.735694
H	1.876220	0.409386	1.767619
H	-0.722071	1.273684	-1.856976
H	1.479179	-0.386023	-1.742707
H	-2.602237	-1.480071	0.365694
H	0.075421	-2.284617	2.044841
O	3.058755	0.491980	-1.183001
H	2.682701	1.375655	-0.980482
H	3.805885	0.636817	-1.769825
O	2.930797	-1.110930	1.083163
H	3.755926	-1.483275	1.404530
H	3.130755	-0.634226	0.252337
O	-1.769953	0.523432	1.895713
H	-2.452845	1.091590	1.505854
H	-1.302338	1.048103	2.553066
O	-0.559840	-3.072035	-1.289602
H	-0.541455	-3.978762	-1.605134
H	-0.190240	-3.057074	-0.386938
O	-3.397763	1.434486	-0.254482
H	-3.349265	0.511979	-0.561816
H	-4.285236	1.755395	-0.433933

45.9, 0.2; 61.8, 4.3; 71.4, 0.8; 75.9, 1.0; 82.7, 4.4; 85.1, 1.1; 102.3, 3.4; 102.6, 2.3; 110.4, 1.4; 114.1, 4.2; 125.1, 1.8; 137.8, 2.6; 150.7, 1.1; 156.8, 6.3; 162.6, 4.0; 171.7, 1.3; 183.1, 12.6; 196.0, 7.0; 202.0, 8.8; 212.1, 2.3; 221.7, 5.7; 229.5, 5.2; 244.1, 11.4; 254.6, 33.2; 268.7, 2.0; 272.3, 17.4; 280.8, 19.3; 283.5, 8.6; 289.9, 6.7; 305.4, 16.1; 334.3, 10.3; 351.6, 47.1; 358.2, 81.7; 366.3, 34.5; 372.7, 33.8; 374.5, 48.8; 384.4, 5.3; 393.0, 24.2; 401.6, 68.9; 424.5, 204.8; 431.7, 82.4; 445.4, 55.3; 457.7, 83.8; 467.2, 32.5; 483.4, 5.4; 505.7, 131.5; 521.7, 49.6; 552.1, 188.2; 568.2, 63.3; 581.3, 160.3; 619.8, 306.0; 647.9, 434.5; 655.9, 561.2; 696.8, 154.6; 729.1, 127.9; 736.8, 206.2; 760.5, 28.3; 781.2, 0.3; 785.3, 213.6; 796.9, 96.6; 806.9, 63.3; 848.9, 97.2; 888.3, 119.6; 1583.3, 155.8; 1585.2, 164.5; 1606.3, 92.6; 1611.1, 41.9; 1615.7, 32.4; 1625.8, 167.7; 1638.7, 45.8; 641.7, 45.9; 1652.2, 73.0; 1653.3, 15.2; 1671.9, 9.9; 3515.8, 487.5; 562.2, 989.9; 3579.6, 236.0; 3619.2, 497.3; 3644.4, 138.8; 3654.9, 147.1; 3679.5, 169.2; 3698.3, 475.8; 3712.3, 207.2; 3726.6, 351.3; 3750.7, 285.9; 780.3, 788.1; 3808.3, 582.6; 3846.4, 227.4; 3901.2, 116.7; 3915.1, 80.2; 3915.9, 152.8; 3928.6, 116.7; 3935.4, 152.6; 3937.2, 161.0; 3941.5, 175.2; 3945.2, 147.1;

-2223.289876850 -2223.005984 -2222.976895 -2223.061174

$[Co(H_2O)_{12}]^+$

Co	0.174562	0.135306	-0.053362
O	0.355439	-2.090727	-0.507244
H	-0.469603	-2.320738	-0.970340
O	-2.729397	2.160361	-0.121508
H	-3.274408	2.949628	-0.173722
O	-0.217453	2.211049	0.936704
H	0.653395	2.647241	0.909052
O	-1.196150	0.549684	-1.775413
H	-1.892386	1.170994	-1.505380
O	-0.881913	-0.300250	1.867145
H	-0.459213	-1.071421	2.282492
O	2.229752	-0.174893	1.040940
H	2.039865	-0.819745	1.742802
H	-1.880089	2.415442	0.295064
H	-1.643739	-0.283112	-1.998125
H	-0.287756	1.754476	1.786887
H	-1.810519	-0.525680	1.692486
H	2.672197	-0.687156	0.339543
H	1.111914	-2.176031	-1.111937
O	-3.394344	-0.428899	0.644761
H	-3.310464	0.517263	0.403007
H	-4.259977	-0.532866	1.049426
O	-2.280265	-1.994739	-1.405619
H	-2.875190	-2.602431	-1.852333
H	-2.777127	-1.600298	-0.661774
O	1.549600	1.014341	-1.724749
H	1.915415	1.803537	-1.290607
H	0.807514	1.281705	-2.282147
O	0.909123	-2.367532	2.176586
H	1.074316	-3.179319	2.661419
H	0.720613	-2.599692	1.246734
O	2.483325	2.502332	0.468662
H	2.645402	1.627816	0.873370
H	3.218652	3.074234	0.702714
O	2.825548	-1.367842	-1.462121
H	3.592281	-1.681987	-1.947387
H	2.549622	-0.518207	-1.855615

54.2, 0.7; 68.0, 0.9; 70.5, 1.8; 75.8, 0.9; 84.6, 1.5; 90.0, 2.2; 97.8, 2.2; 109.6, 4.6; 113.9, 1.2; 120.0, 4.5; 123.7, 1.6; 138.9, 11.1; 141.5, 1.0; 150.7, 3.3; 158.5, 1.3; 168.5, 5.2; 186.3, 1.3; 191.7, 3.9; 194.6, 12.3; 205.4, 12.4; 210.1, 20.6; 215.9, 7.7; 229.6, 1.9; 236.4, 29.4; 250.2, 19.4; 256.5, 18.3; 263.5, 5.6; 271.2, 11.9; 273.1, 20.6; 274.3, 20.7; 279.4, 1.7; 294.5, 11.4; 300.4, 18.3; 335.7, 6.6; 354.4, 11.8; 372.9, 30.3; 380.1, 18.0; 387.6, 4.3; 398.7, 27.4; 414.1, 22.3; 416.7, 105.6; 419.7, 48.6; 431.5, 34.9; 448.2, 108.4; 466.0, 112.0; 480.3, 37.3; 483.2, 62.4; 508.5, 85.0; 521.3, 179.2; 541.1, 53.5; 560.4, 164.6; 575.4, 47.3; 583.5, 155.0; 631.6, 292.5; 644.5, 495.6; 677.0, 731.4; 693.1, 99.2; 696.8, 163.1; 715.6, 134.3; 749.6, 80.8; 757.0, 188.9; 768.7, 46.1; 788.3, 96.9; 798.2, 119.5; 805.7, 209.5; 817.4, 32.9; 848.2, 54.5; 873.0, 122.4; 887.2, 57.3; 1559.0, 103.5; 1574.7, 164.9; 1592.0, 150.3; 1605.4, 23.9; 1609.8, 86.9; 1614.5, 158.5; 1620.4, 24.5; 1626.9, 53.9; 1642.4, 27.2; 1647.8, 28.5; 1663.0, 7.9; 1674.9, 66.8; 3541.2, 455.6; 3588.8, 592.4; 3599.4, 174.6; 3609.1, 39.6; 3625.3, 450.2; 3634.9, 467.8; 3663.4, 95.0; 3673.7, 81.0; 3674.7, 311.0; 3687.4, 268.1; 3703.5, 441.2; 3716.7, 120.4; 3738.4, 205.5; 3757.1, 1481.4; 3769.0, 647.8; 3776.9, 609.9; 3825.8, 273.4; 3858.1, 307.8; 3927.1, 115.5; 3935.9, 149.7; 3936.8, 180.8; 3938.4, 142.1; 3942.8, 140.4; 3948.7, 162.8;

-2299.738068210 -2299.426791 -2299.396198 -2299.483032

$[Co(H_2O)_{13}]^+$

Co	-0.146889	0.011756	-0.203651
O	-0.205652	2.263828	0.254942
H	0.628313	2.629689	-0.087445
O	2.609304	-1.907881	-1.152887
H	3.101932	-2.644325	-1.523207
O	0.015775	-2.267466	-0.438021
H	-0.814870	-2.515830	-0.876028
O	1.208053	0.325644	-1.978811
H	1.869224	-0.384774	-2.014727
O	0.964383	-0.225961	1.781710
H	0.590362	0.459254	2.366986
O	-2.172680	-0.071792	0.902052
H	-1.995901	0.096894	1.839210
H	1.711124	-2.236668	-0.924743
H	1.699663	1.152478	-1.844933
H	-0.099682	-2.574355	0.489687
H	1.903277	-0.027275	1.624785
H	-2.581184	0.745906	0.563902
H	-0.961055	2.626205	-0.239194
O	3.443226	0.108668	0.561065
H	3.269329	-0.656342	-0.028895
H	4.321547	-0.022448	0.928652
O	2.434601	2.440513	-0.635766
H	3.057076	3.150320	-0.812757
H	2.916289	1.751486	-0.137499
O	-1.547951	0.170117	-2.114563
H	-2.011394	-0.685032	-2.118057
H	-0.790720	0.124971	-2.712766
O	-2.697314	-2.058611	-0.979164
H	-2.728475	-1.551421	-0.145021
H	-3.478847	-2.615220	-1.011911
O	-2.728619	2.172044	-0.755691
H	-3.481259	2.702684	-1.026881
H	-2.490318	1.583681	-1.498612
O	-0.786895	1.564616	2.829729
H	-0.921518	2.143186	3.583504
H	-0.643078	2.121733	2.040895
O	-0.315392	-2.590153	2.203065
H	-0.136558	-3.253223	2.872351
H	0.266014	-1.827499	2.369990

51.0, 0.4; 55.3, 0.4; 62.1, 0.5; 71.9, 0.3; 73.6, 0.6; 84.8, 0.6; 86.6, 0.4; 98.4, 2.0; 106.6, 3.4; 111.1, 0.8; 115.3, 3.1; 119.9, 2.5; 129.4, 6.2; 137.9, 0.9; 146.5, 1.1; 159.6, 5.1; 164.0, 3.2; 174.2, 10.9; 192.4, 2.3; 195.1, 11.5; 200.5, 5.6; 211.5, 15.9; 217.5, 9.7; 220.8, 18.8; 233.2, 22.7; 241.5, 4.9; 251.7, 4.3; 255.0, 9.4; 262.3, 10.2; 271.0, 6.3; 275.5, 48.3; 281.2, 1.3; 282.4, 18.4; 288.4, 3.8; 290.5, 30.0; 314.8, 103.1; 325.8, 24.8; 341.0, 2.2; 344.4, 10.0; 349.6, 10.8; 358.0, 53.1; 372.6, 73.6; 379.7, 18.6; 399.2, 38.6; 407.0, 70.1; 423.2, 49.0; 432.8, 35.4; 435.1, 63.5; 452.3, 61.5; 472.4, 209.3; 487.1, 100.2; 492.8, 64.1; 504.4, 5.1; 534.5, 101.8; 545.3, 211.6; 563.6, 85.1; 586.8, 43.6; 624.0, 331.2; 635.4, 364.8; 659.0, 110.6; 694.7, 602.8; 705.4, 117.7; 717.1, 300.5; 732.5, 99.9; 761.7, 247.3; 773.5, 66.4; 785.1, 15.4; 787.1, 55.9; 794.0, 169.2; 804.1, 107.7; 830.3, 52.5; 877.5, 37.2; 884.5, 126.4; 917.7, 96.6; 924.4, 131.4; 1555.1, 97.7; 1562.7, 156.3; 1572.5, 117.5; 1600.0, 11.8; 1603.8, 121.7; 1613.3, 125.2; 1615.0, 19.5; 1617.0, 144.2; 1620.9, 27.9; 1650.7, 35.2; 1657.7, 68.7; 1667.3, 1.4; 1695.4, 61.4; 3463.2, 707.8; 3521.7, 574.5; 3555.0, 353.6; 3595.9, 276.2; 3604.3, 138.5; 3611.3, 293.5; 3637.0, 609.5; 3643.5, 504.9; 3670.5, 109.0; 3682.0, 281.4; 3692.5, 478.1; 3701.5, 263.9; 3707.7, 41.6; 3731.3, 634.5; 3748.8, 325.4; 3756.0, 1232.8; 3778.2, 628.8; 3816.9, 336.2; 3853.7, 334.6; 3927.1, 106.3; 3936.9, 152.3; 3937.7, 147.9; 3945.5, 151.8; 3946.5, 152.7; 3950.9, 157.1; 3961.5, 171.3;

-2376.178026860 -2375.840955 -2375.807807 -2375.900222

$[Co(H_2O)_{14}]^+$

Co	-0.040396	-0.123574	0.332013
O	-0.282418	2.079214	0.914343
H	-1.236460	2.178317	1.079491
O	-2.552381	-2.398347	-0.673609
H	-2.922194	-3.268231	-0.841110
O	0.140066	-2.188113	-0.579638
H	0.779695	-2.651635	-0.012115
O	-1.961667	-0.729652	1.444502
H	-2.427201	-1.412660	0.933772
O	-0.616686	0.451544	-1.739854
H	-0.336874	1.352852	-1.959865
O	2.245957	0.184550	0.300780
H	2.596564	0.569337	-0.524106
H	-1.572412	-2.472554	-0.748112
H	-2.551218	0.039943	1.496602
H	0.657051	-1.959712	-1.385473
H	-1.579253	0.430904	-1.861428
H	2.377005	0.831807	1.014015
H	0.221307	2.188820	1.741119
O	-3.395420	0.097535	-1.457854
H	-3.235583	-0.849326	-1.255693
H	-4.080543	0.125781	-2.130545
O	-3.066617	1.736378	0.794051
H	-3.826541	2.269705	1.040063
H	-3.278470	1.314268	-0.061992
O	0.526025	-0.844625	2.569822
H	1.055987	-1.640086	2.391640
H	-0.404222	-1.100936	2.649498
O	2.626447	1.232066	-2.220219
H	3.401544	1.586087	-2.662803
H	1.993638	1.969198	-2.105569
O	2.276525	-2.449370	1.169652
H	2.558714	-1.597352	0.781764
H	3.055239	-3.002374	1.264203
O	1.690792	1.576402	2.721901
H	2.144204	1.937071	3.487105
H	1.325842	0.703376	2.972247
O	0.618510	2.952628	-1.504223
H	0.464366	3.875054	-1.719510
H	0.346441	2.815001	-0.570577
O	1.935400	-1.508865	-2.492649
H	2.028497	-1.878147	-3.372878
H	2.059297	-0.548777	-2.580134

43.5, 0.6; 58.0, 0.5; 65.9, 0.8; 70.7, 1.0; 74.7, 0.2; 77.6, 2.6; 87.2, 0.3; 87.8, 2.0; 90.2, 2.6; 96.0, 5.1; 100.6, 5.0; 111.1, 0.2; 114.6, 2.0; 120.0, 0.4; 125.2, 3.6; 139.2, 1.7; 153.3, 8.7; 165.7, 4.2; 170.7, 3.3; 181.7, 8.3; 186.6, 6.6; 194.6, 6.8; 200.9, 4.7; 211.3, 18.6; 216.8, 12.5; 218.9, 14.6; 224.7, 13.9; 231.6, 62.3; 239.5, 43.5; 242.5, 22.7; 255.4, 10.9; 258.0, 16.7; 264.1, 4.9; 276.7, 24.6; 280.0, 5.4; 283.0, 19.5; 292.0, 20.8; 301.8, 13.0; 304.4, 5.2; 327.8, 21.7; 333.6, 24.9; 336.8, 7.6; 338.8, 5.8; 350.4, 49.5; 356.9, 6.7; 367.6, 43.8; 394.7, 25.7; 411.1, 27.8; 425.4, 31.1; 434.5, 30.6; 436.1, 155.0; 463.4, 93.2; 470.6, 28.2; 481.4, 35.7; 487.8, 107.8; 496.2, 119.1; 509.2, 120.4; 521.7, 143.0; 547.8, 81.8; 559.5, 48.0; 563.3, 41.3; 594.7, 46.4; 628.4, 151.6; 634.6, 88.3; 651.0, 461.5; 659.0, 594.5; 704.6, 311.4; 715.7, 113.8; 722.6, 173.9; 730.7, 90.1; 758.1, 279.2; 771.0, 84.2; 794.9, 131.3; 797.7, 51.7; 808.6, 91.8; 826.0, 65.5; 860.3, 147.3; 879.4, 43.4; 900.4, 110.6; 930.6, 101.3; 976.8, 161.6; 1559.2, 117.0; 1581.9, 82.7; 1595.5, 121.6; 1612.9, 44.0; 1613.1, 129.9; 1614.1, 128.6; 1620.4, 53.9; 1631.3, 52.4; 1634.5, 33.9; 1644.7, 41.4; 1657.5, 28.0; 1660.8, 15.1; 1676.9, 47.2; 1687.9, 86.0; 3441.2, 984.7; 3507.3, 421.8; 3519.6, 615.2; 3548.4, 374.3; 3577.3, 72.8; 3592.3, 1047.9; 3613.7, 280.0; 3615.5, 363.9; 3651.6, 265.6; 3658.4, 64.2; 3691.1, 190.2; 3695.6, 68.9; 3717.2, 786.0; 3719.6, 321.4; 3726.8, 54.2; 3734.7, 822.2; 3755.7, 970.1; 3778.0, 652.1; 3797.7, 712.3; 3815.7, 462.5; 3934.5, 106.8; 3938.6, 157.3; 3941.8, 127.5; 3943.5, 153.9; 3946.9, 121.6; 3948.2, 246.8; 3949.3, 74.5; 3961.1, 151.9;

-2452.619393980 -2452.256509 -2452.220735 -2452.318837

$[Co(H_2O)_{15}]^+$

Co	-0.121030	0.252863	-0.059331
O	-0.014888	-0.438466	-2.254196
H	-0.881330	-0.832018	-2.442148
O	-2.313651	-0.864748	2.459260
H	-2.808047	-0.719028	3.269194
O	0.006511	0.481515	2.194687

H	0.250232	1.412177	2.330762
O	-2.456938	0.197195	-0.088795
H	-2.681404	-0.157983	0.789804
O	0.409712	-1.874460	0.458234
H	0.926767	-2.303768	-0.240067
O	2.103460	0.947069	-0.295129
H	2.796320	0.264964	-0.224774
H	-1.462900	-0.370938	2.539419
H	-2.682029	-0.490163	-0.738385
H	0.844090	-0.007944	2.359181
H	-0.347567	-2.459073	0.617715
H	2.104719	1.274031	-1.210282
H	0.125320	0.374978	-2.772536
O	-2.136494	-3.026496	0.777673
H	-2.310130	-2.374194	1.488886
H	-2.384352	-3.888045	1.122223
O	-2.380154	-1.974457	-1.826620
H	-3.028975	-2.408881	-2.385997
H	-2.284816	-2.526640	-1.026950
O	-0.374713	2.526399	-0.488904
H	0.102251	2.948717	0.246675
H	-1.308235	2.825115	-0.441904
O	3.652000	-1.325270	0.021339
H	4.596873	-1.468244	-0.069813
H	3.208632	-1.819416	-0.696066
O	1.390694	2.826879	1.606106
H	1.948380	2.226493	1.074438
H	1.967814	3.457304	2.041997
O	1.026669	2.012216	-2.709351
H	1.243036	2.664309	-3.379030
H	0.471386	2.449967	-2.026776
O	1.927137	-2.300294	-1.861372
H	2.030523	-2.953164	-2.556902
H	1.300114	-1.616808	-2.185610
O	2.524380	-0.506069	2.500201
H	2.889534	-0.935978	3.275798
H	2.854304	-0.998326	1.730112
O	-3.025452	2.870957	-0.236866
H	-3.149325	1.906308	-0.259437
H	-3.769555	3.283197	-0.677717

41.3, 0.1; 50.8, 0.4; 59.5, 0.9; 62.3, 0.6; 74.3, 0.4; 75.7, 0.3; 82.3, 2.1; 82.9, 0.2; 89.3, 1.9; 93.2, 1.4; 99.2, 2.0; 103.6, 0.4; 108.4, 2.1; 114.5, 0.3; 116.5, 0.1; 127.7, 1.8; 137.0, 0.3; 145.6, 4.3; 154.5, 4.9; 167.3, 7.1; 172.3, 7.7; 182.1, 6.6; 184.9, 6.5; 191.8, 12.3; 193.5, 4.4; 205.4, 17.2; 208.5, 18.2; 218.1, 39.7; 220.0, 30.1; 225.2, 31.2; 232.0, 28.6; 236.7, 82.3; 244.5, 77.9; 250.8, 33.9; 255.0, 15.9; 257.9, 0.8; 275.6, 13.2; 277.1, 15.7; 284.7, 15.2; 295.7, 4.0; 298.7, 3.3; 301.1, 3.6; 317.3, 32.8; 324.9, 41.2; 328.2, 10.3; 337.4, 20.1; 340.4, 21.3; 345.5, 32.8; 350.3, 18.1; 361.6, 40.2; 388.6, 10.0; 397.7, 115.2; 415.7, 55.3; 420.0, 31.3; 428.5, 58.2; 439.8, 151.0; 453.0, 161.2; 469.7, 18.5; 485.3, 116.3; 489.3, 49.3; 501.1, 16.4; 532.6, 12.2; 544.0, 1.4; 555.3, 68.6; 562.4, 167.1; 587.6, 17.5; 610.8, 145.1; 646.4, 46.9; 658.2, 50.0; 669.0, 554.6; 685.1, 345.6; 702.1, 358.8; 711.5, 9.5; 721.1, 329.0; 749.4, 296.4; 779.4, 25.0; 785.2, 73.4; 808.6, 25.1; 823.4, 82.6; 831.8, 144.5; 845.6, 150.5; 863.0, 200.0; 887.3, 45.2; 906.1, 118.2; 923.2, 169.1; 957.3, 74.7; 967.4, 131.9; 1539.2, 89.5; 1576.3, 50.7; 1586.4, 132.4; 1599.9, 121.1; 1607.4, 162.1; 1610.8, 77.3; 1618.3, 47.6; 1630.1, 138.9; 1638.6, 18.3; 1647.8, 18.4; 1659.5, 15.0; 1667.6, 19.6; 1671.3, 70.3; 1683.3, 27.5; 1690.7, 97.6; 3427.5, 932.5; 3484.4, 950.2; 3506.2, 253.0; 3526.1, 640.8; 3554.8, 301.8; 3559.6, 416.7; 3600.5, 742.9; 3624.3, 247.1; 3632.3, 721.3; 3654.0, 249.7; 3662.0, 128.2; 3665.9, 103.4; 3702.2, 283.8; 3710.4, 419.6; 3725.3, 211.4; 3729.9, 588.1; 3738.7, 916.6; 3752.3, 672.0; 3753.1, 457.5; 3793.4, 511.9; 3796.9, 922.0; 3936.8, 104.5; 3939.1, 161.0; 3942.3, 155.0; 3946.1, 120.6; 3949.8, 103.9; 3950.4, 211.0; 3953.9, 127.8; 3961.5, 157.5; 3973.5, 168.7;

-2529.056422760 -2528.667572 -2528.629080 -2528.733066

$[Co(H_2O)_{16}]^+$

Co	0.720108	0.142760	-0.356434
O	0.011932	-1.765878	-1.383210
H	-0.694844	-1.484768	-1.992539
O	-0.527070	3.559346	-0.200761
H	-0.342510	4.496604	-0.296380
O	1.270824	1.949929	0.977694
H	2.243901	1.929792	0.991148
O	-0.068445	1.481175	-2.017127
H	-0.407808	2.303089	-1.626264
O	-1.257603	0.005137	0.589005
H	-1.308002	-0.879279	0.989494
O	2.278006	-1.157380	0.761553
H	1.874792	-1.599380	1.532803
H	0.232904	3.151029	0.273166
H	-0.825769	0.999446	-2.392118
H	0.965012	1.595242	1.839991
H	-1.498947	0.651442	1.267601
H	2.472295	-1.831160	0.086912
H	0.754040	-2.147543	-1.879401
O	-2.642177	2.338993	1.066729
H	-1.978122	2.912477	0.632424
H	-3.068128	2.867585	1.744747
O	-3.919145	0.456957	-0.585002
H	-4.748513	0.874049	-0.831853
H	-3.460389	1.092734	0.003124
O	2.546172	0.497986	-1.823649
H	3.172747	0.999246	-1.276963
H	1.968777	1.118489	-2.291278
O	0.665992	-2.036657	2.841392
H	0.857753	-2.663865	3.542908
H	-0.047708	-2.431164	2.286663
O	3.854579	1.075679	0.555913
H	3.523595	0.184082	0.788247
H	4.743583	1.164661	0.906267
O	2.674659	-2.217282	-1.825700
H	3.308986	-2.749539	-2.310810
H	2.824002	-1.281706	-2.064478
O	-1.084884	-2.747159	0.970228
H	-2.045912	-2.818882	0.813774
H	-0.679695	-2.643103	0.088418
O	0.186949	0.718593	3.160938
H	0.177705	0.993328	4.080207
H	0.344094	-0.245308	3.159139
H	-3.840696	-1.312522	0.050915
H	-4.514117	-2.688215	0.314658
O	-3.665845	-2.244205	0.269635
O	-2.087721	-0.376949	-2.559984
H	-2.721216	-0.154485	-1.847040
H	-2.614510	-0.563169	-3.340980

40.5, 1.6; 42.3, 2.0; 48.9, 1.0; 52.3, 0.5; 61.2, 1.1; 63.1, 1.8; 67.7, 0.1; 72.7, 0.5; 78.0, 1.3; 86.1, 3.2; 89.6, 0.8; 93.4, 1.7; 102.4, 2.4; 106.5, 0.8; 111.1, 6.0; 123.1, 39.0; 126.7, 2.6; 128.2, 44.1; 133.5, 33.9; 141.5, 6.7; 155.6, 4.2; 164.6, 5.0; 165.8, 3.5; 171.3, 2.5; 183.2, 2.5; 193.0, 9.3; 197.1, 1.6; 202.7, 3.6; 206.4, 4.5; 215.9, 4.9; 220.3, 12.0; 223.7, 20.6; 231.3, 10.7; 237.6, 9.3; 245.1, 13.6; 257.4, 0.9; 258.3, 41.2; 265.9, 21.8; 270.3, 16.4; 274.2, 7.9; 278.3, 0.8; 282.3, 9.5; 291.1, 42.8; 297.6, 37.4; 300.2, 50.9; 321.3, 3.0; 325.8, 3.5; 334.4, 26.0; 349.6, 9.0; 354.2, 16.5; 356.6, 23.5; 365.6, 5.8; 374.8, 84.7; 389.1, 17.7; 394.2, 45.3; 422.0, 75.0; 424.9, 54.9; 435.7, 71.1; 440.8, 36.5; 457.4, 139.8; 474.9, 126.3; 483.7, 39.2; 496.8, 53.3; 511.4, 349.1; 517.6, 128.1; 527.2, 78.6; 529.1, 189.6; 549.1, 114.2; 578.1, 82.9; 581.6, 140.0; 599.0, 60.6; 605.4, 39.0; 625.1, 146.9; 635.4, 280.7; 654.6, 235.1; 685.2, 78.4; 694.7, 141.8; 699.7, 222.2; 721.5, 312.8; 747.0, 50.8; 760.9, 252.1; 776.7, 181.7; 783.1, 156.1; 794.6, 179.8; 809.5, 163.8; 815.4, 11.5; 834.5, 59.4; 854.0, 142.3; 869.1, 206.2; 888.2, 80.4; 899.4, 44.0; 934.0, 29.3; 951.0, 188.2; 1565.9, 120.3; 1586.5, 79.8; 1592.5, 65.4; 1601.4, 80.5; 1608.9, 116.0; 1614.4, 85.9; 1618.6, 14.1; 1621.0, 158.9; 1626.8, 30.9; 1629.8, 110.0; 1637.0, 33.0; 1639.9, 53.6; 1646.4, 19.0; 1658.2, 31.6; 1665.6, 1.2; 1675.5, 72.3; 3440.4, 499.0; 3465.2, 1285.7; 3543.1, 259.9; 3552.0, 420.9; 3571.8, 397.5; 3587.6, 470.1; 3603.7, 97.9; 3611.5, 406.4; 3619.6, 442.5; 3628.4, 430.0; 3641.6, 559.6; 3657.2, 431.5; 3672.3, 267.9; 3687.6, 618.5; 3695.0, 428.5; 3707.1, 14.3; 3711.3, 610.8; 3723.8, 396.1; 3725.6, 510.3; 3755.8, 1106.5; 3774.5, 601.5; 3819.9, 543.9; 3827.7, 443.3; 3933.5, 83.8; 3936.3, 120.6; 3940.4, 145.3; 3942.5, 135.7; 3949.3, 120.9; 3950.2, 186.2; 3950.9, 87.2; 3951.8, 167.8; 3966.7, 152.5;

-2605.495281350 -2605.081281 -2605.040209 -2605.150471

$[Co(H_2O)_{17}]^+$

Co	-0.780996	-0.110496	-0.156303
O	0.017306	0.818727	-2.090264
H	0.562374	0.144863	-2.530259
O	0.191923	-2.940708	1.850807
H	-0.137921	-3.760265	2.226865
O	-1.256948	-0.690232	2.027670
H	-2.186866	-0.426632	2.140389
O	-0.195464	-2.247343	-0.828321
H	0.130037	-2.647305	-0.002976
O	1.363352	0.078332	0.403077
H	1.615511	0.992283	0.181784
O	-1.685750	2.038796	0.286488
H	-1.029622	2.673202	0.629894
H	-0.472709	-2.239383	2.041000
H	0.573901	-2.084456	-1.403239
H	-0.721581	-0.011741	2.490351
H	1.632893	-0.075317	1.320452
H	-1.917489	2.304209	-0.620754
H	-0.740099	1.072012	-2.643081
O	2.625076	-1.688599	2.129295
H	1.829231	-2.257533	2.143521
H	3.055333	-1.784129	2.981318
O	3.878027	-1.305104	-0.346930
H	4.568744	-1.971224	-0.387747
H	3.439026	-1.422643	0.521474
O	-2.953354	-0.408867	-0.842349
H	-3.495428	-0.256368	-0.050711
H	-3.067686	-1.348488	-1.105799
O	0.486947	3.413788	1.342881
H	0.563217	4.338094	1.591171
H	1.084493	3.265786	0.573185
O	-3.630547	0.675888	1.618539
H	-3.077592	1.406780	1.274386
H	-4.381583	1.055563	2.079125
O	-2.518654	1.750849	-2.395329
H	-3.162200	2.131982	-2.996102
H	-2.909374	0.938721	-2.008190
O	1.773096	2.547594	-0.813543
H	2.684006	2.312422	-1.079266
H	1.170854	2.130992	-1.458141
O	0.481750	1.180729	3.040045
H	0.637240	1.402225	3.960571
H	0.516272	2.020304	2.542517
H	4.202852	0.447387	-0.880455
H	5.048766	1.615146	-1.466721
O	4.150997	1.325690	-1.296347
O	-2.745209	-3.017236	-1.397717
H	-2.987893	-3.631377	-2.091892
H	-1.771769	-2.975544	-1.353260
O	1.883174	-1.239492	-2.385115
H	2.550437	-1.127047	-1.679063
H	2.355764	-1.591615	-3.143250

34.0, 1.0; 35.3, 2.4; 44.5, 2.1; 49.5, 0.5; 53.3, 0.3; 58.9, 1.1; 64.7, 0.8; 68.2, 0.8; 74.4, 1.7; 76.4, 1.4; 81.7, 0.2; 85.2, 0.9; 92.6, 0.8; 95.9, 0.9; 110.0, 2.2; 110.7, 0.8; 120.3, 4.0; 127.9, 3.5; 132.3, 0.9; 146.1, 1.6; 151.8, 7.9; 153.3, 1.2; 162.6, 5.6; 171.3, 10.6; 172.4, 5.7; 182.3, 52.0; 188.2, 62.1; 189.4, 7.8; 195.5, 5.9; 201.7, 2.3; 203.4, 12.7; 213.4, 2.7; 220.8, 12.0; 226.8, 5.2; 234.2, 7.1; 236.7, 26.8; 245.8, 30.5; 249.1, 25.4; 257.2, 81.6; 261.3, 64.8; 265.5, 26.0; 268.6, 14.4; 274.9, 8.6; 279.9, 14.8; 281.7, 37.7; 291.5, 18.7; 301.7, 10.5; 306.9, 5.1; 322.1, 2.1; 327.5, 1.3; 334.1, 15.9; 336.3, 13.8; 348.1, 18.5; 351.1, 23.0; 362.4, 4.5; 363.3, 72.3; 368.6, 2.6; 371.5, 66.1; 386.9, 26.5; 417.9, 25.6; 424.9, 111.7; 433.0, 2.4; 449.5, 106.0; 450.8, 105.5; 461.3, 116.1; 469.6, 180.1; 479.3, 39.6; 502.9, 16.4; 512.6, 56.9; 523.5, 231.5; 526.5, 295.4; 544.8, 72.3; 576.4, 31.8; 584.9, 122.3; 587.1, 19.3; 612.3, 82.2; 635.0, 118.8; 649.3, 187.2; 667.0, 7.6; 670.5, 375.9; 685.0, 78.9; 705.3, 428.6; 732.7, 203.0; 743.9, 200.7; 750.2, 89.3; 764.9, 242.0; 791.1, 224.6; 806.0, 24.5; 810.0, 207.7; 814.8, 70.7; 827.2, 45.4; 840.5, 54.5; 850.8, 206.0; 870.2, 169.5; 891.3, 88.2; 909.5, 11.8; 931.5, 96.9; 939.4, 306.4; 950.1, 13.2; 1547.2, 85.2; 1575.4, 68.9; 1586.6, 170.0; 1597.7, 58.9; 1607.8, 179.6; 1610.7, 34.0; 1615.0, 14.2; 1620.3, 154.5; 1626.8, 136.2; 1633.6, 53.6; 1635.1, 32.1; 1641.0, 20.6; 1646.2, 10.7; 1651.6, 5.0; 1658.4, 56.6; 1663.0, 56.9; 1674.7, 19.8; 3446.8, 407.2; 3465.3, 1068.6; 3494.7, 1026.6; 3553.6, 144.8; 3555.8, 370.8; 3561.5, 283.3; 3584.6, 408.5; 3587.5, 355.1; 3603.1, 1199.2; 3616.2, 199.9; 3630.7, 498.1; 3632.2, 513.0; 3653.9, 398.1; 3660.8, 335.4; 3678.8, 227.6; 3687.4, 345.0; 3693.7, 112.8; 3706.5, 502.2; 3710.8, 274.6; 3721.8, 689.0; 3733.0, 1324.2; 3747.9, 606.7; 3785.8, 804.2; 3808.5, 513.2; 3935.3, 75.3; 3940.5, 135.8; 3941.1, 224.5; 3941.8, 54.3; 3951.5, 81.8; 3951.9, 150.3; 3954.0, 185.1; 3955.3, 140.2; 3966.3, 167.8; 3971.3, 151.1;

-2681.935849390 -2681.495852 -2681.452298 -2681.568215

η^1–NL $[CoN_2O]^+$

structure from Co-N2O-7.log

Co	-0.000536	-1.397964	0.000000
N	0.000000	0.529677	0.000000
N	0.000704	1.655650	0.000000
O	0.001194	2.805969	0.000000

187.8, 0.3; 302.9, 1.3; 545.0, 4.9; 593.1, 6.5; 1468.5, 92.7; 2509.0, 581.8;

-1566.984777610 -1566.972005 -1566.966870 -1566.993234

η^1–NL $[Co(H_2O)_1N_2O]^+$

Co	-0.805008	-0.000074	-0.058488
N	2.224940	-0.000021	0.029552
N	1.099268	-0.000240	0.036588
O	3.376252	0.000229	0.023558
O	-2.740970	0.000184	0.092518
H	-3.308135	0.780626	0.093621
H	-3.308364	-0.780091	0.093981

61.6, 4.4; 88.9, 4.6; 150.9, 0.5; 188.7, 0.8; 288.8, 3.3; 334.0, 287.1; 457.3, 1.0; 586.0, 7.6; 607.3, 9.2; 621.0, 65.8; 1456.6, 175.5; 1646.2, 110.8; 2503.1, 639.4; 3822.3, 190.3; 3910.7, 286.7;

-1643.469923220 -1643.431825 -1643.423708 -1643.463866

η^1–NL $[Co(H_2O)_2N_2O]^+$

Co	0.900182	0.000045	-0.000034
O	1.287000	-1.969169	-0.000054
H	0.622744	-2.666374	-0.000015
O	1.286050	1.969502	-0.000088
H	0.621492	2.666417	0.000832
H	2.152464	-2.391538	0.001396
H	2.151329	2.392251	0.000680
N	-2.229375	-0.000204	-0.000041
N	-1.102599	0.000056	-0.000323
O	-3.389190	-0.000449	0.000214

50.3, 0.2; 68.1, 13.3; 100.6, 16.4; 108.7, 2.6; 119.9, 2.3; 184.3, 1.3; 190.2, 0.0; 206.1, 2.5; 293.1, 0.0; 322.6, 0.8; 324.3, 529.7; 410.5, 14.0; 542.5, 2.3; 573.6, 107.8; 576.2, 8.3; 585.0, 9.2; 1412.4, 216.7; 1639.0, 192.6; 1639.7, 11.0; 2463.0, 468.8; 3842.3, 235.5; 3844.6, 23.2; 3937.6, 9.5; 3938.5, 470.4;

-1719.927881560 -1719.865520 -1719.854014 -1719.903455

η^1–NL $[Co(H_2O)_3N_2O]^+$

Co	0.547615	0.000143	0.000207
O	0.702016	-2.076490	0.000025
O	0.715247	2.074081	0.000262
O	2.714981	-0.001451	-0.000007
H	3.283896	-0.014472	0.775817
H	3.286318	-0.010396	-0.774191
H	1.534451	-2.558583	-0.006064
H	-0.009914	-2.723970	0.003277
H	1.553650	2.545485	-0.003475
H	0.010533	2.729012	0.000552
N	-2.549176	0.002315	-0.000337
N	-1.421622	0.001512	-0.000274

```
 O        -3.713363    0.004143    0.000068
---
24.9, 0.8; 52.3, 0.3; 75.6, 7.3; 87.4, 52.8; 131.0,
9.6; 160.9, 5.0; 163.7, 0.7; 179.0, 1.6; 185.3, 8.9;
262.5, 184.4; 264.1, 8.4; 271.1, 2.4; 277.8, 5.3;
303.0, 422.4; 312.6, 0.7; 353.4, 62.1; 355.2, 0.3;
459.4, 113.2; 490.9, 8.6; 517.4, 117.5; 564.3, 7.3;
567.6, 5.8; 1391.8, 302.7; 1616.5, 87.6; 1622.7, 178.4;
1625.6, 43.2; 2449.2, 391.8; 3850.2, 80.5; 3850.8,
107.5; 3853.0, 49.1; 956.4, 133.1; 3956.6, 197.2;
3959.4, 221.1;

 -1796.380937850 -1796.293931 -1796.279343 -
1796.335621
```

η^1–NL $[Co(H_2O)_4N_2O]^+$

```
Co         0.029525    0.313016   -0.101842
 O         3.644808   -1.151625    0.221061
 H         4.235729   -1.584082   -0.405170
 O        -0.333840    2.306717    0.436957
 H         0.400706    2.875702    0.687768
 O         1.993848    1.031748   -0.477798
 H         2.731224    0.420784   -0.301589
 O         0.880654   -1.576411    0.142242
 H         0.440709   -2.393982    0.387885
 H         4.126978   -1.119125    1.054699
 H         1.840831   -1.695821    0.240042
 H        -1.144833    2.718951    0.748396
 H         2.189493    1.478676   -1.306491
 N        -2.896839   -0.618408   -0.042355
 N        -1.822242   -0.276578   -0.064220
 O        -4.008524   -0.971383   -0.023685
---
28.6, 0.5; 39.0, 3.2; 47.9, 2.1; 73.4, 0.9; 112.0, 5.8;
132.0, 0.7; 151.5, 1.5; 174.5, 7.2; 188.8, 3.2; 216.9,
10.1; 229.5, 30.5; 236.1, 46.7; 260.7, 25.0; 277.5,
67.1; 286.5, 15.5; 290.0, 131.0; 321.2, 53.2; 338.6,
6.9; 347.6, 9.7; 385.3, 123.9; 457.8, 151.3; 489.8,
36.2; 542.5, 7.0; 553.9, 9.2; 577.3, 85.3; 590.3,
219.0; 697.8, 133.6; 740.1, 163.8; 1382.5, 362.0;
1610.3, 148.2; 1614.7, 90.3; 1624.4, 105.8; 1658.3,
15.8; 2444.8, 360.8; 3664.7, 123.9; 3704.3, 1022.1;
3843.1, 40.1; 3850.5, 72.6; 3919.3, 198.4; 3935.9,
158.6; 3942.3, 183.6; 3959.6, 175.4;

 -1872.828496790 -1872.714721 -1872.698128 -
1872.759128
```

η^1–NL $[Co(H_2O)_5N_2O]^+$

```
Co         0.174251   -0.000038   -0.002352
 O        -2.749136    2.700990    0.003928
 H        -3.166256    3.107520    0.770820
 O        -0.012126    2.093831    0.000358
 H        -0.877978    2.536638   -0.000337
 O        -1.909026   -0.000356   -0.008370
 H        -2.460260   -0.796647    0.005697
 O        -0.010754   -2.093808   -0.005334
 H         0.678897   -2.761404   -0.008480
 H        -3.169266    3.098761   -0.765927
 H        -0.876295   -2.537254   -0.004042
 H         0.677043    2.761925   -0.001652
 H        -2.461318    0.795206    0.003891
 O        -2.747233   -2.701899    0.007958
 H        -3.161779   -3.107527    0.776727
 H        -3.169692   -3.100847   -0.760020
 N         3.238814    0.000611    0.002531
 O         4.407891    0.000816    0.004748
 N         2.110500    0.000541    0.000400
---
20.1, 20.7; 27.8, 0.5; 33.5, 0.0; 43.1, 0.0; 83.6, 1.8;
89.9, 2.9; 134.2, 0.6; 147.7, 0.7; 160.1, 0.1; 163.0,
11.6; 185.2, 7.5; 203.8, 0.0; 206.9, 0.3; 207.5, 0.6;
221.3, 122.6; 243.1, 31.0; 249.0, 0.0; 278.9, 123.4;
280.9, 0.0; 290.0, 11.0; 290.4, 0.1; 337.7, 21.5;
359.4, 3.8; 429.3, 154.1; 455.4, 154.8; 528.1, 8.4;
545.3, 5.8; 564.0, 104.7; 574.6, 82.5; 613.9, 2.6;
615.9, 241.9; 702.3, 410.3; 717.9, 5.1; 734.2, 170.8;
1371.3, 409.7; 1595.7, 92.9; 1608.7, 223.9; 1610.0,
60.9; 1640.5, 16.6; 1666.6, 4.8; 2436.7, 322.9; 3686.1,
449.1; 3687.3, 95.3; 3730.9, 780.3; 3809.6, 977.0;
3848.8, 41.7; 3853.9, 24.5; 3942.7, 36.4; 3943.2,
297.6; 3950.6, 3.2; 3951.0, 341.6;

 -1949.273394470 -1949.134264 -1949.114729 -
1949.183495
```

η^1–NL $[Co(H_2O)_6N_2O]^+$

```
Co         0.018494    0.218131   -0.005730
 O        -0.053861    1.557362   -1.858244
 H         0.553776    2.238591   -2.161087
 O        -0.765798   -1.170993   -1.579513
 H        -1.615992   -1.511250   -1.245144
 O        -0.043890    1.679369    1.751257
 H        -0.138038    1.104100    2.519692
 O        -0.765402   -1.064149    1.654544
 H        -1.615206   -1.426495    1.343489
 O        -2.113016    1.094151   -0.035257
 H        -2.005733    1.644928   -0.822616
 H        -2.014630    1.694061    0.716253
 H        -0.268312   -1.804511    2.012587
 H         0.565791    2.380149    2.000632
 H        -0.268655   -1.933964   -1.886397
 H        -0.151781    0.927523   -2.582284
 O        -3.005569   -1.477829    0.048245
 H        -3.168598   -0.520152    0.016750
 H        -3.857137   -1.923269    0.061543
 N         3.001494   -0.517220    0.014724
 N         1.896400   -0.280095    0.008396
 O         4.147527   -0.765168    0.021398
---
33.8, 0.7; 40.2, 0.4; 54.8, 0.2; 70.3, 6.4; 95.8, 3.9;
110.5, 1.4; 112.2, 1.6; 117.1, 5.2; 126.5, 12.2; 144.8,
3.1; 174.3, 0.5; 176.1, 0.8; 185.8, 0.1; 194.3, 0.7;
220.9, 10.8; 236.3, 0.3; 252.4, 12.4; 253.2, 15.4;
258.4, 7.8; 260.4, 6.5; 290.4, 0.1; 335.7, 191.7;
339.4, 78.3; 361.6, 205.6; 375.7, 29.9; 404.8, 88.8;
410.5, 22.1; 413.7, 54.1; 425.8, 101.1; 442.4, 0.4;
481.1, 50.4; 493.8, 10.4; 513.3, 4.0; 518.3, 15.6;
522.2, 41.1; 542.8, 356.8; 579.4, 480.0; 654.3, 267.0;
755.6, 224.1; 760.7, 14.3; 1352.3, 428.1; 1572.8,
135.1; 1592.6, 161.3; 1598.0, 39.3; 1632.5, 0.7;
1641.4, 7.1; 1653.6, 221.7; 2415.3, 279.5; 3644.3,
189.4; 3668.5, 427.9; 3732.8, 525.0; 3784.8, 32.2;
3828.1, 136.9; 3831.2, 22.2; 3876.8, 174.4; 3925.7,
69.9; 3928.7, 223.5; 3938.2, 205.0; 3946.5, 61.3;
3948.0, 259.5;

 -2025.717031670 -2025.552431 -2025.530671 -
2025.601686
```

η^1–NL $[Co(H_2O)_7N_2O]^+$

```
Co        -0.169506   -0.071097    0.000794
 O        -1.399786   -0.981157    1.601558
 H        -2.316256   -1.056332    1.280737
 O         0.494847    1.461359    1.519785
 H         1.321777    1.908200    1.275574
 O        -1.397855   -0.978809   -1.602064
 H        -1.183820   -1.810428   -2.031499
 O         0.490104    1.465304   -1.517554
 H         1.317108    1.912038   -1.273256
 O        -1.896169    1.512823    0.001186
 H        -1.561196    1.991198    0.770714
 H        -1.553325    1.990354   -0.765539
 H         0.571766    1.178121   -2.431377
 H        -2.314660   -1.054823   -1.282422
 H         0.577169    1.173085    2.433188
 H        -1.186697   -1.813298    2.030440
 O         2.604722    2.609824   -0.000926
 H         2.735245    3.564233    0.000906
 H         3.490049    2.231142   -0.003520
 N         2.245266   -1.961821   -0.001117
 N         1.350409   -1.269090   -0.000734
 O         3.178887   -2.677594   -0.001531
 O        -3.633672   -0.582319   -0.001486
 H        -4.589128   -0.681309   -0.002587
 H        -3.429714    0.368355   -0.001578
---
25.0, 4.6; 39.4, 0.9; 45.5, 3.5; 54.6, 0.1; 93.0, 3.2;
96.5, 1.1; 110.6, 0.6; 118.8, 0.6; 126.7, 1.4; 134.3,
10.4; 157.0, 0.4; 165.6, 0.1; 171.0, 0.3; 177.2, 0.3;
195.5, 1.6; 208.7, 1.3; 223.8, 4.1; 232.8, 17.0; 250.3,
3.5; 256.3, 10.9; 257.7, 24.5; 261.7, 18.6; 271.5,
22.3; 273.7, 1.7; 291.1, 168.7; 295.4, 1.7; 321.2, 3.5;
323.2, 43.3; 378.3, 12.0; 393.1, 92.8; 396.4, 99.4;
414.1, 25.9; 414.9, 120.4; 446.7, 119.5; 472.9, 88.3;
487.2, 1.2; 487.5, 2.6; 526.3, 168.7; 528.5, 125.2;
```

538.8, 299.5; 565.6, 414.8; 637.4, 218.0; 675.6, 72.0; 734.9, 229.9; 747.7, 0.4; 764.0, 213.1; 1334.4, 473.7; 1574.5, 116.9; 1592.8, 97.1; 1604.0, 158.0; 1622.3, 15.1; 1636.1, 7.4; 1637.9, 29.6; 1646.6, 197.5; 2398.5, 229.1; 3664.9, 110.3; 3676.9, 393.5; 3711.0, 51.5; 3733.4, 1233.2; 3739.0, 24.2; 3800.4, 26.7; 3847.9, 36.5; 3892.1, 204.6; 3929.4, 230.9; 3932.7, 100.9; 3938.1, 92.9; 3940.5, 226.9; 3945.1, 158.7; 3949.5, 158.4;

-2102.159590380 -2101.969282 -2101.944869 -2102.021707

η^1–NL $[Co(H_2O)_8N_2O]^+$

Co	-0.315304	0.195609	0.040528
O	-0.777912	1.889194	1.417236
H	-0.387946	2.710844	1.071328
O	0.352232	-0.992609	1.843042
H	0.806938	-1.830524	1.642180
O	-0.220239	1.551368	-1.701196
H	-0.993235	1.759283	-2.231260
O	0.633071	-1.416069	-1.347459
H	0.726374	-2.255630	-0.864140
O	1.809805	0.975334	0.541836
H	1.734833	0.672278	1.456990
H	2.499408	0.417952	0.134024
H	0.076524	-1.578991	-2.114525
H	0.145478	2.403377	-1.401723
H	-0.197339	-1.131075	2.618285
H	-1.653696	2.107750	1.743344
O	1.856251	-2.933221	0.573570
H	2.648681	-2.453074	0.272797
H	2.134098	-3.820365	0.817275
N	-3.181944	-0.892086	-0.230228
N	-2.126992	-0.488506	-0.163564
O	-4.277985	-1.310519	-0.300056
O	0.936028	3.470914	-0.070900
H	1.353211	4.335495	-0.091309
H	1.605266	2.814031	0.193110
O	3.260790	-0.964596	-0.809911
H	2.522891	-1.029389	-1.441696
H	4.077953	-0.897624	-1.311690

29.5, 0.7; 39.6, 0.3; 43.1, 0.1; 61.0, 1.7; 73.7, 1.9; 88.5, 1.9; 102.4, 1.0; 115.0, 1.1; 118.5, 0.8; 132.4, 6.2; 152.0, 7.6; 164.8, 1.3; 170.9, 1.9; 181.3, 5.7; 182.6, 3.0; 196.7, 1.5; 202.1, 2.1; 216.1, 20.5; 230.4, 3.7; 241.3, 19.7; 245.4, 1.1; 251.4, 6.1; 261.2, 22.5; 266.2, 9.9; 276.3, 110.3; 284.3, 3.9; 299.7, 8.2; 313.0, 33.6; 325.1, 107.5; 338.6, 2.1; 362.6, 35.3; 379.7, 42.7; 386.8, 112.4; 412.3, 227.5; 424.2, 14.0; 439.1, 194.3; 451.8, 44.7; 468.4, 69.2; 491.7, 2.1; 501.6, 263.0; 507.5, 29.2; 540.2, 80.1; 558.2, 87.2; 564.4, 33.9; 594.2, 276.1; 635.1, 136.7; 636.2, 252.4; 730.8, 171.8; 757.0, 35.9; 782.5, 284.6; 829.0, 177.9; 878.3, 70.9; 1337.6, 481.8; 1571.9, 110.6; 1578.3, 116.7; 1586.1, 78.0; 1608.3, 131.0; 1621.9, 69.3; 1624.4, 49.3; 1643.6, 50.9; 1657.1, 120.1; 2400.3, 251.3; 3621.6, 335.7; 3647.6, 236.6; 3656.5, 235.0; 3666.8, 398.3; 3671.0, 66.9; 3716.7, 437.3; 3720.5, 787.5; 3724.4, 445.7; 3838.0, 222.4; 3926.9, 187.9; 3933.7, 197.2; 3936.4, 219.9; 3938.9, 133.5; 3940.0, 71.5; 3945.9, 230.8; 3949.2, 121.7;

-2178.602355980 -2178.385023 -2178.358900 -2178.439042

η^1–NL $[Co(H_2O)_9N_2O]^+$

Co	0.558890	0.143876	-0.211065
O	0.041785	-1.026384	-2.095972
H	-0.503284	-1.812610	-1.905838
O	-0.194348	-1.536118	0.966487
H	-0.786320	-1.314148	1.700203
O	-0.027314	1.517222	1.593817
H	0.658969	1.588804	2.263747
O	1.065647	1.873999	-1.510965
H	1.970705	2.095396	-1.741389
H	0.656607	-1.256350	-2.796777
H	0.620448	2.697701	-1.249971
H	-0.638265	-2.232619	0.457577
H	-0.773354	1.038842	2.012415
O	-1.771849	-2.802518	-0.956794
H	-2.077773	-3.687730	-1.170536
H	-2.544280	-2.289117	-0.652180
O	-0.841719	3.380553	-0.259352
H	-0.594288	3.021620	0.612590
H	-1.180327	4.270741	-0.137160
O	-3.416212	-0.812162	0.116961
H	-4.350239	-0.688816	-0.074310
H	-2.922375	-0.121132	-0.378917
O	-2.096818	-0.127157	2.465076
H	-2.759590	-0.355775	1.783401
H	-2.535443	-0.168043	3.318821
O	-1.607502	0.829315	-0.997982
H	-1.580332	1.802923	-0.948402
H	-1.269930	0.570908	-1.868916
N	3.406741	-0.769411	0.524448
N	2.400574	-0.351947	0.226193
O	4.456810	-1.196215	0.831215

28.4, 0.1; 32.1, 0.1; 54.4, 1.3; 69.9, 0.1; 77.4, 0.1; 82.3, 0.2; 93.3, 0.3; 104.3, 1.1; 108.9, 0.8; 121.8, 0.5; 131.2, 10.3; 139.1, 2.6; 156.7, 3.2; 167.0, 6.0; 170.6, 2.3; 182.0, 0.9; 190.6, 2.1; 196.5, 1.5; 212.3, 10.3; 223.2, 6.0; 233.8, 6.8; 234.2, 10.1; 240.9, 21.0; 257.2, 2.6; 261.7, 26.8; 272.6, 2.3; 280.7, 23.2; 288.6, 45.5; 297.5, 21.0; 302.8, 10.3; 317.2, 47.7; 328.4, 11.5; 354.0, 54.5; 372.6, 74.1; 379.0, 13.2; 397.0, 80.4; 411.4, 22.6; 434.0, 32.7; 443.0, 52.4; 482.1, 99.0; 489.4, 118.0; 502.8, 81.8; 509.7, 85.4; 519.9, 121.4; 525.6, 36.0; 560.9, 178.3; 564.4, 157.9; 626.7, 133.4; 631.3, 194.3; 661.1, 156.2; 691.7, 207.6; 717.1, 429.0; 735.6, 11.0; 785.6, 27.5; 790.3, 324.3; 823.7, 108.2; 862.9, 49.9; 953.3, 146.7; 1346.0, 453.9; 1575.2, 101.0; 1588.8, 157.0; 1612.8, 33.4; 1613.5, 89.6; 1622.5, 197.2; 1629.6, 35.1; 1638.3, 22.6; 1647.4, 49.4; 1668.0, 7.8; 2413.0, 280.3; 3485.1, 412.2; 3562.8, 665.2; 3607.1, 535.7; 3640.0, 786.6; 3645.6, 206.1; 3660.4, 200.8; 3668.9, 222.8; 3721.7, 535.6; 3731.8, 330.4; 3801.5, 45.4; 3804.7, 1029.9; 3917.8, 118.2; 3924.5, 156.4; 3936.3, 168.4; 3938.2, 229.1; 3940.7, 64.6; 3945.4, 256.2; 3948.5, 99.2;

-2255.047346010 -2254.802856 -2254.774867 -2254.858856

η^1–NL $[Co(H_2O)_{10}N_2O]^+$

Co	0.535754	0.021745	0.001170
O	0.195998	-0.181578	-2.321127
H	-0.574805	-0.779323	-2.405392
O	-0.301800	-2.009896	0.119956
H	-0.828262	-2.206400	0.908995
O	0.183616	0.106847	2.326563
H	0.922536	-0.278794	2.806248
O	1.233977	2.113904	-0.113467
H	0.883513	2.535279	-0.912696
H	0.935800	-0.627602	-2.743723
H	0.865630	2.625976	0.622523
H	-0.835160	-2.294869	-0.637082
H	-0.585525	-0.479483	2.479511
O	-2.012940	-1.858992	-2.086282
H	-2.439042	-2.424353	-2.735640
H	-2.704427	-1.542890	-1.471537
O	-0.561224	2.699507	2.001396
H	-0.258590	1.915228	2.493056
H	-0.803222	3.378864	2.635263
O	-3.428114	-0.747048	0.035319
H	-4.354458	-0.490752	0.018653
H	-2.892911	0.079979	-0.016656
O	-2.023317	-1.583556	2.284907
H	-2.707478	-1.342856	1.628813
H	-2.459117	-2.060106	2.996120
O	-1.572663	1.167776	-0.080577
H	-1.445996	1.795040	0.658588
H	-1.434643	1.704440	-0.886469
N	3.469712	-0.975267	0.063812
N	2.387014	-0.656632	0.044332
O	4.595381	-1.308131	0.084020
O	-0.528411	2.438082	-2.312854
H	-0.227161	1.598130	-2.702938
H	-0.763162	3.035338	-3.027060

23.2, 0.1; 34.3, 0.0; 50.2, 0.9; 65.4, 0.2; 71.5, 0.5; 82.6, 0.3; 88.9, 2.8; 100.4, 0.9; 101.5, 1.5; 114.3, 3.8; 118.7, 9.1; 132.0, 1.8; 152.0, 1.4; 154.3, 3.1; 163.5, 1.7; 175.1, 0.1; 178.5, 0.1; 183.2, 3.5; 189.8,

4.8; 197.4, 5.5; 216.3, 8.2; 228.2, 13.1; 229.7, 7.4; 241.7, 8.5; 242.4, 4.5; 247.3, 3.5; 260.3, 25.4; 265.1, 14.2; 283.5, 19.6; 287.3, 52.4; 291.2, 6.0; 320.7, 4.0; 333.0, 36.1; 344.7, 13.3; 352.0, 8.8; 369.5, 4.6; 370.1, 75.3; 387.2, 7.1; 394.8, 14.4; 410.9, 83.3; 420.7, 57.1; 444.7, 23.0; 457.5, 132.0; 461.0, 130.6; 491.6, 111.4; 519.7, 1.9; 522.7, 2.6; 531.9, 30.2; 544.4, 23.3; 554.7, 34.3; 592.6, 217.1; 638.1, 92.9; 661.7, 778.8; 669.0, 225.0; 683.4, 337.7; 730.9, 12.5; 741.5, 174.5; 768.7, 98.1; 776.7, 137.2; 835.0, 10.2; 844.1, 28.2; 862.0, 102.5; 886.9, 225.9; 991.8, 108.3; 1348.0, 456.1; 1569.9, 13.1; 1578.7, 202.0; 1592.7, 68.8; 1619.9, 91.8; 1633.4, 103.0; 1636.6, 56.3; 1641.6, 33.3; 1654.0, 48.8; 1676.1, 2.3; 1699.1, 95.7; 2415.6, 296.1; 3427.4, 688.9; 3557.3, 107.1; 3587.3, 1287.0; 3601.9, 400.9; 3608.2, 512.7; 3629.6, 474.5; 3641.1, 417.3; 3683.6, 384.1; 3688.4, 6.8; 3738.5, 258.1; 3744.0, 490.7; 3813.3, 26.3; 3815.7, 1172.5; 3918.5, 23.7; 3919.0, 219.5; 3924.6, 145.0; 3935.3, 210.5; 3938.1, 129.6; 3946.1, 107.4; 3946.8, 250.4;

-2331.489203500 -2331.217614 -2331.187656 -2331.275828

η^1–NL $[Co(H_2O)_{11}N_2O]^+$

Co	0.508975	0.223931	0.027124
O	0.071526	1.961570	1.544856
H	-0.671285	2.457467	1.142712
O	-0.403382	1.443135	-1.580618
H	-1.023804	0.950154	-2.139780
O	0.396054	-1.438415	-1.621152
H	0.846363	-1.020128	-2.362354
O	1.300007	-1.068099	1.613416
H	0.808011	-1.039557	2.446116
H	0.812185	2.572598	1.595782
H	1.414528	-1.996984	1.355919
H	-0.881200	2.226993	-1.271371
H	-0.546642	-1.454381	-1.876272
O	-2.033116	3.027908	0.069885
H	-2.438012	3.898610	0.094280
H	-2.743574	2.377210	-0.100613
O	1.285216	-3.402122	0.072909
H	1.192286	-2.845005	-0.722434
H	1.933751	-4.084949	-0.114688
O	-3.497081	0.740123	-0.472866
H	-4.405931	0.584156	-0.202544
H	-2.911554	0.223675	0.132419
O	-2.133868	-0.567121	-2.529188
H	-2.826254	-0.216880	-1.936865
H	-2.569553	-0.825850	-3.345347
O	-1.549810	-0.541756	0.800604
H	-1.557105	-1.510182	0.620827
H	-1.428463	-0.456850	1.766066
N	3.394054	1.098744	-0.678276
N	2.325153	0.803432	-0.463371
O	4.505883	1.406440	-0.903023
O	-0.624311	0.010928	3.343185
H	-0.342288	0.891498	3.036506
H	-0.898013	0.085616	4.260095
O	-1.435652	-3.167937	0.192494
H	-0.537376	-3.540183	0.254432
H	-2.054573	-3.875624	0.382279

23.5, 0.1; 25.4, 0.4; 32.2, 0.2; 43.6, 1.5; 70.4, 1.1; 73.8, 0.3; 80.8, 0.1; 85.3, 1.3; 94.6, 1.7; 101.5, 2.4; 111.6, 1.5; 119.8, 0.7; 137.4, 6.1; 140.2, 0.4; 148.1, 4.5; 158.2, 4.8; 167.6, 0.9; 177.2, 2.1; 185.7, 2.6; 193.6, 3.3; 199.3, 2.3; 203.3, 11.3; 214.7, 3.7; 222.8, 7.1; 226.8, 13.1; 231.5, 2.6; 236.2, 44.0; 240.5, 56.9; 259.3, 1.6; 259.9, 22.3; 270.3, 3.4; 279.7, 23.8; 288.5, 20.2; 292.7, 30.5; 305.0, 20.7; 313.4, 27.9; 326.5, 17.2; 348.4, 26.2; 349.6, 48.9; 354.8, 57.6; 358.7, 32.0; 383.8, 0.1; 401.6, 20.4; 407.0, 36.7; 417.9, 17.3; 436.0, 67.5; 453.0, 280.8; 473.9, 52.6; 495.8, 88.9; 512.1, 7.7; 513.9, 9.1; 518.6, 45.1; 530.5, 168.9; 544.5, 19.8; 554.0, 32.4; 572.0, 32.9; 629.2, 244.8; 635.5, 502.3; 662.1, 248.5; 675.4, 450.6; 713.0, 81.2; 732.2, 9.6; 743.8, 91.5; 763.8, 166.7; 794.8, 100.5; 826.6, 82.7; 838.1, 162.1; 867.7, 42.6; 945.9, 212.4; 1037.5, 92.3; 1340.9, 479.1; 1578.4, 94.7; 1585.0, 134.4; 1595.3, 53.3; 1611.6, 4.8; 1620.7, 62.3; 1626.4, 149.4; 1634.1, 72.5; 1637.7, 127.0; 1647.3, 45.2; 1678.9, 56.6; 1685.0, 8.6; 2408.0, 274.2; 3389.7, 984.9; 3498.3, 532.2; 3562.9, 534.7; 3604.3, 698.3; 3620.7, 486.1; 3628.6, 185.8; 3648.9, 882.0; 3668.5, 267.4; 3678.6, 205.1; 3684.4, 203.4; 3726.7, 486.4; 3733.9, 287.2; 3807.6, 619.1; 3825.1, 692.0; 3902.7, 93.2; 3921.2, 114.5; 3928.6, 142.1; 3936.8, 202.5; 3940.2, 126.0; 3944.4, 161.9; 3952.9, 169.2; 3957.8, 172.4;

-2407.928421270 -2407.631702 -2407.598918 -2407.693728

η^1–NL $[Co(H_2O)_{12}N_2O]^+$

Co	0.507483	0.335707	0.042222
O	-1.304684	1.055626	-1.215204
H	-1.569246	0.361811	-1.846604
O	-3.107928	-2.103905	-0.153748
H	-3.927633	-2.600370	-0.228460
O	0.402326	-1.637245	-1.144896
H	0.288049	-2.334785	-0.474334
H	-2.826691	-1.899787	-1.070269
H	1.302274	-1.701042	-1.534492
H	-2.041289	1.097561	-0.575506
O	0.366083	2.343395	0.950380
H	-0.337132	2.409329	1.618400
H	0.201902	3.030413	0.288379
O	-0.992838	-0.490499	1.470997
H	-0.771144	-1.399240	1.724918
H	-1.063934	0.059611	2.266109
O	-1.803169	1.837602	2.656960
H	-2.571627	1.622331	2.097864
H	-2.130224	2.269096	3.449726
O	-3.382303	0.709356	0.657645
H	-4.310611	0.751058	0.413288
H	-3.145945	-0.237019	0.697215
O	-0.735392	-3.130336	0.886458
H	-0.669967	-4.026905	1.223622
H	-1.653806	-2.993103	0.580207
O	-1.865154	-1.352885	-2.488981
H	-0.956387	-1.603549	-2.199451
H	-1.984249	-1.639836	-3.397532
O	1.974909	1.414410	-1.427534
H	2.592744	1.803755	-0.799749
H	1.459181	2.170776	-1.770712
O	0.052324	3.342035	-1.708728
H	-0.657375	2.672718	-1.759191
H	-0.186676	4.083653	-2.268906
O	2.807193	-1.120346	-2.166633
H	2.699570	-0.154504	-2.172872
H	3.412445	-1.358669	-2.870798
N	2.940616	-0.720002	1.643932
N	2.056177	-0.303329	1.076933
O	3.859655	-1.152717	2.236172

24.5, 0.3; 29.0, 0.8; 41.9, 0.6; 52.0, 1.4; 58.1, 0.1; 66.7, 3.1; 76.2, 0.3; 78.3, 0.7; 88.0, 1.7; 100.3, 1.5; 105.2, 3.4; 113.2, 2.8; 129.6, 1.4; 132.0, 5.0; 140.4, 6.9; 147.7, 0.3; 162.5, 1.1; 169.8, 5.7; 173.5, 3.6; 175.5, 2.1; 181.2, 5.8; 185.4, 1.8; 203.9, 4.1; 207.4, 3.0; 215.1, 2.9; 221.8, 7.7; 226.2, 2.3; 230.3, 87.4; 233.0, 31.4; 242.4, 5.0; 246.3, 27.2; 252.2, 10.0; 262.3, 12.7; 270.7, 44.3; 282.5, 15.9; 292.2, 6.5; 297.8, 12.3; 314.4, 12.7; 326.8, 7.9; 331.1, 18.5; 340.8, 54.8; 350.7, 88.3; 358.0, 12.9; 372.0, 76.6; 381.5, 51.4; 388.1, 2.5; 391.5, 3.7; 413.2, 55.0; 424.0, 57.4; 431.2, 43.3; 454.3, 58.6; 467.3, 296.5; 496.7, 121.8; 499.9, 44.9; 508.0, 1.4; 511.5, 133.9; 524.2, 32.4; 541.8, 222.8; 557.1, 156.0; 573.1, 127.2; 617.6, 115.5; 646.3, 194.7; 659.7, 15.5; 667.6, 341.1; 693.4, 104.8; 734.8, 43.8; 766.3, 171.0; 775.5, 123.5; 782.8, 32.3; 810.2, 502.4; 832.5, 77.9; 849.5, 22.0; 867.4, 150.2; 896.3, 206.3; 901.0, 133.6; 990.0, 89.2; 1336.6, 484.2; 1573.7, 68.2; 1575.4, 44.2; 1584.8, 118.6; 1590.9, 157.4; 1593.5, 59.2; 1608.3, 156.1; 1612.4, 62.6; 1624.5, 1.2; 1632.0, 137.3; 1635.2, 23.5; 1667.7, 47.6; 1681.8, 67.5; 2403.7, 260.3; 3426.4, 764.2; 3522.6, 239.4; 3560.3, 447.4; 3581.9, 569.2; 3611.5, 451.5; 3620.8, 605.0; 3650.4, 554.2; 3653.2, 368.6; 3685.0, 507.3; 3686.5, 357.8;
3695.0, 529.3; 3709.8, 370.5; 3719.0, 276.1; 3728.6, 182.9; 3807.3, 725.4; 3821.2, 581.8; 3899.3, 103.7; 3926.4, 114.9; 3935.9, 151.2; 3941.2, 188.2; 3946.1, 133.7; 3948.6, 150.1; 3951.3, 163.8; 3967.1, 173.3;

-2484.370290370 -2484.047523 -2484.012446 -2484.111537

η^1–NL $[Co(H_2O)_{13}N_2O]^+$

Co	-0.328086	0.066185	0.028718
O	1.269109	1.035533	1.392761
H	1.732796	0.326983	1.876646
O	3.811288	-1.229136	-0.275609
H	4.738295	-1.482641	-0.290044
O	0.389960	-2.005401	0.771450
H	0.654610	-2.478001	-0.037911
H	3.526435	-1.288897	0.660468
H	-0.446672	-2.394345	1.113350
H	1.943998	1.396837	0.786865
O	-0.877300	2.238231	-0.479156
H	-0.208623	2.605911	-1.085650
H	-0.810805	2.723585	0.361723
O	1.257072	0.029045	-1.547993
H	1.268833	-0.843979	-1.971319
H	1.097675	0.708198	-2.219368
O	1.289990	2.707860	-2.165343
H	2.121432	2.576082	-1.672805
H	1.450144	3.382320	-2.829491
O	3.254892	1.655047	-0.506460
H	4.156605	1.886672	-0.269075
H	3.263473	0.711053	-0.754929
O	1.771377	-2.633892	-1.544644
H	1.934154	-3.419059	-2.072520
H	2.631615	-2.318211	-1.203962
O	2.529490	-1.314992	2.159608
H	1.720001	-1.764831	1.817932
H	2.772899	-1.721894	2.994542
O	-1.944639	0.308855	1.657869
H	-2.682716	0.657728	1.114643
H	-1.671819	1.062662	2.206141
O	-0.646156	2.716830	2.280700
H	0.219376	2.266983	2.238850
H	-0.596761	3.407567	2.945114
O	-2.047076	-2.422829	1.749933
H	-2.201492	-1.485277	1.966679
H	-2.561346	-2.960458	2.354014
N	-2.688230	-1.214903	-1.496785
N	-1.725343	-0.789694	-1.090533
O	-3.686406	-1.655183	-1.928399
O	-3.521490	1.422487	-0.273084
H	-4.320354	1.940828	-0.385923
H	-2.779299	1.929706	-0.641216

32.1, 1.8; 32.8, 0.4; 44.3, 0.1; 55.4, 1.4; 57.0, 0.5; 60.7, 1.2; 72.5, 0.5; 77.4, 0.1; 84.3, 1.3; 89.2, 3.0; 97.1, 0.2; 110.9, 3.9; 116.5, 1.5; 121.7, 0.9; 127.4, 5.2; 134.4, 1.5; 147.9, 5.8; 149.9, 1.4; 164.7, 0.6; 169.1, 2.6; 171.3, 8.8; 175.9, 7.3; 184.1, 7.2; 188.1, 8.9; 204.4, 3.5; 215.6, 9.1; 217.1, 4.1; 219.1, 6.0; 231.0, 6.5; 234.0, 37.0; 237.1, 7.5; 241.5, 9.8; 249.6, 20.5; 257.6, 51.3; 259.4, 10.8; 265.5, 5.2; 269.3, 40.0; 274.4, 91.5; 280.5, 46.0; 292.1, 14.7; 305.7, 6.9; 317.3, 15.7; 323.7, 43.8; 334.7, 16.1; 347.6, 24.6; 361.1, 15.8; 371.3, 39.5; 380.8, 51.0; 382.0, 73.4; 392.3, 6.2; 405.8, 64.5; 413.5, 69.0; 425.3, 108.3; 427.9, 38.9; 459.2, 170.9; 474.0, 201.2; 498.3, 113.2; 511.6, 98.0; 519.8, 2.3; 526.8, 27.0; 531.6, 8.9; 540.9, 164.3; 555.6, 100.7; 566.7, 136.9; 619.4, 90.0; 650.8, 176.1; 657.2, 52.6; 677.6, 304.5; 691.8, 56.7; 715.9, 84.9; 749.8, 30.4; 771.5, 204.0; 781.3, 150.8; 799.3, 58.7; 809.1, 464.2; 830.9, 8.3; 853.0, 73.7; 875.3, 182.9; 901.6, 194.5; 916.1, 188.7; 926.1, 133.1; 993.0, 88.3; 1351.0, 408.8; 1573.9, 83.0; 1575.0, 56.3; 1579.7, 139.3; 1585.6, 75.2; 1591.1, 148.7; 1595.0, 109.7; 1609.7, 109.7; 1611.1, 43.7; 1631.1, 39.7; 1638.7, 62.2; 1639.9, 47.3; 1681.7, 52.5; 1685.2, 64.4; 2422.1, 291.6; 3407.3, 852.2; 3507.2, 270.7; 3559.0, 371.9; 3560.7, 571.2; 3599.4, 356.5; 3610.1, 166.7; 3626.6, 1342.0; 3648.1, 230.8; 3659.0, 181.9; 3668.6, 611.9; 3678.2, 363.3; 3691.6, 369.7; 3705.1, 555.6; 3718.3, 11.7; 3728.6, 202.2; 3733.0, 615.2; 3757.9, 760.9; 3825.8, 632.9; 3927.4, 113.5; 3936.8, 144.9; 3940.6, 195.8; 3946.4, 149.8; 3947.3, 133.8; 3951.3, 157.7; 3965.5, 161.6; 3969.2, 167.1;

-2560.813336410 -2560.464217 -2560.426828 -2560.530308

η^1–NL $[Co(H_2O)_{14}N_2O]^+$

Co	-0.713000	0.088694	0.003311
O	1.080870	0.159223	1.411378
H	1.867806	-0.037751	0.851996
O	2.923031	2.523684	-1.035089
H	3.742020	2.991023	-1.219765
O	0.690909	-0.551441	-1.664528
H	0.670808	0.101632	-2.385334
H	3.169003	1.587209	-0.832326
H	0.376125	-1.415872	-1.987932
H	1.210705	1.097798	1.641575
O	-1.832622	0.843684	1.919848
H	-1.674215	1.808707	1.972873
H	-1.385587	0.466085	2.683640
O	-0.179648	2.179621	-0.510747
H	-0.093585	2.323790	-1.466799
H	-0.752622	2.862493	-0.136745
O	-0.999941	3.471664	1.760043
H	-0.023766	3.484025	1.817160
H	-1.328446	4.277224	2.165765
O	1.696934	2.931087	1.528134
H	2.465871	3.252222	2.006792
H	1.952443	2.910486	0.582509
O	0.999628	1.896798	-2.938638
H	1.060539	2.229827	-3.836841
H	1.784716	2.218536	-2.450000
O	3.024057	-0.127907	-0.514632
H	2.321848	-0.161467	-1.192582
H	3.016242	-0.998912	-0.057919
O	-1.299023	-2.031819	0.700049
H	-2.238661	-1.920871	0.951481
H	-0.811263	-2.287463	1.504188
O	0.604581	-2.199661	2.637963
H	0.910583	-1.284314	2.477469
H	0.867988	-2.465574	3.521399
O	-0.159650	-3.036268	-1.542650
H	-0.746061	-2.825635	-0.787080
H	-0.553946	-3.758333	-2.036599
N	-3.359999	-0.104570	-1.575882
N	-2.340967	0.032067	-1.108981
O	-4.420369	-0.244539	-2.063011
O	-0.572997	-0.290543	4.006736
H	-1.290422	-0.449039	4.623130
H	-0.252722	-1.148977	3.688115
O	1.947199	-2.413163	0.214304
H	1.489240	-2.402655	1.067218
H	1.288488	-2.658708	-0.453057

24.6, 0.0; 27.2, 0.5; 31.6, 0.5; 51.4, 1.5; 52.7, 2.9; 62.2, 3.2; 64.6, 2.8; 71.8, 0.7; 79.3, 0.9; 84.7, 0.1; 90.8, 2.4; 95.9, 0.8; 98.7, 2.5; 115.4, 1.2; 121.3, 2.7; 127.1, 1.6; 131.6, 4.4; 134.5, 4.4; 148.3, 8.8; 153.3, 2.5; 162.3, 1.2; 167.7, 3.6; 177.5, 0.9; 181.4, 4.0; 186.6, 2.8; 191.8, 5.2; 195.0, 2.1; 198.3, 3.1; 209.4, 0.9; 215.1, 13.7; 231.7, 15.1; 238.0, 10.3; 246.0, 12.7; 252.0, 12.5; 258.3, 6.7; 264.4, 27.6; 266.9, 10.0; 269.9, 2.4; 276.2, 24.3; 282.6, 98.4; 288.4, 16.9; 297.2, 15.9; 307.4, 31.8; 318.4, 27.2; 325.4, 6.2; 330.5, 5.9; 336.8, 7.2; 343.5, 12.5; 359.1, 23.2; 362.4, 57.2; 365.2, 59.4; 372.3, 92.7; 383.8, 41.7; 390.8, 62.1; 400.7, 29.6; 431.7, 80.7; 445.5, 75.8; 448.8, 17.1; 461.0, 39.9; 470.3, 180.1; 487.3, 141.3; 490.3, 11.3; 502.3, 0.2; 505.2, 54.7; 508.1, 290.5; 526.9, 83.2; 534.7, 156.1; 563.0, 62.7; 575.2, 89.1; 585.6, 204.0; 625.0, 55.1; 644.7, 463.1; 654.2, 173.1; 675.3, 36.6; 690.4, 13.9; 699.0, 138.6; 729.5, 100.5; 743.2, 84.2; 754.6, 153.8; 771.3, 188.0; 794.6, 110.8; 810.6, 290.9; 824.4, 55.5; 833.3, 52.7; 871.8, 271.1; 892.3, 285.6; 923.3, 58.0; 978.7, 149.9; 1327.8, 511.1; 1564.4, 55.8; 1578.9, 179.2; 1590.0, 34.4; 1598.1, 113.1; 1603.9, 74.8; 1615.0, 113.4; 1618.8, 94.8; 1622.1, 87.8; 1626.8, 98.7; 1631.3, 75.6; 1635.0, 44.7; 1667.3, 6.4; 1675.8, 85.8; 1689.7, 124.0; 2398.8, 239.7; 3483.8, 330.5; 3523.0, 814.7; 3554.9, 239.8; 3586.0, 625.6; 3608.9, 342.8; 3616.1, 105.3; 3628.5, 646.1; 3647.6, 1022.9; 3652.2, 179.9; 3665.2, 250.5; 3674.1, 67.8; 3694.6, 431.8; 3711.3, 190.9; 3716.4, 572.0; 3727.7, 460.0; 3737.2, 404.3; 3767.6, 457.9; 3804.3, 921.3; 3834.3, 598.7; 3850.2, 217.1; 3924.4, 126.0; 3936.4, 156.0; 3942.4, 132.1; 3948.3, 124.0; 3948.7, 158.9; 3951.0, 112.4; 3951.6, 174.1; 3959.0, 156.1;

-2637.208575580 -2636.874915 -2636.834811 -2636.944576

η^1–NL $[Co(H_2O)_{15}N_2O]^+$

Co	-0.713000	0.088694	0.003311
O	1.080870	0.159223	1.411378
H	1.867806	-0.037751	0.851996
O	2.923031	2.523684	-1.035089
H	3.742020	2.991023	-1.219765
O	0.690909	-0.551441	-1.664528
H	0.670808	0.101632	-2.385334
H	3.169003	1.587209	-0.832326
H	0.376125	-1.415872	-1.987932
H	1.210705	1.097798	1.641575
O	-1.832622	0.843684	1.919848
H	-1.674215	1.808707	1.972873
H	-1.385587	0.466085	2.683640
O	-0.179648	2.179621	-0.510747
H	-0.093585	2.323790	-1.466799
H	-0.752622	2.862493	-0.136745
O	-0.999941	3.471664	1.760043
H	-0.023766	3.484025	1.817160
H	-1.328446	4.277224	2.165765
O	1.696934	2.931087	1.528134
H	2.465871	3.252222	2.006792
H	1.952443	2.910486	0.582509
O	0.999628	1.896798	-2.938638
H	1.060539	2.229827	-3.836841
H	1.784716	2.218536	-2.450000
O	3.078788	-0.058806	-0.435582
H	2.402391	-0.486214	-0.995626
H	3.782964	-0.728497	-0.284095
O	-1.299023	-2.031819	0.700049
H	-2.238661	-1.920871	0.951481
H	-0.811263	-2.287463	1.504188
O	0.604581	-2.199661	2.637963
H	0.910583	-1.284314	2.477469
H	0.867988	-2.465574	3.521399
O	-0.259661	-3.088191	-1.571253
H	-0.846072	-2.877558	-0.815683
H	-0.653957	-3.810256	-2.065202
N	-3.359999	-0.104570	-1.575882
N	-2.340967	0.032067	-1.108981
O	-4.420369	-0.244539	-2.063011
O	-3.773129	-1.060580	1.290717
H	-4.616154	-1.249491	1.707111
H	-3.451023	-0.211355	1.631407
O	4.573159	-2.207299	0.143788
H	5.304892	-2.735853	-0.176885
H	3.774150	-2.766472	0.154409
O	1.973871	-2.949310	0.211796
H	1.515912	-2.938802	1.064710
H	1.315160	-3.194855	-0.455565

26.7, 1.3; 28.3, 0.6; 39.8, 0.8; 42.6, 1.0; 55.1, 2.4; 62.5, 0.4; 64.6, 2.1; 68.7, 2.6; 77.7, 0.9; 82.9, 0.4; 85.9, 4.0; 90.2, 0.6; 94.2, 5.7; 104.5, 1.1; 110.7, 3.9; 117.3, 2.1; 124.0, 1.3; 130.3, 11.0; 141.6, 0.3; 145.3, 4.0; 148.3, 4.3; 165.7, 1.3; 167.9, 1.3; 171.4, 4.4; 175.9, 4.6; 180.1, 1.6; 185.5, 5.1; 192.4, 7.0; 193.7, 11.1; 200.9, 9.7; 206.9, 8.0; 218.1, 11.9; 229.9, 7.2; 230.0, 125.9; 232.2, 28.3; 244.0, 18.0; 248.2, 26.8; 253.7, 7.7; 257.8, 80.6; 267.5, 15.8; 274.3, 8.3; 276.8, 6.0; 289.1, 15.7; 290.2, 16.1; 293.8, 8.0; 302.6, 21.4; 307.8, 14.0; 319.5, 10.5; 322.6, 7.9; 333.9, 39.2; 339.7, 2.7; 359.1, 5.1; 369.9, 17.6; 376.8, 21.5; 379.8, 89.3; 390.8, 60.6; 400.3, 5.3; 403.7, 135.1; 420.3, 100.1; 432.1, 24.9; 452.0, 54.8; 459.0, 59.0; 466.9, 235.2; 487.9, 172.5; 502.1, 63.4; 504.4, 2.8; 512.8, 13.9; 519.7, 72.3; 539.9, 124.8; 543.9, 184.4; 564.6, 189.9; 567.5, 178.4; 586.3, 41.2; 611.5, 76.7; 621.6, 173.6; 631.1, 62.9; 657.7, 216.5; 662.8, 133.1; 706.4, 79.4; 715.0, 118.8; 728.7, 118.6; 764.8, 142.6; 784.8, 155.0; 798.5, 114.5; 815.0, 158.8; 821.1, 33.5; 841.5, 157.2; 847.5, 66.7; 881.5, 236.8; 886.2, 140.6; 896.9, 59.8; 904.3, 237.2; 974.1, 241.9; 1020.4, 108.4; 1340.5, 455.4; 1575.0, 68.6; 1579.9, 248.8; 1582.5, 24.1; 1588.9, 31.1; 1592.7, 125.1; 1602.9, 135.9; 1604.5, 108.2; 1619.6, 43.7; 1624.7, 45.1; 1631.7, 166.9; 1643.8, 10.6; 1651.3, 49.0; 1658.7, 54.0; 1670.5, 28.0; 1697.6, 59.1; 2410.8, 265.5; 3373.9, 975.3; 3443.4, 860.2; 3536.8, 340.5; 3548.9, 320.0; 3559.1, 979.1; 3573.0, 308.6; 3594.1, 1167.5; 3604.0, 156.9; 3608.9, 219.8; 3624.4, 252.6; 3631.0, 270.5; 3655.5, 732.7; 3674.1, 757.0; 3684.7, 712.4; 3692.3, 416.4; 3710.2, 187.3; 3737.9, 351.8; 3748.4, 637.3; 3750.9, 129.3; 3821.0, 613.1; 3837.5, 597.2; 3909.4, 126.8; 3927.5, 71.8; 3930.9, 184.1; 3946.5, 155.5; 3948.4, 131.2; 3950.3, 147.1; 3953.8, 151.6; 3966.2, 181.7; 3974.3, 156.8;

-2713.689875380 -2713.288878 -2713.246663 -2713.360720

η^1–NL $[Co(H_2O)_{16}N_2O]^+$

Co	-0.638760	0.196208	-0.177393
O	1.075309	-0.084424	1.306261
H	1.894205	-0.115948	0.757834
O	3.151757	2.601003	-0.477396
H	3.991033	3.068212	-0.501388
O	0.888318	-0.215504	-1.848606
H	0.939000	0.567712	-2.424082
H	3.364653	1.637613	-0.450037
H	0.531145	-0.971180	-2.349358
H	1.149362	0.762679	1.782202
O	-1.931800	0.716808	1.625222
H	-1.756660	1.632006	1.908204
H	-1.758899	0.132892	2.390452
O	0.017670	2.310792	-0.290791
H	0.173666	2.628749	-1.193338
H	-0.550631	2.940687	0.175793
O	-0.968610	3.307840	2.055982
H	-0.015198	3.226898	2.251190
H	-1.304110	4.066181	2.538995
O	1.703721	2.588696	2.023244
H	2.440252	2.800126	2.602914
H	2.028377	2.722139	1.109409
O	1.396577	2.406094	-2.626844
H	1.563423	2.880672	-3.444258
H	2.132996	2.605830	-2.013622
O	3.186209	-0.062960	-0.411452
H	2.544371	-0.340835	-1.093930
H	3.821077	-0.804721	-0.297126
O	-1.321657	-2.009749	0.136297
H	-2.273242	-1.873947	0.342337
H	-0.921641	-2.445199	0.903053
O	0.579416	-2.552924	2.191224
H	0.924579	-1.642939	2.029874
H	1.235769	-3.039722	2.697122
O	-0.255922	-2.644203	-2.292798
H	-0.853961	-2.547415	-1.523787
H	-0.685558	-3.213168	-2.935266
N	-3.092829	0.373582	-2.047168
N	-2.133175	0.374106	-1.452027
O	-4.090007	0.373327	-2.669808
O	-3.803313	-1.011127	0.550534
H	-4.634012	-1.265474	0.956398
H	-3.471619	-0.226310	1.020685
O	4.444229	-2.401383	-0.011292
H	5.201867	-2.898802	-0.322396
H	3.639149	-2.902863	-0.238486
O	1.853926	-3.068354	-0.438526
H	1.288811	-3.064573	0.344665
H	1.256402	-3.096191	-1.202146
O	-1.584869	-1.295242	3.421708
H	-0.858912	-1.910949	3.231058
H	-1.934774	-1.513116	4.287324

25.7, 0.5; 30.8, 0.3; 34.6, 1.2; 44.2, 1.0; 51.5, 1.3; 57.6, 2.1; 64.3, 3.1; 69.3, 3.2; 72.4, 0.6; 80.4, 3.7; 81.4, 3.2; 87.2, 5.2; 91.4, 6.1; 95.5, 0.7; 103.4, 2.2; 105.2, 3.1; 119.7, 11.6; 124.9, 4.9; 126.2, 3.6; 130.8, 2.8; 138.0, 0.9; 142.9, 3.2; 150.8, 89.7; 157.4, 8.5; 165.4, 23.3; 170.7, 2.7; 173.8, 4.2; 181.7, 5.7; 184.4, 3.5; 187.4, 1.5; 195.1, 4.4; 199.2, 6.2; 206.0, 7.0; 214.7, 9.6; 226.8, 15.6; 228.2, 35.1; 228.6, 16.9; 245.0, 1.9; 247.9, 8.0; 251.6, 40.8; 252.9, 11.3; 258.5, 117.0; 266.2, 21.2; 275.3, 10.6; 276.6, 11.1; 285.0, 2.7; 287.3, 26.2; 293.7, 11.6; 298.4, 33.1; 299.8, 12.4; 308.1, 20.7; 315.5, 16.5; 329.8, 10.0; 335.4, 25.1; 343.2, 3.0; 359.8, 5.9; 367.4, 9.5; 375.1, 110.7; 379.5, 16.0; 393.6, 25.5; 404.8, 16.1; 413.7, 30.5; 428.6, 202.4; 445.3, 136.7; 450.9, 31.3; 454.4, 39.1; 480.2, 146.8; 494.9, 123.9; 497.2, 80.7; 503.0, 10.0; 511.8, 6.7; 518.7, 307.1; 527.7, 41.7; 531.3,

274.1; 544.1, 7.1; 566.9, 101.7; 575.8, 215.0; 597.8, 37.8; 611.2, 147.5; 624.8, 65.6; 636.8, 125.8; 654.7, 33.4; 685.6, 267.6; 706.2, 161.8; 713.5, 75.6; 726.8, 83.8; 750.4, 187.7; 766.0, 141.5; 779.5, 202.3; 797.4, 14.8; 810.9, 28.6; 826.5, 183.5; 852.2, 226.1; 865.0, 146.8; 874.3, 80.7; 889.9, 227.1; 941.9, 63.7; 949.8, 399.0; 978.0, 30.2; 1027.1, 72.0; 1339.1, 463.8; 1575.2, 42.7; 1584.3, 98.4; 1586.6, 171.3; 1591.3, 22.8; 1597.5, 237.0; 1601.7, 90.3; 1604.5, 40.8; 1617.5, 72.6; 1618.1, 1.9; 1622.8, 59.1; 1628.3, 187.2; 1642.8, 4.6; 1652.9, 36.1; 1662.4, 43.0; 1672.7, 70.1; 1699.6, 57.0; 2409.6, 263.1; 3400.6, 938.2; 3421.0, 728.9; 3474.9, 897.3; 3503.9, 848.5; 3545.6, 141.8; 3574.7, 282.9; 3587.3, 187.3; 3598.0, 543.8; 3613.0, 711.2; 3623.3, 474.5; 3636.9, 33.5; 3661.3, 532.9; 3674.8, 881.9; 3690.6, 915.1; 3704.4, 225.0; 3705.7, 273.0; 3717.4, 140.3; 3724.5, 281.0; 3736.6, 631.1; 3751.3, 567.6; 3797.9, 347.3; 3823.5, 669.2; 3850.6, 572.1; 3926.4, 135.7; 3929.4, 76.0; 3933.3, 187.2; 3948.8, 81.2; 3949.1, 199.1; 3951.3, 133.8; 3963.5, 131.0; 3966.9, 221.9; 3970.0, 133.7;

-2790.129295450 -2789.702658 -2789.657764 -2789.777498

η^1–NL $[Co(H_2O)_{17}N_2O]^+$

Co	-0.748363	0.109653	-0.134584
O	0.999545	0.313124	1.220965
H	1.673206	0.823309	0.720605
O	1.635993	3.796570	-0.010849
H	2.185985	4.576247	0.097938
O	0.623557	0.791161	-1.834977
H	0.271213	1.629819	-2.182537
H	2.252045	3.045311	-0.149277
H	0.530151	0.105098	-2.520697
H	0.749446	0.887811	1.964395
O	-1.918227	-0.460580	1.715252
H	-2.207319	0.328713	2.207189
H	-1.347570	-0.992538	2.310121
O	-1.163893	2.322037	0.294159
H	-1.233890	2.825900	-0.534084
H	-1.977031	2.433472	0.808783
O	-2.416985	2.084193	2.744733
H	-1.537244	2.409217	3.013913
H	-3.058630	2.422034	3.373440
O	0.263629	2.673833	2.588974
H	0.916824	3.259919	2.978643
H	0.161159	2.944875	1.656847
O	-0.223531	3.429363	-1.988997
H	-0.364315	4.083390	-2.676948
H	0.488034	3.759078	-1.399495
O	2.881492	1.424516	-0.417215
H	2.400159	1.010224	-1.159494
H	3.737109	0.963668	-0.343219
O	-0.408396	-2.201972	-0.472334
H	-1.328465	-2.497532	-0.301074
H	0.145284	-2.767198	0.098400
O	2.731724	-1.818690	1.047519
H	2.130802	-1.109698	1.349568
H	3.620555	-1.435127	0.985646
O	0.438445	-1.678542	-3.020654
H	0.031121	-2.040396	-2.204872
H	0.076324	-2.156050	-3.769909
N	-3.213722	-0.341997	-1.931703
N	-2.297425	-0.074714	-1.327780
O	-4.167526	-0.618046	-2.562430
O	-3.028132	-2.478683	0.222320
H	-3.646319	-3.138434	0.540798
H	-2.951707	-1.783952	0.901645
O	4.917754	-0.481775	-0.238729
H	5.875392	-0.509903	-0.295981
H	4.555547	-0.900301	-1.043639
O	2.924589	-1.362088	-1.736767
H	2.553847	-1.698102	-0.905500
H	2.283751	-1.579953	-2.429144
O	1.052521	-3.805226	1.349768
H	1.209131	-4.751030	1.308834
H	1.916533	-3.343931	1.315604
O	-0.280604	-2.125170	3.112975
H	0.141867	-2.843316	2.607968
H	-0.364781	-2.436470	4.015973

24.5, 0.5; 30.7, 1.0; 38.4, 1.6; 39.9, 2.6; 49.9, 0.6; 55.1, 0.3; 59.2, 0.2; 68.4, 0.2; 73.5, 1.2; 76.5, 3.6; 79.0, 5.0; 84.0, 0.8; 89.6, 1.5; 94.4, 1.7; 95.8, 3.9; 105.9, 3.3; 109.4, 0.2; 112.1, 4.3; 113.8, 0.9; 123.8, 4.5; 130.3, 5.6; 135.1, 2.8; 143.0, 1.7; 145.7, 1.3; 151.8, 2.7; 168.5, 4.8; 172.2, 14.6; 177.9, 7.3; 182.2, 22.2; 185.8, 13.6; 186.9, 9.7; 192.7, 42.5; 193.6, 1.5; 204.8, 25.4; 208.6, 22.1; 219.0, 22.9; 221.9, 15.0; 232.6, 15.2; 233.5, 1.2; 240.6, 16.3; 244.8, 1.6; 250.9, 7.3; 264.6, 10.5; 270.1, 5.4; 275.5, 10.0; 284.7, 6.6; 286.2, 1.1; 289.1, 69.7; 294.0, 22.7; 302.5, 4.6; 303.4, 18.7; 306.5, 25.5; 311.2, 18.8; 318.1, 6.5; 324.8, 14.4; 327.8, 17.7; 331.7, 50.7; 339.0, 42.8; 348.5, 35.4; 358.5, 35.8; 373.8, 3.9; 380.9, 58.7; 385.0, 31.2; 407.1, 73.5; 422.0, 16.3; 433.1, 35.3; 438.8, 44.9; 448.6, 126.0; 453.5, 17.5; 466.1, 213.6; 475.8, 83.8; 488.5, 152.8; 496.6, 13.9; 506.2, 3.5; 507.9, 34.1; 521.2, 89.6; 533.0, 383.7; 541.5, 148.5; 562.7, 213.6; 571.8, 74.9; 588.7, 45.6; 610.9, 134.3; 625.4, 23.0; 629.4, 25.2; 646.1, 326.6; 654.2, 86.4; 662.4, 370.2; 687.6, 161.8; 715.2, 41.9; 720.9, 26.8; 743.5, 119.4; 753.2, 214.1; 762.9, 155.0; 778.6, 40.4; 792.6, 73.2; 806.5, 146.1; 812.2, 71.5; 829.6, 64.9; 846.1, 430.6; 860.7, 25.6; 869.0, 258.8; 877.2, 79.7; 903.5, 257.2; 922.6, 90.1; 929.8, 139.4; 959.7, 118.7; 1336.5, 462.4; 1573.0, 81.1; 1586.9, 236.5; 1587.5, 24.9; 1590.8, 120.5; 1595.2, 100.0; 1607.3, 182.9; 1608.4, 79.3; 1615.4, 75.9; 1626.5, 46.2; 1635.6, 97.6; 1636.4, 112.2; 1644.3, 56.0; 1646.3, 83.0; 1654.2, 18.4; 1660.4, 7.9; 1683.3, 13.3; 1688.2, 44.6; 2408.2, 254.5; 3489.0, 384.3; 3507.1, 278.1; 3515.1, 1045.3; 3535.9, 532.1; 3548.1, 345.2; 3571.6, 670.9; 3574.0, 252.6; 3615.1, 56.5; 3624.7, 626.1; 3628.3, 658.6; 3636.9, 516.3; 3651.5, 450.6; 3661.7, 631.9; 3667.7, 180.8; 3673.4, 259.8; 3693.9, 292.4; 3696.2, 199.1; 3697.9, 897.3; 3703.4, 121.7; 3725.3, 577.3; 3731.5, 674.5; 3735.4, 410.6; 3777.3, 884.8; 3811.1, 768.4; 3812.6, 368.7; 3937.5, 109.7; 3945.0, 181.6; 3949.9, 135.6; 3950.7, 202.8; 3951.1, 166.7; 3951.5, 81.2; 3952.1, 121.3; 3961.9, 134.6; 3965.9, 158.0;

-2866.569439760 -2866.116266 -2866.069241 -2866.193327

η^1–OL $[CoN_2O]^+$

Co	-1.339725	-0.079239	-0.000011
N	1.716044	0.056044	0.002306
N	2.769542	-0.301249	-0.001225
O	0.596685	0.481985	-0.000910

100.1, 3.6; 274.3, 15.7; 566.9, 6.1; 586.5, 6.1; 1323.3, 161.5; 2442.6, 300.4;

-1566.969470190 -1566.957410 -1566.952089 -1566.986469

η^1–OL $[Co(H_2O)_1N_2O]^+$

Co	-0.744593	-0.058961	-0.000546
N	2.243942	0.005997	0.000761
N	3.256947	0.464211	-0.008170
O	1.172761	-0.527966	0.010935
O	-2.666835	0.235905	-0.004008
H	-3.339734	-0.454167	-0.043487
H	-3.109886	1.091145	0.054663

68.0, 3.5; 92.7, 2.5; 137.5, 1.1; 210.5, 2.6; 280.8, 5.4; 316.2, 283.0; 451.1, 11.6; 566.8, 5.9; 592.4, 3.1; 622.5, 68.4; 1325.3, 157.6; 1640.6, 102.4; 2447.7, 337.2; 3820.1, 181.4; 3911.7, 287.5;

-1643.456937650 -1643.419384 -1643.411239 -1643.452139

η^1–OL $[Co(H_2O)_2N_2O]^+$

Co	1.007823	-0.004545	0.065040
O	1.101852	1.951823	0.038447
H	0.419252	2.515898	-0.341338
O	1.110014	-1.960178	0.018895
H	0.444905	-2.530821	-0.381171
H	1.864860	2.501209	0.247583
H	1.873618	-2.502476	0.244393

```
 N        -2.319071    0.005482   -0.055341
 N        -3.341599   -0.048604    0.390350
 O        -1.235511    0.063450   -0.541168
---
284.6, 18.0; 18.2, 2.1; 50.8, 0.9; 83.2, 10.9; 113.2,
7.5; 124.8, 20.2; 169.0, 0.1; 234.8, 0.9; 292.4, 21.9;
318.5, 468.8; 356.0, 0.1; 469.4, 9.7; 562.9, 0.3;
591.8, 6.0; 601.4, 8.8; 606.3, 146.8; 1335.8, 124.1;
1633.4, 83.4; 1635.4, 129.0; 2413.9, 376.1; 3836.2,
251.4; 3839.0, 10.4; 3930.4, 43.8; 3931.6, 471.8;

 -1719.920252700 -1719.858404 -1719.847499 -
1719.896949
```

η^1–OL $[Co(H_2O)_3N_2O]^+$

```
Co         0.633761   -0.006926   -0.070104
 O         0.592952   -2.010971   -0.174540
 O         0.604514    1.995883   -0.196616
 O         2.753670    0.029415    0.478316
 H         3.107965    0.011854    1.372802
 H         3.504170   -0.000045   -0.123086
 H         1.357180   -2.579709   -0.038930
 H        -0.117835   -2.545242   -0.542377
 H         1.380440    2.547875   -0.057014
 H        -0.091366    2.543089   -0.573348
 N        -2.693880    0.006715    0.086493
 N        -3.654641    0.040206    0.656851
 O        -1.677692   -0.029235   -0.525739
---
8.8, 4.2; 33.8, 0.2; 50.7, 15.6; 63.4, 1.8; 73.7, 3.9;
99.3, 15.2; 124.9, 12.5; 143.8, 5.8; 194.3, 3.4; 247.3,
15.7; 259.1, 42.5; 262.7, 96.7; 274.7, 125.0; 289.3,
363.6; 321.7, 2.3; 337.9, 13.3; 412.8, 23.9; 437.2,
100.4; 517.2, 6.9; 558.7, 165.8; 593.5, 6.5; 604.1,
4.9; 1343.4, 119.1; 1617.2, 89.8; 1619.2, 165.9;
1622.2, 55.6; 2417.9, 451.8; 3847.7, 157.0; 3848.6,
58.9; 3849.5, 18.9; 3950.0, 9.4; 3951.1, 406.5; 3955.7,
182.3;

 -1796.371651430 -1796.285237 -1796.270197 -
1796.329884
```

η^1–OL $[Co(H_2O)_4N_2O]^+$

```
Co        -0.143882    0.428115   -0.174164
 O         0.517764    2.282148    0.261748
 O        -0.756033   -1.456017   -0.482588
 O        -2.183696    1.113387    0.099634
 H        -2.812041    0.397531    0.289590
 H        -2.598840    1.673957   -0.562306
 H        -0.027320    2.944972    0.696974
 H         1.406737    2.635243    0.162497
 H        -1.667482   -1.714925   -0.254613
 H        -0.276738   -2.215985   -0.820824
 N         2.958042   -0.742262    0.107075
 N         3.757187   -1.279717    0.675908
 O         2.114886   -0.172225   -0.500607
 O        -3.376147   -1.466770    0.431038
 H        -3.544376   -1.781218    1.326291
 H        -4.135931   -1.749001   -0.089859
---
9.0, 0.4; 24.2, 1.1; 39.2, 6.2; 56.6, 0.3; 65.9, 0.4;
92.2, 2.9; 101.6, 9.5; 122.5, 3.4; 136.7, 2.2; 161.3,
2.4; 206.1, 15.6; 223.9, 131.9; 249.7, 54.2; 256.5,
127.7; 273.4, 25.6; 288.1, 21.1; 310.1, 45.4; 329.8,
3.2; 347.0, 69.0; 411.2, 19.9; 465.9, 106.3; 512.6,
56.5; 547.6, 46.8; 592.5, 6.9; 605.5, 13.9; 617.5,
377.9; 693.7, 71.2; 713.3, 154.1; 1346.0, 107.8;
1604.9, 126.0; 1614.9, 104.8; 1627.5, 91.9; 1649.4,
30.7; 2415.2, 465.5; 3652.4, 423.6; 3723.9, 585.2;
3842.1, 39.6; 3851.5, 76.9; 3919.6, 181.0; 3935.0,
178.0; 3941.9, 178.6; 3956.5, 212.0;

 -1872.816985030 -1872.704158 -1872.687789 -
1872.749131
```

η^1–OL $[Co(H_2O)_5N_2O]^+$

```
Co         0.054568   -0.000107   -0.149284
 O        -2.580332   -2.784791    0.148270
 H        -3.120606   -3.206660   -0.527937
 O         0.055695   -2.005830   -0.253732
 H        -0.787762   -2.488472   -0.176776
 O        -2.005070   -0.000331    0.423730
 H        -2.547543    0.791389    0.304481
 O         0.054802    2.005585   -0.253725
 H         0.717382    2.573846   -0.653146
 H        -2.794530   -3.234794    0.972601
 H        -0.788306    2.488751   -0.176651
 H         0.717665   -2.574270   -0.653893
 H        -2.547501   -0.792105    0.304655
 O        -2.581620    2.784131    0.148739
 H        -3.122034    3.205450   -0.527698
 H        -2.796149    3.234385    0.972842
 N         3.333880    0.000594    0.159199
 O         2.393181    0.002092   -0.561311
 N         4.223663   -0.000808    0.837435
---
24.2, 0.2; 26.8, 3.3; 43.0, 0.1; 50.5, 18.2; 58.8, 0.3;
64.0, 0.4; 87.0, 4.4; 104.9, 0.2; 108.7, 0.8; 136.0,
1.9; 144.2, 1.5; 180.7, 0.2; 205.6, 25.1; 216.6, 24.9;
227.5, 53.7; 230.3, 15.4; 248.5, 41.6; 270.0, 8.7;
280.4, 25.5; 299.3, 123.2; 303.8, 3.3; 342.0, 0.3;
415.7, 26.4; 447.6, 99.3; 466.1, 167.0; 550.8, 142.0;
565.5, 195.0; 593.9, 12.5; 604.6, 4.7; 617.1, 3.5;
650.0, 299.4; 677.5, 157.9; 733.0, 257.9; 746.6, 0.3;
1346.3, 106.2; 1578.3, 73.9; 1603.2, 231.5; 1605.2,
56.6; 1634.5, 1.6; 1646.4, 36.5; 2413.3, 490.1; 3647.6,
228.3; 3652.7, 892.5; 3750.2, 242.7; 3834.3, 543.9;
3847.6, 37.7; 3863.2, 239.2; 3936.1, 23.5; 3937.0,
345.5; 3949.7, 0.7; 3950.0, 338.3;

 -1949.262221890 -1949.123444 -1949.103622 -
1949.173751
```

η^1–OL $[Co(H_2O)_6N_2O]^+$

```
Co        -0.464927   -0.255080   -0.091923
 O         1.098350   -1.399607   -1.013329
 H         1.870433   -1.682658   -0.495312
 O         0.918769    0.109666    1.516293
 H         0.524370    0.333044    2.363286
 O        -1.741240    1.251776    0.779774
 H        -2.695955    1.116456    0.668630
 O        -2.130853   -1.299149   -0.754290
 H        -2.181943   -2.208505   -1.056343
 H         1.150188   -1.798566   -1.884108
 H        -3.018935   -1.007394   -0.488249
 H         1.651516   -0.508104    1.671412
 H        -1.554017    2.161384    0.530691
 O        -4.320318    0.151035    0.242706
 H        -4.839762   -0.135462    1.001276
 H        -4.949309    0.544917   -0.370938
 O         3.146952   -1.462368    0.900361
 H         3.813740   -0.812004    0.647680
 H         3.621827   -2.187057    1.319202
 N         2.041383    1.548480   -0.661022
 N         3.110348    1.268784   -0.469106
 O         0.915685    1.817431   -0.860815
---
36.3, 16.8; 29.5, 10.2; 47.2, 2.2; 53.4, 2.0; 63.7,
1.5; 79.1, 0.8; 80.5, 2.2; 95.0, 5.3; 99.3, 1.4; 113.4,
4.0; 125.9, 0.9; 133.7, 1.0; 155.1, 4.2; 165.3, 35.1;
186.8, 48.6; 205.1, 33.1; 217.8, 3.9; 232.4, 60.6;
238.9, 19.5; 248.8, 44.5; 272.4, 27.3; 281.6, 69.0;
300.9, 11.1; 306.8, 21.9; 322.5, 9.1; 331.6, 26.7;
347.6, 13.8; 384.9, 97.7; 441.1, 19.2; 448.2, 278.9;
517.2, 126.9; 547.1, 75.9; 573.8, 235.4; 588.5, 145.3;
604.1, 16.3; 611.5, 12.7; 686.2, 61.0; 688.9, 110.1;
696.3, 106.5; 724.2, 200.5; 1379.5, 56.5; 1593.1,
115.5; 1596.9, 198.1; 1603.9, 89.2; 1615.0, 112.9;
1637.2, 25.1; 1645.4, 7.4; 2420.8, 433.5; 3693.1,
235.5; 3698.3, 153.6; 3730.6, 1040.7; 3735.7, 153.2;
3830.6, 29.7; 3848.5, 35.7; 3924.0, 186.0; 3938.0,
186.8; 3942.4, 187.8; 3944.5, 193.6; 3950.7, 151.9;
3951.4, 172.4;

 -2025.705702410 -2025.541844 -2025.519930 -
2025.592499
```

η^1–OL $[Co(H_2O)_7N_2O]^+$

```
Co         0.074603   -0.174207    0.228104
 O        -1.166782    0.543598   -1.600783
 H        -1.468357    1.431919   -1.329384
 O        -0.378887   -2.300639   -0.111164
 H        -1.315399   -2.379775   -0.360758
 O         0.754135    1.894663    0.415589
 H         1.345034    2.253441    1.082144
 O         1.353196   -1.079454    1.785446
```

```
 H         1.117390   -2.009287    1.870479
 O        -2.919283   -1.407875   -0.750622
 H        -2.524781   -0.761891   -1.365143
 H        -3.758307   -1.698087   -1.118021
 H         1.688051   -0.795658    2.639984
 H        -0.012980    2.490189    0.362977
 H         0.124438   -2.761415   -0.788555
 H        -0.622102    0.658370   -2.385550
 O        -1.962745    0.116696    1.319673
 H        -2.540581   -0.495136    0.822499
 H        -2.008776   -0.141212    2.244679
 N         2.893912    0.070060   -0.784525
 N         3.793480    0.571657   -0.345696
 O         1.933486   -0.454014   -1.233940
 O        -1.885894    2.585668    0.079107
 H        -2.496915    3.324967    0.133575
 H        -2.170549    1.906005    0.717363
---
35.6, 0.5; 49.6, 1.5; 53.6, 0.7; 65.9, 0.9; 79.5, 1.0;
81.6, 1.1; 84.8, 0.4; 94.3, 3.9; 106.6, 0.2; 120.1,
2.9; 131.2, 0.2; 138.3, 0.9; 159.7, 3.2; 180.3, 4.0;
192.0, 8.6; 203.2, 1.2; 217.0, 11.8; 228.3, 8.6; 236.2,
30.0; 248.8, 19.5; 262.8, 33.3; 270.0, 2.4; 278.5, 5.2;
284.6, 4.9; 303.0, 22.0; 322.4, 197.3; 368.7, 16.5;
381.6, 76.1; 393.1, 17.4; 396.6, 168.8; 410.8, 90.2;
421.7, 55.7; 432.5, 55.9; 445.4, 50.8; 473.5, 84.0;
481.4, 196.5; 519.3, 162.4; 536.8, 164.4; 598.6, 6.6;
605.1, 5.0; 628.0, 439.3; 712.8, 191.9; 753.0, 56.5;
768.6, 189.0; 794.8, 56.2; 854.8, 84.0; 1348.5, 76.0;
1575.2, 172.2; 1589.0, 108.2; 1602.1, 104.5; 1626.7,
157.9; 1627.1, 1.4; 1629.4, 16.8; 1638.6, 56.8; 2412.5,
426.9; 3596.2, 103.7; 3636.3, 490.8; 3659.6, 349.3;
3669.7, 105.1; 3710.2, 428.5; 3722.0, 672.9; 3845.7,
42.4; 3914.3, 129.3; 3919.5, 231.9; 3923.2, 143.0;
3933.1, 189.4; 3937.4, 182.3; 3940.3, 118.4; 3961.1,
145.7;

 -2102.151480100 -2101.960518 -2101.936328 -
2102.012786
```

η^1–OL $[Co(H_2O)_8N_2O]^+$

```
 Co         0.062659   -0.155602    0.291327
 O         -0.710718   -1.773967   -1.169479
 H         -0.823986   -1.268854   -2.000938
 O         -0.755152   -1.180087    2.069449
 H         -1.658744   -1.448612    1.811519
 O          0.953726    1.161017   -1.179049
 H          0.663899    2.049836   -0.917009
 O          0.511754    1.327920    2.075887
 H         -0.001195    0.752422    2.661507
 O         -2.959256   -1.597188    0.520616
 H         -2.382310   -1.898708   -0.204328
 H         -3.754409   -2.136035    0.508233
 H          1.409031    1.334595    2.424189
 H          0.532814    1.002259   -2.038401
 H         -0.328761   -1.960093    2.435803
 H         -0.179689   -2.547564   -1.378133
 O         -1.924318    0.844671   -0.276378
 H         -2.672545    0.413427    0.161576
 H         -1.846340    1.771653    0.011661
 N          3.062917   -0.788498   -0.178301
 N          3.856755   -0.608384   -0.945693
 O          2.220888   -0.982364    0.633201
 O         -1.151035    0.295298   -2.860226
 H         -1.578350    0.472777   -3.701966
 H         -1.708427    0.662656   -2.149257
 O         -0.557523    3.138477    0.295925
 H         -0.170806    2.818150    1.128836
 H         -0.656617    4.091297    0.369255
---
20.5, 0.2; 45.2, 0.3; 47.0, 0.9; 66.7, 1.3; 76.2, 1.3;
83.4, 4.7; 88.2, 3.4; 100.1, 1.3; 105.0, 5.3; 117.2,
1.2; 122.6, 0.5; 139.5, 1.5; 150.4, 0.4; 157.5, 0.3;
167.1, 6.8; 183.3, 0.8; 195.5, 4.4; 198.0, 8.0; 218.1,
15.3; 236.7, 15.5; 240.3, 5.0; 252.9, 6.5; 269.5, 11.7;
280.7, 8.2; 285.4, 3.7; 310.3, 27.2; 331.6, 10.5;
355.1, 5.9; 367.4, 88.0; 379.5, 73.2; 386.8, 22.1;
397.0, 73.0; 406.8, 51.0; 417.3, 144.0; 430.6, 37.9;
442.0, 105.2; 460.6, 14.5; 473.0, 260.6; 510.6, 114.7;
534.3, 110.9; 546.4, 268.5; 589.9, 8.4; 611.4, 2.2;
635.5, 357.2; 645.3, 382.5; 678.0, 58.8; 722.3, 151.3;
739.3, 161.0; 766.5, 52.7; 815.1, 240.7; 844.5, 61.3;
885.1, 48.7; 1340.9, 90.5; 1540.9, 141.7; 1577.9, 91.1;
1586.4, 198.2; 1593.9, 15.7; 1626.0, 84.5; 1635.3,
49.4; 1639.3, 15.6; 1664.9, 61.5; 2411.0, 449.8;
3574.0, 359.0; 3619.0, 344.9; 3647.2, 411.7; 3681.1,
113.1; 3685.0, 354.4; 3700.0, 63.5; 3731.9, 498.0;
3784.9, 65.0; 3795.6, 394.1; 3820.8, 625.0; 3914.6,
96.4; 3921.8, 137.2; 3922.6, 232.8; 3939.9, 167.2;
3940.5, 184.8; 3942.0, 161.0;

 -2178.593834650 -2178.375661 -2178.349758 -
2178.430175
```

η^1–OL $[Co(H_2O)_9N_2O]^+$

```
Co         0.261964    0.379426   -0.275501
 O         0.220861   -0.662158   -2.268063
 H         0.065918   -1.616311   -2.147565
 O         0.688259   -1.457336    0.761670
 H         0.157303   -1.547678    1.568679
 O        -0.347282    1.365650    1.741319
 H         0.406617    1.628705    2.278168
 O         0.363452    2.302375   -1.300077
 H         1.201859    2.762992   -1.383998
 H         0.849403   -0.551917   -2.985734
 H        -0.283678    2.934727   -0.945958
 H         0.473031   -2.231068    0.214192
 H        -0.775414    0.615882    2.202784
 O        -0.571046   -3.063371   -1.126496
 H        -0.601138   -3.986748   -1.389747
 H        -1.440193   -2.836826   -0.742730
 O        -1.863518    3.022533    0.139334
 H        -1.462105    2.644033    0.943756
 H        -2.431952    3.751151    0.400280
 O        -2.707886   -1.803250    0.166742
 H        -3.633021   -2.051328    0.081541
 H        -2.600954   -0.942707   -0.298133
 O        -1.441184   -1.052469    2.528902
 H        -2.043931   -1.378128    1.829980
 H        -1.779279   -1.367784    3.371133
 O        -1.971374    0.512681   -1.000055
 H        -2.216644    1.432694   -0.788010
 H        -1.666013    0.488255   -1.916805
 N         3.309062   -0.115858    0.462423
 N         4.003326   -0.989548    0.547097
 O         2.569772    0.803521    0.366731
---
22.5, 0.2; 41.5, 0.0; 50.5, 0.1; 57.6, 0.6; 67.0, 0.2;
71.3, 0.1; 82.6, 0.7; 86.5, 1.7; 100.3, 0.6; 102.7,
2.2; 110.9, 1.1; 119.3, 1.9; 127.5, 3.6; 134.7, 0.2;
157.9, 1.8; 173.4, 8.8; 184.5, 5.0; 185.5, 2.7; 198.2,
7.3; 216.8, 7.9; 233.3, 14.6; 234.2, 5.5; 237.4, 7.6;
246.0, 0.9; 264.8, 24.9; 280.8, 1.0; 285.5, 23.2;
299.6, 21.1; 308.9, 49.6; 319.6, 48.9; 330.7, 13.4;
342.3, 19.2; 359.8, 65.5; 388.0, 64.0; 389.4, 32.0;
400.2, 51.4; 422.3, 21.6; 443.4, 42.2; 446.4, 16.8;
482.3, 155.7; 484.2, 240.5; 516.1, 46.0; 524.0, 118.2;
544.6, 214.4; 562.0, 46.5; 578.0, 188.4; 598.2, 12.0;
606.5, 3.2; 636.9, 244.1; 666.2, 137.5; 697.7, 83.0;
717.8, 518.8; 744.6, 18.9; 790.3, 337.1; 806.2, 36.3;
811.1, 12.3; 850.4, 33.3; 941.2, 159.0; 1347.0, 83.3;
1579.3, 118.9; 1595.0, 146.4; 1608.2, 74.8; 1615.4,
3.8; 1618.8, 138.1; 1627.1, 108.3; 1635.9, 41.8;
1642.1, 42.5; 1673.0, 4.7; 2412.5, 440.3; 3486.8,
455.9; 3565.9, 521.2; 3604.4, 585.3; 3638.4, 744.6;
3645.4, 162.6; 3666.3, 3.6; 3669.2, 245.4; 3711.7,
545.0; 3721.8, 420.0; 3777.7, 680.9; 3847.4, 259.5;
3908.4, 132.3; 3920.3, 133.9; 3934.1, 125.0; 3934.6,
216.8; 3939.2, 74.2; 3939.7, 283.0; 3944.6, 113.8;

 -2255.039344540 -2254.794914 -2254.766696 -
2254.852177
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η^1–OL $[Co(H_2O)_{10}N_2O]^+$

```
Co        -0.238355    0.341105   -0.128857
 O        -0.929397    0.026464    2.115847
 H        -0.645073   -0.897412    2.271092
 O        -0.919478   -1.677511   -0.449917
 H        -0.410305   -2.117014   -1.149839
 O         0.509514    0.387071   -2.329804
 H        -0.235450    0.519705   -2.924899
 O        -0.119047    2.475733    0.102742
 H         0.147471    2.686333    1.011128
 H        -1.868998    0.061864    2.320266
 H         0.598701    2.813030   -0.455018
 H        -0.821777   -2.238647    0.336045
```

H	0.825652	-0.527967	-2.468693
O	0.052967	-2.561170	2.004186
H	-0.014943	-3.303425	2.610350
H	0.948614	-2.581152	1.610103
O	2.257985	2.279043	-1.434317
H	1.787940	1.719432	-2.078600
H	2.918162	2.791134	-1.907464
O	2.352215	-2.201927	0.479696
H	3.226698	-2.528458	0.710328
H	2.378434	-1.220155	0.576862
O	1.255425	-2.269179	-2.088889
H	1.789068	-2.370542	-1.275086
H	1.562130	-2.925330	-2.720084
O	2.000550	0.445619	0.628863
H	2.349125	1.080774	-0.026860
H	1.886713	0.955988	1.453829
N	-3.256645	0.163346	-0.624477
N	-4.033572	-0.340961	0.007251
O	-2.426129	0.696389	-1.269116
O	0.927185	1.952800	2.683970
H	0.196163	1.327349	2.837501
H	1.154469	2.361325	3.522674

25.7, 0.3; 37.5, 0.0; 51.5, 0.5; 58.2, 0.0; 69.3, 0.0; 73.5, 1.0; 84.7, 0.8; 88.6, 2.4; 96.1, 1.1; 97.6, 1.8; 108.6, 2.3; 115.5, 1.7; 124.3, 0.2; 136.2, 1.3; 148.5, 0.4; 153.4, 3.8; 175.7, 2.5; 177.8, 4.3; 185.4, 7.5; 190.6, 3.5; 195.1, 5.7; 216.0, 15.0; 224.5, 6.3; 238.5, 5.3; 243.0, 5.2; 246.7, 13.5; 264.5, 14.8; 276.9, 6.7; 289.4, 16.1; 292.1, 4.5; 314.8, 82.8; 338.2, 10.4; 338.6, 2.7; 344.2, 16.4; 356.7, 28.9; 366.9, 69.1; 380.0, 3.2; 396.7, 2.9; 401.1, 1.0; 416.8, 62.5; 433.5, 82.9; 443.6, 5.7; 463.8, 128.8; 472.6, 161.5; 511.7, 86.4; 528.7, 83.1; 554.0, 5.1; 561.6, 56.4; 598.1, 7.3; 603.8, 20.1; 605.0, 161.2; 646.3, 60.2; 666.7, 743.4; 683.0, 226.0; 693.9, 410.9; 732.8, 6.3; 751.1, 209.4; 784.9, 124.4; 788.9, 139.7; 824.5, 3.4; 846.1, 15.1; 857.8, 84.0; 858.8, 138.0; 974.1, 128.4; 1364.0, 66.3; 1572.3, 17.7; 1579.6, 200.4; 1605.6, 65.2; 1624.9, 8.1; 1628.1, 184.7; 1634.0, 77.6; 1640.4, 17.6; 1655.7, 44.1; 1678.6, 5.6; 1696.0, 83.7; 2411.1, 417.0; 3425.4, 696.9; 3555.2, 165.2; 3590.2, 1130.1; 3607.4, 318.9; 3611.2, 387.3; 3635.2, 405.9; 3643.7, 444.0; 3677.2, 369.0; 3687.2, 50.9; 3715.1, 316.6; 3735.5, 414.2; 3779.0, 639.8; 3807.4, 580.9; 3905.4, 107.9; 3907.3, 169.7; 3919.5, 119.8; 3933.4, 190.3; 3936.2, 135.5; 3945.4, 70.5; 3945.9, 276.4;

-2331.481667200 -2331.209933 -2331.179889 -2331.268814

η^1–OL $[Co(H_2O)_{11}N_2O]^+$

Co	-0.015794	0.258868	0.355538
O	-1.046112	0.908393	-1.426499
H	-0.579856	0.549239	-2.198910
O	1.764077	1.147182	-0.568747
H	2.597367	0.744426	-0.284146
O	1.294321	-0.211898	2.213150
H	1.470219	0.604987	2.690086
O	-1.975778	-0.010394	1.607253
H	-2.055624	0.754400	2.185692
H	-1.981447	0.663723	-1.494684
H	-1.764998	-0.774347	2.178961
H	1.712627	1.015772	-1.530410
H	2.139158	-0.463688	1.782493
O	1.090224	-0.025678	-2.999726
H	1.295303	0.036079	-3.935817
H	1.464486	-0.864877	-2.674346
O	-0.603095	-2.093120	2.758450
H	0.198157	-1.544767	2.863916
H	-0.648483	-2.705645	3.496672
O	2.109261	-2.141085	-1.420907
H	2.333848	-3.013216	-1.756680
H	1.283357	-2.241101	-0.891678
O	3.441130	-0.793122	0.582635
H	3.160313	-1.390330	-0.141096
H	4.364416	-0.977874	0.771812
O	-0.167501	-1.991673	-0.001039
H	-0.369553	-2.377242	0.867898
H	-0.934839	-2.172607	-0.593257
N	-0.040894	3.323708	0.231962
N	0.165960	4.043969	-0.598029
O	-0.259653	2.553268	1.104394
O	-2.213236	-2.240269	-1.716819
H	-2.908327	-1.600759	-1.477839
H	-2.641945	-3.001800	-2.111653
O	-3.550075	-0.097643	-0.677120
H	-4.451562	0.231666	-0.657991
H	-3.200132	-0.066886	0.233707

31.0, 1.6; 37.1, 0.2; 44.2, 0.3; 46.4, 1.2; 65.2, 1.5; 68.1, 1.2; 73.4, 0.3; 80.7, 1.2; 85.0, 1.4; 90.9, 2.6; 93.5, 0.6; 99.5, 1.4; 107.8, 0.8; 109.7, 2.2; 121.5, 0.7; 135.9, 0.4; 148.0, 1.4; 157.7, 2.1; 162.1, 0.9; 183.4, 1.8; 188.6, 9.3; 196.7, 3.6; 209.8, 4.8; 218.2, 7.3; 225.0, 18.1; 231.3, 26.5; 240.0, 64.6; 248.0, 10.4; 254.7, 2.9; 266.0, 38.3; 271.5, 15.6; 277.7, 13.7; 295.8, 21.5; 296.5, 12.2; 308.8, 23.2; 319.2, 12.0; 323.7, 21.3; 327.8, 15.8; 337.2, 46.3; 376.4, 31.4; 377.8, 26.0; 398.4, 14.0; 406.2, 26.6; 423.8, 39.1; 430.8, 23.1; 451.5, 120.6; 465.7, 125.2; 481.7, 154.8; 496.8, 11.2; 514.9, 244.1; 518.2, 94.2; 544.0, 42.9; 553.3, 50.9; 595.4, 89.0; 597.2, 5.1; 604.0, 4.0; 642.2, 152.3; 654.5, 369.4; 667.0, 210.7; 689.9, 128.9; 711.3, 534.3; 743.3, 220.7; 765.5, 20.3; 788.7, 32.7; 798.3, 32.1; 810.2, 87.2; 838.4, 158.0; 873.9, 100.2; 923.6, 150.4; 1011.3, 98.4; 1346.9, 80.8; 1578.6, 161.5; 1592.4, 161.8; 1596.7, 106.8; 1603.3, 22.7; 1620.5, 144.5; 1623.0, 49.2; 1626.6, 43.5; 1637.3, 20.7; 1649.8, 39.6; 1659.6, 11.5; 1674.9, 17.4; 2418.8, 404.1; 3415.9, 1076.2; 3486.3, 198.4; 3539.7, 839.3; 3590.6, 890.7; 3596.8, 172.7; 3632.1, 119.7; 3654.7, 338.9; 3664.2, 671.4; 3674.0, 314.6; 3695.9, 12.3; 3724.6, 421.2; 3738.4, 456.9; 3795.7, 983.7; 3808.2, 405.3; 3909.3, 60.2; 3913.0, 228.3; 3925.0, 116.5; 3939.0, 174.3; 3942.5, 215.4; 3944.4, 87.2; 3948.6, 167.6; 3960.2, 163.2;

-2407.923802260 -2407.627049 -2407.594084 -2407.689489

η^1–OL $[Co(H_2O)_{12}N_2O]^+$

Co	-0.598956	-0.265338	-0.401265
O	-1.067542	0.046416	-2.529517
H	-1.290877	0.990545	-2.620373
O	2.643253	1.217428	1.099856
H	2.532033	0.304106	1.422147
O	-2.372085	1.222392	0.253163
H	-2.073185	1.520891	1.140246
H	3.437447	1.172735	0.528254
H	-3.268940	0.895480	0.365730
H	-1.775920	-0.447743	-2.948968
O	1.305617	-1.846288	-0.958258
H	0.554264	-2.417236	-1.143436
H	1.535834	-1.391483	-1.796711
O	-0.441950	-0.706521	1.692625
H	-0.614384	0.070357	2.251570
H	0.425747	-1.063035	1.948116
O	0.747510	1.456031	-0.834149
H	0.247945	2.267905	-1.014876
H	1.367983	1.588944	-0.086860
O	-1.157528	1.815479	2.630830
H	-1.555103	2.050218	3.472897
H	-0.368191	2.396705	2.512003
O	-1.474734	2.718422	-1.853415
H	-2.017588	2.434031	-1.094144
H	-1.829956	3.548368	-2.179562
O	2.329877	0.055056	-2.542145
H	2.218516	0.108831	-3.494731
H	1.710613	0.704128	-2.143775
N	-2.664745	-2.296326	0.644713
N	-3.303328	-2.326633	1.564390
O	-1.996188	-2.240930	-0.328846
O	-0.410678	-2.625553	-2.747826
H	-0.088055	-2.725642	-3.644996
H	-0.682702	-1.700049	-2.632052
O	1.129621	3.130380	2.067659
H	1.875374	2.529734	1.872060
H	1.491013	3.915149	2.483771
O	2.182290	-1.510506	1.569814
H	1.991809	-1.793264	0.653947
H	2.808483	-2.132419	1.947925

45.6, 1.6; 51.9, 0.2; 55.7, 0.8; 64.0, 0.7; 70.0, 1.8; 71.8, 1.7; 73.2, 0.2; 78.4, 1.3; 87.9, 1.0; 91.3, 2.1; 99.2, 0.9; 101.9, 3.3; 107.9, 2.2; 114.8, 2.5; 120.3,

1.0; 135.5, 0.7; 141.5, 1.5; 149.0, 0.2; 165.8, 7.1; 172.9, 5.2; 183.1, 3.2; 188.8, 8.8; 196.8, 8.8; 200.4, 2.8; 210.2, 14.5; 215.3, 2.0; 221.6, 11.1; 240.2, 2.1; 252.2, 28.8; 257.1, 19.8; 267.8, 3.5; 270.9, 8.8; 281.2, 4.5; 292.9, 20.5; 302.6, 26.2; 307.9, 19.0; 311.1, 28.2; 324.0, 56.7; 327.8, 112.4; 335.1, 41.7; 341.6, 12.9; 356.7, 24.9; 365.9, 34.4; 380.2, 45.0; 400.3, 29.6; 407.3, 27.4; 421.5, 20.5; 435.7, 48.0; 438.1, 21.1; 448.2, 138.7; 457.4, 76.8; 486.5, 107.7; 504.9, 86.9; 525.0, 7.5; 556.3, 23.0; 579.2, 35.1; 594.1, 92.3; 599.4, 13.6; 609.9, 4.6; 638.1, 98.8; 643.6, 242.7; 654.8, 37.6; 669.1, 624.6; 691.3, 406.4; 697.1, 264.9; 745.7, 331.2; 795.7, 46.0; 805.1, 56.8; 822.6, 126.6; 832.2, 131.7; 847.3, 48.1; 864.3, 63.9; 873.9, 63.8; 907.8, 77.3; 926.5, 194.8; 1045.9, 102.2; 1359.9, 70.2; 1579.4, 165.5; 1585.7, 130.7; 1590.7, 86.4; 1592.2, 107.3; 1615.6, 93.9; 1624.3, 22.2; 1633.4, 37.9; 1639.7, 66.6; 1658.8, 91.3; 1668.9, 34.1; 1675.7, 30.6; 1698.1, 13.5; 2418.7, 376.6; 3258.8, 958.1; 3498.7, 380.2; 3547.8, 231.0; 3559.1, 1471.4; 3578.5, 470.4; 3608.4, 60.0; 3619.1, 111.9; 3635.5, 183.5; 3650.9, 153.2; 3663.5, 832.0; 3672.2, 769.7; 3714.1, 293.9; 3725.1, 599.6; 3770.8, 837.3; 3772.9, 58.0; 3785.6, 693.6; 3900.1, 102.0; 3907.4, 172.0; 3927.3, 111.4; 3938.7, 162.4; 3942.9, 193.0; 3945.9, 172.4; 3946.5, 123.7; 3959.5, 194.5;

-2484.326851650 -2484.040089 -2484.005633 -2484.102631

η^1–OL $[Co(H_2O)_{13}N_2O]^+$

Co	-0.590321	-0.314408	-0.418275
O	-1.017393	0.083553	-2.555732
H	-1.323594	1.003529	-2.637251
O	2.633685	1.130392	1.166119
H	2.476156	0.325713	1.694289
O	-2.394000	1.186284	0.271869
H	-2.068577	1.497365	1.141881
H	3.370401	0.908149	0.570049
H	-3.289575	0.867292	0.412923
H	-1.649011	-0.476589	-3.012742
O	0.932648	-1.733689	-1.135402
H	1.646561	-2.103469	-0.596170
H	1.384218	-1.302169	-1.877195
O	-0.440188	-0.749135	1.686226
H	-0.592527	0.049205	2.216901
H	0.417033	-1.105981	1.973475
O	3.445787	-2.336955	0.175571
H	3.934556	-1.585346	-0.217523
H	3.938973	-3.137468	-0.020210
O	0.723082	1.478024	-0.812508
H	0.208515	2.287665	-0.955792
H	1.306578	1.575772	-0.037519
O	-1.074954	1.849309	2.610096
H	-1.445224	2.098509	3.460337
H	-0.305534	2.441113	2.449293
O	-1.525743	2.713071	-1.828156
H	-2.060620	2.383596	-1.081201
H	-1.922307	3.530417	-2.137463
O	2.302318	0.241627	-2.649294
H	2.204972	0.413775	-3.588590
H	1.648894	0.800814	-2.175664
N	-2.675320	-2.357684	0.664615
N	-3.236008	-2.472303	1.607797
O	-2.081361	-2.216028	-0.341521
O	4.309596	0.065171	-0.848540
H	5.194808	0.345569	-1.095153
H	3.735057	0.186130	-1.637339
O	1.142398	3.270277	1.955938
H	1.903459	2.676242	1.823524
H	1.480008	4.106863	2.281475
O	2.210481	-1.371744	2.379848
H	2.711122	-1.900380	1.725147
H	2.474515	-1.672983	3.252753

26.1, 0.0; 36.7, 0.5; 40.7, 0.5; 47.0, 1.0; 52.6, 0.7; 54.4, 1.2; 61.1, 1.9; 64.1, 0.7; 70.5, 1.2; 74.3, 1.2; 79.8, 0.1; 84.7, 3.5; 90.3, 0.1; 93.7, 0.1; 99.3, 0.2; 104.7, 1.0; 112.9, 1.6; 122.0, 0.6; 134.2, 0.5; 149.2, 2.8; 157.6, 4.2; 159.5, 0.6; 185.1, 8.8; 192.0, 9.1; 198.1, 3.1; 204.8, 0.8; 210.1, 1.1; 211.8, 1.0; 219.5, 20.6; 232.8, 13.3; 236.1, 14.9; 248.6, 84.4; 253.2, 1.6; 257.9, 51.0; 267.3, 12.6; 272.9, 13.9; 276.1, 24.4; 283.4, 6.8; 296.3, 10.3; 302.4, 6.3; 310.3, 10.2; 313.0, 17.2; 314.9, 14.3; 327.7, 11.8; 336.4, 86.7; 341.9, 22.3; 354.1, 21.9; 364.3, 17.1; 386.8, 49.0; 393.0, 135.0; 402.5, 24.8; 420.8, 58.5; 428.3, 91.9; 451.3, 45.1; 461.2, 107.7; 471.6, 197.2; 484.2, 36.3; 498.5, 20.1; 514.0, 47.8; 537.9, 56.8; 547.8, 33.9; 579.6, 166.2; 595.8, 43.1; 600.8, 6.7; 601.8, 24.6; 606.9, 8.5; 630.9, 156.0; 639.1, 183.2; 679.0, 43.1; 706.8, 108.6; 715.6, 719.7; 731.9, 174.5; 749.5, 223.1; 781.4, 98.3; 787.7, 366.7; 806.9, 52.6; 833.9, 116.2; 836.2, 54.4; 847.4, 42.2; 861.3, 85.2; 892.7, 93.8; 946.7, 109.1; 1352.4, 59.7; 1548.1, 103.1; 1584.3, 117.7; 1604.3, 182.4; 1610.7, 107.0; 1613.6, 44.0; 1623.5, 85.2; 1626.0, 69.8; 1638.3, 8.6; 1641.9, 42.0; 1647.1, 59.6; 1665.1, 12.2; 1676.9, 96.3; 1693.8, 31.0; 2412.3, 397.2; 3472.3, 358.8; 3480.5, 773.5; 3547.3, 796.1; 3560.5, 250.7; 3575.6, 494.7; 3605.6, 864.6; 3632.3, 170.3; 3641.7, 181.3; 3647.1, 304.5; 3684.3, 534.7; 3697.6, 303.3; 3704.9, 329.7; 3726.5, 867.6; 3728.6, 424.7; 3758.6, 425.3; 3778.1, 631.6; 3788.8, 717.1; 3920.2, 122.9; 3932.8, 147.3; 3937.3, 120.4; 3938.6, 123.7; 3939.7, 165.7; 3940.2, 208.9; 3944.2, 128.5; 3951.3, 137.8; 3957.9, 173.1;

-2560.797446750 -2560.454065 -2560.415834 -2560.522999

η^1–OL $[Co(H_2O)_{14}N_2O]^+$

Co	0.180974	-0.585118	-0.678776
O	-0.015809	-0.920266	1.605543
H	0.263499	-0.041992	1.924346
O	-1.194023	3.314747	1.222362
H	-1.304720	4.126743	1.723669
O	1.081395	1.403678	-0.967626
H	0.495858	2.007793	-1.458885
H	-0.399662	2.863619	1.587026
H	1.964702	1.365127	-1.383360
H	-0.984560	-0.969327	1.715023
O	-0.357537	-2.645033	-0.982991
H	-1.318553	-2.763101	-1.047132
H	-0.015996	-3.253428	-0.311819
O	-1.468215	0.055183	-1.806894
H	-1.741400	0.974856	-1.672005
H	-2.240416	-0.520541	-1.680061
O	-3.085633	-2.061322	-0.947234
H	-3.169012	-1.847774	0.001932
H	-3.900548	-2.484961	-1.226064
O	-2.826392	-1.024804	1.604029
H	-3.317874	-1.230698	2.403416
H	-3.052012	-0.098564	1.355666
O	-1.131321	2.881163	-1.539319
H	-1.386914	3.565234	-2.162579
H	-1.199652	3.259230	-0.643413
O	0.929412	1.712782	1.731247
H	1.062361	1.631543	0.760603
H	1.835227	1.745559	2.070457
O	2.350182	-1.218356	-0.151936
H	2.891473	-1.140757	-0.948118
H	2.264919	-2.157292	0.095371
O	1.248360	-3.305131	1.196988
H	0.829503	-2.554958	1.662392
H	1.473891	-3.975586	1.844795
O	3.715000	0.884231	-1.457326
H	4.394998	1.211724	-2.050430
H	3.997252	1.082476	-0.546672
O	-3.212470	1.459324	0.659295
H	-2.577811	2.145575	0.938229
H	-4.052268	1.900278	0.514415
O	3.574088	0.774115	1.322023
H	3.159094	-0.063787	1.032666
H	4.286003	0.538717	1.922184
N	1.484796	-1.011901	-3.879010
N	2.088949	-1.258832	-4.923926
O	0.817875	-0.739314	-2.725532

34.0, 0.4; 39.5, 0.3; 45.0, 0.6; 47.4, 0.9; 52.2, 1.5; 58.3, 1.7; 64.4, 0.5; 68.4, 0.6; 72.3, 0.4; 75.0, 0.0; 81.7, 0.4; 86.2, 1.4; 88.7, 0.9; 94.9, 0.7; 101.9, 0.1; 106.2, 1.6; 114.0, 1.3; 115.1, 0.7; 128.9, 0.9; 139.0, 0.2; 143.5, 2.1; 152.6, 4.8; 170.7, 10.4; 176.2, 1.3; 179.9, 1.3; 185.7, 4.1; 193.3, 3.5; 200.7, 5.9; 204.3, 8.8; 208.0, 7.9; 230.1, 14.0; 233.8, 13.0; 240.6, 3.6; 244.8, 0.6; 250.6, 91.4; 263.0, 12.6; 271.3, 19.8;

277.7, 26.2; 280.2, 40.0; 286.1, 4.0; 289.4, 6.7; 300.1, 4.9; 303.9, 4.2; 306.6, 49.5; 311.9, 2.6; 325.8, 25.9; 329.2, 28.5; 344.1, 22.2; 358.6, 16.7; 359.8, 23.2; 362.5, 23.3; 373.1, 40.1; 399.5, 75.4; 411.6, 60.9; 421.9, 67.8; 428.7, 176.3; 444.6, 107.9; 450.7, 156.0; 467.6, 8.5; 481.8, 110.4; 485.4, 52.4; 490.8, 32.9; 517.0, 142.5; 542.8, 2.7; 554.5, 3.2; 578.2, 231.0; 590.3, 163.2; 603.2, 3.4; 612.1, 9.5; 614.9, 101.6; 621.6, 218.1; 637.4, 320.6; 677.6, 393.3; 687.9, 30.4; 719.6, 419.2; 734.0, 34.2; 747.4, 98.4; 756.9, 169.8; 774.5, 62.3; 787.4, 138.7; 795.6, 35.2; 812.5, 243.5; 817.6, 208.3; 825.1, 83.9; 866.3, 78.2; 907.9, 52.5; 946.9, 206.0; 964.0, 74.2; 1360.1, 76.1; 1553.7, 92.7; 1580.2, 174.6; 1585.1, 133.8; 1593.3, 83.8; 1597.5, 35.2; 1602.0, 77.9; 1604.8, 62.6; 1614.8, 67.7; 1620.4, 50.3; 1640.6, 14.3; 1645.5, 44.2; 1654.0, 62.4; 1659.1, 11.0; 1686.9, 63.8; 2415.1, 410.9; 3445.0, 333.8; 3467.6, 903.3; 3518.8, 907.9; 3573.0, 190.1; 3589.6, 397.8; 3618.4, 127.0; 3622.9, 395.9; 3630.7, 485.2; 3651.4, 313.3; 3674.5, 457.5; 3679.4, 133.3; 3691.1, 209.5; 3693.1, 519.8; 3702.5, 1282.9; 3714.5, 217.9; 3728.8, 444.5; 3795.4, 742.4; 3819.9, 596.6; 3822.2, 203.3; 3846.7, 377.3; 3934.1, 127.2; 3934.6, 137.6; 3938.4, 159.9; 3946.5, 103.1; 3947.0, 124.5; 3950.4, 164.3; 3953.3, 206.2; 3955.9, 129.0;

-2637.170082610 -2636.867485 -2636.827245 -2636.937681

η^1–OL $[Co(H_2O)_{15}N_2O]^+$

Co	-0.617887	0.238793	-0.009530
O	-1.726980	1.605037	1.383589
H	-1.631944	1.257885	2.284670
O	2.688365	-1.647149	0.370252
H	2.587365	-1.643843	-0.599577
O	-2.214744	-1.272086	0.728512
H	-2.086400	-2.149633	0.327215
H	3.447267	-1.065878	0.545116
H	-3.081715	-0.904069	0.468045
H	-1.335154	2.499592	1.329793
O	0.930171	1.756939	-0.728001
H	1.500106	1.562804	-1.485147
H	1.551295	1.879950	0.014920
O	-0.214087	-1.154746	-1.611043
H	-0.449958	-2.065037	-1.362302
H	0.663980	-1.196878	-2.022790
O	3.484593	1.163006	-1.978435
H	3.971784	1.056252	-1.135902
H	3.986596	1.776839	-2.520316
O	0.747202	-0.226504	1.766092
H	0.171695	-0.590594	2.463673
H	1.316712	-0.928402	1.402629
O	-1.025264	-3.510684	-0.349540
H	-1.306640	-4.363561	-0.687686
H	-0.318119	-3.671406	0.312320
O	-1.513930	-0.514696	3.221572
H	-1.939242	-0.974666	2.467016
H	-1.887832	-0.864777	4.032532
O	-4.067186	0.597003	0.252051
H	-4.955892	0.878353	0.475114
H	-3.442050	1.211309	0.676498
O	-0.332959	3.790949	0.608046
H	-0.656901	4.646707	0.319228
H	-0.012993	3.322080	-0.182184
O	2.323315	1.914853	1.673898
H	2.104586	2.723178	2.145303
H	1.700761	1.208918	1.963553
N	-2.634165	0.475809	-2.315079
N	-3.292978	-0.289029	-2.800741
O	-1.934677	1.270784	-1.794145
O	4.410105	0.614451	0.570986
H	5.303549	0.671752	0.919720
H	3.840183	1.183598	1.130826
O	1.013627	-3.532353	1.453111
H	1.810327	-3.072864	1.132552
H	1.306304	-4.224908	2.048917
O	2.469732	-1.305649	-2.414655
H	2.918983	-0.440197	-2.495660
H	2.798028	-1.870594	-3.118350

30.9, 0.2; 37.1, 0.2; 39.6, 1.1; 41.7, 0.4; 49.6, 0.2; 53.1, 0.2; 55.9, 0.5; 62.0, 0.1; 64.5, 1.3; 67.7, 0.5; 78.4, 1.1; 83.1, 0.6; 84.8, 0.7; 88.8, 1.1; 91.3, 3.2; 96.8, 0.0; 104.4, 1.3; 107.7, 1.8; 113.2, 2.9; 120.8, 0.0; 127.4, 1.0; 134.8, 0.2; 147.6, 0.6; 151.7, 3.7; 153.6, 7.5; 168.2, 6.4; 180.8, 7.4; 194.1, 2.7; 199.8, 6.1; 209.1, 3.9; 211.7, 11.2; 214.9, 12.1; 234.0, 13.4; 242.1, 18.0; 249.3, 12.8; 252.6, 2.0; 255.9, 42.3; 258.9, 10.6; 260.2, 23.8; 270.2, 23.9; 275.2, 24.2; 280.3, 22.1; 285.5, 67.7; 292.8, 0.5; 295.2, 44.0; 303.2, 38.3; 305.7, 96.8; 311.2, 17.5; 314.7, 13.3; 318.2, 15.1; 323.4, 20.2; 334.0, 119.9; 356.4, 36.2; 360.7, 59.1; 364.9, 12.1; 373.6, 54.2; 408.7, 38.6; 412.1, 24.5; 432.0, 88.7; 443.5, 85.8; 455.5, 97.6; 465.8, 61.3; 479.5, 81.6; 489.8, 19.3; 496.0, 148.7; 504.6, 12.8; 515.3, 182.6; 542.7, 115.9; 558.3, 80.5; 574.0, 85.4; 590.1, 28.8; 597.3, 14.3; 609.7, 92.8; 611.1, 70.6; 626.5, 45.6; 641.6, 88.8; 662.0, 110.9; 678.6, 390.6; 700.7, 323.9; 705.8, 78.0; 735.1, 175.3; 749.4, 23.0; 753.8, 464.2; 776.0, 196.2; 792.7, 288.5; 808.4, 102.4; 827.4, 30.1; 841.1, 47.7; 854.7, 60.5; 872.1, 251.2; 884.5, 55.9; 908.2, 137.4; 932.8, 66.1; 944.7, 114.1; 1358.4, 62.7; 1555.6, 122.8; 1577.9, 68.6; 1586.1, 28.9; 1604.0, 167.6; 1606.2, 203.5; 1608.9, 19.3; 1610.3, 142.4; 1615.4, 63.8; 1623.7, 37.0; 1633.4, 12.4; 1635.4, 28.6; 1638.2, 44.5; 1651.1, 25.5; 1669.1, 81.5; 1691.6, 35.6; 2413.8, 415.5; 3456.0, 541.3; 3516.5, 230.0; 3533.8, 601.0; 3540.0, 493.7; 3570.1, 566.8; 3582.4, 632.1; 3615.2, 544.9; 3617.0, 556.5; 3638.0, 68.4; 3645.7, 255.0; 3651.4, 419.5; 3669.2, 49.5; 3677.1, 153.2; 3691.1, 596.2; 3708.4, 467.8; 3718.2, 1578.1; 3727.6, 599.1; 3746.1, 669.4; 3763.1, 332.6; 3772.9, 685.4; 3824.0, 368.7; 3932.3, 170.8; 3934.9, 113.2; 3938.5, 179.4; 3941.8, 150.2; 3948.7, 126.5; 3955.0, 68.1; 3955.4, 280.8; 3955.9, 115.3; 3968.8, 158.2;

-2713.681777820 -2713.281186 -2713.238386 -2713.354949

η^1–OL $[Co(H_2O)_{16}N_2O]^+$

Co	-0.638494	0.079627	-0.099341
O	-1.423835	1.942429	0.878416
H	-1.266239	1.892281	1.834839
O	2.462872	-2.072873	0.661760
H	2.301802	-2.303638	-0.271291
O	-2.350628	-0.923994	1.097549
H	-2.343201	-1.889057	0.969787
H	3.266072	-1.524433	0.651123
H	-3.188370	-0.543942	0.771551
H	-1.009748	2.743340	0.513370
O	1.009550	1.187909	-1.238380
H	1.540282	0.739780	-1.913759
H	1.654970	1.399857	-0.529054
O	-0.527353	-1.733439	-1.265809
H	-0.837616	-2.499563	-0.752773
H	0.312221	-1.994057	-1.678156
O	3.360043	-0.050890	-2.354299
H	3.879625	0.003913	-1.524123
H	3.899771	0.331016	-3.050877
O	0.727843	-0.154481	1.688384
H	0.181616	-0.222286	2.490733
H	1.202851	-0.988857	1.528908
O	-1.492997	-3.511917	0.657640
H	-1.908491	-4.372626	0.570141
H	-0.745194	-3.610117	1.286523
O	-1.410365	0.438051	3.245084
H	-1.949452	-0.145107	2.671948
H	-1.778537	0.406094	4.130136
O	-3.978128	0.997308	0.197331
H	-4.794562	1.458971	0.395205
H	-3.238538	1.589477	0.421122
O	-0.144846	3.633873	-0.914236
H	-0.637083	4.101146	-1.593022
H	0.210814	2.816863	-1.320923
O	2.518435	1.727677	0.979827
H	2.339040	2.667835	1.189589
H	1.881393	1.186220	1.489514
N	-2.784844	-0.050795	-2.293578
N	-3.563073	-0.828256	-2.504510
O	-1.960763	0.761052	-2.059185
O	4.371973	-0.016401	0.204520
H	5.282321	0.040652	0.505478
H	3.880520	0.739916	0.601439
O	0.713346	-3.450462	2.256240
H	1.523966	-3.166387	1.796592

H	0.980082	-4.021746	2.978966
O	2.062226	-2.414265	-2.105597
H	2.590681	-1.652443	-2.418316
H	2.285037	-3.167976	-2.657210
O	1.489040	4.214101	1.229650
H	1.777775	5.088312	1.497310
H	0.969642	4.310552	0.412910

25.8, 0.1; 32.6, 0.2; 37.3, 0.6; 40.4, 1.6; 44.8, 0.2; 50.4, 1.0; 51.1, 0.2; 54.5, 0.0; 59.5, 0.3; 60.8, 2.2; 61.8, 1.1; 69.6, 0.3; 79.3, 0.6; 81.7, 1.5; 84.7, 0.4; 89.4, 0.7; 98.1, 0.0; 105.0, 0.9; 107.1, 0.9; 112.2, 1.6; 125.8, 0.3; 126.2, 0.0; 138.1, 0.0; 145.6, 0.3; 153.8, 1.7; 157.3, 7.6; 162.6, 3.5; 177.1, 3.7; 187.9, 16.5; 198.3, 27.4; 201.2, 9.0; 205.2, 13.1; 212.3, 3.7; 213.9, 15.9; 223.9, 75.1; 231.5, 7.6; 235.8, 10.0; 242.5, 12.0; 244.8, 85.8; 251.0, 12.3; 256.6, 5.8; 259.8, 16.3; 264.4, 24.5; 275.7, 14.9; 276.3, 92.0; 277.2, 29.9; 284.8, 17.5; 291.9, 53.3; 292.6, 16.9; 303.9, 31.9; 309.7, 19.9; 312.3, 1.1; 314.9, 3.8; 320.4, 31.4; 331.7, 29.5; 342.4, 64.7; 353.8, 49.3; 357.9, 9.6; 367.6, 36.3; 392.2, 11.5; 404.1, 32.4; 422.8, 126.5; 432.2, 53.6; 439.1, 51.9; 462.5, 22.0; 473.0, 156.8; 475.6, 38.5; 492.1, 46.8; 503.7, 170.2; 508.7, 108.1; 528.4, 19.0; 545.8, 142.8; 571.0, 45.5; 583.2, 99.5; 597.3, 58.4; 600.0, 21.5; 609.5, 14.6; 614.7, 21.9; 635.2, 143.5; 641.4, 97.4; 651.5, 69.7; 676.8, 64.3; 688.9, 348.9; 693.0, 277.7; 706.5, 169.1; 714.7, 250.5; 733.2, 302.6; 751.2, 194.5; 771.2, 152.3; 787.1, 77.6; 802.9, 326.8; 815.8, 66.7; 825.7, 142.9; 842.0, 67.6; 856.2, 18.2; 871.2, 155.6; 881.1, 159.7; 923.7, 59.7; 956.3, 132.4; 986.7, 163.6; 1358.2, 65.7; 1545.8, 142.7; 1559.0, 48.5; 1577.0, 50.6; 1600.0, 31.6; 1603.5, 187.1; 1606.8, 150.2; 1607.0, 98.9; 1615.2, 23.2; 1617.7, 147.3; 1628.0, 24.3; 1630.9, 12.6; 1634.5, 39.4; 1655.5, 59.0; 1658.6, 1.9; 1667.0, 102.2; 1692.4, 40.0; 2413.7, 423.0; 3438.6, 789.7; 3471.7, 222.8; 3516.5, 416.4; 3542.0, 577.2; 3558.6, 675.7; 3575.6, 87.6; 3591.6, 990.5; 3603.3, 908.4; 3610.6, 534.1; 3631.7, 151.0; 3642.7, 385.0; 3658.3, 390.5; 3665.8, 313.6; 3672.5, 159.0; 3692.4, 553.2; 3701.3, 64.3; 3712.3, 211.6; 3720.4, 1313.9; 3731.4, 831.1; 3754.3, 552.1; 3760.0, 469.9; 3789.8, 801.4; 3795.1, 435.1; 3935.9, 135.4; 3939.1, 151.1; 3943.0, 158.8; 3946.6, 135.6; 3947.6, 131.6; 3958.0, 79.8; 3958.6, 215.7; 3964.7, 182.5; 3968.0, 150.1;

-2790.124125540 -2789.698310 -2789.652846 -2789.775806

η^1–OL $[Co(H_2O)_{17}N_2O]^+$

Co	-0.638494	0.079627	-0.099341
O	-1.423835	1.942429	0.878416
H	-1.266239	1.892281	1.834839
O	2.462872	-2.072873	0.661760
H	2.301802	-2.303638	-0.271291
O	-2.350628	-0.923994	1.097549
H	-2.343201	-1.889057	0.969787
H	3.266072	-1.524433	0.651123
H	-3.188370	-0.543942	0.771551
H	-1.009748	2.743340	0.513370
O	1.009550	1.187909	-1.238380
H	1.540282	0.739780	-1.913759
H	1.654970	1.399857	-0.529054
O	-0.527353	-1.733439	-1.265809
H	-0.837616	-2.499563	-0.752773
H	0.312221	-1.994057	-1.678156
O	3.360043	-0.050890	-2.354299
H	3.879625	0.003913	-1.524123
H	3.899771	0.331016	-3.050877
O	0.727843	-0.154481	1.688384
H	0.181616	-0.222286	2.490733
H	1.202851	-0.988857	1.528908
O	-1.492997	-3.511917	0.657640
H	-1.908491	-4.372626	0.570141
H	-0.745194	-3.610117	1.286523
O	-1.280290	0.565105	3.167324
H	-1.649379	0.093340	2.392479
H	-2.012281	0.929736	3.668445
O	-3.978128	0.997308	0.197331
H	-4.794562	1.458971	0.395205
H	-3.238538	1.589477	0.421122
O	-0.144846	3.633873	-0.914236
H	-0.637083	4.101146	-1.593022
H	0.210814	2.816863	-1.320923
O	2.518435	1.727677	0.979827
H	2.339040	2.667835	1.189589
H	1.881393	1.186220	1.489514
N	-2.784844	-0.050795	-2.293578
N	-3.563073	-0.828256	-2.504510
O	-1.960763	0.761052	-2.059185
O	4.371973	-0.016401	0.204520
H	5.282321	0.040652	0.505478
H	3.880520	0.739916	0.601439
O	0.645200	-3.495141	2.202821
H	1.371954	-3.076276	1.707382
H	0.291045	-2.835718	2.802473
O	2.062226	-2.414265	-2.105597
H	2.590681	-1.652443	-2.418316
H	2.285037	-3.167976	-2.657210
O	1.489040	4.214101	1.229650
H	1.777775	5.088312	1.497310
H	0.969642	4.310552	0.412910
O	-0.798767	-2.001855	3.859584
H	-0.387415	-2.166746	4.711171
H	-1.146216	-1.107164	3.839402

27.0, 0.6; 30.2, 0.8; 32.4, 0.3; 40.5, 1.5; 49.8, 0.7; 50.4, 1.5; 53.4, 0.9; 58.1, 1.0; 61.2, 1.5; 66.2, 1.0; 67.2, 0.2; 69.9, 1.4; 77.1, 0.9; 82.0, 1.8; 84.1, 0.5; 89.7, 0.2; 94.0, 0.2; 99.0, 0.8; 102.0, 0.5; 105.5, 1.3; 115.4, 1.2; 123.4, 0.7; 125.6, 0.4; 134.8, 0.5; 141.5, 1.0; 143.6, 0.7; 149.2, 1.1; 155.1, 3.2; 174.9, 1.4; 183.5, 5.2; 189.6, 19.1; 194.4, 20.7; 202.8, 6.7; 206.5, 6.2; 212.4, 15.5; 219.2, 8.0; 229.1, 22.1; 234.0, 10.8; 236.0, 85.7; 243.2, 7.6; 248.7, 29.5; 255.6, 83.9; 258.6, 3.8; 259.6, 23.8; 260.6, 61.0; 269.8, 25.6; 276.3, 31.4; 279.7, 10.6; 287.9, 30.4; 288.6, 33.9; 297.2, 23.7; 301.3, 41.8; 305.1, 38.3; 313.2, 6.6; 319.2, 9.9; 325.4, 11.6; 330.4, 14.5; 338.5, 5.2; 354.9, 81.4; 361.3, 13.1; 368.4, 34.0; 388.1, 7.2; 393.6, 26.9; 398.1, 30.7; 410.9, 54.4; 433.9, 56.9; 443.2, 66.5; 458.1, 31.6; 471.5, 93.1; 475.9, 58.5; 491.3, 52.2; 499.5, 38.9; 510.4, 28.6; 529.6, 74.6; 531.5, 81.2; 552.8, 150.2; 566.3, 15.8; 584.6, 5.4; 592.8, 217.3; 599.7, 37.8; 608.8, 6.4; 617.4, 196.3; 633.6, 1.3; 639.6, 309.4; 640.0, 53.6; 660.6, 288.0; 671.4, 64.6; 680.3, 361.6; 693.3, 180.6; 712.5, 114.7; 713.2, 177.3; 725.3, 142.6; 759.1, 338.7; 768.9, 121.0; 785.8, 85.3; 800.2, 241.0; 820.4, 160.6; 823.6, 94.2; 837.8, 85.2; 857.7, 11.1; 885.4, 198.6; 908.8, 70.4; 933.2, 119.8; 975.7, 148.9; 992.1, 126.7; 1001.4, 164.2; 1359.0, 64.0; 1550.3, 86.7; 1584.7, 66.6; 1596.1, 67.0; 1601.1, 80.6; 1605.6, 167.0; 1608.2, 225.2; 1618.4, 86.4; 1624.0, 22.6; 1627.0, 23.4; 1630.4, 47.4; 1637.2, 40.3; 1640.2, 44.8; 1655.6, 55.4; 1658.7, 7.4; 1668.3, 95.7; 1680.4, 47.8; 1708.9, 23.5; 2414.4, 415.2; 3394.1, 509.5; 3452.9, 417.7; 3469.7, 357.7; 3476.0, 713.6; 3522.9, 733.4; 3548.0, 737.8; 3574.3, 737.1; 3584.6, 862.1; 3600.6, 568.4; 3605.5, 149.4; 3612.2, 460.9; 3618.9, 445.2; 3657.6, 328.0; 3662.8, 842.0; 3671.3, 684.0; 3677.9, 191.2; 3692.7, 484.0; 3707.3, 215.1; 3717.2, 623.8; 3734.1, 378.1; 3738.4, 972.6; 3759.8, 245.0; 3785.8, 478.0; 3806.4, 431.1; 3818.0, 730.1; 3935.9, 132.4; 3936.2, 125.2; 3939.0, 145.6; 3944.0, 184.9; 3945.1, 113.3; 3948.1, 155.3; 3950.3, 117.2; 3964.6, 175.5; 3972.4, 159.0;

-2866.540132460 -2866.110654 -2866.063151 -2866.190036

PES of $[Co(H_2O)_8N_2O]^+$

^{3}N1

Co	-0.315304	0.195609	0.040528
O	-0.777912	1.889194	1.417236
H	-0.387946	2.710844	1.071328
O	0.352232	-0.992609	1.843042
H	0.806938	-1.830524	1.642180
O	-0.220239	1.551368	-1.701196
H	-0.993235	1.759283	-2.231260
O	0.633071	-1.416069	-1.347459
H	0.726374	-2.255630	-0.864140
O	1.809805	0.975334	0.541836
H	1.734833	0.672278	1.456990

H	2.499408	0.417952	0.134024
H	0.076524	-1.578991	-2.114525
H	0.145478	2.403377	-1.401723
H	-0.197339	-1.131075	2.618285
H	-1.653696	2.107750	1.743344
O	1.856251	-2.933221	0.573570
H	2.648681	-2.453074	0.272797
H	2.134098	-3.820365	0.817275
N	-3.181944	-0.892086	-0.230228
N	-2.126992	-0.488506	-0.163564
O	-4.277985	-1.310519	-0.300056
O	0.936028	3.470914	-0.070900
H	1.353211	4.335495	-0.091309
H	1.605266	2.814031	0.193110
O	3.260790	-0.964596	-0.809911
H	2.522891	-1.029389	-1.441696
H	4.077953	-0.897624	-1.311690

29.5, 0.7; 39.6, 0.3; 43.1, 0.1; 61.0, 1.7; 73.7, 1.9; 88.5, 1.9; 102.4, 1.0; 115.0, 1.1; 118.5, 0.8; 132.4, 6.2; 152.0, 7.6; 164.8, 1.3; 170.9, 1.9; 181.3, 5.7; 182.6, 3.0; 196.7, 1.5; 202.1, 2.1; 216.1, 20.5; 230.4, 3.7; 241.3, 19.7; 245.4, 1.1; 251.4, 6.1; 261.2, 22.5; 266.2, 9.9; 276.3, 110.3; 284.3, 3.9; 299.7, 8.2; 313.0, 33.6; 325.1, 107.5; 338.6, 2.1; 362.6, 35.3; 379.7, 42.7; 386.8, 112.4; 412.3, 227.5; 424.2, 14.0; 439.1, 194.3; 451.8, 44.7; 468.4, 69.2; 491.7, 2.1; 501.6, 263.0; 507.5, 29.2; 540.2, 80.1; 558.2, 87.2; 564.4, 33.9; 594.2, 276.1; 635.1, 136.7; 636.2, 252.4; 730.8, 171.8; 757.0, 35.9; 782.5, 284.6; 829.0, 177.9; 878.3, 70.9; 1337.6, 481.8; 1571.9, 110.6; 1578.3, 116.7; 1586.1, 78.0; 1608.3, 131.0; 1621.9, 69.3; 1624.4, 49.3; 1643.6, 50.9; 1657.1, 120.1; 2400.3, 251.3; 3621.6, 335.7; 3647.6, 236.6; 3656.5, 235.0; 3666.8, 398.3; 3671.0, 66.9; 3716.7, 437.3; 3720.5, 787.5; 3724.4, 445.7; 3838.0, 222.4; 3926.9, 187.9; 3933.7, 197.2; 3936.4, 219.9; 3938.9, 133.5; 3940.0, 71.5; 3945.9, 230.8; 3949.2, 121.7;

-2178.602355980 -2178.385023 -2178.358900 -2178.439042

$^{3}TS_{N1-2}$

Co	0.524448	-0.201668	-0.232609
O	-0.057159	-2.309602	0.102342
H	0.167324	-2.978665	-0.550101
O	2.183858	-0.813566	-1.468166
H	2.143188	-0.787649	-2.427419
O	1.282925	1.831396	-0.034148
H	0.900758	2.583354	-0.493014
O	-0.685413	0.220868	1.571521
H	-1.415197	-0.413465	1.664840
H	-1.011976	-2.380229	0.277948
H	-1.117202	1.092243	1.466516
H	2.984919	-0.327550	-1.197848
H	2.250107	1.883194	-0.114008
O	-2.156326	2.409551	0.764100
H	-2.405677	3.228362	1.200284
H	-2.934709	2.114719	0.274632
O	1.932553	-0.594498	1.529498
H	1.310778	-0.203328	2.162664
H	1.901389	-1.545078	1.687579
O	-2.695764	-1.678878	0.906220
H	-3.248591	-1.150133	0.308556
H	-3.300067	-2.229071	1.413837
N	-2.113852	0.300574	-1.447629
N	-0.981187	0.168793	-1.338316
O	-3.260295	0.396958	-1.057107
O	3.829604	0.780884	0.067445
H	3.533099	0.317799	0.868664
H	4.755180	1.010055	0.185288

-259.7, 586.5; 55.0, 0.3; 58.4, 0.4; 69.1, 0.6; 71.0, 0.6; 98.5, 3.7; 108.4, 1.4; 116.7, 3.7; 120.9, 3.7; 123.4, 8.6; 30.9, 0.8; 133.9, 6.1; 148.4, 7.6; 168.1, 3.2; 173.4, 3.7; 179.2, 3.3; 194.0, 0.2; 218.7, 3.4; 222.9, 5.0; 241.2, 73.0; 249.9, 4.0; 254.1, 23.9; 263.8, 3.8; 278.9, 109.9; 284.2, 46.8; 300.5, 1.6; 305.8, 14.3; 312.1, 167.2; 328.1, 37.2; 331.4, 40.3; 344.0, 27.0; 348.7, 23.7; 354.8, 32.5; 365.5, 39.5; 377.1, 97.8; 401.2, 178.6; 409.7, 23.1; 418.1, 153.5; 424.6, 98.6; 442.7, 54.7; 480.0, 32.7; 517.5, 72.0; 554.3, 171.0; 577.7, 113.2; 601.3, 445.9; 624.6, 104.5; 643.8, 194.6; 717.6, 103.4; 742.0, 190.8; 761.3, 70.5; 771.2, 86.5; 837.5, 249.3; 1217.3, 730.8; 1580.6, 137.4; 1598.7, 108.6; 1607.1, 168.7; 1610.2, 33.8; 1629.7, 122.1; 1631.7, 62.8; 1640.5, 162.5; 1679.6, 19.8; 2165.4, 115.6; 3614.0, 378.5; 3651.1, 335.6; 3682.8, 148.3; 3699.0, 190.1; 3720.6, 104.0; 3740.8, 687.3; 3765.1, 253.8; 3768.5, 163.5; 3816.4, 45.2; 3900.1, 164.8; 3923.9, 235.8; 3929.7, 132.5; 3936.2, 149.9; 3942.3, 252.2; 3945.8, 106.6; 3954.1, 181.7;

-2178.593110900 -2178.377580 -2178.351806 -2178.429558

$^{3}N2$

Co	-0.496882	0.508821	0.115313
O	0.241065	2.182915	-0.994596
H	-0.175825	2.325354	-1.850099
O	-2.338212	0.637508	-0.942532
H	-3.016314	1.178934	-0.526368
O	-1.206732	-1.091829	1.358319
H	-0.447337	-1.635866	1.636013
O	1.157317	0.691824	1.327951
H	1.940806	1.054832	0.873448
H	1.201355	2.087600	-1.147788
H	1.429494	-0.144208	1.752736
H	-2.716601	-0.247401	-1.106998
H	-1.776483	-1.668588	0.821615
O	1.447767	-1.985598	1.801609
H	1.835672	-2.589210	2.441698
H	1.950198	-2.080975	0.970470
O	-2.443824	-2.084610	-1.009138
H	-1.606914	-2.097971	-1.500266
H	-2.987138	-2.804345	-1.343206
O	2.866341	1.360115	-0.718587
H	2.970161	0.409483	-0.919975
H	3.710672	1.786333	-0.891429
N	1.208672	-1.398513	-1.340137
N	0.157939	-0.869082	-1.220648
O	2.328030	-1.352646	-0.770845
O	-1.512974	1.916131	1.420645
H	-1.088980	2.776982	1.507174
H	-1.683446	1.593549	2.312429

64.5, 1.2; 80.4, 6.0; 87.5, 0.3; 92.7, 0.7; 103.2, 3.9; 113.0, 0.1; 125.3, 0.6; 132.7, 1.7; 139.7, 8.0; 143.5, 3.5; 150.2, 3.2; 156.7, 28.6; 180.4, 4.5; 181.8, 6.9; 191.8, 5.3; 212.5, 7.4; 223.6, 7.8; 229.9, 4.4; 238.5, 0.5; 250.9, 1.4; 261.3, 2.9; 266.6, 6.1; 287.2, 6.9; 321.9, 32.8; 328.8, 18.9; 335.9, 70.8; 338.4, 8.6; 352.7, 48.7; 353.7, 67.3; 374.0, 9.8; 384.8, 58.5; 398.9, 33.3; 405.5, 137.8; 419.8, 119.3; 430.7, 163.7; 436.2, 93.7; 446.1, 81.9; 480.7, 207.3; 516.8, 48.0; 534.7, 27.7; 575.0, 56.4; 615.4, 15.4; 649.3, 125.5; 667.8, 466.2; 693.1, 33.2; 719.4, 74.3; 735.5, 421.5; 775.0, 189.5; 798.0, 88.4; 810.4, 37.2; 858.9, 315.8; 884.0, 5.9; 1179.4, 306.3; 1577.6, 134.2; 1593.8, 120.8; 1603.7, 227.0; 1604.7, 131.3; 1623.2, 108.8; 1625.4, 49.2; 1649.1, 24.4; 1685.2, 5.0; 1831.2, 251.2; 3594.1, 181.8; 3596.9, 16.5; 3619.7, 135.3; 3630.1, 280.1; 3641.0, 137.3; 3678.5, 377.1; 3695.6,1011.5; 3734.4, 318.2; 3765.9, 557.1; 3835.9, 91.3; 3911.8, 204.9; 3912.8, 166.0; 3925.7, 229.0; 3927.0, 182.7; 3932.6, 182.8; 3944.7, 172.7;

-2178.600774630 -2178.382354 -2178.357810 -2178.432176

$^{5}N2$

Co	0.532502	-0.510443	0.113355
O	-0.129788	-2.211279	-1.020254
H	0.297731	-2.331494	-1.874057
O	2.366679	-0.504903	-0.951250
H	3.093096	-1.012447	-0.576539
O	1.160047	1.104951	1.390752
H	0.370890	1.602854	1.674293
O	-1.124966	-0.795377	1.328233
H	-1.887793	-1.167111	0.844594
H	-1.090400	-2.125408	-1.184440
H	-1.431664	0.026771	1.758451
H	2.681077	0.407774	-1.109422
H	1.695704	1.720712	0.861301
O	-1.538695	1.857928	1.841750
H	-1.954316	2.421435	2.500790

H	-2.045706	1.958896	1.012963
O	2.308318	2.199980	-0.975129
H	1.454186	2.159540	-1.440098
H	2.792831	2.957434	-1.315705
O	-2.763813	-1.440643	-0.774035
H	-2.883598	-0.483654	-0.945805
H	-3.596982	-1.876350	-0.975370
N	-1.265629	1.463126	-1.292683
N	-0.214078	0.921714	-1.228684
O	-2.396300	1.296351	-0.752603
O	1.568029	-1.866496	1.369561
H	1.168743	-2.741756	1.433338
H	1.720535	-1.553206	2.268486

66.0, 0.6; 84.5, 3.4; 87.0, 1.7; 93.3, 1.8; 102.9, 1.3; 104.6, 5.7; 125.3, 0.2; 135.8, 2.9; 140.1, 0.2; 147.9, 1.4; 151.6, 1.9; 164.9, 35.2; 180.1, 0.5; 187.4, 10.8; 191.5, 6.6; 215.2, 6.9; 225.4, 8.0; 231.5, 12.4; 237.9, 29.0; 241.4, 11.0; 263.8, 7.0; 269.9, 4.7; 275.4, 3.6; 293.0, 14.7; 320.3, 35.8; 331.5, 10.3; 343.5, 41.4; 348.6, 57.2; 366.6, 63.1; 372.6, 25.8; 383.8, 42.9; 394.4, 41.8; 406.2, 55.4; 428.1, 220.9; 439.0, 130.5; 455.4, 89.6; 470.2, 120.7; 484.7, 189.0; 536.1, 79.7; 571.7, 5.5; 583.6, 94.1; 627.0, 16.7; 676.3, 94.4; 692.7, 475.5; 717.4, 19.2; 735.1, 54.2; 753.3, 483.7; 786.5, 150.7; 815.5, 107.8; 823.4, 28.2; 875.4, 354.8; 893.3, 21.6; 1159.9, 223.5; 1576.4, 112.9; 1598.5, 117.1; 1608.2, 182.0; 1608.8, 198.9; 1625.6, 133.3; 1628.4, 21.2; 1653.0, 26.2; 1690.2, 5.9; 1834.6, 370.9; 3554.9, 192.7; 3585.7, 56.7; 3597.3, 216.3; 3605.5, 412.2; 3628.1, 143.9; 3663.9, 574.5; 3680.3, 560.2; 3701.0, 634.3; 3747.6, 701.7; 3829.0, 92.7; 3910.5, 182.6; 3913.8, 177.7; 3923.9, 226.8; 3925.3, 177.7; 3930.3, 169.3; 3936.0, 185.5;

-2178.586089730 -2178.367464 -2178.343063 -2178.417649

$^{3}TS_{N2-3}$

Co	0.435027	-0.599158	0.123538
O	-0.520330	-2.158851	-0.953599
H	-0.189194	-2.397816	-1.824318
O	2.196882	-0.766884	-1.030644
H	2.830152	-1.447992	-0.783486
O	1.251585	0.989360	1.264932
H	0.521303	1.599961	1.512877
O	-1.189740	-0.576017	1.338288
H	-2.015946	-0.854259	0.888049
H	-1.474774	-1.930188	-1.051135
H	-1.364840	0.307772	1.728127
H	2.680911	0.076460	-1.119082
H	1.908301	1.507637	0.773194
O	-1.199526	2.102136	1.652811
H	-1.548729	2.782388	2.233659
H	-1.755155	2.091870	0.811917
O	3.035441	1.879699	-0.808849
H	2.645948	2.474574	-1.459603
H	3.933346	2.200509	-0.670901
O	-2.948974	-1.033104	-0.657124
H	-2.932679	-0.029890	-0.756607
H	-3.844309	-1.335857	-0.827221
N	-1.100735	1.487292	-1.516296
N	-0.214136	0.827425	-1.305255
O	-2.512568	1.536871	-0.532538
O	1.345154	-2.036492	1.378072
H	0.832045	-2.845765	1.488252
H	1.568583	-1.718917	2.260807

-555.6, 215.9; 67.9, 0.1; 75.9, 1.6; 85.0, 4.2; 101.9, 1.0; 106.2, 8.8; 112.0, 1.2; 126.2, 7.4; 135.6, 0.9; 141.7, 1.9; 150.0, 2.1; 153.7, 0.1; 156.9, 3.2; 173.4, 0.7; 205.7, 7.8; 209.7, 6.9; 226.7, 7.0; 236.1, 4.5; 255.2, 1.9; 277.2, 6.7; 279.7, 10.7; 289.2, 6.8; 299.4, 21.2; 308.1, 6.6; 311.1, 15.1; 315.9, 18.6; 333.3, 9.3; 350.1, 61.8; 354.0, 38.7; 361.1, 75.6; 393.2, 78.9; 403.7, 19.9; 408.9, 3.8; 415.6, 86.7; 419.3, 46.6; 429.4, 49.9; 461.3, 162.5; 480.9, 256.3; 550.9, 136.1; 572.3, 6.5; 583.1, 63.4; 587.1, 6.1; 601.4, 148.6; 642.3, 156.3; 686.0, 22.3; 710.8, 274.7; 787.6, 33.4; 834.2, 284.3; 864.1, 408.4; 947.4, 259.2; 964.2, 137.6; 992.5, 65.7; 1007.5, 5.6; 1610.8, 83.3; 1613.8, 159.0; 1623.1, 139.2; 1630.5, 221.6; 1636.5, 12.7; 1643.8, 52.8; 1663.7, 9.2; 1704.9, 8.3; 2104.6, 232.4; 2981.0,1221.2; 3079.7, 674.2; 3455.5, 278.1; 3492.4, 79.6; 3555.4, 859.2; 3587.3,1061.6; 3634.9, 487.5; 3756.6, 597.0; 3825.0, 96.6; 3842.5, 28.1; 3912.9, 171.1; 3915.4, 172.3; 3929.7, 181.6; 3935.6, 169.2; 3936.7, 119.8; 3941.4, 169.6;

-2178.569083440 -2178.352758 -2178.329021 -2178.401818

$^{5}TS_{N2-3}$

Co	0.526352	-0.664626	0.083704
O	-0.378722	-1.834413	-1.320282
H	-0.023398	-1.928138	-2.208481
O	2.358299	-0.585772	-1.011893
H	3.022404	-1.261093	-1.168695
O	1.142724	0.868580	1.287721
H	0.368972	1.382610	1.626915
O	-1.222234	-0.901292	1.284774
H	-2.008341	-1.093892	0.733762
H	-1.352353	-1.654158	-1.379190
H	-1.430582	-0.066390	1.752831
H	2.784263	0.290309	-1.040941
H	1.768755	1.485179	0.872700
O	-1.311003	1.758256	1.876477
H	-1.679356	2.356831	2.530712
H	-1.847812	1.850248	1.025088
O	2.888856	2.106769	-0.584732
H	2.418135	2.676093	-1.204284
H	3.721699	2.553642	-0.398806
O	-2.853423	-0.987381	-0.899440
H	-2.869039	0.020904	-0.831641
H	-3.723247	-1.284985	-1.176849
N	-1.151882	1.701817	-1.309465
N	-0.245663	1.041598	-1.175537
O	-2.522569	1.547404	-0.416790
O	1.146432	-2.205426	1.320106
H	0.442086	-2.411735	1.948688
H	1.992268	-2.308243	1.765667

-646.2, 195.2; 58.3, 1.7; 72.2, 2.0; 82.9, 1.9; 91.1, 16.4; 96.2, 5.8; 106.9, 5.3; 112.9, 8.6; 123.8, 1.2; 126.2, 8.2; 133.0, 4.6; 143.6, 6.8; 158.7, 11.8; 166.1, 11.3; 180.7, 34.4; 189.7, 0.2; 207.1, 7.5; 218.0, 11.6; 239.9, 68.1; 247.6, 19.2; 257.8, 4.3; 276.5, 2.2; 280.1, 35.8; 290.7, 11.0; 310.9, 15.5; 318.5, 20.3; 331.4, 7.7; 344.3, 72.8; 347.9, 45.5; 352.1, 35.9; 366.4, 81.3; 382.1, 29.6; 385.7, 22.0; 391.8, 47.4; 405.6, 46.0; 413.9, 230.6; 418.7, 58.0; 469.8, 135.9; 554.6, 38.8; 567.7, 50.7; 593.6, 26.6; 600.7, 63.5; 604.3, 42.7; 662.9, 210.2; 678.7, 200.3; 697.3, 70.5; 790.1, 83.4; 852.3, 320.3; 855.6, 326.4; 940.6, 185.3; 983.8, 232.9; 1019.3, 14.4; 1032.6, 51.0; 1600.6, 154.7; 1609.2, 143.5; 1615.1, 176.7; 1621.1, 47.3; 1634.1, 72.5; 1645.2, 71.4; 1663.5, 10.0; 1706.0, 15.6; 2072.2, 187.3; 2923.9,1265.8; 3030.2, 846.7; 3361.2, 515.1; 3411.6, 557.7; 3577.2, 515.2; 3616.6, 922.6; 3657.4, 376.0; 3732.0, 717.6; 3814.7, 95.1; 3841.0, 27.3; 3922.0, 164.9; 3936.0, 174.4; 3937.0, 128.2; 3941.4, 145.0; 3943.0, 151.3; 3946.1, 265.4;

-2178.564225220 -2178.349413 -2178.325021 -2178.400237

$^{3}N3$

Co	0.658281	-0.055070	-0.086113
O	1.802526	-1.196012	-1.580755
H	1.313303	-1.526894	-2.339491
O	1.369726	1.577419	-1.129279
H	2.199382	1.464841	-1.603106
O	-0.284487	1.303247	1.275392
H	-1.172132	0.992700	1.548271
O	-0.289215	-1.592967	0.405556
H	0.989587	-2.694819	0.613775
H	2.078357	-1.989525	-1.078341
H	-1.010381	-1.476541	1.032081
H	1.313135	2.477300	-0.761000
H	-0.309841	2.252301	1.091948
O	-2.569418	-0.053010	1.838836
H	-2.980124	-0.152121	2.701176
H	-3.226077	-0.342887	1.184267
O	0.605703	3.854257	0.271826
H	0.098676	4.533555	-0.184871
H	1.174477	4.327061	0.888520

O	1.966068	-2.878538	0.548669
H	2.139627	-3.790766	0.788536
N	-2.423810	0.171557	-1.862055
N	-1.359731	0.240795	-1.615613
O	-4.112597	-1.163866	-0.284865
O	2.304606	-0.269822	1.193759
H	2.486580	-1.233150	1.219697
H	2.138429	0.013362	2.098052
H	-4.865096	-0.899641	-0.843901

29.2, 2.3; 33.9, 2.2; 41.5, 3.2; 50.1, 1.4; 64.6, 1.5; 76.4, 1.2; 82.8, 1.0; 88.1, 2.0; 98.2, 3.4; 101.8, 4.1; 115.3, 2.7; 119.6, 1.8; 121.0, 2.0; 137.8, 3.5; 141.6, 0.6; 160.8, 11.1; 185.7, 0.4; 188.8, 14.1; 205.3, 18.6; 215.4, 8.2; 234.0, 8.2; 246.1, 9.4; 252.2, 17.5; 261.4, 83.4; 270.8, 133.1; 276.7, 10.9; 278.2, 18.4; 283.2, 34.6; 293.1, 29.6; 297.2, 58.1; 316.0, 29.0; 322.9, 18.4; 329.5, 33.2; 361.6, 21.3; 382.8, 151.1; 398.6, 56.4; 406.6, 41.4; 424.6, 59.9; 447.4, 195.9; 523.6, 54.2; 536.4, 28.5; 552.6, 92.6; 574.0, 50.0; 593.6, 134.6; 601.8, 303.3; 609.9, 277.3; 679.9, 47.2; 694.9, 197.7; 729.1, 356.0; 762.9, 87.0; 821.5, 152.3; 873.4, 101.3; 885.2, 251.9; 981.7, 27.4; 1586.4, 139.0; 1597.3, 181.3; 1601.0, 88.3; 1623.0, 99.6; 1630.8, 57.0; 1643.4, 32.4; 1662.2, 23.6; 2452.8, 2.1; 3273.4, 704.8; 3559.9, 231.4; 3575.7, 640.7; 3623.2, 886.2; 3665.9, 419.3; 3728.7, 398.5; 3755.3, 26.6; 3812.2, 566.0; 3852.4, 12.2; 3891.0, 153.4; 3913.9, 165.7; 3919.6, 224.2; 3921.2, 113.7; 3946.6, 161.3; 3951.0, 173.9; 3954.5, 142.5;

-2178.605903320 -2178.394256 -2178.366619 -2178.451429

^{5}N3

Co	0.232575	-0.402704	0.039169
O	-0.883312	-1.944306	-0.846817
H	-0.812387	-2.025152	-1.803146
O	1.275543	-0.128495	-1.732677
H	2.212584	-0.342473	-1.567505
O	1.459191	0.946108	0.802540
H	1.148247	1.498957	1.527911
O	-1.098583	-0.286079	1.680675
H	-0.724155	-0.642809	2.494452
H	-1.839120	-1.953421	-0.604471
H	-1.201292	0.690301	1.804294
O	1.428470	-1.952249	0.861584
H	2.366581	-1.738920	0.686962
H	1.262959	-2.846806	0.548451
N	-2.397657	1.393427	-1.667221
O	0.773365	2.429377	-0.714439
N	-1.583326	0.933961	-1.099589
O	-0.943596	2.394430	1.501781
H	-0.465126	2.646508	0.684399
H	-1.407969	3.169219	1.826537
H	1.582094	2.937097	-0.557854
H	1.237497	0.850170	-1.775297
O	-3.287876	-1.530311	0.195591
H	-4.145959	-1.954995	0.269830
H	-3.064223	-1.164534	1.058855
O	3.511303	-0.480297	-0.081037
H	3.095761	0.265275	0.402438
H	4.465804	-0.392543	-0.023359

47.6, 0.1; 54.6, 0.7; 60.1, 2.5; 63.8, 0.8; 70.0, 2.8; 83.6, 0.3; 88.9, 2.0; 109.0, 5.5; 115.7, 3.0; 123.6, 1.9; 132.8, 5.6; 151.0, 3.5; 164.0, 2.9; 164.3, 0.3; 169.7, 7.7; 179.1, 0.9; 196.1, 3.5; 212.3, 9.2; 232.1, 0.7; 240.7, 48.8; 249.1, 77.4; 255.7, 2.7; 276.7, 54.2; 298.7, 61.4; 303.1, 18.9; 307.6, 46.0; 315.2, 21.6; 321.3, 40.6; 342.8, 6.6; 349.2, 103.3; 357.1, 34.4; 374.0, 23.1; 405.2, 126.4; 411.1, 18.9; 432.3, 135.0; 447.5, 6.0; 455.5, 10.5; 470.6, 63.1; 502.1, 101.7; 523.0, 106.1; 537.0, 54.3; 548.8, 181.5; 586.2, 27.6; 608.3, 178.1; 625.2, 267.7; 641.0, 128.5; 737.7, 277.2; 750.8, 250.6; 791.6, 28.4; 811.9, 117.8; 839.0, 118.0; 856.0, 207.7; 865.8, 80.7; 970.7, 123.4; 1584.6, 130.9; 1587.4, 108.7; 1620.4, 128.9; 1626.0, 37.3; 1627.1, 71.9; 1636.0, 109.9; 1672.8, 55.7; 2461.5, 3.0; 3413.3, 411.8; 3461.8, 906.2; 3536.3, 445.9; 3560.1, 507.9; 3576.9, 135.9; 3615.3, 297.1; 3693.5, 661.3; 3834.7, 141.6; 3838.8, 61.7; 3875.7, 138.1; 3881.0, 146.2; 3908.4, 154.3; 3914.1, 167.5; 3941.8, 247.4; 3944.4, 119.1; 3969.7, 221.3;

-2178.616166950 -2178.402000 -2178.376065 -2178.455601

^{2}N4

Co	0.450878	-0.124916	-0.014936
O	0.013244	-2.242427	0.040937
H	0.429815	-2.944436	-0.464362
O	1.067162	1.938357	0.041456
H	0.251463	2.479472	0.012163
O	-1.000859	0.119885	1.467126
H	-1.746074	-0.472931	1.252872
H	-0.955490	-2.339839	-0.067323
H	-1.361415	1.018344	1.348825
H	1.555187	2.206794	0.826415
O	-1.579489	2.430041	0.016324
H	-2.249401	3.090099	-0.175318
H	-1.565410	1.757413	-0.704935
O	1.719308	-0.414535	1.498612
H	1.228333	-0.711889	2.275964
H	2.437505	-1.040210	1.352181
O	-2.535939	-1.469696	-0.184257
H	-2.186164	-0.836149	-0.855135
H	-3.429120	-1.730783	-0.418344
O	-0.863274	0.245839	-1.306154
H	-0.535875	0.251624	-2.208110
O	2.104074	-0.260298	-1.334848
H	2.393162	0.638315	-1.537306
H	2.165962	-0.770418	-2.147875

23.4, 4.5; 82.0, 0.9; 93.1, 3.1; 105.5, 9.5; 120.1, 8.9; 139.7, 3.9; 154.2, 6.0; 160.2, 6.4; 185.8, 4.2; 194.8, 10.4; 198.4, 8.0; 209.6, 57.5; 225.4, 17.8; 251.8, 13.5; 266.1, 34.5; 277.2, 4.5; 289.6, 13.8; 294.1, 44.7; 306.3, 10.5; 311.6, 4.2; 321.8, 49.2; 349.3, 44.7; 364.5, 7.6; 375.1, 9.1; 388.5, 48.8; 391.7, 61.9; 418.4, 50.7; 464.5, 26.4; 468.4, 228.9; 514.8, 24.7; 520.7, 90.8; 532.6, 229.1; 544.8, 157.8; 564.4, 73.6; 576.8, 145.8; 591.8, 97.4; 681.5, 18.8; 718.7, 366.1; 759.9, 540.3; 854.8, 122.4; 869.8, 73.3; 883.7, 128.1; 898.6, 85.2; 972.4, 3.7; 1570.9, 19.9; 1593.6, 218.9; 1603.5, 51.3; 1607.1, 156.5; 1630.8, 117.5; 1644.5, 80.4; 1686.2, 38.9; 3417.2, 484.7; 3455.5, 272.3; 3579.0, 291.1; 3593.2, 300.6; 3652.2, 746.5; 3703.1, 674.8; 3809.1, 101.3; 3823.5, 73.3; 3907.2, 155.6; 3920.3, 161.1; 3933.1, 43.7; 3937.8, 143.6; 3943.4, 226.1; 3945.4, 124.9; 3950.3, 163.7;

-1993.357182070 -1993.161661 -1993.141456 -1993.206739

^{4}N4

Co	-0.431862	0.125508	-0.072310
O	-0.098324	2.214668	0.085009
H	-0.554473	2.931134	-0.362363
O	-1.001045	-1.945750	0.068131
H	-0.170679	-2.467341	0.040002
O	1.028977	-0.122259	1.521503
H	1.751765	0.504847	1.343712
H	0.868930	2.363259	0.000467
H	1.426197	-0.999927	1.380108
H	-1.473198	-2.201119	0.867066
O	1.650815	-2.397012	0.000395
H	2.318696	-3.060036	-0.187978
H	1.654441	-1.718435	-0.716445
O	-1.791162	0.312299	1.570679
H	-1.334586	0.574774	2.378742
H	-2.619793	0.799331	1.527332
O	2.478805	1.585848	-0.137227
H	2.198174	0.924531	-0.814676
H	3.353205	1.915760	-0.355090
O	0.959833	-0.222699	-1.364440
H	0.728071	-0.230763	-2.295109
O	-2.189678	0.224452	-1.380024
H	-2.469513	-0.673446	-1.593019
H	-2.322722	0.752341	-2.172580

79.9, 0.4; 87.4, 1.9; 95.0, 6.8; 106.5, 2.4; 114.2, 1.4; 136.8, 4.1; 154.3, 1.0; 163.7, 0.5; 179.6, 2.9; 183.7, 1.7; 205.8, 4.9; 223.1, 45.7; 234.2, 33.0; 242.2, 1.0; 260.7, 35.3; 271.6, 14.7; 273.7, 18.9;

287.0, 36.1; 291.2, 8.7; 293.0, 10.7; 300.4, 41.5; 320.6, 32.8; 339.0, 15.8; 374.0, 87.8; 387.1, 38.3; 407.1, 164.0; 413.8, 64.4; 435.9, 168.6; 455.7, 150.7; 485.1, 69.3; 493.7, 105.6; 504.3, 11.6; 537.4, 108.6; 549.8, 51.2; 562.1, 160.1; 574.6, 96.1; 603.8, 63.8; 710.4, 430.8; 745.7, 478.3; 774.4, 83.9; 826.1, 228.1; 868.2, 67.4; 893.7, 114.4; 950.9, 15.3; 1580.0, 25.3; 1599.1, 238.8; 1600.1, 74.5; 1613.5, 112.3; 1630.0, 137.2; 1640.8, 71.2; 1680.3, 35.7; 3404.8, 514.9; 3442.9, 276.6; 3540.8, 471.9; 3570.5, 603.1; 3679.5, 387.9; 3740.5, 578.1; 3833.7, 95.5; 3838.4, 60.8; 3907.3, 156.3; 3939.0, 137.7; 3941.9, 59.4; 3945.4, 148.4; 3948.9, 210.8; 3949.8, 121.2; 3952.5, 193.5;

-1993.388877070 -1993.194373 -1993.173914 -1993.239369

^{3}O1

Co	0.062659	-0.155602	0.291327
O	-0.710718	-1.773967	-1.169479
H	-0.823986	-1.268854	-2.000938
O	-0.755152	-1.180087	2.069449
H	-1.658744	-1.448612	1.811519
O	0.953726	1.161017	-1.179049
H	0.663899	2.049836	-0.917009
O	0.511754	1.327920	2.075887
H	-0.001195	0.752422	2.661507
O	-2.959256	-1.597188	0.520616
H	-2.382310	-1.898708	-0.204328
H	-3.754409	-2.136035	0.508233
H	1.409031	1.334595	2.424189
H	0.532814	1.002259	-2.038401
H	-0.328761	-1.960093	2.435803
H	-0.179689	-2.547564	-1.378133
O	-1.924318	0.844671	-0.276378
H	-2.672545	0.413427	0.161576
H	-1.846340	1.771653	0.011661
N	3.062917	-0.788498	-0.178301
N	3.856755	-0.608384	-0.945693
O	2.220888	-0.982364	0.633201
O	-1.151035	0.295298	-2.860226
H	-1.578350	0.472777	-3.701966
H	-1.708427	0.662656	-2.149257
O	-0.557523	3.138477	0.295925
H	-0.170806	2.818150	1.128836
H	-0.656617	4.091297	0.369255

20.5, 0.2; 45.2, 0.3; 47.0, 0.9; 66.7, 1.3; 76.2, 1.3; 83.4, 4.7; 88.2, 3.4; 100.1, 1.3; 105.0, 5.3; 117.2, 1.2; 122.6, 0.5; 139.5, 1.5; 150.4, 0.4; 157.5, 0.3; 167.1, 6.8; 183.3, 0.8; 195.5, 4.4; 198.0, 8.0; 218.1, 15.3; 236.7, 15.5; 240.3, 5.0; 252.9, 6.5; 269.5, 11.7; 280.7, 8.2; 285.4, 3.7; 310.3, 27.2; 331.6, 10.5; 355.1, 5.9; 367.4, 88.0; 379.5, 73.2; 386.8, 22.1; 397.0, 73.0; 406.8, 51.0; 417.3, 144.0; 430.6, 37.9; 442.0, 105.2; 460.6, 14.5; 473.0, 260.6; 510.6, 114.7; 534.3, 110.9; 546.4, 268.5; 589.9, 8.4; 611.4, 2.2; 635.5, 357.2; 645.3, 382.5; 678.0, 58.8; 722.3, 151.3; 739.3, 161.0; 766.5, 52.7; 815.1, 240.7; 844.5, 61.3; 885.1, 48.7; 1340.9, 90.5; 1540.9, 141.7; 1577.9, 91.1; 1586.4, 198.2; 1593.9, 15.7; 1626.0, 84.5; 1635.3, 49.4; 1639.3, 15.6; 1664.9, 61.5; 2411.0, 449.8; 3574.0, 359.0; 3619.0, 344.9; 3647.2, 411.7; 3681.1, 113.1; 3685.0, 354.4; 3700.0, 63.5; 3731.9, 498.0; 3784.9, 65.0; 3795.6, 394.1; 3820.8, 625.0; 3914.6, 96.4; 3921.8, 137.2; 3922.6, 232.8; 3939.9, 167.2; 3940.5, 184.8; 3942.0, 161.0;

-2178.593834650 -2178.375661 -2178.349758 -2178.430175

^{3}TS$_{01\text{-}2}$

Co	-0.300512	0.604679	0.339564
O	-1.282513	1.399781	2.148788
H	-0.770820	1.632105	2.928505
O	-1.734321	1.793168	-0.781878
H	-2.341841	1.211966	-1.269012
O	1.222302	1.817086	-0.413562
H	2.155737	1.736259	-0.154955
O	1.183145	-0.509294	1.458458
H	1.056858	-1.469633	1.473442
H	-1.851049	0.659984	2.397115
H	2.116272	-0.320046	1.269908
H	-2.273051	2.353770	-0.215445
H	1.079092	2.642454	-0.882707
O	3.563248	0.566707	0.332049
H	3.706415	0.068829	-0.485781
H	4.431069	0.781590	0.687285
O	-2.789935	-0.582643	-1.823383
H	-3.498630	-0.850114	-2.415290
H	-1.957162	-0.849852	-2.236583
O	-1.844276	-0.920102	0.825163
H	-2.416518	-1.009161	0.045495
H	-1.414928	-1.780299	0.958368
N	1.135451	-0.857771	-1.906839
N	2.271583	-0.784079	-1.919047
O	-0.007581	-0.761197	-1.496018
O	-0.034012	-3.091391	1.340296
H	0.170961	-3.727952	0.648269
H	-0.136250	-3.610200	2.145063

-481.2,1417.2; 38.5, 3.0; 55.9, 1.4; 60.9, 1.0; 73.2, 4.5; 83.7, 6.3; 84.8, 1.1; 94.9, 5.9; 103.9, 2.9; 105.0, 5.7; 110.2, 2.0; 117.4, 10.0; 126.8, 2.9; 146.7, 6.5; 153.6, 9.9; 160.1, 40.2; 175.8, 0.4; 180.6, 0.6; 191.6, 6.2; 221.5, 10.7; 223.9, 3.1; 231.2, 9.6; 238.5, 6.5; 241.6, 5.9; 249.7, 30.2; 255.4, 13.2; 273.2, 115.8; 290.1, 8.3; 303.1, 47.1; 309.4, 15.9; 318.8, 88.3; 329.3, 101.5; 348.2, 44.0; 363.8, 53.9; 368.0, 94.7; 397.5, 206.9; 410.6, 18.2; 421.6, 65.1; 433.2, 63.0; 459.4, 94.5; 479.7, 136.8; 510.3, 40.7; 556.0, 134.2; 578.1, 150.5; 602.3, 154.4; 635.3, 361.3; 651.8, 179.6; 683.8, 231.9; 696.7, 87.3; 728.2, 219.3; 761.8, 92.6; 782.2, 52.7; 1117.3, 515.9; 1573.1, 338.3; 1586.4, 56.5; 1589.5, 182.7; 1595.7, 127.5; 1613.5, 35.5; 1623.7, 74.6; 1627.2, 54.5; 1656.0, 7.3; 2186.0, 801.0; 3688.1, 8.6; 3694.1, 125.9; 3708.2, 125.6; 3711.9, 237.8; 3764.7, 273.7; 3779.8, 243.0; 3800.0, 365.2; 3810.4, 631.1; 3816.7, 79.6; 3855.3, 2.0; 3918.3, 160.0; 3931.6, 205.7; 3942.6, 163.9; 3943.6, 222.3; 3949.0, 165.3; 3956.1, 133.8;

-2178.577898930 -2178.364078 -2178.337195 -2178.418568

^{3}O2

Co	0.727843	-0.306537	0.106074
O	0.727807	0.823550	1.871304
H	-0.201106	1.052553	2.087968
O	-0.890351	-1.397984	0.988585
H	-1.454239	-0.857739	1.570377
O	0.586776	-1.608584	-1.507770
H	1.071750	-1.354330	-2.299594
O	2.588281	0.412965	-0.692302
H	2.608690	1.360724	-0.903639
H	1.250440	1.628936	1.937646
H	3.426221	0.165404	-0.289357
H	-1.477875	-1.808866	0.330171
H	-0.353966	-1.739396	-1.751658
O	-2.973339	0.680637	-0.503322
H	-2.075170	1.007966	-0.766950
H	-3.627154	1.250850	-0.917521
O	2.021293	-1.748140	1.098006
H	1.956544	-2.632537	0.719826
H	1.812016	-1.842508	2.034377
N	0.048187	2.320659	-1.122474
N	1.127067	2.740193	-1.027740
O	-0.405401	1.072682	-0.788315
O	-2.031280	0.825862	2.124048
H	-2.596082	1.057266	2.866467
H	-2.550151	0.964038	1.305342
O	-2.156601	-1.810159	-1.417945
H	-2.757111	-2.434105	-1.834823
H	-2.648820	-0.974346	-1.279431

32.2, 1.1; 55.5, 7.3; 80.5, 4.8; 86.5, 0.0; 92.3, 6.7; 109.0, 0.2; 111.3, 6.0; 117.8, 0.2; 133.1, 1.9; 143.9, 1.6; 148.2, 2.4; 150.2, 2.1; 159.0, 0.3; 181.2, 0.7; 192.8, 3.5; 207.2, 28.7; 219.2, 11.1; 225.7, 2.7; 233.2, 11.0; 242.4, 17.9; 260.6, 5.8; 271.9, 2.5; 289.5, 27.8; 294.7, 22.2; 320.7, 4.8; 330.1, 31.2; 335.5, 19.6; 345.9, 27.0; 352.6, 28.5; 369.7, 37.2; 378.9, 49.7; 389.1, 60.2; 418.2, 57.3; 425.3, 199.6; 465.7, 69.2; 478.8, 138.6; 483.8, 272.4; 510.9, 139.4; 534.9, 134.4; 555.2, 9.4; 571.1, 54.2; 588.7, 129.0; 612.2, 77.5; 614.8, 22.7; 639.8, 45.0; 698.1, 448.2;

728.1, 244.8; 748.2, 285.6; 782.2, 190.5; 812.8, 5.8; 848.5, 79.6; 873.6, 275.8; 965.0, 88.4; 1580.3, 164.7; 1601.6, 53.3; 1613.3, 56.4; 1616.1, 90.0; 1621.5, 120.0; 1635.9, 180.2; 1655.6, 21.3; 1688.8, 7.8; 1839.5, 137.1; 3335.6, 814.7; 3535.9, 75.3; 3563.8,1139.3; 3584.0, 202.3; 3614.0, 582.0; 3672.9, 311.0; 3716.4, 139.4; 3729.2, 972.4; 3832.2, 85.7; 3904.4, 138.6; 3906.6, 176.9; 3919.6, 248.2; 3921.2, 80.3; 3929.1, 232.3; 3932.1, 91.3; 3935.7, 166.2;

-2178.595209530 -2178.378552 -2178.353632 -2178.429878

^{5}O2

Co	0.728201	-0.277047	0.104206
O	0.732501	0.904345	1.850906
H	-0.198734	1.134943	2.055467
O	-0.892977	-1.351062	1.032795
H	-1.455812	-0.792628	1.597890
O	0.600731	-1.689031	-1.432319
H	1.100968	-1.500366	-2.232780
O	2.624131	0.350376	-0.699252
H	2.696249	1.286364	-0.941302
H	1.245845	1.718020	1.880488
H	3.449208	0.067909	-0.292182
H	-1.482021	-1.780964	0.387966
H	-0.338388	-1.820675	-1.680759
O	-2.987146	0.659257	-0.527585
H	-2.090862	0.980574	-0.805854
H	-3.645091	1.210578	-0.960233
O	1.987912	-1.682783	1.175939
H	1.835913	-2.590183	0.887270
H	1.808560	-1.671467	2.123253
N	0.051829	2.269601	-1.241571
N	1.144411	2.641698	-1.097038
O	-0.429507	1.035337	-0.829616
O	-2.033969	0.909198	2.093039
H	-2.600609	1.163815	2.826383
H	-2.554267	1.013372	1.270254
O	-2.152485	-1.860297	-1.358711
H	-2.754768	-2.501161	-1.746256
H	-2.644832	-1.019688	-1.254482

42.7, 1.7; 63.4, 4.5; 83.7, 6.2; 90.2, 0.5; 94.5, 3.9; 108.8, 0.3; 120.7, 0.2; 123.2, 4.2; 131.5, 0.7; 139.6, 2.7; 149.1, 3.0; 150.2, 2.4; 161.9, 1.9; 172.1, 3.1; 192.4, 5.1; 198.7, 23.4; 219.6, 14.5; 222.3, 3.4; 232.3, 9.6; 246.1, 18.3; 261.2, 5.6; 270.2, 4.4; 290.4, 22.8; 295.1, 18.0; 317.8, 5.5; 330.8, 23.3; 340.0, 35.7; 350.3, 24.6; 359.9, 26.4; 376.6, 28.6; 392.2, 35.1; 402.5, 71.1; 425.7, 26.4; 429.2, 279.1; 463.0, 103.6; 472.9, 84.4; 501.6, 172.4; 514.3, 219.4; 544.0, 134.8; 564.4, 123.3; 567.9, 63.2; 578.8, 56.5; 595.3, 16.3; 610.6, 71.9; 624.3, 47.3; 646.4, 210.9; 695.4, 475.3; 748.0, 313.4; 780.2, 148.3; 812.9, 7.4; 847.7, 90.7; 872.5, 301.1; 963.7, 87.6; 1579.1, 161.0; 1601.7, 35.9; 1613.1, 38.9; 1616.6, 132.1; 1623.4, 107.2; 1637.2, 199.2; 1657.3, 15.8; 1690.8, 7.1; 1809.1, 87.7; 3329.5, 826.4; 3539.4, 78.0; 3567.2,1122.2; 3587.1, 195.5; 3615.5, 567.5; 3675.4, 307.2; 3732.5, 954.5; 3748.3, 120.9; 3830.5, 82.1; 3905.9, 72.5; 3906.8, 245.9; 3921.0, 255.8; 3922.3, 73.6; 3929.5, 227.6; 3932.5, 91.4; 3933.2, 169.5;

-2178.592269720 -2178.375631 -2178.350778 -2178.426953

^{3}TS$_{O2-3}$

Co	0.701043	-0.319565	0.095568
O	0.706195	0.650224	1.964422
H	-0.222121	0.889518	2.174447
O	-0.936877	-1.456684	0.884999
H	-1.492016	-0.949745	1.503906
O	0.583632	-1.559984	-1.582079
H	1.080788	-1.257839	-2.349095
O	2.616335	0.405143	-0.602382
H	2.729762	1.343471	-0.808150
H	1.252399	1.424868	2.127431
H	3.431473	0.072628	-0.214245
H	-1.530156	-1.791068	0.188810
H	-0.357942	-1.635517	-1.846040
O	-2.940608	0.784389	-0.477769
H	-2.017840	1.089037	-0.701026
H	-3.560818	1.408204	-0.864825
O	1.965245	-1.847222	0.996880
H	1.845771	-2.703003	0.568944
H	1.750432	-1.982532	1.926982
N	0.146804	2.491849	-1.011086
N	1.231869	2.816038	-0.927795
O	-0.377621	1.074433	-0.732291
O	-2.050616	0.708006	2.159880
H	-2.630784	0.896754	2.902314
H	-2.545355	0.913807	1.339165
O	-2.175649	-1.657727	-1.557158
H	-2.789479	-2.233821	-2.020654
H	-2.643280	-0.816329	-1.372137

-578.2, 203.9; 38.4, 0.7; 65.8, 3.8; 85.7, 0.8; 87.5, 11.0; 89.1, 1.1; 106.8, 0.3; 112.8, 0.9; 118.1, 2.0; 126.5, 0.8; 136.1, 3.4; 144.7, 1.6; 149.9, 3.3; 160.3, 0.9; 163.6, 7.6; 191.1, 2.8; 194.2, 16.2; 202.4, 12.1; 220.9, 7.6; 232.9, 5.8; 245.4, 14.3; 256.8, 3.3; 272.4, 2.0; 289.3, 42.5; 295.7, 19.2; 314.8, 14.3; 322.9, 16.9; 339.1, 6.4; 342.6, 48.2; 348.8, 44.5; 363.0, 58.0; 377.3, 63.0; 397.3, 24.7; 415.9, 254.6; 425.6, 75.1; 442.7, 71.3; 467.9, 28.3; 492.6, 274.1; 511.7, 96.7; 538.7, 115.2; 553.0, 109.9; 557.9, 37.0; 568.1, 29.1; 583.4, 79.5; 608.8, 14.1; 621.9, 111.3; 702.3, 410.1; 758.7, 333.5; 781.5, 165.2; 820.1, 8.8; 848.6, 87.4; 872.9, 305.8; 989.1, 94.3; 1583.7, 167.3; 1601.7, 22.5; 1614.5, 48.9; 1617.2, 108.4; 1622.5, 126.4; 1637.5, 220.0; 1657.5, 7.4; 1691.7, 6.2; 1971.9, 117.1; 3235.2,1007.0; 3522.5, 118.3; 3552.8,1094.9; 3575.3, 275.7; 3599.9, 472.6; 3668.6, 345.5; 3725.7, 948.8; 3781.1, 78.3; 3830.5, 84.0; 3904.7, 156.9; 3916.0, 150.5; 3924.1, 136.9; 3930.1, 194.6; 3930.7, 219.1; 3933.6, 169.6; 3933.8, 85.1;

-2178.593117410 -2178.378249 -2178.353277 -2178.429537

^{5}TS$_{O2-3}$

Co	0.714443	-0.272136	0.094127
O	0.710549	0.706962	1.969240
H	-0.220636	0.942609	2.167836
O	-0.925924	-1.425283	0.909232
H	-1.488440	-0.914605	1.517838
O	0.611642	-1.578864	-1.549579
H	1.123843	-1.338502	-2.328074
O	2.654964	0.379865	-0.575753
H	2.790982	1.315908	-0.779423
H	1.247907	1.489513	2.124622
H	3.452409	0.027607	-0.168166
H	-1.513052	-1.781126	0.218938
H	-0.326753	-1.667070	-1.819116
O	-2.980416	0.742380	-0.489701
H	-2.073137	1.073572	-0.722017
H	-3.622561	1.340818	-0.881254
O	1.934238	-1.805187	1.048294
H	1.775206	-2.666761	0.645388
H	1.700752	-1.900923	1.978901
N	0.131507	2.390052	-1.161694
N	1.223855	2.695756	-0.999977
O	-0.421210	1.080798	-0.715540
O	-2.060222	0.746139	2.156742
H	-2.638574	0.937243	2.900057
H	-2.564801	0.929957	1.338069
O	-2.152084	-1.705171	-1.534757
H	-2.756079	-2.303452	-1.982836
H	-2.636837	-0.870879	-1.365909

-521.5, 200.0; 41.2, 0.6; 61.5, 5.2; 83.4, 2.3; 83.7, 0.9; 88.0, 9.5; 99.3, 0.7; 108.0, 0.1; 119.7, 1.2; 125.0, 1.5; 140.3, 3.9; 147.4, 2.1; 154.1, 5.5; 158.2, 2.7; 161.4, 3.2; 189.8, 4.6; 194.7, 22.1; 209.0, 11.2; 214.4, 3.7; 226.7, 7.6; 242.6, 14.8; 255.5, 8.5; 270.1, 3.5; 287.0, 24.4; 293.2, 16.7; 313.8, 19.5; 321.7, 17.8; 326.3, 14.0; 338.3, 9.5; 343.6, 58.0; 357.6, 53.9; 373.6, 97.9; 410.7, 16.9; 416.4, 56.7; 424.9, 280.3; 444.1, 39.2; 467.7, 31.4; 496.8, 48.4; 510.8, 314.0; 531.4, 110.3; 546.6, 115.0; 559.3, 88.7; 571.7, 31.7; 579.6, 59.7; 596.3, 15.3; 611.5, 113.6; 691.3, 419.7; 746.0, 265.8; 775.3, 209.7; 810.3, 4.7; 837.3, 90.8; 862.3, 315.0; 960.4, 93.9; 1576.9, 169.8; 1604.2, 20.6; 1612.5, 33.0; 1617.6, 121.0; 1622.0, 130.3; 1638.1, 217.6; 1660.1, 11.9; 1689.6, 9.7;

1897.6, 82.5; 3301.1, 878.2; 3537.9, 80.0; 3563.8,1075.2; 3586.6, 215.7; 3613.8, 563.0; 3673.7, 308.5; 3730.4, 953.1; 3778.1, 74.7; 3829.8, 81.1; 3909.0, 153.5; 3913.8, 160.0; 3923.5, 155.0; 3927.3, 175.7; 3930.7, 217.7; 3932.3, 174.2; 3933.7, 88.1;

-2178.591665160 -2178.377098 -2178.352008 -2178.429046

^{3}O3

Co	-0.931730	-0.390126	-0.069721
O	0.305638	-1.845492	-0.773969
H	1.193951	-1.685340	-0.385554
O	-0.319925	-0.905844	1.936933
H	0.642407	-1.060950	1.871474
O	-2.354000	0.905103	0.566607
H	-2.427041	1.586351	-0.133384
O	-1.653452	-0.258602	-2.114153
H	-1.720507	0.687470	-2.349830
H	0.389382	-1.734905	-1.729515
H	-2.485571	-0.683126	-2.346058
H	-0.391157	-0.091648	2.467123
H	-1.997479	1.388849	1.340983
O	-1.509093	2.382504	-1.591086
H	-1.437728	3.255231	-1.985743
H	-0.648463	2.137509	-1.181358
O	-2.328814	-1.857461	0.115156
H	-3.032537	-1.647573	0.741240
H	-1.960414	-2.715007	0.361235
O	0.224906	0.843584	-0.222610
O	2.178782	-0.721409	0.753650
H	3.132486	-0.643439	0.823882
H	1.811942	0.092368	0.342017
O	-0.448213	1.843857	2.233747
H	-0.153015	2.600279	2.746880
H	0.045854	1.811176	1.387453
N	6.282944	0.459536	-0.757244
N	5.349622	0.132780	-0.288836

19.3, 0.0; 21.3, 0.0; 72.3, 4.1; 82.9, 0.9; 87.4, 1.0; 94.2, 1.6; 102.4, 0.9; 116.6, 7.1; 127.5, 0.1; 138.9, 7.2; 152.8, 2.7; 162.8, 1.6; 176.2, 7.8; 185.9, 0.4; 198.1, 1.6; 206.2, 11.3; 213.8, 4.3; 214.5, 4.9; 240.3, 5.3; 245.3, 18.6; 273.2, 22.4; 281.3, 7.0; 294.6, 4.3; 307.0, 34.2; 319.2, 44.9; 335.7, 4.7; 348.4, 19.4; 366.7, 12.2; 379.2, 7.2; 380.8, 31.1; 395.8, 50.7; 416.7, 107.0; 437.9, 124.1; 444.8, 57.8; 463.4, 125.4; 510.6, 190.5; 516.5, 211.5; 529.8, 154.8; 542.0, 32.9; 565.3, 122.1; 595.0, 14.1; 663.0, 69.1; 665.3, 129.3; 700.2, 308.2; 731.7, 218.0; 746.1, 117.6; 760.8, 588.6; 804.7, 31.9; 812.9, 40.9; 885.2, 107.7; 936.5, 5.0; 975.9, 139.8; 1013.4, 100.4; 1550.0, 29.2; 1562.2, 33.7; 1584.7, 410.5; 1605.9, 99.9; 1621.1, 122.2; 1630.3, 55.4; 1672.0, 27.4; 1699.0, 52.0; 2463.8, 4.2; 3428.1, 160.4; 3480.4, 351.1; 3513.1, 541.7; 3524.5, 84.2; 3581.0, 317.3; 3617.1, 274.5; 3657.3,1008.8; 3662.3, 456.3; 3729.3, 590.3; 3813.3, 126.9; 3854.6, 602.9; 3866.6, 145.0; 3914.7, 179.0; 3919.6, 181.8; 3938.5, 164.4; 3941.7, 201.1;

-2178.631521620 -2178.414027 -2178.389525 -2178.466984

^{5}O3

Co	0.085794	-0.635632	0.026948
O	-0.015209	-0.717767	2.189157
H	-0.588154	0.041966	2.420784
O	-2.040682	-0.666750	0.164572
H	-2.339187	-0.112818	0.909856
O	-0.257253	-1.115020	-2.034955
H	0.544823	-1.081043	-2.565927
O	2.104459	-1.340408	-0.208961
H	2.812473	-0.685103	-0.132458
H	0.808308	-0.597785	2.670927
H	2.419124	-2.193519	0.103333
H	-2.426480	-0.268089	-0.638333
H	-0.856317	-0.417001	-2.367389
O	-1.459834	2.692460	-0.201853
H	-0.559094	2.271825	-0.208329
H	-1.343967	3.641243	-0.301660
O	-0.156348	-2.805481	0.275910
H	-0.641733	-3.183684	-0.466308
H	-0.672313	-2.998069	1.067124
N	4.022937	2.214209	-0.126615
N	3.747281	1.156476	-0.097357
O	0.485456	0.993870	-0.122384
O	-1.980361	1.245198	2.129333
H	-2.554643	1.599476	2.813441
H	-1.849467	1.950510	1.461071
O	-2.243927	0.827250	-2.128476
H	-2.904765	1.043074	-2.791863
H	-2.046962	1.649475	-1.632816

15.2, 0.0; 39.0, 0.6; 63.1, 2.7; 67.2, 2.0; 80.5, 1.3; 89.2, 0.6; 95.7, 1.2; 111.8, 10.3; 116.1, 0.6; 134.3, 1.4; 136.3, 1.5; 150.5, 1.1; 160.1, 0.3; 165.0, 6.2; 177.1, 4.9; 183.7, 13.4; 192.4, 11.9; 198.7, 18.3; 204.8, 14.8; 214.3, 2.2; 227.8, 1.5; 241.0, 1.5; 256.3, 5.9; 279.3, 13.2; 295.6, 7.0; 304.1, 25.8; 310.2, 41.2; 324.9, 32.2; 334.6, 16.8; 345.9, 34.8; 351.4, 47.8; 368.8, 62.7; 381.8, 87.1; 411.2, 211.9; 418.3, 78.5; 451.9, 46.9; 459.0, 73.2; 503.5, 266.4; 520.2, 188.1; 532.1, 150.1; 563.5, 29.3; 573.8, 22.4; 588.0, 38.5; 604.2, 135.6; 606.6, 44.9; 707.4, 326.5; 747.1, 184.8; 787.4, 329.7; 811.1, 44.6; 821.4, 22.3; 860.3, 54.9; 879.7, 256.7; 945.5, 95.8; 1576.8, 81.0; 1580.2, 72.2; 605.1, 58.9; 1613.8, 122.3; 1622.4, 143.9; 1635.2, 213.1; 1654.5, 18.2; 1696.0, 2.7; 2466.9, 3.5; 3283.3, 751.7; 3535.3, 177.8; 3580.5, 846.0; 3594.5, 430.7; 3604.0, 41.7; 3655.9, 526.6; 3700.7, 978.6; 3779.3, 306.9; 3829.5, 76.8; 3910.6, 168.0; 3921.0, 175.5; 3925.5, 140.3; 3931.2, 214.0; 3934.2, 89.6; 3935.0, 160.4; 3939.7, 250.6;

-2178.664117170 -2178.447872 -2178.421841 -2178.502849

^{3}O4

Co	-0.052121	-0.400327	0.172323
O	1.130421	-1.767403	-0.729853
H	1.889593	-1.304530	-1.151634
O	1.677800	0.348842	1.215886
H	2.399841	0.336596	0.561188
O	-1.331816	0.771075	1.199247
H	-2.080807	0.948798	0.593728
O	-1.697289	-1.510385	-0.711544
H	-2.321703	-0.865982	-1.097731
H	0.627975	-2.195121	-1.434485
H	-2.201612	-2.124253	-0.168507
H	1.526098	1.296554	1.381745
H	-0.905141	1.645340	1.322324
O	-2.595323	0.985569	-1.230695
H	-3.176305	1.509656	-1.787534
H	-1.660589	1.151157	-1.487986
O	-0.220307	-1.741689	1.688866
H	-0.493760	-1.359929	2.531814
H	0.580472	-2.257855	1.844056
O	0.082315	0.733403	-1.087093
O	2.688224	0.255525	-1.398774
H	3.340332	0.562976	-2.032810
H	1.806622	0.645750	-1.607154
O	0.417736	2.764891	0.727662
H	0.522241	3.717529	0.662590
H	0.339929	2.383495	-0.171933

83.6, 3.4; 93.6, 0.2; 114.8, 6.6; 123.7, 0.4; 135.6, 9.3; 151.7, 3.4; 158.9, 2.5; 173.7, 7.9; 179.2, 0.8; 196.0, 1.5; 202.2, 9.5; 210.2, 3.9; 214.4, 4.8; 238.1, 1.7; 244.5, 14.7; 269.7, 11.3; 277.9, 10.9; 292.2, 8.7; 302.2, 11.1; 313.1, 73.4; 330.9, 2.7; 349.0, 19.4; 363.3, 15.4; 370.6, 23.9; 378.7, 13.3; 387.6, 76.5; 410.7, 98.8; 415.6, 25.3; 436.3, 108.2; 443.1, 79.5; 467.4, 203.7; 504.4, 191.6; 509.2, 192.3; 527.2, 69.4; 532.5, 137.2; 586.7, 22.3; 662.5, 78.9; 665.1, 122.2; 698.4, 339.5; 728.7, 199.0; 747.2, 91.2; 759.9, 598.9; 801.3, 29.9; 810.0, 40.4; 878.4, 117.2; 939.0, 1.5; 970.0, 138.9; 996.1, 96.6; 1550.7, 24.8; 1557.6, 29.2; 1583.1, 437.9; 1606.1, 92.1; 1619.0, 122.3; 1630.8, 64.7; 1671.3, 28.4; 1698.3, 52.2; 3420.3, 139.6; 3485.6, 274.1; 3513.2, 663.1; 3529.0, 29.2; 3580.0, 144.1; 3608.0, 482.2; 3649.6, 863.0; 3672.7, 454.8; 3729.6, 575.4; 3813.3, 124.2; 3863.5, 185.3; 3912.5, 182.6; 3919.6, 183.8; 3937.4, 137.1; 3939.2, 227.9; 3941.8, 184.5;

-2069.138439850 -2068.926394 -2068.905705 -
2068.971009

^{5}O4

Co	0.007785	-0.350616	0.074820
O	1.490743	-1.729438	-0.545709
H	2.200054	-1.209201	-0.973808
O	1.539886	0.585963	1.244012
H	2.311123	0.655497	0.654376
O	-1.538632	0.593356	1.235562
H	-2.293086	0.660820	0.623282
O	-1.427525	-1.723809	-0.708508
H	-2.150723	-1.205132	-1.111046
H	1.172519	-2.372216	-1.188839
H	-1.814672	-2.348122	-0.085996
H	1.253573	1.506832	1.384540
H	-1.246337	1.514940	1.366612
O	-2.725490	0.574668	-1.339789
H	-3.409815	0.940039	-1.906847
H	-1.860861	0.908755	-1.648606
O	-0.109562	-1.738063	1.759867
H	-0.497845	-1.342561	2.548710
H	0.740784	-2.112042	2.017393
O	0.010819	0.799446	-1.177382
O	2.763868	0.532922	-1.295564
H	3.470226	0.878862	-1.847523
H	1.913505	0.878334	-1.629026
O	-0.003902	2.829963	0.732174
H	-0.006889	3.790975	0.732154
H	0.006610	2.520802	-0.192803

76.6, 1.8; 85.2, 0.1; 98.3, 3.1; 104.7, 1.1; 123.8,
4.7; 135.1, 0.7; 152.4, 5.2; 158.6, 5.3; 171.0, 0.5;
182.2, 5.2; 183.6, 0.4; 189.3, 1.5; 199.9, 5.1; 226.9,
23.0; 241.4, 17.4; 246.2, 9.6; 251.5, 57.6; 267.2, 2.3;
272.6, 5.3; 277.1, 5.2; 282.1, 29.3; 325.3, 44.2;
332.9, 55.2; 354.0, 7.0; 357.7, 0.4; 368.3, 47.6;
374.3, 13.7; 394.7, 47.2; 404.9, 107.1; 410.1, 13.9;
430.8, 238.5; 457.7, 155.3; 465.6, 106.7; 489.2, 226.4;
508.5, 116.1; 563.4, 15.9; 572.2, 103.3; 592.1, 83.8;
632.1, 177.6; 657.1, 393.7; 695.6, 589.2; 752.2, 48.7;
791.0, 31.4; 792.2, 122.6; 821.3, 58.4; 841.0, 37.4;
860.6, 265.7; 861.1, 56.4; 1564.9, 21.6; 1571.4, 21.9;
1588.3, 457.5; 1602.0, 84.6; 1616.5, 118.0; 1625.7,
81.8; 1665.1, 30.8; 1689.8, 44.6; 3591.5, 102.9;
3602.1, 95.3; 3633.0, 117.1; 3640.2, 427.6; 3642.5,
55.2; 3653.8, 93.2; 3695.8, 519.7; 3732.2, 730.3;
3751.0, 533.6; 3828.7, 93.6; 3896.8, 194.9; 3904.4,
182.7; 3933.6, 156.6; 3934.5, 248.4; 3936.5, 170.3;
3937.0, 170.0;

-2069.168103240 -2068.957898 -2068.935990 -
2069.004576