Supporting Information

Mechanistic Details of the Cobalt-Mediated Dehydrogenative Dimerization of Aminoquinoline-Directed Benzamides

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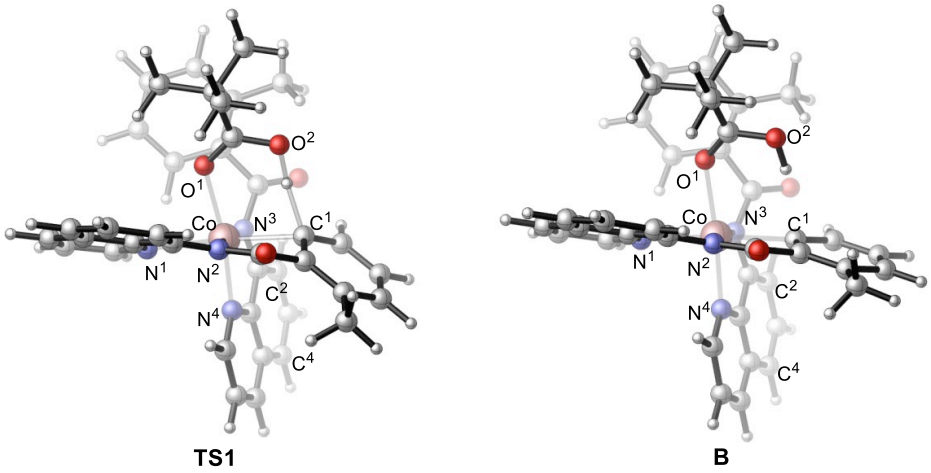
Contents

1. Geometry and spin density analyses of the transition state **TS1** and intermediate **B** ("**t**" stands for triplet, and "**q**" stands for quintet)



		spin density (|e|)					bond distances (Å)							
		Co	N^3	C^1	C^2	C^4	Co-N^1	Co-N^2	Co-N^3	Co-N^4	Co-O^1	Co-C^1	O^1-H	C^1-H
TS1	triplet	1.90	-0.01	-0.09	0.02	0.02	2.03	1.90	2.00	2.17	2.19	2.14	1.36	1.29
	quintet	2.66	0.41	0.15	0.26	0.28	2.18	2.05	2.10	2.12	2.16	2.28	1.13	1.53
B	triplet	2.00	0.01	-0.18	0	0	2.03	1.90	2.00	2.17	2.19	2.14	1.36	1.29
	quintet	2.75	0.21	0.53	0.10	0.09	2.14	2.11	2.04	2.10	2.21	2.28	0.99	2.00

Figure S1. Geometry and spin density analyses of the transition state **TS1** and intermediate **B** ("**t**" stands for triplet, and "**q**" stands for quintet)

2. Dimetallic reaction pathway

Since bimetallic catalysis has grown fast in the field of C-C and C-X coupling reactions,[1-3] here, we also investigated the bimetallic cobalt complex mediated reaction pathway (**Figure S2**). The *dimetallic* mechanism starts from the intermediate **B**, but proceeds via the: (a) BQN-to-$PivO^-$ ligand exchange, (b) dimerization of the resulted (PivO)Co(BQN), **20,** complex to form the (BQN)Co$(PivO)_2$Co(BQN), **21,** intermediate, and (c) C–C coupling to form biaryl product.

At first, we have explored the BQN-to-$PivO^-$ exchange process. We found that it is endergonic by 18.9 kcal/mol indicating that aminoquinoline is a better bidentate ligand than pivalate. The dimerization of **20t** forms the bimetallic species **21** with a quintet ground electronic state (**21q**). This dimerization process is a slightly exergonic because of presence of weak π-π interaction between the two aryl rings of substrates. In **21q,** the Co–Co bond distance (3.46 Å) is too long (**Figure S3**), and each cobalt atom has about two (Co^1: 2.01 |e|; Co^2: 1.99 |e|) unpaired spins.

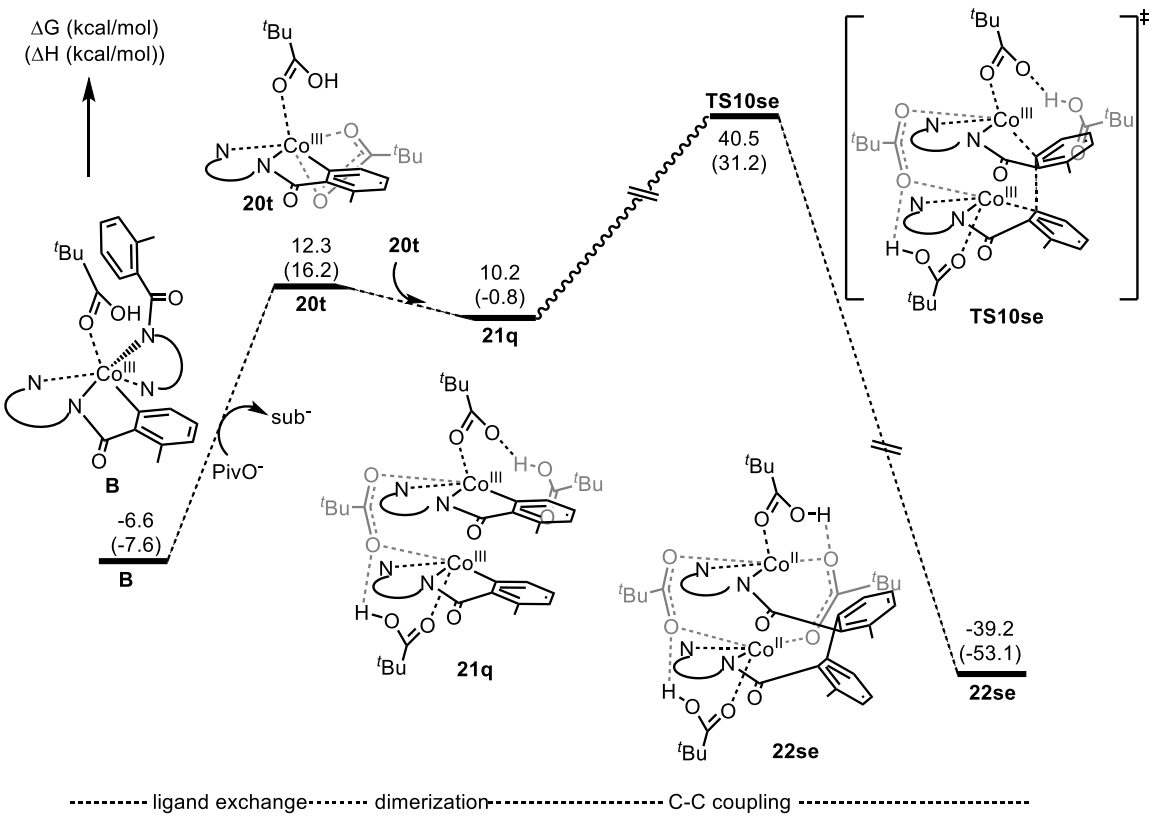


Figure S2. Potential energy surface for the *dimetallic* reaction pathway.

In **21q**, the C-C coupling occurs via the transition state **TS10**, where two Co-C bonds are going to be broken and one C-C bond is going to be formed. We located a septet state **TS10**, **TS10se**. Unfortunately, all attempts to locate its other spin states were unsuccessful. Careful examination of the structure of **TS10se** (**Figure S3**) indicates that the two cobalt-carbon bonds are "asymmetric" with a Co^1-C^1 =2.36 Å and Co^2-C^2 = 1.97 Å bond distances. The "asymmetric" property of Co-centers is also reflected in their spin densities: Co^1 has a 2.66 |e| unpaired spin, while Co^2 has 2.16 |e| unpaired spin. The performed IRC calculation from **TS10se** leads to the product, **22se**, with a C^1-C^2 = 1.51 Å bond. This species with the Co^1 = 2.70 |e| and Co^2: 2.73 |e| spins were characterized as a Co^{II}-Co^{II} complex. As seen in **Figure S2,** transition state **TS10se** has a 47.1 kcal/mol free energy relative to complex **B**. This barrier is prohibitively high that enables us to conclude that dimetallic mechanism of the studied reaction cannot be operative.

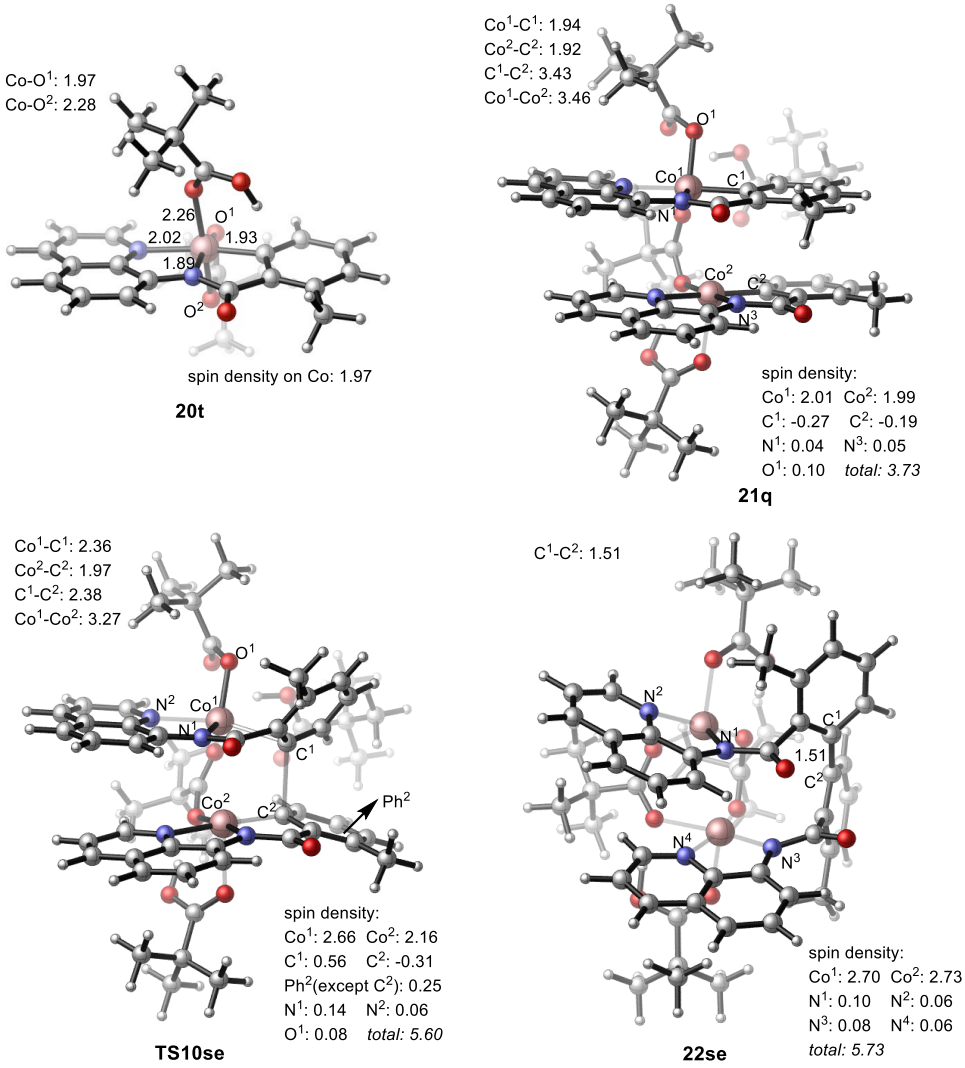


Figure S3. Geometries (in Å) and spin densities (in |e|) of the key intermediates and transition states of the dimetallic reaction pathway.

3. The second C-H bond activation via the "outer-sphere" mechanism

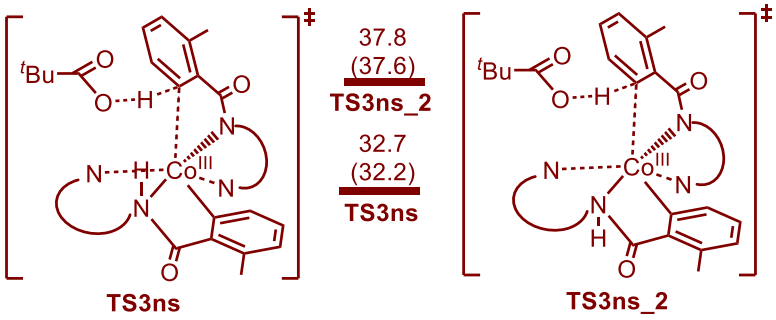


Figure S4. The second C-H bond activation via the "outer-sphere mechanism", transition states **TS3ns** and **TS3ns_2**.

As it can be seen from Figure S4, transition states associated with the "outer-sphere" mechanism, **TS3ns** and **TS3ns_2**, are higher in free energy than that associated with the "inner-sphere" mechanism (**TS3**, 26.2 kcal/mol).

4. Potential energy surface for the C-C coupling in the complex **D** via the release of PivOH.

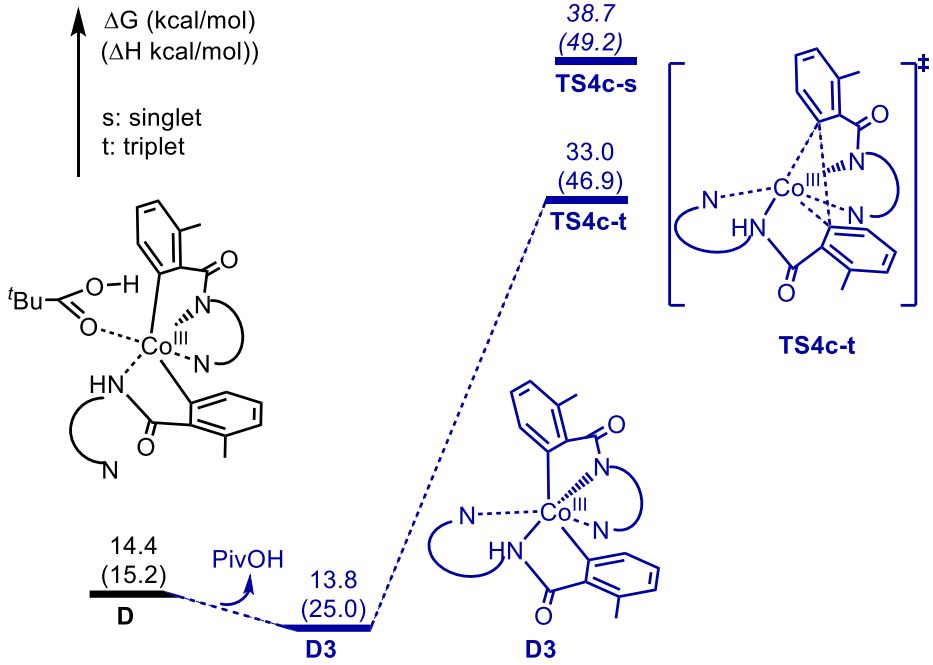


Figure S5. Potential energy surface for the C-C coupling in the complex **D** via the release of PivOH.

5. Potential energy surface for the second amide nitrogen protonation and the following C-C coupling.

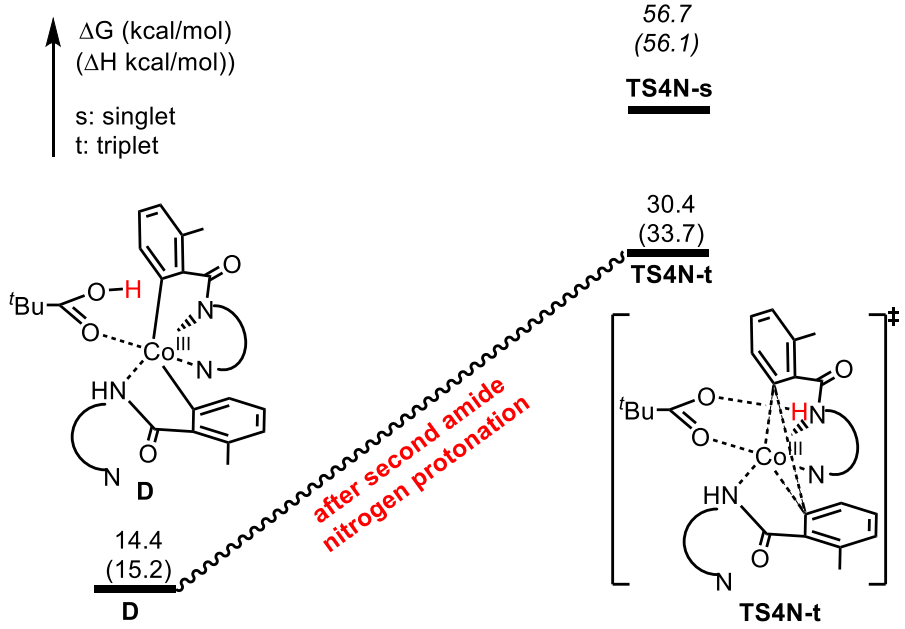
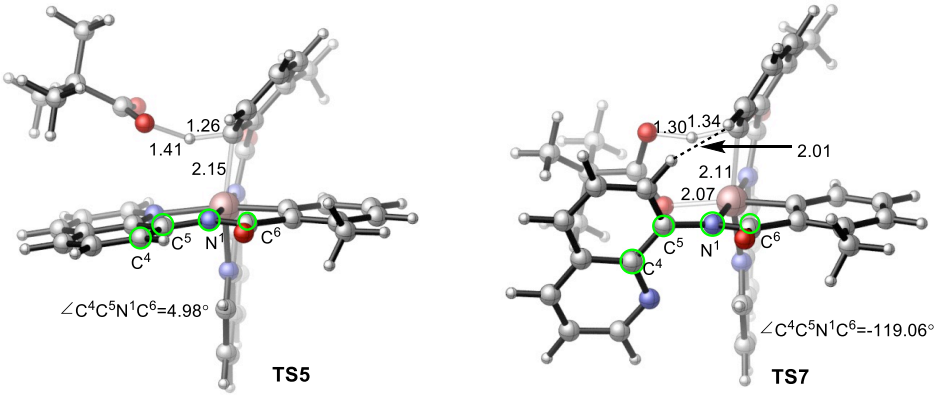


Figure S6. Potential energy surface for the second amide nitrogen protonation and the following C-C coupling.

6. Computational analyses of the transition states **TS5s** and **TS7s**



ΔG≠ = 22.2 kcal/mol
ΔE≠ = 26.4 kcal/mol
ΔE(dist-cat) = 8.7 kcal/mol
ΔE(dist-sub) = 43.8 kcal/mol
ΔE(int-cat) = 26.1 kcal/mol

ΔG≠ = 27.4 kcal/mol
ΔE≠ = 32.4 kcal/mol
ΔE(dist-cat) = 62.5 kcal/mol
ΔE(dist-sub) = 63.3 kcal/mol
ΔE(int-cat) = 93.4 kcal/mol

Figure S7. Computational analyses of the transition states **TS5s** and **TS7s**

As seen in Figure S7, transition state **TS7** is unfavorable compared with transition state **TS5** for several reasons: (1) in **TS7** the H(quinolone)-H(aryl) distance is only 2.01 Å, indicating that there should be a large steric repulsion between these atoms; and (2) in **TS7** one of the quinolone moiety rotated near vertically to the rest benzamide part ($\angle C^4C^5N^1C^6$ = -119.06°), which interrupted the "global" conjugation of the entire substrate and made it unfavorable (in **TS5,** $\angle C^4C^5N^1C^6$ = 4.98°).

7. Synthetic procedures and characterization of cobalt complexes.

Synthesis of 2-methyl-N-(quinolin-8-yl)benzamide. Prepared using a modified literature procedure.[8] A two-neck RB flask was charged with 2-methylbenzoyl chloride (6.52 mL, 50 mmol) and a magnetic stir bar. The acid chloride was diluted with CH_2Cl_2 (50 mL) under an N_2 atmosphere and cooled to 0ºC. A solution of 8-aminoquinoline (7.2090 g, 50.05 mmol) and triethylamine (7.62mL, 54.5 mmol) in CH_2Cl_2 (40 mL) was added dropwise to the acid chloride solution. The mixture was allowed to warm to room temperature and then stirred for 18 h. The reaction mixture was quenched with a saturated $NaHCO_3$ solution (7.5 g in 90 mL DI H_2O) and extracted three times with CH_2Cl_2. The extracts were combined and dried of $MgSO_4$ and filtered through Celite® and activated charcoal. Filtrate was dried in vacuo to obtain a light-yellow power. A crystalline product can be obtained by layering a concentrated toluene solution of the compound with hexanes (10.57 g, 81%). ^{1}H NMR (δ, $CDCl_3$, 600 MHz) 10.22 (br s, 1H), 8.96 (d, J = 7.6 Hz, 1H), 8.77 (dt, J = 4.1, 1.3 Hz, 1H), 8.17 (dt, J = 8.3, 1.4 Hz, 1H), 7.71 – 7.67 (m, 1H), 7.60 (t, J = 7.9 Hz, 1H), 7.55 (dt, J = 8.3, 1.3 Hz, 1H), 7.45 (ddd, J = 8.2, 4.2, 1.2 Hz, 1H), 7.40 (tt, J = 7.5, 1.2 Hz, 1H), 7.35 – 7.30 (m, 2H), 2.61 (s, 3H).

Synthesis of 1 ($Co^{II}(BQN)_2$). Under an inert atmosphere, a 20 mL scintillation vial was charged with 2-methyl-*N*-(quinolin-8-yl)benzamine (0.2750 g, 1.05 mmol), potassium hydride (44.5 g, 1.11 mmol), a stir bar, and 10 mL of dimethylformamide. The solution was stirred at ambient temperature for 1 h. To this homogenous dark yellow solution, $CoBr_2$ (0.972 g, 0.518 mmol) was added as a solid and the solution immediately changed to a deep burgundy color. The resulting homogenous solution was concentrated to dryness under reduced pressure to yield a dark maroon solid. The solid was extracted into a CH_2Cl_2 and filtered through a plug of Celite®. The solution was layered with petroleum ether and yielded needle-shaped dark red crystals of the product (282.0 mg, 93.7%). This product decomposes slowly in air. ^{1}H NMR (δ, $CDCl_3$, 400 MHz): -21.31 (s), -19.72 (s), -9.67 (s), -8.30 (s), 26.27 (s), 40.06 (s), 42.88 (br), 46.13 (br), 66.08 (s). $\lambda_{max}(CH_2Cl_2)$, nm (ε, M^{-1} cm^{-1}): 617 (190), 590 (288), 535 (316), 400 (6730). IR (diamond ATR, cm^{-1}): υ(CO) = 1605 MS (+ESI) calculated 581.14, found 581.14, μ_{eff} = 4.41(1) μ_B (Evans Method, CD_2Cl_2, 400 MHz). EA: $(C_{34}H_{26}CoN_4O_2)_4$ + CH_2Cl_2 calcd. C 68.25, H 4.43, N 9.30 %; exp. C 68.47, H 4.60, N 9.37 %.

Synthesis of 2 $(PPh_4)[Co^{II}(OPiv)_2(BQN)]$. Under an inert atmosphere a 20 mL scintillation vial was charged with pivalic acid (102.2 mg, 1.00 mmol), (2-methylbenzoyl)(quinolin-8-yl)amide (133.4 mg, 0.509 mmol), potassium hydride (59.7 mg, 1.49 mmol), a magnetic stir bar, and 2 mL DMF. The solution was stirred for 2 h. Cobalt bromide (93.9 mg, 0.500 mmol) was added to the stirring solution and, after 20 min, tetraphenylphosphonium bromide (206.1 mg, 0.492 mmol) was added and the solution was stirred for an additional 12 h. The resulting solution was concentrated in vacuo, dissolved in CH_3CN, and filtered through a frit to afford a dark green solution. A concentrated solution of the product in CH3CN was layered with diethyl ether, which afforded red, block crystals (232.1 mg, 51% yield). Product is stable to air. ^{1}H NMR (δ, $CDCl_3$, 400 MHz): -12.54, -12.25, -11.22, -5.59, -3.51, 7.69, 7.79, 7.90 11.54, 16.70, 32.57, 33.43. IR (diamond ATR, cm^{-1}): υ(CO) = 1618, 1588, MS (-ESI) calculated [M-PPh_4] 522.16, found 522.16, μ_{eff} = 4.22(9) μ_B (Evans Method, CD_2Cl_2, 400 MHz). EA: $C_{51}H_{51}CoN_2O_5P$ calcd. C 71.07, H 5.96, N 3.25 %; exp. C 70.79, H 6.21, N 3.49 %.

Synthesis of 3 $(PPh_4)[Co^{II}(OAc)_2(BQN)]$. Under an inert atmosphere a 20 mL scintillation vial was charged with (2-methylbenzoyl)(quinolin-8-yl)amide (130.8 mg, 0.499 mmol), potassium hydride (26.3 mg, 0.656 mmol), a magnetic stir bar, and 2 mL DMF. The solution was stirred for 1 h. Cobalt acetate (87.7 mg, 0.495 mmol) and tetraphenylphosphonium bromide (214.2 mg, 0.511 mmol) were added to the stirring solution and stirred for an additional 12 h. The resulting solution was concentrated in vacuo, dissolved in CH_3CN, and filtered through a frit to afford a dark green solution. A concentrated solution of the product in CH_3CN was layered with diethyl ether, which afforded red, block crystals (99.6 mg, 26% yield). ^{1}H NMR (δ, $CDCl_3$, 400 MHz): -14.47, -10.77 -5.18, 7.69, 7.79, 7.9010.60, 14.97, 33.40, 35.00. IR (diamond ATR, cm^{-1}): υ(CO) = 1612, 1582, 1562, MS (-ESI) calculated [M-PPh_4] 438.06, found 438.06, μ_{eff} = 4.21(8) μ_B (Evans Method, CD_2Cl_2, 400 MHz). EA: $(C_{45}H_{39}CoN_2O_5P)_3$ + CH_2Cl_2 calcd. C 67.55, H 4.96, N 3.48 %; exp. C 67.71, H 4.74, N 3.61%.

Synthesis of 4 $(Co^{III}(H_2O)(BQN)(BQNN))$. Under an inert atmosphere a 20 mL

scintillation vial was charged with complex 2 (84.8 mg, 0.094 mmol), (2-methylbenzoyl)(quinolin-8-yl)amide (25.3 mg, 0.096 mmol), FcBF4 (55.0 mg, 0.202 mmol), a magnetic stir bar, and 2 mL CH3CN. The solution was stirred for 18 h. The solution was filtered through Celite® and concentrated in vacuo. The complex was isolated by column chromatography on silica gel using appropriate eluent (34.8 mg, 62% yield). 1H NMR (δ, CDCl3, 400 MHz): 10.27 – 10.15 (m, 2H), 8.93 (d, J = 7.5 Hz, 2H), 8.76 (d, J = 4.1 Hz, 2H), 8.17 (dd, J = 8.3, 1.7 Hz, 2H), 7.72 – 7.64 (m, 5H), 7.61 – 7.53 (m, 4H), 7.44 (dd, J = 8.3, 4.2 Hz, 2H), 7.37 (t, J = 6.5 Hz, 3H), 7.31 (s, 2H). 13C NMR(δ, CDCl3, MHz): 205.08, 195.50,168.59, 165.48, 148.28, 147.49, 139.28, 137.73, 136.68, 136.37, 136.16, 134.92, 134.51, 134.41, 131.72, 131.37, 130.32, 129.40, 129.24, 129.09, 128.82, 128.75, 128.52, 128.01, 127.84, 127.55, 127.44, 127.27, 127.12, 126.52, 126.01, 125.32, 122.59, 122.41, 121.91, 121.77, 121.71, 121.67, 121.11, 120.26, 119.15, 118.62, 20.00, 19.71.IR (diamond ATR, cm-1): υ(CO) = 1595, 1594, MS (ESI+) calculated ([M-H2O] + H+) 580.138, found 581.137

Synthesis of 5 (Co^{III}(PivO)(BQN-BQN)). Under an inert atmosphere, a 20 mL scintillation vial was charged with 1 (0.0495 g, 0.085 mmol), silver carbonate (0.2241 g, 0.813 mmol), sodium pivalate (0.0120 g, 0.097 mmol), a stir bar, and 10 mL of CH_2Cl_2. The solution was heated to 65ºC and stirred for 40h. The mixture was allowed to cool to room temperature and filtered through Celite®. A dark grey solid remained on the Celite® and afforded a dark orange solution. The solution was concentrated to dryness. A crystalline product can be obtained by layering concentrated benzene solution of the mixture with petroleum ether and yielded dark orange block crystals (24.1 mg, 42% yield). ^{1}H NMR (δ, $CDCl_3$, 400 MHz): 8.85 (dd, J = 5.1, 1.3 Hz, 1H), 8.69 (dd, J = 7.9, 1.1 Hz, 1H), 8.32 (dd, J = 8.3, 1.3 Hz, 1H), 7.60 (dd, J = 8.3, 5.1 Hz, 1H), 7.38 (t, J = 8.0 Hz, 1H), 7.26 (dd, J = 8.1, 1.0 Hz, 1H), 6.36 – 6.30 (m, 2H), 6.18 (dd, J = 7.2, 1.3 Hz, 1H), 2.01 (s, 3H). ^{13}C NMR (δ, $CDCl_3$, 600 MHz): 200.44, 178.67, 150.98, 149.34, 147.67, 142.02, 138.42, 136.53, 134.95, 129.77, 127.72, 127.14, 126.76, 124.84, 121.67, 121.25, 117.80, 38.94, 29.72, 27.44, 25.34, 20.57, λ_{max} (CH_2Cl_2), nm (ε, M^{-1} cm^{-1}): 530 (873), 426 (8409). IR (diamond ATR, cm^{-1}): υ(CO) = 1605, MS (-ESI) calculated 680.18, found 679.54.

Synthesis of 6 (Co^{II}(BQN-BQN)). Under an inert atmosphere a 20 mL scintillation vial was charged with 1 (0.0467 g, 0.080 mmol), silver oxide (0.1884 g, 0.813 mmol), a stir bar, and 10 mL of CH_2Cl_2. The solution was heated to 65ºC and stirred for 72h. The mixture was allowed to cool to room temperature and filtered through Celite®. The remaining solution was dried in vacuo. A concentrated solution of the product in benzene was layered with petroleum ether, which afforded small, dark red crystals (17.2 mg, 37% yield). The crystals are stable to air. ^{1}H NMR (δ, $CDCl_3$, 400 MHz): -33.78 (s), -15.05 (s), -13.46 (s), -1.40 (s), 34.84 (s), 45.48 (s), 79.41 (br), 81.26 (br). λ_{max} (CH_2Cl_2), nm (ε, M-1 cm-1): 393 (11918), 533 (1080), 588 (664). IR (diamond ATR, cm^{-1}): υ(CO) = 1597, MS (+ESI) calculated 579.12, found 579.12, μ_{eff} 4.13(9) μ_B (Evans Method, CD_2Cl_2, 400 MHz). EA: $(C_{34}H_{24}CoN_4O_2)_3$ + DMF calcd. C 69.61, H 4.40, N 10.05 %; exp. C 69.31, H 4.48, N 9.61 %.

Synthesis of 6^{OMe} (Co^{II}(BQN^{OMe}-BQN^{OMe})). Under an inert atmosphere, a 20 mL scintillation vial was charged with a stir bar, benzylquinolinamide (BQN, 0.200 mmol), KH (0.220 mmol), and 3 mL of DMF. The mixture was stirred for 0.5 h. Next, $CoBr_2$ (0.100 mmol) and the mixture was stirred for 1 h. Solvent was removed under vacuum. The mixture was redissolved in 3 mL DCE and silver carbonate was added (1.00 mmol), removed from the glovebox, heated to 100 ºC, and stirred for 21 h. After 21 h, the solution was cooled to room temperature (25 ºC), trimethoxybenzene (0.10 mmol) was added as internal standard, and the solution was filtered through Celite®. The resulting solution was concentrated in vacuo and an NMR in $CDCl_3$ was taken. The products were isolated and purified by column chromatography (25% v/v hexanes/ethyl acetate).). ^{1}H NMR (δ, $CDCl_3$, 400 MHz): -33.23 (s), -15.97 (s), -15.22 (s), -2.09 (s), -1.01 (s), 33.68 (s), 46.42 (s), 81.47 (s), 83.46 (s). λ_{max} (CH_2Cl_2), nm (ε, M-1 cm-1): 406 (15868), 545 (765), 587 (514). IR (diamond ATR, cm^{-1}): υ(CO) = 1606, MS (+ESI) calculated [M+H$^+$] 640.144, found 640.157, μ_{eff} 1.88(8) μ_B (Evans Method, CD_2Cl_2, 400 MHz).

Synthesis of 7 (Co^{III}(BQN) (BQN-BQN)). In air, a 20 mL screw-top vial was charged with 1 (0.0581 g, 0.10 mmol), (2-methylbenzoyl)(quinolin-8-yl)amide (0.1346 g, 0.51 mmol), silver carbonate (0.2764 g, 1.0 mmol), a stir bar, and 5 mL dichloroethane. The solution was heated to 100ºC and stirred for 19h. The mixture was cooled to room temperate and filtered through Celite®. The product was purified by column chromatography (40% v/v hexanes/ethyl acetate). Green block crystals were obtained by layering a concentrated solution of compound in CH_2Cl_2 and petroleum ether (32.9 mg, 48% yield). ^{1}H NMR (δ, $CDCl_3$, 400 MHz): 9.46 (d, J = 8.0 Hz, 1H), 8.71 (d, J = 5.3 Hz, 1H), 8.38 (d, J = 8.0 Hz, 1H), 8.07 (dd, J = 13.3, 8.2 Hz, 2H), 7.88 (d, J = 7.6 Hz, 1H), 7.72 (d, J = 8.2 Hz, 1H), 7.65 (t, J = 8.1 Hz, 1H), 7.48 (d, J = 5.3 Hz, 1H), 7.36 – 7.31 (m, 2H), 7.21 (dd, J = 8.2, 5.2 Hz, 1H), 7.16 (td, J = 9.3, 8.8, 3.6 Hz, 3H), 7.07 (t, J = 6.7 Hz, 3H), 7.01 – 6.93 (m, 2H), 6.85 (d, J = 7.9 Hz, 1H), 6.64 (dd, J = 12.1, 5.7 Hz, 2H), 6.57 (d, J = 7.4 Hz, 1H), 6.49 (t, J = 7.6 Hz, 1H), 6.38 (d, J = 8.1 Hz, 1H), 6.08 (d, J = 7.7 Hz, 1H), 2.29 (s, 3H), 1.14 (s, 3H), 1.12 (s, 3H). ^{13}C NMR (δ, $CDCl_3$, 600 MHz): 180.60, 180.26, 178.87, 152.16, 150.42, 149.90, 149.46, 148.74, 148.52, 145.05, 144.81, 141.48, 141.04, 139.12, 138.53, 137.82, 137.80, 137.70, 136.85, 136.43, 136.28, 132.40, 130.71, 130.15, 129.84, 129.61, 129.23, 129.02, 128.80, 128.66, 128.48, 127.24, 126.71, 126.35, 126.23, 125.84, 125.49, 122.89, 122.53, 121.55, 121.05, 119.71, 119.06, 117.69, 115.35, 20.73, 19.39, 18.17. λ_{max} (CH_2Cl_2), nm (ε, M^{-1} cm^{-1}): 648 (436), 430 (10346), MS (-ESI) calc. for $C_{51}H_{37}ClCoN_6O_3$ 875.19, found 875.20, IR (diamond ATR, cm^{-1}): υ(CO) = 1594.

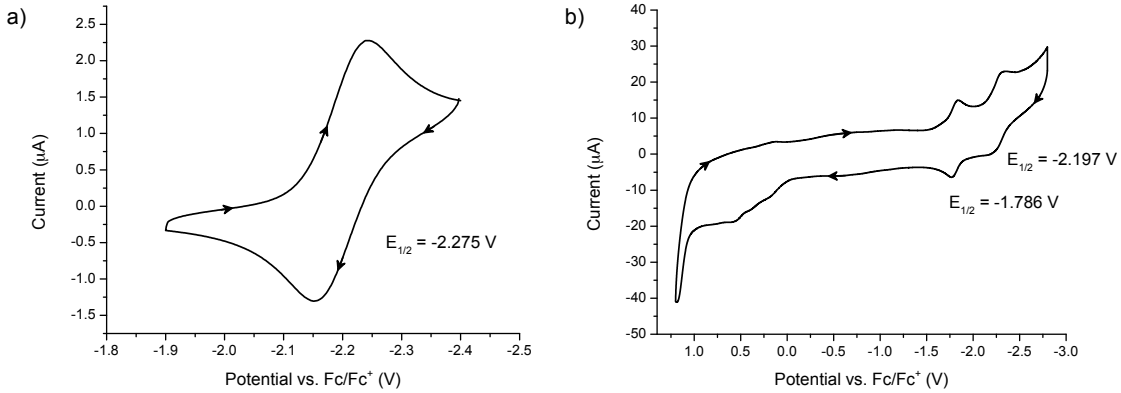
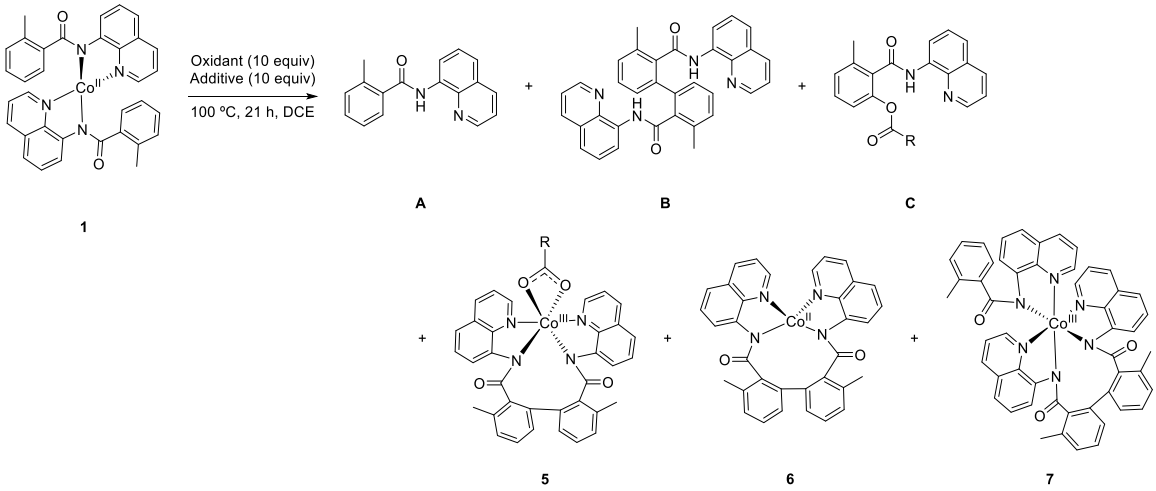


Figure S8. Cyclic voltammogram of $\mathbf{Co^{II}(BNQ)_2}$ with 0.1M $TBAPF_6$ as the supporting electrolyte in a) acetonitrile and b) dimethylformamide. Referenced vs. Fc/Fc^+ with an Ag/Ag^+ counter electrode, a Pt-wire auxiliary electrode, and a glass-carbon working electrode.

8. General procedure for reaction condition screen for biaryl homocoupling of 1.

Under an inert atmosphere, a 20 mL scintillation vial was charged with a stir bar, 1 (0.047 g, 0.10 mmol), oxidant (1.0 mmol), additive (1.0 mmol) and 5 mL of CH_2Cl_2. The mixture was heated to 100 ºC and stirred for 24 h. After 24 h, the mixture was cooled to room temperature (ca. 25 ºC), removed from the glovebox, and filtered through Celite®. The resulting solution was concentrated in vacuo and an NMR in $CDCl_3$ was taken. The products were isolated and purified by column chromatography (25% v/v hexanes/ethyl acetate).

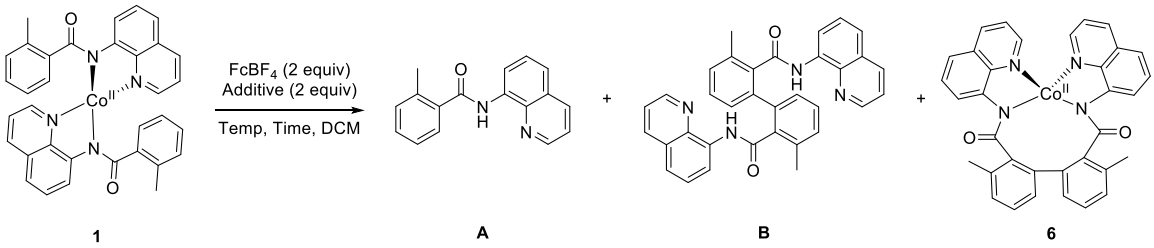
Table S1. Reaction condition screen for stoichiometric biaryl coupling from the $Co^{II}(BNQ)_2$ complex.



Entry	Oxidant	Additive	Yield A	Yield B	Yield C	Yield 2	Yield 3	Yield 4	Total [c–c]
1	Ag_2CO_3	Na_2CO_3	13%	—	—	—	15%	44%	59%
2	Ag_2CO_3	NaOAc	9%	2%	5%	—	18%	58%	78%
3	Ag_2CO_3	NaOPiv	—	—	61%	14%	15%	—	29%
4	Ag_2CO_3	Et_3N	29%	34%	—	—	—	—	34%
5[a]	Ag_2CO_3	Et_3N	20%	17%	—	36%	—	—	53%
6[b]	Ag_2CO_3	Et_3N	43%	47%	—	8%	—	—	55%
7[c]	Ag_2CO_3	Et_3N	25%	20%	—	—	—	—	20%
8	Ag_2CO_3	—	7%	3%	—	20%	49%	—	72%
9	Ag_2O	—	8%	—	—	—	37%	—	37%
10	$K_2S_2O_8$	NaOPiv	15%	—	—	—	—	—	0%
11	O_2 (sat.)	NaOPiv	—	—	—	—	—	—	0%

[a]Reaction was run in 1.40 mL Et_3N (100 equiv) with 0.5 mL DCE to solubilize the cobalt complex. [b]Reaction was run under inert conditions. [c]Reaction was run for 42 h.

Table S2. Reaction condition screen for stoichiometric biaryl coupling from the $Co^{II}(BNQ)_2$ complex with an outer-sphere oxidant.



1 A B 6

Entry	Additve	Time	Temp.	Yield A	Yield B	Yield 6	Total [c-c]
1	NaOPiv	21h	25 °C	21%	22%	11%	33%
2	NaOPiv	21h	60 °C	36%	31%	33%	64%
3[a,b]	NaOPiv	3h	25 °C	47%	—	10%	10%
4	Et_3N	3h	25 °C	18%	—	—	0%

[a]Yields determined using 1,3,5-trimethoxybenzene as the internal standard [b]72% of the starting complex was recovered.

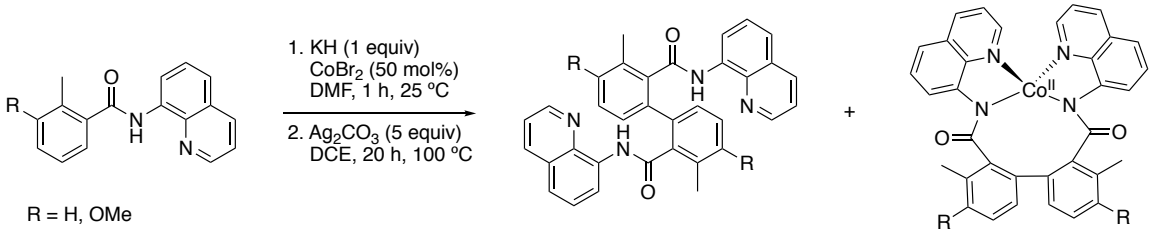
9. Effect of an aryl substituent

Under an inert atmosphere, a 20 mL scintillation vial was charged with a stir bar, benzylquinolinamide (BQN, 0.200 mmol), KH (0.220 mmol), and 3 mL of DMF. The mixture was stirred for 0.5 h. Next, $CoBr_2$ (0.100 mmol) and the mixture was stirred

for 1 h. Solvent was removed under vacuum. The mixture was redissolved in 3 mL DCE and silver carbonate was added (1.00 mmol), removed from the glovebox, heated to 100 ºC, and stirred for 21 h. After 21 h, the solution was cooled to room temperature (25 ºC), trimethoxybenzene (0.10 mmol) was added as internal standard, and the solution was filtered through Celite®. The resulting solution was concentrated in vacuo and an NMR in $CDCl_3$ was taken. The products were isolated and purified by column chromatography (25% v/v hexanes/ethyl acetate).

When the reaction was performed with 2-methyl-N-(quinolin-8-yl)benzamide, di-BQNH and Co^{II}(BQN-BQN) were isolated in a 7% and 87% yield respectively (Scheme S1). When the reaction was performed with 3-methoxy-2-methyl-N-(quinolin-8-yl)benzamide Crude NMR showed a mixture of di-$BNQH^{OMe}$, $Co^{II}(BNQ^{OMe})_2$, and $Co^{II}(BQN^{OMe}$-$BQN^{OMe})$. $BQNH^{OMe}$, di-$BNQH^{OMe}$ and $Co^{II}(BQN^{OMe}$-$BQN^{OMe})$ were isolated in a 45%, 7%, and 16% yield respectively (Scheme S1).

Scheme S1. Stoichiometric cross-coupling of BQN with different aryl substituents.



R = H	7%	87%
R = OMe	7%	16%

10. ^{1}H and ^{13}C NMR Spectra

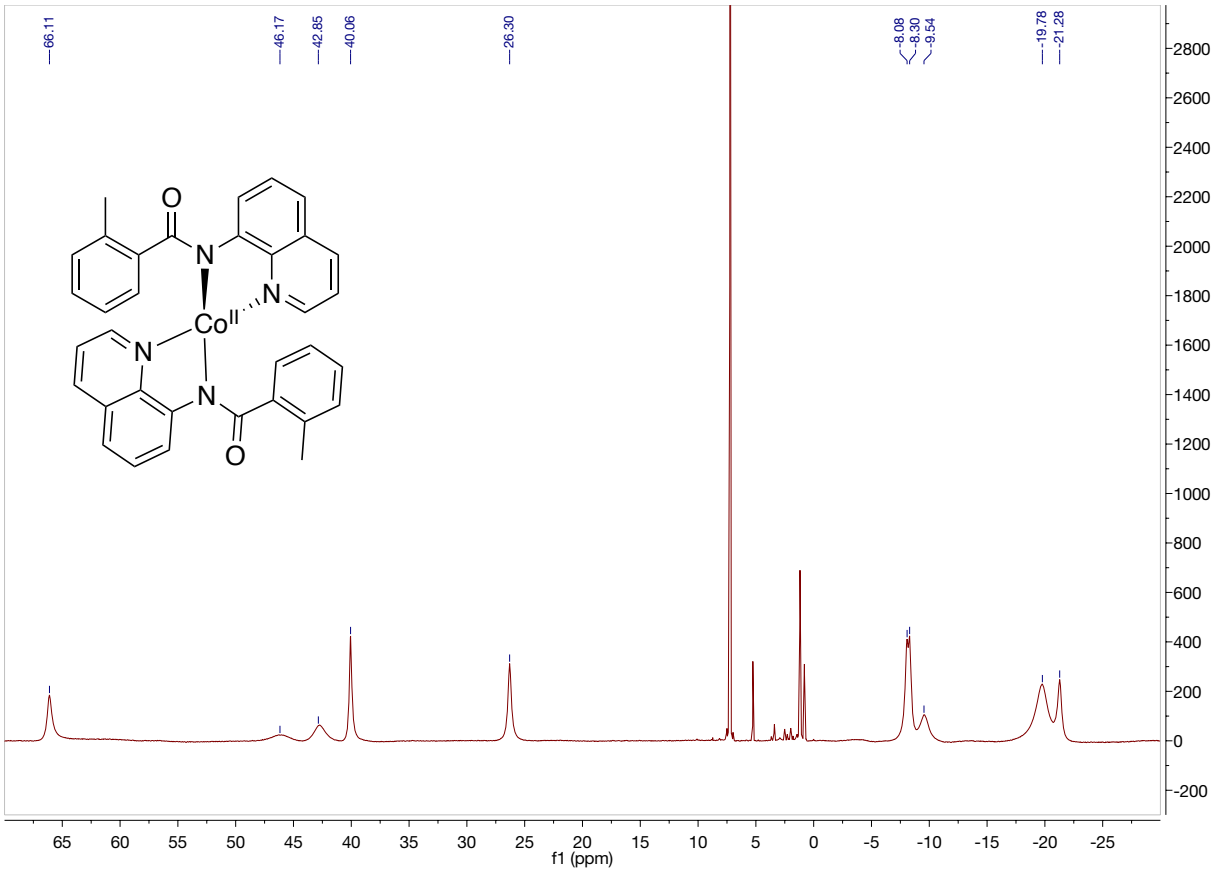


Figure S9: ^{1}H NMR spectrum of **$Co^{II}(BNQ)_2$ (1)** ($CDCl_3$, 400 MHz)

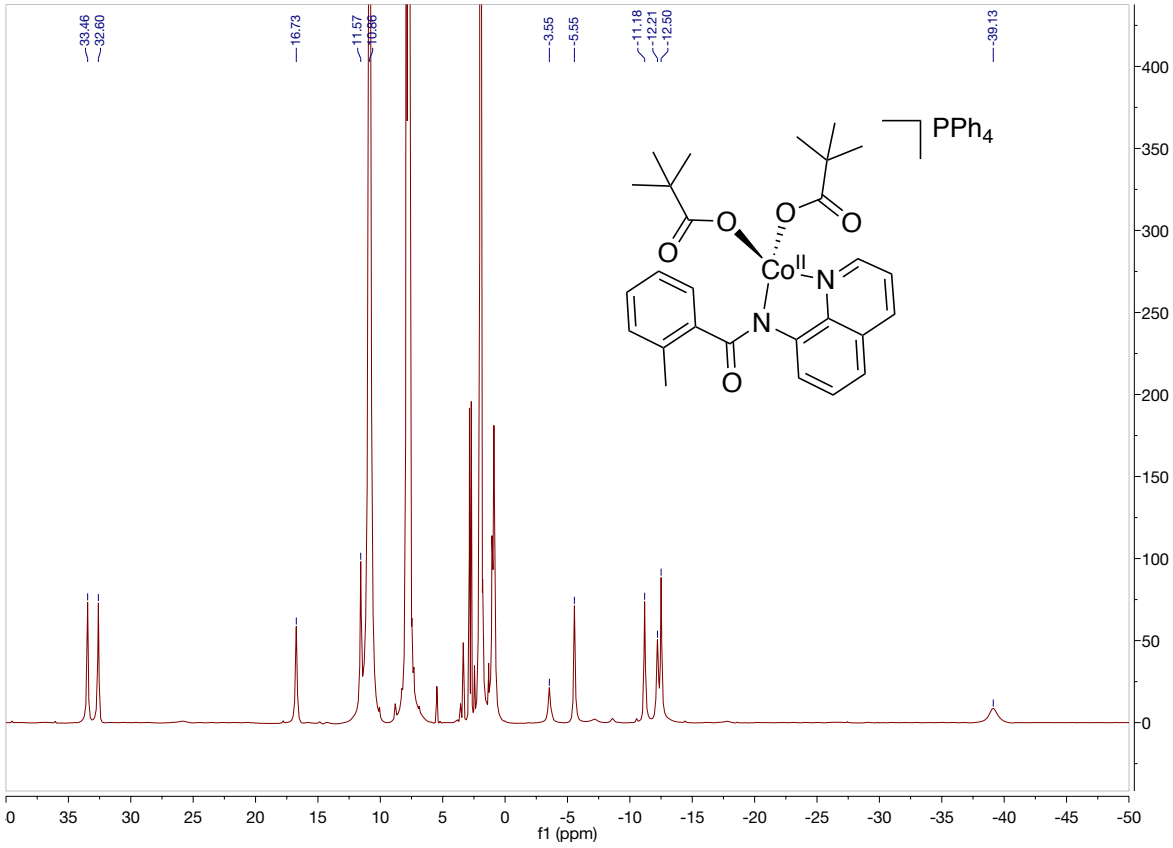


Figure S10: ^{1}H NMR spectrum of **$(PPh_4)[Co^{II}(OPiv)_2(BQN)]$** (**2**) ($CDCl_3$, 400 MHz)

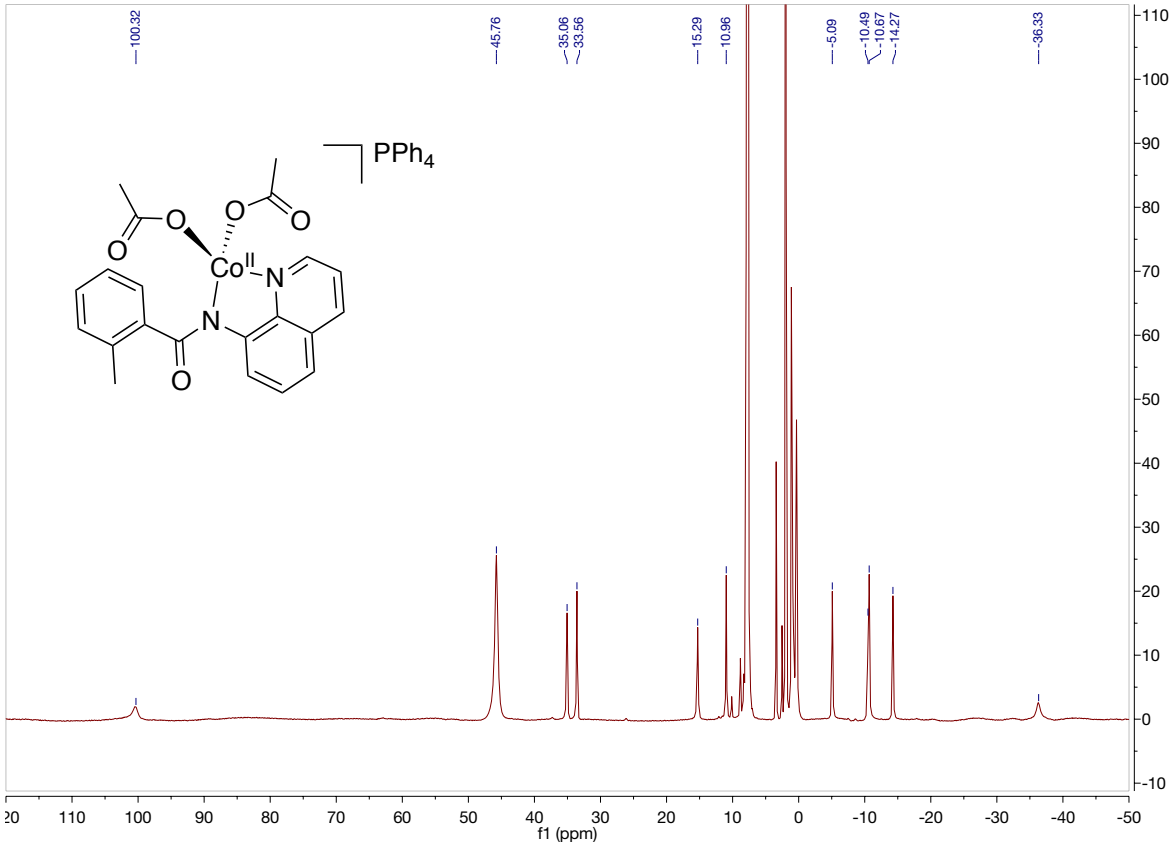


Figure S11: ^{1}H NMR spectrum of **(PPh$_4$)[Co^{II}(OAc)$_2$(BQN)]** (**3**) (CDCl$_3$, 400 MHz)

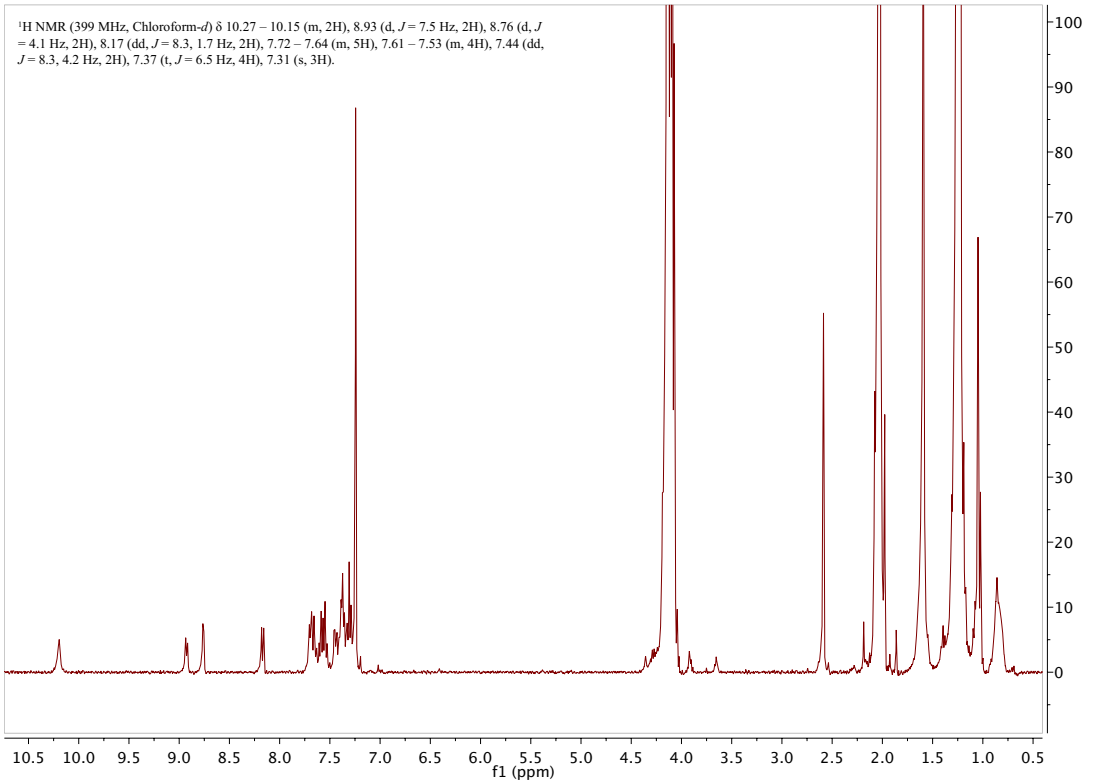


Figure S12: ^{1}H NMR spectrum of **$Co^{III}(H_2O)$(BQN)(BQNN)** (**4**) ($CDCl_3$, 400 MHz)

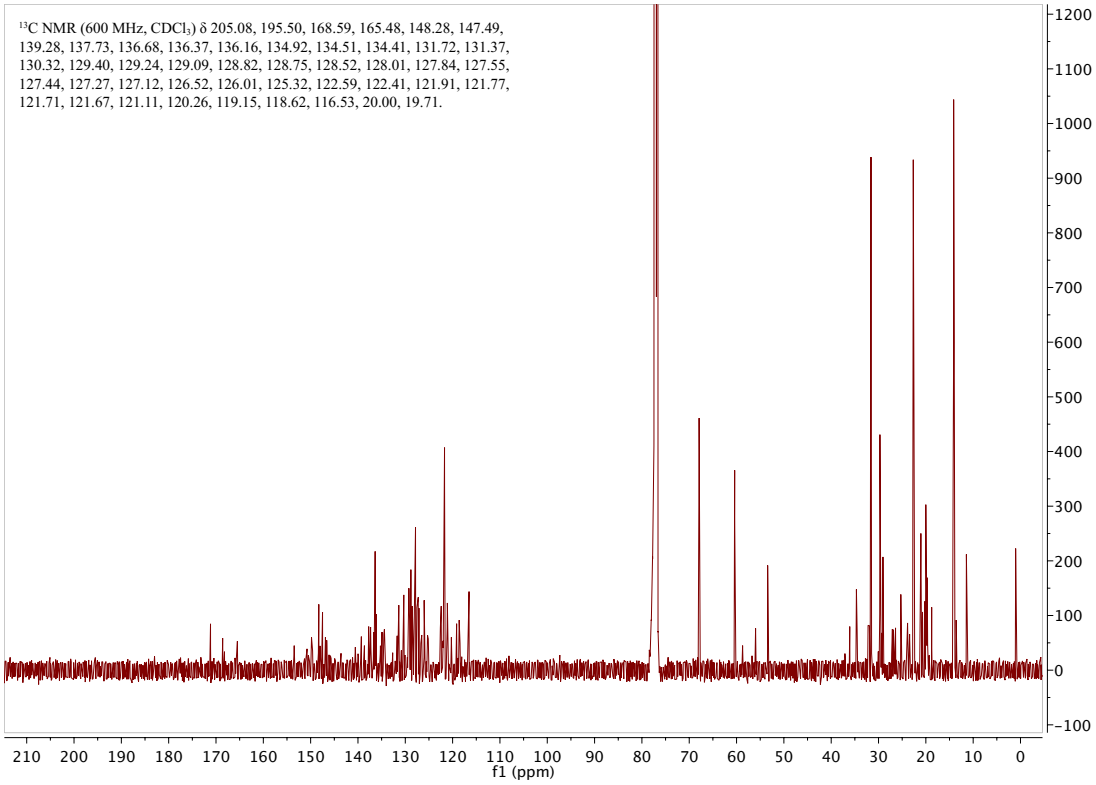


Figure S13: ^{13}C NMR spectrum of **$Co^{III}(H_2O)$(BQN)(BQNN)** (**4**) ($CDCl_3$, 600 MHz)

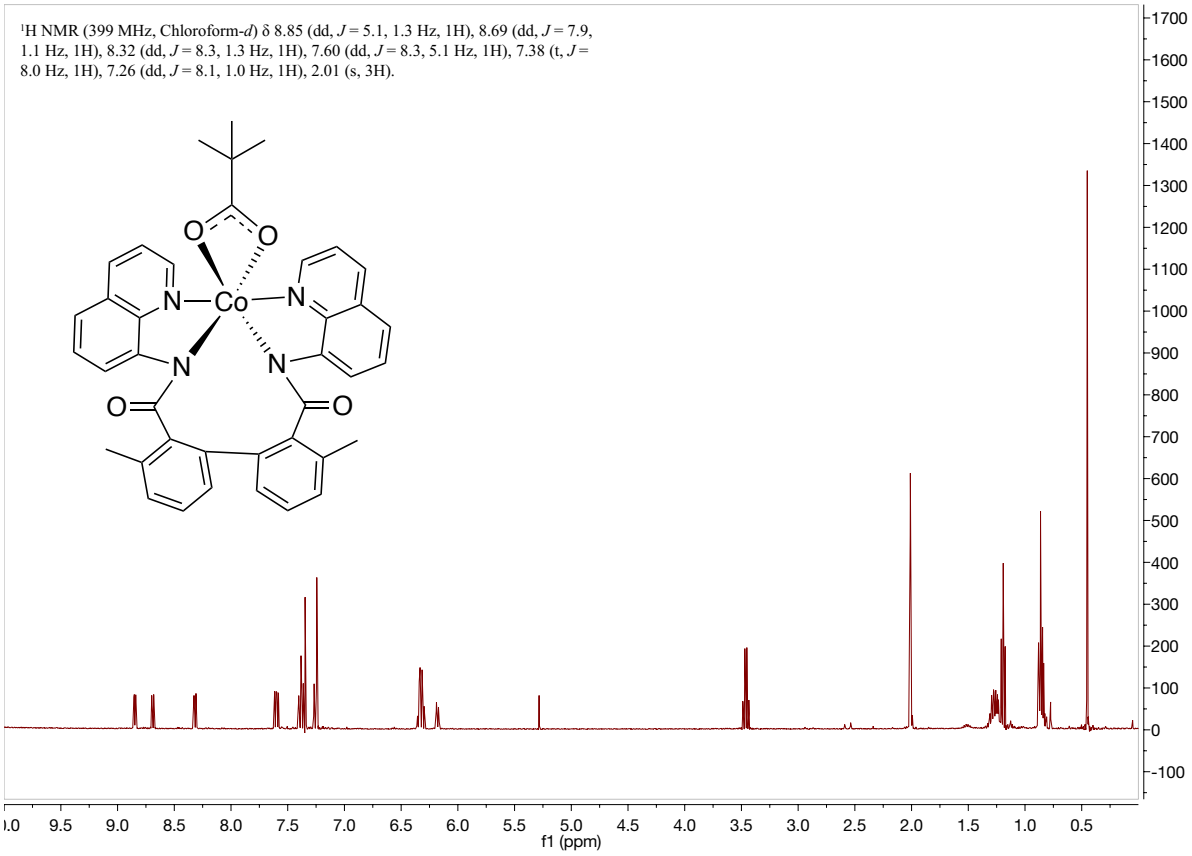


Figure S14: ^{1}H NMR spectrum of **Co^{III}(PivO)(BQN-BQN)** (**5**) ($CDCl_3$, 400 MHz)

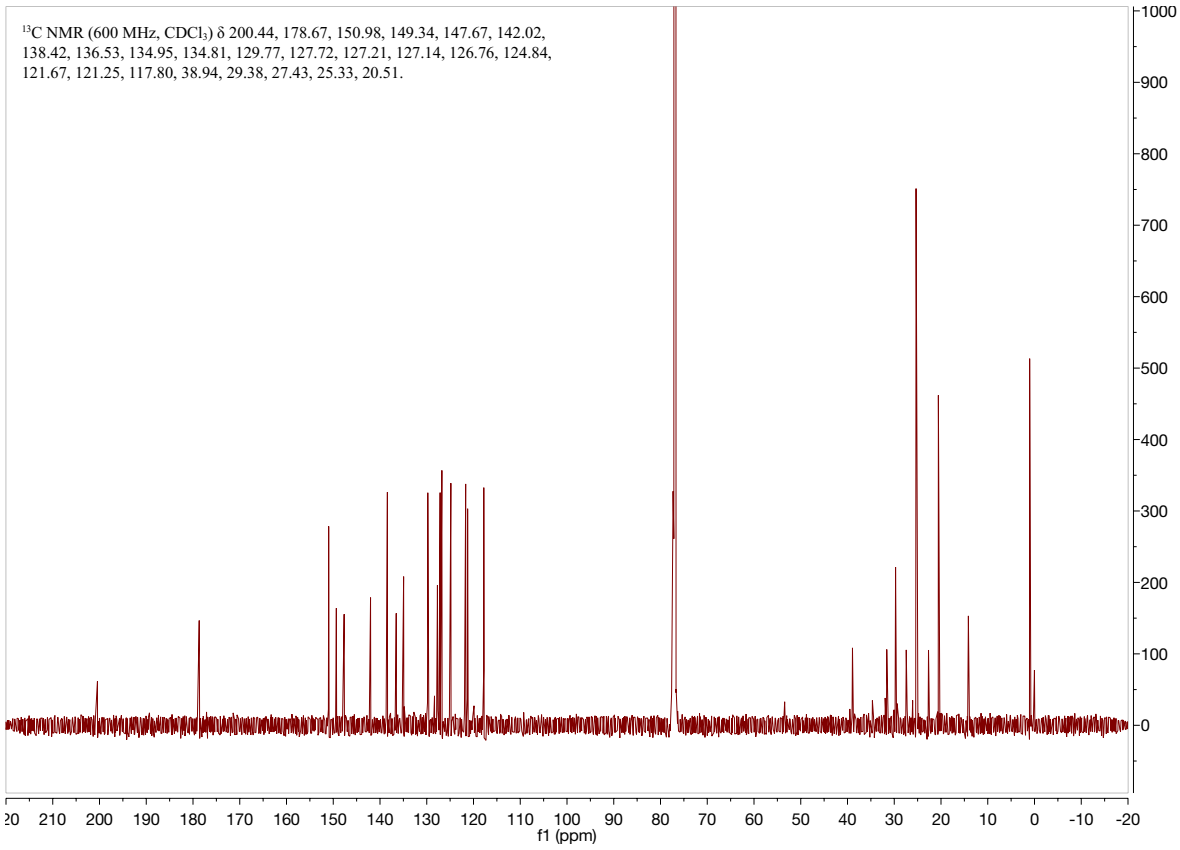


Figure S15: ^{13}C NMR spectrum of **Co^{III}(PivO)(BQN-BQN)** (**5**) ($CDCl_3$, 600 MHz)

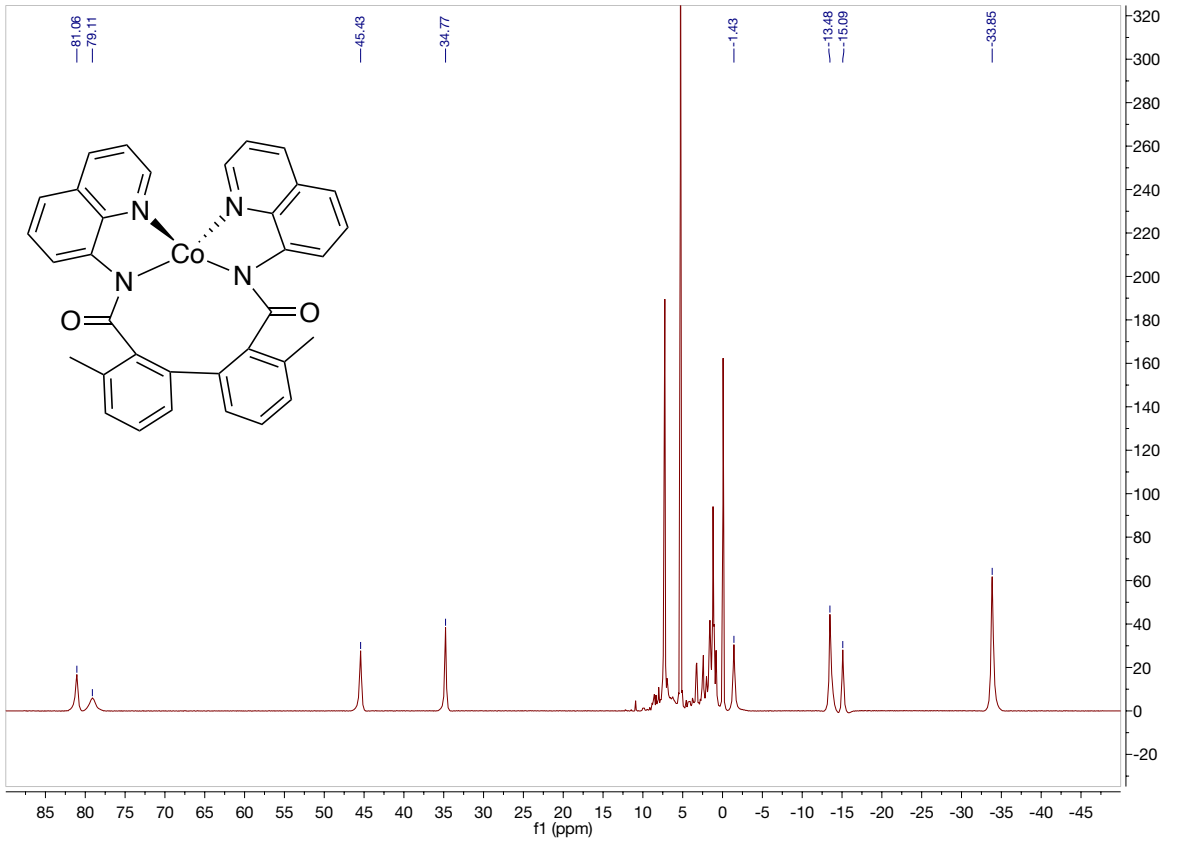


Figure S16: ^{1}H NMR spectrum of **Co^{II}(BQN-BQN)** (**6**) ($CDCl_3$, 400 MHz)

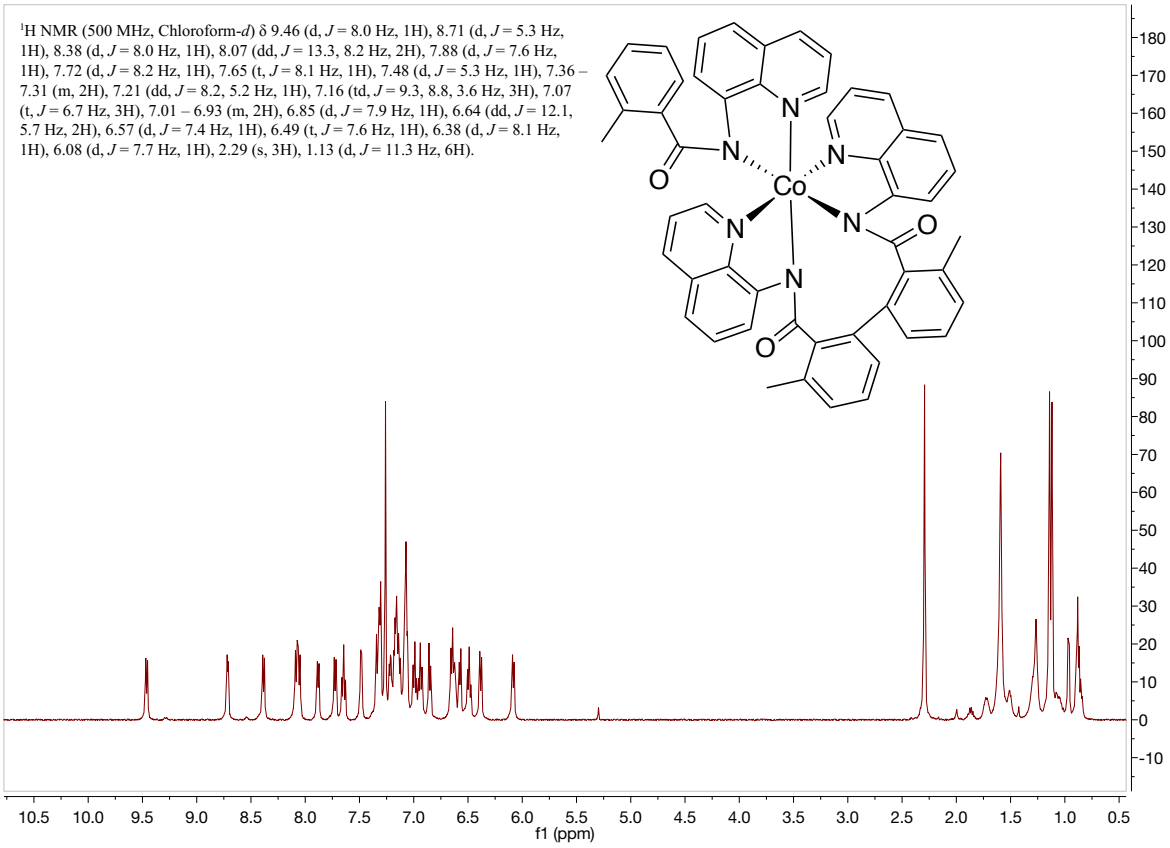


Figure S17: ^{1}H NMR spectrum of **Co^{III}(BQN)(BQN-BQN)** (**7**) ($CDCl_3$, 400 MHz)

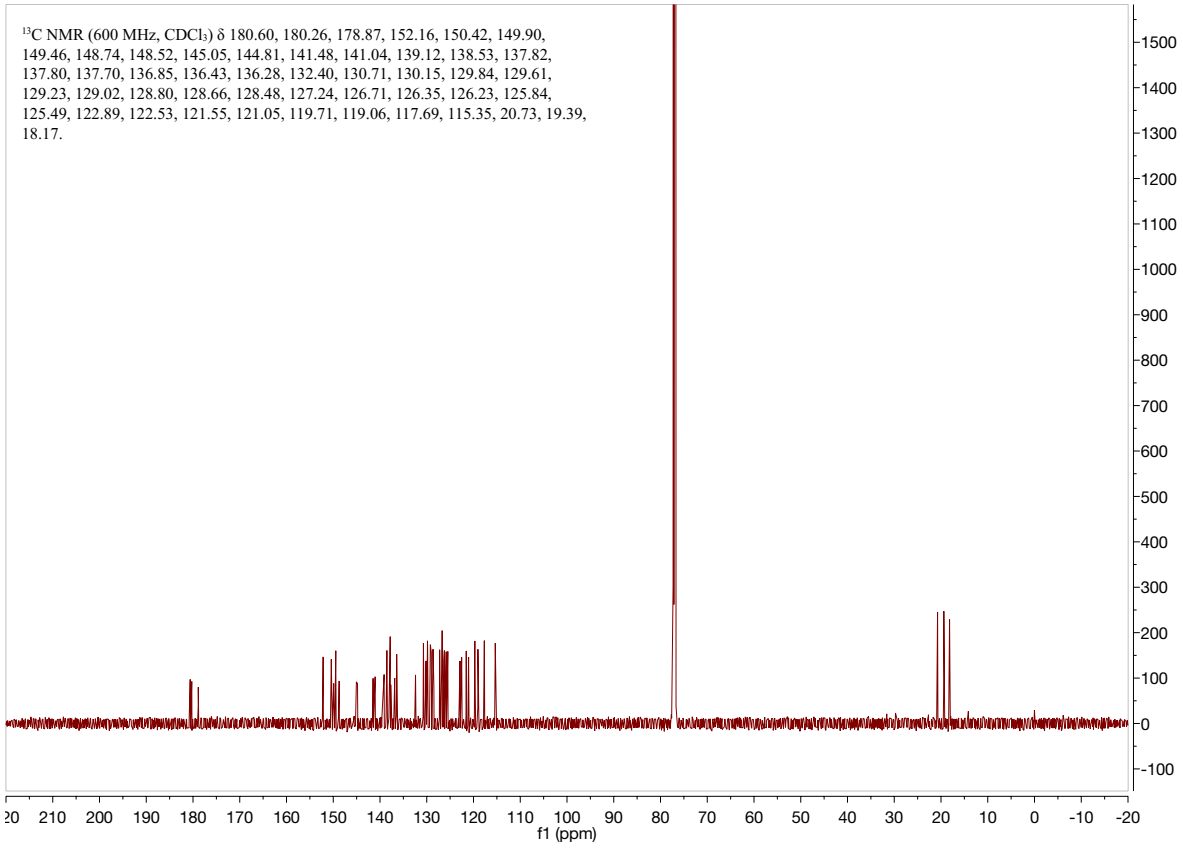


Figure S18: ^{13}C NMR spectrum of **Co^{III}(BQN)(BQN-BQN)** (**7**) ($CDCl_3$, 600 MHz)

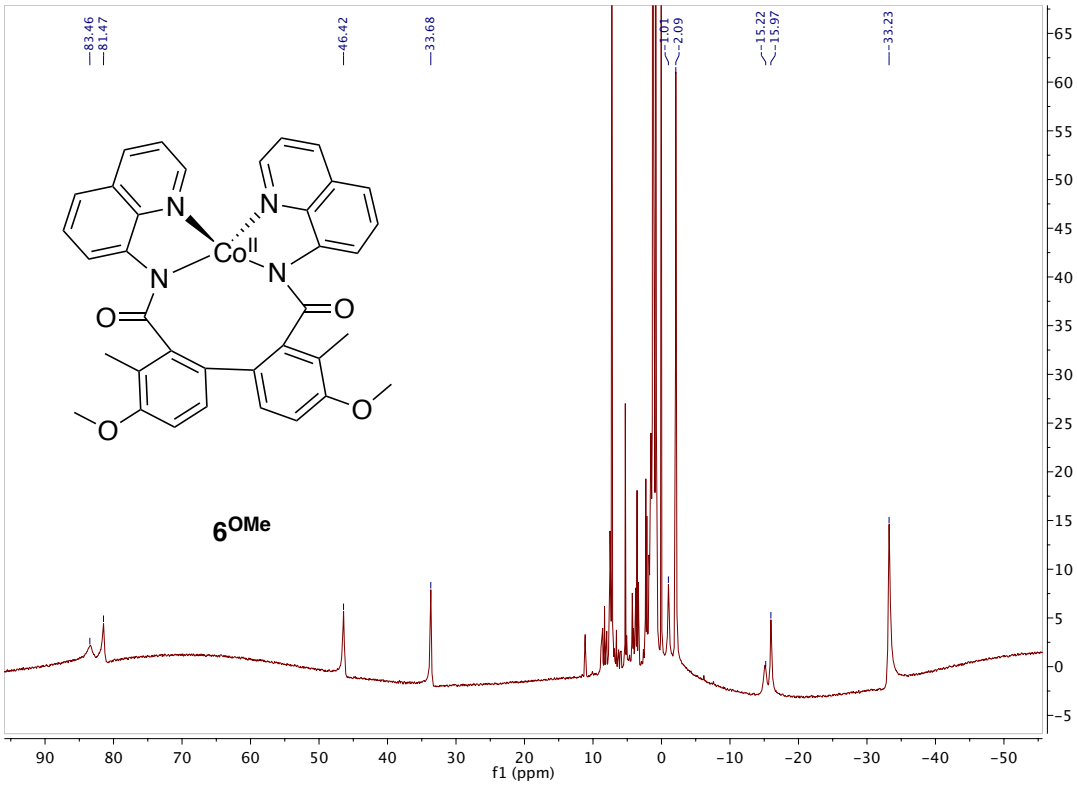


Figure S19. ^{1}H NMR spectrum of **Co^{II}(BQN^{OMe}-BQN^{OMe})** (**6^{OMe}**) ($CDCl_3$, 400 MHz)

11. X-Ray crystallographic data

Table S3. Crystal data for **$Co^{II}(BNQ)_2$ (1)**

	$Co^{II}(BNQ)_2$ (1)
Empirical formula	$C_{34}H_{26}CoN_4O_2$
Formula weight	581.52
T (K)	100.01
λ (Å)	0.71073
Crystal size (mm^3)	0.38 x 0.34 x 0.29
Crystal system	Orthorhombic
Space group	Pbca
a (Å)	12.1904
b (Å)	15.2935
c (Å)	23.3304
α (º)	90
β (º)	90
γ (º)	90
V ($Å^3$)	5420.00
Z	8
ρ_{calcd} (Mg/m^3)	1.425
GOF on F^2	1.033
*R*1, *wR*2 [$I > 2\alpha(I)$]	0.0355, 0.1006
CCDC #	1848074

Table S4. Crystal data for **(PPh$_4$)[Co^{II}(OPiv)$_2$(BQN)]** (**2**) and **(PPh$_4$)[Co^{II}(OAc)$_2$(BQN)]** (**3**).

	(PPh$_4$)[Co^{II}(OPiv)$_2$(BQN)] (2)	**(PPh$_4$)[Co^{II}(OAc)$_2$(BQN)] (3)**
Empirical formula	$C_{55}H_{61}CoN_2O_6P$	$C_{45}H_{39}CoN_2O_5P$
Formula weight	935.95	777.68
T (K)	101	155
λ (Å)	0.71073	0.71073
Crystal size (mm^3)	0.40 x 0.29 x 0.18	0.34 x 0.27 x 0.13
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	P-1
a (Å)	13.1076	10.5354
b (Å)	22.2355	12.5903
c (Å)	16.9979	15.1966
α (º)	90	79.8711
β (º)	101.0538	86.4335
γ (º)	90	78.9990
V (Å^3)	4862.18	1947.00
Z	4	2
ρ_{calcd} (Mg/m^3)	1.279	1.327
GOF on F^2	1.051	1.040
$R1$, $wR2$ [$I > 2\alpha(I)$]	0.0466, 0.1230	0.0475, 0.1280
CCDC #	1862102	1862295

Table S5. Crystal data for **$Co^{III}(H_2O)(BQN)(BQNN)$ (4)** and **$Co^{III}(py)(BQN)(BQNN)$ (4^{py})**

	$Co^{III}(H_2O)$ (BQN)(BQNN)	**$Co^{III}(py)$ (BQN)(BQNN)**
Empirical formula	$C_{38}H_{30}CoN_5O_2$	$C_{39}H_{30}CoN_5O_2$
Formula weight	670.63	659.61
T (K)	100(2)	100(2)
λ (Å)	1.54184	0.71073
Crystal size (mm^3)	0.24 x 0.11 x 0.09	0.31 x 0.13 x 0.13
Crystal system	Triclinic	Monoclinic
Space group	*P*-1	$P2_1/c$
a (Å)	12.5135(5)	12.7185(3)
b (Å)	16.2562(4)	9.1380(2)
c (Å)	17.4421(8)	30.1522(7)
α (º)	87.763(3)	90
β (º)	69.624(4)	97.574(2)
γ (º)	70.719(3)	90
V ($Å^3$)	3627.9(2)	3473.79(14)
Z	4	4
ρ_{calcd} (Mg/m^3)	1.228	1.261
GOF on F^2	1.029	1.034
*R*1, *wR*2 [$I > 2\alpha(I)$]	0.0932, 0.2364	0.0493, 0.1285
CCDC #	1988219	1862100

Table S6. Crystal data for **Co^{III}(PivO)(BQN-BQN)** (**5**) and **Co^{III}(BQN)(BQN-BQN)** (**7**)**.**

	Co^{III}(PivO)(BQN-BQN) (5)	**Co^{III}(BNQ)(BQN-BQN) (7)**
Empirical formula	$C_{45}H_{39}CoN_4O_4$	$C_{53}H_{41}Cl_4CoN_6O_3$
Formula weight	758.73	1010.65
T (K)	100	101
λ (Å)	0.71973	1.54184
Crystal size (mm^3)	0.30 x 0.20 x 0.18	0.44 x 0.12 x 0.08
Crystal system	Triclinic	Monoclinic
Space group	*P*-1	$P2_1/c$
a (Å)	10.9148	11.6863
b (Å)	12.2160	20.5971
c (Å)	14.5150	19.6222
α (º)	77.378	90
β (º)	74.686	106.514
γ (º)	89.375	90
V ($Å^3$)	1819.28	4528.3
Z	2	4
ρ_{calcd} (Mg/m^3)	1.385	1.482
GOF on F^2	1.056	1.017
*R*1, *wR*2 [$I > 2\alpha(I)$]	0.0393, 0.1124	0.0670, 0.1965
CCDC #	1848433	1862101

Table S7. Crystal data for **Co^{II}(BQN-BQN)** (**6**) and **Co^{II}(BQN^{OMe}-BQN^{OMe})** (6^{OMe})

	Co^{II}(BQN-BQN) (6)	**Co^{II}(BQN^{OMe}-BQN^{OMe}) (6^{OMe})**
Empirical formula	$C_{34}H_{24}CoN_4O_2$	$C_{36}H_{28}CoN_4O_4$
Formula weight	579.50	639.577
T (K)	100	106(1)
λ (Å)	1.54184	0.71073
Crystal size (mm^3)	0.2 x 0.1 x 0.04	0.21 x 0.14 x 0.14
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$C2/c$
a (Å)	11.1507	12.0679(2)
b (Å)	16.6952	16.0420(2)
c (Å)	14.6913	15.5043(2)
α (º)	90	90
β (º)	99.221	92.0380(1)
γ (º)	90	90
V ($Å^3$)	2699.64	2999.63(7)
Z	4	1
ρ_{calcd} (Mg/m^3)	1.426	1.416
GOF on F^2	1.064	1.057
*R*1, *wR*2 [$I > 2\alpha(I)$]	0.0817, 0.2325	0.0418, 0.1285
CCDC #	1850726	1862100

12. Basis set and density functional effect.

To validate impact of the used density functional (B3LYP-D3BJ) to the calculated rate-limiting steps of the *charge neutral* and *anionic* mechanisms of the Co-mediated dehydrogenative dimerization of AQ-directed benzamides we recalculated geometries and energies of the C–H activation and C–C coupling transition states and associated pre-reaction complexes at the M06/BS1 level of theory. We found that at the M06/BS1 level rate-determining step of the *charge neutral* pathway is the second C–H bond activation with a 31.3 kcal/mol activation barrier, since a barrier required for Its C–C coupling step is 24.1 kcal/mol. Meantime, the rate-limiting C–C coupling free energy barrier for the For the *anionic* pathway is 24.4 kcal/mol.

Table S8. Free energy barriers of the rate-limiting steps of the *charge neutral* and *anionic* mechanisms of the Co-mediated dehydrogenative dimerization of AQ-directed benzamides calculated by the M06 density functional.

Basis sets/Activation barrier (kcal/mol)	Neutral pathway (C-H activation)	Neutral pathway (C-C coupling)	Anionic pathway
6-31G(d,p)/Lanl2dz, BS1	31.3	24.1	24.4
6-311++G(d,p)/SDD, BS2	31.8	22.9	26.5

We also have validated the impact of the used basis sets (i.e. BS1) to the calculated critical energy barriers. For this reason, we performed single-point energy calculations (at the previously optimized geometries, at the B3LYP-D3BJ/BS1 and M06/BS1 levels of theory, respectively) of the C–H activation and C–C coupling transition states and associated pre-reaction complexes of the *charge neutral* and *anionic* pathways of the of the Co-mediated dehydrogenative dimerization of AQ-directed benzamides at the B3LYP-D3BJ/BS2 and M06/BS2 levels, where basis set BS2 = [6-311++G(d,p)] (for all atoms except Co) + SDD (and associated ECP for Co) and is larger than BS1. We found that at the M06/BS2//M06/BS1 level, the rate-determining C–H bond activation step of the *charge neutral* pathway requires a 31.8 kcal/mol free energy barrier. However, the free energy barrier required for the rate-limiting C–C coupling for the *anionic* pathway increased by 2.1 kcal, i.e. to 26.5 kcal/mol.

Table S9. Free energy barriers of the rate-limiting steps of the *charge neutral* and *anionic* mechanisms of the Co-mediated dehydrogenative dimerization of AQ-directed benzamides calculated by the B3LYP-D3BJ density functional.

Basis sets/Activation barrier (kcal/mol)	Neutral pathway (C-H activation)	Neutral pathway (C-C coupling)	Anionic pathway
6-31G(d,p)/Lanl2dz, BS1	32.8	32.6	29.5
6-311++G(d,p)/SDD, BS2	33.2	33.5	32.3

13. Meta-C-H activation: barriers and transition states.

We have examined the meta-C-H activation process. However, because of the significant aminoquinoline (AQ) ring constrains in the metallacycle structures, direct search for the meta-C-H activation transition states (TSs) in these metallacycles were failed: All our efforts led to dissociation of the coordinated AQ ligand. These results prompted us to extend our investigations and identify the meta-C-H TSs along with the dissociation of the binding ligand (see Figure S20). As you can see from the Table S10,

the calculated meta-C-H activation barriers are prohibitively high.

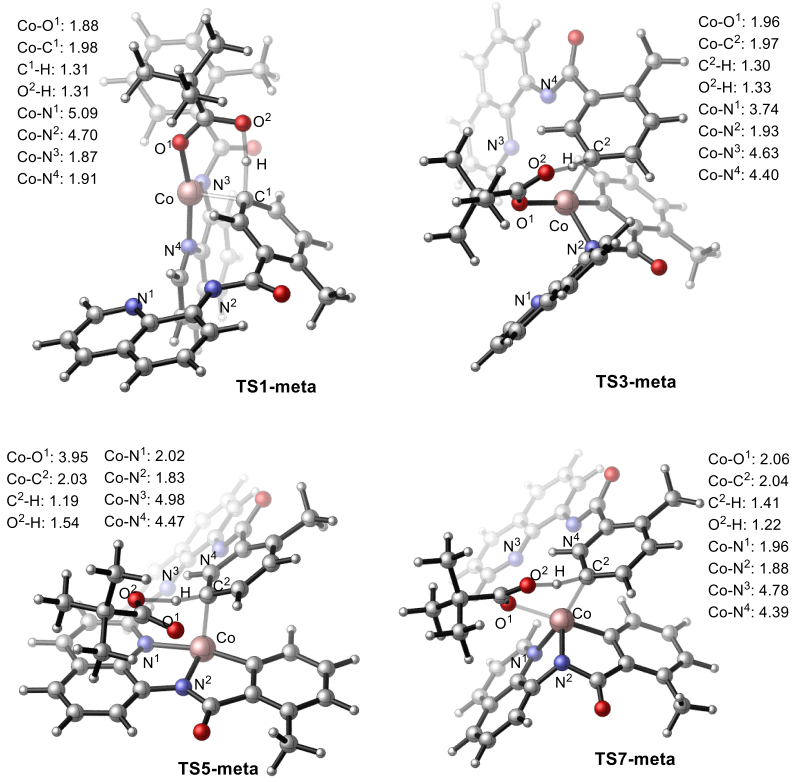
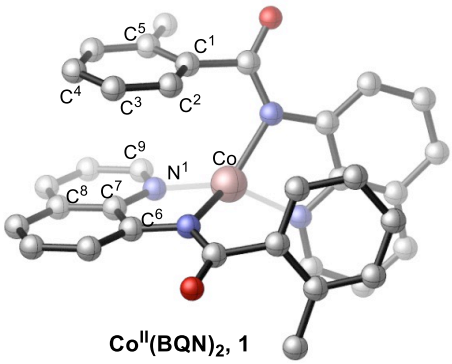


Figure S20. Geometries and key bond distances (in Å) for the meta-C-H activation TSs.

Table S10. Activation Barriers for the ortho- and meta-C-H Activation for **TS1**, **TS3**, **TS5**, and **TS7**.

TS	$\Delta G^{\neq}$ (ortho-C-H)	$\Delta G^{\neq}$ (meta-C-H)
TS1	5.1 kcal/mol	76.2 kcal/mol
TS3	32.8 kcal/mol	110.0 kcal/mol
TS5	22.2 kcal/mol	92.7 kcal/mol
TS7	27.4 kcal/mol	77.9kcal/mol

14. Distances between aryl ring and quinoline moiety in **$Co^{II}(BQN)_2$** showing the π-π stacking interactions.



$Co^{II}(BQN)_2$, 1

Bond distances (Å):

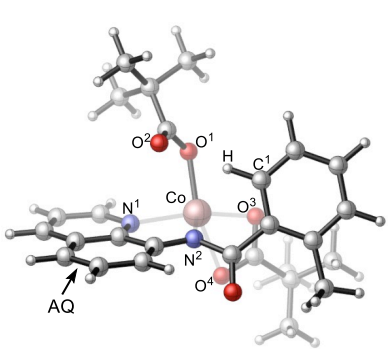
C^1-N^1: 3.37 C^2-C^6: 3.57 C^3-C^6: 3.44
C^3-C^7: 3.48 C^4-C^7: 3.59 C^4-C^8: 3.61
C^5-C^9: 3.42

Figure S21. Calculated key distances between the aryl ring and the aminoquinoline moiety (hydrogen atoms are omitted for clarity).

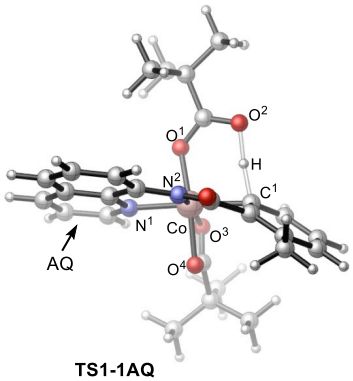
15. C-H activation on Co(III) species with one AQ ligand and two $PivO^-$ ligands.

We have calculated C-H activation in the Co(III) species with one AQ ligand and two $PivO^-$, i.e., in the Co(III)(BQNH)$(PivO)_2$ species. In general, we found that in this species the C-H cleavage occurs with a slightly larger energy barrier.

As shown in Figure S22, the same-state-to-same-state C-H activation barrier in Co(III)(BQNH)$(PivO)_2$ (with one AQ ligand, called as **1a-1AQ**) is 5.6 kcal/mol, while that is 5.1 kcal/mol in the species **1a** (with two AQ ligand). Moreover, if we consider the more stable quintet spin state of the pre-reaction complex (**1a-1AQ**, Figure S22), then the activation barrier increases to 13.6 kcal/mol. Thus, in the Co(III) complex with one AQ ligand, the C-H activation occurs with higher energy barrier.



1a-1AQ



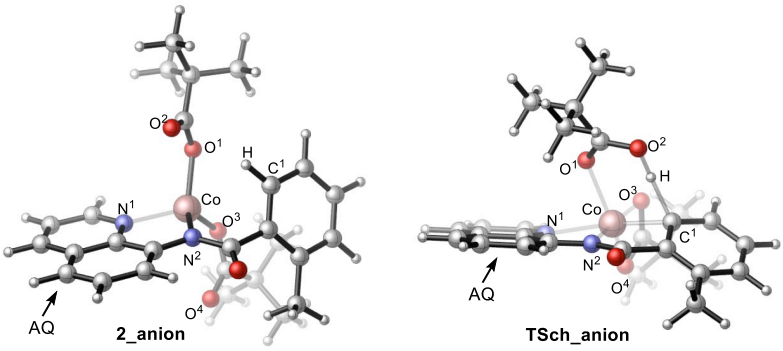
TS1-1AQ

		ΔG(ΔH) (kcal/mol)	spin density (|e|)						bond distances (Å)							
			Co	N^2	O^1	O^3	O^4	ΣAQ	Co-N^1	Co-N^2	Co-O^1	Co-O^3	Co-O^4	Co-C^1	O^2-H	C^1-H
1a-1AQ	singlet	0.0(0.0)	-	-	-	-	-	-	1.91	1.89	1.88	1.98	1.96	2.38	2.11	1.09
	triplet	0.1(5.2)	1.77	0.03	0.02	-0.03	0.01	0.14	2.10	1.86	1.87	1.98	1.98	2.95	2.17	1.09
	quintet	-8.0(-2.8)	2.71	0.48	0.08	0.06	0.06	0.58	2.15	2.13	1.96	2.06	2.21	3.30	2.31	1.09
TS1-1AQ	singlet	5.6(4.9)	-	-	-	-	-	-	1.96	1.89	1.92	1.98	1.96	2.07	1.31	1.30
	triplet	11.7(13.7)	1.84	0.06	0.10	0.01	0.06	0.02	1.98	1.87	2.08	1.96	2.33	2.08	1.38	1.27
	quintet	17.5(22.3)	2.67	0.43	0.05	0.06	0.06	0.54	2.15	2.09	2.13	2.10	2.19	2.22	1.16	1.49

Figure S22. Energies, spin densities and bond distances for the singlet, triplet, and quintet spin states for the intermediate (**1a-1AQ**) and transition state (**TS1-1AQ**) with one AQ ligand.

16. C-H activation on the Co(II) species with closed-shell BQN ligand.

We have calculated the C-H cleavage barrier in the Co(II) complex with closed-shell BQN ligand (complex **2**). The counter cation, PPh_4^+, is not included to these model calculations. For the corresponding quartet and doublet spin state species, we found that the C-H cleavage occurs with over 30.8 kcal/mol activation barriers, which are much higher than that (only 5.1 kcal/mol) reported for **1a**.



		ΔG(ΔH) (kcal/mol)	spin density (|e|) Co	N^2	O^1	O^3	O^4	ΣAQ	bond distances (Å) Co-N^1	Co-N^2	Co-O^1	Co-O^3	Co-O^4	Co-C^1	O^2-H	C^1-H
2_anion	doublet	16.9(14.7)	0.97	-0.02	0	-0.01	-0.01	0.06	2.15	1.95	1.95	2.01	2.04	2.91	2.19	1.09
	quartet	0.0(0.0)	2.68	0.07	0.07	0.08	0.01	0.06	2.08	2.03	1.97	1.95	3.16	3.07	2.61	1.09
TSch_anion	doublet	31.4(28.5)	1.02	-0.02	0.03	-0.01	0.02	0.02	1.97	1.92	2.28	1.95	2.61	2.07	1.28	1.37
	quartet	30.8(29.2)	2.65	0.07	0.03	0.04	0.05	0.04	2.19	2.06	2.23	2.25	2.14	2.18	1.10	1.60

Figure S23. Energies, spin densities and bond distances for the doublet and quartet spin states for the intermediate (**2_anion**) and transition state (**TSch_anion**) for Co(II) complexes with closed-shell BQN ligand.

17. C-C coupling after the dissociation of PivOH from the complex D'.

We have calculated the C-C coupling after the dissociation of pivalic acid (PivOH) from **D'** (see **TS6**). The results show that this process (Figure S24, red pathway) is by 4.2 kcal/mol less favorable than that without pivalic acid dissociation (Figure S24, black pathway).

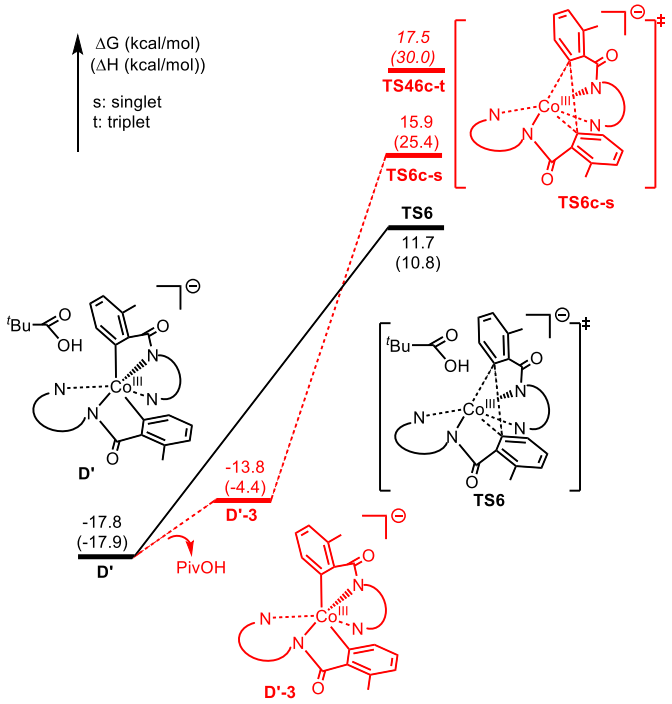


Figure S24. Comparison of the C-C coupling process from complex **D'** with (in black) and without (in red) presence of PivOH.

18. The calculated total energies (in hartree) and cartesian coordinates (in Å) for all reported structures.

1-q

Energy = -2172.52262291 ZPE = -2171.864445
H = -2171.819964, G = -2171.942912

C	-2.177630	1.970234	0.659149
C	-2.983502	3.140528	0.589029
C	-4.314473	3.109772	1.005892
C	-4.893858	1.946920	1.508361
C	-4.136453	0.743717	1.604801
C	-2.787392	0.750541	1.174385
N	-2.011702	-0.352380	1.206489
C	-2.514364	-1.489511	1.678536
C	-3.834306	-1.590715	2.151408
C	-4.650716	-0.475750	2.105143
N	-0.891454	1.873528	0.323424
H	-4.908688	4.014900	0.939086
H	-5.929186	1.945825	1.833851
H	-5.680585	-0.524028	2.444948
H	-4.197871	-2.539384	2.528583
H	-1.846102	-2.343918	1.655562
C	-0.197169	2.919144	-0.344119
C	1.109512	3.274904	0.261910
C	2.164012	3.795352	-0.524097
C	1.276066	3.094697	1.643953
C	3.357367	4.126817	0.128732
C	2.468998	3.441798	2.272446
C	3.513785	3.961706	1.506737
H	0.455952	2.685966	2.225574
H	4.185819	4.510888	-0.459941
H	2.582154	3.305170	3.343295
H	4.454758	4.230503	1.977759
O	-0.658086	3.423673	-1.359613
H	-2.552812	4.052959	0.196614
C	2.064384	3.939035	-2.021738
H	1.717124	3.003626	-2.470607
H	1.343488	4.710496	-2.303703
H	3.038371	4.193170	-2.447783
C	0.844812	-2.881481	0.025520
C	1.293760	-4.136601	-0.391445
C	2.313672	-4.816000	0.311413
C	2.905941	-4.285367	1.438554
C	2.479747	-3.018256	1.912129
C	1.457057	-2.317746	1.204854
N	1.027957	-1.087299	1.620662
C	1.547607	-0.534195	2.705755
C	2.553007	-1.161475	3.470224
C	3.018837	-2.393851	3.066560
N	-0.128214	-2.089081	-0.559550
H	2.636171	-5.786068	-0.056931
H	3.688209	-4.817795	1.970707
H	3.801673	-2.900942	3.623815
H	2.948555	-0.664841	4.349112
H	1.173012	0.449464	2.970115
C	-0.974759	-2.513197	-1.531592
C	-2.012302	-1.458404	-1.858019
C	-3.378950	-1.716997	-1.618422
C	-1.601351	-0.195992	-2.316398
C	-4.288910	-0.667666	-1.790431
C	-2.531269	0.833240	-2.496465
C	-3.875595	0.600974	-2.212746
H	-0.549958	-0.036830	-2.544454
H	-5.340578	-0.843662	-1.577982
H	-2.191397	1.813844	-2.812562
H	-4.605687	1.398084	-2.319955
O	-1.012365	-3.628374	-2.080661
H	0.844231	-4.579986	-1.267873
C	-3.851436	-3.077037	-1.161802
H	-4.919872	-3.065222	-0.930952
H	-3.660898	-3.831105	-1.930321
H	-3.313867	-3.408448	-0.267226
Co	-0.140598	-0.134213	0.136127
C	2.123379	-0.046020	-1.819351
O	1.353889	0.542312	-0.956237
O	1.731107	-0.482981	-2.910476
C	3.631951	-0.144332	-1.469357
C	4.071365	-1.609720	-1.657518
H	5.149385	-1.709533	-1.485236
H	3.551905	-2.269304	-0.954323
H	3.844762	-1.949374	-2.671310
C	4.388547	0.755796	-2.469101
H	4.117586	1.808425	-2.331983
H	5.471085	0.664461	-2.322767
H	4.149353	0.470682	-3.497411
C	3.926082	0.311296	-0.034138
H	5.006649	0.288590	0.152360
H	3.563562	1.325883	0.139993
H	3.444645	-0.346100	0.692714

1-s

Energy = -2172.52822239 ZPE = -2171.865903
H = -2171.823172 G = -2171.938722

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C	-3.804484	3.424199	1.566428
C	-4.578973	2.305575	1.802724
C	-4.015166	1.022511	1.592568
C	-2.672171	0.940962	1.126343
N	-2.085032	-0.263327	0.861543
C	-2.739688	-1.394435	1.091438
C	-4.061412	-1.399611	1.574409
C	-4.698439	-0.199149	1.811212
N	-0.532289	1.838494	0.583158
H	-4.229207	4.411514	1.722972
H	-5.606003	2.389555	2.142464
H	-5.723708	-0.177487	2.168965
H	-4.558630	-2.348063	1.740503
H	-2.210003	-2.312718	0.873016
C	0.212726	2.831800	-0.037233
C	1.682575	2.862052	0.256096
C	2.631592	3.179221	-0.740615
C	2.086460	2.714035	1.587323
C	3.965493	3.338278	-0.348849
C	3.420179	2.884171	1.960618
C	4.363900	3.200190	0.984500
H	1.335243	2.492753	2.337028
H	4.709616	3.573858	-1.105280
H	3.714258	2.776208	3.000461
H	5.407635	3.335947	1.253130
O	-0.289937	3.718287	-0.739304
H	-1.900451	4.241911	0.955096
C	2.249191	3.302239	-2.196738
H	1.753669	2.389195	-2.543252
H	1.552541	4.128889	-2.350981
H	3.134930	3.461974	-2.817539
C	0.461681	-2.777490	0.118332
C	0.817576	-4.089634	-0.178797
C	1.557880	-4.848042	0.760361
C	1.940100	-4.341642	1.986674
C	1.582602	-3.012582	2.334232

C	0.853183	-2.250073	1.385337
N	0.474794	-0.962244	1.656129
C	0.750687	-0.394726	2.818800
C	1.459013	-1.095262	3.816695
C	1.881533	-2.385517	3.571441
N	-0.269369	-1.867987	-0.634179
H	1.828633	-5.866063	0.496830
H	2.499550	-4.944366	2.694487
H	2.439757	-2.935153	4.323343
H	1.666878	-0.600518	4.758010
H	0.412707	0.624490	2.947785
C	-0.972160	-2.150684	-1.771204
C	-1.879026	-1.005965	-2.149482
C	-3.267635	-1.217234	-2.267101
C	-1.351939	0.301194	-2.201945
C	-4.088991	-0.090018	-2.401147
C	-2.198910	1.411807	-2.323950
C	-3.572225	1.211248	-2.413702
H	-0.268078	0.421231	-2.276567
H	-5.163878	-0.234439	-2.474154
H	-1.772409	2.409360	-2.312602
H	-4.247671	2.057564	-2.495118
O	-0.955677	-3.231201	-2.371736
H	0.525154	-4.514226	-1.128110
C	-3.874260	-2.598142	-2.189160
H	-4.959889	-2.553795	-2.305692
H	-3.457121	-3.255389	-2.955134
H	-3.656877	-3.068552	-1.223301
Co	-0.268273	-0.092485	0.130371
C	2.148264	-0.222919	-1.522811
O	1.577771	0.090884	-0.399083
O	1.615107	-0.199763	-2.640328
C	3.626686	-0.669255	-1.394005
C	3.673909	-2.148466	-1.837715
H	4.707422	-2.512090	-1.815895
H	3.076990	-2.779317	-1.171386
H	3.285956	-2.259546	-2.853842
C	4.477973	0.182601	-2.353850
H	4.475853	1.233122	-2.049671
H	5.515453	-0.169869	-2.351997
H	4.087820	0.117578	-3.372571
C	4.148651	-0.541910	0.043481
H	5.193209	-0.871818	0.089393
H	4.094572	0.491103	0.392677
H	3.562244	-1.160975	0.728279

1-t

Energy = -2172.52526585 ZPE = -2171.864091 H = -2171.821058 G = -2171.938126

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C	2.438325	-3.313065	0.901499
C	3.779987	-3.440652	1.325391
C	4.545721	-2.350370	1.691682
C	3.975677	-1.050360	1.639471
C	2.638780	-0.926509	1.183407
N	2.028229	0.281982	1.063920
C	2.656495	1.387245	1.446763
C	3.973239	1.352382	1.939715
C	4.637637	0.142836	2.016127
N	0.519271	-1.737921	0.531692
H	4.212630	-4.435415	1.367348
H	5.571871	-2.470887	2.023055
H	5.663510	0.095964	2.368945
H	4.453474	2.278717	2.232005
H	2.108139	2.314074	1.330832
C	-0.314161	-2.748978	-0.016644
C	-1.714974	-2.783961	0.483033
C	-2.748560	-3.397774	-0.265131
C	-1.989577	-2.240171	1.747004
C	-4.032021	-3.420046	0.297457
C	-3.268531	-2.286101	2.291530
C	-4.297356	-2.877797	1.556373
H	-1.177432	-1.777962	2.293755
H	-4.841884	-3.871530	-0.269147
H	-3.460869	-1.860703	3.271718
H	-5.305681	-2.916811	1.958431
O	0.126558	-3.564667	-0.820907
H	1.878404	-4.197103	0.630192
C	-2.530992	-3.984556	-1.638318
H	-2.013862	-3.268050	-2.281805
H	-1.906268	-4.880003	-1.589578
H	-3.488806	-4.246269	-2.096202
C	-0.584884	2.777662	-0.154190
C	-1.037398	3.927043	-0.798763
C	-2.014036	4.755553	-0.200252
C	-2.550553	4.472230	1.037714
C	-2.116115	3.316149	1.736859
C	-1.140805	2.468200	1.136512
N	-0.699031	1.338603	1.760989
C	-1.151756	1.031390	2.964083
C	-2.109834	1.817574	3.640118
C	-2.595939	2.948017	3.020406
N	0.366353	1.873859	-0.619194
H	-2.343683	5.638205	-0.740338
H	-3.295908	5.119004	1.490146
H	-3.343856	3.569758	3.504406
H	-2.452063	1.517544	4.624173
H	-0.754213	0.128046	3.416249
C	1.291553	2.171198	-1.587808
C	2.243259	1.038953	-1.872516
C	3.637938	1.248856	-1.788038
C	1.736567	-0.240445	-2.148073
C	4.477767	0.138905	-1.934599
C	2.597578	-1.331185	-2.300376
C	3.971751	-1.142199	-2.180052
H	0.665815	-0.392715	-2.277229
H	5.551625	0.279379	-1.841396
H	2.180492	-2.317603	-2.475765
H	4.653345	-1.982758	-2.272318
O	1.406066	3.263463	-2.160612
H	-0.627241	4.182990	-1.764286
C	4.225665	2.611879	-1.508855
H	5.306518	2.546182	-1.359777
H	4.021169	3.301044	-2.332171
H	3.785812	3.063090	-0.613578
Co	0.267221	0.129903	0.230486
C	-1.969883	-0.287326	-1.587878
O	-1.524589	0.006427	-0.409939
O	-1.328349	-0.850985	-2.486610
C	-3.419373	0.193215	-1.848899
C	-3.281500	1.467626	-2.712869
H	-4.273113	1.866614	-2.955305
H	-2.722898	2.242542	-2.178332
H	-2.758750	1.246363	-3.648328
C	-4.185668	-0.884074	-2.634029
H	-4.345864	-1.774879	-2.020019
H	-5.165904	-0.501159	-2.939329
H	-3.629284	-1.178871	-3.526581

C	-4.157745	0.527388	-0.543721
H	-5.178731	0.857575	-0.768629
H	-4.214143	-0.348040	0.109226
H	-3.648333	1.324337	0.003262

20q

Energy = -1678.48279594 ZPE = -1677.950014 H = -1677.913006 G = -1678.023115

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C	-2.661052	1.299027	-2.268842
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C	-2.274225	3.701263	-2.184223
C	-1.094109	3.514110	-1.408104
C	-0.704616	2.195997	-1.061421
N	0.414506	1.943095	-0.347193
C	1.170592	2.956657	0.063784
C	0.862326	4.298222	-0.227275
C	-0.271224	4.577623	-0.966007
N	-1.039736	-0.131282	-1.045470
H	-3.917328	2.768779	-3.195493
H	-2.574538	4.709528	-2.452092
H	-0.539734	5.600324	-1.212593
H	1.513116	5.088683	0.128341
H	2.043135	2.682736	0.648108
C	-1.622495	-1.395309	-1.319324
C	-0.698097	-2.507222	-0.969408
C	-0.955714	-3.834863	-1.406088
C	0.421584	-2.171435	-0.157629
C	-0.055309	-4.826437	-1.003656
C	1.278181	-3.215891	0.220650
C	1.046080	-4.529302	-0.193770
H	-0.883724	-1.912093	1.453671
H	-0.220590	-5.850732	-1.328037
H	2.141620	-2.998619	0.847392
H	1.718535	-5.329741	0.107194
O	-2.764211	-1.529739	-1.758663
H	-3.260000	0.459567	-2.590024
C	-2.129484	-4.218192	-2.275770
H	-2.042651	-5.259647	-2.598628
H	-3.074588	-4.094651	-1.738795
H	-2.202064	-3.579091	-3.160442
Co	0.711962	-0.142775	0.182533
C	-1.657108	-0.326994	2.140555
O	-0.658882	0.344838	1.879309
O	-1.709611	-1.637252	1.922071
C	-2.959359	0.269757	2.655052
C	-3.530111	-0.590571	3.799302
H	-4.476769	-0.159697	4.139278
H	-3.715268	-1.615815	3.471022
H	-2.843580	-0.618796	4.651543
C	-2.713012	1.710516	3.124936
H	-2.307226	2.322526	2.315434
H	-3.656248	2.153082	3.458595
H	-2.005093	1.738096	3.958679
C	-3.935325	0.264427	1.449933
H	-4.898687	0.676299	1.765638
H	-3.553307	0.880578	0.629921
H	-4.095254	-0.748990	1.072916
C	3.213880	0.118109	0.126139
O	2.692660	-0.064040	-1.003817
O	2.477087	0.197527	1.180477
C	4.731632	0.261586	0.303412
C	5.206055	-0.843003	1.271051
H	6.284551	-0.756391	1.442900
H	4.691140	-0.763222	2.231703
H	5.007815	-1.838057	0.856925
C	5.451700	0.130546	-1.045364
H	5.117816	0.901166	-1.746006
H	6.533218	0.235301	-0.905774
H	5.255245	-0.843486	-1.502420
C	5.007141	1.648243	0.922900
H	6.081031	1.779859	1.094174
H	4.671837	2.449991	0.254803
H	4.485762	1.755333	1.877779

20s

Energy = -1678.52738508 ZPE = -1677.99001 H = -1677.954826 G = -1678.056216

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C	-3.633424	0.921312	-2.770984
C	-3.665036	2.169175	-2.181653
C	-2.646105	2.527078	-1.261465
C	-1.620766	1.582891	-0.974948
N	-0.614676	1.862971	-0.093579
C	-0.572162	3.035327	0.516120
C	-1.544364	4.033409	0.287510
C	-2.573426	3.777558	-0.593487
N	-0.552238	-0.519160	-1.173683
H	-4.411813	0.643470	-3.476012
H	-4.453460	2.879916	-2.408460
H	-3.337852	4.525226	-0.785375
H	-1.470206	4.980866	0.809265
H	0.250984	3.184055	1.207569
C	-0.225829	-1.757777	-1.664298
C	0.937576	-2.318001	-0.898081
C	1.511980	-3.587095	-1.141426
C	1.417470	-1.487372	0.137526
C	2.572185	-3.982056	-0.313323
C	2.470010	-1.911007	0.948575
C	3.044894	-3.165209	0.717547
H	-0.258089	-2.395528	0.961642
H	3.031915	-4.953204	-0.477461
H	2.840371	-1.268458	1.741366
H	3.865134	-3.510878	1.341784
O	-0.813760	-2.340791	-2.585454
H	-2.618072	-0.990875	-2.970606
C	1.028653	-4.506870	-2.236245
H	1.632880	-5.417875	-2.268238
H	-0.019422	-4.781022	-2.085833
H	1.070514	-4.015910	-3.212122
Co	0.537140	0.213320	0.186839
C	-1.509151	-1.217858	1.744489
O	-0.796614	-0.217386	1.572838
O	-1.148327	-2.431636	1.384814
C	-2.904815	-1.107677	2.331701
C	-3.112424	-2.178069	3.420910
H	-4.135503	-2.109366	3.801900
H	-2.957906	-3.184224	3.024533
H	-2.425421	-2.025252	4.259236
C	-3.120350	0.303809	2.897867
H	-2.988051	1.063352	2.123155
H	-4.136998	0.382157	3.293430
H	-2.417210	0.517294	3.708083
C	-3.875110	-1.355086	1.145620
H	-4.903983	-1.250676	1.502568
H	-3.713103	-0.629280	0.342325
H	-3.748525	-2.360228	0.735511

C	2.523032	1.407553	0.223894
O	1.988973	0.971469	-0.854225
O	1.896412	1.131895	1.303518
C	3.817960	2.196381	0.235170
C	4.827712	1.412805	1.103082
H	5.773441	1.961510	1.151740
H	4.447291	1.281230	2.119258
H	5.026259	0.423231	0.678443
C	4.353425	2.371137	-1.193052
H	3.637960	2.910773	-1.819842
H	5.288209	2.939693	-1.167493
H	4.551222	1.402834	-1.661260
C	3.525713	3.569990	0.878528
H	4.450216	4.152869	0.937000
H	2.802122	4.137111	0.283390
H	3.125791	3.450588	1.888944

20t

Energy = -1678.52346142 ZPE = -1677.987667 H = -1677.951549 G = -1678.056629

C	-1.700767	0.328077	-1.546603
C	-2.853290	0.073630	-2.284614
C	-3.785302	1.111204	-2.531874
C	-3.599383	2.394961	-2.063901
C	-2.434023	2.698546	-1.311435
C	-1.493818	1.661685	-1.065918
N	-0.354373	1.883567	-0.343226
C	-0.103141	3.085347	0.152186
C	-0.980558	4.171075	-0.045451
C	-2.137202	3.976807	-0.773051
N	-0.696527	-0.565255	-1.177239
H	-4.674997	0.874474	-3.107745
H	-4.327250	3.176188	-2.258169
H	-2.831663	4.795592	-0.937922
H	-0.737028	5.138350	0.378779
H	0.812237	3.178665	0.727280
C	-0.622111	-1.900117	-1.544538
C	0.531163	-2.542670	-0.844108
C	0.883037	-3.905368	-0.962938
C	1.251489	-1.683156	0.004509
C	1.970754	-4.353218	-0.200083
C	2.325231	-2.148854	0.758284
C	2.678934	-3.498508	0.649653
H	-0.491635	-2.207304	1.338135
H	2.264482	-5.397219	-0.269063
H	2.871553	-1.477328	1.412026
H	3.511202	-3.888287	1.229939
O	-1.401775	-2.468899	-2.311213
H	-3.029591	-0.922564	-2.663032
C	0.134754	-4.863106	-1.856649
H	0.577894	-5.861358	-1.807805
H	-0.918468	-4.927498	-1.568894
H	0.141960	-4.521447	-2.895372
Co	0.625047	0.142452	-0.026775
C	-1.597555	-0.802443	1.940886
O	-0.710310	0.037655	1.791757
O	-1.402519	-2.093263	1.679980
C	-3.007105	-0.471468	2.409229
C	-3.287771	-1.243462	3.717652
H	-4.304231	-1.021338	4.056167
H	-3.200497	-2.322253	3.566403
H	-2.592313	-0.945455	4.508865
C	-3.124036	1.042748	2.636334
H	-2.928718	1.595538	1.713100
H	-4.135977	1.282450	2.975753
H	-2.413563	1.385766	3.393184
C	-3.993966	-0.922596	1.306234
H	-5.015170	-0.691349	1.624090
H	-3.801468	-0.399156	0.364694
H	-3.921181	-1.997646	1.125353
C	2.892525	1.122229	-0.008827
O	2.529148	0.725075	-1.144804
O	2.093913	0.967139	0.994618
C	4.249702	1.777054	0.246584
C	5.029456	0.863063	1.217709
H	6.011202	1.298636	1.430672
H	4.488538	0.745390	2.160431
H	5.184901	-0.130392	0.783177
C	5.022774	1.940038	-1.069309
H	4.474974	2.575073	-1.771526
H	5.995959	2.401645	-0.872984
H	5.189448	0.972522	-1.550622
C	4.008656	3.152335	0.903617
H	4.967253	3.634565	1.121618
H	3.441723	3.812080	0.237339
H	3.452117	3.044632	1.838145

21n

Energy = -3357.04215266 ZPE = -3355.973102 H = -3355.899557 G = -3356.086562

C	-1.992124	1.880143	2.074035
C	-2.203434	2.550899	3.308197
C	-1.802296	3.880496	3.469655
C	-1.211890	4.593944	2.433786
C	-0.983995	3.978255	1.169003
C	-1.329188	2.614569	1.001121
N	-1.119516	1.954705	-0.160896
C	-0.603951	2.614026	-1.194496
C	-0.264517	3.975906	-1.134005
C	-0.442881	4.658406	0.053902
N	-2.388325	0.654825	1.722372
H	-1.964773	4.366141	4.426441
H	-0.916991	5.628986	2.573335
H	-0.165054	5.702915	0.146555
H	0.159950	4.460609	-2.004887
H	-0.451274	2.036900	-2.097057
C	-3.097939	-0.258701	2.533471
C	-3.812272	-1.263140	1.704587
C	-4.740612	-2.169133	2.287363
C	-3.522912	-1.257937	0.314151
C	-5.395955	-3.057648	1.429023
C	-4.232929	-2.154028	-0.496289
C	-5.153950	-3.050233	0.051127
H	-6.113432	-3.760731	1.844813
H	-4.051040	-2.173630	-1.569026
H	-5.682939	-3.754849	-0.587683
O	-3.091514	-0.205711	3.764416
H	-2.670287	2.007480	4.117264
C	-5.050464	-2.213356	3.764968
H	-5.373335	-1.237035	4.138349
H	-5.835568	-2.947182	3.970042
H	-4.161832	-2.474933	4.346979
Co	-1.883054	-0.081789	-0.180318
C	0.310096	-2.186790	0.531648
O	-0.466430	-1.283107	0.921572
O	1.487372	-1.903745	0.099950
C	-0.149026	-3.650975	0.504130
C	-0.906938	-3.827955	-0.832246

H	-1.294311	-4.850316	-0.899989
H	-1.741349	-3.128398	-0.907185
H	-0.236977	-3.657068	-1.678723
C	1.039910	-4.624199	0.549205
H	1.647753	-4.466021	1.442716
H	0.666298	-5.653467	0.563713
H	1.682286	-4.518767	-0.329094
C	-1.103095	-3.917955	1.681142
H	-1.489315	-4.940751	1.616066
H	-0.581117	-3.810018	2.635889
H	-1.943371	-3.222513	1.666742
O	-3.347316	1.046016	-1.679597
C	-3.825309	0.537725	-2.694095
O	-3.224849	-0.448751	-3.347607
C	-5.176804	0.974178	-3.256854
C	-5.456571	0.349405	-4.631645
H	-6.427875	0.694846	-4.999709
H	-4.692154	0.635703	-5.360057
H	-5.478460	-0.741901	-4.575496
C	-6.242152	0.513505	-2.233630
H	-6.233274	-0.574419	-2.114463
H	-6.058140	0.964110	-1.254537
H	-7.235891	0.816326	-2.578261
C	-5.180938	2.513148	-3.354036
H	-4.960798	2.963269	-2.383104
H	-4.434976	2.864362	-4.075146
H	-6.164463	2.859871	-3.686073
C	2.161253	2.477766	1.602521
C	2.067176	3.426011	2.624746
C	2.375905	4.784189	2.391428
C	2.775742	5.248721	1.155151
C	2.877822	4.331307	0.078826
C	2.562438	2.958895	0.305980
N	2.609824	2.044564	-0.699161
C	2.952538	2.413674	-1.922384
C	3.289429	3.747002	-2.238121
C	3.252795	4.697147	-1.239088
N	1.996141	1.101536	1.694922
H	2.284661	5.480213	3.220892
H	3.003693	6.297139	0.989589
H	3.498990	5.734341	-1.449729
H	3.566528	4.005594	-3.254252
H	2.944300	1.630144	-2.672289
C	1.551850	0.511707	2.854841
C	2.036420	-0.901303	3.028690
C	1.353265	-1.887619	3.787304
C	3.260881	-1.255448	2.496485
C	1.971022	-3.137510	3.939401
C	3.904101	-2.464940	2.627964
C	3.221708	-3.430638	3.383338
H	1.455385	-3.906566	4.508089
H	4.871811	-2.672659	2.181270
H	3.661948	-4.413740	3.530220
O	0.880487	1.061292	3.738573
H	1.735964	3.114081	3.603961
C	-0.006527	-1.629738	4.385447
H	-0.404197	-2.537564	4.848072
H	0.037095	-0.834588	5.132410
H	-0.705234	-1.297085	3.614824
Co	1.996757	0.089388	-0.095761
C	0.148610	-0.581751	-2.538043
O	1.082475	0.024190	-1.954008
O	-1.013239	-0.757238	-2.033237
C	0.405600	-1.043164	-3.985501
C	-0.448819	-2.263855	-4.366970
H	-0.245379	-2.537131	-5.407498
H	-0.209683	-3.127439	-3.740685
H	-1.518459	-2.065820	-4.278900
C	0.026342	0.161290	-4.880948
H	0.616958	1.044585	-4.616742
H	0.219322	-0.079575	-5.931448
H	-1.035585	0.407077	-4.777067
C	1.897884	-1.381664	-4.155898
H	2.091517	-1.712126	-5.181512
H	2.524886	-0.513170	-3.945599
H	2.197164	-2.183875	-3.473023
O	3.912658	-0.551152	-0.808120
C	4.290273	-1.676401	-1.174363
O	3.585424	-2.770343	-1.007499
C	5.650032	-1.843712	-1.846432
C	5.870514	-3.278546	-2.346578
H	6.853527	-3.350218	-2.822246
H	5.832617	-3.997620	-1.524196
H	5.112111	-3.562886	-3.081620
C	5.714850	-0.847766	-3.024768
H	4.970854	-1.094632	-3.789098
H	5.530028	0.172997	-2.681421
H	6.705648	-0.890722	-3.487094
C	6.717373	-1.473288	-0.790386
H	6.562079	-0.456410	-0.420460
H	6.686544	-2.161898	0.060719
H	7.712967	-1.533983	-1.240505
H	2.707968	-2.557641	-0.534890
H	-2.350734	-0.652104	-2.885429

21q

Energy = -3357.1022719 ZPE = -3356.028056 H = -3355.955952 G = -3356.136186

C	3.287160	0.573617	1.440606
C	4.235920	0.613973	2.459010
C	5.237943	-0.381208	2.540829
C	5.323046	-1.416685	1.633498
C	4.378696	-1.492734	0.577292
C	3.370986	-0.494349	0.491677
N	2.426316	-0.514290	-0.496596
C	2.431101	-1.486097	-1.396628
C	3.395107	-2.512828	-1.388596
C	4.363567	-2.513476	-0.406984
N	2.227097	1.450440	1.220842
H	5.956791	-0.319285	3.352394
H	6.096400	-2.173909	1.712742
H	5.113476	-3.297590	-0.369284
H	3.351122	-3.289814	-2.142157
H	1.650376	-1.448896	-2.145914
C	1.936053	2.579159	1.979515
C	0.812454	3.323980	1.352625
C	0.234967	4.498587	1.877330
C	0.343374	2.767997	0.155354
C	-0.804711	5.080785	1.140157
C	-0.691550	3.351844	-0.567209
C	-1.259001	4.525924	-0.059964
H	-1.272616	5.986164	1.517612
H	-1.070647	2.906158	-1.477801
H	-2.067041	5.010780	-0.600602
O	2.542594	2.913226	2.999126
H	4.189188	1.403926	3.193326
C	0.681794	5.107401	3.181684
H	1.743589	5.366552	3.159712

H	0.099874	6.004994	3.408549
H	0.560294	4.391283	3.999683
Co	1.266294	1.166107	-0.355907
C	-4.290167	1.807501	-1.263615
O	-3.311417	1.958022	-1.977431
O	-4.619148	0.650924	-0.679623
C	-5.260409	2.939972	-0.904730
C	-6.718591	2.454368	-1.021788
H	-7.399765	3.276329	-0.778117
H	-6.942368	2.119993	-2.040437
H	-6.916137	1.625677	-0.338539
C	-4.963256	3.361165	0.553034
H	-3.928416	3.700868	0.659685
H	-5.624690	4.185111	0.840030
H	-5.129646	2.530157	1.244213
C	-5.019098	4.125243	-1.851217
H	-5.677431	4.956605	-1.580769
H	-3.983250	4.467452	-1.796830
H	-5.223371	3.847104	-2.889780
O	2.829040	2.141012	-1.574086
C	3.192349	1.747915	-2.689059
O	2.370003	1.129760	-3.521256
C	4.632299	1.850612	-3.167002
C	5.240131	0.441107	-2.942665
H	6.289494	0.449696	-3.252230
H	5.196897	0.157003	-1.886473
H	4.711583	-0.315865	-3.528147
C	4.686475	2.218965	-4.661190
H	4.161870	1.481384	-5.272537
H	4.236435	3.200444	-4.841490
H	5.730340	2.258973	-4.986611
C	5.387518	2.886122	-2.320291
H	4.952039	3.883341	-2.435478
H	5.360117	2.623123	-1.260099
H	6.432084	2.927901	-2.642434
C	1.022690	-2.833407	1.472022
C	2.078174	-3.432196	2.155112
C	2.618279	-4.659842	1.703527
C	2.138231	-5.311051	0.587168
C	1.066242	-4.735104	-0.142135
C	0.521517	-3.498752	0.305732
N	-0.502367	-2.883590	-0.354931
C	-1.016949	-3.441194	-1.440991
C	-0.539443	-4.663909	-1.956062
C	0.497642	-5.304330	-1.309255
N	0.368464	-1.640248	1.767613
H	3.444095	-5.090991	2.261836
H	2.566366	-6.251144	0.254089
H	0.887885	-6.246162	-1.684299
H	-0.994017	-5.080410	-2.847681
H	-1.841058	-2.908690	-1.898550
C	0.619267	-0.851550	2.883584
C	-0.356507	0.271744	2.947503
C	-0.402445	1.239576	3.974198
C	-1.282718	0.304665	1.900513
C	-1.410267	2.210526	3.889956
C	-2.276163	1.267735	1.826155
C	-2.329591	2.232120	2.838774
H	-1.472615	2.968653	4.665951
H	-2.993831	1.261919	1.017902
H	-3.092682	3.003939	2.808959
O	1.506975	-1.069793	3.709955
H	2.486670	-2.943506	3.026113
C	0.577655	1.263070	5.120788
H	0.315318	2.055811	5.827330
H	0.600528	0.306445	5.648363
H	1.589850	1.447637	4.751937
Co	-1.092963	-1.164830	0.646155
C	-0.846076	0.119827	-2.143800
O	-1.500135	-0.357004	-1.194403
O	0.270173	0.757300	-1.986262
C	-1.282900	-0.091579	-3.604794
C	-1.210791	1.245486	-4.371931
H	-1.518116	1.081063	-5.409838
H	-1.882443	1.979822	-3.923144
H	-0.198204	1.656669	-4.384988
C	-0.283741	-1.101015	-4.226775
H	-0.285513	-2.053515	-3.687867
H	-0.576181	-1.303799	-5.261461
H	0.738300	-0.713903	-4.242762
C	-2.705051	-0.664398	-3.691755
H	-2.926680	-0.917029	-4.733763
H	-2.826597	-1.558155	-3.079566
H	-3.432739	0.069358	-3.347442
O	-2.866404	-1.806877	1.053537
C	-3.641611	-2.432607	0.219853
O	-4.000564	-1.965780	-0.874048
C	-4.170349	-3.795523	0.714484
C	-4.794212	-4.579333	-0.448670
H	-5.198025	-5.530854	-0.086260
H	-5.602127	-4.012426	-0.917247
H	-4.046651	-4.797108	-1.218683
C	-3.029491	-4.611387	1.353026
H	-2.265895	-4.870786	0.613479
H	-2.547607	-4.046527	2.154132
H	-3.425966	-5.543996	1.768986
C	-5.242919	-3.485278	1.783714
H	-4.808095	-2.922990	2.615322
H	-6.062334	-2.895582	1.358355
H	-5.662704	-4.417938	2.176373
H	-4.028361	-0.116395	-0.903931
H	1.481598	1.021006	-3.072815

21s

Energy = -3357.05633278 ZPE = -3355.979789 H = -3355.909122 G = -3356.085633

C	-2.184212	1.146290	-2.637004
C	-2.373669	2.093768	-3.641850
C	-1.350669	2.351036	-4.588243
C	-0.153205	1.666508	-4.601162
C	0.082606	0.674388	-3.613875
C	-0.913892	0.464607	-2.605477
N	-0.731116	-0.413969	-1.594631
C	0.318008	-1.233277	-1.608793
C	1.325922	-1.140301	-2.592480
C	1.223968	-0.151677	-3.564170
N	-3.066766	0.732194	-1.661029
H	-1.537605	3.107590	-5.345292
H	0.600961	1.859144	-5.357149
H	2.006434	-0.031097	-4.306983
H	2.148160	-1.844087	-2.589244
H	0.324249	-2.007764	-0.854011
C	-4.323771	1.235275	-1.439320
C	-4.876466	0.707496	-0.154931
C	-6.187397	0.962866	0.304541
C	-3.976316	-0.049200	0.615175
C	-6.553924	0.427158	1.548476
C	-4.360774	-0.568814	1.845868

C	-5.659861	-0.327737	2.309948
H	-7.557795	0.608203	1.924351
H	-3.668963	-1.152765	2.441020
H	-5.975070	-0.726617	3.271305
O	-4.915708	2.019407	-2.196676
H	-3.316356	2.618117	-3.696753
C	-7.184868	1.783068	-0.478603
H	-7.331667	1.379512	-1.484137
H	-8.149086	1.811088	0.037357
H	-6.828115	2.807570	-0.617751
Co	-2.276457	-0.234929	-0.237819
C	-1.521986	2.025911	1.582332
O	-1.953653	1.530317	0.478984
O	-0.594301	1.571854	2.281346
C	-2.224226	3.324503	2.038478
C	-1.146879	4.346356	2.446489
H	-1.614321	5.257804	2.834602
H	-0.492402	3.929832	3.215636
H	-0.525064	4.622806	1.587127
C	-3.122222	3.904571	0.936502
H	-3.907325	3.198440	0.658423
H	-3.589918	4.831729	1.286707
H	-2.544358	4.130472	0.034714
C	-3.083520	2.939790	3.263935
H	-3.601420	3.823675	3.652485
H	-3.835716	2.191216	2.992117
H	-2.458389	2.525467	4.060563
O	-2.940911	-1.927985	-1.027266
C	-3.239536	-2.982375	-0.439546
O	-2.829266	-3.271494	0.772189
C	-4.197359	-3.976647	-1.073377
C	-3.868411	-5.415688	-0.640019
H	-4.592332	-6.102865	-1.088038
H	-2.868184	-5.709040	-0.974676
H	-3.913985	-5.526088	0.445608
C	-5.598905	-3.564247	-0.548600
H	-5.650605	-3.639676	0.541271
H	-5.836487	-2.535459	-0.836156
H	-6.352583	-4.230112	-0.979556
C	-4.150323	-3.843977	-2.604202
H	-4.393306	-2.827210	-2.920598
H	-3.157015	-4.094369	-2.990176
H	-4.874653	-4.531563	-3.050362
C	4.681547	-1.297899	-1.150850
C	5.955010	-1.430212	-1.706658
C	6.656936	-2.653002	-1.604640
C	6.126955	-3.757851	-0.970912
C	4.835565	-3.667806	-0.393147
C	4.129481	-2.433361	-0.478313
N	2.886777	-2.274106	0.069335
C	2.304924	-3.300683	0.669225
C	2.921129	-4.562155	0.789890
C	4.184594	-4.739893	0.268250
N	3.841843	-0.193272	-1.197492
H	7.645269	-2.714200	-2.051041
H	6.675988	-4.692020	-0.909257
H	4.690781	-5.697256	0.351869
H	2.396308	-5.366154	1.293027
H	1.318008	-3.120478	1.071491
C	4.216704	1.063724	-1.625622
C	3.098848	2.019921	-1.426719
C	3.074049	3.336236	-1.936550
C	1.990262	1.483691	-0.755770
C	1.891303	4.071267	-1.764064
C	0.824593	2.215672	-0.618673
C	0.777277	3.517412	-1.133142
H	1.841973	5.086447	-2.149130
H	-0.046407	1.778039	-0.163751
H	-0.138402	4.096251	-1.040237
O	5.310709	1.337574	-2.134291
H	6.393778	-0.588943	-2.220815
C	4.246725	3.951668	-2.660960
H	4.011002	4.972077	-2.975860
H	5.137104	3.974247	-2.026270
H	4.521324	3.363477	-3.541255
Co	2.274340	-0.309991	-0.149868
C	-0.224847	-1.076639	1.777543
O	0.775446	-0.618739	1.177968
O	-1.397763	-1.203334	1.261155
C	-0.080238	-1.585596	3.232929
C	-1.040021	-0.797917	4.151523
H	-0.976961	-1.202557	5.167282
H	-0.783604	0.261546	4.168761
H	-2.072890	-0.887410	3.808555
C	-0.473918	-3.080869	3.289151
H	0.139655	-3.705164	2.633282
H	-0.336143	-3.447502	4.310849
H	-1.522373	-3.233113	3.023780
C	1.362784	-1.404167	3.727788
H	1.460669	-1.823126	4.734062
H	2.085813	-1.898681	3.075176
H	1.620782	-0.345031	3.778249
O	3.328146	0.316674	1.286912
C	3.132272	1.225987	2.119623
O	1.992190	1.774224	2.418247
C	4.330712	1.825524	2.842414
C	4.032734	1.935002	4.350417
H	4.886869	2.396696	4.854209
H	3.147096	2.546256	4.536404
H	3.871144	0.945891	4.791155
C	5.581885	0.969846	2.592590
H	5.450684	-0.044696	2.980178
H	5.806791	0.899947	1.525358
H	6.436494	1.425583	3.100508
C	4.520992	3.235544	2.224450
H	4.685029	3.172075	1.143607
H	3.647911	3.866871	2.407523
H	5.396892	3.707511	2.679126
H	1.151298	1.403064	2.028082
H	-2.244289	-2.523232	1.109197

21se

Energy = -3357.06421811 ZPE = -3355.992689 H = -3355.919636 G = -3356.103666

C	-2.954931	-1.048660	1.495842
C	-3.840239	-1.069800	2.569112
C	-5.082201	-0.396098	2.483299
C	-5.467660	0.295010	1.354986
C	-4.589487	0.351296	0.241560
C	-3.333047	-0.307223	0.331204
N	-2.433001	-0.276586	-0.696564
C	-2.734884	0.358983	-1.821016
C	-3.963753	1.017597	-2.003134
C	-4.882278	1.019715	-0.971273
N	-1.719305	-1.685181	1.388392
H	-5.746168	-0.434656	3.341642
H	-6.424891	0.803277	1.303585
H	-5.831566	1.535769	-1.076460

H	-4.162972	1.525512	-2.938790
H	-1.982417	0.340592	-2.600229
C	-1.132251	-2.492353	2.361061
C	0.114835	-3.092282	1.816451
C	0.968127	-3.962641	2.524177
C	0.414086	-2.712919	0.502165
C	2.095274	-4.443300	1.842691
C	1.535701	-3.190824	-0.165199
C	2.373968	-4.075369	0.522519
H	2.772268	-5.118089	2.359805
H	1.769452	-2.866210	-1.172220
H	3.256786	-4.475352	0.031216
O	-1.600050	-2.689731	3.483217
H	-3.569275	-1.605612	3.466082
C	0.714801	-4.356476	3.956847
H	-0.257839	-4.842110	4.072915
H	1.495594	-5.033018	4.315001
H	0.692352	-3.470055	4.597358
Co	-0.853258	-1.491377	-0.253702
C	4.899367	-0.743913	-0.628259
O	3.904676	-0.856868	-1.332382
O	5.118875	0.310454	0.157294
C	5.994642	-1.808794	-0.518404
C	7.376234	-1.155624	-0.727087
H	8.159300	-1.916925	-0.648265
H	7.449434	-0.696222	-1.718665
H	7.564715	-0.384119	0.022861
C	5.913718	-2.421145	0.898966
H	4.939264	-2.890445	1.067750
H	6.684985	-3.189840	1.013604
H	6.070096	-1.657387	1.665473
C	5.754550	-2.895315	-1.575899
H	6.513485	-3.678483	-1.483200
H	4.767813	-3.349119	-1.456421
H	5.809401	-2.479588	-2.586447
O	-1.922306	-3.030422	-1.386324
C	-2.142068	-3.042035	-2.603729
O	-1.371530	-2.403809	-3.468301
C	-3.355674	-3.725445	-3.215187
C	-4.324365	-2.585472	-3.622176
H	-5.231349	-3.020489	-4.052496
H	-4.612092	-1.982753	-2.754612
H	-3.867561	-1.926806	-4.365582
C	-2.939209	-4.534461	-4.459278
H	-2.467572	-3.895665	-5.209366
H	-2.238108	-5.332053	-4.193103
H	-3.826118	-4.995533	-4.904300
C	-4.020822	-4.634284	-2.171680
H	-3.338633	-5.424581	-1.844603
H	-4.327523	-4.064569	-1.290770
H	-4.907198	-5.103199	-2.608816
C	-2.142314	2.574656	1.572438
C	-3.264885	2.835918	2.360269
C	-4.346612	3.594195	1.857734
C	-4.349473	4.119152	0.583169
C	-3.233903	3.882768	-0.260769
C	-2.147171	3.102878	0.232502
N	-1.071329	2.817791	-0.551778
C	-1.003068	3.285418	-1.790327
C	-2.023380	4.075164	-2.353175
C	-3.133912	4.368311	-1.587635
N	-1.000614	1.866451	1.911181
H	-5.198954	3.764313	2.509228
H	-5.183507	4.707626	0.214159
H	-3.944298	4.966862	-1.993938
H	-1.923974	4.435537	-3.370664
H	-0.108834	3.027835	-2.346709
C	-0.866004	1.144212	3.078661
C	0.397584	0.340271	3.070879
C	0.920180	-0.351324	4.187297
C	1.077278	0.283584	1.860298
C	2.140407	-1.024055	4.009425
C	2.245533	-0.428734	1.660886
C	2.801239	-1.063162	2.779933
H	2.569391	-1.553847	4.855958
H	2.689455	-0.506912	0.678504
H	3.731800	-1.613787	2.684189
O	-1.667656	1.137595	4.021057
H	-3.296086	2.442666	3.364415
C	0.206255	-0.427460	5.513423
H	0.837125	-0.917784	6.260834
H	-0.084844	0.560030	5.878162
H	-0.716796	-1.004264	5.399604
Co	0.462059	1.813709	0.460967
C	0.906421	0.016425	-2.094197
O	1.132153	0.891674	-1.234975
O	0.166339	-1.022966	-1.877198
C	1.468780	0.174934	-3.514352
C	2.077897	-1.159098	-3.993519
H	2.471279	-1.031041	-5.007204
H	2.893288	-1.466542	-3.336439
H	1.331090	-1.957064	-4.024176
C	0.288384	0.567702	-4.436669
H	-0.195161	1.491406	-4.102854
H	0.664440	0.737347	-5.450175
H	-0.468954	-0.219301	-4.490555
C	2.534535	1.282010	-3.527623
H	2.951365	1.376232	-4.535473
H	2.107721	2.246781	-3.240271
H	3.335345	1.048102	-2.824743
O	1.726587	3.248870	0.579590
C	2.876967	3.404773	-0.006433
O	3.712964	2.511270	-0.191982
C	3.154550	4.847395	-0.478536
C	4.538756	4.935536	-1.134596
H	4.731050	5.960891	-1.468527
H	5.325564	4.646441	-0.432195
H	4.604831	4.270683	-2.000524
C	2.060315	5.234863	-1.495978
H	2.080904	4.571476	-2.368162
H	1.068009	5.173743	-1.042718
H	2.221360	6.259129	-1.849288
C	3.079538	5.786668	0.742977
H	2.098062	5.724189	1.219870
H	3.841335	5.527083	1.486433
H	3.251552	6.822262	0.430201
H	4.417522	1.008093	0.032710
H	-0.661019	-1.906291	-2.965180

21t

Energy = -3357.07732638 ZPE = -3356.002148 H = -3355.930821 G = -3356.110764

C	3.129513	-0.479691	-2.773285
C	3.695946	-1.115519	-3.880815
C	3.052648	-1.074788	-5.138389
C	1.866060	-0.399545	-5.339189
C	1.260542	0.271943	-4.246280
C	1.882194	0.205469	-2.965110

N	1.334668	0.809205	-1.867292
C	0.246697	1.548869	-2.008205
C	-0.425588	1.687884	-3.240653
C	0.067124	1.032413	-4.347786
N	3.627065	-0.410836	-1.487323
H	3.523752	-1.588167	-5.972230
H	1.394010	-0.363139	-6.316110
H	-0.437732	1.101025	-5.307370
H	-1.324194	2.293201	-3.289981
H	-0.131499	2.016454	-1.111625
C	4.758988	-1.029654	-1.029551
C	4.847143	-0.931886	0.457173
C	5.920024	-1.447531	1.218343
C	3.741131	-0.326351	1.077172
C	5.837321	-1.332831	2.613805
C	3.677102	-0.238927	2.464536
C	4.733522	-0.742771	3.231529
H	6.650075	-1.720126	3.223199
H	2.814847	0.200270	2.950260
H	4.693233	-0.680772	4.316549
O	5.592018	-1.608082	-1.747092
H	4.636252	-1.632553	-3.760898
C	7.125181	-2.111942	0.595596
H	7.617116	-1.451652	-0.123769
H	7.846918	-2.397971	1.366491
H	6.836424	-3.003342	0.031786
Co	2.427516	0.273717	-0.189267
C	1.152113	-2.236030	0.697455
O	1.758450	-1.521758	-0.173083
O	0.280577	-1.810967	1.490291
C	1.604564	-3.711553	0.758107
C	0.386546	-4.641642	0.890732
H	0.718779	-5.684367	0.933854
H	-0.182395	-4.427713	1.797141
H	-0.288470	-4.534730	0.034939
C	2.440418	-4.098272	-0.472139
H	3.323470	-3.462661	-0.563905
H	2.764761	-5.141147	-0.385473
H	1.861178	-3.998718	-1.395297
C	2.485033	-3.812379	2.027365
H	2.839174	-4.841551	2.152620
H	3.354849	-3.152002	1.953717
H	1.913374	-3.530932	2.916753
O	3.393621	1.997790	-0.362057
C	3.711432	2.794502	0.537438
O	3.081519	2.866396	1.685061
C	4.936589	3.680533	0.395922
C	4.710575	5.047721	1.064705
H	5.621794	5.647247	0.980210
H	3.897116	5.594710	0.577113
H	4.466106	4.938392	2.123631
C	6.066070	2.904185	1.125969
H	5.833547	2.777025	2.186922
H	6.210421	1.913912	0.682448
H	7.000968	3.465930	1.038645
C	5.292792	3.849073	-1.089285
H	5.465516	2.880809	-1.564431
H	4.489957	4.357833	-1.632035
H	6.202109	4.450559	-1.178489
C	-5.167108	1.535413	-0.649641
C	-6.532267	1.659496	-0.892645
C	-7.159901	2.926268	-0.808719
C	-6.463313	4.075242	-0.500033
C	-5.069196	3.991973	-0.246744
C	-4.439756	2.717623	-0.304195
N	-3.105785	2.560351	-0.055937
C	-2.355572	3.622572	0.205443
C	-2.889019	4.924675	0.260686
C	-4.241354	5.103954	0.048069
N	-4.383281	0.385828	-0.727721
H	-8.227086	2.982006	-1.002100
H	-6.958565	5.039621	-0.450444
H	-4.682407	6.095342	0.096688
H	-2.235037	5.760995	0.478726
H	-1.304081	3.435072	0.391601
C	-4.769701	-0.791490	-1.350698
C	-3.563322	-1.625899	-1.579406
C	-3.523847	-2.850742	-2.276181
C	-2.383100	-1.039355	-1.126224
C	-2.256400	-3.400432	-2.522056
C	-1.130117	-1.558192	-1.390539
C	-1.084012	-2.761634	-2.109140
H	-2.187554	-4.340146	-3.063229
H	-0.226827	-1.075024	-1.052641
H	-0.118513	-3.204105	-2.336820
O	-5.919086	-1.065641	-1.697481
H	-7.105491	0.782077	-1.152697
C	-4.775034	-3.539219	-2.760695
H	-4.527702	-4.470633	-3.276578
H	-5.447306	-3.767464	-1.927860
H	-5.341800	-2.895113	-3.438614
Co	-2.621825	0.524000	-0.000566
C	0.027537	1.041889	1.552111
O	-0.832165	0.801268	0.664720
O	1.276798	1.060770	1.277239
C	-0.365261	1.339298	3.018207
C	-0.264956	0.011835	3.806705
H	-0.441388	0.219084	4.867563
H	-1.009874	-0.705408	3.462743
H	0.718366	-0.448127	3.694212
C	0.608278	2.364870	3.633677
H	0.643502	3.290149	3.049276
H	0.270527	2.618966	4.642745
H	1.622485	1.969248	3.718205
C	-1.797455	1.885631	3.136456
H	-2.040983	2.011983	4.196183
H	-1.900174	2.861672	2.656745
H	-2.528161	1.200098	2.708421
O	-3.089200	-0.823478	1.702847
C	-3.079468	-2.020407	2.023440
O	-2.013052	-2.776016	1.990394
C	-4.353736	-2.698695	2.528865
C	-4.140537	-4.195356	2.796696
H	-5.074539	-4.638831	3.155866
H	-3.838550	-4.720136	1.885893
H	-3.367783	-4.358629	3.552373
C	-4.758146	-1.971184	3.831560
H	-3.991669	-2.089946	4.604797
H	-4.904230	-0.903196	3.648967
H	-5.693960	-2.392301	4.212048
C	-5.447662	-2.495214	1.460080
H	-5.601054	-1.433471	1.256472
H	-5.177038	-2.986132	0.520371
H	-6.390096	-2.926479	1.811215
H	-1.138927	-2.309498	1.726859
H	2.332762	2.194875	1.683630

22n

Energy = -3357.11078072 ZPE = -3356.037496 H = -3355.966768 G = -3356.141539

C	-2.352992	-1.727396	-1.417449
C	-2.807798	-2.718898	-2.352881
C	-3.632103	-3.750209	-1.944942
C	-4.033499	-3.875867	-0.607110
C	-3.670012	-2.895711	0.350710
C	-2.847366	-1.804786	-0.067004
N	-2.486603	-0.816555	0.794766
C	-2.914085	-0.873061	2.085402
C	-3.693438	-1.906103	2.570169
C	-4.067383	-2.947360	1.707208
N	-1.551131	-0.646855	-1.701119
H	-3.953189	-4.491356	-2.670261
H	-4.657227	-4.708191	-0.294563
H	-4.677972	-3.774251	2.055316
H	-3.995102	-1.906539	3.612156
H	-2.609995	-0.047218	2.709778
C	-0.853294	-0.580719	-2.889607
C	-0.377124	0.760253	-3.411430
C	-1.446471	1.532238	-3.932941
C	0.973299	1.094987	-3.722401
C	-1.187751	2.568784	-4.834536
C	1.156999	2.076005	-4.724150
C	0.109441	2.801640	-5.275625
H	-2.015382	3.151017	-5.230428
H	2.158715	2.276686	-5.083910
H	0.310400	3.548052	-6.038398
O	-0.730401	-1.511107	-3.694491
H	-2.482925	-2.651172	-3.377885
C	-2.892115	1.235506	-3.577644
H	-3.088748	1.380131	-2.511457
H	-3.560646	1.893728	-4.138767
H	-3.166749	0.202201	-3.815988
Co	-1.385516	0.678466	-0.098707
C	1.021356	2.318725	-0.426261
O	-0.161406	2.101487	-0.799391
O	1.816373	1.387564	-0.058876
C	1.451940	3.793768	-0.371681
C	2.945281	3.965626	-0.066995
H	3.204106	5.028986	-0.091903
H	3.195495	3.587512	0.927959
H	3.565377	3.442164	-0.796746
C	1.081763	4.474225	-1.705092
H	0.015089	4.362042	-1.910435
H	1.320352	5.541369	-1.650496
H	1.629605	4.044227	-2.545819
C	0.617151	4.433513	0.762472
H	0.843612	5.502641	0.830304
H	-0.452570	4.307035	0.577650
H	0.852111	3.973359	1.723818
C	0.380397	-3.094497	-0.914544
C	-0.004891	-4.108607	-1.821139
C	-0.733495	-5.220930	-1.388376
C	-1.133202	-5.360621	-0.067110
C	-0.779095	-4.373637	0.886080
C	-0.028752	-3.236376	0.459399
N	0.331044	-2.254745	1.334364
C	-0.001825	-2.371575	2.632315
C	-0.733394	-3.449626	3.127580
C	-1.144936	-4.448127	2.252719
N	1.115102	-1.959207	-1.206009
H	-1.012523	-5.976954	-2.116201
H	-1.704395	-6.225261	0.256606
H	-1.725930	-5.295713	2.602333
H	-0.984257	-3.485349	4.181982
H	0.339466	-1.570732	3.273919
C	1.767420	-1.808207	-2.407242
C	2.623795	-0.569617	-2.461706
C	3.921755	-0.789568	-1.930507
C	2.258542	0.671778	-3.033751
C	4.848833	0.251434	-1.903850
C	3.236091	1.694129	-2.949019
C	4.496597	1.499868	-2.403353
H	5.839851	0.081066	-1.493128
H	2.993960	2.688993	-3.294510
H	5.198629	2.327765	-2.365545
O	1.836108	-2.620842	-3.334028
H	0.280556	-4.006349	-2.854562
C	4.331930	-2.159779	-1.432518
H	5.355646	-2.140398	-1.050612
H	3.679430	-2.504973	-0.627092
H	4.279674	-2.896649	-2.239961
Co	1.351891	-0.663084	0.429632
C	0.114109	1.118005	2.691317
O	1.061886	0.380988	2.338919
O	-0.844044	1.461740	1.905430
C	0.054523	1.605034	4.155262
C	-0.048003	3.141967	4.203026
H	-0.188244	3.468009	5.238791
H	0.867250	3.610142	3.828696
H	-0.890761	3.512048	3.613829
C	-1.205464	0.990649	4.806865
H	-1.216982	-0.100147	4.709973
H	-1.223131	1.235122	5.873644
H	-2.120284	1.387579	4.358001
C	1.310156	1.148289	4.913663
H	1.275109	1.515380	5.944623
H	1.386057	0.057716	4.939043
H	2.215561	1.533893	4.437610
C	-5.136074	2.817329	0.888743
C	-5.884858	1.477320	1.112968
H	-5.638921	1.045844	2.088364
H	-6.964121	1.653684	1.074760
H	-5.621742	0.750718	0.338581
C	-5.461216	3.370436	-0.510400
H	-6.535048	3.565874	-0.586251
H	-4.929924	4.310065	-0.694608
H	-5.179339	2.659036	-1.289847
C	-5.524789	3.830395	1.976813
H	-5.330633	3.435961	2.976796
H	-4.966872	4.765109	1.863438
H	-6.592062	4.058218	1.896386
C	-3.658758	2.454481	0.958391
O	-3.080013	1.958176	-0.021535
O	-3.077470	2.626018	2.123424
H	-2.130085	2.236207	2.110748
C	5.269739	-0.460044	2.485008
C	5.313097	-1.977942	2.709914
H	5.386035	-2.514909	1.760182
H	6.184154	-2.232378	3.321039
H	4.414061	-2.325871	3.226226
C	5.128982	0.278713	3.836073
H	5.984652	0.035519	4.473458
H	5.099297	1.361610	3.691955
H	4.216305	-0.026884	4.357742
C	6.547550	0.012207	1.757312
H	6.667471	-0.502865	0.798730

H	6.521471	1.088286	1.570404
H	7.421976	-0.214117	2.375028
C	4.061233	-0.097006	1.631292
O	3.253299	-0.954723	1.241160
O	3.953251	1.179450	1.352308
H	3.135816	1.363274	0.780544

22q

Energy = -3357.17350583 ZPE = -3356.095024 H = -3356.02493 G = -3356.197746

C	-2.499558	0.234205	-2.359351
C	-2.969294	0.297192	-3.674812
C	-3.740658	-0.742796	-4.235645
C	-4.065899	-1.875249	-3.522750
C	-3.617312	-1.993906	-2.185311
C	-2.843690	-0.941229	-1.603330
N	-2.384070	-1.036411	-0.320301
C	-2.644011	-2.126339	0.393030
C	-3.397448	-3.204615	-0.103167
C	-3.883943	-3.133588	-1.389469
N	-1.727279	1.188387	-1.697089
H	-4.074381	-0.638901	-5.264575
H	-4.650268	-2.677668	-3.962340
H	-4.464103	-3.948503	-1.813017
H	-3.569442	-4.070094	0.526290
H	-2.233502	-2.153099	1.391217
C	-1.243546	2.283740	-2.348323
C	-0.531832	3.269238	-1.454262
C	-1.419556	4.153272	-0.787260
C	0.870483	3.437072	-1.370865
C	-0.915538	5.181780	0.008801
C	1.318050	4.489977	-0.538867
C	0.459407	5.344334	0.138499
H	-1.601547	5.853043	0.518519
H	2.381198	4.632130	-0.409406
H	0.867806	6.131567	0.765671
O	-1.423642	2.614628	-3.529999
H	-2.708115	1.157494	-4.269379
C	-2.919432	4.006451	-0.945569
H	-3.273844	3.077452	-0.491606
H	-3.440034	4.841621	-0.469504
H	-3.203830	3.983094	-2.002344
Co	-1.388052	0.757678	0.296612
C	1.201322	1.757488	1.419480
O	-0.038484	1.912799	1.308837
O	1.867913	0.935585	0.683691
C	1.960384	2.494250	2.544227
C	2.487968	1.408745	3.513843
H	3.005940	1.894919	4.346602
H	1.672374	0.813598	3.922985
H	3.184759	0.730282	3.018349
C	3.168188	3.293065	2.012191
H	2.845593	4.201591	1.507374
H	3.799595	3.587530	2.856663
H	3.783852	2.712908	1.322593
C	1.005770	3.431964	3.298824
H	1.552104	3.951607	4.092859
H	0.575723	4.176318	2.624929
H	0.184224	2.871116	3.753213
C	0.233870	-1.942825	-2.138822
C	-0.288968	-2.198569	-3.409737
C	-0.819802	-3.466756	-3.738844
C	-0.856529	-4.510426	-2.840181
C	-0.343703	-4.303512	-1.536194
C	0.183685	-3.021936	-1.202957
N	0.671909	-2.761387	0.044095
C	0.703632	-3.717925	0.964676
C	0.208093	-5.011068	0.713169
C	-0.322266	-5.297230	-0.527554
N	0.854097	-0.783283	-1.646312
H	-1.222066	-3.604217	-4.738248
H	-1.271389	-5.477613	-3.105382
H	-0.723217	-6.282787	-0.746390
H	0.247085	-5.756020	1.499710
H	1.121766	-3.441244	1.923045
C	1.037156	0.282303	-2.483820
C	2.154448	1.275748	-2.236717
C	3.411873	0.738388	-2.616002
C	1.996778	2.677075	-2.046667
C	4.496253	1.587753	-2.850695
C	3.100901	3.487191	-2.400854
C	4.328631	2.966381	-2.788552
H	5.455029	1.163211	-3.135786
H	2.989626	4.564719	-2.372651
H	5.145505	3.635936	-3.041668
O	0.504084	0.411583	-3.594075
H	-0.313266	-1.404500	-4.135771
C	3.594571	-0.747649	-2.862437
H	4.619440	-0.957606	-3.179653
H	3.374490	-1.342015	-1.973747
H	2.923286	-1.099629	-3.654254
Co	1.242172	-0.930700	0.287289
C	-0.065726	-0.985019	2.819370
O	1.053332	-1.154573	2.258089
O	-1.067186	-0.453602	2.235089
C	-0.263354	-1.485946	4.260260
C	-0.798119	-0.333566	5.137795
H	-0.979991	-0.701822	6.152285
H	-0.078928	0.488429	5.203634
H	-1.737451	0.068626	4.751161
C	-1.312433	-2.622613	4.203722
H	-0.991369	-3.427385	3.533513
H	-1.444788	-3.048876	5.202924
H	-2.285196	-2.258772	3.862564
C	1.050819	-2.027562	4.842815
H	0.881745	-2.375398	5.866698
H	1.430190	-2.867583	4.254925
H	1.826359	-1.258260	4.864123
C	-5.439933	0.942762	1.801906
C	-5.786524	0.269016	0.447567
H	-5.521523	-0.793438	0.453170
H	-6.862395	0.353075	0.267520
H	-5.253749	0.753156	-0.375278
C	-5.774975	2.445341	1.738472
H	-6.847022	2.571759	1.560198
H	-5.524553	2.943980	2.680541
H	-5.227126	2.936356	0.931464
C	-6.206476	0.262202	2.945275
H	-5.998752	-0.810008	2.980764
H	-5.938514	0.694083	3.914123
H	-7.281236	0.400411	2.793968
C	-3.935350	0.773285	1.948680
O	-3.150161	1.429174	1.242503
O	-3.526224	-0.143107	2.793219
H	-2.515584	-0.258983	2.701757
C	5.771096	-1.582148	0.690807
C	5.686135	-3.090670	0.421587
H	5.276326	-3.289436	-0.572993

H	6.686051	-3.531609	0.478007
H	5.046335	-3.587981	1.155689
C	6.315317	-1.318259	2.113967
H	7.316973	-1.749253	2.208494
H	6.377222	-0.246361	2.318163
H	5.673941	-1.779594	2.872771
C	6.681966	-0.901138	-0.353784
H	6.307668	-1.065827	-1.368958
H	6.745377	0.175542	-0.181013
H	7.689079	-1.324916	-0.290061
C	4.379422	-0.963893	0.610389
O	3.353548	-1.632998	0.448560
O	4.362363	0.349383	0.743032
H	3.400279	0.670592	0.716565

22s

Energy = -3357.12666708 ZPE = -3356.044919 H = -3355.976145 G = -3356.142774

C	-2.454531	1.017920	-1.775808
C	-3.110938	1.740258	-2.775565
C	-4.224890	1.199792	-3.453508
C	-4.717110	-0.060684	-3.179672
C	-4.106117	-0.822488	-2.154809
C	-2.998813	-0.261975	-1.454386
N	-2.395892	-0.931030	-0.428943
C	-2.830592	-2.131956	-0.069681
C	-3.900534	-2.766821	-0.726994
C	-4.534616	-2.115360	-1.762558
N	-1.363113	1.417352	-0.998138
H	-4.695762	1.802136	-4.225457
H	-5.562651	-0.471259	-3.722118
H	-5.369185	-2.577237	-2.281961
H	-4.206543	-3.755181	-0.404760
H	-2.314544	-2.604537	0.752747
C	-0.518327	2.367238	-1.507955
C	0.351996	3.269838	-0.641822
C	-0.434318	4.221752	0.061774
C	1.747306	3.517066	-0.856560
C	0.116048	5.449041	0.444289
C	2.195502	4.827573	-0.567514
C	1.410786	5.780532	0.066700
H	-0.501576	6.165543	0.978891
H	3.200527	5.112974	-0.849344
H	1.815292	6.767434	0.271237
O	-0.544102	2.743411	-2.688486
H	-2.744929	2.715600	-3.056844
C	-1.899525	3.984426	0.363109
H	-2.049141	3.063915	0.925136
H	-2.304050	4.822485	0.937981
H	-2.494056	3.894329	-0.553211
Co	-1.156820	0.218216	0.516726
C	1.070481	1.418440	1.670570
O	-0.187069	1.413983	1.637544
O	1.773809	0.797459	0.797338
C	1.755931	2.091775	2.863152
C	2.122973	0.938402	3.829803
H	2.600032	1.351676	4.723713
H	1.227568	0.397112	4.143242
H	2.810606	0.226738	3.366198
C	3.030364	2.839926	2.448516
H	2.788930	3.681616	1.796708
H	3.524171	3.230073	3.344275
H	3.735791	2.192523	1.925955
C	0.782850	3.063269	3.551551
H	1.278254	3.527132	4.410392
H	0.472157	3.852312	2.860881
H	-0.112048	2.545189	3.904075
C	-0.007066	-0.934861	-2.735690
C	-0.626406	-0.681098	-3.958924
C	-1.427168	-1.670917	-4.575882
C	-1.613179	-2.922974	-4.025567
C	-1.017682	-3.217567	-2.773616
C	-0.265191	-2.196282	-2.129596
N	0.256543	-2.371174	-0.881981
C	0.188567	-3.558847	-0.295029
C	-0.490372	-4.641873	-0.887812
C	-1.117709	-4.461812	-2.103912
N	0.874736	-0.130621	-2.005410
H	-1.901372	-1.427554	-5.522288
H	-2.208449	-3.679861	-4.526168
H	-1.684490	-5.267807	-2.560765
H	-0.529719	-5.590593	-0.364994
H	0.669884	-3.643006	0.669558
C	1.609285	0.799259	-2.680015
C	2.807482	1.350941	-1.960907
C	3.971933	0.580750	-2.219587
C	2.861733	2.549458	-1.216526
C	5.199731	0.978580	-1.696357
C	4.133950	2.873824	-0.675601
C	5.274746	2.121904	-0.907092
H	6.089429	0.390410	-1.902455
H	4.232973	3.722497	-0.015539
H	6.216967	2.423980	-0.458917
O	1.490292	1.081549	-3.881559
H	-0.494681	0.280815	-4.425241
C	3.905801	-0.662843	-3.080388
H	4.883341	-1.150046	-3.127460
H	3.187024	-1.378920	-2.674762
H	3.590689	-0.417079	-4.098711
Co	0.965715	-0.747151	-0.126447
C	-0.085402	-1.630061	2.379483
O	0.967836	-1.568253	1.690227
O	-1.158393	-1.024555	2.037428
C	-0.140471	-2.507350	3.633961
C	-0.714086	-1.700416	4.817740
H	-0.814362	-2.357009	5.687246
H	-0.056105	-0.873818	5.098220
H	-1.699922	-1.289034	4.588856
C	-1.097655	-3.681888	3.315885
H	-0.752828	-4.265907	2.456839
H	-1.147564	-4.353011	4.178358
H	-2.108997	-3.322508	3.105427
C	1.257738	-3.040395	3.977402
H	1.204577	-3.657591	4.879236
H	1.658270	-3.651895	3.165016
H	1.959070	-2.221225	4.157545
C	-5.418776	0.835169	1.984222
C	-6.183170	-0.323035	1.299855
H	-6.062506	-1.258034	1.852484
H	-7.249051	-0.078165	1.258036
H	-5.827524	-0.476864	0.276332
C	-5.599119	2.130285	1.178865
H	-6.659409	2.399224	1.150975
H	-5.043774	2.957350	1.630033
H	-5.242943	2.006984	0.152414
C	-5.918548	1.017573	3.432379
H	-5.791405	0.100171	4.012195
H	-5.377447	1.824975	3.936883

H	-6.981766	1.276625	3.421222
C	-3.943997	0.453431	2.005200
O	-3.081854	1.072120	1.381623
O	-3.666652	-0.632340	2.720866
H	-2.697763	-0.839837	2.610642
C	5.010692	-2.532285	0.654406
C	4.911319	-3.602425	-0.442340
H	5.032432	-3.158861	-1.434867
H	5.696932	-4.350441	-0.298830
H	3.941458	-4.105778	-0.414491
C	4.785994	-3.172528	2.045750
H	5.558102	-3.926065	2.229862
H	4.837296	-2.421082	2.838385
H	3.809001	-3.663175	2.097057
C	6.386267	-1.839408	0.610229
H	6.551741	-1.359560	-0.358601
H	6.472200	-1.077695	1.388250
H	7.174274	-2.583367	0.762916
C	3.897901	-1.506020	0.471156
O	2.929767	-1.706165	-0.268053
O	4.032013	-0.415408	1.204259
H	3.229889	0.171805	1.060714

22se

Energy = -3357.18674837 ZPE = -3356.110415 H = -3356.039395 G = -3356.21494

C	-2.657909	1.123425	-2.282409
C	-3.248495	1.742078	-3.388035
C	-4.310503	1.135742	-4.094287
C	-4.803259	-0.103727	-3.748984
C	-4.237281	-0.780717	-2.640763
C	-3.189307	-0.155972	-1.896813
N	-2.635209	-0.769767	-0.811724
C	-3.023731	-1.990717	-0.475862
C	-4.035926	-2.686789	-1.165186
C	-4.652298	-2.072494	-2.231169
N	-1.628473	1.629834	-1.488348
H	-4.733424	1.666282	-4.943058
H	-5.604579	-0.574134	-4.310596
H	-5.446970	-2.570414	-2.779826
H	-4.311162	-3.685120	-0.844628
H	-2.515498	-2.436140	0.368158
C	-0.874775	2.680978	-1.916937
C	-0.021581	3.314958	-0.846988
C	-0.738936	4.184117	0.013874
C	1.382426	3.218589	-0.778569
C	-0.050604	4.941633	0.959488
C	2.023685	3.956800	0.243159
C	1.330687	4.814092	1.085680
H	-0.599322	5.620502	1.606865
H	3.091608	3.839594	0.384020
H	1.866492	5.376558	1.844713
O	-0.902592	3.234474	-3.026580
H	-2.863069	2.693990	-3.717933
C	-2.243384	4.316248	-0.091639
H	-2.739251	3.406577	0.258016
H	-2.598886	5.157733	0.509279
H	-2.558939	4.479257	-1.127209
Co	-1.341721	0.567351	0.265302
C	1.053569	1.429645	2.005823
O	-0.157165	1.499515	1.696347
O	1.941364	0.897534	1.233508
C	1.494297	1.874474	3.412216
C	1.532334	0.579715	4.261735
H	1.882957	0.818666	5.270910
H	0.536570	0.139099	4.340432
H	2.197611	-0.165532	3.819456
C	2.901249	2.497725	3.411804
H	2.951878	3.380765	2.773316
H	3.159153	2.801707	4.431411
H	3.658322	1.784580	3.079147
C	0.473912	2.848838	4.020718
H	0.770742	3.100770	5.044059
H	0.414964	3.770691	3.438662
H	-0.522735	2.401751	4.048009
C	0.078070	-1.885250	-1.967657
C	-0.801645	-2.014436	-3.038720
C	-1.367821	-3.267301	-3.369852
C	-1.075332	-4.413610	-2.663586
C	-0.162885	-4.341251	-1.580619
C	0.414320	-3.079610	-1.244134
N	1.319281	-2.960969	-0.232929
C	1.677034	-4.025829	0.465239
C	1.150815	-5.310191	0.211616
C	0.231633	-5.461416	-0.805636
N	0.725071	-0.723542	-1.517665
H	-2.068211	-3.309722	-4.198851
H	-1.525361	-5.367684	-2.920585
H	-0.194655	-6.435634	-1.028768
H	1.472169	-6.152073	0.814718
H	2.390954	-3.856145	1.265021
C	0.949504	0.310689	-2.384194
C	2.212643	1.131496	-2.162110
C	3.331752	0.492981	-2.765268
C	2.322084	2.459951	-1.680750
C	4.518418	1.200835	-2.961947
C	3.524700	3.148266	-1.971015
C	4.601536	2.543990	-2.602797
H	5.363603	0.706609	-3.432920
H	3.606129	4.192995	-1.693646
H	5.502295	3.115310	-2.806922
O	0.370537	0.498061	-3.458396
H	-1.072782	-1.135430	-3.600771
C	3.259907	-0.953562	-3.211604
H	4.171065	-1.237381	-3.743901
H	3.144345	-1.617783	-2.349564
H	2.409281	-1.130454	-3.876558
Co	1.633263	-0.893484	0.283188
C	-0.413508	-1.694018	2.383964
O	0.798361	-1.606283	2.072400
O	-1.345240	-1.057545	1.774299
C	-0.826964	-2.657444	3.512671
C	-1.609018	-1.899786	4.606007
H	-1.948978	-2.609196	5.367364
H	-0.978536	-1.156042	5.102034
H	-2.488123	-1.390327	4.206570
C	-1.735277	-3.734804	2.874916
H	-1.229957	-4.237383	2.042570
H	-1.990017	-4.492028	3.623172
H	-2.668285	-3.301801	2.503964
C	0.413195	-3.322361	4.127953
H	0.108069	-3.999782	4.932102
H	0.961957	-3.899282	3.379495
H	1.094273	-2.574529	4.542791
C	-5.503106	1.005594	1.718067
C	-6.047636	0.522829	0.347889
H	-5.970783	-0.564373	0.250204
H	-7.101373	0.804097	0.258814

H	-5.494486	0.981640	-0.476465
C	-5.573888	2.539969	1.794929
H	-6.617516	2.860800	1.724379
H	-5.166514	2.906385	2.742755
H	-5.011824	3.001175	0.980173
C	-6.306061	0.366065	2.862805
H	-6.292053	-0.724284	2.799329
H	-5.903240	0.657883	3.837879
H	-7.346086	0.702044	2.808987
C	-4.048155	0.558684	1.742875
O	-3.146579	1.248720	1.245446
O	-3.827600	-0.635572	2.249341
H	-2.842423	-0.868930	2.143740
C	6.093179	-0.798774	0.199094
C	6.176519	-1.806464	-0.959454
H	5.845685	-1.349474	-1.895882
H	7.212755	-2.134529	-1.083822
H	5.552102	-2.681874	-0.768371
C	6.555657	-1.468036	1.518642
H	7.600800	-1.777074	1.419906
H	6.481084	-0.772574	2.360428
H	5.953796	-2.354419	1.742039
C	6.962730	0.435197	-0.098152
H	6.611369	0.953149	-0.994818
H	6.948377	1.143253	0.733335
H	7.996534	0.117155	-0.264089
C	4.639616	-0.403891	0.428646
O	3.713264	-1.210818	0.221286
O	4.451953	0.797654	0.915147
H	3.464258	0.948413	1.115966

30bt

Energy = -2172.51637808 ZPE = -2171.854705 H = -2171.81085 G = -2171.931954

C	-3.338718	-0.661183	-0.726738
C	-4.080047	-1.795874	-0.446388
C	-5.342138	-1.673950	0.183477
C	-5.859720	-0.447101	0.538066
C	-5.124071	0.735348	0.258611
C	-3.859034	0.636084	-0.392001
N	-3.098574	1.723946	-0.702692
C	-3.554210	2.919239	-0.374299
C	-4.790114	3.129645	0.284316
C	-5.571350	2.039512	0.595649
N	-2.062141	-0.633386	-1.286570
H	-5.902991	-2.578716	0.396685
H	-6.823789	-0.367357	1.031079
H	-6.526727	2.160493	1.098489
H	-5.103088	4.138147	0.531973
H	-2.922652	3.767608	-0.630035
C	-1.274488	-1.649775	-1.737012
C	0.098856	-1.203185	-2.229091
C	0.111102	-0.506504	-3.496730
C	1.339568	-1.744808	-1.712723
C	1.305869	-0.362741	-4.188545
C	2.520990	-1.575802	-2.491163
C	2.509109	-0.901494	-3.694576
H	1.303093	0.154447	-5.143400
H	3.444498	-1.997937	-2.109415
H	3.425350	-0.795303	-4.266777
O	-1.655791	-2.817595	-1.810549
H	-3.681572	-2.767459	-0.701850
C	-1.167305	0.029190	-4.104880
H	-1.940224	-0.744434	-4.163241
H	-1.586316	0.854500	-3.520614
H	-0.980571	0.397506	-5.115925
C	3.212372	1.327763	0.546116
C	4.411804	1.581735	1.220521
C	4.842850	2.900308	1.480834
C	4.115312	4.002503	1.081048
C	2.900784	3.807315	0.376512
C	2.460835	2.477502	0.096682
N	1.306104	2.249661	-0.601395
C	0.560278	3.271004	-1.003290
C	0.911916	4.613031	-0.752122
C	2.081137	4.875741	-0.072086
N	2.612297	0.095614	0.322870
H	5.777837	3.040937	2.016898
H	4.455589	5.012333	1.289481
H	2.388863	5.897963	0.130598
H	0.265572	5.411627	-1.099481
H	-0.351018	3.017623	-1.537553
C	3.255301	-1.076078	0.524076
C	2.353338	-2.302288	0.551613
C	2.445566	-3.148546	1.680378
C	1.453634	-2.624885	-0.498560
C	1.670117	-4.313206	1.724587
C	0.733435	-3.831873	-0.443200
C	0.836511	-4.666706	0.666319
H	1.726550	-4.950888	2.602681
H	0.080125	-4.090435	-1.264386
H	0.262359	-5.587548	0.705241
O	4.474090	-1.252903	0.718743
H	5.007690	0.742899	1.549753
C	3.330857	-2.809513	2.859059
H	3.171890	-1.778502	3.191980
H	3.123784	-3.476656	3.699966
H	4.386379	-2.889193	2.590077
Co	0.957235	0.274614	-0.901284
H	-1.674696	0.304481	-1.262652
C	-1.608764	0.075854	2.958753
C	-0.641386	-0.142492	4.147573
H	0.271338	0.450330	4.025735
H	-1.130154	0.170174	5.075472
H	-0.361469	-1.195208	4.238743
C	-2.881922	-0.774209	3.152225
H	-3.398874	-0.447387	4.059866
H	-3.568419	-0.658690	2.309122
H	-2.639387	-1.834330	3.255095
C	-1.971846	1.562051	2.835056
H	-1.082299	2.172881	2.660508
H	-2.664520	1.731005	2.007878
H	-2.450852	1.898393	3.759490
C	-0.869002	-0.378099	1.706041
O	-0.675151	-1.697633	1.661623
O	-0.457692	0.385038	0.838756
H	-0.098645	-1.925093	0.904458

Ag2CO3

Energy = -557.957158949 ZPE = -555.372006 H = -555.363982 G = -555.407473

C	-0.000029	1.012585	-0.000023
O	1.126282	1.634776	-0.000198
O	-1.126526	1.634587	0.000210
O	0.000045	-0.312221	-0.000082

AgOPiv

Energy = -493.589320787 ZPE = -492.113236 H = -

492.102261 G = -492.150509

C	-0.708576	0.051708	-0.000564
O	-0.101574	-1.066270	-0.000349
O	-0.120279	1.171810	-0.000446
C	-2.256524	0.003794	-0.000164
C	-2.709606	-0.767848	-1.256611
H	-2.402286	-0.246801	-2.170407
H	-2.272773	-1.769382	-1.270411
H	-3.801465	-0.860080	-1.272144
C	-2.707870	-0.758013	1.263029
H	-2.270715	-1.759301	1.284318
H	-2.399686	-0.229517	2.172238
H	-3.799669	-0.850567	1.280534
C	-2.857767	1.415727	-0.005188
H	-2.541161	1.981186	0.875659
H	-2.542110	1.974471	-0.890703
H	-3.952312	1.358017	-0.004480

B

Energy = -2172.54118572 ZPE = -2171.877591 H = -2171.835217 G = -2171.949166

C	-2.669433	-1.355131	-0.912574
C	-3.570166	-2.271818	-1.460941
C	-4.954220	-2.000878	-1.495612
C	-5.488014	-0.834605	-0.984752
C	-4.618193	0.126413	-0.415624
C	-3.218578	-0.147388	-0.389171
N	-2.334330	0.748107	0.144054
C	-2.764533	1.895996	0.650181
C	-4.131290	2.237735	0.660252
C	-5.051551	1.359735	0.132664
N	-1.275814	-1.438174	-0.888248
H	-5.612727	-2.742908	-1.938195
H	-6.555370	-0.640071	-1.011474
H	-6.110914	1.599313	0.128260
H	-4.431841	3.188648	1.084836
H	-2.009461	2.556299	1.053080
C	-0.692655	-2.682536	-0.941740
C	0.746498	-2.757613	-1.364801
C	1.659358	-3.589528	-0.682077
C	1.142837	-2.087555	-2.528205
C	2.959113	-3.698654	-1.192311
C	2.432439	-2.230071	-3.037538
C	3.347114	-3.037526	-2.360749
H	0.427314	-1.450050	-3.032692
H	3.680810	-4.316309	-0.663914
H	2.721123	-1.710435	-3.946389
H	4.360833	-3.150920	-2.734179
O	-1.286018	-3.748548	-0.708136
H	-3.202501	-3.204859	-1.862162
C	1.281455	-4.348623	0.568946
H	2.175458	-4.666327	1.112270
H	0.663223	-3.749259	1.242455
H	0.690756	-5.234788	0.319318
C	0.632503	2.737933	0.004283
C	1.309499	3.916356	0.320586
C	1.703329	4.811009	-0.701644
C	1.428629	4.576741	-2.033501
C	0.731728	3.396332	-2.400670
C	0.352983	2.478537	-1.380568
N	-0.296692	1.312674	-1.672884
C	-0.637008	1.037969	-2.919866
C	-0.318661	1.899356	-3.992269
C	0.373155	3.062925	-3.733008
N	0.174067	1.755627	0.864633
H	2.234898	5.714429	-0.416162
H	1.730002	5.279928	-2.803572
H	0.643792	3.739052	-4.539113
H	-0.614382	1.629681	-4.999906
H	-1.172430	0.106506	-3.070722
C	0.353644	1.716607	2.220993
C	-0.176526	0.429566	2.775313
C	-0.190171	0.122130	4.152926
C	-0.637314	-0.496660	1.810815
C	-0.687157	-1.134937	4.532119
C	-1.134789	-1.735844	2.223292
C	-1.151544	-2.050977	3.589638
H	1.234978	-1.436081	1.716594
H	-0.705598	-1.396054	5.587048
H	-1.503938	-2.455564	1.500659
H	-1.529509	-3.016311	3.916702
O	0.884833	2.612133	2.897140
H	1.526408	4.132202	1.356307
C	0.309814	1.073225	5.214151
H	0.168768	0.644531	6.210455
H	1.370354	1.298434	5.071638
H	-0.208058	2.034605	5.163512
Co	-0.507839	0.186208	0.012738
C	2.369911	-0.520112	0.524745
O	1.448219	-0.213697	-0.236999
O	2.197460	-1.278181	1.595944
C	3.774297	0.032455	0.355196
C	4.830630	-1.068480	0.565099
H	5.828568	-0.623650	0.506321
H	4.721543	-1.542043	1.543744
H	4.748609	-1.839624	-0.204433
C	3.915152	0.676171	-1.032232
H	3.195576	1.488250	-1.163474
H	4.924211	1.084913	-1.139512
H	3.749215	-0.059672	-1.822772
C	3.915133	1.117076	1.458167
H	4.899410	1.586231	1.366186
H	3.151397	1.893133	1.356146
H	3.830054	0.677854	2.455645

BQNH

Energy = -841.052121483 ZPE = -840.779763 H = -840.762995 G = -840.82419

C	1.235563	-0.716704	-0.142968
C	1.589336	-2.036923	-0.371646
C	2.954408	-2.410492	-0.403578
C	3.962525	-1.492356	-0.210909
C	3.634588	-0.131583	0.026268
C	2.264534	0.266792	0.061517
N	1.875398	1.553848	0.282751
C	2.811843	2.466033	0.472343
C	4.198155	2.179179	0.458126
C	4.604439	0.882934	0.235292
N	-0.069491	-0.218809	-0.092310
H	3.199658	-3.452687	-0.585140
H	5.006453	-1.790497	-0.236334
H	5.658944	0.621568	0.216453
H	4.915188	2.976651	0.621140
H	2.471499	3.485112	0.646533
C	-1.257398	-0.893913	-0.229452
C	-2.474050	-0.012825	-0.190494
C	-3.649524	-0.448225	0.463656
C	-2.451899	1.229275	-0.845202

C	-4.761112	0.404108	0.448966
C	-3.575994	2.053419	-0.859638
C	-4.734823	1.638054	-0.203865
H	-5.666636	0.091191	0.961926
H	-3.545407	3.006099	-1.379193
H	-5.618132	2.270063	-0.199753
O	-1.329223	-2.115481	-0.374272
H	0.814402	-2.774298	-0.521316
C	-3.738431	-1.776651	1.178225
H	-4.647318	-1.827089	1.783489
H	-3.746027	-2.603303	0.462831
H	-2.875972	-1.943538	1.830014
H	-0.091885	0.775866	0.112832
H	-1.555293	1.542713	-1.372228

BQN

Energy = -840.530392241 ZPE = -840.272647 H = -840.256939 G = -840.315034

C	1.155384	-0.638909	-0.047797
C	1.465328	-2.013566	-0.109159
C	2.789047	-2.491828	-0.078575
C	3.870864	-1.639276	0.002609
C	3.637406	-0.241400	0.054520
C	2.295228	0.276302	0.028613
N	2.058944	1.619213	0.070493
C	3.083379	2.450858	0.138288
C	4.436634	2.041380	0.173743
C	4.703931	0.692843	0.131268
N	-0.092742	-0.073511	-0.023607
H	2.954310	-3.566849	-0.122571
H	4.891514	-2.012476	0.023821
H	5.726779	0.323228	0.154452
H	5.231070	2.779330	0.231896
H	2.844185	3.514694	0.167911
C	-1.217716	-0.781405	-0.216028
C	-2.479502	0.067650	-0.102026
C	-3.742895	-0.494156	0.208742
C	-2.395238	1.450931	-0.336941
C	-4.858920	0.356279	0.264749
C	-3.516410	2.277255	-0.290903
C	-4.762191	1.725011	0.012362
H	-5.827785	-0.070571	0.515496
H	-3.417969	3.341985	-0.486748
H	-5.649583	2.351111	0.058259
O	-1.356510	-2.004676	-0.488254
H	0.640161	-2.706736	-0.184372
C	-3.949100	-1.963713	0.505508
H	-4.954165	-2.135328	0.905449
H	-3.814682	-2.570411	-0.393320
H	-3.212774	-2.334746	1.222689
H	-1.413782	1.858736	-0.548963

B-q

Energy = -2172.4859705 ZPE = -2171.827624 H = -2171.783362 G = -2171.905987

C	-2.739391	1.546188	0.823825
C	-3.700996	2.560294	0.845358
C	-5.027957	2.299879	1.250180
C	-5.442432	1.039020	1.629654
C	-4.508728	-0.029382	1.616287
C	-3.166985	0.233296	1.218577
N	-2.235736	-0.754909	1.176461
C	-2.557259	-1.997516	1.507330
C	-3.855986	-2.345355	1.926053
C	-4.825570	-1.363005	1.976850
N	-1.387754	1.683136	0.526000
H	-5.736089	3.123123	1.258021
H	-6.466180	0.850899	1.937322
H	-5.838925	-1.600730	2.287851
H	-4.077439	-3.372035	2.194582
H	-1.760709	-2.729996	1.421888
C	-0.946485	2.803781	-0.170345
C	0.459652	3.232228	0.116228
C	1.292777	3.751812	-0.900071
C	0.921503	3.163999	1.436758
C	2.574659	4.182874	-0.538005
C	2.196765	3.609627	1.779843
C	3.027956	4.120525	0.782933
H	0.260813	2.760855	2.195683
H	3.232754	4.576591	-1.308286
H	2.536072	3.554080	2.809726
H	4.027727	4.468224	1.026725
O	-1.642750	3.428218	-0.979699
H	-3.426555	3.561671	0.543608
C	0.864668	3.812439	-2.347644
H	1.718839	4.038141	-2.991752
H	0.431254	2.862293	-2.672905
H	0.095479	4.573538	-2.500129
C	1.351233	-2.486437	0.621685
C	2.200032	-3.576266	0.397855
C	3.196375	-3.931884	1.335202
C	3.376538	-3.242525	2.515674
C	2.536513	-2.135600	2.799875
C	1.539543	-1.756374	1.851566
N	0.722554	-0.688296	2.077981
C	0.818715	-0.003329	3.206752
C	1.765484	-0.314882	4.204021
C	2.625653	-1.370381	3.991374
N	0.346764	-1.995329	-0.192497
H	3.834200	-4.782174	1.108913
H	4.140927	-3.531003	3.230596
H	3.376116	-1.632678	4.732054
H	1.807664	0.279163	5.110055
H	0.126612	0.824020	3.326542
C	-0.026345	-2.585138	-1.361400
C	-1.079142	-1.788516	-2.098945
C	-1.815650	-2.316285	-3.189153
C	-1.302968	-0.464330	-1.704851
C	-2.740556	-1.470690	-3.822242
C	-2.216292	0.370271	-2.339130
C	-2.938486	-0.149150	-3.421073
H	0.477092	0.204165	-2.323991
H	-3.317798	-1.863416	-4.655543
H	-2.366738	1.396550	-2.015985
H	-3.656475	0.475803	-3.946825
O	0.417897	-3.649841	-1.828614
H	2.078843	-4.147823	-0.509681
C	-1.662977	-3.734761	-3.688862
H	-0.673274	-3.894821	-4.124255
H	-1.750867	-4.457660	-2.874159
H	-2.423127	-3.954589	-4.444550
Co	-0.410544	-0.101644	0.366114
C	2.123260	0.402760	-1.406957
O	1.571570	0.578446	-0.322429
O	1.442049	0.256461	-2.538797
C	3.632076	0.293456	-1.568764
C	4.108299	1.330575	-2.607490
H	5.190452	1.238288	-2.741753

H	3.624280	1.173627	-3.574527
H	3.890585	2.348052	-2.270049
C	4.309916	0.531752	-0.211872
H	3.971279	-0.198797	0.528209
H	5.393886	0.434443	-0.325529
H	4.086540	1.531266	0.169406
C	3.932403	-1.140313	-2.069339
H	5.014006	-1.260478	-2.186007
H	3.578651	-1.887975	-1.352305
H	3.454949	-1.330660	-3.033754

B-t

Energy = -2172.52076082 ZPE = -2171.859923 H = -2171.816324 G = -2171.935402

C	-3.019531	0.874676	0.934463
C	-4.026226	1.633011	1.534488
C	-5.379714	1.235569	1.481039
C	-5.781396	0.088881	0.827421
C	-4.802541	-0.719845	0.200581
C	-3.430871	-0.326145	0.263363
N	-2.460982	-1.078062	-0.319676
C	-2.761399	-2.190124	-0.965657
C	-4.089399	-2.655435	-1.076877
C	-5.099975	-1.920994	-0.495013
N	-1.642625	1.129743	1.007426
H	-6.119527	1.862396	1.970994
H	-6.825997	-0.203828	0.786616
H	-6.133416	-2.249793	-0.560608
H	-4.293673	-3.575471	-1.613128
H	-1.925915	-2.725888	-1.406456
C	-1.215938	2.428746	1.181788
C	0.198338	2.608536	1.657915
C	1.057189	3.544906	1.043672
C	0.630360	1.890302	2.778866
C	2.347414	3.695130	1.566054
C	1.908675	2.073284	3.302783
C	2.775164	2.974185	2.684307
H	-0.047630	1.180782	3.237406
H	3.030894	4.390711	1.086050
H	2.226798	1.511103	4.175822
H	3.781020	3.119879	3.067985
O	-1.911306	3.437410	0.984436
H	-3.766954	2.547237	2.048970
C	0.636459	4.360112	-0.157327
H	0.107275	3.755523	-0.899679
H	-0.057545	5.152768	0.136048
H	1.505515	4.815380	-0.639600
C	1.121216	-2.517359	-0.196655
C	2.045818	-3.488394	-0.578473
C	2.586037	-4.380388	0.379005
C	2.218107	-4.345574	1.707385
C	1.267241	-3.383002	2.138251
C	0.740227	-2.468052	1.185237
N	-0.159881	-1.504005	1.543193
C	-0.603313	-1.438318	2.788418
C	-0.146429	-2.314705	3.793743
C	0.793331	-3.271812	3.470251
N	0.496876	-1.563118	-0.988721
H	3.310094	-5.116860	0.042653
H	2.635352	-5.042716	2.427139
H	1.173298	-3.953134	4.226241
H	-0.531912	-2.218625	4.802337
H	-1.333553	-0.661507	2.988874
C	0.713475	-1.376696	-2.332669
C	-0.011103	-0.153738	-2.794546
C	-0.021732	0.298796	-4.131865
C	-0.681534	0.564313	-1.785669
C	-0.727547	1.478772	-4.409131
C	-1.392313	1.726607	-2.086064
C	-1.400690	2.183351	-3.410273
H	1.299308	1.757400	-1.453320
H	-0.747838	1.850672	-5.430084
H	-1.921635	2.279088	-1.318402
H	-1.937313	3.094513	-3.661231
O	1.419135	-2.096441	-3.052095
H	2.342523	-3.552319	-1.614763
C	0.694300	-0.426636	-5.245339
H	0.539874	0.086940	-6.198289
H	1.767431	-0.491892	-5.046113
H	0.344078	-1.458333	-5.336820
Co	-0.523263	-0.233675	-0.018593
C	2.547336	0.856251	-0.360568
O	1.681698	0.447867	0.401255
O	2.268461	1.653091	-1.400975
C	4.013332	0.456885	-0.275130
C	4.905996	1.714153	-0.267236
H	5.957596	1.411396	-0.249585
H	4.736992	2.324934	-1.157521
H	4.707464	2.327187	0.615799
C	4.232944	-0.373279	0.998077
H	3.623608	-1.280787	0.985055
H	5.286046	-0.661944	1.069260
H	3.966417	0.203379	1.888048
C	4.315051	-0.397319	-1.532117
H	5.347403	-0.757678	-1.481938
H	3.649528	-1.263148	-1.596486
H	4.196706	0.192599	-2.444767

C

Energy = -2172.52316383 ZPE = -2171.862428 H = -2171.820374 G = -2171.933623

C	-0.089721	2.671933	0.822625
C	-0.576102	3.920160	1.232120
C	0.296161	4.944946	1.646516
C	1.667668	4.779039	1.676546
C	2.212197	3.535198	1.279704
C	1.327369	2.491291	0.871515
N	1.801503	1.266351	0.489573
C	3.109105	1.042805	0.461404
C	4.047667	2.023586	0.837134
C	3.602037	3.257841	1.252396
N	-0.811581	1.625485	0.267447
H	-0.135037	5.895640	1.947946
H	2.330492	5.577394	1.993957
H	4.302876	4.030141	1.555858
H	5.103843	1.783481	0.795751
H	3.444653	0.068107	0.136691
C	-2.192443	1.602323	0.512505
C	-3.119986	1.186265	-0.591981
C	-4.524952	1.112838	-0.393480
C	-2.604144	0.956394	-1.875694
C	-5.332296	0.826322	-1.506100
C	-3.421226	0.680597	-2.965547
C	-4.803067	0.621787	-2.779388
H	-1.535643	0.969857	-1.996335
H	-6.407878	0.764730	-1.363285
H	-2.983500	0.508089	-3.944351
H	-5.464876	0.408884	-3.614113

O	-2.663828	2.005458	1.583652
H	-1.641285	4.106270	1.228922
C	-5.214668	1.323882	0.934641
H	-6.278897	1.085947	0.846651
H	-4.778000	0.705178	1.721937
H	-5.110576	2.357390	1.274858
C	2.235150	-1.547002	-1.495067
C	3.166841	-2.486067	-1.893779
C	3.773616	-2.388403	-3.170164
C	3.462405	-1.360603	-4.032809
C	2.512941	-0.377273	-3.650926
C	1.874542	-0.493256	-2.381724
N	0.947731	0.419184	-1.952668
C	0.702867	1.483094	-2.699536
C	1.291881	1.684282	-3.966975
C	2.177655	0.746681	-4.448685
N	1.542216	-1.552673	-0.241553
H	4.501951	-3.138720	-3.460720
H	3.942768	-1.281425	-5.003202
H	2.641585	0.864662	-5.423586
H	1.037313	2.570051	-4.537589
H	0.014277	2.208350	-2.278639
C	2.218633	-1.883349	0.990715
C	1.357564	-1.521688	2.133850
C	1.535271	-2.072911	3.426470
C	0.359502	-0.562110	1.862501
C	0.664883	-1.638349	4.429435
C	-0.475167	-0.130697	2.891652
C	-0.320577	-0.680219	4.168094
H	0.683327	-2.329716	-0.300180
H	0.762079	-2.050639	5.430212
H	-1.235644	0.619732	2.711127
H	-0.976268	-0.358338	4.973810
O	3.336606	-2.374128	1.026399
H	3.440913	-3.286181	-1.219984
C	2.603989	-3.093022	3.734584
H	2.485984	-3.478774	4.750723
H	2.570023	-3.933022	3.034011
H	3.603052	-2.657626	3.638621
Co	0.362196	0.028877	0.032314
C	-1.367250	-2.315536	-0.154833
O	-1.243673	-1.052651	-0.271165
O	-0.399967	-3.129343	-0.250745
C	-2.776034	-2.855037	0.131804
C	-3.320419	-2.107579	1.366902
H	-4.331305	-2.459246	1.598772
H	-2.685748	-2.277984	2.243010
H	-3.354469	-1.033960	1.180514
C	-3.665411	-2.564043	-1.093494
H	-3.288477	-3.079966	-1.983693
H	-4.683972	-2.918988	-0.903074
H	-3.704585	-1.495788	-1.301872
C	-2.727194	-4.365406	0.404218
H	-3.737869	-4.735061	0.607249
H	-2.325913	-4.909995	-0.454666
H	-2.096735	-4.591265	1.269153

C'

Energy = -2172.05877666 ZPE = -2171.409342 H = -2171.367059 G = -2171.481229

C	2.554688	1.538582	-0.837722
C	3.404880	2.553317	-1.292821
C	4.776330	2.313842	-1.514017
C	5.356172	1.081385	-1.282460
C	4.543277	0.020444	-0.815696
C	3.152456	0.260276	-0.601293
N	2.323096	-0.727766	-0.154564
C	2.801936	-1.937967	0.093077
C	4.162636	-2.257186	-0.093326
C	5.027015	-1.285096	-0.544607
N	1.175096	1.597942	-0.672425
H	5.390158	3.134894	-1.875098
H	6.415336	0.911639	-1.449101
H	6.080418	-1.502484	-0.697894
H	4.503588	-3.263755	0.122027
H	2.086927	-2.668176	0.448345
C	0.590278	2.822945	-0.462786
C	-0.861667	2.979689	-0.822938
C	-1.763523	3.647742	0.032838
C	-1.267462	2.598523	-2.105336
C	-3.056573	3.898820	-0.440017
C	-2.555015	2.872638	-2.567749
C	-3.455693	3.526606	-1.727401
H	-0.560466	2.080716	-2.742410
H	-3.767474	4.394449	0.216767
H	-2.850506	2.574263	-3.569830
H	-4.465665	3.743102	-2.065018
O	1.197894	3.832546	-0.062921
H	3.003009	3.539759	-1.474286
C	-1.377468	4.041452	1.438335
H	-2.230931	4.475939	1.967374
H	-1.048633	3.155722	1.989311
H	-0.556841	4.762277	1.432844
C	-0.663699	-2.703707	-0.367103
C	-1.310832	-3.932970	-0.206148
C	-1.797733	-4.640812	-1.327858
C	-1.649253	-4.175145	-2.619351
C	-0.986445	-2.939330	-2.835355
C	-0.509861	-2.206441	-1.709859
N	0.115288	-1.002794	-1.854237
C	0.336560	-0.511132	-3.059123
C	-0.086793	-1.173842	-4.232694
C	-0.754620	-2.373815	-4.117110
N	-0.129066	-1.887348	0.604289
H	-2.302592	-5.588197	-1.157195
H	-2.023342	-4.737107	-3.469809
H	-1.103777	-2.902924	-4.999772
H	0.111449	-0.728011	-5.201404
H	0.860295	0.438602	-3.092369
C	-0.170002	-2.099180	1.957249
C	0.434173	-0.939548	2.677772
C	0.632800	-0.910059	4.076705
C	0.780148	0.158657	1.863504
C	1.203769	0.245000	4.627932
C	1.365283	1.287060	2.439876
C	1.569411	1.327208	3.822662
H	1.369938	0.291957	5.701921
H	1.642587	2.139198	1.828918
H	2.015097	2.208650	4.279944
O	-0.630072	-3.117373	2.506405
H	-1.433810	-4.327338	0.791663
C	0.259533	-2.058871	4.985818
H	0.527015	-1.830783	6.022544
H	-0.811596	-2.273842	4.935179
H	0.760112	-2.984505	4.687280
Co	0.460387	-0.169652	0.004601
C	-2.280088	0.422003	0.900133
O	-1.412993	0.281780	-0.045358

O	-2.090442	0.907286	2.023608
C	-3.695523	-0.134032	0.562449
C	-4.759802	0.889967	0.991803
H	-5.767188	0.472729	0.872835
H	-4.616046	1.168807	2.038746
H	-4.690595	1.798787	0.385919
C	-3.853625	-0.469537	-0.927246
H	-3.127172	-1.224514	-1.236530
H	-4.862340	-0.856133	-1.121305
H	-3.699167	0.418936	-1.545718
C	-3.848865	-1.421923	1.402573
H	-4.833902	-1.874553	1.233826
H	-3.083344	-2.158030	1.137969
H	-3.747787	-1.197016	2.468535

C1

Energy = -2172.52845393 ZPE = -2171.865182 H = -2171.823014 G = -2171.937057

C	-0.035035	2.666955	-0.966277
C	0.397600	3.934164	-1.378005
C	-0.508611	4.897370	-1.860517
C	-1.863660	4.646741	-1.963019
C	-2.354758	3.381063	-1.566201
C	-1.435000	2.404169	-1.076220
N	-1.860987	1.164850	-0.682689
C	-3.149540	0.853481	-0.746069
C	-4.117724	1.764229	-1.212083
C	-3.723670	3.017350	-1.621857
N	0.725738	1.672615	-0.365991
H	-0.118450	5.866256	-2.159896
H	-2.553770	5.395168	-2.338653
H	-4.449124	3.737763	-1.988594
H	-5.156618	1.456388	-1.240370
H	-3.438781	-0.136151	-0.424143
C	2.104156	1.709605	-0.592179
C	3.037455	1.337262	0.526067
C	4.440718	1.253760	0.322225
C	2.531107	1.187963	1.825606
C	5.258331	1.048163	1.445023
C	3.358563	0.993161	2.925886
C	4.739563	0.932932	2.734161
H	1.462861	1.209476	1.955746
H	6.332943	0.979177	1.298083
H	2.929374	0.886595	3.917759
H	5.408719	0.783998	3.576815
O	2.578202	2.130937	-1.656588
H	1.449096	4.181501	-1.327486
C	5.116901	1.372353	-1.024643
H	6.167947	1.079405	-0.943837
H	4.632778	0.750391	-1.780668
H	5.064802	2.396803	-1.402614
C	-2.278678	-1.431792	1.515281
C	-3.216911	-2.348653	1.976345
C	-3.834479	-2.168848	3.236822
C	-3.550311	-1.084453	4.038775
C	-2.610506	-0.117554	3.597440
C	-1.954944	-0.312732	2.347201
N	-1.041945	0.585616	1.864669
C	-0.820486	1.706129	2.533393
C	-1.426858	1.985060	3.776729
C	-2.302049	1.067201	4.313995
N	-1.574023	-1.476071	0.301321
H	-4.558715	-2.907693	3.566928
H	-4.043941	-0.947434	4.995849
H	-2.779921	1.247238	5.272733
H	-1.195601	2.913666	4.286108
H	-0.140734	2.410252	2.065639
C	-2.022226	-2.144947	-0.839938
C	-1.158808	-1.801430	-2.003916
C	-1.194352	-2.509642	-3.228469
C	-0.295847	-0.703934	-1.817130
C	-0.336595	-2.076923	-4.246689
C	0.532295	-0.281808	-2.854798
C	0.509179	-0.978933	-4.067495
H	-0.360190	-2.557328	0.661486
H	-0.334609	-2.607017	-5.195692
H	1.192011	0.568875	-2.728691
H	1.158116	-0.665321	-4.882014
O	-2.992153	-2.907450	-0.867111
H	-3.477652	-3.193401	1.355756
C	-2.100597	-3.694413	-3.463600
H	-1.898536	-4.143980	-4.439998
H	-1.970389	-4.456340	-2.689654
H	-3.153573	-3.401695	-3.421205
Co	-0.414845	0.046117	-0.051743
C	1.454890	-2.216780	0.417720
O	1.247482	-0.991071	0.376170
O	0.502250	-3.084553	0.656454
C	2.847492	-2.784531	0.176469
C	3.389237	-2.129230	-1.111996
H	4.405436	-2.487260	-1.302490
H	2.764381	-2.377818	-1.975668
H	3.409977	-1.044273	-1.009890
C	3.729159	-2.392566	1.381710
H	3.351391	-2.838806	2.307716
H	4.747002	-2.759634	1.217373
H	3.766150	-1.311022	1.503303
C	2.803842	-4.312754	0.022137
H	3.816180	-4.682904	-0.166240
H	2.424015	-4.795662	0.926131
H	2.167451	-4.609501	-0.816453

C1'

Energy = -1825.450386 ZPE = -1824.93664 H = -1824.903271 G = -1824.999459

C	-0.243530	-2.785879	0.315450
C	-0.511411	-4.106449	0.667158
C	-0.060917	-5.163180	-0.159134
C	0.644796	-4.941541	-1.325218
C	0.931448	-3.610348	-1.725168
C	0.479848	-2.549925	-0.894760
N	0.710279	-1.239836	-1.227127
C	1.363729	-0.926896	-2.338065
C	1.845247	-1.925226	-3.208653
C	1.632345	-3.253803	-2.905643
N	-0.591260	-1.610495	0.965958
H	-0.282774	-6.182432	0.143482
H	0.981096	-5.766586	-1.944782
H	1.994468	-4.036606	-3.565517
H	2.375368	-1.627764	-4.105848
H	1.505226	0.128909	-2.530643
C	-1.496797	-1.514206	1.977434
C	-1.825372	-0.066066	2.259759
C	-3.158113	0.395668	2.193020
C	-0.775954	0.845843	2.485861
C	-3.380235	1.772428	2.302480
C	-1.026315	2.219973	2.596947
C	-2.332735	2.683285	2.485646

H	0.229494	0.473840	2.647212
H	-4.399384	2.143644	2.232584
H	-0.203427	2.906057	2.770995
H	-2.547514	3.745201	2.557224
O	-2.041513	-2.453272	2.573804
H	-1.067550	-4.307685	1.571489
C	-4.314336	-0.548098	1.968578
H	-5.267304	-0.016009	2.024109
H	-4.244487	-1.014087	0.980121
H	-4.309187	-1.355795	2.703111
C	1.998531	2.024445	-0.259181
C	2.698151	3.165285	-0.653634
C	4.030220	3.373731	-0.226939
C	4.695154	2.477040	0.584300
C	4.023096	1.303958	1.014259
C	2.679087	1.090044	0.594487
N	1.976539	-0.015941	0.985765
C	2.545632	-0.925057	1.761982
C	3.874302	-0.796707	2.218209
C	4.604426	0.312760	1.846668
N	0.706444	1.648607	-0.599677
H	4.539628	4.274448	-0.557944
H	5.719057	2.652053	0.899323
H	5.628997	0.440282	2.184783
H	4.298907	-1.566419	2.852762
H	1.927216	-1.775432	2.032320
C	-0.186426	2.408805	-1.322975
C	-1.456063	1.643306	-1.538666
C	-2.550658	2.128750	-2.288554
C	-1.485878	0.358013	-0.961684
C	-3.646796	1.271625	-2.463338
C	-2.574503	-0.483845	-1.178639
C	-3.658571	-0.019126	-1.930155
H	-4.500674	1.620705	-3.038531
H	-2.587013	-1.487019	-0.764842
H	-4.518154	-0.663306	-2.098684
O	0.025848	3.554261	-1.743636
H	2.205955	3.887582	-1.287972
C	-2.577929	3.509003	-2.901617
H	-3.524190	3.678034	-3.423766
H	-2.450043	4.284012	-2.140852
H	-1.753756	3.645585	-3.607306
Co	0.076315	-0.021153	0.074448

C1-q

Energy = -2172.48535811 ZPE = -2171.827079 H = -2171.783038 G = -2171.904593

C	-1.190561	-2.619209	-1.178162
C	-1.427705	-3.981719	-1.376090
C	-2.645828	-4.445068	-1.918989
C	-3.662365	-3.583083	-2.271820
C	-3.477898	-2.189463	-2.083505
C	-2.248726	-1.716070	-1.536378
N	-2.031489	-0.387395	-1.322535
C	-2.970016	0.496265	-1.638818
C	-4.205189	0.118670	-2.198934
C	-4.457307	-1.220267	-2.413380
N	-0.002591	-2.030823	-0.751339
H	-2.774358	-5.514755	-2.057297
H	-4.596342	-3.947726	-2.687494
H	-5.404247	-1.546899	-2.834055
H	-4.937017	0.880084	-2.443619
H	-2.746168	1.536419	-1.431415
C	1.007772	-2.830542	-0.236194
C	2.407021	-2.419046	-0.579457
C	3.489257	-2.675071	0.292597
C	2.645380	-1.881081	-1.851461
C	4.777453	-2.343442	-0.145951
C	3.937953	-1.577042	-2.278168
C	5.009270	-1.805532	-1.414274
H	1.797206	-1.723822	-2.510096
H	5.617392	-2.510195	0.523375
H	4.104321	-1.168788	-3.270618
H	6.023016	-1.566138	-1.722172
O	0.810363	-3.853131	0.433636
H	-0.666017	-4.699129	-1.104888
C	3.301377	-3.268991	1.668722
H	4.216869	-3.169723	2.258505
H	2.483904	-2.778979	2.205116
H	3.037546	-4.327574	1.603391
C	-1.031441	2.902787	-0.136348
C	-1.672080	4.126678	0.043962
C	-1.376248	5.234020	-0.783682
C	-0.438177	5.158509	-1.790003
C	0.235135	3.932035	-2.019680
C	-0.082456	2.800623	-1.208642
N	0.507006	1.585898	-1.424589
C	1.434294	1.465760	-2.364178
C	1.835693	2.539580	-3.184793
C	1.225783	3.763262	-3.020054
N	-1.138213	1.758253	0.666775
H	-1.898142	6.169228	-0.602338
H	-0.204091	6.018235	-2.410226
H	1.495755	4.609409	-3.645657
H	2.604404	2.382453	-3.932851
H	1.884955	0.486550	-2.469197
C	-2.251733	1.531845	1.446601
C	-2.160265	0.244612	2.214152
C	-2.912963	0.003049	3.393452
C	-1.336952	-0.767213	1.732624
C	-2.774249	-1.248048	4.010246
C	-1.210379	-2.014393	2.316834
C	-1.948320	-2.245187	3.486573
H	0.198328	1.855065	1.554183
H	-3.332254	-1.445444	4.921882
H	-0.583943	-2.790966	1.889981
H	-1.877756	-3.207745	3.987803
O	-3.250143	2.260562	1.517045
H	-2.398398	4.224861	0.837012
C	-3.835684	1.033802	4.001831
H	-4.156622	0.716479	4.998277
H	-3.351792	2.010899	4.078954
H	-4.721164	1.184104	3.378161
Co	-0.215860	-0.059950	-0.246518
C	1.976086	1.142823	1.489869
O	1.604960	0.115310	0.893932
O	1.142548	2.055412	1.918574
C	3.457987	1.419847	1.724496
C	4.032504	0.268935	2.575055
H	5.107828	0.418621	2.713816
H	3.562537	0.234856	3.563588
H	3.876515	-0.688164	2.079028
C	4.122242	1.424839	0.328068
H	3.721523	2.232019	-0.295108
H	5.200020	1.581342	0.437247
H	3.956081	0.475879	-0.184327
C	3.679963	2.767179	2.426518
H	4.753479	2.931491	2.562562

H	3.276923	3.594128	1.835512
H	3.201362	2.787900	3.409422

C1-q'

Energy = -1825.40074586 ZPE = -1824.891906 H = -1824.856954 G = -1824.959815

C	-2.498418	-1.598556	-0.580536
C	-3.427599	-2.358090	-1.293438
C	-4.744068	-2.541779	-0.812908
C	-5.172176	-1.987767	0.374531
C	-4.266857	-1.210907	1.142417
C	-2.933334	-1.019605	0.669084
N	-2.028166	-0.280938	1.380604
C	-2.385906	0.269833	2.529794
C	-3.682038	0.134715	3.070814
C	-4.615188	-0.603131	2.375919
N	-1.187324	-1.310318	-0.940263
H	-5.431749	-3.138585	-1.405905
H	-6.185825	-2.135444	0.734626
H	-5.623366	-0.729662	2.760854
H	-3.922712	0.608621	4.016011
H	-1.621040	0.844150	3.045348
C	-0.508484	-1.966343	-1.921172
C	0.911513	-1.457150	-2.060301
C	2.011248	-2.328893	-1.911653
C	1.128215	-0.093159	-2.305717
C	3.299073	-1.786195	-1.983284
C	2.422776	0.427490	-2.387225
C	3.512046	-0.423816	-2.214807
H	0.271889	0.562360	-2.428593
H	4.153587	-2.442955	-1.841523
H	2.571167	1.487762	-2.568897
H	4.525110	-0.034394	-2.257538
O	-0.918235	-2.892142	-2.641256
H	-3.119679	-2.812356	-2.223860
C	1.812879	-3.797831	-1.627224
H	2.772044	-4.318310	-1.562952
H	1.291213	-3.933064	-0.673432
H	1.199338	-4.266716	-2.400019
C	0.982982	2.721404	0.293906
C	1.796505	3.870405	0.483385
C	1.342852	5.139414	0.105646
C	0.096856	5.325130	-0.477364
C	-0.763454	4.212558	-0.699569
C	-0.329669	2.917573	-0.310403
N	-1.092127	1.816709	-0.497297
C	-2.284272	1.945099	-1.071686
C	-2.798476	3.184315	-1.495456
C	-2.037861	4.321541	-1.304620
N	1.257268	1.446870	0.622286
H	1.987894	5.996309	0.271403
H	-0.233560	6.315575	-0.774891
H	-2.401236	5.296573	-1.615243
H	-3.776352	3.230151	-1.961101
H	-2.852439	1.029548	-1.200173
C	2.538803	0.981099	1.027351
C	2.522934	-0.459680	1.386096
C	3.717402	-1.136679	1.764712
C	1.268337	-1.120841	1.334173
C	3.603152	-2.481181	2.125864
C	1.212090	-2.461745	1.742028
C	2.366465	-3.141281	2.126105
H	4.497761	-3.025309	2.418435
H	0.261994	-2.993182	1.715442
H	2.322400	-4.190193	2.411939
O	3.535209	1.704078	1.054574
H	2.772766	3.744184	0.926027
C	5.081656	-0.490145	1.786464
H	5.844717	-1.218251	2.077548
H	5.338890	-0.081775	0.804648
H	5.116481	0.354785	2.479928
Co	-0.163799	-0.083939	0.322315

C1-t

Energy = -2172.51055608 ZPE = -2171.850222 H = -2171.806732 G = -2171.926481

C	-0.067790	2.870464	0.273263
C	-0.624909	4.141906	0.443344
C	0.176217	5.271724	0.705666
C	1.549925	5.187402	0.818836
C	2.170324	3.923530	0.669782
C	1.361529	2.776160	0.402975
N	1.916080	1.543524	0.271620
C	3.222791	1.374578	0.373518
C	4.099802	2.453124	0.615397
C	3.571273	3.716864	0.767081
N	-0.757603	1.721006	-0.106787
H	-0.313660	6.235033	0.818073
H	2.157569	6.064617	1.017370
H	4.217109	4.568069	0.964147
H	5.166770	2.272687	0.684376
H	3.590327	0.358390	0.267230
C	-2.130621	1.687050	0.181659
C	-3.061290	1.106917	-0.842879
C	-4.466857	1.077019	-0.637374
C	-2.542193	0.628973	-2.055904
C	-5.271312	0.562740	-1.667198
C	-3.356069	0.117104	-3.059179
C	-4.737408	0.085915	-2.863233
H	-1.473313	0.638732	-2.189333
H	-6.347531	0.534711	-1.519204
H	-2.916464	-0.251953	-3.981160
H	-5.396164	-0.306222	-3.632908
O	-2.581543	2.159818	1.233024
H	-1.697522	4.267726	0.370326
C	-5.160884	1.564787	0.613450
H	-6.241339	1.418514	0.524072
H	-4.807397	1.037843	1.503206
H	-4.959267	2.623317	0.794719
C	2.185717	-1.914971	-1.265497
C	3.010860	-2.998483	-1.540718
C	3.515059	-3.203315	-2.847581
C	3.225464	-2.341077	-3.883721
C	2.397513	-1.214276	-3.641962
C	1.862122	-1.024759	-2.335289
N	1.064012	0.044184	-2.035103
C	0.829756	0.966268	-2.957174
C	1.319961	0.860318	-4.274902
C	2.086038	-0.233859	-4.617704
N	1.604727	-1.585274	-0.030632
H	4.153058	-4.063767	-3.026387
H	3.630041	-2.500471	-4.878313
H	2.472120	-0.347997	-5.626592
H	1.086427	1.636307	-4.994838
H	0.228605	1.811336	-2.637610
C	2.244023	-1.837168	1.179341
C	1.482884	-1.186558	2.283216
C	1.660806	-1.490240	3.651582

C	0.550366	-0.219599	1.887018
C	0.862736	-0.801261	4.573526
C	-0.220695	0.478179	2.808208
C	-0.060863	0.163158	4.163507
H	0.274413	-2.702393	0.229538
H	0.968334	-1.024489	5.631863
H	-0.939031	1.227718	2.497965
H	-0.665807	0.678093	4.905684
O	3.279325	-2.492380	1.319355
H	3.276762	-3.677661	-0.743016
C	2.656953	-2.519320	4.128680
H	2.557489	-2.678713	5.205892
H	2.519843	-3.474554	3.614183
H	3.681936	-2.205328	3.912075
Co	0.416291	0.059398	-0.049168
C	-1.551649	-2.330620	0.397291
O	-1.400963	-1.223854	-0.130272
O	-0.552380	-3.182100	0.536717
C	-2.903404	-2.761150	0.950630
C	-3.269536	-1.722919	2.037894
H	-4.259781	-1.952593	2.443372
H	-2.546812	-1.738738	2.860244
H	-3.282957	-0.715401	1.617595
C	-3.925263	-2.687867	-0.204047
H	-3.685917	-3.414017	-0.988361
H	-4.924517	-2.918376	0.178664
H	-3.941201	-1.690242	-0.645140
C	-2.858453	-4.173860	1.548832
H	-3.847427	-4.435189	1.937930
H	-2.579345	-4.916400	0.795819
H	-2.138744	-4.235541	2.369748

C1-t'

Energy = -1825.44490374 ZPE = -1824.933217 H = -1824.898997 G = -1824.999581

C	1.885423	2.077257	-0.458835
C	2.591778	3.113600	-1.067783
C	3.814936	3.574542	-0.527638
C	4.362515	3.031703	0.614913
C	3.682933	1.975197	1.273193
C	2.450087	1.503810	0.735129
N	1.763214	0.489238	1.332929
C	2.226298	-0.078527	2.433653
C	3.435870	0.327507	3.035997
C	4.157303	1.348061	2.454309
N	0.681552	1.507643	-0.879056
H	4.329814	4.383151	-1.038413
H	5.300866	3.397143	1.020394
H	5.093672	1.683941	2.890784
H	3.778752	-0.166077	3.938279
H	1.625807	-0.883552	2.847248
C	-0.139319	2.078015	-1.819424
C	-1.379902	1.263306	-2.091941
C	-2.661371	1.852740	-2.015423
C	-1.252041	-0.099030	-2.404470
C	-3.775833	1.025970	-2.197080
C	-2.378061	-0.903296	-2.595044
C	-3.645898	-0.338852	-2.473516
H	-0.262781	-0.527987	-2.520554
H	-4.768666	1.460786	-2.115545
H	-2.258305	-1.956201	-2.831235
H	-4.533885	-0.950288	-2.604641
O	0.059151	3.148714	-2.408084
H	2.188369	3.569363	-1.959312
C	-2.845622	3.321553	-1.720522
H	-3.907009	3.576227	-1.662228
H	-2.378321	3.590651	-0.768485
H	-2.372519	3.935048	-2.490896
C	-0.177622	-2.854873	0.330333
C	-0.581632	-4.148825	0.649621
C	0.164748	-5.262104	0.194514
C	1.302549	-5.123607	-0.572866
C	1.746420	-3.822773	-0.926204
C	1.000111	-2.700750	-0.469676
N	1.362810	-1.419968	-0.778995
C	2.436015	-1.200859	-1.523995
C	3.237922	-2.252880	-2.013483
C	2.893727	-3.554734	-1.715498
N	-0.765888	-1.647272	0.695310
H	-0.179759	-6.255809	0.466083
H	1.862612	-5.989097	-0.912584
H	3.491508	-4.384526	-2.081735
H	4.107922	-2.022741	-2.617920
H	2.667137	-0.163513	-1.740742
C	-2.020186	-1.517745	1.273102
C	-2.317960	-0.078201	1.539002
C	-3.473073	0.385949	2.204302
C	-1.330546	0.819208	1.106846
C	-3.569368	1.765472	2.440107
C	-1.432528	2.181293	1.365443
C	-2.564317	2.649861	2.043228
H	-4.446333	2.150219	2.954034
H	-0.660654	2.869108	1.036617
H	-2.667526	3.711277	2.253830
O	-2.769127	-2.458730	1.547188
H	-1.470917	-4.294023	1.244759
C	-4.577932	-0.535324	2.661807
H	-5.371729	0.032664	3.154867
H	-5.007686	-1.084671	1.819291
H	-4.201483	-1.294218	3.353360
Co	0.105057	-0.050008	0.151407

C2

Energy = -2172.497545 ZPE = -2171.8355 H = -2171.792391 G = -2171.909814

C	-1.474034	2.734800	0.199769
C	-2.067507	3.977697	-0.004069
C	-1.742975	5.061896	0.843921
C	-0.849794	4.937461	1.888892
C	-0.231470	3.684082	2.133367
C	-0.555823	2.593749	1.280650
N	-0.001569	1.353230	1.460733
C	0.868755	1.149713	2.438576
C	1.235721	2.179455	3.329172
C	0.692860	3.436558	3.178832
N	-1.658089	1.556436	-0.502479
H	-2.217084	6.020994	0.657359
H	-0.612936	5.779759	2.530795
H	0.966412	4.244518	3.850865
H	1.948915	1.958972	4.114830
H	1.319717	0.169053	2.523798
C	-2.689096	1.302664	-1.352192
C	-2.738949	-0.153500	-1.723669
C	-3.926398	-0.893169	-1.542420
C	-1.552233	-0.786811	-2.146657
C	-3.877093	-2.271363	-1.775737
C	-1.550577	-2.167420	-2.402235
C	-2.707226	-2.910553	-2.201193

H	-0.673246	-0.194092	-2.427580
H	-4.775494	-2.861279	-1.614498
H	-0.649338	-2.654956	-2.757480
H	-2.710152	-3.981662	-2.377836
O	-3.524939	2.125820	-1.748582
H	-2.774263	4.098283	-0.811901
C	-5.201328	-0.246017	-1.060686
H	-5.047569	0.224091	-0.083871
H	-5.524714	0.541631	-1.744510
H	-5.999340	-0.985908	-0.960272
C	1.922510	-1.724754	-0.163375
C	2.069702	-1.911423	-1.516964
C	3.353743	-2.130185	-2.068431
C	4.476249	-2.151050	-1.268886
C	4.355527	-1.939861	0.129286
C	3.060816	-1.728814	0.692080
N	2.860479	-1.514719	2.023806
C	3.914452	-1.498827	2.820190
C	5.240316	-1.697487	2.364364
C	5.457157	-1.917455	1.022648
N	0.651231	-1.494245	0.467293
H	3.445422	-2.270553	-3.140385
H	5.461201	-2.314006	-1.696024
H	6.460140	-2.071651	0.635061
H	6.060887	-1.671682	3.072826
H	3.723578	-1.319505	3.875992
C	-0.328725	-2.622409	0.461952
C	-1.583793	-2.163361	1.071100
C	-2.538684	-3.052125	1.622864
C	-1.771205	-0.766678	1.076591
C	-3.644942	-2.479891	2.254935
C	-2.884183	-0.230822	1.722440
C	-3.808064	-1.090474	2.320610
H	-4.390793	-3.128843	2.705304
H	-3.045290	0.842502	1.738586
H	-4.677162	-0.680295	2.828675
O	-0.031058	-3.708552	0.019532
H	1.211821	-1.836876	-2.168665
C	-2.386968	-4.548909	1.536279
H	-3.180812	-5.052249	2.093845
H	-2.426949	-4.877180	0.492801
H	-1.418642	-4.879562	1.924142
Co	-0.467621	0.172524	0.028547
C	1.502121	1.176314	-2.067362
O	1.004390	0.644624	-3.076397
O	1.074715	1.056654	-0.859888
C	2.740859	2.101058	-2.187712
C	3.807829	1.660267	-1.166983
H	4.681062	2.320815	-1.220932
H	3.406257	1.691478	-0.151504
H	4.142277	0.637439	-1.366455
C	3.315627	2.043178	-3.608724
H	2.568180	2.344222	-4.347486
H	4.181647	2.709233	-3.696426
H	3.636656	1.026646	-3.857186
C	2.271245	3.534080	-1.856621
H	3.112734	4.234777	-1.906306
H	1.508072	3.872153	-2.567062
H	1.842760	3.572639	-0.850869
H	0.876048	-1.358016	1.461193

C2-q'

Energy = -2171.97918803 ZPE = -2171.335433 H = -2171.290804 G = -2171.415638

C	-1.987347	2.488767	-1.074175
C	-2.331052	3.427982	-2.048675
C	-2.742281	4.732439	-1.692879
C	-2.827920	5.139590	-0.378215
C	-2.494158	4.223985	0.653027
C	-2.077165	2.902617	0.307178
N	-1.748398	1.986814	1.266528
C	-1.815725	2.322328	2.543967
C	-2.216647	3.604417	2.978741
C	-2.552540	4.548341	2.033051
N	-1.551937	1.185880	-1.269932
H	-2.995460	5.428999	-2.487827
H	-3.145798	6.144569	-0.116851
H	-2.864425	5.546520	2.328665
H	-2.252630	3.826638	4.039736
H	-1.537509	1.551149	3.257623
C	-1.712462	0.504400	-2.439663
C	-1.234511	-0.927001	-2.326845
C	-2.116105	-2.001615	-2.575224
C	0.085746	-1.177750	-1.922900
C	-1.639816	-3.303229	-2.384664
C	0.543821	-2.488674	-1.748797
C	-0.326330	-3.553050	-1.971503
H	0.796470	-0.365550	-1.769995
H	-2.317696	-4.138120	-2.547554
H	1.570845	-2.628201	-1.422792
H	0.006453	-4.577629	-1.825740
O	-2.215527	0.925499	-3.496188
H	-2.283849	3.135991	-3.087629
C	-3.553145	-1.762916	-2.972479
H	-4.085828	-1.239108	-2.170540
H	-3.617235	-1.135800	-3.864647
H	-4.072238	-2.707528	-3.158056
C	1.432838	-0.928038	1.861765
C	2.327547	-1.706469	2.645865
C	3.562921	-1.188526	3.041993
C	3.969300	0.088416	2.675707
C	3.126245	0.910356	1.877204
C	1.861673	0.410766	1.474024
N	1.005067	1.136514	0.726391
C	1.368974	2.348977	0.324363
C	2.601259	2.930618	0.667848
C	3.480867	2.210778	1.451934
N	0.198271	-1.250776	1.455926
H	4.220238	-1.803722	3.648579
H	4.936448	0.470632	2.987511
H	4.442702	2.624724	1.739946
H	2.844998	3.925459	0.312573
H	0.648976	2.883169	-0.287168
C	-0.383400	-2.536354	1.575697
C	-1.837294	-2.517276	1.265420
C	-2.628641	-3.695504	1.365614
C	-2.385784	-1.269623	0.873675
C	-3.995507	-3.575026	1.098955
C	-3.768208	-1.207510	0.644910
C	-4.568285	-2.345244	0.750483
H	-4.625969	-4.458359	1.169455
H	-4.221365	-0.264100	0.341977
H	-5.636643	-2.292124	0.548859
O	0.260492	-3.539640	1.890709
H	2.029771	-2.704230	2.931684
C	-2.074982	-5.052156	1.732100
H	-2.873205	-5.800917	1.745043
H	-1.305817	-5.367297	1.020669

H	-1.586458	-5.038602	2.710604
Co	-0.970201	0.144200	0.378486
C	3.680753	-0.299903	-1.255777
O	3.477025	-1.369695	-0.612755
O	2.812646	0.478687	-1.734134
C	5.187542	0.049168	-1.544031
C	5.348545	1.520118	-1.950853
H	6.393223	1.744207	-2.204480
H	4.718178	1.753343	-2.811940
H	5.045406	2.183844	-1.134064
C	6.052739	-0.248856	-0.310094
H	5.893289	-1.276299	0.023513
H	7.118647	-0.104809	-0.530426
H	5.789236	0.414241	0.521030
C	5.629863	-0.863857	-2.706648
H	6.683272	-0.695147	-2.965668
H	5.505998	-1.916471	-2.432516
H	5.027319	-0.673616	-3.602703

C2'

Energy = -2172.02837793 ZPE = -2171.379883 H = -2171.336824 G = -2171.454192

C	2.065601	-2.038751	-1.417001
C	2.619246	-2.864182	-2.393562
C	3.243325	-4.077560	-2.020951
C	3.336873	-4.488638	-0.705242
C	2.796788	-3.671226	0.321578
C	2.165490	-2.454227	-0.052157
N	1.633043	-1.609647	0.885488
C	1.696892	-1.906451	2.175176
C	2.306574	-3.096239	2.623794
C	2.848922	-3.972065	1.707147
N	1.421230	-0.824201	-1.554287
H	3.661418	-4.702870	-2.804735
H	3.821516	-5.423046	-0.440992
H	3.321867	-4.893630	2.033812
H	2.336884	-3.301416	3.687674
H	1.252816	-1.190518	2.854712
C	1.454774	-0.027570	-2.657314
C	0.922808	1.339536	-2.306822
C	1.693029	2.497305	-2.549412
C	-0.292886	1.430575	-1.595311
C	1.239512	3.705977	-2.010313
C	-0.732088	2.662813	-1.084967
C	0.053356	3.794523	-1.269677
H	-1.014272	0.611716	-1.573631
H	1.835666	4.601779	-2.168535
H	-1.702088	2.680848	-0.591889
H	-0.259238	4.755716	-0.870597
O	1.909946	-0.327491	-3.770731
H	2.565918	-2.560534	-3.429445
C	2.993329	2.447796	-3.315875
H	3.753100	1.896008	-2.751854
H	2.869844	1.933485	-4.270710
H	3.376068	3.456099	-3.495862
C	-1.195966	0.131612	2.102454
C	-1.933332	0.464879	3.238383
C	-3.131639	-0.223684	3.538024
C	-3.617482	-1.239493	2.740295
C	-2.904047	-1.603815	1.568681
C	-1.703769	-0.909646	1.255924
N	-0.975728	-1.202128	0.137645
C	-1.389760	-2.146094	-0.688968
C	-2.558313	-2.897323	-0.448514
C	-3.309963	-2.625516	0.672933
N	0.007763	0.661746	1.670240
H	-3.679700	0.062958	4.431558
H	-4.538276	-1.758775	2.987279
H	-4.220313	-3.181183	0.879936
H	-2.854596	-3.664747	-1.154737
H	-0.775438	-2.314263	-1.567115
C	0.685224	1.707674	2.242376
C	2.004346	1.896400	1.558877
C	2.965707	2.853272	1.955807
C	2.261270	1.001568	0.502255
C	4.198475	2.849198	1.288432
C	3.510357	0.996740	-0.116538
C	4.477907	1.925352	0.278147
H	4.955810	3.574489	1.576299
H	3.727818	0.287602	-0.909354
H	5.451457	1.936120	-0.206775
O	0.283397	2.384228	3.202458
H	-1.576082	1.255799	3.881545
C	2.718535	3.857348	3.057577
H	3.580951	4.521064	3.172311
H	1.830709	4.461887	2.852276
H	2.524197	3.360039	4.012039
Co	0.759440	-0.118130	0.109308
C	-3.921070	0.758992	-1.036933
O	-3.654311	1.691957	-0.226412
O	-3.111678	0.134687	-1.776589
C	-5.443091	0.386300	-1.161114
C	-5.642436	-0.892516	-1.984212
H	-6.709832	-1.131794	-2.082949
H	-5.215389	-0.782206	-2.984506
H	-5.141005	-1.740462	-1.507731
C	-6.043273	0.203993	0.243233
H	-5.852681	1.093093	0.848791
H	-7.126777	0.032881	0.191930
H	-5.589039	-0.650413	0.755731
C	-6.139701	1.572618	-1.857600
H	-7.221056	1.403943	-1.945698
H	-5.975194	2.491766	-1.287247
H	-5.740086	1.723776	-2.867917

C2-t'

Energy = -2172.02159241 ZPE = -2171.374936 H = -2171.330992 G = -2171.454977

C	-2.023096	2.117098	-1.349018
C	-2.432372	2.901958	-2.427402
C	-2.847223	4.240447	-2.237939
C	-2.871865	4.832345	-0.993148
C	-2.464550	4.078996	0.137072
C	-2.042276	2.729459	-0.045086
N	-1.635804	1.971512	1.011325
C	-1.628729	2.470436	2.234865
C	-2.035926	3.793892	2.507945
C	-2.448439	4.590064	1.461001
N	-1.575719	0.794898	-1.382394
H	-3.154268	4.811025	-3.109948
H	-3.195400	5.860362	-0.861948
H	-2.764072	5.615071	1.634675
H	-2.014657	4.163766	3.526943
H	-1.281296	1.806541	3.021454
C	-1.751990	-0.033397	-2.466461
C	-1.196308	-1.416237	-2.254372
C	-1.995014	-2.555911	-2.502032
C	0.114365	-1.565847	-1.774397

C	-1.460585	-3.810742	-2.188658
C	0.634500	-2.831318	-1.484580
C	-0.167279	-3.954792	-1.673279
H	0.792035	-0.719417	-1.677098
H	-2.074255	-4.694347	-2.348492
H	1.656171	-2.883294	-1.113635
H	0.209833	-4.947194	-1.439344
O	-2.322687	0.272402	-3.523087
H	-2.435827	2.469735	-3.416428
C	-3.394826	-2.451930	-3.060281
H	-4.025716	-1.814308	-2.433822
H	-3.387045	-2.002973	-4.056566
H	-3.862740	-3.438604	-3.117940
C	1.261131	-0.144976	2.143170
C	2.038329	-0.469952	3.251262
C	3.245819	0.224905	3.501092
C	3.698853	1.232067	2.674830
C	2.941822	1.584592	1.526710
C	1.728652	0.891145	1.273504
N	0.950171	1.171403	0.187614
C	1.339706	2.090888	-0.677586
C	2.521876	2.838607	-0.499421
C	3.315306	2.588957	0.598098
N	0.043172	-0.693695	1.749571
H	3.827046	-0.052449	4.375952
H	4.627927	1.754167	2.881379
H	4.234744	3.144789	0.758353
H	2.793733	3.587926	-1.234084
H	0.692432	2.250132	-1.532699
C	-0.536375	-1.827430	2.295769
C	-1.895296	-2.033839	1.711940
C	-2.785708	-3.053545	2.113330
C	-2.269405	-1.084685	0.748050
C	-4.064465	-3.054088	1.538258
C	-3.553237	-1.086267	0.211645
C	-4.452083	-2.079270	0.615729
H	-4.772144	-3.826130	1.829536
H	-3.848571	-0.338326	-0.516401
H	-5.457567	-2.099334	0.202525
O	-0.019362	-2.537080	3.163481
H	1.714123	-1.259003	3.913772
C	-2.412807	-4.110906	3.124558
H	-3.238402	-4.814022	3.267752
H	-1.525442	-4.666298	2.808029
H	-2.156552	-3.663827	4.089371
Co	-0.837504	0.138500	0.299297
C	3.791288	-0.877401	-1.183075
O	3.524181	-1.858195	-0.429608
O	2.978873	-0.195199	-1.864356
C	5.317704	-0.522002	-1.309325
C	5.529750	0.788080	-2.078117
H	6.600143	1.011097	-2.182998
H	5.086078	0.729505	-3.075661
H	5.052520	1.624318	-1.558272
C	5.935466	-0.411791	0.095004
H	5.736682	-1.323784	0.662936
H	7.021181	-0.256489	0.039780
H	5.501706	0.426781	0.649789
C	5.988297	-1.686692	-2.065209
H	7.071861	-1.532978	-2.154399
H	5.810785	-2.627689	-1.536249
H	5.578731	-1.784007	-3.078200

di-BQNH

Energy = -1680.92852448 ZPE = -1680.4037 H = -1680.370662 G = -1680.467268

C	2.196213	1.549423	-0.709715
C	3.159285	2.539375	-0.611542
C	4.422779	2.371083	-1.225714
C	4.727830	1.234194	-1.940024
C	3.766462	0.195958	-2.054637
C	2.489787	0.342359	-1.429227
N	1.542913	-0.637413	-1.473850
C	1.813275	-1.749512	-2.133862
C	3.038548	-1.986566	-2.799498
C	4.011258	-1.013956	-2.754409
N	0.930866	1.625008	-0.114781
H	5.156418	3.166012	-1.131794
H	5.696545	1.113577	-2.415793
H	4.970360	-1.157824	-3.244221
H	3.196020	-2.922606	-3.324176
H	1.030723	-2.505937	-2.140710
C	0.605285	2.265443	1.050502
C	-0.650571	1.715659	1.681343
C	-1.820500	2.495815	1.705598
C	-0.624892	0.413106	2.225561
C	-2.976629	1.945805	2.269882
C	-1.799438	-0.098969	2.797851
C	-2.967633	0.659436	2.810289
H	-3.891676	2.531567	2.281581
H	-1.791181	-1.096560	3.223661
H	-3.872435	0.249245	3.249016
O	1.270774	3.162797	1.567131
H	2.934844	3.437884	-0.054056
C	-1.842442	3.873124	1.084866
H	-0.995909	4.473935	1.426787
H	-1.772406	3.806509	-0.007559
H	-2.768586	4.399902	1.326974
C	-2.196174	-1.549996	-0.708159
C	-3.159059	-2.540103	-0.609128
C	-4.422667	-2.372586	-1.223357
C	-4.727939	-1.236312	-1.938584
C	-3.766763	-0.197958	-2.054019
C	-2.490049	-0.343530	-1.428496
N	-1.543438	0.636395	-1.473969
C	-1.814062	1.747850	-2.134863
C	-3.039389	1.984126	-2.800638
C	-4.011882	1.011346	-2.754763
N	-0.930740	-1.625087	-0.113393
H	-5.156119	-3.167618	-1.128804
H	-5.696678	-1.116281	-2.414466
H	-4.971026	1.154567	-3.244708
H	-3.197088	2.919717	-3.326043
H	-1.031682	2.504450	-2.142388
C	-0.604985	-2.264533	1.052413
C	0.650884	-1.714151	1.682755
C	1.820881	-2.494191	1.707697
C	0.625066	-0.411179	2.225933
C	2.976954	-1.943582	2.271627
C	1.799488	0.101491	2.797845
C	2.967762	-0.656751	2.810989
H	3.892063	-2.529267	2.283853
H	1.791108	1.099405	3.222841
H	3.872503	-0.246151	3.249460
O	-1.270337	-3.161553	1.569836
H	-2.934341	-3.438144	-0.050961
C	1.843103	-3.871950	1.087897
H	0.995730	-4.472126	1.428840

H	1.774857	-3.805903	-0.004687
H	2.768600	-4.399033	1.331814
H	-0.224622	-0.986204	-0.485900
H	0.224560	0.986015	-0.486823

5-q

Energy = -2171.32653618 ZPE = -2170.689795 H = -2170.646802 G = -2170.766018

Co	-0.009867	0.670717	-0.197200
O	-0.787400	-2.256547	-3.136459
O	0.542800	2.444337	0.982999
O	0.201913	-0.961936	3.486865
O	0.012983	2.673524	-1.153168
N	2.090607	0.628846	-0.698123
N	-0.972355	-0.640996	-1.458237
N	0.852373	-0.588481	1.304099
N	-2.026942	1.067925	0.295741
C	-4.556334	-0.448064	-2.621216
H	-5.190975	-0.852389	-3.405201
C	-2.312583	-0.302969	-1.652640
C	1.982326	-2.523501	-1.874770
C	2.690927	-3.747102	0.109692
C	0.419904	-2.919677	-0.034475
C	-4.262634	0.890445	-0.638657
C	-2.872717	0.570329	-0.650686
C	-2.650133	-0.981355	3.552865
H	-2.232312	0.022135	3.432851
H	-2.180323	-1.409839	4.441990
H	-3.723827	-0.886584	3.732901
C	4.281064	0.148170	0.225066
C	1.415127	-3.627250	0.654069
H	1.188602	-4.054101	1.626731
C	5.029257	-0.445452	1.280903
C	2.971550	-3.188046	-1.139860
H	3.972081	-3.273913	-1.555165
C	4.380750	-1.074587	2.337586
C	0.704091	-2.379271	-1.307423
C	2.987417	-1.144305	2.397462
H	2.501212	-1.641883	3.225746
C	-0.420777	-1.721760	-2.077264
C	2.188147	-0.552016	1.383750
C	-3.180837	-0.777964	-2.636161
H	-2.788476	-1.423370	-3.407547
C	2.864828	0.097659	0.272686
C	-5.104989	0.360379	-1.650005
H	-6.163224	0.603382	-1.645593
C	0.030078	-1.177168	2.292740
C	-4.728019	1.729467	0.405842
H	-5.783134	1.986127	0.445886
C	-1.116697	-1.958911	1.740018
C	-2.486594	1.860261	1.251697
H	-1.742640	2.243820	1.942020
C	-2.395458	-1.836463	2.334119
C	0.374569	3.178820	-0.045181
C	-3.468470	-2.504613	1.733733
H	-4.460220	-2.399945	2.164276
C	-3.290422	-3.289283	0.594840
H	-4.140541	-3.795819	0.147502
C	-2.024924	-3.423338	0.029158
H	-1.878792	-4.027065	-0.860687
C	-0.930493	-2.755127	0.586333
C	-3.848516	2.212029	1.351101
H	3.469116	-4.269587	0.657651
H	4.965716	-1.528745	3.130364
H	6.113375	-0.407751	1.244098
C	4.873413	0.785294	-0.891764
C	4.065304	1.333402	-1.868797
C	2.668119	1.240961	-1.727915
H	5.955305	0.838662	-0.966099
H	4.485440	1.831717	-2.734764
H	1.991235	1.686441	-2.448451
C	2.288181	-1.960634	-3.242141
H	3.360495	-1.991861	-3.451256
H	1.761173	-2.525857	-4.016407
H	1.953090	-0.922503	-3.328112
C	0.645499	4.684510	0.079942
C	2.144142	4.855100	0.411804
H	2.386590	5.916521	0.532445
H	2.396929	4.331505	1.337561
H	2.771586	4.452544	-0.391825
C	-0.212451	5.234185	1.237269
H	-1.280515	5.104979	1.028253
H	0.017357	4.712402	2.169505
H	-0.020703	6.303614	1.377039
C	0.308745	5.414871	-1.226920
H	0.898515	5.021499	-2.059384
H	-0.748615	5.297804	-1.482142
H	0.522556	6.484525	-1.124872
H	-4.180147	2.855966	2.158037

5

Energy = -2171.34222069 ZPE = -2170.701082 H = -2170.659888 G = -2170.770951

Co	0.031607	0.735551	-0.008750
O	-0.271932	-1.660890	-3.322005
O	0.478435	2.390315	1.014589
O	0.040526	-1.650112	3.326877
O	-0.199955	2.434456	-1.046162
N	1.892938	0.683327	-0.495248
N	-0.654147	-0.399904	-1.423269
N	0.571821	-0.461618	1.417561
N	-1.819640	0.915428	0.479981
C	-4.212025	-0.266443	-2.662283
H	-4.809667	-0.579353	-3.513773
C	-2.005787	-0.128810	-1.636690
C	2.315320	-2.355764	-1.835970
C	2.767105	-3.710415	0.134970
C	0.542835	-2.815589	-0.205783
C	-4.040191	0.752514	-0.484343
C	-2.638574	0.527622	-0.538183
C	-3.005528	-1.426250	3.151924
H	-2.428692	-0.525775	3.369814
H	-2.829474	-2.119400	3.982095
H	-4.066844	-1.164058	3.147344
C	4.073475	0.284478	0.491110
C	1.439933	-3.584125	0.544674
H	1.095510	-4.066881	1.454169
C	4.803463	-0.204608	1.603846
C	3.195652	-3.108112	-1.047648
H	4.227602	-3.222563	-1.368798
C	4.113279	-0.715196	2.684360
C	0.997258	-2.178945	-1.378353
C	2.700569	-0.786702	2.721558
H	2.197771	-1.203294	3.581039
C	-0.006485	-1.370967	-2.148330
C	1.944325	-0.343236	1.637672
C	-2.816929	-0.498351	-2.708705
H	-2.373213	-0.981683	-3.565878

C	2.655162	0.220556	0.535509
C	-4.830556	0.333895	-1.584461
H	-5.902827	0.500074	-1.567719
C	-0.185977	-1.343618	2.149128
C	-4.544331	1.385269	0.680921
H	-5.611186	1.571634	0.762908
C	-1.273294	-2.038852	1.383399
C	-2.305571	1.515189	1.555558
H	-1.584034	1.816744	2.304752
C	-2.602370	-2.064455	1.843079
C	0.194781	3.086318	-0.021317
C	-3.561825	-2.721059	1.061649
H	-4.599416	-2.718947	1.384967
C	-3.204678	-3.375423	-0.117244
H	-3.964078	-3.875934	-0.710903
C	-1.872353	-3.400961	-0.528392
H	-1.584660	-3.926497	-1.433828
C	-0.894055	-2.732293	0.216320
C	-3.686876	1.760124	1.694070
H	3.465694	-4.287766	0.733569
H	4.665457	-1.081079	3.545359
H	5.887737	-0.161121	1.593873
C	4.654883	0.840173	-0.677300
C	3.853090	1.294301	-1.703606
C	2.451930	1.207921	-1.574587
H	5.736526	0.904734	-0.751154
H	4.275853	1.719269	-2.606375
H	1.774863	1.576458	-2.335305
C	2.790522	-1.777047	-3.148574
H	3.868563	-1.596574	-3.127122
H	2.579840	-2.473102	-3.968466
H	2.288718	-0.840451	-3.396721
C	0.355829	4.594191	-0.017574
C	1.864762	4.885830	0.156328
H	2.028237	5.967689	0.179402
H	2.239983	4.455751	1.088677
H	2.444264	4.469496	-0.674578
C	-0.433009	5.156821	1.183673
H	-1.502654	4.942172	1.087067
H	-0.078233	4.721782	2.121377
H	-0.305197	6.242606	1.231474
C	-0.158916	5.190119	-1.335543
H	0.385223	4.782414	-2.191816
H	-1.222271	4.976027	-1.477142
H	-0.024487	6.276050	-1.324547
H	-4.050731	2.242309	2.593751

5-t

Energy = -2171.32531902 ZPE = -2170.68872 H = -2170.645684 G = -2170.764437

Co	-0.004249	0.678013	-0.199611
O	-0.749848	-2.221597	-3.166459
O	0.542100	2.471752	0.987437
O	0.201927	-1.026845	3.484888
O	-0.060298	2.675492	-1.132204
N	2.102087	0.674298	-0.663528
N	-0.954607	-0.626708	-1.470810
N	0.861765	-0.592725	1.318578
N	-2.027651	1.026154	0.322393
C	-4.551229	-0.489502	-2.599670
H	-5.184612	-0.893459	-3.384882
C	-2.303274	-0.313863	-1.648046
C	2.031214	-2.449946	-1.908272
C	2.754203	-3.696161	0.056957
C	0.470087	-2.905062	-0.079717
C	-4.267667	0.821445	-0.596816
C	-2.871909	0.529090	-0.625388
C	-2.647862	-1.090435	3.532222
H	-2.240039	-0.080061	3.439529
H	-2.181850	-1.534533	4.415743
H	-3.724157	-1.011490	3.704204
C	4.288662	0.194047	0.265447
C	1.474774	-3.608859	0.598694
H	1.252571	-4.057925	1.562288
C	5.035602	-0.417449	1.312120
C	3.029467	-3.109502	-1.181557
H	4.032717	-3.170667	-1.594640
C	4.387421	-1.082085	2.348255
C	0.749020	-2.337849	-1.342488
C	2.996099	-1.169783	2.396349
H	2.509558	-1.692172	3.209007
C	-0.387756	-1.690534	-2.103992
C	2.194458	-0.554898	1.394695
C	-3.169312	-0.789982	-2.632566
H	-2.770142	-1.413599	-3.418341
C	2.872653	0.128786	0.301180
C	-5.107589	0.291034	-1.609999
H	-6.170473	0.512329	-1.592933
C	0.041895	-1.219386	2.285270
C	-4.740144	1.634866	0.464970
H	-5.799609	1.870390	0.518058
C	-1.089260	-2.005849	1.707507
C	-2.493903	1.795102	1.293647
H	-1.752083	2.181828	1.984736
C	-2.373067	-1.914719	2.296638
C	0.315427	3.196136	-0.034587
C	-3.432768	-2.585351	1.675735
H	-4.428351	-2.504151	2.102463
C	-3.236928	-3.343066	0.521736
H	-4.077037	-3.852101	0.058636
C	-1.966498	-3.447053	-0.038897
H	-1.806732	-4.029145	-0.940662
C	-0.885137	-2.774503	0.538287
C	-3.861646	2.119803	1.409715
H	3.539578	-4.215047	0.597963
H	4.972937	-1.549158	3.133053
H	6.119402	-0.365270	1.285154
C	4.883742	0.865185	-0.830045
C	4.077997	1.430384	-1.798998
C	2.680912	1.318551	-1.672859
H	5.965591	0.930567	-0.894213
H	4.499857	1.955439	-2.648173
H	2.004237	1.772920	-2.388284
C	2.329326	-1.858209	-3.265040
H	3.400796	-1.880513	-3.479373
H	1.801006	-2.409817	-4.048175
H	1.989637	-0.819810	-3.327948
C	0.524790	4.713086	0.080323
C	2.017555	4.950826	0.394740
H	2.215162	6.022374	0.508037
H	2.302304	4.442934	1.319863
H	2.653625	4.571869	-0.413574
C	-0.343122	5.228387	1.246310
H	-1.406944	5.052534	1.049936
H	-0.080006	4.718871	2.176573
H	-0.196312	6.305418	1.382044
C	0.140314	5.423606	-1.224251
H	0.736837	5.053852	-2.062802

H	-0.913739	5.259024	-1.466380
H	0.307846	6.502075	-1.128100
H	-4.198338	2.744858	2.229343

6-d

Energy = -1824.86033217 ZPE = -1824.358961 H = -1824.325265 G = -1824.423763

C	2.550346	0.421521	0.973231
C	3.836415	0.007902	1.316033
C	4.950096	0.849879	1.089305
C	4.823221	2.104609	0.530581
C	3.533147	2.571658	0.171131
C	2.411353	1.726580	0.404415
N	1.141044	2.120595	0.083461
C	0.936430	3.306942	-0.478382
C	1.992035	4.197230	-0.754517
C	3.281282	3.832687	-0.424712
N	1.357908	-0.299286	1.058827
H	5.934928	0.483656	1.364882
H	5.687890	2.737290	0.357352
H	4.113871	4.502145	-0.621135
H	1.774531	5.152666	-1.217867
H	-0.091371	3.557231	-0.715470
C	1.263106	-1.462187	1.771866
C	0.010449	-2.260757	1.498015
C	-0.956665	-2.454791	2.500692
C	-0.142646	-2.836244	0.223996
C	-2.085330	-3.225038	2.194593
C	-1.275160	-3.610207	-0.052252
C	-2.243823	-3.802110	0.932233
H	-2.847533	-3.374183	2.955050
H	-1.399576	-4.039300	-1.041838
H	-3.125324	-4.399259	0.717013
O	2.097831	-1.897395	2.577493
H	3.976967	-0.966795	1.758604
C	-0.788520	-1.821715	3.862022
H	0.126331	-2.177782	4.344081
H	-0.698229	-0.732004	3.777487
H	-1.639428	-2.042859	4.511130
C	-2.621294	0.162419	-0.979564
C	-3.721985	-0.380685	-1.642320
C	-5.009157	0.188946	-1.497247
C	-5.242014	1.298071	-0.711329
C	-4.156710	1.883255	-0.011267
C	-2.863977	1.302552	-0.151175
N	-1.782904	1.804819	0.516464
C	-1.921041	2.860672	1.312073
C	-3.161772	3.499390	1.497515
C	-4.271979	3.011095	0.839081
N	-1.293178	-0.280302	-0.979523
H	-5.835838	-0.271576	-2.030777
H	-6.235042	1.724990	-0.613222
H	-5.243015	3.480401	0.968244
H	-3.225450	4.358109	2.155712
H	-1.022808	3.206641	1.812911
C	-0.839951	-1.102604	-1.972020
C	0.574748	-1.608772	-1.833547
C	1.555016	-1.208048	-2.760407
C	0.877350	-2.535688	-0.823599
C	2.837321	-1.759562	-2.656593
C	2.165504	-3.080714	-0.748429
C	3.140975	-2.696878	-1.666585
H	3.606109	-1.448838	-3.359524
H	2.399894	-3.783498	0.045249
H	4.140612	-3.117440	-1.605542
O	-1.483966	-1.459236	-2.971433
H	-3.584157	-1.240164	-2.279958
C	1.236552	-0.178300	-3.819368
H	0.442008	-0.533296	-4.481760
H	0.876401	0.751313	-3.362031
H	2.118277	0.058902	-4.420054
Co	-0.191148	0.679232	0.391762

6-quar

Energy = -1824.88233945 ZPE = -1824.380744 H = -1824.347144 G = -1824.445696

C	2.586071	0.424017	1.182581
C	3.717502	0.101638	1.932690
C	4.949727	0.762866	1.722527
C	5.097273	1.753380	0.776561
C	3.978665	2.122577	-0.013345
C	2.731041	1.462075	0.193035
N	1.633313	1.792299	-0.554362
C	1.712318	2.731812	-1.488344
C	2.906154	3.428259	-1.755246
C	4.030319	3.122162	-1.016978
N	1.323067	-0.164752	1.253634
H	5.799782	0.471823	2.333150
H	6.047616	2.254961	0.623267
H	4.967991	3.640799	-1.195972
H	2.924287	4.187057	-2.529073
H	0.801257	2.937167	-2.042040
C	1.039872	-1.233255	2.049678
C	-0.310817	-1.857517	1.765278
C	-1.331690	-1.778305	2.733234
C	-0.531369	-2.518902	0.539462
C	-2.567099	-2.373648	2.455826
C	-1.776043	-3.116891	0.296851
C	-2.788107	-3.044141	1.250391
H	-3.364241	-2.309224	3.191858
H	-1.948427	-3.614520	-0.652272
H	-3.752069	-3.504863	1.054679
O	1.759840	-1.728588	2.930225
H	3.636906	-0.670783	2.682499
C	-1.104650	-1.031636	4.027174
H	-0.258415	-1.452500	4.576898
H	-0.864949	0.020645	3.831930
H	-1.992055	-1.063665	4.664141
C	-2.582906	0.412791	-1.191563
C	-3.712070	0.087578	-1.943874
C	-4.944953	0.749573	-1.740049
C	-5.095434	1.743599	-0.798249
C	-3.979241	2.115811	-0.006345
C	-2.730902	1.454743	-0.206518
N	-1.635531	1.788113	0.542945
C	-1.717514	2.730945	1.473273
C	-2.912369	3.427899	1.734231
C	-4.034163	3.118967	0.993555
N	-1.319748	-0.176644	-1.256378
H	-5.793097	0.456184	-2.352205
H	-6.046261	2.245677	-0.649651
H	-4.972479	3.638062	1.167769
H	-2.933002	4.189467	2.505266
H	-0.808048	2.938737	2.028677
C	-1.037446	-1.254305	-2.040430
C	0.310993	-1.879604	-1.747470
C	1.332742	-1.816176	-2.715603
C	0.528142	-2.527539	-0.513824

C	2.565435	-2.413566	-2.430505
C	1.770000	-3.128259	-0.263611
C	2.782882	-3.071108	-1.217358
H	3.363178	-2.361265	-3.166852
H	1.939724	-3.615562	0.691331
H	3.744670	-3.533829	-1.015755
O	-1.757481	-1.757822	-2.916295
H	-3.629230	-0.687961	-2.690202
C	1.109881	-1.083909	-4.018490
H	0.261113	-1.506402	-4.562998
H	0.876446	-0.027920	-3.836017
H	1.997037	-1.128947	-4.654998
Co	0.000823	0.666053	-0.004704

1-d

Energy = -1827.30404233 ZPE = -1825.552782 H = -1825.517981 G = -1825.62042

C	-1.543035	2.326215	0.282074
C	-2.128842	3.590642	0.255151
C	-3.359538	3.827550	0.913057
C	-4.020773	2.842134	1.615139
C	-3.457126	1.541458	1.679189
C	-2.232392	1.293020	0.997358
N	-1.647536	0.056982	1.009119
C	-2.197078	-0.927843	1.703374
C	-3.396491	-0.763034	2.424711
C	-4.029103	0.461655	2.399161
N	-0.347815	1.907724	-0.307602
H	-3.784026	4.826302	0.863343
H	-4.956923	3.043535	2.126478
H	-4.962377	0.616074	2.933267
H	-3.806631	-1.602058	2.975039
H	-1.675286	-1.876990	1.676469
C	0.534818	2.764322	-0.903353
C	1.754695	2.049998	-1.427301
C	3.049716	2.438806	-1.028651
C	1.584411	0.933745	-2.260413
C	4.126120	1.632232	-1.420710
C	2.671795	0.151553	-2.656490
C	3.947696	0.493516	-2.211630
H	0.593690	0.718696	-2.644989
H	5.127008	1.899189	-1.091538
H	2.518295	-0.709431	-3.299671
H	4.805916	-0.111053	-2.489400
O	0.427380	3.996491	-0.999904
H	-1.627960	4.390863	-0.268545
C	3.296258	3.673995	-0.194711
H	2.572725	3.775467	0.618092
H	4.301495	3.659001	0.234495
H	3.194391	4.576151	-0.806022
C	1.557893	-2.287580	0.332039
C	2.167964	-3.540874	0.319566
C	3.405348	-3.746227	0.975609
C	4.049877	-2.740380	1.663962
C	3.461577	-1.450109	1.713947
C	2.231269	-1.232838	1.031178
N	1.625745	-0.007220	1.026887
C	2.156763	0.995883	1.709265
C	3.358423	0.861477	2.432877
C	4.013797	-0.351508	2.420676
N	0.351814	-1.900141	-0.258517
H	3.848484	-4.737319	0.936160
H	4.990983	-2.917919	2.175042
H	4.950339	-0.482206	2.955394
H	3.753316	1.714157	2.973279
H	1.618765	1.935594	1.668385
C	-0.515830	-2.786264	-0.832575
C	-1.753853	-2.113364	-1.368253
C	-3.037645	-2.526689	-0.958231
C	-1.614999	-1.016172	-2.231641
C	-4.136745	-1.763500	-1.374083
C	-2.723672	-0.276730	-2.649544
C	-3.990210	-0.643177	-2.196886
H	-0.630416	-0.781229	-2.620142
H	-5.129903	-2.050074	-1.038030
H	-2.593936	0.570069	-3.316400
H	-4.865122	-0.072072	-2.492866
O	-0.383017	-4.017883	-0.904023
H	1.680794	-4.357652	-0.191138
C	-3.250989	-3.744413	-0.090119
H	-2.512820	-3.815473	0.712601
H	-4.249746	-3.735148	0.354230
H	-3.144804	-4.659587	-0.681204
Co	-0.004712	0.005475	-0.137132

1-quar

Energy = -1827.32847823 ZPE = -1825.571101 H = -1825.535889 G = -1825.639044

C	-2.031803	1.930868	-0.080173
C	-2.864919	2.919695	-0.598453
C	-4.231177	2.987912	-0.238630
C	-4.797799	2.096922	0.646200
C	-3.990485	1.077357	1.213321
C	-2.616399	0.991664	0.842942
N	-1.812810	0.006939	1.351551
C	-2.300520	-0.872391	2.216323
C	-3.639875	-0.845162	2.647944
C	-4.478865	0.124265	2.140783
N	-0.684140	1.719735	-0.377856
H	-4.841455	3.772263	-0.677307
H	-5.845803	2.161556	0.921701
H	-5.521792	0.167635	2.441971
H	-3.990708	-1.586702	3.356383
H	-1.609842	-1.630902	2.570781
C	0.106158	2.645314	-0.994401
C	1.517968	2.151036	-1.219650
C	2.605768	2.793302	-0.593129
C	1.740027	1.042131	-2.045301
C	3.888777	2.274682	-0.799049
C	3.029034	0.547865	-2.253637
C	4.106177	1.163095	-1.618838
H	0.893177	0.560796	-2.521404
H	4.732041	2.743166	-0.298182
H	3.182167	-0.321028	-2.885759
H	5.112744	0.777502	-1.751171
O	-0.213176	3.793373	-1.337865
H	-2.448939	3.643950	-1.283261
C	2.388424	3.979690	0.314946
H	1.696878	3.729360	1.128201
H	3.328579	4.314016	0.760836
H	1.937401	4.812144	-0.231664
C	2.031556	-1.931365	-0.081798
C	2.863976	-2.920555	-0.600536
C	4.230239	-2.989842	-0.240879
C	4.797548	-2.099541	0.644210
C	3.990958	-1.079607	1.211736
C	2.616893	-0.992850	0.841535
N	1.814053	-0.007753	1.350531

C	2.302446	0.870963	2.215498
C	3.641802	0.842672	2.647026
C	4.480089	-0.127172	2.139503
N	0.683983	-1.719314	-0.379177
H	4.839934	-3.774463	-0.679892
H	5.845534	-2.164982	0.919606
H	5.523014	-0.171382	2.440611
H	3.993198	1.583727	3.355693
H	1.612372	1.629907	2.570191
C	-0.106872	-2.644234	-0.995938
C	-1.518553	-2.149389	-1.220791
C	-2.606495	-2.791568	-0.594384
C	-1.740398	-1.040157	-2.046108
C	-3.889363	-2.272595	-0.800093
C	-3.029343	-0.545556	-2.254248
C	-4.106577	-1.160758	-1.619576
H	-0.893447	-0.558844	-2.522079
H	-4.732699	-2.741005	-0.299295
H	-3.182305	0.323565	-2.886104
H	-5.113058	-0.774898	-1.751737
O	0.211873	-3.792298	-1.340021
H	2.447440	-3.644305	-1.285544
C	-2.389375	-3.978258	0.313313
H	-1.697580	-3.728401	1.126500
H	-3.329546	-4.312393	0.759301
H	-1.938745	-4.810711	-0.233622
Co	0.000375	0.000148	0.367592

CoOPiv2-d

Energy = -838.060705763 ZPE = -837.786821 H = -837.767705 G = -837.83456

C	-2.312948	0.027042	0.008241
O	-1.627451	-1.056606	0.004472
O	-1.633509	1.111424	0.005842
C	-3.829208	-0.000890	0.002755
C	-4.273552	-0.673819	-1.316586
H	-3.948708	-0.091502	-2.185112
H	-3.858905	-1.681752	-1.399787
H	-5.365569	-0.742904	-1.341250
C	-4.295522	-0.851992	1.204072
H	-3.879666	-1.861259	1.152084
H	-3.987609	-0.398635	2.152030
H	-5.387623	-0.923359	1.199525
C	-4.393359	1.423843	0.096755
H	-4.075622	1.913911	1.021419
H	-4.059014	2.037592	-0.744020
H	-5.486995	1.385867	0.084353
Co	0.000003	0.028020	-0.000435
C	2.312955	0.026999	-0.008949
O	1.627436	-1.056630	-0.005333
O	1.633536	1.111399	-0.006651
C	3.829207	-0.000919	-0.002449
C	4.272314	-0.668982	1.319843
H	3.946445	-0.083579	2.185907
H	3.857814	-1.676714	1.406289
H	5.364324	-0.737740	1.345876
C	4.296713	-0.856376	-1.200136
H	3.880741	-1.865417	-1.144958
H	3.989816	-0.406430	-2.150047
H	5.388806	-0.927771	-1.194195
C	4.393382	1.423494	-0.101035
H	4.076422	1.910215	-1.027740
H	4.058264	2.040207	0.737245
H	5.487009	1.385628	-0.087567

CoOPiv2-quar

Energy = -838.076737519 ZPE = -837.804355 H = -837.784434 G = -837.854561

C	-2.416232	0.031380	0.019031
O	-1.750709	-1.061377	0.014736
O	-1.764573	1.128765	0.021812
C	-3.940152	-0.004319	0.001321
C	-4.369756	-0.659034	-1.331625
H	-4.037356	-0.063391	-2.188578
H	-3.949803	-1.663878	-1.425087
H	-5.461395	-0.731853	-1.371299
C	-4.416913	-0.874939	1.183264
H	-3.993876	-1.880516	1.121000
H	-4.121801	-0.434555	2.141671
H	-5.508811	-0.952668	1.167396
C	-4.520596	1.412547	0.109923
H	-4.214437	1.893343	1.043425
H	-4.184355	2.041152	-0.718955
H	-5.614173	1.366001	0.088115
Co	-0.000110	0.033409	0.001305
C	2.416247	0.032207	-0.017961
O	1.750185	-1.060323	-0.013025
O	1.765094	1.129741	-0.020280
C	3.940171	-0.004462	-0.002364
C	4.371791	-0.665177	1.326871
H	4.041437	-0.073003	2.186999
H	3.951241	-1.670083	1.416772
H	5.463453	-0.738946	1.364185
C	4.414388	-0.870346	-1.188947
H	3.991020	-1.876003	-1.130091
H	4.117692	-0.425777	-2.144938
H	5.506280	-0.948588	-1.175410
C	4.521380	1.412471	-0.106045
H	4.213855	1.897437	-1.036927
H	4.187101	2.037781	0.726118
H	5.614963	1.365082	-0.086377

C-q

Energy = -2172.48833307 ZPE = -2171.82981 H = -2171.78564 G = -2171.90769

C	-0.623275	-2.724728	-1.197170
C	-0.653073	-4.108349	-1.388840
C	-1.773063	-4.743535	-1.967680
C	-2.887726	-4.036267	-2.366779
C	-2.912364	-2.629284	-2.185473
C	-1.788468	-1.983416	-1.593587
N	-1.772076	-0.636738	-1.373728
C	-2.809015	0.102681	-1.749224
C	-3.950912	-0.448121	-2.360890
C	-4.003924	-1.810664	-2.567403
N	0.447186	-1.965566	-0.742641
H	-1.743701	-5.821277	-2.099366
H	-3.743285	-4.532577	-2.813740
H	-4.876189	-2.269916	-3.023881
H	-4.769514	0.201804	-2.648087
H	-2.747935	1.165443	-1.547589
C	1.577511	-2.592203	-0.226757
C	2.886599	-1.963432	-0.590680
C	4.028480	-2.094540	0.232588
C	2.992025	-1.323764	-1.834983
C	5.231343	-1.537177	-0.221420
C	4.203707	-0.796807	-2.278397
C	5.328929	-0.899121	-1.459368

H	2.106147	-1.263179	-2.458578
H	6.111378	-1.606737	0.412538
H	4.266771	-0.312471	-3.248299
H	6.280304	-0.484400	-1.779791
O	1.537205	-3.621117	0.458150
H	0.195826	-4.705593	-1.086237
C	3.997525	-2.795766	1.569990
H	4.901699	-2.570139	2.142376
H	3.125197	-2.499814	2.158132
H	3.925877	-3.878970	1.439378
C	-1.546985	2.827701	0.016040
C	-2.416389	3.889553	0.176065
C	-2.317218	5.031588	-0.653137
C	-1.337546	5.123413	-1.616528
C	-0.433255	4.048140	-1.815145
C	-0.559431	2.873851	-1.011997
N	0.241104	1.780127	-1.214919
C	1.199235	1.846603	-2.128579
C	1.427513	2.984396	-2.930528
C	0.600968	4.074905	-2.784683
N	-1.523307	1.678815	0.848581
H	-3.013002	5.851059	-0.504403
H	-1.243936	6.010377	-2.235578
H	0.728085	4.959998	-3.401232
H	2.234803	2.973104	-3.653634
H	1.821034	0.965396	-2.232588
C	-2.677395	1.048946	1.306503
C	-2.373924	-0.205807	2.053531
C	-3.216016	-0.686095	3.087542
C	-1.269103	-0.958389	1.653651
C	-2.875123	-1.904831	3.684563
C	-0.944340	-2.176821	2.229998
C	-1.765422	-2.644050	3.264336
H	-0.685686	1.681429	1.499120
H	-3.494494	-2.285573	4.492227
H	-0.100014	-2.764150	1.883651
H	-1.538530	-3.593306	3.743873
O	-3.811915	1.438126	1.042807
H	-3.172957	3.839053	0.947998
C	-4.438378	0.073030	3.547178
H	-4.826155	-0.348659	4.478423
H	-4.217645	1.132245	3.708010
H	-5.227076	0.034985	2.790379
Co	-0.083245	-0.104071	-0.164457
C	1.667222	1.360764	1.675384
O	1.496455	0.274885	1.003880
O	0.736371	2.027181	2.183489
C	3.124714	1.835613	1.838088
C	3.886458	0.778719	2.662498
H	4.933137	1.079566	2.783199
H	3.449066	0.666634	3.660936
H	3.860621	-0.187831	2.160251
C	3.749255	1.947464	0.432745
H	3.226176	2.698404	-0.170436
H	4.799471	2.250139	0.511102
H	3.700193	0.991337	-0.089482
C	3.171931	3.194407	2.549940
H	4.211506	3.522947	2.658528
H	2.627124	3.954875	1.982621
H	2.721603	3.134996	3.544495

C-q'

Energy = -2172.00195166 ZPE = -2171.356518 H = -2171.312556 G = -2171.433861

C	2.370884	1.957048	-0.845466
C	3.193401	3.085513	-0.907092
C	4.480719	3.028131	-1.483183
C	5.000077	1.859465	-2.002906
C	4.216458	0.679111	-1.950949
C	2.913180	0.733407	-1.371587
N	2.134060	-0.376657	-1.275579
C	2.567889	-1.539740	-1.732188
C	3.834063	-1.684624	-2.336960
C	4.652262	-0.579100	-2.440126
N	1.049134	1.919578	-0.413775
H	5.073145	3.938702	-1.513203
H	5.992581	1.826277	-2.441807
H	5.637791	-0.657964	-2.891255
H	4.147502	-2.656226	-2.703083
H	1.894006	-2.379915	-1.597919
C	0.578853	2.917884	0.413402
C	-0.868810	3.288370	0.236700
C	-1.717119	3.539472	1.337230
C	-1.331267	3.502697	-1.066204
C	-3.009510	4.008201	1.078186
C	-2.621017	3.982425	-1.306020
C	-3.462812	4.238080	-0.225031
H	-0.657621	3.307368	-1.894638
H	-3.678643	4.190517	1.915514
H	-2.960106	4.151567	-2.324024
H	-4.471917	4.605813	-0.389371
O	1.270658	3.539736	1.234274
H	2.836240	4.023605	-0.503211
C	-1.278508	3.258019	2.753075
H	-2.096375	3.433391	3.457719
H	-0.963255	2.213505	2.838839
H	-0.425568	3.880327	3.032756
C	-0.909313	-2.719162	-0.729590
C	-1.459101	-4.009207	-0.695047
C	-2.397877	-4.430742	-1.661510
C	-2.819411	-3.613462	-2.691099
C	-2.290599	-2.301297	-2.783253
C	-1.345772	-1.860421	-1.807501
N	-0.824510	-0.603168	-1.851698
C	-1.169969	0.231450	-2.818562
C	-2.089978	-0.120797	-3.827660
C	-2.649682	-1.380164	-3.801358
N	-0.006228	-2.142204	0.131483
H	-2.798101	-5.438568	-1.582386
H	-3.541008	-3.953384	-3.427855
H	-3.369717	-1.683495	-4.556789
H	-2.347585	0.598876	-4.596990
H	-0.713524	1.214944	-2.781818
C	0.579376	-2.807700	1.166046
C	1.505983	-1.923949	1.959699
C	2.283952	-2.385543	3.051977
C	1.578718	-0.579401	1.605335
C	3.085918	-1.450012	3.725216
C	2.361355	0.350467	2.272644
C	3.128347	-0.104352	3.353925
H	3.688633	-1.788417	4.564841
H	2.371683	1.396906	1.978719
H	3.755943	0.590217	3.908728
O	0.411960	-4.008441	1.459411
H	-1.152476	-4.677182	0.095469
C	2.288881	-3.822502	3.522578
H	2.978614	-3.945511	4.363826
H	1.290271	-4.142964	3.830552

H	2.583092	-4.504435	2.720211
Co	0.327192	-0.014974	-0.133452
C	-2.044666	-0.194866	1.708723
O	-1.226944	0.487936	0.972611
O	-1.738220	-0.762794	2.765351
C	-3.533834	-0.219745	1.260239
C	-4.331873	0.559795	2.326959
H	-5.405743	0.521386	2.107743
H	-4.161135	0.132116	3.318923
H	-4.028319	1.612167	2.346449
C	-3.745669	0.423955	-0.115452
H	-3.234019	-0.140224	-0.897506
H	-4.815694	0.444962	-0.358344
H	-3.364008	1.445337	-0.132756
C	-4.001620	-1.687559	1.234647
H	-5.071346	-1.744347	0.999177
H	-3.455423	-2.260556	0.477891
H	-3.830391	-2.159669	2.205588

C-t

Energy = -2172.50539983 ZPE = -2171.846139 H = -2171.802738 G = -2171.921189

C	-0.489412	2.839223	-0.283867
C	-1.147662	4.074494	-0.284972
C	-0.434930	5.288875	-0.246290
C	0.945500	5.328666	-0.202103
C	1.664757	4.109561	-0.177032
C	0.943811	2.875897	-0.196248
N	1.594816	1.681023	-0.133160
C	2.918766	1.638329	-0.108445
C	3.706812	2.806006	-0.128937
C	3.080367	4.033101	-0.145958
N	-1.070022	1.594112	-0.455936
H	-0.997646	6.218204	-0.263401
H	1.485778	6.269861	-0.191706
H	3.659720	4.952001	-0.139381
H	4.787272	2.718962	-0.115850
H	3.379919	0.659445	-0.062040
C	-2.413722	1.455497	-0.112159
C	-3.267773	0.579493	-0.983755
C	-4.665746	0.451530	-0.769581
C	-2.682820	-0.094704	-2.067508
C	-5.398009	-0.349673	-1.660771
C	-3.424879	-0.889390	-2.933089
C	-4.799758	-1.015722	-2.728816
H	-1.617744	-0.006074	-2.205507
H	-6.468744	-0.452350	-1.505363
H	-2.935102	-1.403713	-3.754773
H	-5.403246	-1.628051	-3.392935
O	-2.907659	2.047904	0.858578
H	-2.229161	4.098065	-0.325881
C	-5.423940	1.123698	0.351839
H	-6.488404	0.880352	0.283443
H	-5.053335	0.809485	1.330738
H	-5.304692	2.209328	0.321588
C	2.459557	-2.018204	-0.879975
C	3.441330	-2.984890	-0.944586
C	4.016986	-3.338309	-2.189529
C	3.619019	-2.719994	-3.354303
C	2.622294	-1.709497	-3.321178
C	2.027236	-1.367665	-2.070102
N	1.074860	-0.387434	-1.973882
C	0.737384	0.294410	-3.058501
C	1.267710	0.017356	-4.335785
C	2.198122	-0.989938	-4.466911
N	1.819179	-1.596131	0.322021
H	4.784502	-4.105011	-2.216020
H	4.067344	-2.985105	-4.306918
H	2.626598	-1.231363	-5.435238
H	0.938467	0.601013	-5.187628
H	0.018530	1.093360	-2.905630
C	2.572320	-1.193654	1.448651
C	1.694508	-0.489460	2.421240
C	1.951441	-0.452230	3.811413
C	0.605937	0.213057	1.891132
C	1.066200	0.277347	4.611712
C	-0.253774	0.961674	2.681741
C	-0.014565	0.972904	4.061172
H	0.998331	-2.233783	0.633281
H	1.228112	0.305892	5.685600
H	-1.089554	1.505971	2.255105
H	-0.681171	1.532176	4.712447
O	3.783936	-1.330895	1.548401
H	3.775147	-3.462003	-0.031486
C	3.128428	-1.172962	4.422327
H	3.053877	-1.177764	5.512711
H	3.191864	-2.206865	4.070415
H	4.068646	-0.691974	4.137318
Co	0.299432	0.071189	-0.044658
C	-1.198688	-2.299405	0.959454
O	-1.175140	-1.219419	0.265625
O	-0.188204	-3.008691	1.192338
C	-2.574607	-2.705630	1.515047
C	-3.130665	-1.513737	2.322436
H	-4.121730	-1.761582	2.718315
H	-2.476495	-1.271144	3.167209
H	-3.213425	-0.624633	1.695842
C	-3.502735	-3.004418	0.319626
H	-3.125891	-3.849643	-0.267557
H	-4.503683	-3.264703	0.681393
H	-3.584573	-2.136404	-0.334629
C	-2.449200	-3.943399	2.413573
H	-3.435113	-4.224417	2.799640
H	-2.039080	-4.792741	1.860191
H	-1.788891	-3.748495	3.263878

C-t'

Energy = -2172.03350728 ZPE = -2171.386271 H = -2171.342999 G = -2171.46199

C	-2.807354	1.399019	0.631772
C	-3.785251	2.379413	0.836813
C	-5.115616	2.044187	1.159950
C	-5.534095	0.733468	1.278723
C	-4.593513	-0.303782	1.069174
C	-3.240601	0.030942	0.746287
N	-2.314116	-0.937107	0.523373
C	-2.640980	-2.214104	0.607331
C	-3.947500	-2.637202	0.934393
C	-4.915388	-1.683327	1.160486
N	-1.450287	1.627867	0.431675
H	-5.826750	2.850967	1.318074
H	-6.561992	0.485285	1.525374
H	-5.933504	-1.971788	1.408277
H	-4.169607	-3.696986	0.998086
H	-1.843385	-2.921590	0.403330
C	-1.060986	2.814449	-0.138970
C	0.332103	3.287702	0.189290
C	1.224716	3.761108	-0.797133

C	0.688244	3.356609	1.540349
C	2.461169	4.266637	-0.378042
C	1.921525	3.872818	1.942121
C	2.816892	4.323920	0.972833
H	-0.019334	3.003376	2.282359
H	3.164901	4.617086	-1.129499
H	2.176559	3.920572	2.997181
H	3.784813	4.724870	1.261444
O	-1.781404	3.535654	-0.854135
H	-3.512556	3.422110	0.746409
C	0.925492	3.652048	-2.273217
H	1.601041	4.287646	-2.854213
H	1.076131	2.615548	-2.596618
H	-0.105132	3.933485	-2.491508
C	1.128763	-2.485180	0.859416
C	1.918943	-3.635965	0.922001
C	2.552852	-4.011821	2.128465
C	2.418324	-3.280666	3.290834
C	1.620855	-2.106356	3.280592
C	0.990546	-1.709823	2.065805
N	0.232462	-0.575688	1.994355
C	0.036343	0.160349	3.073647
C	0.611396	-0.162872	4.321609
C	1.405925	-1.285229	4.417985
N	0.440444	-1.977669	-0.223228
H	3.163541	-4.910844	2.129893
H	2.908405	-3.585531	4.210486
H	1.871819	-1.556649	5.361513
H	0.426979	0.475171	5.178931
H	-0.593251	1.032129	2.935359
C	0.386928	-2.531774	-1.474209
C	-0.430994	-1.662744	-2.376695
C	-0.753253	-1.993101	-3.712220
C	-0.876073	-0.451464	-1.824801
C	-1.528422	-1.079856	-4.440817
C	-1.657197	0.440814	-2.550881
C	-1.975708	0.115955	-3.874674
H	-1.788149	-1.314255	-5.470334
H	-1.996554	1.375135	-2.117971
H	-2.575979	0.801639	-4.468449
O	0.922610	-3.598108	-1.820843
H	2.037684	-4.232244	0.029281
C	-0.296090	-3.274224	-4.370245
H	-0.672868	-3.333303	-5.395897
H	0.795031	-3.342826	-4.388438
H	-0.639303	-4.152296	-3.816035
Co	-0.338712	-0.166794	0.016865
C	2.327549	0.463833	-1.250333
O	1.452937	0.675988	-0.330070
O	2.120465	0.486374	-2.475681
C	3.777932	0.172296	-0.765562
C	4.711885	1.212947	-1.412876
H	5.759292	1.000475	-1.166152
H	4.596652	1.201204	-2.499869
H	4.475796	2.221742	-1.055512
C	3.908713	0.232412	0.762127
H	3.258517	-0.502927	1.241174
H	4.944051	0.023678	1.060322
H	3.634574	1.220130	1.142722
C	4.145336	-1.239881	-1.267164
H	5.176863	-1.490774	-0.990910
H	3.482414	-1.994929	-0.831228
H	4.051703	-1.292318	-2.355333

D

Energy = -2172.50422707 ZPE = -2171.841816 H = -2171.798871 G = -2171.915795

C	-1.468511	-2.149829	0.115242
C	-1.494778	-2.718708	1.368677
C	-2.727437	-2.923087	2.035600
C	-3.922405	-2.553767	1.459852
C	-3.929782	-1.970378	0.165940
C	-2.693462	-1.784626	-0.521518
N	-2.619657	-1.251549	-1.770626
C	-3.736596	-0.864860	-2.356984
C	-5.013732	-0.983593	-1.755322
C	-5.107422	-1.542990	-0.500628
N	-0.270016	-1.810652	-0.603409
H	-2.715193	-3.369577	3.024565
H	-4.863082	-2.699388	1.982281
H	-6.068988	-1.658958	-0.008755
H	-5.893708	-0.640196	-2.287983
H	-3.639665	-0.435675	-3.352142
C	0.760526	-2.846462	-0.819123
C	2.008783	-2.235444	-1.292377
C	3.022335	-2.992977	-1.935718
C	2.167309	-0.859145	-1.008743
C	4.185903	-2.318209	-2.307043
C	3.355942	-0.226006	-1.379952
C	4.351707	-0.953687	-2.031697
H	4.976549	-2.863738	-2.814759
H	3.495190	0.826849	-1.157792
H	5.273641	-0.460241	-2.330516
O	0.529828	-4.015176	-0.576907
H	-0.576374	-2.997266	1.863399
C	2.873532	-4.467301	-2.219934
H	2.842680	-5.043559	-1.290345
H	1.936652	-4.683614	-2.742836
H	3.706162	-4.828540	-2.829162
C	1.069817	2.693686	-0.641573
C	1.294108	4.065850	-0.498423
C	0.901785	4.968252	-1.511690
C	0.307528	4.545371	-2.682476
C	0.067581	3.160811	-2.874666
C	0.423072	2.245125	-1.840739
N	0.189675	0.900204	-1.954341
C	-0.301771	0.430372	-3.090788
C	-0.662247	1.258037	-4.174151
C	-0.497778	2.619705	-4.056861
N	1.410826	1.677357	0.231288
H	1.090898	6.027250	-1.358449
H	0.028568	5.247605	-3.461949
H	-0.780461	3.288195	-4.865209
H	-1.068734	0.808858	-5.073289
H	-0.439318	-0.640715	-3.171593
C	1.966430	1.863244	1.467834
C	2.104765	0.556335	2.178113
C	2.777341	0.422705	3.414584
C	1.533662	-0.551479	1.503012
C	2.892513	-0.864668	3.955878
C	1.716977	-1.821746	2.067771
C	2.381162	-1.976453	3.287465
H	3.403763	-0.995336	4.906208
H	1.375390	-2.713789	1.556420
H	2.506460	-2.968954	3.713081
O	2.315342	2.957153	1.943273
H	1.779786	4.423194	0.396703
C	3.376096	1.590880	4.162835

H	3.865024	1.246357	5.078886
H	4.106301	2.124685	3.548841
H	2.612357	2.328227	4.424063
Co	0.689500	-0.037471	-0.172940
H	-0.613701	-1.523886	-1.529374
C	-2.844334	1.741167	1.911640
C	-3.561970	2.024970	0.583242
H	-3.917146	1.100175	0.120339
H	-4.425354	2.671118	0.767646
H	-2.896231	2.524693	-0.124745
C	-2.319378	3.062212	2.528434
H	-3.163304	3.731830	2.719844
H	-1.800989	2.877075	3.473098
H	-1.628182	3.566329	1.844765
C	-3.789371	1.028785	2.899165
H	-4.142420	0.078564	2.487355
H	-3.292052	0.827288	3.850672
H	-4.658593	1.665356	3.090098
C	-1.615081	0.886359	1.647462
O	-1.150274	0.732309	0.517860
O	-1.057300	0.364101	2.730798
H	-0.225882	-0.093838	2.465391

D’

Energy = -2172.05573653 ZPE = -2171.406846 H = -2171.364093 G = -2171.48205

C	1.523298	2.644319	-0.382461
C	1.617566	4.040191	-0.359130
C	2.427100	4.718302	-1.296862
C	3.152773	4.055118	-2.268291
C	3.087669	2.639218	-2.334546
C	2.274955	1.945009	-1.392754
N	2.167820	0.582279	-1.403048
C	2.829057	-0.125529	-2.303573
C	3.657308	0.478867	-3.274606
C	3.785253	1.851243	-3.288048
N	0.799083	1.813012	0.439759
H	2.475117	5.803146	-1.244706
H	3.769133	4.595696	-2.980327
H	4.416431	2.343837	-4.022814
H	4.179326	-0.143539	-3.993446
H	2.697385	-1.201470	-2.248698
C	-0.037131	2.203563	1.448587
C	-0.617644	0.998718	2.127141
C	-1.524145	1.075078	3.211902
C	-0.184957	-0.246580	1.605912
C	-1.956230	-0.128273	3.786071
C	-0.642958	-1.424107	2.212813
C	-1.516416	-1.363488	3.301434
H	-2.313851	-0.202155	0.861118
H	-2.654518	-0.094729	4.619145
H	-0.325832	-2.387549	1.824292
H	-1.872545	-2.279979	3.767529
O	-0.281485	3.382134	1.770558
H	1.059604	4.585577	0.388114
C	-2.064802	2.382022	3.741517
H	-1.262369	3.055337	4.051771
H	-2.617195	2.909764	2.958634
H	-2.735426	2.205755	4.588691
C	0.069460	-2.398614	-1.210161
C	-0.148514	-3.708917	-1.652415
C	-1.193586	-3.994972	-2.557788
C	-2.034062	-3.016635	-3.055159
C	-1.852017	-1.673125	-2.638784
C	-0.815058	-1.376925	-1.708493
N	-0.604956	-0.106355	-1.248263
C	-1.356359	0.888447	-1.689417
C	-2.391164	0.689767	-2.629453
C	-2.640924	-0.582808	-3.093759
N	1.034686	-1.926615	-0.351313
H	-1.331262	-5.025882	-2.874393
H	-2.826018	-3.255959	-3.758500
H	-3.438028	-0.767303	-3.808934
H	-2.981582	1.537657	-2.958358
H	-1.145063	1.866317	-1.272564
C	2.002203	-2.671794	0.266864
C	2.830468	-1.797428	1.156506
C	3.939788	-2.267204	1.898040
C	2.423502	-0.443185	1.211822
C	4.630993	-1.343304	2.693983
C	3.140137	0.446946	2.017916
C	4.239320	-0.002169	2.754544
H	5.488183	-1.680735	3.272606
H	2.836711	1.489289	2.068865
H	4.796966	0.690779	3.382171
O	2.176209	-3.897465	0.116614
H	0.501115	-4.492786	-1.291085
C	4.404127	-3.706099	1.867327
H	5.287460	-3.838279	2.500564
H	3.618420	-4.385091	2.210787
H	4.646394	-4.027610	0.850338
Co	0.942406	-0.061772	0.075782
C	-3.986740	0.528074	0.317076
O	-3.192779	-0.521558	0.568753
O	-3.618243	1.684708	0.432051
C	-5.413493	0.122389	-0.064982
C	-5.957319	1.140005	-1.082198
H	-7.009444	0.927662	-1.296996
H	-5.874428	2.158072	-0.695103
H	-5.398664	1.086382	-2.022225
C	-5.474549	-1.299887	-0.646855
H	-5.135717	-2.042809	0.078804
H	-6.506291	-1.536308	-0.927756
H	-4.846231	-1.388079	-1.537708
C	-6.236104	0.193285	1.243962
H	-7.278789	-0.072700	1.041107
H	-5.843646	-0.503242	1.992045
H	-6.211174	1.202898	1.665092

D’-AQBr

Energy = -2197.17598093 ZPE = -2196.547882 H = -2196.501956 G = -2196.628048

C	1.875071	-0.036725	-2.201832
C	2.231292	-0.318443	-3.525223
C	3.244343	-1.256935	-3.802635
C	3.927028	-1.937316	-2.811282
C	3.604406	-1.690657	-1.454347
C	2.576755	-0.739280	-1.155042
N	2.202565	-0.445132	0.123747
C	2.793689	-1.042606	1.142319
C	3.819058	-1.994673	0.964153
C	4.203652	-2.299856	-0.319406
N	0.923362	0.836583	-1.736146
H	3.496666	-1.450748	-4.841814
H	4.701410	-2.653098	-3.057526
H	4.279290	-2.463392	1.824783
H	2.448592	-0.760881	2.131507
C	0.088087	1.604966	-2.504433

C	-0.786538	2.445489	-1.624572
C	-1.771653	3.332051	-2.123368
C	-0.558606	2.293465	-0.234200
C	-2.492350	4.093381	-1.193796
C	-1.301175	3.078053	0.658494
C	-2.256265	3.977682	0.179197
H	-2.518745	1.239468	-0.505556
H	-3.257202	4.778017	-1.552528
H	-1.142399	2.975113	1.727773
H	-2.834501	4.581606	0.875380
O	0.060084	1.617535	-3.748204
H	1.715319	0.195484	-4.322777
C	-2.101016	3.452585	-3.591919
H	-1.225226	3.733880	-4.181407
H	-2.435936	2.487894	-3.983869
H	-2.892731	4.192227	-3.748191
C	-0.478030	0.140896	2.566419
C	-0.923393	0.016927	3.887720
C	-1.925441	-0.916814	4.215124
C	-2.503050	-1.754778	3.278771
C	-2.084773	-1.674618	1.928561
C	-1.087369	-0.710527	1.574162
N	-0.651153	-0.548262	0.290782
C	-1.118915	-1.322074	-0.671403
C	-2.080800	-2.325452	-0.430008
C	-2.552731	-2.474081	0.850817
N	0.487935	0.977094	2.062324
H	-2.250467	-0.982497	5.250097
H	-3.263569	-2.471011	3.563608
H	-2.437971	-2.938631	-1.247160
H	-0.743606	-1.136130	-1.670312
C	1.220923	1.889758	2.777789
C	2.118984	2.656301	1.858759
C	3.038919	3.634753	2.304169
C	1.983548	2.339261	0.486774
C	3.817631	4.284755	1.337123
C	2.777575	3.011496	-0.447062
C	3.691054	3.979488	-0.021797
H	4.533178	5.039941	1.654672
H	2.679808	2.779196	-1.504026
H	4.309922	4.503213	-0.748067
O	1.152976	2.060857	4.009609
H	-0.480995	0.646814	4.645362
C	3.214793	3.999449	3.760747
H	3.992714	4.761165	3.874893
H	2.283649	4.377305	4.192442
H	3.484330	3.126001	4.361361
Co	0.730244	0.942333	0.164595
C	-3.910098	0.295001	-1.394464
O	-3.417226	0.902675	-0.306497
O	-3.278273	0.172520	-2.430650
C	-5.357522	-0.174416	-1.221562
C	-5.523187	-1.526139	-1.938542
H	-6.575400	-1.827783	-1.925404
H	-5.188404	-1.458194	-2.976093
H	-4.941899	-2.307267	-1.438709
C	-5.754992	-0.302080	0.258223
H	-5.685746	0.658402	0.774173
H	-6.787833	-0.658795	0.329382
H	-5.111634	-1.015126	0.780220
C	-6.231087	0.898768	-1.914384
H	-7.287057	0.617629	-1.845737
H	-6.104950	1.876273	-1.437163
H	-5.964267	0.993335	-2.971136
Br	5.639770	-3.634367	-0.557569
Br	-3.924264	-3.857502	1.170726

D'-AQCl

Energy = -3091.24231211 ZPE = -3090.612924 H = -3090.567525 G = -3090.691588

C	-1.823143	0.795036	-2.212549
C	-2.094707	1.256467	-3.505346
C	-3.030243	2.290177	-3.708801
C	-3.715383	2.894523	-2.670629
C	-3.473719	2.464568	-1.342897
C	-2.528299	1.416478	-1.118519
N	-2.238500	0.948483	0.130719
C	-2.843366	1.463424	1.186439
C	-3.792443	2.499458	1.079627
C	-4.095300	2.986160	-0.172539
N	-0.955326	-0.193328	-1.817330
H	-3.217390	2.622430	-4.726553
H	-4.429119	3.687076	-2.859155
H	-4.267187	2.898534	1.967587
H	-2.570054	1.042136	2.147996
C	-0.130268	-0.918163	-2.636403
C	0.640029	-1.919314	-1.830019
C	1.581687	-2.814765	-2.392388
C	0.353703	-1.916388	-0.441878
C	2.199062	-3.733808	-1.533340
C	0.993732	-2.855080	0.378424
C	1.904536	-3.762910	-0.167236
H	2.408313	-1.004380	-0.441540
H	2.927534	-4.430259	-1.941658
H	0.789533	-2.866146	1.444922
H	2.402894	-4.487478	0.473365
O	-0.032810	-0.778318	-3.869258
H	-1.573784	0.806250	-4.337482
C	1.966904	-2.794993	-3.852674
H	1.098434	-2.931074	-4.501553
H	2.396694	-1.825670	-4.121597
H	2.701783	-3.577647	-4.066323
C	0.271814	-0.101727	2.593481
C	0.654937	-0.157482	3.939047
C	1.697505	0.660685	4.416447
C	2.377651	1.554653	3.609184
C	2.023735	1.652747	2.241835
C	0.985448	0.811555	1.735384
N	0.607485	0.827730	0.422988
C	1.182410	1.666436	-0.420153
C	2.197487	2.558461	-0.020881
C	2.611942	2.535253	1.290788
N	-0.717074	-0.807427	1.952360
H	1.970700	0.586654	5.465809
H	3.168236	2.178195	4.008251
H	2.647369	3.228288	-0.742683
H	0.849160	1.621957	-1.449798
C	-1.538440	-1.747190	2.521140
C	-2.436912	-2.337418	1.480167
C	-3.434477	-3.299016	1.766362
C	-2.218678	-1.867923	0.163601
C	-4.208593	-3.772872	0.698448
C	-3.012475	-2.365180	-0.874404
C	-4.003563	-3.312948	-0.606234
H	-4.982549	-4.511839	0.893607
H	-2.854613	-2.011770	-1.889831
H	-4.621926	-3.700309	-1.413932
O	-1.541233	-2.067219	3.724992

H	0.134155	-0.835378	4.599224
C	-3.695465	-3.827810	3.158578
H	-4.516853	-4.551430	3.147124
H	-2.805532	-4.308458	3.574670
H	-3.945532	-3.020565	3.853028
Co	-0.863250	-0.534640	0.063438
C	3.935845	-0.064900	-1.080266
O	3.305375	-0.766254	-0.128143
O	3.412533	0.236394	-2.139754
C	5.388557	0.263199	-0.723639
C	5.721248	1.666202	-1.261376
H	6.785646	1.877280	-1.117327
H	5.488202	1.738436	-2.326156
H	5.149218	2.434399	-0.731531
C	5.644706	0.194310	0.791240
H	5.464947	-0.810747	1.179702
H	6.685571	0.464218	0.998006
H	4.997925	0.887488	1.335589
C	6.248132	-0.797334	-1.452753
H	7.309273	-0.613205	-1.255506
H	6.004668	-1.806537	-1.104422
H	6.083086	-0.755321	-2.533452
Cl	-5.275944	4.280483	-0.313081
Cl	3.897614	3.625968	1.788571

D'-AQMe

Energy = -2250.70581691 ZPE = -2250.001209 H = -2249.955209 G = -2250.079246

C	-1.666647	1.557849	-1.953266
C	-1.844337	2.328789	-3.107287
C	-2.707750	3.443063	-3.089343
C	-3.405815	3.825764	-1.958238
C	-3.257224	3.080199	-0.759182
C	-2.387510	1.951848	-0.769003
N	-2.185745	1.182395	0.343391
C	-2.810941	1.486282	1.466611
C	-3.689606	2.583858	1.564623
C	-3.928410	3.391176	0.467741
N	-0.879293	0.443607	-1.777163
H	-2.824672	4.019066	-4.004026
H	-4.060593	4.689328	-1.984511
H	-4.176227	2.786095	2.513762
H	-2.608065	0.837228	2.312642
C	-0.052143	-0.116080	-2.711074
C	0.615524	-1.332310	-2.140967
C	1.533238	-2.131165	-2.866420
C	0.253720	-1.641678	-0.805707
C	2.048571	-3.269461	-2.232357
C	0.793590	-2.791675	-0.213462
C	1.678661	-3.603472	-0.926008
H	2.344019	-0.845236	-0.588773
H	2.757214	-3.896736	-2.768175
H	0.530234	-3.043511	0.809737
H	2.098309	-4.493441	-0.461214
O	0.123123	0.306093	-3.870299
H	-1.309431	2.053856	-4.004655
C	2.001963	-1.786884	-4.260302
H	1.165380	-1.688585	-4.955918
H	2.512448	-0.819250	-4.260811
H	2.693342	-2.549726	-4.632591
C	0.101839	-0.567103	2.582502
C	0.391621	-0.941852	3.899878
C	1.428676	-0.301938	4.608059
C	2.188062	0.715696	4.058807
C	1.932546	1.136839	2.727712
C	0.905697	0.474815	1.994637
N	0.615187	0.801116	0.698139
C	1.279259	1.779976	0.110065
C	2.288476	2.507193	0.771927
C	2.636857	2.199323	2.073200
N	-0.875636	-1.055451	1.746541
H	1.629069	-0.620829	5.628013
H	2.969748	1.191013	4.640290
H	2.794814	3.305148	0.238765
H	1.015672	1.985638	-0.921025
C	-1.779637	-2.038955	2.045687
C	-2.653712	-2.308624	0.860103
C	-3.717535	-3.241073	0.871259
C	-2.340010	-1.558051	-0.297797
C	-4.457970	-3.400936	-0.308153
C	-3.103297	-1.747235	-1.454408
C	-4.157952	-2.663759	-1.458191
H	-5.281130	-4.112028	-0.323370
H	-2.870747	-1.177745	-2.350433
H	-4.751765	-2.810705	-2.358716
O	-1.870810	-2.629342	3.140539
H	-0.197380	-1.721719	4.360045
C	-4.084890	-4.060500	2.087987
H	-4.943350	-4.704923	1.872272
H	-3.248197	-4.683143	2.416978
H	-4.328320	-3.421107	2.941398
Co	-0.903099	-0.336539	-0.027899
C	3.960628	0.108633	-0.906298
O	3.230214	-0.747921	-0.181629
O	3.540455	0.661039	-1.909370
C	5.388885	0.280706	-0.378274
C	5.774599	1.766626	-0.491221
H	6.827454	1.899829	-0.222735
H	5.620925	2.129232	-1.510169
H	5.170132	2.379270	0.184358
C	5.530871	-0.200228	1.075049
H	5.330253	-1.270775	1.162206
H	6.550170	-0.009991	1.426893
H	4.833402	0.324192	1.733545
C	6.291375	-0.565463	-1.307037
H	7.336721	-0.470570	-0.995205
H	6.016419	-1.624624	-1.264172
H	6.205414	-0.227857	-2.343983
C	-4.865191	4.566269	0.552956
H	-4.345677	5.501011	0.313029
H	-5.686990	4.465754	-0.165081
H	-5.293549	4.659244	1.553428
C	3.719024	2.960873	2.791149
H	3.332795	3.421967	3.707025
H	4.538458	2.297150	3.089529
H	4.133282	3.749385	2.158900

D'-AQNH2

Energy = -2282.79333008 ZPE = -2282.110596 H = -2282.064968 G = -2282.18842

C	-1.680939	1.902502	-1.631781
C	-1.841054	2.877842	-2.622210
C	-2.693074	3.978581	-2.403449
C	-3.405364	4.139024	-1.229129
C	-3.287139	3.167787	-0.200605
C	-2.417816	2.061889	-0.402829
N	-2.222821	1.094055	0.545625
C	-2.870255	1.186202	1.696378

C	-3.761842	2.225720	1.990767
C	-3.995953	3.229243	1.051315
N	-0.889570	0.775643	-1.659976
H	-2.785942	4.726542	-3.186812
H	-4.028815	5.016590	-1.094629
H	-4.274132	2.238108	2.947753
H	-2.677675	0.389967	2.409005
C	-0.047969	0.407096	-2.671134
C	0.632982	-0.885728	-2.328524
C	1.570390	-1.523633	-3.176919
C	0.265074	-1.439927	-1.076395
C	2.096170	-2.753686	-2.758772
C	0.815611	-2.673759	-0.701836
C	1.717913	-3.329569	-1.542160
H	2.343190	-0.682859	-0.667794
H	2.819816	-3.261192	-3.392672
H	0.545863	-3.112915	0.254392
H	2.145518	-4.285522	-1.245873
O	0.132010	1.036478	-3.732640
H	-1.294009	2.771700	-3.547632
C	2.052331	-0.918361	-4.474128
H	1.224619	-0.706879	-5.154989
H	2.542331	0.040896	-4.283462
H	2.764864	-1.586723	-4.968561
C	0.093619	-1.021583	2.438187
C	0.384387	-1.641037	3.659563
C	1.418856	-1.147503	4.478488
C	2.181167	-0.049120	4.124501
C	1.930192	0.607306	2.891753
C	0.895092	0.113324	2.052879
N	0.588350	0.684933	0.846599
C	1.254565	1.762035	0.461954
C	2.283388	2.336371	1.219085
C	2.658018	1.761308	2.431076
N	-0.886799	-1.347316	1.527493
H	1.613162	-1.645101	5.425284
H	2.943211	0.316810	4.804333
H	2.804978	3.207722	0.836962
H	0.977332	2.171556	-0.503199
C	-1.779334	-2.378038	1.634636
C	-2.647584	-2.434907	0.414747
C	-3.701999	-3.364130	0.251067
C	-2.336812	-1.483265	-0.585867
C	-4.436823	-3.314383	-0.941736
C	-3.095554	-1.466811	-1.761244
C	-4.140354	-2.377701	-1.937214
H	-5.253136	-4.018074	-1.090309
H	-2.865524	-0.741656	-2.537866
H	-4.729901	-2.364443	-2.852487
O	-1.866779	-3.165153	2.599537
H	-0.206577	-2.492937	3.963095
C	-4.066140	-4.392733	1.298078
H	-4.914149	-4.999475	0.963631
H	-3.222804	-5.052690	1.519473
H	-4.325187	-3.919511	2.249776
Co	-0.918469	-0.315392	-0.086065
C	3.972168	0.289621	-0.839096
O	3.233854	-0.663462	-0.258649
O	3.558476	1.005022	-1.735936
C	5.408223	0.346077	-0.306715
C	5.841375	1.820547	-0.230671
H	6.896492	1.887730	0.052759
H	5.701792	2.317144	-1.193469
H	5.252081	2.360088	0.517602
C	5.548421	-0.323174	1.070312
H	5.276920	-1.380442	1.029102
H	6.586593	-0.245839	1.410420
H	4.907723	0.160992	1.811961
C	6.273638	-0.402650	-1.348077
H	7.325320	-0.378724	-1.044012
H	5.965486	-1.449986	-1.433292
H	6.185584	0.064263	-2.333521
N	3.664096	2.305629	3.198148
H	4.159685	1.692081	3.828012
H	4.267090	2.976098	2.742617
N	-4.840523	4.281079	1.326438
H	-5.282808	4.738931	0.542691
H	-5.465397	4.157405	2.110906

D'-AQOH

Energy = -2322.51305771 ZPE = -2321.855239 H = -2321.810098 G = -2321.935021

C	-1.739228	1.968430	-1.532788
C	-1.935596	2.989381	-2.470186
C	-2.828891	4.047172	-2.199243
C	-3.541557	4.131191	-1.017322
C	-3.371650	3.117025	-0.041951
C	-2.478429	2.042906	-0.299157
N	-2.268627	1.032927	0.601158
C	-2.916225	1.048157	1.753287
C	-3.821820	2.065483	2.106669
C	-4.051352	3.099312	1.214209
N	-0.915370	0.868953	-1.616169
H	-2.955513	4.821244	-2.951971
H	-4.222517	4.951605	-0.824065
H	-4.326910	2.031861	3.067098
H	-2.709122	0.220064	2.424004
C	-0.051620	0.584371	-2.636181
C	0.665831	-0.703086	-2.356556
C	1.639610	-1.256790	-3.221868
C	0.297426	-1.341800	-1.145937
C	2.202115	-2.490185	-2.865637
C	0.883532	-2.575918	-0.832760
C	1.823520	-3.149450	-1.692509
H	2.368661	-0.582868	-0.589735
H	2.954485	-2.934168	-3.513472
H	0.614491	-3.078836	0.091709
H	2.280059	-4.105428	-1.443625
O	0.120711	1.280247	-3.656070
H	-1.388818	2.949708	-3.401152
C	2.116426	-0.561888	-4.475249
H	1.291945	-0.356882	-5.162303
H	2.553219	0.409922	-4.227909
H	2.870126	-1.168306	-4.988033
C	0.086767	-1.139750	2.378526
C	0.398929	-1.822908	3.560588
C	1.438766	-1.367792	4.397934
C	2.184093	-0.239459	4.108044
C	1.896445	0.483429	2.924179
C	0.865179	0.029059	2.060267
N	0.556074	0.669824	0.889791
C	1.213933	1.767761	0.559263
C	2.238969	2.311421	1.354412
C	2.589041	1.666953	2.526569
N	-0.885621	-1.429746	1.448110
H	1.653577	-1.927934	5.304556
H	2.975841	0.100876	4.764795
H	2.759546	3.205848	1.028187

H	0.936438	2.225257	-0.383490
C	-1.756898	-2.483555	1.491054
C	-2.613408	-2.490624	0.262062
C	-3.647664	-3.429591	0.037923
C	-2.313192	-1.479964	-0.682213
C	-4.372359	-3.328964	-1.157765
C	-3.060258	-1.414209	-1.863084
C	-4.085000	-2.334576	-2.098391
H	-5.173212	-4.039027	-1.352563
H	-2.838180	-0.643253	-2.596602
H	-4.666230	-2.283031	-3.017515
O	-1.834090	-3.322223	2.411571
H	-0.174091	-2.702381	3.816310
C	-4.000137	-4.520874	1.023712
H	-4.838158	-5.119343	0.651692
H	-3.148204	-5.180877	1.209753
H	-4.268244	-4.106379	1.999856
Co	-0.926999	-0.309510	-0.105636
C	3.997371	0.394966	-0.751303
O	3.271075	-0.593391	-0.209559
O	3.543960	1.192589	-1.553642
C	5.460820	0.355275	-0.303056
C	6.098736	1.730188	-0.549218
H	7.161705	1.699978	-0.289558
H	6.000495	2.026582	-1.596071
H	5.617275	2.498315	0.065160
C	5.587977	-0.034283	1.181713
H	5.131253	-1.006392	1.379414
H	6.647657	-0.089024	1.453128
H	5.110584	0.703743	1.832125
C	6.145215	-0.717435	-1.184982
H	7.205461	-0.792107	-0.921581
H	5.681535	-1.697377	-1.037665
H	6.072325	-0.457516	-2.246036
O	-4.900810	4.124867	1.459172
H	-5.306914	4.015629	2.330847
O	3.585247	2.091256	3.343457
H	3.991958	2.890531	2.978898

D'-ArBr

Energy = -2197.1810963 ZPE = -2196.553199 H = -2196.506945 G = -2196.63485

C	0.873254	-1.804852	-2.576050
C	0.776906	-2.090934	-3.941492
C	1.459113	-3.199914	-4.489738
C	2.240286	-4.043107	-3.723299
C	2.369094	-3.793848	-2.332416
C	1.686107	-2.677584	-1.770049
N	1.768732	-2.382654	-0.437572
C	2.496763	-3.142260	0.363858
C	3.206489	-4.268039	-0.107903
C	3.142498	-4.589666	-1.446621
N	0.285805	-0.783719	-1.861532
H	1.359481	-3.388615	-5.555589
H	2.756481	-4.890497	-4.164239
H	3.679062	-5.449746	-1.837954
H	3.789837	-4.861326	0.587871
H	2.516421	-2.846005	1.407697
C	-0.547036	0.173783	-2.366999
C	-0.963004	1.117625	-1.269107
C	-1.885614	2.179972	-1.474667
C	-0.374909	0.849563	-0.011501
C	-2.134576	2.977381	-0.352140
C	-0.667095	1.702776	1.059529
C	-1.542930	2.774461	0.893333
H	-2.472882	0.078730	0.399408
H	-0.227505	1.523716	2.035743
H	-1.780724	3.430549	1.723669
O	-0.900345	0.268298	-3.555759
H	0.171884	-1.450102	-4.566052
C	-2.578729	2.379433	-2.799134
H	-1.853560	2.536073	-3.599527
H	-3.131870	1.473040	-3.055924
H	-3.268468	3.221965	-2.765432
C	0.113777	-1.396016	2.673923
C	0.066964	-1.505402	4.067729
C	-0.962979	-2.241496	4.694295
C	-1.953352	-2.887140	3.979148
C	-1.946379	-2.808826	2.562879
C	-0.922192	-2.054561	1.922791
N	-0.871872	-1.924331	0.561576
C	-1.770374	-2.534129	-0.194461
C	-2.809233	-3.316007	0.355797
C	-2.901452	-3.442299	1.724092
N	1.034175	-0.734852	1.888993
H	-0.965525	-2.299736	5.779735
H	-2.732392	-3.454613	4.479177
H	-3.699707	-4.024532	2.176150
H	-3.528239	-3.787023	-0.305212
H	-1.681545	-2.374378	-1.262231
C	2.107142	-0.019075	2.340253
C	2.829205	0.603830	1.176231
C	4.017140	1.369651	1.327467
C	2.227875	0.371643	-0.080197
C	4.550572	1.880985	0.138934
C	2.821299	0.915245	-1.222331
C	3.987096	1.673204	-1.119435
H	2.376417	0.749984	-2.199223
H	4.453275	2.098273	-2.002167
O	2.440315	0.106716	3.533476
H	0.833524	-1.019299	4.653263
C	4.645810	1.603125	2.680554
H	5.561912	2.186821	2.599078
H	3.948721	2.121270	3.343300
H	4.868365	0.652187	3.170123
Co	0.684891	-0.737441	0.008349
C	-4.229645	-0.234971	-0.258123
O	-3.386483	0.057505	0.746975
O	-3.849947	-0.514730	-1.381501
C	-5.690968	-0.159239	0.183557
C	-6.594091	-0.557448	-0.991166
H	-7.644513	-0.498309	-0.689108
H	-6.440395	0.105653	-1.846883
H	-6.384527	-1.579927	-1.318606
C	-5.905948	-1.117012	1.375199
H	-5.266906	-0.846085	2.218937
H	-6.950759	-1.071656	1.699656
H	-5.678696	-2.150635	1.095025
C	-5.982527	1.295419	0.616879
H	-7.030503	1.386620	0.921008
H	-5.348744	1.588445	1.457399
H	-5.801093	1.996466	-0.204446
Br	6.228823	2.991299	0.142031
Br	-3.440001	4.502546	-0.429561

D'-ArCl

Energy = -3091.24566004 ZPE = -3090.616256 H = -3090.570718 G = -3090.695831

C	1.031751	-1.528877	-2.495909
C	0.938386	-1.883870	-3.845504
C	1.651851	-2.996747	-4.343486
C	2.463011	-3.777000	-3.542138
C	2.591274	-3.455911	-2.166025
C	1.876256	-2.335401	-1.653948
N	1.957615	-1.972479	-0.338355
C	2.714788	-2.667829	0.493709
C	3.456912	-3.792857	0.072715
C	3.394732	-4.182468	-1.247920
N	0.413732	-0.494967	-1.827965
H	1.552803	-3.240313	-5.398244
H	3.003322	-4.628442	-3.944800
H	3.955686	-5.043783	-1.600446
H	4.063221	-4.332223	0.792376
H	2.731906	-2.319140	1.521239
C	-0.431924	0.425301	-2.379726
C	-0.879336	1.402733	-1.326148
C	-1.825476	2.430198	-1.580472
C	-0.292823	1.203568	-0.054328
C	-2.113903	3.274565	-0.497440
C	-0.620122	2.090978	0.978227
C	-1.522540	3.129448	0.759388
H	-2.375478	0.404470	0.322964
H	-0.183207	1.963095	1.963576
H	-1.788464	3.814600	1.558201
O	-0.771393	0.467448	-3.575703
H	0.311430	-1.292412	-4.496592
C	-2.516750	2.562913	-2.915308
H	-1.791771	2.711858	-3.717603
H	-3.041607	1.632404	-3.144828
H	-3.231402	3.385719	-2.916824
C	0.302159	-0.902787	2.735685
C	0.278959	-0.957242	4.133523
C	-0.711081	-1.708277	4.804835
C	-1.684320	-2.421640	4.131601
C	-1.700321	-2.400503	2.713346
C	-0.716340	-1.632915	2.027469
N	-0.688609	-1.557958	0.661385
C	-1.572271	-2.232815	-0.055455
C	-2.573096	-3.030054	0.541998
C	-2.641098	-3.104894	1.915598
N	1.184549	-0.239412	1.911078
H	-0.696075	-1.722735	5.891675
H	-2.432850	-2.998909	4.665907
H	-3.409111	-3.699257	2.402998
H	-3.282358	-3.554517	-0.088704
H	-1.505953	-2.111800	-1.129841
C	2.235765	0.534556	2.316256
C	2.924063	1.127510	1.118288
C	4.080530	1.943877	1.220526
C	2.323199	0.812225	-0.120631
C	4.596467	2.424670	0.007200
C	2.889778	1.322727	-1.291661
C	4.025039	2.128230	-1.232659
H	2.445438	1.093932	-2.255839
H	4.471998	2.529841	-2.137009
O	2.576242	0.726424	3.498961
H	1.033587	-0.417720	4.686911
C	4.714472	2.271205	2.552311
H	5.604117	2.888969	2.431836
H	4.003239	2.790860	3.198893
H	4.983705	1.356489	3.085811
Co	0.820288	-0.344984	0.035580
C	-4.088837	-0.058828	-0.360924
O	-3.298826	0.358449	0.642671
O	-3.655884	-0.402978	-1.446685
C	-5.567365	-0.029410	0.026343
C	-6.401959	-0.603846	-1.125972
H	-7.464677	-0.575974	-0.865242
H	-6.253216	-0.027646	-2.043180
H	-6.123244	-1.641174	-1.333380
C	-5.772268	-0.865385	1.307688
H	-5.186399	-0.464271	2.138098
H	-6.830343	-0.853382	1.589374
H	-5.471037	-1.906277	1.151046
C	-5.957242	1.443080	0.289239
H	-7.016916	1.501661	0.558614
H	-5.365740	1.865736	1.105107
H	-5.796721	2.057928	-0.602675
Cl	6.048456	3.466307	-0.029528
Cl	-3.303496	4.595845	-0.653342

D'-ArMe

Energy = -2250.69527672 ZPE = -2249.990897 H = -2249.944913 G = -2250.0696

C	1.181659	-1.907838	-2.084059
C	1.129071	-2.596232	-3.301877
C	1.878539	-3.778337	-3.489340
C	2.688183	-4.309357	-2.503107
C	2.775483	-3.648342	-1.250684
C	2.023408	-2.454812	-1.050323
N	2.063534	-1.771298	0.132454
C	2.814405	-2.214381	1.127035
C	3.592020	-3.387843	1.016862
C	3.572043	-4.098073	-0.164378
N	0.527643	-0.757067	-1.711503
H	1.809948	-4.282824	-4.449996
H	3.256973	-5.219544	-2.668038
H	4.160854	-5.004329	-0.278470
H	4.191930	-3.712491	1.860331
H	2.797136	-1.618189	2.033883
C	-0.334957	-0.033522	-2.489421
C	-0.829476	1.165270	-1.731122
C	-1.793112	2.070297	-2.241492
C	-0.260428	1.317878	-0.442231
C	-2.156063	3.181136	-1.448715
C	-0.630940	2.435520	0.312429
C	-1.555235	3.350532	-0.192525
H	-2.337851	0.606988	0.019246
H	-0.209997	2.583377	1.302987
H	-1.840545	4.210907	0.410989
O	-0.652287	-0.315520	-3.660309
H	0.504799	-2.205851	-4.092244
C	-2.463598	1.825773	-3.575547
H	-1.733474	1.785130	-4.387172
H	-2.957160	0.850212	-3.565623
H	-3.206329	2.590168	-3.808047
C	0.316114	0.004515	2.803371
C	0.260376	0.303895	4.170309
C	-0.724789	-0.283486	4.993636
C	-1.663332	-1.174687	4.508470
C	-1.647190	-1.512457	3.130877
C	-0.669265	-0.911346	2.287507
N	-0.614325	-1.180339	0.947829
C	-1.465200	-2.039025	0.410826
C	-2.454634	-2.694860	1.175445
C	-2.548842	-2.426560	2.523204

N	1.201164	0.460708	1.853880
H	-0.734720	-0.022212	6.048963
H	-2.407826	-1.622150	5.160153
H	-3.309064	-2.905782	3.134130
H	-3.134805	-3.384164	0.687292
H	-1.379495	-2.187353	-0.658993
C	2.225563	1.344698	2.065173
C	2.933856	1.629368	0.773579
C	4.072776	2.465608	0.673486
C	2.368830	0.992892	-0.356714
C	4.651894	2.662689	-0.599897
C	2.962315	1.203400	-1.602054
C	4.084134	2.025933	-1.713871
H	2.547815	0.726803	-2.486536
H	4.537532	2.183491	-2.691829
O	2.525813	1.841577	3.168967
H	0.987295	0.989355	4.580704
C	4.666285	3.135864	1.895496
H	5.559810	3.712883	1.653114
H	3.939662	3.802652	2.368403
H	4.923780	2.399168	2.661213
Co	0.884115	-0.125240	0.059546
C	-4.050345	-0.099826	-0.427626
O	-3.247066	0.603937	0.384513
O	-3.646056	-0.705214	-1.405077
C	-5.513159	-0.026786	0.014780
C	-6.363252	-0.921244	-0.897243
H	-7.414140	-0.869028	-0.595146
H	-6.284947	-0.605465	-1.941113
H	-6.037014	-1.963774	-0.838188
C	-5.626260	-0.495643	1.481040
H	-5.016553	0.124388	2.142343
H	-6.669602	-0.434291	1.807681
H	-5.294152	-1.532986	1.588536
C	-5.967822	1.445740	-0.103622
H	-7.016706	1.534970	0.198225
H	-5.364258	2.095099	0.535362
H	-5.879275	1.801844	-1.135908
C	5.870495	3.541315	-0.802827
H	5.693785	4.576196	-0.485908
H	6.740306	3.182103	-0.239445
H	6.154513	3.567391	-1.858933
C	-3.199589	4.182120	-1.900514
H	-2.943112	4.648771	-2.858554
H	-4.184742	3.715983	-2.026639
H	-3.310595	4.983053	-1.163899

D'-ArNH2

Energy = -2282.77292751 ZPE = -2282.090227 H = -2282.044746 G = -2282.168144

C	-1.238761	1.872555	-2.099493
C	-1.220276	2.545596	-3.326925
C	-1.989094	3.715083	-3.515445
C	-2.786024	4.248598	-2.520612
C	-2.839678	3.603247	-1.258243
C	-2.067982	2.422281	-1.056737
N	-2.077209	1.754846	0.135607
C	-2.814327	2.202342	1.138345
C	-3.609062	3.364244	1.027906
C	-3.621029	4.058072	-0.163039
N	-0.559877	0.735431	-1.724165
H	-1.946013	4.207124	-4.484002
H	-3.370109	5.148983	-2.686080
H	-4.223393	4.955238	-0.278308
H	-4.196536	3.692989	1.878536
H	-2.772341	1.619014	2.052735
C	0.290324	0.012436	-2.513206
C	0.826961	-1.169999	-1.749165
C	1.795456	-2.070545	-2.253177
C	0.280425	-1.309853	-0.447052
C	2.174254	-3.164751	-1.441598
C	0.668869	-2.415795	0.315767
C	1.590636	-3.338708	-0.178048
H	2.313576	-0.577115	0.039611
H	0.256551	-2.553752	1.311300
H	1.890831	-4.191361	0.429782
O	0.559410	0.286563	-3.700045
H	-0.607122	2.153416	-4.124757
C	2.503811	-1.906391	-3.578330
H	2.285857	-2.744853	-4.256536
H	2.202335	-0.988358	-4.073620
H	3.590411	-1.900521	-3.423313
C	-0.266276	0.032522	2.794254
C	-0.181889	-0.251245	4.163173
C	0.809123	0.357996	4.963394
C	1.726147	1.257181	4.453157
C	1.680644	1.580649	3.072856
C	0.697029	0.957183	2.252480
N	0.616620	1.211962	0.911523
C	1.445498	2.077529	0.352135
C	2.438281	2.755149	1.092992
C	2.559250	2.500968	2.441200
N	-1.160155	-0.448849	1.863599
H	0.840999	0.107166	6.020830
H	2.475706	1.721628	5.086976
H	3.323372	2.995730	3.034616
H	3.100401	3.448880	0.586647
H	1.339100	2.214402	-0.717358
C	-2.174640	-1.333483	2.107383
C	-2.901282	-1.653450	0.828372
C	-4.025550	-2.510570	0.740964
C	-2.358436	-1.018762	-0.315871
C	-4.620236	-2.704668	-0.527067
C	-2.966299	-1.242934	-1.551698
C	-4.086472	-2.068409	-1.657300
H	-2.567803	-0.764598	-2.442548
H	-4.558383	-2.229787	-2.626178
O	-2.449257	-1.797597	3.233995
H	-0.891056	-0.942204	4.594307
C	-4.637128	-3.240389	1.917137
H	-4.744988	-4.309032	1.690668
H	-4.034827	-3.116645	2.812653
H	-5.648787	-2.865097	2.134643
Co	-0.879013	0.121864	0.059642
C	4.031997	0.107641	-0.432965
O	3.227317	-0.573763	0.396197
O	3.628005	0.705794	-1.414666
C	5.496886	0.026091	0.002258
C	6.359864	0.843523	-0.968067
H	7.410991	0.790210	-0.666800
H	6.271442	0.462265	-1.989210
H	6.053966	1.893692	-0.975807
C	5.626746	0.585736	1.435297
H	5.003314	0.024865	2.135696
H	6.669204	0.519266	1.764030
H	5.320882	1.635877	1.476154
C	5.922346	-1.459244	-0.022173
H	6.975961	-1.546953	0.263475

H	5.321576	-2.049613	0.673878
H	5.802377	-1.888634	-1.022565
N	3.203242	-4.035431	-1.863864
N	-5.711859	-3.595200	-0.671659
H	-6.363093	-3.569075	0.104454
H	-6.221568	-3.441654	-1.534221
H	3.205533	-4.220136	-2.859911
H	3.205230	-4.913530	-1.358395

D'-ArOH

Energy = -2322.49893882 ZPE = -2321.842056 H = -2321.796571 G = -2321.919784

C	-1.272730	2.348324	-1.547955
C	-1.238109	3.328212	-2.547164
C	-2.058680	4.473801	-2.454878
C	-2.922638	4.686152	-1.397254
C	-2.993993	3.722016	-0.358683
C	-2.169698	2.562773	-0.440780
N	-2.189855	1.597877	0.526858
C	-2.991009	1.725285	1.571392
C	-3.841777	2.840475	1.734404
C	-3.841886	3.830710	0.775459
N	-0.554484	1.179196	-1.457438
H	-2.002443	5.211294	-3.251756
H	-3.545748	5.574005	-1.346158
H	-4.486157	4.700327	0.873999
H	-4.480727	2.901859	2.608887
H	-2.955215	0.917131	2.295318
C	0.376971	0.734763	-2.355911
C	0.933563	-0.585160	-1.906920
C	1.976321	-1.250471	-2.592137
C	0.349388	-1.100398	-0.723897
C	2.399342	-2.484903	-2.068920
C	0.783398	-2.349511	-0.267095
C	1.794292	-3.040947	-0.937474
H	2.292115	-0.394265	0.168692
H	0.349821	-2.778518	0.631770
H	2.143474	-4.003973	-0.566925
O	0.708304	1.325474	-3.400850
H	-0.572502	3.190931	-3.386928
C	2.683139	-0.663103	-3.791115
H	1.981461	-0.443777	-4.598552
H	3.142248	0.290251	-3.514619
H	3.457749	-1.338556	-4.156916
C	-0.356256	-0.709071	2.717119
C	-0.289963	-1.358453	3.956019
C	0.660986	-0.963735	4.922156
C	1.555145	0.067995	4.706506
C	1.525874	0.759754	3.468500
C	0.578944	0.361307	2.481925
N	0.511477	0.977814	1.262445
C	1.320191	1.988284	0.986590
C	2.280960	2.455617	1.909852
C	2.388054	1.839075	3.136729
N	-1.207665	-0.945328	1.662321
H	0.681287	-1.495845	5.870058
H	2.275618	0.359163	5.464999
H	3.127531	2.168034	3.861934
H	2.930351	3.278496	1.632121
H	1.225096	2.415430	-0.004531
C	-2.175640	-1.911978	1.609506
C	-2.844488	-1.895549	0.266952
C	-3.923797	-2.748398	-0.063994
C	-2.306012	-0.963090	-0.649989
C	-4.453567	-2.636507	-1.362164
C	-2.866092	-0.889612	-1.926244
C	-3.932543	-1.719032	-2.281328
H	-2.470705	-0.184070	-2.651974
H	-4.368607	-1.660395	-3.278280
O	-2.461483	-2.696183	2.535640
H	-0.980884	-2.164159	4.156899
C	-4.518026	-3.748756	0.902627
H	-5.352699	-4.282723	0.446353
H	-3.766316	-4.472402	1.229329
H	-4.865564	-3.254082	1.813844
Co	-0.903544	0.097571	0.084706
C	4.008614	0.296551	-0.287347
O	3.223710	-0.506296	0.448577
O	3.573301	1.159230	-1.029348
C	5.491393	-0.006618	-0.071011
C	6.327791	0.876993	-1.005857
H	7.393276	0.682112	-0.847249
H	6.090187	0.672963	-2.053931
H	6.136101	1.937322	-0.819932
C	5.836994	0.294882	1.404217
H	5.238983	-0.320697	2.081119
H	6.896153	0.084798	1.586416
H	5.651618	1.347366	1.644434
C	5.740133	-1.500620	-0.377171
H	6.810004	-1.719960	-0.294422
H	5.199449	-2.137823	0.326678
H	5.408097	-1.763134	-1.387077
O	-5.508873	-3.461030	-1.705608
O	3.451558	-3.125197	-2.695937
H	-5.759707	-3.272801	-2.619293
H	3.676364	-3.915945	-2.188439

D1

Energy = -2172.50366193 ZPE = -2171.84002 H = -2171.797245 G = -2171.913785

C	-2.227658	-1.529734	0.134567
C	-2.275202	-2.164005	1.354814
C	-3.491127	-2.255642	2.071468
C	-4.649806	-1.695067	1.581112
C	-4.631319	-1.018028	0.335357
C	-3.410848	-0.945468	-0.405457
N	-3.326791	-0.318119	-1.612835
C	-4.411766	0.253435	-2.103962
C	-5.665156	0.246087	-1.446404
C	-5.770920	-0.390922	-0.230989
N	-1.014492	-1.383457	-0.628297
H	-3.495739	-2.765598	3.029433
H	-5.579803	-1.754285	2.138507
H	-6.714605	-0.419587	0.306365
H	-6.516287	0.737981	-1.904166
H	-4.304243	0.753382	-3.064370
C	-0.437401	-2.606060	-1.223487
C	0.864092	-2.310377	-1.838871
C	1.418528	-3.145251	-2.841929
C	1.546071	-1.177596	-1.333273
C	2.673273	-2.796105	-3.344396
C	2.813172	-0.882809	-1.846626
C	3.361242	-1.681524	-2.851624
H	3.121069	-3.404133	-4.125587
H	3.374599	-0.034533	-1.471970
H	4.340775	-1.438591	-3.256605
O	-1.013025	-3.672933	-1.144883
H	-1.372055	-2.571928	1.785107

C	0.704405	-4.366905	-3.366767
H	0.637180	-5.141319	-2.596760
H	-0.324714	-4.138034	-3.659975
H	1.231784	-4.778535	-4.231252
C	2.328828	2.045945	-0.317120
C	3.438248	2.888975	-0.307415
C	3.525016	3.972508	-1.211090
C	2.522073	4.251484	-2.113845
C	1.374226	3.419328	-2.155602
C	1.290486	2.305463	-1.269730
N	0.220103	1.448397	-1.280907
C	-0.784817	1.692962	-2.110953
C	-0.795355	2.784084	-3.005785
C	0.284326	3.636369	-3.035875
N	2.065016	0.964421	0.529826
H	4.407914	4.604208	-1.174435
H	2.591023	5.096605	-2.791681
H	0.314508	4.478371	-3.721647
H	-1.650815	2.926491	-3.656606
H	-1.628925	1.012806	-2.076261
C	2.959820	0.478588	1.473415
C	2.522916	-0.852764	1.973878
C	3.202088	-1.535847	3.011155
C	1.434027	-1.429508	1.280663
C	2.784672	-2.837257	3.314311
C	1.097408	-2.755191	1.575454
C	1.760021	-3.448768	2.591625
H	3.284311	-3.383311	4.110305
H	0.336098	-3.279762	1.011619
H	1.477901	-4.474471	2.817133
O	3.984390	1.068534	1.837721
H	4.224612	2.710998	0.410055
C	4.347742	-0.929928	3.787642
H	5.211023	-0.747146	3.141718
H	4.077802	0.043081	4.206874
H	4.650535	-1.594892	4.602004
Co	0.625322	-0.210879	0.021318
H	-1.269158	-0.799940	-1.433095
C	-2.199359	2.532016	2.090196
C	-3.074698	1.580637	2.928660
H	-2.630785	1.404005	3.913955
H	-4.062642	2.027726	3.075555
H	-3.196785	0.618732	2.428087
C	-2.858557	2.759311	0.705709
H	-3.835873	3.231901	0.842405
H	-2.246297	3.412043	0.074999
H	-2.999768	1.810052	0.183729
C	-1.998948	3.871533	2.813156
H	-1.500056	3.730790	3.776595
H	-1.397515	4.561206	2.215664
H	-2.973575	4.334219	2.996516
C	-0.876096	1.837928	1.796051
O	-0.836733	0.665603	1.414803
O	0.214561	2.577924	1.909518
H	0.972541	2.022087	1.582221

D1-q

Energy = -2172.4437743 ZPE = -2171.784609 H = -2171.740082 G = -2171.862562

C	-3.262871	-0.330765	-1.111901
C	-4.448032	-0.682910	-0.484017
C	-5.456260	0.284317	-0.265435
C	-5.299300	1.592486	-0.664813
C	-4.099831	1.987250	-1.312542
C	-3.068040	1.025731	-1.545324
N	-1.889670	1.348999	-2.151419
C	-1.700292	2.603282	-2.521249
C	-2.655813	3.630913	-2.337672
C	-3.854591	3.317852	-1.739645
N	-2.210466	-1.209410	-1.370261
H	-6.370462	-0.024428	0.232515
H	-6.075615	2.331262	-0.489769
H	-4.616415	4.075618	-1.579141
H	-2.432511	4.639658	-2.667711
H	-0.747055	2.835328	-2.991204
C	-1.969556	-2.450804	-0.828684
C	-0.633355	-3.026891	-1.193186
C	-0.562379	-4.389132	-1.571215
C	0.513911	-2.206796	-1.097305
C	0.694089	-4.917875	-1.887510
C	1.753999	-2.802283	-1.407903
C	1.848354	-4.135041	-1.807039
H	0.767163	-5.956394	-2.200936
H	2.668787	-2.214263	-1.329008
H	2.814442	-4.570466	-2.051696
O	-2.782254	-3.037232	-0.107370
H	-4.585629	-1.702818	-0.156240
C	-1.783295	-5.278198	-1.658517
H	-2.163382	-5.520233	-0.662083
H	-2.605658	-4.789761	-2.190306
H	-1.544430	-6.211334	-2.176483
C	3.467714	0.746221	-0.028503
C	4.767466	1.057217	0.361641
C	5.659371	1.714903	-0.518073
C	5.288899	2.074197	-1.794351
C	3.976995	1.776306	-2.243804
C	3.067995	1.119938	-1.360569
N	1.798280	0.810482	-1.766224
C	1.399431	1.101552	-2.997552
C	2.231918	1.753697	-3.927216
C	3.513554	2.090914	-3.545798
N	2.467077	0.131812	0.748537
H	6.662178	1.936457	-0.164704
H	5.980246	2.575229	-2.464736
H	4.184569	2.592963	-4.237022
H	1.857575	1.976056	-4.919945
H	0.384580	0.807000	-3.245267
C	2.733746	-0.473621	1.955709
C	1.485209	-1.040674	2.598250
C	1.064357	-0.632383	3.890271
C	0.682145	-1.938860	1.927212
C	-0.139953	-1.154509	4.382307
C	-0.500254	-2.485060	2.379736
C	-0.916820	-2.060027	3.649256
H	-0.481689	-0.839145	5.364395
H	-1.095109	-3.168088	1.781618
H	-1.847836	-2.434839	4.066663
O	3.823157	-0.552839	2.531407
H	5.092917	0.783962	1.354144
C	1.857382	0.377165	4.684739
H	2.889687	0.046008	4.817289
H	1.890673	1.336224	4.155354
H	1.404709	0.546506	5.664945
Co	0.774634	-0.342882	-0.376599
H	-1.470645	-0.801821	-1.929592
C	-1.608697	2.223372	2.327696
C	-2.834808	1.297661	2.322650
H	-2.606830	0.348150	2.816165

H	-3.655484	1.780791	2.861121
H	-3.166160	1.081608	1.307721
C	-1.924408	3.537455	1.570452
H	-2.758720	4.044567	2.064853
H	-1.061816	4.210430	1.571357
H	-2.211433	3.335953	0.535339
C	-1.176548	2.533687	3.773512
H	-0.919215	1.614574	4.307745
H	-0.312955	3.201512	3.801331
H	-2.005373	3.016677	4.299780
C	-0.473321	1.560586	1.564167
O	-0.670141	0.678916	0.714972
O	0.731781	2.027272	1.836563
H	1.416185	1.467509	1.366021

D1-t

Energy = -2172.49200828 ZPE = -2171.830721 H = -2171.787125 G = -2171.906135

C	-3.118557	-0.904024	-0.834862
C	-3.963009	-1.763943	-0.150431
C	-5.173258	-1.281379	0.402875
C	-5.551353	0.036564	0.278155
C	-4.712622	0.942224	-0.423123
C	-3.486130	0.476451	-0.985611
N	-2.632995	1.293667	-1.662430
C	-2.954994	2.567548	-1.795722
C	-4.147498	3.130382	-1.281668
C	-5.023056	2.315350	-0.600466
N	-1.886232	-1.255935	-1.390049
H	-5.810183	-1.979130	0.937928
H	-6.481193	0.397505	0.707178
H	-5.947891	2.707944	-0.187231
H	-4.352581	4.185321	-1.427491
H	-2.245421	3.195215	-2.331546
C	-1.300983	-2.498022	-1.485052
C	0.117827	-2.472508	-1.969026
C	0.523977	-3.403422	-2.956317
C	1.037882	-1.581982	-1.387131
C	1.865579	-3.410856	-3.347786
C	2.383790	-1.644202	-1.780191
C	2.792397	-2.544482	-2.762697
H	2.189656	-4.108647	-4.115221
H	3.119340	-0.988159	-1.320825
H	3.834355	-2.576582	-3.070732
O	-1.880777	-3.536575	-1.165654
H	-3.691832	-2.804663	-0.050592
C	-0.449263	-4.368885	-3.594458
H	-0.766728	-5.132120	-2.879008
H	-1.359165	-3.862409	-3.932242
H	0.007369	-4.863803	-4.455619
C	3.051093	1.612070	0.130599
C	4.267996	2.186202	0.477372
C	4.801979	3.258086	-0.276099
C	4.141524	3.774144	-1.369847
C	2.899453	3.212570	-1.765708
C	2.358838	2.127226	-1.015423
N	1.173444	1.530422	-1.372969
C	0.508540	1.980730	-2.429446
C	0.966046	3.058012	-3.214339
C	2.157228	3.667741	-2.884087
N	2.381771	0.582529	0.805762
H	5.754342	3.682300	0.027941
H	4.554864	4.600756	-1.939322
H	2.540894	4.496002	-3.473040
H	0.378316	3.384102	-4.064907
H	-0.427975	1.482124	-2.653677
C	3.034163	-0.419433	1.518159
C	2.046289	-1.471312	1.913216
C	2.248983	-2.342478	3.008670
C	0.842629	-1.497677	1.182985
C	1.197704	-3.197426	3.362218
C	-0.193376	-2.346762	1.563740
C	-0.011747	-3.191032	2.662777
H	1.324623	-3.867538	4.208490
H	-1.135050	-2.355230	1.029299
H	-0.816421	-3.853447	2.972170
O	4.237538	-0.439242	1.789792
H	4.804045	1.798292	1.332058
C	3.529525	-2.356426	3.809842
H	4.374847	-2.682565	3.197530
H	3.787403	-1.355735	4.168772
H	3.436995	-3.027226	4.668562
Co	0.757261	-0.084319	-0.161225
H	-1.421949	-0.475975	-1.840804
C	-1.865383	1.603548	2.934880
C	-2.774153	0.354852	2.948893
H	-2.261996	-0.497895	3.406879
H	-3.676497	0.567916	3.529694
H	-3.067489	0.073170	1.936749
C	-2.587638	2.770636	2.223748
H	-3.515758	3.002427	2.755285
H	-1.965894	3.672099	2.212963
H	-2.835204	2.504874	1.195078
C	-1.475374	2.004143	4.364806
H	-0.950289	1.191655	4.875235
H	-0.827685	2.884666	4.370287
H	-2.380431	2.238659	4.933457
C	-0.645949	1.261918	2.090526
O	-0.781897	0.781470	0.953960
O	0.530418	1.506314	2.622714
H	1.255790	1.227318	1.977252

D-t'

Energy = -2172.0086182 ZPE = -2171.362189 H = -2171.318305 G = -2171.44123

C	0.615059	-2.554893	-1.319493
C	0.710846	-3.855042	-1.827161
C	-0.157902	-4.304889	-2.846594
C	-1.131627	-3.494039	-3.393337
C	-1.275370	-2.165903	-2.913220
C	-0.416472	-1.703617	-1.872108
N	-0.537137	-0.439785	-1.361221
C	-1.439205	0.391470	-1.856751
C	-2.315229	0.024351	-2.900367
C	-2.236026	-1.250706	-3.417261
N	1.390626	-1.955092	-0.353962
H	-0.043764	-5.323094	-3.210141
H	-1.786855	-3.849725	-4.182944
H	-2.903732	-1.570501	-4.213049
H	-3.043096	0.740438	-3.265894
H	-1.488312	1.367226	-1.387972
C	2.346347	-2.565823	0.404632
C	2.941189	-1.588185	1.387678
C	4.071467	-1.891361	2.187534
C	2.334901	-0.315034	1.470405
C	4.562247	-0.894896	3.042705
C	2.846030	0.656596	2.331359
C	3.964865	0.367180	3.114475

H	5.431005	-1.112029	3.659926
H	2.361142	1.627436	2.389003
H	4.370660	1.118063	3.789373
O	2.704644	-3.757479	0.324462
H	1.470052	-4.509316	-1.422733
C	4.775041	-3.229615	2.148675
H	4.104372	-4.041388	2.442608
H	5.108253	-3.476109	1.136681
H	5.642493	-3.225306	2.816526
C	0.903256	2.903839	-0.589526
C	0.623815	4.262937	-0.783171
C	1.300853	5.010899	-1.771141
C	2.265628	4.453659	-2.587312
C	2.595738	3.082219	-2.429854
C	1.918562	2.312979	-1.435779
N	2.211126	0.993884	-1.239643
C	3.131374	0.400354	-1.981983
C	3.844073	1.080810	-2.992329
C	3.575006	2.415010	-3.210877
N	0.336431	2.029569	0.298999
H	1.046324	6.061683	-1.887611
H	2.776022	5.042331	-3.343890
H	4.106592	2.970509	-3.979193
H	4.588075	0.550080	-3.576724
H	3.302465	-0.650760	-1.767974
C	-0.494375	2.362221	1.318478
C	-0.852141	1.139114	2.133730
C	-1.835273	1.159111	3.156048
C	-0.172534	-0.061965	1.821841
C	-2.088202	-0.030658	3.853520
C	-0.446928	-1.228092	2.545086
C	-1.403940	-1.213002	3.560886
H	-2.846302	-0.030229	4.633202
H	0.088282	-2.143062	2.304478
H	-1.625682	-2.118785	4.121024
O	-0.913314	3.504192	1.599844
H	-0.124272	4.727239	-0.156245
C	-2.658808	2.382552	3.485654
H	-2.033843	3.212998	3.821661
H	-3.182300	2.738039	2.594195
H	-3.394718	2.148944	4.262032
Co	0.914419	-0.032810	0.180933
C	-5.300482	-0.417766	-0.027884
C	-6.163232	0.641289	-0.727669
H	-5.732699	0.919431	-1.694659
H	-7.170203	0.247564	-0.898486
H	-6.239828	1.547888	-0.122192
C	-5.913513	-0.788817	1.342850
H	-6.914251	-1.209092	1.198473
H	-5.296459	-1.528858	1.859653
H	-6.003183	0.093942	1.984806
C	-5.181434	-1.678884	-0.907405
H	-4.712040	-1.445001	-1.867727
H	-4.582601	-2.449179	-0.416283
H	-6.179406	-2.085539	-1.102138
C	-3.913666	0.166873	0.246085
O	-3.623905	1.346617	0.145656
O	-3.039597	-0.768997	0.648404
H	-2.191054	-0.336325	0.878362

E

Energy = -2172.47093528 ZPE = -2171.809393 H = -2171.765977 G = -2171.885026

C	-2.183652	-1.472233	-0.238140
C	-2.416519	-2.272675	0.855663
C	-3.711618	-2.354657	1.419573
C	-4.763851	-1.637306	0.893469
C	-4.555720	-0.806913	-0.238014
C	-3.251805	-0.728150	-0.816782
N	-2.978145	0.044741	-1.905742
C	-3.957281	0.757053	-2.433500
C	-5.280631	0.759202	-1.930037
C	-5.576268	-0.024514	-0.837718
N	-0.879099	-1.311353	-0.823237
H	-3.866372	-2.991123	2.285200
H	-5.755217	-1.695134	1.332926
H	-6.580014	-0.051068	-0.422990
H	-6.036944	1.371920	-2.408216
H	-3.702905	1.367856	-3.297251
C	-0.270570	-2.538091	-1.436172
C	1.172650	-2.404535	-1.528898
C	1.837676	-2.802340	-2.720139
C	1.873040	-1.720133	-0.445263
C	3.171435	-2.453677	-2.893077
C	3.256636	-1.406766	-0.698927
C	3.862266	-1.743146	-1.885887
H	3.682686	-2.723193	-3.812246
H	3.843485	-0.927660	0.075906
H	4.906499	-1.482570	-2.040484
O	-0.996925	-3.425950	-1.856983
H	-1.598248	-2.827723	1.295107
C	1.109786	-3.532224	-3.825576
H	0.750556	-4.507644	-3.486779
H	0.223790	-2.980159	-4.156752
H	1.767560	-3.677126	-4.686413
C	2.538617	1.804747	0.219366
C	3.676594	2.545275	0.509709
C	4.087768	3.576250	-0.367680
C	3.375199	3.885970	-1.507821
C	2.209891	3.143311	-1.835906
C	1.809317	2.085904	-0.973710
N	0.717977	1.286419	-1.236353
C	-0.013033	1.562677	-2.312573
C	0.297557	2.609552	-3.206344
C	1.409390	3.389465	-2.980376
N	1.956333	0.785970	0.970636
H	4.981515	4.142320	-0.122115
H	3.690671	4.691338	-2.163876
H	1.679735	4.191722	-3.660811
H	-0.346524	2.776207	-4.062536
H	-0.897444	0.957394	-2.477583
C	2.594245	0.038549	1.908243
C	1.826707	-1.246787	2.125990
C	1.488831	-1.640258	3.439693
C	1.484533	-2.056310	0.997672
C	0.849599	-2.866004	3.631221
C	0.878230	-3.309094	1.256281
C	0.570226	-3.706479	2.549726
H	0.586353	-3.177142	4.638292
H	0.686630	-3.983715	0.430179
H	0.117192	-4.678516	2.721151
O	3.652528	0.292161	2.493933
H	4.232494	2.326141	1.411202
C	1.790743	-0.743967	4.618479
H	2.868041	-0.608903	4.740512
H	1.361814	0.253878	4.473136
H	1.377143	-1.161102	5.539726
Co	0.551129	-0.189135	0.110459

H	-1.050545	-0.714610	-1.640601
C	-2.293487	2.901156	1.514807
C	-3.587114	2.152141	1.874796
H	-3.599909	1.879518	2.935244
H	-4.452029	2.792814	1.677006
H	-3.685992	1.239454	1.286468
C	-2.306566	3.285610	0.012654
H	-3.145740	3.960598	-0.183633
H	-1.380291	3.794558	-0.272770
H	-2.419999	2.397875	-0.614496
C	-2.137191	4.161383	2.381254
H	-2.079542	3.906046	3.444141
H	-1.237355	4.721161	2.115838
H	-3.004374	4.812987	2.234453
C	-1.107676	1.954942	1.665523
O	-1.169996	0.755327	1.402905
O	0.036851	2.542897	2.011265
H	0.755944	1.872751	1.875122

E'

Energy = -2172.01981138 ZPE = -2171.371483 H = -2171.328239 G = -2171.446588

C	0.773777	2.266854	-0.684862
C	1.409249	3.505897	-0.715950
C	2.588817	3.672537	-1.477504
C	3.150866	2.633057	-2.196700
C	2.559226	1.342544	-2.153071
C	1.380558	1.174462	-1.379467
N	0.754261	-0.049776	-1.227067
C	1.311606	-1.118797	-1.814951
C	2.459918	-1.026864	-2.623149
C	3.080700	0.193492	-2.807919
N	-0.416241	1.905319	-0.057322
H	3.057255	4.653183	-1.503481
H	4.050175	2.784068	-2.786701
H	3.970015	0.283206	-3.424250
H	2.855233	-1.929216	-3.077841
H	0.808409	-2.062086	-1.636286
C	-0.775122	2.392716	1.154626
C	-1.889143	1.576082	1.792368
C	-3.137845	2.190141	1.998144
C	-1.710066	0.197352	2.083678
C	-4.215114	1.414524	2.447555
C	-2.810361	-0.546044	2.543563
C	-4.057372	0.052814	2.704056
H	-5.185235	1.883936	2.590247
H	-2.678293	-1.600418	2.765307
H	-4.901221	-0.537580	3.050753
O	-0.289937	3.377079	1.746136
H	0.985649	4.330974	-0.158913
C	-3.335099	3.661750	1.708288
H	-2.642669	4.270240	2.295181
H	-3.134685	3.891468	0.655843
H	-4.359957	3.971831	1.929742
C	-2.889263	-1.942994	-0.934067
C	-3.577899	-3.142130	-1.099722
C	-4.874227	-3.140557	-1.665492
C	-5.501868	-1.972932	-2.056627
C	-4.844277	-0.725738	-1.880888
C	-3.539614	-0.728677	-1.316778
N	-2.832909	0.430067	-1.072323
C	-3.402266	1.596885	-1.391014
C	-4.681550	1.684863	-1.971272
C	-5.407062	0.535227	-2.217109
N	-1.621929	-1.726635	-0.393396
H	-5.385422	-4.091023	-1.796222
H	-6.496381	-1.991670	-2.493480
H	-6.399735	0.580571	-2.656032
H	-5.086022	2.663861	-2.207860
H	-2.811226	2.477203	-1.167909
C	-1.199865	-2.436207	0.680292
C	-0.112265	-1.732047	1.474418
C	1.148782	-2.339091	1.602681
C	-0.360905	-0.463374	2.070051
C	2.154336	-1.681504	2.330966
C	0.669940	0.162543	2.788766
C	1.920230	-0.439127	2.915769
H	3.133750	-2.145055	2.410434
H	0.482135	1.130478	3.242061
H	2.711841	0.061650	3.465812
O	-1.636906	-3.533467	1.079723
H	-3.113464	-4.065837	-0.782874
C	1.494477	-3.655511	0.940626
H	1.630151	-4.443497	1.691224
H	0.718609	-3.992586	0.253040
H	2.438464	-3.551631	0.396595
Co	-1.019973	0.121329	-0.555341
C	6.155886	-0.313753	0.071376
C	7.188666	-1.400231	-0.256668
H	6.993101	-1.844537	-1.236733
H	8.192953	-0.965129	-0.267604
H	7.165208	-2.202554	0.485944
C	6.434019	0.286001	1.468149
H	7.435947	0.727106	1.485208
H	5.707093	1.063987	1.713770
H	6.389474	-0.485358	2.244538
C	6.196644	0.802767	-0.993693
H	6.013443	0.396207	-1.993145
H	5.443610	1.569322	-0.797984
H	7.185931	1.272285	-0.993660
C	4.758995	-0.937032	0.090982
O	4.512718	-2.116242	-0.093854
O	3.806980	-0.028110	0.363540
H	2.946976	-0.485570	0.409168

E-q

Energy = -2172.48306436 ZPE = -2171.823083 H = -2171.779552 G = -2171.898197

C	-3.270409	0.714865	-1.130253
C	-4.390834	-0.035507	-1.433017
C	-5.564105	0.110722	-0.652330
C	-5.622286	0.986369	0.409609
C	-4.487095	1.774715	0.738530
C	-3.301100	1.648404	-0.040681
N	-2.166788	2.358023	0.215789
C	-2.165149	3.192134	1.239663
C	-3.287944	3.390713	2.080088
C	-4.444713	2.688018	1.824709
N	-2.032111	0.637754	-1.773086
H	-6.431254	-0.491915	-0.903855
H	-6.525067	1.083279	1.004974
H	-5.325719	2.815279	2.447372
H	-3.222900	4.088979	2.907368
H	-1.238599	3.734560	1.417965
C	-1.507282	-0.384684	-2.509604
C	-0.005538	-0.261928	-2.738403
C	0.418945	0.804269	-3.581388
C	0.943994	-1.226072	-2.260889

C	1.767687	0.903765	-3.928093
C	2.287761	-1.088316	-2.677054
C	2.695264	-0.039191	-3.487505
H	2.088312	1.716816	-4.572308
H	3.012064	-1.822064	-2.345130
H	3.735561	0.038295	-3.786978
O	-2.184168	-1.289555	-2.989622
H	-4.355911	-0.741097	-2.251140
C	-0.554482	1.824265	-4.133735
H	-1.489046	1.362754	-4.464021
H	-0.812174	2.582447	-3.386464
H	-0.111582	2.343435	-4.986318
C	3.296276	0.410191	0.980645
C	4.533196	0.117509	1.585863
C	5.382871	1.157287	1.965434
C	5.019866	2.490764	1.761776
C	3.784509	2.824919	1.164580
C	2.916461	1.757644	0.765764
N	1.689095	2.022167	0.160146
C	1.293581	3.333926	-0.033700
C	2.087521	4.394736	0.338595
C	3.345893	4.167651	0.937846
N	2.319561	-0.566796	0.620284
H	6.338197	0.923582	2.427776
H	5.687786	3.293797	2.063558
H	3.983268	4.994881	1.233623
H	1.734065	5.407146	0.165303
H	0.319717	3.459023	-0.494515
C	2.646270	-1.813041	0.156938
C	1.435468	-2.659241	-0.216899
C	1.143301	-3.758535	0.617788
C	0.628068	-2.383543	-1.352471
C	0.046807	-4.570622	0.310547
C	-0.436125	-3.250622	-1.652023
C	-0.728370	-4.328327	-0.823235
H	-0.190178	-5.408502	0.960580
H	-1.028726	-3.070467	-2.537286
H	-1.557488	-4.985821	-1.066844
O	3.779317	-2.294135	0.048541
H	4.813707	-0.916100	1.737136
C	1.973708	-4.042191	1.848722
H	3.025324	-4.182619	1.587871
H	1.922000	-3.205408	2.553959
H	1.613134	-4.936012	2.363006
Co	0.755771	0.370784	-0.240122
H	-1.413794	1.366388	-1.432308
C	-1.969509	-1.546628	2.529374
C	-3.024735	-1.976077	1.495991
H	-2.638918	-2.771177	0.850732
H	-3.908570	-2.351867	2.019768
H	-3.326069	-1.141353	0.863815
C	-2.503026	-0.360588	3.373602
H	-3.410940	-0.675396	3.896894
H	-1.767338	-0.043324	4.118722
H	-2.751522	0.494207	2.739212
C	-1.596045	-2.729470	3.440497
H	-1.178907	-3.554092	2.854301
H	-0.862629	-2.439566	4.195763
H	-2.495242	-3.089037	3.949193
C	-0.741059	-1.019847	1.807732
O	-0.833474	-0.481300	0.683890
O	0.392739	-1.123631	2.456119
H	1.174146	-0.849903	1.860128

E-s

Energy = -2172.47093528 ZPE = -2171.809393 H = -2171.765977 G = -2171.885026

C	-2.183652	-1.472233	-0.238140
C	-2.416519	-2.272675	0.855663
C	-3.711618	-2.354657	1.419573
C	-4.763851	-1.637306	0.893469
C	-4.555720	-0.806913	-0.238014
C	-3.251805	-0.728150	-0.816782
N	-2.978145	0.044741	-1.905742
C	-3.957281	0.757053	-2.433500
C	-5.280631	0.759202	-1.930037
C	-5.576268	-0.024514	-0.837718
N	-0.879099	-1.311353	-0.823237
H	-3.866372	-2.991123	2.285200
H	-5.755217	-1.695134	1.332926
H	-6.580014	-0.051068	-0.422990
H	-6.036944	1.371920	-2.408216
H	-3.702905	1.367856	-3.297251
C	-0.270570	-2.538091	-1.436172
C	1.172650	-2.404535	-1.528898
C	1.837676	-2.802340	-2.720139
C	1.873040	-1.720133	-0.445263
C	3.171435	-2.453677	-2.893077
C	3.256636	-1.406766	-0.698927
C	3.862266	-1.743146	-1.885887
H	3.682686	-2.723193	-3.812246
H	3.843485	-0.927660	0.075906
H	4.906499	-1.482570	-2.040484
O	-0.996925	-3.425950	-1.856983
H	-1.598248	-2.827723	1.295107
C	1.109786	-3.532224	-3.825576
H	0.750556	-4.507644	-3.486779
H	0.223790	-2.980159	-4.156752
H	1.767560	-3.677126	-4.686413
C	2.538617	1.804747	0.219366
C	3.676594	2.545275	0.509709
C	4.087768	3.576250	-0.367680
C	3.375199	3.885970	-1.507821
C	2.209891	3.143311	-1.835906
C	1.809317	2.085904	-0.973710
N	0.717977	1.286419	-1.236353
C	-0.013033	1.562677	-2.312573
C	0.297557	2.609552	-3.206344
C	1.409390	3.389465	-2.980376
N	1.956333	0.785970	0.970636
H	4.981515	4.142320	-0.122115
H	3.690671	4.691338	-2.163876
H	1.679735	4.191722	-3.660811
H	-0.346524	2.776207	-4.062536
H	-0.897444	0.957394	-2.477583
C	2.594245	0.038549	1.908243
C	1.826707	-1.246787	2.125990
C	1.488831	-1.640258	3.439693
C	1.484533	-2.056310	0.997672
C	0.849599	-2.866004	3.631221
C	0.878230	-3.309094	1.256281
C	0.570226	-3.706479	2.549726
H	0.586353	-3.177142	4.638292
H	0.686630	-3.983715	0.430179
H	0.117192	-4.678516	2.721151
O	3.652528	0.292161	2.493933
H	4.232494	2.326141	1.411202
C	1.790743	-0.743967	4.618479

H	2.868041	-0.608903	4.740512
H	1.361814	0.253878	4.473136
H	1.377143	-1.161102	5.539726
Co	0.551129	-0.189135	0.110459
H	-1.050545	-0.714610	-1.640601
C	-2.293487	2.901156	1.514807
C	-3.587114	2.152141	1.874796
H	-3.599909	1.879518	2.935244
H	-4.452029	2.792814	1.677006
H	-3.685992	1.239454	1.286468
C	-2.306566	3.285610	0.012654
H	-3.145740	3.960598	-0.183633
H	-1.380291	3.794558	-0.272770
H	-2.419999	2.397875	-0.614496
C	-2.137191	4.161383	2.381254
H	-2.079542	3.906046	3.444141
H	-1.237355	4.721161	2.115838
H	-3.004374	4.812987	2.234453
C	-1.107676	1.954942	1.665523
O	-1.169996	0.755327	1.402905
O	0.036851	2.542897	2.011265
H	0.755944	1.872751	1.875122

E-t

Energy = -2172.52830396 ZPE = -2171.86683 H = -2171.823228 G = -2171.942555

C	-3.443842	0.130782	-1.105831
C	-4.440768	-0.807401	-1.310057
C	-5.680923	-0.677789	-0.639385
C	-5.930826	0.365031	0.224867
C	-4.931103	1.348751	0.448117
C	-3.680414	1.246133	-0.230119
N	-2.674954	2.152397	-0.064881
C	-2.869978	3.158965	0.767720
C	-4.068768	3.349359	1.496567
C	-5.095654	2.447499	1.331104
N	-2.160664	0.091916	-1.650990
H	-6.443754	-1.430635	-0.813173
H	-6.881954	0.448777	0.741915
H	-6.031987	2.559887	1.870562
H	-4.161720	4.195494	2.168690
H	-2.046503	3.860814	0.884134
C	-1.499183	-0.960166	-2.213832
C	-0.014029	-0.723402	-2.472278
C	0.283673	0.149502	-3.581635
C	1.026878	-1.580852	-1.950476
C	1.561143	0.155292	-4.128420
C	2.294023	-1.557080	-2.596159
C	2.560156	-0.708771	-3.652694
H	1.774865	0.817047	-4.962623
H	3.067451	-2.222260	-2.229122
H	3.539359	-0.716479	-4.121311
O	-2.058661	-1.991720	-2.582863
H	-4.254205	-1.646000	-1.965523
C	-0.782773	1.036878	-4.186827
H	-1.674761	0.464859	-4.462409
H	-1.106602	1.817574	-3.491564
H	-0.403289	1.526207	-5.086527
C	3.356680	0.827754	0.645947
C	4.672998	0.789727	1.100170
C	5.379076	1.981216	1.383422
C	4.801162	3.223647	1.231472
C	3.467810	3.317899	0.755908
C	2.754937	2.121811	0.443682
N	1.479945	2.165725	-0.063365
C	0.878895	3.339700	-0.227860
C	1.501025	4.564890	0.086745
C	2.793000	4.551856	0.566265
N	2.497313	-0.257216	0.435992
H	6.402394	1.904429	1.740272
H	5.348257	4.132408	1.463502
H	3.308557	5.478374	0.802998
H	0.961223	5.493446	-0.062754
H	-0.130246	3.303366	-0.628518
C	2.927151	-1.546941	0.321415
C	1.784646	-2.551120	0.250548
C	1.648779	-3.460986	1.317503
C	0.865107	-2.565321	-0.826802
C	0.603741	-4.392277	1.284839
C	-0.145376	-3.537741	-0.847234
C	-0.277172	-4.440672	0.205421
H	0.486160	-5.085991	2.113208
H	-0.827123	-3.572871	-1.685565
H	-1.068534	-5.184504	0.181610
O	4.098433	-1.954305	0.294864
H	5.147031	-0.171282	1.240393
C	2.571290	-3.400037	2.513668
H	3.616043	-3.508381	2.213702
H	2.476851	-2.430818	3.017017
H	2.324731	-4.180603	3.237765
Co	0.857472	0.368603	-0.768623
H	-1.607250	0.865497	-1.296757
C	-1.588769	-0.987260	2.807268
C	-2.632483	-1.786680	2.007938
H	-2.187972	-2.691961	1.582814
H	-3.453405	-2.080882	2.669483
H	-3.040349	-1.194016	1.188770
C	-2.228043	0.309373	3.360411
H	-3.051644	0.052309	4.034243
H	-1.498111	0.901138	3.922164
H	-2.626442	0.925692	2.550302
C	-1.031365	-1.842576	3.958309
H	-0.536571	-2.738730	3.570822
H	-0.307371	-1.285664	4.557357
H	-1.852487	-2.156672	4.610712
C	-0.469147	-0.548407	1.866715
O	-0.673728	-0.311323	0.672051
O	0.717581	-0.401243	2.425950
H	1.397796	-0.246393	1.680464

E-t'

Energy = -2172.05422214 ZPE = -2171.406884 H = -2171.362983 G = -2171.485405

C	1.553511	-0.715500	2.215905
C	2.495190	-1.458163	2.933300
C	3.661896	-0.851001	3.451789
C	3.925255	0.491700	3.282242
C	3.004626	1.290959	2.555654
C	1.829214	0.687134	2.020755
N	0.925796	1.402971	1.280690
C	1.137435	2.698762	1.078701
C	2.264938	3.379583	1.579879
C	3.197740	2.676676	2.313081
N	0.362673	-1.159680	1.647464
H	4.365662	-1.470723	4.001963
H	4.823647	0.948384	3.687557
H	4.084614	3.165919	2.706836
H	2.386639	4.438388	1.376322

H	0.385654	3.213613	0.488511
C	-0.104398	-2.419710	1.807781
C	-1.469906	-2.621719	1.178228
C	-2.594109	-2.728139	2.022314
C	-1.616972	-2.688893	-0.219539
C	-3.858694	-2.890459	1.447247
C	-2.898627	-2.855299	-0.768077
C	-4.013561	-2.952714	0.059795
H	-4.730424	-2.964799	2.092897
H	-3.009811	-2.885929	-1.847365
H	-5.002222	-3.080660	-0.372248
O	0.420582	-3.373746	2.416047
H	2.313168	-2.511270	3.088140
C	-2.432109	-2.625431	3.521197
H	-1.741487	-3.388231	3.891709
H	-2.005157	-1.653405	3.797738
H	-3.391048	-2.734203	4.034701
C	-2.655898	1.261533	-1.370039
C	-3.474786	1.581531	-2.461302
C	-4.449099	2.600248	-2.380512
C	-4.650955	3.331596	-1.229621
C	-3.853392	3.053539	-0.090788
C	-2.863889	2.025124	-0.162226
N	-2.072585	1.723694	0.914295
C	-2.218635	2.412310	2.043443
C	-3.168211	3.440826	2.198917
C	-3.985229	3.757994	1.134816
N	-1.643428	0.301393	-1.310868
H	-5.052990	2.806176	-3.260988
H	-5.403464	4.113308	-1.177449
H	-4.730597	4.544592	1.215870
H	-3.242119	3.964711	3.146277
H	-1.548067	2.139083	2.853317
C	-1.481538	-0.598823	-2.311372
C	-0.358099	-1.601599	-2.122924
C	0.723491	-1.592160	-3.030126
C	-0.434478	-2.593903	-1.124200
C	1.727990	-2.556537	-2.897020
C	0.597832	-3.537696	-1.006121
C	1.675622	-3.517921	-1.886855
H	2.568823	-2.541308	-3.585579
H	0.543368	-4.281316	-0.217254
H	2.469024	-4.254392	-1.793527
O	-2.149058	-0.711655	-3.363053
H	-3.350337	1.025958	-3.377445
C	0.820249	-0.537284	-4.108331
H	-0.055134	-0.568668	-4.762023
H	0.860154	0.462653	-3.664310
H	1.722132	-0.675154	-4.711358
Co	-0.678573	0.273982	0.585470
C	4.294746	1.008446	-1.753239
C	4.624411	2.398406	-2.314600
H	4.376834	3.180274	-1.589906
H	5.693125	2.463721	-2.542332
H	4.059360	2.597992	-3.228708
C	4.633009	-0.085261	-2.792584
H	5.703615	-0.058358	-3.020951
H	4.380288	-1.077877	-2.411384
H	4.080963	0.073636	-3.725001
C	5.084833	0.756803	-0.452875
H	4.841488	1.506439	0.305375
H	4.861232	-0.227662	-0.036347
H	6.158660	0.812253	-0.660596
C	2.791431	0.923130	-1.479293
O	1.970148	1.745383	-1.850158
O	2.463352	-0.190708	-0.811600
H	1.493504	-0.202002	-0.661481

F-q

Energy = -491.521764213 ZPE = -491.386181 H = -491.375395 G = -491.424179

C	-0.146567	0.022693	-0.001507
O	0.496321	-1.081744	-0.001704
O	0.513387	1.113740	-0.001812
C	-1.675075	0.011326	0.000042
C	-2.143299	-0.750801	-1.258420
H	-1.822033	-0.238676	-2.171842
H	-1.737459	-1.765482	-1.271211
H	-3.236460	-0.811205	-1.269771
C	-2.139635	-0.741789	1.265414
H	-1.733689	-1.756345	1.284325
H	-1.815740	-0.223046	2.174161
H	-3.232753	-0.802170	1.280359
C	-2.230430	1.442307	-0.004155
H	-1.897206	1.997225	0.877247
H	-1.900200	1.990861	-0.890683
H	-3.325009	1.414594	-0.002263
Co	2.319738	0.001328	0.000354

F-s

Energy = -491.488831502 ZPE = -491.352741 H = -491.343137 G = -491.386448

C	-0.094518	0.022984	0.000375
O	0.575405	-1.069389	0.000462
O	0.594361	1.100776	0.000554
C	-1.614462	0.011720	-0.000133
C	-2.079506	-0.749284	-1.261235
H	-1.757563	-0.234883	-2.172740
H	-1.672296	-1.763448	-1.275075
H	-3.172423	-0.811188	-1.272584
C	-2.080206	-0.744060	1.263946
H	-1.672817	-1.758087	1.282367
H	-1.759016	-0.225693	2.173466
H	-3.173122	-0.806160	1.274785
C	-2.163275	1.445309	-0.003228
H	-1.830030	1.997086	0.880134
H	-1.829697	1.993346	-0.888806
H	-3.257629	1.420638	-0.003411
Co	2.183639	0.000640	-0.000171

F-t

Energy = -491.545263612 ZPE = -491.409903 H = -491.399984 G = -491.445237

C	-0.133314	0.025404	-0.000484
O	0.489201	-1.085928	-0.000353
O	0.507747	1.123158	-0.000379
C	-1.670235	0.011107	-0.000081
C	-2.139200	-0.750409	-1.257714
H	-1.821140	-0.235185	-2.170942
H	-1.724538	-1.761445	-1.272523
H	-3.232504	-0.819285	-1.271676
C	-2.137888	-0.742835	1.262673
H	-1.723127	-1.753743	1.283223
H	-1.818978	-0.222005	2.172416
H	-3.231170	-0.811750	1.278120
C	-2.235851	1.437916	-0.004030
H	-1.905144	1.994452	0.877360
H	-1.906463	1.989024	-0.889345

H	-3.331100	1.407092	-0.003180
Co	2.319167	0.001034	0.000008

HOPiv

Energy = -347.054090746 ZPE = -346.906939 H = -346.898734 G = -346.937488

C	-0.570422	0.029707	-0.000043
C	-1.098529	-0.685479	1.262962
H	-0.741846	-0.193405	2.173960
H	-2.192800	-0.661679	1.269689
H	-0.770562	-1.727913	1.282194
C	-1.099392	-0.688832	-1.260746
H	-2.193671	-0.665220	-1.266705
H	-0.743482	-0.199094	-2.173304
H	-0.771272	-1.731255	-1.277518
C	-1.011312	1.501028	-0.001814
H	-0.642901	2.028640	0.882244
H	-0.643306	2.026370	-0.887397
H	-2.104807	1.553402	-0.001637
C	0.951848	-0.131478	-0.000201
O	1.518560	-1.208663	-0.000141
O	1.630630	1.034751	-0.000160
H	2.577973	0.811778	-0.000068

NaOPiv

Energy = -508.958114038 ZPE = -508.711313 H = -508.700433 G = -508.74762

C	-0.423159	0.028159	-0.007001
O	-1.009219	-1.099390	-0.008774
O	-1.026368	1.143624	-0.009061
C	1.130199	0.010623	0.000991
C	1.592230	-0.739796	1.266198
H	1.276075	-0.212071	2.173633
H	1.166205	-1.745786	1.291122
H	2.685281	-0.821076	1.288967
C	1.607100	-0.754173	-1.249859
H	1.181882	-1.760614	-1.268037
H	1.301314	-0.237279	-2.167022
H	2.700389	-0.835045	-1.258994
C	1.708376	1.431597	-0.003638
H	1.387316	1.983744	-0.891413
H	1.376011	1.994021	0.873385
H	2.804278	1.396393	0.003406
Na	-3.025684	0.002308	0.005226

OPiv

Energy = -346.553675072 ZPE = -346.420057 H = -346.411144 G = -346.452523

C	-0.523560	0.010156	-0.000030
C	-0.993145	-0.748411	1.255157
H	-0.698088	-0.216531	2.168507
H	-2.085741	-0.859641	1.272086
H	-0.537475	-1.741788	1.282882
C	-0.994051	-0.749768	-1.254039
H	-2.086661	-0.860994	-1.270072
H	-0.699638	-0.218900	-2.168187
H	-0.538396	-1.743172	-1.280995
C	-1.110285	1.426886	-0.000558
H	-0.778566	1.986044	0.879443
H	-0.779381	1.985079	-0.881490
H	-2.208554	1.398983	-0.000070
C	1.051778	0.032002	-0.000537
O	1.608782	-1.101983	-0.000102
O	1.619728	1.157699	-0.000155

TS1-q

Energy = -2172.48189731 ZPE = -2171.828445 H = -2171.784851 G = -2171.90529

Imaginary frequency: -794.27

C	-2.203971	-2.159544	-0.505519
C	-2.875643	-3.394335	-0.368185
C	-4.202012	-3.541262	-0.798298
C	-4.906044	-2.486635	-1.361091
C	-4.283030	-1.216745	-1.514977
C	-2.936895	-1.060427	-1.095115
N	-2.285906	0.119171	-1.199986
C	-2.909496	1.177241	-1.705014
C	-4.240421	1.116582	-2.158216
C	-4.926031	-0.079954	-2.062674
N	-0.914905	-1.902224	-0.171283
H	-4.684366	-4.506673	-0.685146
H	-5.932440	-2.617147	-1.688895
H	-5.956137	-0.159057	-2.396898
H	-4.709645	2.003613	-2.567987
H	-2.329916	2.094781	-1.732626
C	-0.203230	-2.802996	0.657352
C	1.200343	-3.073954	0.255180
C	2.184846	-3.424019	1.210191
C	1.532506	-2.988214	-1.104831
C	3.483051	-3.666418	0.743169
C	2.824780	-3.250635	-1.547842
C	3.806065	-3.586909	-0.613511
H	0.760259	-2.711918	-1.812973
H	4.258537	-3.918970	1.461061
H	3.064594	-3.183179	-2.604303
H	4.824157	-3.783860	-0.936563
O	-0.722192	-3.280460	1.663753
H	-2.358836	-4.235112	0.076125
C	1.901055	-3.497261	2.691173
H	2.829952	-3.632601	3.251079
H	1.413417	-2.582502	3.040731
H	1.223811	-4.322503	2.924101
C	0.915404	2.675312	-0.904362
C	1.580800	3.898872	-0.787322
C	2.521499	4.310461	-1.758564
C	2.819250	3.541778	-2.864410
C	2.167094	2.292566	-3.034563
C	1.228968	1.856259	-2.051932
N	0.591229	0.653349	-2.163604
C	0.813869	-0.114118	-3.217864
C	1.714037	0.241695	-4.244664
C	2.393340	1.436230	-4.143163
N	-0.023558	2.129892	-0.053329
H	3.018451	5.267354	-1.622182
H	3.539302	3.872911	-3.606609
H	3.103455	1.738582	-4.908101
H	1.862265	-0.426305	-5.085939
H	0.264108	-1.049767	-3.257326
C	-0.543148	2.750442	1.040301
C	-1.545869	1.867261	1.749824
C	-2.708528	2.417236	2.335016
C	-1.294922	0.474363	1.768851
C	-3.623473	1.532042	2.922946
C	-2.234844	-0.369567	2.380507
C	-3.394671	0.153849	2.954201
H	0.166071	0.130737	2.079858
H	-4.534611	1.933478	3.361105
H	-2.056902	-1.441938	2.405996

H	-4.122105	-0.503101	3.426124
O	-0.282058	3.899391	1.442644
H	1.356983	4.528412	0.061561
C	-3.014938	3.898346	2.318783
H	-2.320696	4.451177	2.956961
H	-2.902516	4.319598	1.315355
H	-4.036534	4.085108	2.663552
Co	-0.368344	0.119035	-0.284640
C	2.052910	0.076074	1.459545
O	1.693407	-0.146417	0.289017
O	1.227317	0.086525	2.466777
C	3.504591	0.436332	1.776503
C	4.007959	-0.401135	2.966747
H	5.022397	-0.088813	3.235109
H	3.362194	-0.273784	3.838781
H	4.036570	-1.464135	2.709249
C	4.386171	0.202251	0.541473
H	4.045440	0.806622	-0.303388
H	5.421212	0.475381	0.771193
H	4.362480	-0.847884	0.237655
C	3.497119	1.939574	2.146444
H	4.517884	2.268220	2.367723
H	3.112652	2.544458	1.317992
H	2.872652	2.121411	3.025120

TS1-s

Energy = -2172.51805871 ZPE = -2171.859976 H = -2171.818121 G = -2171.93056

Imaginary frequency: -996.27

C	-1.721357	-2.191540	-1.013580
C	-2.172014	-3.454944	-1.402092
C	-3.495983	-3.649476	-1.847629
C	-4.408195	-2.614373	-1.916462
C	-4.002243	-1.315350	-1.527152
C	-2.663694	-1.123918	-1.073726
N	-2.220137	0.103917	-0.672046
C	-3.025949	1.155001	-0.719077
C	-4.359531	1.050391	-1.161899
C	-4.845431	-0.176047	-1.558219
N	-0.420315	-1.830717	-0.663794
H	-3.797388	-4.649896	-2.144923
H	-5.424467	-2.776430	-2.260779
H	-5.870950	-0.284104	-1.899242
H	-4.979329	1.939364	-1.179625
H	-2.610448	2.099368	-0.394896
C	0.400354	-2.799355	-0.117601
C	1.881079	-2.651314	-0.313154
C	2.795522	-3.027403	0.695975
C	2.350022	-2.288090	-1.581279
C	4.160430	-3.019919	0.381851
C	3.711545	-2.304755	-1.880984
C	4.622097	-2.675099	-0.891454
H	1.630394	-2.007452	-2.340248
H	4.876426	-3.296963	1.151467
H	4.055059	-2.030693	-2.874107
H	5.687538	-2.690433	-1.102509
O	-0.022028	-3.817485	0.452029
H	-1.497067	-4.298613	-1.358893
C	2.348592	-3.413501	2.086821
H	3.203050	-3.449625	2.768395
H	1.628108	-2.692050	2.480842
H	1.858325	-4.390065	2.082036
C	0.194618	2.792706	-0.452724
C	0.513454	4.138151	-0.286125
C	1.063396	4.874369	-1.362948
C	1.287477	4.312677	-2.603788
C	0.964749	2.947023	-2.819088
C	0.436995	2.198213	-1.732905
N	0.118225	0.875881	-1.868503
C	0.244034	0.268851	-3.034953
C	0.739253	0.945458	-4.170228
C	1.111441	2.268573	-4.057253
N	-0.367356	1.914848	0.458562
H	1.307641	5.919779	-1.198263
H	1.697046	4.898103	-3.420717
H	1.509831	2.806554	-4.912597
H	0.829047	0.410909	-5.108878
H	-0.047461	-0.774460	-3.061485
C	-0.882584	2.227146	1.683953
C	-1.537032	1.017139	2.286704
C	-2.613423	1.104879	3.184719
C	-1.062712	-0.235916	1.814192
C	-3.215913	-0.101591	3.581729
C	-1.698968	-1.416329	2.235032
C	-2.773093	-1.344221	3.120518
H	0.231096	-0.301936	1.971811
H	-4.058570	-0.060708	4.267520
H	-1.342339	-2.377943	1.878447
H	-3.270289	-2.250103	3.455994
O	-0.867052	3.350736	2.207187
H	0.328810	4.607631	0.669389
C	-3.152850	2.418762	3.697949
H	-4.057270	2.259018	4.291311
H	-2.411370	2.933686	4.314419
H	-3.386691	3.099106	2.874287
Co	-0.355238	0.095985	-0.126415
C	2.084345	0.232474	1.323073
O	1.563868	0.183799	0.170037
O	1.472424	-0.145512	2.373061
C	3.465975	0.872493	1.475337
C	4.311145	0.073652	2.482163
H	5.266917	0.581976	2.645220
H	3.795789	-0.016080	3.441346
H	4.517224	-0.931530	2.104821
C	4.178222	0.973183	0.119283
H	3.590791	1.564642	-0.587779
H	5.151512	1.456632	0.253305
H	4.337320	-0.016403	-0.314463
C	3.185997	2.293378	2.027643
H	4.134300	2.823836	2.162564
H	2.565993	2.869450	1.333055
H	2.673611	2.245762	2.992597

TS1-t

Energy = -2172.48692415 ZPE = -2171.83181 H = -2171.789773 G = -2171.903595

Imaginary frequency: -1011.16

C	-2.164319	2.003011	0.754857
C	-2.791363	3.243702	0.875366
C	-4.148337	3.347825	1.249497
C	-4.924392	2.236273	1.505910
C	-4.338231	0.951505	1.396596
C	-2.964384	0.844148	1.024122
N	-2.359454	-0.366758	0.897620
C	-3.035483	-1.478546	1.125665
C	-4.395362	-1.469957	1.503243
C	-5.039602	-0.258897	1.634828
N	-0.800208	1.797377	0.503391

H	-4.584294	4.339317	1.332465
H	-5.968668	2.327520	1.787721
H	-6.087224	-0.215124	1.919430
H	-4.909935	-2.408078	1.678789
H	-2.490342	-2.408852	0.995542
C	-0.099009	2.789486	-0.181063
C	1.365111	2.915886	0.105380
C	2.286671	3.254754	-0.912166
C	1.798163	2.797108	1.430041
C	3.626365	3.433064	-0.548553
C	3.134805	2.991847	1.775502
C	4.055171	3.305245	0.776113
H	1.067709	2.565647	2.194009
H	4.350907	3.677535	-1.320975
H	3.450085	2.899787	2.810623
H	5.102816	3.455148	1.021247
O	-0.638637	3.581825	-0.964291
H	-2.231979	4.147185	0.675855
C	1.879896	3.387021	-2.361076
H	1.325259	2.504016	-2.691081
H	1.228829	4.251533	-2.508745
H	2.761235	3.494024	-2.999327
C	0.871953	-2.580201	0.679820
C	1.511636	-3.805426	0.532988
C	2.379192	-4.275620	1.549940
C	2.601450	-3.566816	2.712147
C	1.950462	-2.318567	2.905206
C	1.109979	-1.830655	1.870728
N	0.463845	-0.631196	1.974306
C	0.555338	0.077043	3.086450
C	1.352916	-0.341118	4.172706
C	2.060760	-1.521302	4.073285
N	-0.012182	-1.954515	-0.196019
H	2.873414	-5.231116	1.402340
H	3.257966	-3.950307	3.486716
H	2.695182	-1.857111	4.888376
H	1.404748	0.276161	5.062086
H	-0.011051	1.000502	3.110983
C	-0.660502	-2.556559	-1.250187
C	-1.555505	-1.569916	-1.930076
C	-2.739273	-1.939536	-2.588523
C	-1.179818	-0.210301	-1.779854
C	-3.550067	-0.898644	-3.070222
C	-2.025247	0.800406	-2.271143
C	-3.206046	0.449560	-2.919893
H	0.067954	-0.012025	-2.023363
H	-4.481254	-1.153733	-3.569721
H	-1.748108	1.842618	-2.146953
H	-3.866306	1.218022	-3.311679
O	-0.545513	-3.743464	-1.568399
H	1.336809	-4.394708	-0.355592
C	-3.174276	-3.376310	-2.745612
H	-4.164117	-3.432097	-3.205927
H	-2.464761	-3.936797	-3.359572
H	-3.208932	-3.884840	-1.777340
Co	-0.330531	-0.118521	0.177667
C	2.135959	-0.092747	-1.515138
O	1.782578	0.122690	-0.329761
O	1.332250	-0.023786	-2.513907
C	3.581807	-0.519254	-1.814778
C	4.167970	0.402027	-2.901369
H	5.175402	0.067907	-3.171814
H	3.543624	0.391265	-3.798200
H	4.235973	1.432972	-2.541309
C	4.436054	-0.459452	-0.540678
H	4.024305	-1.110763	0.235327
H	5.457260	-0.787219	-0.764310
H	4.476437	0.557702	-0.141986
C	3.514358	-1.972609	-2.336775
H	4.522021	-2.331217	-2.572982
H	3.083606	-2.639196	-1.581596
H	2.901516	-2.032973	-3.239977

TS2-q

Energy = -2172.4837234 ZPE = -2171.829421 H = -2171.78564 G = -2171.906659

Imaginary frequency: -905.99

C	0.009912	2.957920	1.181352
C	-0.354827	4.106530	1.887668
C	0.611938	5.031906	2.337811
C	1.959123	4.847611	2.111028
C	2.385151	3.694003	1.404720
C	1.412952	2.754450	0.950017
N	1.777740	1.621190	0.283094
C	3.059557	1.390000	0.026335
C	4.082519	2.272017	0.422483
C	3.743830	3.414627	1.116016
N	-0.846911	2.027807	0.596019
H	0.271630	5.910831	2.877785
H	2.696472	5.563107	2.461049
H	4.509032	4.110987	1.447378
H	5.113685	2.036007	0.185617
H	3.292465	0.470061	-0.496644
C	-2.196699	2.044056	0.909547
C	-3.128399	1.652446	-0.197682
C	-4.365110	1.020972	0.065550
C	-2.802082	2.032810	-1.506498
C	-5.215988	0.767593	-1.017790
C	-3.671470	1.789042	-2.569431
C	-4.884354	1.146139	-2.320855
H	-1.859363	2.543892	-1.673358
H	-6.159044	0.259163	-0.834759
H	-3.405092	2.098805	-3.575674
H	-5.571833	0.937416	-3.135476
O	-2.651779	2.389608	2.008825
H	-1.398562	4.291354	2.098170
C	-4.781223	0.596456	1.454226
H	-5.651862	-0.063796	1.410062
H	-3.970264	0.071607	1.967291
H	-5.027024	1.464472	2.070759
C	2.213234	-1.744535	-1.080490
C	3.296564	-2.588441	-1.281080
C	3.772329	-2.861369	-2.584899
C	3.167303	-2.321407	-3.698363
C	2.060514	-1.449008	-3.539962
C	1.602435	-1.138934	-2.223662
N	0.577633	-0.255279	-2.017813
C	-0.047052	0.271090	-3.061549
C	0.309440	-0.016187	-4.395386
C	1.371181	-0.860650	-4.630457
N	1.574431	-1.482468	0.151835
H	4.621617	-3.527977	-2.700311
H	3.522024	-2.550695	-4.698482
H	1.690190	-1.087850	-5.643687
H	-0.245479	0.441020	-5.206555
H	-0.865973	0.944320	-2.838891
C	2.287721	-1.469664	1.340665
C	1.423504	-1.120591	2.512156

C	1.716534	-1.551027	3.831752
C	0.326212	-0.292180	2.305670
C	0.862322	-1.126558	4.857557
C	-0.510075	0.154927	3.312370
C	-0.226587	-0.285054	4.612990
H	0.488844	-2.207953	0.170776
H	1.058862	-1.459413	5.873279
H	-1.337002	0.830251	3.117476
H	-0.858471	0.033415	5.438716
O	3.501161	-1.663984	1.446591
H	3.773279	-3.045085	-0.425291
C	2.895489	-2.440162	4.151012
H	2.820131	-2.824238	5.172139
H	2.961571	-3.285082	3.460082
H	3.835994	-1.891072	4.050952
Co	0.107329	0.322609	-0.000122
C	-1.487067	-2.175291	-0.296072
O	-1.545979	-0.938248	-0.060722
O	-0.453198	-2.894114	-0.044284
C	-2.690433	-2.860082	-0.950478
C	-3.907066	-2.704127	-0.017213
H	-4.791171	-3.149513	-0.485238
H	-3.738321	-3.208806	0.940260
H	-4.109423	-1.650910	0.173051
C	-2.951400	-2.116236	-2.279793
H	-2.094896	-2.209855	-2.957097
H	-3.826883	-2.546194	-2.777442
H	-3.135714	-1.055960	-2.100105
C	-2.409262	-4.345287	-1.217275
H	-3.280968	-4.803090	-1.696374
H	-1.546385	-4.472598	-1.877001
H	-2.204211	-4.884064	-0.287985

TS2-s

Energy = -2172.5231586 ZPE = -2171.863642 H = -2171.82208 G = -2171.933789

Imaginary frequency: -159.13

C	-0.082578	2.679892	0.811909
C	-0.563586	3.934685	1.207609
C	0.312548	4.959582	1.613373
C	1.683096	4.787106	1.648535
C	2.222334	3.536795	1.265187
C	1.333456	2.493360	0.864302
N	1.803114	1.263048	0.494071
C	3.109648	1.032587	0.473455
C	4.051701	2.012085	0.843769
C	3.610867	3.252531	1.245183
N	-0.809711	1.630860	0.267660
H	-0.114746	5.915367	1.904079
H	2.349147	5.585196	1.959843
H	4.314415	4.024358	1.543534
H	5.106760	1.766123	0.808839
H	3.441578	0.053244	0.159459
C	-2.189224	1.615562	0.515907
C	-3.121397	1.184153	-0.578934
C	-4.523169	1.092745	-0.366812
C	-2.615038	0.964625	-1.868141
C	-5.338012	0.800938	-1.472451
C	-3.439667	0.684489	-2.951337
C	-4.818876	0.609163	-2.751963
H	-1.547823	0.992269	-1.998996
H	-6.411256	0.725035	-1.319276
H	-3.009789	0.521610	-3.935254
H	-5.486294	0.392483	-3.581234
O	-2.658192	2.038750	1.580661
H	-1.627824	4.125797	1.200760
C	-5.201473	1.289953	0.969424
H	-6.258751	1.018041	0.897125
H	-4.735051	0.691155	1.754918
H	-5.126215	2.328761	1.301235
C	2.235402	-1.545478	-1.485835
C	3.169303	-2.483540	-1.883856
C	3.775229	-2.387278	-3.160654
C	3.462091	-1.362280	-4.025991
C	2.511251	-0.379811	-3.645561
C	1.873676	-0.494170	-2.375774
N	0.946506	0.418611	-1.947994
C	0.700072	1.480972	-2.696561
C	1.287788	1.680004	-3.964891
C	2.174094	0.742218	-4.445248
N	1.540793	-1.549144	-0.235436
H	4.504830	-3.137006	-3.449727
H	3.941872	-1.284522	-4.996774
H	2.637298	0.858769	-5.420671
H	1.032151	2.564482	-4.537039
H	0.012014	2.206943	-2.276145
C	2.206066	-1.891608	0.994856
C	1.343858	-1.526123	2.137367
C	1.513071	-2.081198	3.429278
C	0.352730	-0.559874	1.865269
C	0.642237	-1.642843	4.430535
C	-0.482815	-0.125041	2.892289
C	-0.336081	-0.677858	4.168334
H	0.661812	-2.342854	-0.302813
H	0.733576	-2.057947	5.430728
H	-1.238059	0.630493	2.710907
H	-0.992284	-0.353306	4.972576
O	3.318442	-2.396811	1.036609
H	3.445169	-3.281745	-1.208704
C	2.573073	-3.109792	3.739533
H	2.449932	-3.494522	4.755485
H	2.533592	-3.949441	3.038858
H	3.575825	-2.682715	3.645213
Co	0.361848	0.030604	0.034911
C	-1.364792	-2.313772	-0.166125
O	-1.246555	-1.052011	-0.270463
O	-0.388855	-3.121680	-0.265888
C	-2.767628	-2.869540	0.111493
C	-3.321280	-2.135713	1.350802
H	-4.330264	-2.496605	1.576185
H	-2.688293	-2.308374	2.227646
H	-3.362521	-1.061149	1.171647
C	-3.655564	-2.575984	-1.114226
H	-3.272370	-3.082311	-2.007191
H	-4.671754	-2.940047	-0.928927
H	-3.702224	-1.506500	-1.314344
C	-2.706160	-4.381504	0.372330
H	-3.714223	-4.760678	0.570304
H	-2.298995	-4.916360	-0.489890
H	-2.075925	-4.608826	1.237019

TS2-t

Energy = -2172.504207 ZPE = -2171.848432 H = -2171.805393 G = -2171.922950

Imaginary frequency: -960.02

C	-0.149035	2.775972	0.849819
C	-0.685243	3.988282	1.297201
C	0.135982	5.021639	1.790731

C	1.509228	4.894450	1.866892
C	2.107854	3.682836	1.444884
C	1.277570	2.629108	0.952429
N	1.810802	1.440214	0.563308
C	3.119182	1.244432	0.599109
C	4.014155	2.240221	1.040657
C	3.506424	3.446868	1.471032
N	-0.846597	1.748954	0.228348
H	-0.335914	5.946042	2.112219
H	2.134016	5.700932	2.237348
H	4.167058	4.229653	1.833051
H	5.079258	2.037853	1.044809
H	3.478208	0.272505	0.278596
C	-2.215825	1.652089	0.491312
C	-3.120604	1.261111	-0.641720
C	-4.525339	1.145341	-0.468577
C	-2.574845	1.059220	-1.918888
C	-5.303541	0.830215	-1.594214
C	-3.362685	0.743166	-3.019276
C	-4.744027	0.630283	-2.855158
H	-1.505555	1.134416	-2.030272
H	-6.379419	0.738023	-1.471165
H	-2.903490	0.586705	-3.990962
H	-5.382704	0.386582	-3.699478
O	-2.686883	1.909086	1.608424
H	-1.756045	4.141424	1.257880
C	-5.243145	1.343619	0.846435
H	-6.315031	1.164874	0.720039
H	-4.862383	0.671687	1.619217
H	-5.094874	2.355273	1.232299
C	2.207205	-1.717892	-1.566948
C	3.057531	-2.714972	-2.006332
C	3.637255	-2.645428	-3.296753
C	3.380901	-1.585396	-4.138920
C	2.522161	-0.537157	-3.716477
C	1.918127	-0.620720	-2.427176
N	1.089998	0.363595	-1.957977
C	0.889264	1.447718	-2.691805
C	1.443035	1.612175	-3.978621
C	2.244785	0.616342	-4.492865
N	1.558552	-1.692064	-0.301772
H	4.298542	-3.444208	-3.617451
H	3.836005	-1.530758	-5.123058
H	2.683873	0.709437	-5.481911
H	1.230891	2.515586	-4.538672
H	0.266288	2.213702	-2.240841
C	2.295436	-1.933316	0.877173
C	1.478207	-1.548638	2.058510
C	1.670073	-2.081197	3.353949
C	0.502162	-0.570507	1.839188
C	0.835669	-1.609844	4.373607
C	-0.304367	-0.080771	2.856841
C	-0.132160	-0.630126	4.133485
H	0.575877	-2.436911	-0.276257
H	0.948314	-2.014366	5.375681
H	-1.049606	0.686063	2.676448
H	-0.761752	-0.285929	4.949983
O	3.448311	-2.348654	0.909787
H	3.286956	-3.543463	-1.348595
C	2.722905	-3.123431	3.641247
H	2.619131	-3.504823	4.660336
H	2.653829	-3.962920	2.942934
H	3.727054	-2.707162	3.521142
Co	0.322854	0.064746	-0.015857
C	-1.455191	-2.354768	-0.121852
O	-1.352260	-1.108776	-0.302980
O	-0.457580	-3.153746	-0.162811
C	-2.849338	-2.915509	0.177957
C	-3.376854	-2.170431	1.424039
H	-4.389303	-2.513105	1.662045
H	-2.738566	-2.355516	2.295030
H	-3.401163	-1.094388	1.242863
C	-3.754863	-2.605671	-1.032337
H	-3.396406	-3.117060	-1.932733
H	-4.774043	-2.952087	-0.830184
H	-3.784636	-1.533472	-1.229838
C	-2.796589	-4.426584	0.438350
H	-3.803756	-4.800777	0.650265
H	-2.405006	-4.964031	-0.429903
H	-2.155354	-4.658381	1.293624

TS3ns

Energy = -2172.47137784 ZPE = -2171.814095 H = -2171.771804 G = -2171.886562

Imaginary frequency: -889.79

C	1.217331	2.770614	-0.981824
C	1.505782	4.101165	-1.285324
C	0.844250	4.744942	-2.355624
C	-0.098079	4.102664	-3.133312
C	-0.424858	2.750964	-2.854338
C	0.232660	2.100766	-1.772780
N	-0.045948	0.801683	-1.437703
C	-0.928877	0.115577	-2.149213
C	-1.613577	0.680126	-3.244063
C	-1.369144	1.991069	-3.589804
N	1.776728	1.962113	-0.008967
H	1.094202	5.780960	-2.565440
H	-0.593367	4.610831	-3.954414
H	-1.890178	2.452308	-4.423617
H	-2.325405	0.071869	-3.789829
H	-1.120182	-0.908422	-1.856008
C	2.767528	2.328535	0.855510
C	3.318063	1.122485	1.551820
C	4.696733	1.032419	1.837479
C	2.452583	0.013218	1.721509
C	5.197634	-0.206549	2.262094
C	3.012530	-1.208453	2.146627
C	4.371713	-1.323470	2.408393
H	1.326622	0.022717	2.299499
H	6.259871	-0.297010	2.473935
H	2.363025	-2.060892	2.323499
H	4.791176	-2.269756	2.737716
O	3.209402	3.478267	0.996311
H	2.238967	4.627596	-0.692341
C	5.651263	2.191569	1.664409
H	5.590620	2.611488	0.656339
H	5.407668	3.009427	2.347046
H	6.679803	1.870582	1.850754
C	-1.488085	-1.106007	0.850897
C	-2.516240	-2.022817	0.871265
C	-3.822398	-1.608439	1.235870
C	-4.078909	-0.309592	1.614322
C	-3.031249	0.648283	1.626951
C	-1.730510	0.244131	1.220963
N	-0.681508	1.122564	1.185818
C	-0.861511	2.366018	1.589160
C	-2.115266	2.849181	2.028738
C	-3.196627	1.999463	2.033191

N	-0.088789	-1.402208	0.564571
H	-4.621332	-2.342502	1.234856
H	-5.076160	-0.004239	1.915827
H	-4.176450	2.342586	2.351521
H	-2.203889	3.880951	2.347954
H	0.006023	3.013313	1.545012
C	0.283198	-2.422438	-0.455157
C	1.591728	-2.120081	-1.039969
C	2.300228	-3.073060	-1.824249
C	2.080775	-0.808951	-0.840558
C	3.507366	-2.662243	-2.388307
C	3.279022	-0.430165	-1.445418
C	3.987175	-1.357359	-2.209003
H	4.081388	-3.367339	-2.982795
H	3.662791	0.574283	-1.305293
H	4.927329	-1.068988	-2.672906
O	-0.475205	-3.329035	-0.739441
H	-2.324177	-3.054186	0.613372
C	1.795578	-4.475355	-2.054949
H	2.550458	-5.074852	-2.570067
H	1.535743	-4.969169	-1.113647
H	0.881817	-4.469029	-2.656901
Co	0.922250	0.282177	0.204194
C	0.015635	0.300093	4.121602
O	0.397579	-0.540585	3.214019
O	0.421155	1.468706	4.210869
C	-0.978990	-0.255463	5.174650
C	-1.984342	0.845885	5.549952
H	-2.645034	0.504380	6.355008
H	-1.460878	1.746224	5.879047
H	-2.607379	1.115268	4.690499
C	-1.723324	-1.494377	4.654320
H	-1.023071	-2.287641	4.382154
H	-2.402606	-1.878284	5.424588
H	-2.316895	-1.255140	3.767358
C	-0.134318	-0.632963	6.411428
H	-0.776753	-1.018233	7.211632
H	0.599014	-1.407802	6.161792
H	0.405191	0.240064	6.791574
H	0.328528	-1.667999	1.466012

TS3ns_2

Energy = -2172.46260515 ZPE = -2171.805663 H = -2171.76319 G = -2171.878455

Imaginary frequency: -703.83

C	1.139657	2.774248	-0.588136
C	1.540441	4.105695	-0.469491
C	1.088667	5.067709	-1.399876
C	0.255741	4.742344	-2.452293
C	-0.167976	3.398816	-2.614156
C	0.273048	2.425824	-1.672275
N	-0.094424	1.107926	-1.768050
C	-0.862164	0.722006	-2.776368
C	-1.339071	1.616839	-3.754982
C	-1.000229	2.949362	-3.669890
N	1.473375	1.700361	0.209570
H	1.415204	6.096258	-1.275752
H	-0.076781	5.493249	-3.161727
H	-1.357705	3.662246	-4.407038
H	-1.965447	1.239197	-4.554767
H	-1.123729	-0.328075	-2.841572
C	2.517579	1.668155	1.089787
C	2.748450	0.264887	1.562272
C	4.039680	-0.224495	1.830010
C	1.606506	-0.577707	1.589338
C	4.161797	-1.590510	2.127471
C	1.787573	-1.937663	1.922546
C	3.054068	-2.444494	2.181435
H	0.617223	-0.159688	2.221133
H	5.152389	-1.994945	2.320679
H	0.918604	-2.584047	2.003572
H	3.191980	-3.492511	2.431986
O	3.228200	2.632139	1.403378
H	2.200939	4.383150	0.338669
C	5.276322	0.639461	1.756477
H	5.345079	1.142196	0.786998
H	5.250329	1.431271	2.508697
H	6.177419	0.037544	1.903138
C	-1.475092	-1.825327	0.376994
C	-2.145247	-3.006728	0.612025
C	-3.276016	-3.012047	1.466457
C	-3.750052	-1.846289	2.028745
C	-3.088292	-0.615458	1.786280
C	-1.920541	-0.617432	0.976945
N	-1.195136	0.521313	0.753776
C	-1.612762	1.667983	1.253698
C	-2.796154	1.772935	2.019924
C	-3.516344	0.635884	2.302837
N	-0.361214	-1.651449	-0.544443
H	-3.784068	-3.952077	1.654724
H	-4.633024	-1.853836	2.660641
H	-4.410118	0.679611	2.918074
H	-3.097421	2.742100	2.399476
H	-0.978222	2.527266	1.081021
C	0.688389	-2.701176	-0.731267
C	1.860901	-2.096566	-1.373719
C	2.836559	-2.872753	-2.050128
C	1.977259	-0.696070	-1.228519
C	3.912172	-2.186396	-2.616435
C	3.071417	-0.050503	-1.805044
C	4.026235	-0.795150	-2.500405
H	4.673181	-2.744877	-3.154333
H	3.186863	1.023784	-1.703120
H	4.877576	-0.292541	-2.953061
O	0.505301	-3.846338	-0.380719
H	-1.807997	-3.921166	0.144037
C	2.742168	-4.373846	-2.161591
H	3.522850	-4.761847	-2.820773
H	2.848426	-4.844246	-1.179026
H	1.767844	-4.689863	-2.547093
Co	0.564021	0.090470	-0.193904
C	-0.120238	1.103339	3.911098
O	-0.216905	-0.059411	3.363667
O	0.431781	2.092212	3.395771
C	-0.708348	1.226078	5.344352
C	-1.415225	2.584547	5.485596
H	-1.758654	2.735690	6.515605
H	-0.737274	3.397087	5.214936
H	-2.289037	2.640068	4.827045
C	-1.688827	0.086453	5.657372
H	-1.199269	-0.886656	5.573261
H	-2.084001	0.192598	6.674766
H	-2.532089	0.094100	4.959542
C	0.494002	1.165892	6.310945
H	0.160563	1.277043	7.349419
H	1.018450	0.207640	6.223185
H	1.205700	1.966540	6.087310
H	-0.749492	-1.522524	-1.480422

TS3-q

Energy = -2172.43855544 ZPE = -2171.784454 H = -2171.740457 G = -2171.862838

Imaginary frequency: -1066.54

C	1.663300	3.230592	-0.745906
C	2.425818	4.391382	-0.894521
C	2.071319	5.365834	-1.855440
C	0.972808	5.221872	-2.678621
C	0.168212	4.057149	-2.568672
C	0.523165	3.068963	-1.608451
N	-0.205786	1.930073	-1.454979
C	-1.288931	1.724542	-2.192808
C	-1.716742	2.651873	-3.163367
C	-0.987164	3.809396	-3.351895
N	1.850161	2.179240	0.132735
H	2.688498	6.255678	-1.937597
H	0.711070	5.984228	-3.405710
H	-1.290940	4.541473	-4.094847
H	-2.607050	2.444530	-3.746348
H	-1.825011	0.800306	-2.001016
C	2.893375	2.072452	1.033853
C	2.819578	0.782806	1.801978
C	3.963395	0.160331	2.340338
C	1.541980	0.184214	1.892676
C	3.786785	-1.095895	2.946768
C	1.411254	-1.062780	2.518083
C	2.536050	-1.708882	3.035070
H	0.363383	0.994242	2.181258
H	4.657967	-1.605110	3.351500
H	0.432085	-1.529345	2.590421
H	2.444855	-2.687087	3.499145
O	3.793716	2.905310	1.188281
H	3.289712	4.535124	-0.262385
C	5.347033	0.762233	2.267340
H	5.604731	1.045321	1.242665
H	5.408387	1.680079	2.858286
H	6.094910	0.054803	2.636423
C	-1.631681	-2.648654	0.311880
C	-1.654860	-3.380116	1.488329
C	-2.890203	-3.724523	2.087010
C	-4.092318	-3.349874	1.528972
C	-4.103249	-2.598051	0.324298
C	-2.867955	-2.241351	-0.295732
N	-2.806218	-1.531538	-1.457502
C	-3.940315	-1.160130	-2.024862
C	-5.217630	-1.455296	-1.490703
C	-5.294408	-2.172667	-0.318606
N	-0.476461	-2.250233	-0.361278
H	-2.876344	-4.297562	3.009044
H	-5.035403	-3.617530	1.995689
H	-6.254565	-2.419372	0.125844
H	-6.109281	-1.114914	-2.005825
H	-3.858345	-0.593574	-2.950589
C	0.802959	-2.750895	-0.241016
C	1.778132	-2.069459	-1.155361
C	2.732836	-2.834419	-1.865156
C	1.728401	-0.672315	-1.291727
C	3.598796	-2.156233	-2.731748
C	2.612794	-0.022138	-2.158438
C	3.541032	-0.769698	-2.886644
H	4.329175	-2.728152	-3.297930
H	2.589482	1.058455	-2.262257
H	4.225265	-0.272352	-3.569360
O	1.106218	-3.653821	0.536017
H	-0.723519	-3.700031	1.932962
C	2.829379	-4.336198	-1.725944
H	3.516334	-4.748694	-2.469556
H	3.182226	-4.611904	-0.728697
H	1.853930	-4.816398	-1.851271
Co	0.674002	0.593602	-0.056964
C	-1.560467	1.053981	1.743230
O	-0.648802	1.460909	2.562134
O	-1.284301	0.491826	0.653099
C	-3.016268	1.229222	2.172599
C	-3.929302	1.236133	0.937564
H	-4.972311	1.345017	1.250968
H	-3.681133	2.068992	0.271436
H	-3.831245	0.311358	0.370834
C	-3.340538	0.012870	3.072738
H	-2.698581	0.001401	3.958918
H	-4.383247	0.068372	3.402188
H	-3.202092	-0.925929	2.531165
C	-3.181258	2.534868	2.970744
H	-4.220179	2.631660	3.301854
H	-2.533801	2.547281	3.850172
H	-2.938533	3.406898	2.354310
H	-0.678086	-1.664981	-1.166226

TS3-s

Energy = -2172.48231398 ZPE = -2171.82498 H = -2171.782658 G = -2171.89701

Imaginary frequency: -1021.73

C	0.832488	2.764544	-0.508315
C	0.990069	4.133911	-0.297971
C	0.429488	5.061276	-1.206537
C	-0.259993	4.663007	-2.333495
C	-0.430277	3.277752	-2.590716
C	0.090935	2.341467	-1.654963
N	-0.058718	0.989916	-1.824913
C	-0.617978	0.535072	-2.935486
C	-1.139339	1.391347	-3.926937
C	-1.068826	2.754631	-3.743443
N	1.326985	1.710988	0.238517
H	0.564073	6.120846	-1.008382
H	-0.664018	5.387408	-3.033565
H	-1.479992	3.437907	-4.480826
H	-1.594929	0.959066	-4.810313
H	-0.676695	-0.537394	-3.064937
C	2.222202	1.819031	1.260248
C	2.584889	0.464152	1.780509
C	3.831147	0.203697	2.379831
C	1.624873	-0.557210	1.555639
C	4.109956	-1.123305	2.740113
C	1.958856	-1.868515	1.939468
C	3.190397	-2.151179	2.523793
H	0.430469	-0.189270	1.964012
H	5.070445	-1.353125	3.194399
H	1.267394	-2.685629	1.775016
H	3.437999	-3.168710	2.812696
O	2.703286	2.879749	1.690286
H	1.554493	4.472361	0.558154
C	4.873016	1.272158	2.614329
H	5.079796	1.832825	1.698632
H	4.525926	2.006487	3.345651
H	5.804748	0.826854	2.974227
C	-1.600857	-2.069505	0.242181
C	-1.558633	-2.577360	1.519351

C	-2.758362	-2.800572	2.238122
C	-3.985821	-2.502738	1.689332
C	-4.061482	-1.975224	0.373978
C	-2.857876	-1.773529	-0.364117
N	-2.845058	-1.287127	-1.634534
C	-3.995391	-0.962182	-2.194176
C	-5.245474	-1.103480	-1.543499
C	-5.276087	-1.617575	-0.266434
N	-0.442471	-1.732143	-0.542039
H	-2.695054	-3.200314	3.244840
H	-4.901260	-2.660983	2.251430
H	-6.215751	-1.749139	0.262418
H	-6.155098	-0.812947	-2.057483
H	-3.949409	-0.568153	-3.207323
C	0.584515	-2.769115	-0.787941
C	1.784378	-2.161515	-1.378121
C	2.756192	-2.926206	-2.072954
C	1.946877	-0.779656	-1.141126
C	3.879226	-2.247701	-2.549285
C	3.089562	-0.140225	-1.621846
C	4.044706	-0.874279	-2.327093
H	4.637730	-2.798163	-3.098932
H	3.233697	0.920268	-1.442236
H	4.933133	-0.377474	-2.709752
O	0.387330	-3.927021	-0.481416
H	-0.613680	-2.790174	1.996452
C	2.606744	-4.410203	-2.299432
H	3.395004	-4.781189	-2.959552
H	2.656117	-4.956527	-1.352665
H	1.635650	-4.654014	-2.741560
Co	0.519840	0.039025	-0.171170
C	-1.387402	0.817174	1.850570
O	-0.586083	0.275811	2.682835
O	-1.210521	0.777995	0.602421
C	-2.579778	1.608406	2.400393
C	-3.653129	1.785131	1.315112
H	-4.486229	2.374256	1.712546
H	-3.247295	2.299675	0.441092
H	-4.043115	0.817527	0.986554
C	-3.169603	0.892860	3.627845
H	-2.412981	0.757835	4.404182
H	-3.993716	1.483402	4.041532
H	-3.556744	-0.093716	3.353784
C	-2.007660	2.987382	2.807724
H	-2.809727	3.621403	3.200012
H	-1.242010	2.878792	3.581626
H	-1.558140	3.493572	1.946477
H	-0.843067	-1.481301	-1.456750

TS3-t

Energy = -2172.46397432 ZPE = -2171.808285 H = -2171.764933 G = -2171.883822

Imaginary frequency: -1016.96

C	0.711119	3.054339	-0.301527
C	0.478491	4.385297	0.025590
C	-0.333164	5.189787	-0.810514
C	-0.903222	4.700078	-1.966984
C	-0.678814	3.348109	-2.341935
C	0.121694	2.532973	-1.497573
N	0.368925	1.215510	-1.792586
C	-0.129363	0.683935	-2.898212
C	-0.922732	1.427554	-3.796668
C	-1.202861	2.747488	-3.515214
N	1.455095	2.109861	0.390917
H	-0.504665	6.223197	-0.524333
H	-1.521123	5.329798	-2.599179
H	-1.820257	3.338972	-4.185031
H	-1.304276	0.945012	-4.689078
H	0.107754	-0.356565	-3.083645
C	2.328430	2.341483	1.419004
C	3.005050	1.054756	1.816061
C	4.281378	1.024203	2.401956
C	2.294625	-0.143764	1.520782
C	4.834065	-0.239936	2.671917
C	2.889826	-1.385649	1.814391
C	4.155747	-1.429417	2.392045
H	1.056589	-0.098159	1.923492
H	5.824811	-0.288680	3.116784
H	2.347147	-2.302912	1.608631
H	4.620779	-2.382428	2.627026
O	2.559078	3.436362	1.942197
H	0.924979	4.792883	0.921718
C	5.069001	2.270996	2.728278
H	5.132575	2.938817	1.864856
H	4.581467	2.844974	3.520798
H	6.081447	2.013401	3.050410
C	-2.044029	-2.486636	0.104285
C	-2.308641	-3.240057	1.235666
C	-3.618598	-3.276903	1.771403
C	-4.654462	-2.571739	1.199544
C	-4.413211	-1.783916	0.042724
C	-3.102204	-1.741486	-0.519239
N	-2.798291	-1.010514	-1.627435
C	-3.756272	-0.296825	-2.188294
C	-5.088017	-0.260195	-1.707815
C	-5.413621	-1.008918	-0.599537
N	-0.802129	-2.373681	-0.521412
H	-3.797247	-3.876195	2.659017
H	-5.654243	-2.601799	1.622236
H	-6.424339	-1.010398	-0.200985
H	-5.827550	0.349946	-2.215169
H	-3.475862	0.289434	-3.060976
C	0.389874	-2.958774	-0.203776
C	1.518454	-2.543884	-1.108674
C	2.231752	-3.542059	-1.811624
C	1.868462	-1.191057	-1.222337
C	3.287921	-3.143084	-2.637123
C	2.930672	-0.822452	-2.057441
C	3.638771	-1.797310	-2.762554
H	3.838083	-3.897275	-3.193416
H	3.208306	0.223845	-2.162178
H	4.460378	-1.509053	-3.412988
O	0.540829	-3.757259	0.725346
H	-1.508296	-3.799220	1.698349
C	1.864057	-5.003241	-1.691908
H	2.469242	-5.614120	-2.366345
H	2.008360	-5.357881	-0.668005
H	0.808793	-5.169917	-1.935893
Co	1.171007	0.309411	-0.181141
C	-0.957754	0.513033	1.719293
O	-0.100473	0.122433	2.581105
O	-0.796653	0.376770	0.471969
C	-2.200744	1.246172	2.239785
C	-3.104669	1.674262	1.075909
H	-3.975254	2.213208	1.464633
H	-2.567945	2.331268	0.385826
H	-3.458209	0.812024	0.509817
C	-2.959247	0.317371	3.207567

H	-2.311022	0.001956	4.029509
H	-3.822898	0.843718	3.627790
H	-3.322079	-0.576534	2.691720
C	-1.691570	2.496910	2.992449
H	-2.542271	3.061455	3.388648
H	-1.040133	2.214109	3.822833
H	-1.128921	3.155126	2.320819
H	-0.818792	-1.711164	-1.290260

TS4b-q

Energy = -2172.43054465 ZPE = -2171.77207 H = -2171.728261 G = -2171.848975

Imaginary frequency: -277.91

C	-3.133758	-0.820289	-0.876259
C	-3.973392	-1.817397	-0.400131
C	-5.206545	-1.486663	0.206679
C	-5.612614	-0.178953	0.350408
C	-4.774028	0.867519	-0.113453
C	-3.525426	0.557085	-0.737205
N	-2.679000	1.521957	-1.198871
C	-3.029125	2.786618	-1.043330
C	-4.238451	3.200617	-0.436725
C	-5.109609	2.239511	0.020357
N	-1.898111	-1.042876	-1.490240
H	-5.838925	-2.293478	0.564475
H	-6.559890	0.068369	0.819823
H	-6.050564	2.511943	0.490094
H	-4.459676	4.258202	-0.343034
H	-2.331065	3.536355	-1.408394
C	-1.222099	-2.231258	-1.668161
C	0.161291	-2.105749	-2.227374
C	0.546439	-2.982639	-3.262446
C	1.079283	-1.174184	-1.628073
C	1.843232	-2.871020	-3.784561
C	2.384446	-1.110053	-2.223534
C	2.751714	-1.927373	-3.277162
H	2.140461	-3.519422	-4.604387
H	3.107518	-0.409162	-1.813527
H	3.744424	-1.846982	-3.713391
O	-1.716353	-3.322444	-1.365558
H	-3.673828	-2.849220	-0.503773
C	-0.396781	-4.005254	-3.857504
H	-0.560705	-4.833795	-3.162943
H	-1.382601	-3.578003	-4.064973
H	0.007427	-4.406402	-4.790927
C	3.009626	2.102626	0.108126
C	4.204424	2.669827	0.551563
C	4.599864	3.961632	0.134113
C	3.838741	4.714543	-0.733497
C	2.618459	4.181473	-1.223269
C	2.200357	2.886834	-0.792810
N	1.028296	2.340878	-1.244201
C	0.280735	2.996073	-2.122973
C	0.624101	4.275345	-2.601211
C	1.783234	4.865397	-2.142134
N	2.486165	0.856897	0.438860
H	5.537405	4.360598	0.511086
H	4.156687	5.701185	-1.055901
H	2.075690	5.853762	-2.485680
H	-0.022292	4.773510	-3.314865
H	-0.618303	2.484036	-2.449968
C	3.172211	-0.111939	1.097495
C	2.372107	-1.382897	1.331799
C	2.423543	-1.992886	2.613108
C	1.633015	-2.009764	0.317102
C	1.778784	-3.222266	2.801595
C	1.030221	-3.252506	0.502364
C	1.111795	-3.864688	1.758731
H	1.806156	-3.683919	3.784868
H	0.485564	-3.732809	-0.303236
H	0.638306	-4.828714	1.925470
O	4.343957	-0.050882	1.501925
H	4.832079	2.098311	1.219485
C	3.136443	-1.346001	3.779679
H	2.873388	-0.287488	3.870701
H	2.875641	-1.847807	4.715440
H	4.219802	-1.385500	3.644278
Co	0.745135	0.443124	-0.440269
H	-1.471866	-0.197353	-1.851085
C	-1.956744	0.400534	3.086934
C	-0.979939	0.301710	4.288144
H	-0.071420	0.885043	4.106884
H	-1.471071	0.698472	5.181670
H	-0.694966	-0.736627	4.478418
C	-3.220450	-0.436334	3.364248
H	-3.734151	-0.026558	4.239005
H	-3.909669	-0.405100	2.516326
H	-2.970627	-1.479884	3.567901
C	-2.325320	1.866948	2.818431
H	-1.434962	2.471285	2.628669
H	-2.988011	1.955483	1.953934
H	-2.843140	2.275161	3.691208
C	-1.193098	-0.162140	1.900373
O	-1.100395	-1.479117	1.889278
O	-0.655497	0.561273	1.055329
H	-0.470682	-1.793185	1.203947

TS4b-s

Energy = -2172.46616405 ZPE = -2171.80471 H = -2171.76223 G = -2171.878204

Imaginary frequency: -145.70

C	-2.401913	-0.775799	-0.588844
C	-2.671359	-1.834228	0.249202
C	-3.825246	-1.822334	1.069288
C	-4.696897	-0.755515	1.058128
C	-4.448166	0.349325	0.202554
C	-3.297995	0.333003	-0.642721
N	-3.002557	1.345849	-1.502913
C	-3.801202	2.396236	-1.534044
C	-4.956035	2.522685	-0.723444
C	-5.280555	1.496661	0.135274
N	-1.207548	-0.674727	-1.384180
H	-4.009460	-2.668489	1.723444
H	-5.574146	-0.744346	1.698040
H	-6.162754	1.552530	0.766705
H	-5.567629	3.415507	-0.793694
H	-3.534018	3.190436	-2.228176
C	-0.921515	-1.791257	-2.342434
C	0.502097	-1.942857	-2.546023
C	1.008510	-2.519397	-3.746606
C	1.387494	-1.465544	-1.485800
C	2.380632	-2.521713	-3.956001
C	2.789896	-1.459422	-1.805130
C	3.255707	-1.964862	-2.996401
H	2.782701	-2.934188	-4.876591
H	3.493770	-1.080034	-1.074134
H	4.323747	-1.946630	-3.200298
O	-1.857402	-2.392204	-2.852839

H	-1.989174	-2.672339	0.299878
C	0.093485	-3.073288	-4.812734
H	-0.481505	-3.924948	-4.438324
H	-0.644192	-2.330866	-5.133596
H	0.671273	-3.391579	-5.684549
C	2.575728	1.661153	0.243327
C	3.687388	2.282886	0.811375
C	4.056521	3.586306	0.409456
C	3.350425	4.283427	-0.549393
C	2.216272	3.682990	-1.155801
C	1.829503	2.374207	-0.748975
N	0.741528	1.729569	-1.287659
C	0.041486	2.351060	-2.228411
C	0.355709	3.645232	-2.694179
C	1.434952	4.310825	-2.158579
N	2.074288	0.400444	0.503854
H	4.926077	4.043551	0.873273
H	3.647045	5.282938	-0.852102
H	1.699426	5.309687	-2.493803
H	-0.262832	4.093445	-3.463729
H	-0.824694	1.836705	-2.624329
C	2.662460	-0.538709	1.278744
C	1.875594	-1.824655	1.229295
C	1.870918	-2.698431	2.339370
C	1.090175	-2.105121	0.060258
C	1.105297	-3.871299	2.267841
C	0.376791	-3.322690	0.034760
C	0.374699	-4.186373	1.123594
H	1.092966	-4.546480	3.118582
H	-0.148505	-3.616272	-0.865973
H	-0.188074	-5.114003	1.075123
O	3.708723	-0.419908	1.938307
H	4.259858	1.751748	1.557890
C	2.612731	-2.392229	3.620753
H	2.394008	-1.380284	3.972127
H	2.329940	-3.103433	4.401369
H	3.693397	-2.436210	3.470192
Co	0.506470	-0.112766	-0.437138
H	-1.380835	0.143738	-1.979646
C	-1.719894	1.461926	3.336246
C	-0.636459	1.934260	4.336195
H	0.148689	2.501936	3.826053
H	-1.095676	2.584621	5.087236
H	-0.175443	1.085141	4.847998
C	-2.808474	0.659885	4.077646
H	-3.305997	1.311663	4.802325
H	-3.560788	0.282320	3.379164
H	-2.380199	-0.190079	4.613889
C	-2.339020	2.666716	2.611985
H	-1.576679	3.242365	2.081275
H	-3.088294	2.345051	1.883391
H	-2.825632	3.320912	3.341544
C	-1.016362	0.574439	2.318067
O	-0.661428	-0.620782	2.800412
O	-0.761213	0.924886	1.172124
H	-0.157591	-1.100811	2.114925

TS4b-t

Energy = -2172.4718655 ZPE = -2171.812256 H = -2171.768619 G = -2171.889695

Imaginary frequency: -289.45

C	-3.028733	-0.966484	-0.766730
C	-3.714181	-1.991710	-0.136502
C	-4.970353	-1.744051	0.466201
C	-5.545691	-0.493088	0.447289
C	-4.866394	0.581262	-0.184525
C	-3.598314	0.350311	-0.799521
N	-2.893108	1.337942	-1.417302
C	-3.405115	2.555385	-1.439772
C	-4.653102	2.890914	-0.863079
C	-5.380078	1.902548	-0.239715
N	-1.766826	-1.096147	-1.362854
H	-5.482381	-2.569024	0.951707
H	-6.510759	-0.311969	0.910643
H	-6.341363	2.117880	0.218155
H	-5.014789	3.911874	-0.916658
H	-2.811094	3.324573	-1.929198
C	-1.123639	-2.252668	-1.732015
C	0.295373	-2.078438	-2.201621
C	0.607943	-2.540990	-3.499590
C	1.300909	-1.519548	-1.362758
C	1.922820	-2.429036	-3.960022
C	2.620820	-1.452237	-1.861142
C	2.920841	-1.888751	-3.145222
H	2.166042	-2.769896	-4.962161
H	3.409483	-1.053700	-1.235141
H	3.940869	-1.814987	-3.511965
O	-1.652172	-3.363613	-1.662366
H	-3.292408	-2.985960	-0.121249
C	-0.456759	-3.125575	-4.401369
H	-0.819714	-4.079102	-4.008845
H	-1.326349	-2.463843	-4.478162
H	-0.064346	-3.286982	-5.408191
C	3.013855	1.835597	0.304381
C	4.199534	2.455767	0.701334
C	4.517115	3.762457	0.268496
C	3.683608	4.476360	-0.566836
C	2.474552	3.883300	-1.014877
C	2.138483	2.565836	-0.580341
N	0.989013	1.944674	-1.002485
C	0.173684	2.580013	-1.835094
C	0.427012	3.884033	-2.307395
C	1.571138	4.531352	-1.894957
N	2.549249	0.588362	0.673320
H	5.447473	4.209307	0.608391
H	3.937502	5.479218	-0.896428
H	1.797773	5.536402	-2.240272
H	-0.276865	4.353900	-2.985520
H	-0.722263	2.043326	-2.127755
C	3.315416	-0.409251	1.178790
C	2.490764	-1.662732	1.374709
C	2.806872	-2.560822	2.417633
C	1.331847	-1.869393	0.564662
C	1.952725	-3.648642	2.658662
C	0.507161	-2.973108	0.843373
C	0.812100	-3.848326	1.889728
H	2.184692	-4.334577	3.468343
H	-0.364375	-3.182840	0.241471
H	0.154721	-4.689106	2.091850
O	4.529980	-0.365637	1.445717
H	4.874868	1.913472	1.348123
C	4.005647	-2.377450	3.321987
H	4.050958	-1.364077	3.728946
H	3.967555	-3.090299	4.150328
H	4.938225	-2.521968	2.771617
Co	0.850995	-0.005805	-0.220552
H	-1.402130	-0.210602	-1.698075
C	-2.021223	1.078656	3.062898

C	-1.188844	1.451927	4.312687
H	-0.277587	1.990749	4.032403
H	-1.784436	2.102706	4.960085
H	-0.905900	0.561854	4.880061
C	-3.287059	0.301197	3.484391
H	-3.908468	0.941699	4.117846
H	-3.878679	0.005628	2.613233
H	-3.028637	-0.597966	4.048908
C	-2.401077	2.342576	2.279498
H	-1.511434	2.894581	1.964692
H	-2.977275	2.094190	1.386784
H	-3.009518	2.994657	2.913076
C	-1.155316	0.181565	2.190411
O	-0.832494	-0.973507	2.756548
O	-0.766822	0.503756	1.066781
H	-0.278530	-1.496741	2.135389

TS4-q

Energy = -2172.43586925 ZPE = -2171.777628 H = -2171.733982 G = -2171.853748

Imaginary frequency: -281.02

C	-3.242805	-0.530284	-1.135360
C	-4.313248	-1.297694	-0.701928
C	-5.435301	-0.685409	-0.096858
C	-5.503791	0.677946	0.079863
C	-4.428618	1.494542	-0.357269
C	-3.289163	0.897684	-0.980338
N	-2.223399	1.632125	-1.409363
C	-2.245892	2.939571	-1.219584
C	-3.320954	3.627034	-0.609353
C	-4.411998	2.902906	-0.187155
N	-2.076990	-1.047167	-1.705958
H	-6.253566	-1.317358	0.234998
H	-6.363992	1.142206	0.552653
H	-5.260898	3.390364	0.284244
H	-3.271552	4.703453	-0.486049
H	-1.376403	3.496941	-1.559265
C	-1.576518	-2.327771	-1.610138
C	-0.132349	-2.477371	-1.977411
C	0.246594	-3.578249	-2.773321
C	0.832912	-1.554239	-1.437097
C	1.596838	-3.714901	-3.128411
C	2.189918	-1.745328	-1.865861
C	2.560205	-2.791703	-2.691554
H	1.893768	-4.541369	-3.768538
H	2.954653	-1.056312	-1.513432
H	3.595434	-2.904406	-3.004392
O	-2.271255	-3.278517	-1.235837
H	-4.271580	-2.370238	-0.820159
C	-0.748382	-4.591163	-3.297171
H	-1.091058	-5.251207	-2.495380
H	-1.643934	-4.111003	-3.702327
H	-0.297297	-5.201841	-4.084135
C	3.043073	1.740712	-0.018907
C	4.255411	2.224170	0.457216
C	4.895324	3.324584	-0.159475
C	4.349753	3.954551	-1.256471
C	3.116525	3.492553	-1.784016
C	2.457887	2.392570	-1.156332
N	1.267130	1.913691	-1.639072
C	0.727436	2.453261	-2.724719
C	1.313787	3.539106	-3.403558
C	2.498561	4.059108	-2.926772
N	2.298176	0.682330	0.533105
H	5.840171	3.671495	0.248193
H	4.849483	4.793150	-1.731281
H	2.975567	4.899060	-3.423798
H	0.827175	3.948140	-4.281525
H	-0.210290	2.016014	-3.052400
C	2.905838	-0.394969	1.136965
C	1.913128	-1.448298	1.587154
C	1.845516	-1.779318	2.964350
C	1.056978	-2.089469	0.689895
C	0.928715	-2.754606	3.370931
C	0.169919	-3.080545	1.092631
C	0.105646	-3.408874	2.449075
H	0.859852	-3.005910	4.426053
H	-0.475482	-3.580584	0.378735
H	-0.588470	-4.173119	2.790310
O	4.115834	-0.541727	1.331153
H	4.714863	1.738035	1.306464
C	2.696960	-1.057660	3.983570
H	3.759568	-1.149907	3.748437
H	2.458785	0.012653	3.990350
H	2.518551	-1.447768	4.988870
Co	0.607600	0.256768	-0.549879
H	-1.459543	-0.336065	-2.075493
C	-1.762621	0.679468	3.129154
C	-2.760630	-0.415411	2.716642
H	-2.268277	-1.391799	2.668758
H	-3.565661	-0.469434	3.455738
H	-3.198805	-0.207552	1.740054
C	-2.460036	2.062786	3.136885
H	-3.277246	2.048644	3.864629
H	-1.760972	2.855755	3.419299
H	-2.878281	2.297054	2.153722
C	-1.168641	0.371269	4.516356
H	-0.637112	-0.585334	4.507300
H	-0.471059	1.148821	4.835261
H	-1.978534	0.310075	5.249626
C	-0.658206	0.765153	2.087454
O	-0.839241	0.394379	0.916953
O	0.474800	1.295101	2.500964
H	1.172297	1.214565	1.776098

TS4-s

Energy = -2172.46801024 ZPE = -2171.806529 H = -2171.764175 G = -2171.878924

Imaginary frequency: -188.58

C	-2.548257	-0.734133	-0.348784
C	-2.899641	-1.695513	0.570072
C	-4.117430	-1.596050	1.282476
C	-4.971824	-0.533140	1.085843
C	-4.636947	0.475369	0.146048
C	-3.417426	0.367795	-0.591513
N	-3.040137	1.292891	-1.518804
C	-3.827454	2.332505	-1.728731
C	-5.047685	2.539909	-1.041452
C	-5.449126	1.610271	-0.109132
N	-1.293995	-0.761286	-1.058281
H	-4.367547	-2.369042	2.002340
H	-5.900439	-0.451109	1.642758
H	-6.379380	1.731660	0.438724
H	-5.644190	3.419469	-1.257341
H	-3.491883	3.054001	-2.470840
C	-1.119003	-1.894602	-2.024896
C	0.283891	-2.179126	-2.236278
C	0.726378	-2.768825	-3.454567

C	1.206075	-1.820190	-1.167282
C	2.091395	-2.907727	-3.667670
C	2.599855	-1.963026	-1.483896
C	3.014921	-2.478656	-2.691014
H	2.449925	-3.330877	-4.601255
H	3.345352	-1.692845	-0.746174
H	4.079990	-2.568466	-2.891246
O	-2.106110	-2.403158	-2.536231
H	-2.225555	-2.518635	0.768402
C	-0.240430	-3.192594	-4.534678
H	-0.893363	-3.998683	-4.188401
H	-0.903995	-2.371612	-4.824394
H	0.302207	-3.532480	-5.420774
C	2.876013	0.989301	0.381335
C	4.185353	1.335636	0.698613
C	4.762887	2.505131	0.151397
C	4.055438	3.344905	-0.682634
C	2.715596	3.025902	-1.025791
C	2.139717	1.831379	-0.508256
N	0.859840	1.436919	-0.820410
C	0.123533	2.234446	-1.586549
C	0.606917	3.447596	-2.121328
C	1.900077	3.836524	-1.855430
N	2.127549	-0.090020	0.854391
H	5.788639	2.747214	0.414015
H	4.502907	4.250548	-1.080326
H	2.303952	4.758213	-2.264440
H	-0.051005	4.049573	-2.738164
H	-0.897613	1.925399	-1.781753
C	2.651808	-1.159950	1.527288
C	1.679430	-2.302854	1.526017
C	1.615664	-3.195698	2.613118
C	0.821785	-2.440800	0.389548
C	0.694065	-4.250210	2.555772
C	-0.045696	-3.552030	0.365202
C	-0.121348	-4.432048	1.439062
H	0.630269	-4.944087	3.389305
H	-0.640877	-3.753558	-0.517508
H	-0.805955	-5.274450	1.397542
O	3.774423	-1.229218	2.044035
H	4.746451	0.707694	1.375293
C	2.483930	-3.041552	3.841329
H	3.523942	-3.293732	3.618382
H	2.490225	-2.009876	4.203137
H	2.127983	-3.692253	4.644592
Co	0.461277	-0.420521	-0.057902
H	-1.332185	0.059678	-1.673155
C	-1.454688	2.584763	2.698451
C	-2.746923	1.915260	3.204177
H	-2.558092	1.332790	4.112155
H	-3.490024	2.683137	3.441029
H	-3.161453	1.247817	2.446802
C	-1.759320	3.404791	1.419884
H	-2.472348	4.200137	1.658408
H	-0.851340	3.866785	1.018388
H	-2.192399	2.768028	0.645519
C	-0.851380	3.491598	3.780981
H	-0.596254	2.921597	4.679405
H	0.054448	3.988799	3.425152
H	-1.579849	4.259767	4.058603
C	-0.487608	1.491084	2.258739
O	-0.848909	0.543846	1.562122
O	0.779575	1.657948	2.621646
H	1.303978	0.944473	2.172551

TS4-t

Energy = -2172.48187301 ZPE = -2171.822243 H = -2171.779017 G = -2171.897295

Imaginary frequency: -281.52

C	-3.199634	-0.708271	-0.903535
C	-4.132320	-1.549504	-0.319067
C	-5.323754	-1.018039	0.230004
C	-5.593202	0.331358	0.200235
C	-4.662857	1.218798	-0.401317
C	-3.457468	0.702791	-0.965806
N	-2.525059	1.499429	-1.557742
C	-2.745106	2.801169	-1.594782
C	-3.903193	3.415630	-1.061627
C	-4.860340	2.621965	-0.471945
N	-1.965829	-1.112184	-1.425876
H	-6.032066	-1.702545	0.686534
H	-6.507348	0.731538	0.628295
H	-5.764557	3.052459	-0.051001
H	-4.019949	4.491982	-1.125190
H	-1.977035	3.412215	-2.064651
C	-1.446324	-2.377085	-1.518024
C	0.007872	-2.445048	-1.899591
C	0.337656	-3.183630	-3.058082
C	1.021133	-1.839997	-1.106504
C	1.680907	-3.297269	-3.429136
C	2.366019	-2.013838	-1.498771
C	2.686884	-2.716070	-2.654997
H	1.939498	-3.851413	-4.326739
H	3.164633	-1.602633	-0.893061
H	3.728005	-2.822772	-2.946426
O	-2.103186	-3.394619	-1.290091
H	-3.942127	-2.612047	-0.287187
C	-0.734199	-3.826696	-3.910150
H	-1.217107	-4.647735	-3.373782
H	-1.523107	-3.112971	-4.170453
H	-0.308649	-4.215465	-4.838354
C	3.139474	1.548189	0.166890
C	4.376268	2.048162	0.556113
C	4.944922	3.166718	-0.095793
C	4.301004	3.798875	-1.137746
C	3.043373	3.313196	-1.581528
C	2.462193	2.184436	-0.929302
N	1.261157	1.659140	-1.342483
C	0.627299	2.214574	-2.367895
C	1.124969	3.338893	-3.058089
C	2.326978	3.884701	-2.663488
N	2.444174	0.490297	0.760282
H	5.910899	3.531160	0.241626
H	4.742217	4.657978	-1.633767
H	2.741427	4.748356	-3.176007
H	0.559246	3.751077	-3.886118
H	-0.316511	1.757162	-2.645059
C	3.071289	-0.608823	1.301101
C	2.041369	-1.641403	1.678833
C	2.158663	-2.347651	2.894525
C	0.877150	-1.762173	0.872826
C	1.077823	-3.133109	3.316674
C	-0.187804	-2.542213	1.338137
C	-0.089879	-3.209719	2.558662
H	1.147518	-3.670371	4.258523
H	-1.097736	-2.642942	0.765664
H	-0.928347	-3.804289	2.911375
O	4.288767	-0.763944	1.461045

H	4.902099	1.563241	1.367400
C	3.384648	-2.236002	3.772911
H	4.263936	-2.655026	3.277342
H	3.627894	-1.191469	3.990474
H	3.227218	-2.760953	4.718977
Co	0.766419	-0.082410	-0.304739
H	-1.430384	-0.335320	-1.797496
C	-1.778759	1.249899	3.041219
C	-2.724772	0.035605	2.930901
H	-2.221148	-0.882950	3.250300
H	-3.597531	0.192528	3.572176
H	-3.064615	-0.103205	1.903711
C	-2.493611	2.519698	2.524313
H	-3.388562	2.707040	3.126191
H	-1.842849	3.397474	2.598559
H	-2.796825	2.397501	1.482896
C	-1.322045	1.444785	4.494260
H	-0.792971	0.561308	4.863594
H	-0.655164	2.305192	4.591999
H	-2.196722	1.612190	5.130576
C	-0.600052	1.000327	2.106457
O	-0.789425	0.634120	0.937714
O	0.598393	1.207899	2.607243
H	1.309311	0.990658	1.909607

TS5-q

Energy = -2171.95127091 ZPE = -2171.311927 H = -2171.268002 G = -2171.390933

Imaginary frequency: -1326.36

C	-0.901186	-0.493376	2.800595
C	-0.761256	-0.447604	4.189377
C	-1.102237	-1.562239	4.990395
C	-1.583072	-2.737466	4.451822
C	-1.741819	-2.838162	3.045078
C	-1.401128	-1.719958	2.229135
N	-1.524309	-1.769973	0.873950
C	-1.965061	-2.866178	0.281250
C	-2.331092	-4.018468	1.009191
C	-2.217368	-3.999903	2.383628
N	-0.624881	0.500804	1.875072
H	-0.974488	-1.479857	6.066471
H	-1.836255	-3.585844	5.080466
H	-2.486132	-4.871474	2.974446
H	-2.689565	-4.896402	0.483059
H	-2.018359	-2.829001	-0.803161
C	-0.332078	1.801225	2.205878
C	-0.301810	2.685542	0.986863
C	-0.846476	3.986559	1.029503
C	0.180023	2.117688	-0.214861
C	-0.922230	4.701365	-0.175721
C	0.080942	2.879140	-1.394397
C	-0.467662	4.159498	-1.381205
H	1.379702	1.420013	-0.264930
H	-1.355715	5.698977	-0.167183
H	0.448852	2.458532	-2.328090
H	-0.545731	4.739694	-2.297790
O	-0.184029	2.246469	3.354019
H	-0.390518	0.458948	4.644123
C	-1.383302	4.615329	2.295907
H	-2.110217	3.962160	2.789004
H	-0.585978	4.781053	3.024797
H	-1.867605	5.571847	2.077226
C	0.424078	-1.636620	-2.380774
C	0.695203	-2.262734	-3.603372
C	1.792262	-3.142012	-3.747035
C	2.643035	-3.436413	-2.702488
C	2.417981	-2.826575	-1.441668
C	1.326823	-1.919325	-1.291135
N	1.087920	-1.292305	-0.108247
C	1.853018	-1.535077	0.941919
C	2.937829	-2.436178	0.892410
C	3.219844	-3.072169	-0.296848
N	-0.616140	-0.781841	-2.061372
H	1.958052	-3.601343	-4.718382
H	3.476093	-4.122439	-2.824142
H	4.054995	-3.763255	-0.374669
H	3.535741	-2.604628	1.781277
H	1.624765	-0.973503	1.839163
C	-1.617373	-0.458788	-2.935101
C	-2.657671	0.426691	-2.300441
C	-3.803140	0.905578	-2.982618
C	-2.452567	0.774727	-0.966079
C	-4.691843	1.721702	-2.264779
C	-3.333024	1.589806	-0.264571
C	-4.471533	2.061844	-0.927841
H	-5.577038	2.100423	-2.770385
H	-3.132453	1.871043	0.765445
H	-5.182676	2.700708	-0.408443
O	-1.710740	-0.834087	-4.118832
H	0.043068	-2.067634	-4.440926
C	-4.108574	0.585995	-4.428233
H	-5.040926	1.069138	-4.737166
H	-3.301775	0.916761	-5.087750
H	-4.197190	-0.491918	-4.588346
Co	-0.677499	0.005658	-0.081434
C	3.332396	1.164407	0.523394
O	2.571789	1.191363	-0.530661
O	2.932349	1.262718	1.690641
C	4.847667	1.054419	0.216917
C	5.561429	0.366457	1.390599
H	6.644250	0.347992	1.222043
H	5.357963	0.890690	2.326973
H	5.215967	-0.666603	1.502476
C	5.100830	0.276493	-1.085049
H	4.609278	0.760210	-1.931963
H	6.176835	0.222547	-1.289331
H	4.714805	-0.744905	-1.012249
C	5.363957	2.503017	0.067576
H	6.439732	2.506323	-0.143039
H	4.852698	3.015591	-0.754064
H	5.193001	3.073460	0.986687

TS5-s

Energy = -2172.01663612 ZPE = -2171.372967 H = -2171.330784 G = -2171.445776

Imaginary frequency: -866.90

C	1.170468	2.789104	-0.792564
C	1.519611	4.135012	-0.925879
C	0.972966	4.910537	-1.973123
C	0.086967	4.390374	-2.897122
C	-0.295306	3.027198	-2.801213
C	0.248608	2.242684	-1.746701
N	-0.075782	0.922265	-1.595445
C	-0.906671	0.338124	-2.443987
C	-1.485606	1.043283	-3.520365
C	-1.185541	2.377243	-3.695372
N	1.602263	1.861822	0.130934
H	1.266112	5.954443	-2.046170

H	-0.319805	5.003209	-3.695482
H	-1.621785	2.941979	-4.514480
H	-2.160672	0.523409	-4.190895
H	-1.120143	-0.708001	-2.260561
C	2.612420	2.047366	1.029647
C	3.031727	0.729810	1.612957
C	4.375982	0.477007	1.953158
C	2.059515	-0.302037	1.630876
C	4.727996	-0.839310	2.287907
C	2.467738	-1.606138	1.965391
C	3.791885	-1.878424	2.287724
H	0.952882	-0.115823	2.210017
H	5.763242	-1.054839	2.542360
H	1.722593	-2.396286	1.984438
H	4.104604	-2.887530	2.543533
O	3.171788	3.128710	1.278767
H	2.213515	4.566571	-0.219236
C	5.447309	1.543666	1.929123
H	5.495259	2.036525	0.953503
H	5.236971	2.334332	2.653634
H	6.426709	1.109804	2.151745
C	-1.453069	-1.531982	0.536668
C	-2.340672	-2.605778	0.645459
C	-3.602231	-2.433593	1.258922
C	-4.016076	-1.218152	1.766474
C	-3.147203	-0.099484	1.678007
C	-1.871664	-0.265298	1.070859
N	-0.982214	0.767617	0.977720
C	-1.301560	1.959492	1.446953
C	-2.551846	2.218628	2.050456
C	-3.464804	1.194568	2.168432
N	-0.198371	-1.510553	-0.041276
H	-4.262890	-3.294069	1.327046
H	-4.990075	-1.102113	2.232305
H	-4.429886	1.360724	2.639490
H	-2.767189	3.213576	2.423945
H	-0.544210	2.728287	1.357903
C	0.393341	-2.543252	-0.719001
C	1.684190	-2.088654	-1.323965
C	2.518407	-2.921279	-2.105615
C	2.027198	-0.745135	-1.065836
C	3.693484	-2.361410	-2.625475
C	3.199079	-0.215999	-1.606995
C	4.030367	-1.026259	-2.385318
H	4.351748	-2.981605	-3.229624
H	3.469777	0.817419	-1.412517
H	4.948194	-0.620421	-2.806138
O	-0.076134	-3.690319	-0.837882
H	-2.045144	-3.567384	0.252331
C	2.197183	-4.369602	-2.395171
H	2.979197	-4.819997	-3.014670
H	2.100207	-4.947866	-1.471905
H	1.236390	-4.470374	-2.907601
Co	0.727707	0.161093	0.013434
C	0.034946	0.737960	4.086984
O	0.080690	-0.286100	3.307941
O	0.604603	1.825885	3.885742
C	-0.771394	0.542643	5.404038
C	-1.571703	1.822312	5.699839
H	-2.082059	1.744005	6.667319
H	-0.908624	2.690244	5.718585
H	-2.329357	1.993104	4.927703
C	-1.720354	-0.662172	5.319251
H	-1.167415	-1.583253	5.119399
H	-2.268072	-0.782044	6.262265
H	-2.448962	-0.532610	4.512941
C	0.269347	0.314299	6.520780
H	-0.223831	0.198860	7.493437
H	0.856467	-0.591048	6.328553
H	0.959019	1.162083	6.579759

TS5-t

Energy = -2171.98050987 ZPE = -2171.33946 H = -2171.296987 G = -2171.415224

Imaginary frequency: -1178.71

C	-1.871692	1.711049	-1.817859
C	-2.257526	2.328799	-3.011200
C	-2.764987	3.647676	-3.014074
C	-2.899001	4.388217	-1.857373
C	-2.518019	3.809697	-0.619027
C	-2.008102	2.477069	-0.601170
N	-1.628945	1.876550	0.559234
C	-1.722003	2.527308	1.703954
C	-2.214177	3.849493	1.786273
C	-2.608736	4.483053	0.627684
N	-1.383542	0.431889	-1.643691
H	-3.052183	4.086452	-3.966244
H	-3.285527	5.402922	-1.877226
H	-2.990500	5.500309	0.652587
H	-2.272742	4.343892	2.750030
H	-1.389626	1.988591	2.587428
C	-1.315864	-0.519638	-2.616008
C	-0.947288	-1.848177	-2.005904
C	-1.560512	-3.053075	-2.396677
C	-0.054336	-1.785028	-0.896190
C	-1.273976	-4.206264	-1.646245
C	0.215438	-2.982642	-0.202441
C	-0.396482	-4.180454	-0.560618
H	1.112727	-1.171355	-1.114978
H	-1.758126	-5.140575	-1.924177
H	0.948134	-2.946884	0.598283
H	-0.190049	-5.096188	-0.010933
O	-1.546848	-0.357889	-3.830660
H	-2.162408	1.774446	-3.933466
C	-2.562342	-3.178189	-3.526854
H	-3.527599	-3.526342	-3.139349
H	-2.708652	-2.235385	-4.048939
H	-2.226197	-3.925011	-4.256092
C	1.322246	0.524552	2.168484
C	2.049561	0.604062	3.354946
C	3.202332	1.420797	3.439864
C	3.649100	2.174938	2.375940
C	2.936265	2.130118	1.148304
C	1.787091	1.296323	1.049703
N	1.075061	1.194908	-0.110877
C	1.440716	1.892541	-1.172573
C	2.549533	2.762581	-1.157383
C	3.296163	2.873995	-0.003411
N	0.167132	-0.201166	1.915849
H	3.743732	1.449488	4.381675
H	4.531836	2.801835	2.457759
H	4.165049	3.525204	0.036117
H	2.805388	3.318763	-2.052318
H	0.840889	1.754338	-2.064314
C	-0.524673	-0.948806	2.843666
C	-1.804572	-1.433293	2.249763
C	-2.776527	-2.168735	2.967546
C	-2.011692	-1.077941	0.905006

C	-3.956032	-2.512945	2.295271
C	-3.200564	-1.419385	0.263545
C	-4.171756	-2.138142	0.965872
H	-4.719989	-3.077502	2.824499
H	-3.365278	-1.141150	-0.771189
H	-5.102437	-2.413597	0.474509
O	-0.158732	-1.165903	4.008834
H	1.722624	0.028404	4.208091
C	-2.591972	-2.581736	4.409299
H	-3.460482	-3.147625	4.759949
H	-1.695024	-3.194299	4.536971
H	-2.450777	-1.712064	5.057427
Co	-0.542487	-0.069992	0.138175
C	3.246264	-1.200875	-0.742614
O	2.312807	-0.927684	-1.597760
O	3.063625	-1.633767	0.405963
C	4.699666	-1.006588	-1.255247
C	5.229282	-2.414269	-1.604495
H	6.270504	-2.360972	-1.943916
H	5.183568	-3.069904	-0.729469
H	4.634486	-2.869178	-2.404671
C	4.755575	-0.104467	-2.496436
H	4.360671	0.890699	-2.271289
H	5.791485	0.005034	-2.839535
H	4.161107	-0.521433	-3.312987
C	5.551004	-0.401782	-0.125261
H	6.600557	-0.326658	-0.433073
H	5.198103	0.601381	0.135195
H	5.488357	-1.020966	0.772294

TS6-s

Energy = -2172.00709942 ZPE = -2171.360924 H = -2171.318292 G = -2171.435176

Imaginary frequency: -77.71

C	0.905990	-1.976494	1.146285
C	1.596165	-2.782742	2.056724
C	2.822738	-3.380910	1.689941
C	3.390326	-3.199849	0.442444
C	2.719082	-2.396663	-0.517258
C	1.477560	-1.804766	-0.161101
N	0.738026	-1.060906	-1.047980
C	1.221593	-0.846204	-2.266612
C	2.460038	-1.370061	-2.694363
C	3.200263	-2.151179	-1.831825
N	-0.274904	-1.287796	1.317470
H	3.334453	-3.999620	2.423050
H	4.338240	-3.661697	0.182155
H	4.146677	-2.585093	-2.142798
H	2.801868	-1.167507	-3.703995
H	0.592018	-0.259272	-2.925818
C	-1.095375	-1.351118	2.403852
C	-2.274606	-0.453233	2.199688
C	-2.840941	0.242800	3.287045
C	-2.687044	-0.176861	0.831766
C	-3.795187	1.238664	3.043762
C	-3.661326	0.856998	0.656782
C	-4.184547	1.548979	1.730468
H	-4.225063	1.783210	3.880253
H	-4.017362	1.081516	-0.343103
H	-4.919579	2.332149	1.557510
O	-0.906636	-2.038090	3.432135
H	1.175949	-2.933137	3.041164
C	-2.411562	-0.008216	4.717625
H	-2.667147	-1.021072	5.038896
H	-1.326632	0.074617	4.831575
H	-2.890370	0.709156	5.391321
C	-1.154819	2.027430	-1.790317
C	-1.423097	2.941763	-2.809898
C	-0.876228	4.244502	-2.759135
C	-0.074010	4.668029	-1.716448
C	0.208202	3.777770	-0.646419
C	-0.336391	2.464227	-0.692832
N	-0.137394	1.555064	0.313216
C	0.591410	1.902221	1.364949
C	1.184183	3.178474	1.487411
C	0.994921	4.111173	0.489083
N	-1.581900	0.719594	-1.666820
H	-1.096662	4.929588	-3.573905
H	0.340025	5.672000	-1.698006
H	1.434025	5.102560	0.560690
H	1.774101	3.409656	2.368410
H	0.701200	1.142307	2.133275
C	-2.688311	0.206215	-2.256097
C	-3.053559	-1.123105	-1.638125
C	-3.590819	-2.152168	-2.439826
C	-2.776908	-1.342473	-0.242107
C	-3.866757	-3.396762	-1.859030
C	-3.072376	-2.625495	0.284933
C	-3.603796	-3.630113	-0.507261
H	-4.276367	-4.191659	-2.476472
H	-2.909647	-2.807467	1.341749
H	-3.821679	-4.602174	-0.072203
O	-3.371154	0.738024	-3.153958
H	-2.054586	2.636960	-3.632778
C	-3.823148	-1.977100	-3.923841
H	-4.594284	-1.230249	-4.123150
H	-2.909981	-1.633568	-4.415931
H	-4.118014	-2.928623	-4.376360
Co	-0.884556	-0.248546	-0.165148
C	0.003981	-5.154360	-3.290763
C	0.102655	-5.279115	-4.816951
H	0.813032	-4.554566	-5.224696
H	0.438888	-6.285440	-5.086413
H	-0.867152	-5.098861	-5.289680
C	-1.021109	-6.166279	-2.734854
H	-0.718664	-7.184030	-3.002815
H	-1.090016	-6.097648	-1.646649
H	-2.017677	-5.984455	-3.151255
C	1.386500	-5.393216	-2.643567
H	2.122042	-4.671503	-3.013191
H	1.335174	-5.294134	-1.556615
H	1.739234	-6.400647	-2.888328
C	-0.456612	-3.741246	-2.928838
O	-0.662740	-2.846016	-3.729668
O	-0.600524	-3.590439	-1.604380
H	-0.869860	-2.669307	-1.408951

TS6-s-AQBr

Energy = -2197.1281906 ZPE = -2196.502813 H = -2196.456967 G = -2196.583711

Imaginary frequency: -104.27

C	0.890785	-1.980233	1.245733
C	1.553499	-2.791824	2.170831
C	2.759216	-3.428097	1.812546
C	3.335803	-3.283310	0.563886
C	2.695553	-2.476422	-0.410330
C	1.465152	-1.839716	-0.065060
N	0.737730	-1.086279	-0.951928

C	1.219910	-0.882417	-2.171852
C	2.438864	-1.438718	-2.608072
C	3.145078	-2.232830	-1.736133
N	-0.271732	-1.261143	1.404183
H	3.255177	-4.051617	2.551741
H	4.268323	-3.777302	0.319849
H	2.783138	-1.256872	-3.618538
H	0.604959	-0.288389	-2.836724
C	-1.105101	-1.304854	2.480356
C	-2.287596	-0.414363	2.239535
C	-2.857709	0.315128	3.301938
C	-2.706071	-0.194870	0.869838
C	-3.832330	1.281863	3.022451
C	-3.703380	0.800855	0.655301
C	-4.238034	1.527142	1.703103
H	-4.267567	1.852255	3.838580
H	-4.069055	0.973905	-0.351117
H	-4.992642	2.284072	1.502290
O	-0.935131	-1.969798	3.523250
H	1.126814	-2.915958	3.155967
C	-2.412530	0.130597	4.737391
H	-2.647188	-0.872515	5.101313
H	-1.328243	0.238448	4.837049
H	-2.897413	0.866954	5.385306
C	-1.134316	1.970213	-1.794110
C	-1.395708	2.847574	-2.848021
C	-0.844873	4.145707	-2.840046
C	-0.044044	4.608442	-1.812683
C	0.233522	3.762036	-0.709513
C	-0.318728	2.442659	-0.705531
N	-0.135340	1.563385	0.326536
C	0.589580	1.929718	1.372030
C	1.196585	3.199747	1.466801
C	1.011448	4.088243	0.433942
N	-1.564826	0.670419	-1.632554
H	-1.057044	4.803484	-3.678731
H	0.369818	5.609167	-1.837272
H	1.784450	3.456248	2.339438
H	0.692295	1.195367	2.165218
C	-2.659392	0.135041	-2.235911
C	-3.031347	-1.177122	-1.595768
C	-3.597003	-2.212900	-2.368627
C	-2.712310	-1.379341	-0.202696
C	-3.850769	-3.452691	-1.767076
C	-2.981798	-2.663829	0.342754
C	-3.534543	-3.675346	-0.423888
H	-4.281038	-4.253626	-2.361971
H	-2.782814	-2.840654	1.394169
H	-3.729373	-4.646089	0.024860
O	-3.316806	0.645589	-3.163397
H	-2.022814	2.514287	-3.662626
C	-3.882247	-2.055326	-3.845380
H	-4.648510	-1.299293	-4.027577
H	-2.983090	-1.732194	-4.375516
H	-4.209786	-3.008457	-4.271541
Co	-0.878839	-0.265453	-0.107861
C	0.019804	-5.048620	-3.428573
C	0.094872	-5.071006	-4.961079
H	0.796260	-4.317604	-5.330185
H	0.430202	-6.055397	-5.302702
H	-0.882862	-4.863731	-5.405549
C	-0.994216	-6.098531	-2.924703
H	-0.696388	-7.094693	-3.268016
H	-1.042307	-6.105323	-1.833252
H	-1.998737	-5.889884	-3.308164
C	1.412893	-5.324279	-2.820394
H	2.146469	-4.588823	-3.164240
H	1.382192	-5.284811	-1.728754
H	1.757718	-6.318204	-3.124469
C	-0.443280	-3.665869	-2.968898
O	-0.669665	-2.722266	-3.706140
O	-0.568946	-3.599950	-1.634383
H	-0.867484	-2.702431	-1.382230
Br	4.817861	-3.061463	-2.383987
Br	1.858371	5.868958	0.581279

TS6-s-AQCl

Energy = -3091.19439116 ZPE = -3090.567324 H = -3090.522216 G = -3090.645297

Imaginary frequency: -101.72

C	0.889822	-1.982590	1.251203
C	1.552358	-2.792784	2.177969
C	2.758909	-3.429722	1.822287
C	3.336149	-3.287174	0.573364
C	2.693621	-2.481479	-0.400452
C	1.465460	-1.844455	-0.058848
N	0.739993	-1.091938	-0.949013
C	1.227375	-0.893251	-2.168492
C	2.444977	-1.452950	-2.599453
C	3.155045	-2.249062	-1.727870
N	-0.272825	-1.262754	1.407412
H	3.253965	-4.051467	2.563670
H	4.269304	-3.781295	0.331044
H	2.794632	-1.277730	-3.609715
H	0.614682	-0.299999	-2.836144
C	-1.107924	-1.305862	2.481824
C	-2.288890	-0.413772	2.239419
C	-2.854647	0.321347	3.300231
C	-2.708321	-0.196747	0.869387
C	-3.825973	1.291042	3.019531
C	-3.702980	0.801859	0.653697
C	-4.232972	1.533560	1.699941
H	-4.257587	1.865718	3.834598
H	-4.069846	0.973017	-0.352618
H	-4.985238	2.292541	1.497942
O	-0.940819	-1.971387	3.525149
H	1.124960	-2.915342	3.163052
C	-2.407375	0.139785	4.735483
H	-2.642953	-0.861959	5.102487
H	-1.322696	0.246138	4.832969
H	-2.889751	0.878754	5.382322
C	-1.133119	1.967495	-1.794335
C	-1.392092	2.844657	-2.849184
C	-0.842174	4.143606	-2.840877
C	-0.044512	4.607186	-1.811051
C	0.228236	3.758787	-0.708137
C	-0.321219	2.441272	-0.704182
N	-0.139165	1.563511	0.330216
C	0.582916	1.935952	1.376384
C	1.186021	3.206375	1.469214
C	1.006030	4.099542	0.435568
N	-1.563033	0.667037	-1.633191
H	-1.052871	4.800282	-3.680872
H	0.368847	5.608391	-1.834805
H	1.771513	3.470165	2.341886
H	0.684655	1.203544	2.171515
C	-2.659387	0.133256	-2.233640
C	-3.031470	-1.179115	-1.593188

C	-3.593679	-2.215870	-2.367198
C	-2.716860	-1.380411	-0.199163
C	-3.845721	-3.456450	-1.766512
C	-2.984650	-2.665357	0.345635
C	-3.532111	-3.678567	-0.422659
H	-4.272885	-4.258248	-2.362526
H	-2.788693	-2.841196	1.397808
H	-3.725677	-4.649831	0.025534
O	-3.319318	0.644501	-3.159237
H	-2.016983	2.510717	-3.665312
C	-3.878201	-2.057785	-3.844056
H	-4.648104	-1.305267	-4.025711
H	-2.980353	-1.729648	-4.373148
H	-4.200935	-3.011908	-4.271715
Co	-0.876489	-0.267132	-0.106793
C	0.018472	-5.044614	-3.438682
C	0.059628	-5.072995	-4.972402
H	0.743514	-4.313103	-5.360316
H	0.398302	-6.055042	-5.317448
H	-0.930267	-4.878892	-5.395551
C	-0.971091	-6.104139	-2.907958
H	-0.669608	-7.098107	-3.254400
H	-0.994408	-6.107434	-1.815742
H	-1.986384	-5.908512	-3.269298
C	1.428499	-5.301013	-2.861008
H	2.144946	-4.559598	-3.228113
H	1.423150	-5.254138	-1.769181
H	1.777312	-6.293100	-3.166465
C	-0.446292	-3.663710	-2.974777
O	-0.674961	-2.719102	-3.709976
O	-0.566296	-3.599823	-1.639775
H	-0.859590	-2.701306	-1.384523
Cl	4.646906	-2.997640	-2.283174
Cl	1.749309	5.690548	0.548892

TS6-s-AQMe

Energy = -2250.65636309 ZPE = -2249.954276 H = -2249.908506 G = -2250.031356

Imaginary frequency: -69.14

C	0.896664	-1.985488	1.147925
C	1.569592	-2.800633	2.063503
C	2.783972	-3.418488	1.698802
C	3.355855	-3.250587	0.450186
C	2.704620	-2.438908	-0.517175
C	1.474072	-1.824647	-0.159399
N	0.740943	-1.068356	-1.041715
C	1.228489	-0.864744	-2.258648
C	2.454198	-1.412261	-2.685646
C	3.202338	-2.212725	-1.841828
N	-0.275593	-1.281599	1.317991
H	3.286415	-4.044544	2.432215
H	4.294932	-3.735618	0.208545
H	2.792068	-1.215540	-3.698704
H	0.610907	-0.268321	-2.921056
C	-1.100052	-1.339587	2.402817
C	-2.273075	-0.435946	2.195610
C	-2.831323	0.271709	3.279709
C	-2.684216	-0.163073	0.825295
C	-3.777238	1.274514	3.033346
C	-3.651931	0.878659	0.647528
C	-4.166595	1.580430	1.718238
H	-4.200276	1.827933	3.867516
H	-4.007847	1.101482	-0.352835
H	-4.895467	2.368845	1.542385
O	-0.918789	-2.027836	3.432126
H	1.143642	-2.941695	3.046774
C	-2.398980	0.026397	4.710512
H	-2.656551	-0.983869	5.038046
H	-1.313301	0.106304	4.820747
H	-2.872894	0.749176	5.381945
C	-1.148884	2.037623	-1.789253
C	-1.416898	2.946097	-2.813783
C	-0.879740	4.250030	-2.758106
C	-0.089857	4.680298	-1.707272
C	0.192228	3.798175	-0.629444
C	-0.343037	2.480837	-0.684276
N	-0.151806	1.565484	0.318452
C	0.561143	1.918575	1.376857
C	1.141788	3.197080	1.505922
C	0.973159	4.151646	0.519109
N	-1.570028	0.726859	-1.670261
H	-1.095415	4.934701	-3.574590
H	0.309593	5.688367	-1.702152
H	1.719006	3.425017	2.397204
H	0.668851	1.161168	2.148153
C	-2.678429	0.214547	-2.256136
C	-3.044149	-1.115200	-1.637202
C	-3.570299	-2.147634	-2.442142
C	-2.784913	-1.329847	-0.237862
C	-3.847132	-3.392099	-1.861611
C	-3.080916	-2.611983	0.289302
C	-3.598022	-3.621472	-0.506662
H	-4.246908	-4.189982	-2.481723
H	-2.929915	-2.789481	1.348676
H	-3.816805	-4.593425	-0.071784
O	-3.365198	0.745358	-3.151625
H	-2.039372	2.634669	-3.641014
C	-3.792630	-1.974198	-3.927875
H	-4.572393	-1.237462	-4.131900
H	-2.880687	-1.618442	-4.413083
H	-4.071860	-2.928940	-4.383515
Co	-0.877662	-0.239901	-0.165722
C	0.019965	-5.157153	-3.300814
C	0.060519	-5.300237	-4.828129
H	0.737213	-4.565532	-5.272894
H	0.408066	-6.302534	-5.098202
H	-0.931408	-5.147946	-5.263621
C	-0.959036	-6.183051	-2.691678
H	-0.646877	-7.197307	-2.961706
H	-0.984309	-6.104006	-1.602422
H	-1.975673	-6.026458	-3.068019
C	1.433394	-5.357725	-2.708598
H	2.138042	-4.633735	-3.129633
H	1.428990	-5.232119	-1.623128
H	1.793014	-6.364712	-2.944898
C	-0.448414	-3.746397	-2.938920
O	-0.655783	-2.852171	-3.740431
O	-0.591254	-3.594665	-1.614451
H	-0.855611	-2.672008	-1.419318
C	4.492761	-2.839805	-2.296512
H	5.331280	-2.526920	-1.663687
H	4.438760	-3.933055	-2.235475
H	4.722496	-2.567139	-3.329204
C	1.579822	5.523705	0.644701
H	2.256427	5.734648	-0.191526
H	0.805853	6.299906	0.630111
H	2.144753	5.622909	1.574530

TS6-s-AQNH2

Energy = -2282.74216601 ZPE = -2282.061572 H = -2282.016224 G = -2282.137638

Imaginary frequency: -14.52

C	0.920270	-2.031835	0.981650
C	1.589502	-2.871951	1.877880
C	2.797906	-3.492236	1.500744
C	3.360424	-3.312200	0.249939
C	2.703314	-2.487032	-0.700999
C	1.491892	-1.850653	-0.328104
N	0.763330	-1.063579	-1.186682
C	1.243982	-0.860159	-2.408424
C	2.435691	-1.430168	-2.872195
C	3.174810	-2.272044	-2.043636
N	-0.244256	-1.320992	1.176138
H	3.304362	-4.126735	2.223879
H	4.307582	-3.785801	0.013674
H	2.755495	-1.244543	-3.892996
H	0.634595	-0.235979	-3.054219
C	-1.054492	-1.389677	2.277542
C	-2.200980	-0.450394	2.126163
C	-2.678915	0.275327	3.237944
C	-2.644253	-0.130990	0.767955
C	-3.563573	1.341472	3.042122
C	-3.550964	0.982448	0.643580
C	-3.975138	1.696112	1.741521
H	-3.920225	1.907875	3.898420
H	-3.925698	1.247214	-0.339812
H	-4.655213	2.534930	1.604524
O	-0.863929	-2.113416	3.283153
H	1.164689	-3.025865	2.859628
C	-2.212192	-0.019562	4.648835
H	-2.507253	-1.022511	4.967531
H	-1.120521	0.004813	4.723571
H	-2.626796	0.712079	5.349651
C	-1.182273	2.148979	-1.757793
C	-1.485989	3.099876	-2.730939
C	-1.006007	4.420219	-2.601044
C	-0.248971	4.821742	-1.515512
C	0.052346	3.894389	-0.482283
C	-0.405601	2.556938	-0.619248
N	-0.173427	1.586670	0.321703
C	0.509281	1.915648	1.409821
C	1.006226	3.206034	1.643002
C	0.785963	4.220304	0.712693
N	-1.551412	0.815211	-1.718363
H	-1.235032	5.138543	-3.383940
H	0.124317	5.839714	-1.471154
H	1.546491	3.413092	2.561968
H	0.646771	1.119561	2.136174
C	-2.685109	0.323453	-2.265500
C	-3.027282	-1.033025	-1.677076
C	-3.491317	-2.064774	-2.522797
C	-2.862839	-1.258439	-0.269767
C	-3.795528	-3.314293	-1.971036
C	-3.181476	-2.541968	0.230345
C	-3.639539	-3.550900	-0.604114
H	-4.145705	-4.110961	-2.622239
H	-3.092408	-2.720306	1.296796
H	-3.885396	-4.525511	-0.190329
O	-3.425888	0.883240	-3.097693
H	-2.090036	2.807500	-3.578859
C	-3.615428	-1.870784	-4.017203
H	-4.341241	-1.092232	-4.258519
H	-2.655333	-1.564401	-4.441358
H	-3.912575	-2.805975	-4.500528
Co	-0.833152	-0.204186	-0.258306
C	0.054005	-5.288766	-3.142478
C	0.144649	-5.511661	-4.657808
H	0.837143	-4.800979	-5.117126
H	0.498731	-6.526857	-4.864108
H	-0.831726	-5.381806	-5.133828
C	-0.952189	-6.276124	-2.513768
H	-0.635594	-7.304851	-2.715389
H	-1.016819	-6.136700	-1.432221
H	-1.953529	-6.138197	-2.935643
C	1.444675	-5.468294	-2.492485
H	2.178561	-4.792390	-2.942579
H	1.410186	-5.261867	-1.420148
H	1.790726	-6.496490	-2.642444
C	-0.418798	-3.858735	-2.871149
O	-0.602708	-3.010699	-3.726453
O	-0.599672	-3.634434	-1.561877
H	-0.848242	-2.696820	-1.425194
N	1.292974	5.490326	0.901470
H	0.785995	6.251533	0.472533
H	1.585855	5.708504	1.844170
N	4.346231	-2.856930	-2.478042
H	4.610729	-3.729919	-2.044655
H	4.495340	-2.859518	-3.477748

TS6-s-AQOH

Energy = -2322.46206838 ZPE = -2321.806446 H = -2321.761679 G = -2321.882268

Imaginary frequency: -39.10

C	0.878657	-2.023726	1.075149
C	1.534789	-2.875951	1.970434
C	2.725986	-3.530733	1.590094
C	3.293679	-3.366480	0.339656
C	2.653596	-2.516468	-0.597713
C	1.453437	-1.856177	-0.232691
N	0.744012	-1.065030	-1.103648
C	1.227498	-0.876169	-2.324321
C	2.421121	-1.465350	-2.778162
C	3.126755	-2.297594	-1.926859
N	-0.276533	-1.296442	1.262031
H	3.209623	-4.184873	2.311384
H	4.209075	-3.875829	0.062270
H	2.759032	-1.288518	-3.794739
H	0.629281	-0.250313	-2.977868
C	-1.096767	-1.355024	2.353523
C	-2.253579	-0.431610	2.167742
C	-2.782316	0.282665	3.263161
C	-2.669593	-0.133342	0.798758
C	-3.696372	1.318146	3.036884
C	-3.606147	0.946859	0.643394
C	-4.085125	1.652096	1.725780
H	-4.094057	1.876514	3.880219
H	-3.963220	1.193983	-0.350975
H	-4.788151	2.467217	1.565453
O	-0.914201	-2.060044	3.372670
H	1.108422	-3.021297	2.952969
C	-2.345223	0.008926	4.687574
H	-2.623126	-0.999292	5.004866
H	-1.257023	0.062090	4.790619
H	-2.797063	0.733812	5.372024
C	-1.163904	2.099760	-1.769615
C	-1.446911	3.034247	-2.766373

C	-0.941887	4.349919	-2.672207
C	-0.167823	4.766593	-1.604878
C	0.122193	3.850163	-0.561912
C	-0.372768	2.522665	-0.647906
N	-0.161604	1.585426	0.331246
C	0.533072	1.932494	1.404037
C	1.081331	3.217639	1.581157
C	0.881391	4.177362	0.603056
N	-1.562326	0.777900	-1.688832
H	-1.171447	5.052501	-3.469193
H	0.215209	5.778865	-1.547879
H	1.644758	3.445939	2.481142
H	0.654101	1.160639	2.158692
C	-2.680655	0.276635	-2.261141
C	-3.038940	-1.065122	-1.656228
C	-3.530875	-2.098105	-2.483268
C	-2.833351	-1.283216	-0.250840
C	-3.825431	-3.344011	-1.916355
C	-3.145030	-2.564703	0.263287
C	-3.630025	-3.574846	-0.553282
H	-4.197665	-4.142192	-2.553118
H	-3.031116	-2.740875	1.327603
H	-3.865610	-4.547199	-0.128336
O	-3.388496	0.820728	-3.131405
H	-2.061049	2.733853	-3.604107
C	-3.697131	-1.916687	-3.975359
H	-4.458964	-1.168700	-4.203550
H	-2.762423	-1.573178	-4.425581
H	-3.970912	-2.865678	-4.445667
Co	-0.867786	-0.214811	-0.199539
C	0.054105	-5.225044	-3.221274
C	0.191097	-5.388642	-4.740695
H	0.906039	-4.668752	-5.148782
H	0.541614	-6.398778	-4.975602
H	-0.767807	-5.228498	-5.242009
C	-0.982561	-6.225163	-2.664647
H	-0.670727	-7.248607	-2.897771
H	-1.079070	-6.128013	-1.580723
H	-1.968622	-6.058201	-3.111259
C	1.420167	-5.447324	-2.534406
H	2.179355	-4.765969	-2.930545
H	1.352255	-5.284554	-1.456200
H	1.757906	-6.473526	-2.714007
C	-0.423741	-3.805467	-2.908733
O	-0.617279	-2.934093	-3.738202
O	-0.606517	-3.620067	-1.593055
H	-0.881271	-2.694295	-1.431901
O	4.258685	-2.952974	-2.287875
H	4.478419	-2.745502	-3.207285
O	1.363480	5.442651	0.681017
H	1.851892	5.557077	1.508492

TS6-s-ArBr

Energy = -2197.13307011 ZPE = -2196.506974 H = -2196.461257 G = -2196.586156

Imaginary frequency: -47.43

C	0.916059	-1.949604	1.009185
C	1.618800	-2.768310	1.897119
C	2.853538	-3.341030	1.515519
C	3.416209	-3.125771	0.271994
C	2.731629	-2.310271	-0.667178
C	1.486293	-1.736965	-0.293165
N	0.738558	-0.987569	-1.164294
C	1.201167	-0.759638	-2.385826
C	2.441013	-1.265135	-2.832625
C	3.198253	-2.041815	-1.981633
N	-0.278232	-1.284236	1.202023
H	3.372818	-3.970534	2.233663
H	4.367122	-3.572824	-0.002180
H	4.147292	-2.460855	-2.304618
H	2.771134	-1.049978	-3.843290
H	0.560469	-0.166472	-3.029675
C	-1.100982	-1.414518	2.281690
C	-2.284937	-0.506216	2.126066
C	-2.923135	0.082697	3.242488
C	-2.634115	-0.136294	0.752511
C	-3.892422	1.057201	2.980480
C	-3.614256	0.901886	0.605176
C	-4.226087	1.487481	1.690269
H	-3.915059	1.216563	-0.387681
H	-4.968342	2.265719	1.547715
O	-0.909223	-2.188844	3.246332
H	1.200845	-2.954565	2.875967
C	-2.554359	-0.241562	4.673882
H	-3.426619	-0.639779	5.204675
H	-1.755731	-0.975496	4.719560
H	-2.257676	0.669925	5.204042
C	-1.160474	2.138585	-1.766866
C	-1.454375	3.104522	-2.727697
C	-0.907433	4.404167	-2.618566
C	-0.081607	4.770275	-1.573207
C	0.228525	3.822555	-0.562216
C	-0.315180	2.512656	-0.669566
N	-0.085693	1.548294	0.276285
C	0.671913	1.834282	1.325004
C	1.264159	3.104133	1.505065
C	1.044474	4.092268	0.568870
N	-1.582478	0.821914	-1.706317
H	-1.148974	5.132814	-3.387901
H	0.330557	5.772873	-1.507826
H	1.483230	5.079308	0.686111
H	1.878707	3.284795	2.380664
H	0.808049	1.031041	2.042520
C	-2.692725	0.337547	-2.301789
C	-3.021135	-1.041013	-1.758117
C	-3.506137	-2.051661	-2.618027
C	-2.766650	-1.292312	-0.365006
C	-3.782601	-3.295347	-2.034650
C	-3.091904	-2.573623	0.135573
C	-3.596379	-3.569511	-0.684487
H	-2.964131	-2.780983	1.192060
H	-3.835120	-4.546995	-0.281232
O	-3.421123	0.923951	-3.125789
H	-2.106132	2.845195	-3.550357
C	-3.641154	-1.867896	-4.110589
H	-4.669064	-2.067306	-4.430921
H	-3.377359	-0.860100	-4.416123
H	-2.991275	-2.586787	-4.618001
Co	-0.899297	-0.199200	-0.237045
C	0.091508	-5.286186	-3.065497
C	-0.017205	-5.579863	-4.567911
H	0.553059	-4.853313	-5.152319
H	0.371236	-6.581136	-4.779397
H	-1.058863	-5.535660	-4.900167
C	-0.736948	-6.305682	-2.257453
H	-0.374881	-7.318042	-2.465279
H	-0.651154	-6.121455	-1.184148
H	-1.795705	-6.255800	-2.530057

C	1.570539	-5.335031	-2.614158
H	2.174309	-4.609230	-3.168225
H	1.666039	-5.109175	-1.548801
H	1.977729	-6.334637	-2.798591
C	-0.413349	-3.868618	-2.795071
O	-0.630681	-3.027039	-3.649369
O	-0.557962	-3.627790	-1.482118
H	-0.822722	-2.694854	-1.355605
Br	-4.854609	1.962302	4.484353
Br	-4.437809	-4.802253	-3.160585

TS6-s-ArCl

Energy = -3091.19814619 ZPE = -3090.570562 H = -3090.525548 G = -3090.647563

Imaginary frequency: -49.17

C	0.915275	-1.957939	1.030268
C	1.615413	-2.776577	1.920336
C	2.849888	-3.351231	1.540892
C	3.414325	-3.137405	0.297856
C	2.731862	-2.322481	-0.643354
C	1.486133	-1.748441	-0.272044
N	0.739183	-0.999173	-1.144660
C	1.205875	-0.770423	-2.364895
C	2.446618	-1.276345	-2.808731
C	3.201624	-2.054402	-1.956915
N	-0.276518	-1.288168	1.221374
H	3.367855	-3.980424	2.260289
H	4.365392	-3.585335	0.025555
H	4.151176	-2.473777	-2.278013
H	2.779052	-1.060620	-3.818561
H	0.566782	-0.177789	-3.010640
C	-1.100886	-1.413621	2.299021
C	-2.281946	-0.501528	2.139245
C	-2.898855	0.112328	3.250956
C	-2.646308	-0.152295	0.766204
C	-3.872238	1.090474	2.997036
C	-3.628970	0.881245	0.614944
C	-4.221282	1.488710	1.698591
H	-3.945157	1.175497	-0.379395
H	-4.965780	2.265669	1.555359
O	-0.916576	-2.184415	3.267967
H	1.196135	-2.960092	2.899220
C	-2.512526	-0.178890	4.685062
H	-3.372508	-0.581875	5.232756
H	-1.702180	-0.899508	4.739287
H	-2.225703	0.746668	5.196258
C	-1.167351	2.115136	-1.772681
C	-1.459698	3.070915	-2.744447
C	-0.913659	4.371885	-2.648535
C	-0.090074	4.749955	-1.605614
C	0.218254	3.813496	-0.583616
C	-0.324505	2.502006	-0.677445
N	-0.096893	1.548452	0.279730
C	0.657883	1.847158	1.326996
C	1.249103	3.119259	1.494383
C	1.031356	4.096561	0.546368
N	-1.588598	0.798982	-1.700166
H	-1.153890	5.091893	-3.426432
H	0.321551	5.753425	-1.550455
H	1.469239	5.085178	0.653397
H	1.861234	3.310402	2.369515
H	0.792520	1.052025	2.054013
C	-2.701713	0.311077	-2.288768
C	-3.029435	-1.063249	-1.736608
C	-3.520588	-2.076684	-2.586011
C	-2.763232	-1.309562	-0.343534
C	-3.790875	-3.327900	-2.006820
C	-3.077726	-2.593820	0.159756
C	-3.584949	-3.591288	-0.654573
H	-2.939712	-2.799219	1.215261
H	-3.815540	-4.571177	-0.250653
O	-3.431361	0.893658	-3.115076
H	-2.109649	2.802275	-3.565529
C	-3.677420	-1.905138	-4.078169
H	-4.709721	-2.107969	-4.382896
H	-3.419124	-0.899547	-4.395768
H	-3.034581	-2.626850	-4.591036
Co	-0.899173	-0.212517	-0.225669
C	0.101494	-5.257071	-3.110781
C	0.112780	-5.488973	-4.627548
H	0.746451	-4.754889	-5.132362
H	0.496036	-6.490594	-4.846929
H	-0.895383	-5.405380	-5.044171
C	-0.820994	-6.282260	-2.418313
H	-0.466671	-7.296420	-2.630627
H	-0.828615	-6.136929	-1.335584
H	-1.849603	-6.193853	-2.782293
C	1.534402	-5.367000	-2.540173
H	2.202199	-4.641070	-3.014875
H	1.546012	-5.180870	-1.463316
H	1.928297	-6.371384	-2.727508
C	-0.404493	-3.843338	-2.823000
O	-0.628952	-2.992426	-3.666113
O	-0.556679	-3.624466	-1.507213
H	-0.831002	-2.696147	-1.365796
Cl	-4.694305	1.911032	4.345171
Cl	-4.389934	-4.657823	-3.013563

TS6-s-ArMe

Energy = -2250.64918097 ZPE = -2249.947343 H = -2249.901594 G = -2250.024357

Imaginary frequency: -88.04

C	0.906601	-1.935661	1.090597
C	1.607575	-2.752526	1.983030
C	2.830141	-3.345870	1.596113
C	3.382736	-3.152379	0.343850
C	2.698886	-2.341215	-0.599645
C	1.463046	-1.749977	-0.221749
N	0.712053	-1.003308	-1.094761
C	1.171245	-0.791927	-2.322430
C	2.402398	-1.314993	-2.772287
C	3.158743	-2.092375	-1.920893
N	-0.271741	-1.247412	1.286854
H	3.349879	-3.972654	2.316593
H	4.326201	-3.613443	0.066588
H	4.100559	-2.525028	-2.247191
H	2.726659	-1.113003	-3.787804
H	0.531309	-0.201300	-2.969117
C	-1.099144	-1.364575	2.360122
C	-2.285399	-0.455932	2.189635
C	-2.893568	0.190689	3.284783
C	-2.676902	-0.153942	0.821235
C	-3.902187	1.156771	3.065110
C	-3.686674	0.837713	0.659621
C	-4.265896	1.467202	1.744220
H	-4.034539	1.083999	-0.337870
H	-5.035628	2.217701	1.571807
O	-0.921329	-2.127097	3.337285

H	1.197386	-2.918392	2.969003
C	-2.467992	-0.052755	4.719623
H	-3.305354	-0.454507	5.304982
H	-1.645069	-0.758531	4.787047
H	-2.180814	0.889557	5.202292
C	-1.170160	2.098081	-1.775255
C	-1.461187	3.033172	-2.770062
C	-0.890910	4.325689	-2.722467
C	-0.042143	4.720652	-1.705969
C	0.266636	3.809155	-0.661875
C	-0.302097	2.505164	-0.704484
N	-0.075260	1.577950	0.278287
C	0.706182	1.895885	1.300424
C	1.324163	3.160883	1.417824
C	1.105956	4.112326	0.443843
N	-1.606972	0.791932	-1.664810
H	-1.131713	5.026185	-3.518158
H	0.388376	5.717680	-1.688248
H	1.563617	5.095612	0.511196
H	1.957066	3.367601	2.274725
H	0.842671	1.120064	2.048349
C	-2.723433	0.295452	-2.249394
C	-3.046218	-1.072207	-1.690852
C	-3.567542	-2.093508	-2.507973
C	-2.711142	-1.317278	-0.306812
C	-3.816931	-3.374471	-1.961087
C	-2.996170	-2.610434	0.195836
C	-3.533342	-3.600553	-0.609773
H	-2.807725	-2.824652	1.242277
H	-3.727762	-4.583245	-0.185064
O	-3.446074	0.881441	-3.083072
H	-2.128400	2.751641	-3.572562
C	-3.787996	-1.915913	-3.994626
H	-4.823692	-2.151579	-4.267857
H	-3.577976	-0.901568	-4.321257
H	-3.141198	-2.609840	-4.542848
Co	-0.908951	-0.206268	-0.182693
C	0.092963	-5.254650	-3.151914
C	0.115872	-5.496427	-4.666831
H	0.752495	-4.764673	-5.171551
H	0.502006	-6.498884	-4.877594
H	-0.888785	-5.416029	-5.092431
C	-0.830080	-6.279823	-2.459509
H	-0.459148	-7.293205	-2.645677
H	-0.863200	-6.114005	-1.380329
H	-1.852094	-6.215500	-2.846633
C	1.521338	-5.359473	-2.570507
H	2.190661	-4.633380	-3.042428
H	1.524822	-5.168899	-1.494541
H	1.919320	-6.363516	-2.751398
C	-0.426510	-3.841902	-2.875255
O	-0.691225	-3.013563	-3.729562
O	-0.543599	-3.604474	-1.561495
H	-0.857744	-2.688490	-1.418175
C	-4.571011	1.868210	4.216854
H	-5.033523	1.167070	4.923439
H	-3.861593	2.469186	4.801608
H	-5.354236	2.542414	3.857943
C	-4.341165	-4.497861	-2.821262
H	-5.307144	-4.253524	-3.280479
H	-3.654950	-4.723675	-3.647412
H	-4.470418	-5.412728	-2.236283

TS6-s-ArNH2

Energy = -2282.72844507 ZPE = -2282.048192 H = -2282.003009 G = -2282.123745

Imaginary frequency: -82.54

C	0.902258	-1.938510	1.220219
C	1.584441	-2.745680	2.136802
C	2.813284	-3.345016	1.781509
C	3.391918	-3.165932	0.538631
C	2.730204	-2.362584	-0.427269
C	1.486282	-1.767115	-0.082528
N	0.758153	-1.021989	-0.976571
C	1.252595	-0.809802	-2.190754
C	2.492395	-1.339203	-2.608240
C	3.222952	-2.120756	-1.738351
N	-0.278518	-1.247944	1.383434
H	3.317434	-3.964555	2.519251
H	4.340635	-3.630709	0.286373
H	4.170569	-2.558241	-2.040595
H	2.843597	-1.138816	-3.615175
H	0.631234	-0.220115	-2.855363
C	-1.120656	-1.339079	2.446830
C	-2.312290	-0.448671	2.230360
C	-2.934795	0.215939	3.306592
C	-2.693628	-0.193805	0.853537
C	-3.964610	1.147668	3.045796
C	-3.715657	0.778127	0.658874
C	-4.324744	1.425966	1.713906
H	-4.058313	0.990772	-0.348287
H	-5.109207	2.155220	1.517611
O	-0.955332	-2.064212	3.454891
H	1.154658	-2.897473	3.116778
C	-2.511528	0.047445	4.751008
H	-3.281937	-0.482894	5.329978
H	-1.594502	-0.528121	4.841072
H	-2.382137	1.027910	5.225530
C	-1.133512	2.005739	-1.800757
C	-1.404232	2.899362	-2.839895
C	-0.818147	4.185306	-2.847398
C	0.028789	4.616562	-1.844124
C	0.318237	3.749991	-0.757074
C	-0.268235	2.452681	-0.741383
N	-0.059990	1.570969	0.285899
C	0.720992	1.926856	1.295527
C	1.355898	3.187484	1.357740
C	1.155464	4.094304	0.338416
N	-1.585087	0.711296	-1.639526
H	-1.044313	4.851058	-3.676671
H	0.472022	5.607928	-1.869028
H	1.625901	5.073665	0.361560
H	1.987495	3.426162	2.207413
H	0.844708	1.184903	2.079754
C	-2.687586	0.191981	-2.235399
C	-3.020875	-1.155411	-1.643539
C	-3.557230	-2.183675	-2.440505
C	-2.668322	-1.372613	-0.257538
C	-3.807603	-3.450643	-1.862825
C	-2.944145	-2.666039	0.262114
C	-3.500764	-3.666556	-0.509942
H	-2.743430	-2.866329	1.309258
H	-3.696388	-4.642577	-0.069741
O	-3.386036	0.747198	-3.111394
H	-2.067495	2.588734	-3.634858
C	-3.795761	-2.049364	-3.927898
H	-4.866466	-2.119354	-4.168745
H	-3.441621	-1.097159	-4.311395

H	-3.286555	-2.863490	-4.455500
Co	-0.900542	-0.246880	-0.122491
C	0.048873	-5.100915	-3.343580
C	0.067889	-5.224270	-4.873134
H	0.733794	-4.480560	-5.319374
H	0.416016	-6.221418	-5.161208
H	-0.931525	-5.072234	-5.291421
C	-0.924474	-6.133746	-2.735728
H	-0.629261	-7.143132	-3.041920
H	-0.913197	-6.084644	-1.644111
H	-1.950534	-5.949387	-3.071084
C	1.469477	-5.310355	-2.772480
H	2.170872	-4.577218	-3.183871
H	1.475355	-5.206895	-1.684549
H	1.827442	-6.312544	-3.031404
C	-0.414726	-3.694647	-2.958466
O	-0.639384	-2.793135	-3.747588
O	-0.533260	-3.557063	-1.630725
H	-0.824843	-2.646395	-1.416340
N	-4.269242	-4.516872	-2.655104
N	-4.568188	1.865647	4.099915
H	-5.443276	2.298103	3.828312
H	-4.708963	1.322291	4.943504
H	-4.921938	-4.255643	-3.383723
H	-4.638117	-5.289580	-2.114861

TS6-s-ArOH

Energy = -2322.45239912 ZPE = -2321.797841 H = -2321.752588 G = -2321.875213

Imaginary frequency: -84.80

C	0.862476	-2.006697	1.314191
C	1.536927	-2.815694	2.233362
C	2.773883	-3.404373	1.887474
C	3.364454	-3.210561	0.652511
C	2.708817	-2.404656	-0.315659
C	1.456600	-1.822505	0.019678
N	0.729987	-1.073997	-0.875815
C	1.243939	-0.838272	-2.079293
C	2.493504	-1.352912	-2.484630
C	3.217254	-2.144275	-1.617432
N	-0.322598	-1.318987	1.468932
H	3.274902	-4.025293	2.626028
H	4.320477	-3.664651	0.408474
H	4.171122	-2.572172	-1.913370
H	2.856726	-1.135734	-3.483783
H	0.624930	-0.251646	-2.747629
C	-1.179650	-1.425791	2.514937
C	-2.372687	-0.536903	2.283722
C	-2.956960	0.167774	3.352652
C	-2.781517	-0.316363	0.911568
C	-3.972940	1.099104	3.069260
C	-3.804627	0.647434	0.703895
C	-4.377185	1.345189	1.751334
H	-4.170908	0.824748	-0.301430
H	-5.161703	2.074253	1.556241
O	-1.038419	-2.151098	3.524171
H	1.097426	-2.975530	3.207973
C	-2.521327	0.031336	4.795877
H	-3.218428	-0.606485	5.354265
H	-1.535096	-0.418851	4.880151
H	-2.529191	1.009229	5.285926
C	-1.201490	1.924724	-1.727073
C	-1.461844	2.804671	-2.780379
C	-0.907996	4.104966	-2.778446
C	-0.104025	4.563626	-1.752237
C	0.171915	3.711682	-0.650032
C	-0.382067	2.400307	-0.643931
N	-0.187235	1.530915	0.396849
C	0.548705	1.914422	1.430343
C	1.149909	3.190678	1.503692
C	0.962647	4.084676	0.470363
N	-1.629355	0.622130	-1.567868
H	-1.124070	4.759482	-3.619279
H	0.315364	5.565446	-1.770672
H	1.407414	5.075721	0.501798
H	1.744752	3.451918	2.373032
H	0.661187	1.182477	2.225667
C	-2.714616	0.081877	-2.180637
C	-3.055722	-1.254220	-1.574659
C	-3.593810	-2.275112	-2.382462
C	-2.714163	-1.475298	-0.187856
C	-3.811532	-3.539372	-1.807647
C	-2.952919	-2.782137	0.318361
C	-3.483558	-3.785522	-0.469154
H	-2.743696	-2.992665	1.361572
H	-3.653641	-4.774558	-0.047730
O	-3.389404	0.604058	-3.092149
H	-2.092034	2.472609	-3.593431
C	-3.875997	-2.082922	-3.856167
H	-4.754217	-1.450642	-4.011955
H	-3.035117	-1.585330	-4.340556
H	-4.043892	-3.044956	-4.342327
Co	-0.934163	-0.319670	-0.044904
C	-0.119504	-4.965046	-3.547847
C	-0.125324	-4.944723	-5.082016
H	0.589560	-4.212701	-5.467827
H	0.144121	-5.932716	-5.469012
H	-1.114654	-4.679931	-5.466340
C	-1.156251	-5.980662	-3.020619
H	-0.925945	-6.978825	-3.408012
H	-1.144176	-6.019363	-1.928662
H	-2.167925	-5.708494	-3.337412
C	1.288370	-5.322642	-3.020589
H	2.032826	-4.596600	-3.363992
H	1.306930	-5.334466	-1.927908
H	1.580119	-6.312909	-3.386012
C	-0.482945	-3.573999	-3.026012
O	-0.678164	-2.595836	-3.726290
O	-0.552411	-3.547444	-1.687429
H	-0.792326	-2.644636	-1.388805
O	-4.540569	1.763124	4.133380
O	-4.334531	-4.535945	-2.604531
H	-5.172029	2.411902	3.795007
H	-4.347077	-5.361075	-2.101579

TS6-t

Energy = -2171.99849058 ZPE = -2171.353505 H = -2171.310096 G = -2171.431208

Imaginary frequency: -234.77

C	0.742167	-2.953417	-0.070123
C	0.882492	-4.322157	-0.323012
C	0.031971	-5.268843	0.290938
C	-0.972740	-4.899760	1.162542
C	-1.153663	-3.524861	1.465763
C	-0.291464	-2.558456	0.865581
N	-0.403272	-1.229904	1.158865
C	-1.349013	-0.808896	1.982370
C	-2.262470	-1.689542	2.600560

C	-2.154329	-3.040902	2.348426
N	1.457430	-1.909147	-0.610613
H	0.177989	-6.320967	0.058823
H	-1.623806	-5.638187	1.621184
H	-2.829910	-3.749639	2.820396
H	-3.020292	-1.297676	3.270531
H	-1.362177	0.258453	2.179354
C	2.626945	-2.025286	-1.295470
C	3.196288	-0.665056	-1.620332
C	4.039213	-0.468011	-2.736976
C	2.803926	0.442581	-0.805176
C	4.454083	0.834659	-3.048974
C	3.239318	1.732858	-1.160737
C	4.047063	1.925842	-2.275758
H	5.091181	0.994390	-3.915294
H	2.949894	2.580530	-0.548397
H	4.370486	2.929371	-2.542953
O	3.204822	-3.085205	-1.617202
H	1.658867	-4.641201	-1.003980
C	4.480685	-1.600876	-3.638819
H	5.139927	-2.294040	-3.110121
H	3.631282	-2.200462	-3.977785
H	5.007299	-1.208345	-4.514349
C	-0.488582	2.516826	0.296293
C	-1.058585	3.718947	0.728504
C	-2.203918	4.250616	0.095734
C	-2.809807	3.625364	-0.976240
C	-2.260647	2.413278	-1.470109
C	-1.100785	1.866843	-0.842466
N	-0.517113	0.719421	-1.297499
C	-1.040074	0.079443	-2.329913
C	-2.195109	0.535258	-3.003191
C	-2.796871	1.698674	-2.573366
N	0.580845	1.843372	0.836256
H	-2.617764	5.182295	0.473852
H	-3.692108	4.044853	-1.450775
H	-3.683212	2.082796	-3.071757
H	-2.587377	-0.027784	-3.843438
H	-0.527665	-0.830737	-2.631848
C	1.533568	2.406749	1.621395
C	2.614295	1.407210	1.951610
C	3.378657	1.524843	3.136815
C	2.778767	0.277242	1.085365
C	4.296000	0.514907	3.453279
C	3.703715	-0.721121	1.462182
C	4.447912	-0.602688	2.628393
H	4.873516	0.591847	4.370830
H	3.844653	-1.587189	0.825498
H	5.149444	-1.387103	2.902496
O	1.573018	3.590602	2.017690
H	-0.603224	4.234555	1.562474
C	3.181006	2.653875	4.123839
H	3.429783	3.622294	3.685454
H	2.132400	2.712413	4.428512
H	3.797395	2.491814	5.013889
Co	1.050222	-0.013023	0.066898
C	0.568717	-1.079462	5.931643
C	-0.306193	-0.263321	6.892401
H	-1.316040	-0.136506	6.491081
H	-0.378327	-0.776391	7.856641
H	0.115058	0.731902	7.057802
C	1.998740	-1.225242	6.500146
H	1.961934	-1.741144	7.465357
H	2.634110	-1.799486	5.821180
H	2.461475	-0.244553	6.654331
C	-0.049174	-2.474236	5.696167
H	-1.050025	-2.392781	5.260546
H	0.566548	-3.069197	5.017585
H	-0.131737	-3.006070	6.649793
C	0.673371	-0.340932	4.596884
O	0.227925	0.771870	4.376400
O	1.336804	-1.059286	3.677703
H	1.438745	-0.520830	2.867855

TS7

Energy = -2172.00718979 ZPE = -2171.364284 H = -2171.321917 G = -2171.437451

Imaginary frequency: -1207.52

C	0.890851	2.729018	-0.692092
C	1.111844	4.106632	-0.645629
C	0.622290	4.940761	-1.677929
C	-0.066228	4.443455	-2.766827
C	-0.304169	3.046236	-2.859942
C	0.156836	2.208266	-1.808880
N	-0.049742	0.856708	-1.825631
C	-0.633160	0.283666	-2.862741
C	-1.101046	1.040607	-3.959961
C	-0.955569	2.410963	-3.949767
N	1.311088	1.745482	0.179146
H	0.808053	6.009344	-1.607392
H	-0.419653	5.098308	-3.557577
H	-1.321817	3.015746	-4.774984
H	-1.578856	0.530155	-4.788967
H	-0.755892	-0.787096	-2.800754
C	2.157327	1.922497	1.228870
C	2.520560	0.596805	1.831669
C	3.741149	0.389859	2.504249
C	1.616787	-0.468288	1.580048
C	4.046945	-0.918819	2.909021
C	1.974052	-1.758147	2.001859
C	3.180491	-1.985904	2.660085
H	0.358348	-0.188532	1.954400
H	4.988120	-1.102601	3.422183
H	1.304560	-2.586856	1.801769
H	3.453028	-2.988579	2.979992
O	2.617258	3.012091	1.621001
H	1.668478	4.519764	0.183081
C	4.735614	1.496782	2.771672
H	4.991324	2.031374	1.852513
H	4.320453	2.248525	3.448073
H	5.651957	1.091883	3.211789
C	-1.531578	-2.093668	0.228774
C	-1.521538	-2.899745	1.359102
C	-2.695857	-3.211057	2.077487
C	-3.915854	-2.710990	1.678791
C	-3.991827	-1.904371	0.514846
C	-2.803804	-1.610095	-0.237176
N	-2.858735	-0.898523	-1.397724
C	-4.021232	-0.434677	-1.807935
C	-5.242607	-0.630697	-1.116221
C	-5.220742	-1.374704	0.039842
N	-0.334347	-1.724978	-0.414732
H	-2.624791	-3.838160	2.961886
H	-4.823718	-2.928546	2.234917
H	-6.131742	-1.568923	0.600425
H	-6.163967	-0.209221	-1.505116
H	-4.012787	0.128956	-2.741229
C	0.448663	-2.688385	-0.968713

C	1.751345	-2.115190	-1.441696
C	2.713744	-2.846163	-2.174573
C	1.977281	-0.774627	-1.081818
C	3.897972	-2.188275	-2.536342
C	3.164240	-0.143768	-1.458422
C	4.123627	-0.854394	-2.184997
H	4.651886	-2.730324	-3.103083
H	3.342060	0.891087	-1.181554
H	5.052062	-0.369993	-2.481498
O	0.136004	-3.891461	-1.090852
H	-0.572951	-3.292013	1.703860
C	2.516136	-4.289197	-2.580474
H	3.371583	-4.645244	-3.163812
H	2.387225	-4.932482	-1.706037
H	1.605628	-4.415287	-3.173215
Co	0.512738	0.025358	-0.151133
C	-1.431719	0.793758	1.863866
O	-0.657628	0.171801	2.674972
O	-1.222408	0.848189	0.628888
C	-2.626192	1.546219	2.465527
C	-3.594911	1.985155	1.358545
H	-4.433333	2.537946	1.796525
H	-3.093697	2.630492	0.632553
H	-3.993278	1.121606	0.820129
C	-3.347888	0.642555	3.482569
H	-2.662718	0.316557	4.268795
H	-4.176598	1.189404	3.945587
H	-3.753733	-0.248316	2.993637
C	-2.039308	2.784240	3.181239
H	-2.844591	3.372150	3.634732
H	-1.341533	2.483459	3.967902
H	-1.503896	3.426918	2.473459

TS10se

Energy = -3357.04813507 ZPE = -3355.977679 H = -3355.905093 G = -3356.087898

Imaginary frequency: -284.00

C	-3.454036	-0.295135	1.664222
C	-4.366636	-0.320644	2.715302
C	-5.480747	0.551144	2.718267
C	-5.710409	1.454142	1.701444
C	-4.804089	1.515870	0.611314
C	-3.685850	0.636946	0.601143
N	-2.775104	0.657338	-0.418237
C	-2.908622	1.519478	-1.415712
C	-3.988595	2.420423	-1.485348
C	-4.932592	2.411253	-0.480095
N	-2.317354	-1.081577	1.503577
H	-6.168024	0.502691	3.557747
H	-6.567412	2.119789	1.721061
H	-5.774202	3.097316	-0.504933
H	-4.055532	3.109666	-2.318643
H	-2.138118	1.489149	-2.177561
C	-1.956182	-2.146244	2.306796
C	-0.840057	-2.897159	1.662306
C	-0.452237	-4.201472	2.018932
C	-0.223585	-2.232432	0.577008
C	0.513238	-4.827455	1.213559
C	0.729903	-2.879521	-0.221036
C	1.076871	-4.189646	0.100507
H	0.821474	-5.840528	1.456519
H	1.232665	-2.369054	-1.030852
H	1.806460	-4.715097	-0.508574
O	-2.500694	-2.459024	3.368810
H	-4.207557	-1.007792	3.532879
C	-1.047587	-4.934792	3.195951
H	-2.135945	-4.998629	3.113932
H	-0.636339	-5.945207	3.266216
H	-0.845218	-4.404356	4.130444
Co	-1.367381	-0.792275	-0.116062
C	4.258825	-2.140228	-1.235878
O	3.425308	-2.282806	-2.117724
O	4.460536	-0.999332	-0.573469
C	5.212851	-3.253808	-0.779243
C	6.663160	-2.764732	-0.991546
H	7.364234	-3.553957	-0.700791
H	6.846152	-2.520078	-2.043378
H	6.870006	-1.876079	-0.390746
C	4.982349	-3.551717	0.717449
H	3.973528	-3.939181	0.894281
H	5.694800	-4.311199	1.055471
H	5.123275	-2.653210	1.323364
C	4.957650	-4.515889	-1.614733
H	5.638524	-5.313000	-1.300138
H	3.931158	-4.871860	-1.492989
H	5.116879	-4.322157	-2.678977
O	-2.777967	-2.198428	-1.125133
C	-3.327307	-1.944529	-2.203591
O	-2.728727	-1.242020	-3.151897
C	-4.765785	-2.334690	-2.508259
C	-5.591657	-1.028920	-2.375863
H	-6.645670	-1.248592	-2.571077
H	-5.511307	-0.612511	-1.366684
H	-5.255480	-0.273411	-3.090621
C	-4.879668	-2.891129	-3.940294
H	-4.540635	-2.160966	-4.678592
H	-4.284230	-3.802476	-4.056589
H	-5.924470	-3.138274	-4.151610
C	-5.251978	-3.366328	-1.479849
H	-4.660146	-4.285078	-1.531758
H	-5.178865	-2.971521	-0.463358
H	-6.297291	-3.618029	-1.681808
C	-0.970319	2.738822	1.027167
C	-2.050922	3.377774	1.631074
C	-2.599157	4.554036	1.069451
C	-2.101067	5.112793	-0.087978
C	-0.999168	4.499414	-0.738858
C	-0.433495	3.318179	-0.175921
N	0.636335	2.697279	-0.746533
C	1.169135	3.186945	-1.855596
C	0.666737	4.342447	-2.491107
C	-0.413005	4.993273	-1.931737
N	-0.319413	1.584217	1.444456
H	-3.446455	5.015808	1.567866
H	-2.537366	6.011814	-0.512174
H	-0.822245	5.888093	-2.392329
H	1.137340	4.702386	-3.399181
H	2.032810	2.652703	-2.235479
C	-0.515437	0.994552	2.667929
C	0.597755	0.012393	2.950772
C	1.288149	0.069008	4.187034
C	1.114477	-0.802051	1.933897
C	2.460573	-0.687527	4.326750
C	2.260420	-1.572536	2.087334
C	2.962581	-1.475696	3.288889
H	2.997570	-0.647482	5.270328
H	2.607358	-2.217368	1.294059
H	3.883426	-2.036079	3.423608

O	-1.387724	1.263380	3.497919
H	-2.471751	2.955038	2.531218
C	0.821289	0.945215	5.327071
H	1.522763	0.889913	6.163343
H	0.736720	1.990826	5.014443
H	-0.170857	0.646088	5.671688
Co	1.319325	0.988679	0.415942
C	0.652340	-0.201867	-2.256103
O	1.542546	0.084836	-1.431323
O	-0.564980	-0.474562	-1.905736
C	0.948530	-0.254001	-3.759476
C	0.743916	-1.712768	-4.229839
H	0.928843	-1.776646	-5.306961
H	1.443750	-2.379990	-3.719421
H	-0.275942	-2.058929	-4.040767
C	-0.037995	0.689036	-4.485618
H	0.045515	1.713807	-4.108187
H	0.197020	0.703247	-5.554333
H	-1.076767	0.368188	-4.377605
C	2.391611	0.186741	-4.044437
H	2.585565	0.109980	-5.119463
H	2.559842	1.222326	-3.740561
H	3.096030	-0.446015	-3.505675
O	3.070576	1.728081	0.832533
C	3.861791	2.200465	-0.080313
O	4.106296	1.612472	-1.149874
C	4.524496	3.550187	0.258624
C	5.338522	4.066451	-0.935165
H	5.814269	5.020301	-0.682220
H	6.117433	3.353593	-1.218323
H	4.696560	4.222902	-1.807585
C	3.428737	4.569659	0.633481
H	2.773051	4.776192	-0.218646
H	2.812018	4.191429	1.452471
H	3.886634	5.515200	0.944088
C	5.448632	3.317412	1.473974
H	4.876252	2.946806	2.328641
H	6.230470	2.586306	1.239395
H	5.937037	4.255136	1.761033
H	3.965859	-0.218299	-0.939846
H	-1.828676	-0.954963	-2.812424

TS1-meta

Energy = -2172.39472976 ZPE = -2171.741018 H = -2171.697702 G = -2171.81735

Imaginary frequency: -996.94

C	-1.540000	1.831749	1.350503
C	-2.119935	3.025090	1.766959
C	-3.395297	3.013249	2.381164
C	-4.113140	1.848444	2.574409
C	-3.562094	0.614315	2.142768
C	-2.281004	0.638721	1.540092
N	-1.683289	-0.490961	1.065862
C	-2.291236	-1.671332	1.151129
C	-3.558842	-1.780716	1.759419
C	-4.191267	-0.653838	2.246205
N	-0.252216	1.622553	0.834628
H	-3.816626	3.960169	2.704317
H	-5.091656	1.863713	3.042943
H	-5.175174	-0.723917	2.700912
H	-4.015131	-2.761928	1.814693
H	-1.819990	-2.551422	0.715694
C	0.413819	2.697857	0.201163
C	1.897113	2.723742	0.337728
C	2.710675	3.382052	-0.616249
C	2.470395	2.176821	1.497881
C	4.082938	3.471505	-0.349802
C	3.834555	2.296175	1.749079
C	4.643279	2.951033	0.819117
H	1.825108	1.669338	2.206051
H	4.725335	3.962890	-1.075307
H	4.260636	1.880940	2.656911
H	5.710319	3.050431	0.995221
O	-0.207025	3.599151	-0.359075
H	-1.599802	3.963494	1.628457
C	2.165368	3.954647	-1.902505
H	1.511027	3.236827	-2.403941
H	1.570680	4.851791	-1.713112
H	2.982856	4.211250	-2.581441
C	-2.653146	-5.140467	-1.285903
C	-3.143520	-6.055603	-2.232822
C	-3.288468	-7.427606	-1.943344
C	-2.962287	-7.946412	-0.708093
C	-2.469377	-7.075290	0.297412
C	-2.307937	-5.674669	0.025260
N	-1.841835	-4.819820	0.981706
C	-1.539208	-5.294342	2.177408
C	-1.660244	-6.655506	2.540637
C	-2.124957	-7.539208	1.594154
N	-2.454484	-3.791154	-1.466934
H	-3.669373	-8.086411	-2.720538
H	-3.077637	-9.004216	-0.487934
H	-2.237043	-8.596331	1.822818
H	-1.392106	-6.980268	3.540998
H	-1.178769	-4.569872	2.907979
C	-2.854988	-3.131305	-2.561108
C	-2.518604	-1.653656	-2.421907
C	-3.443249	-0.623514	-2.729154
C	-1.285661	-1.302973	-1.882729
C	-3.119460	0.713395	-2.413852
C	-0.965424	0.033941	-1.535987
C	-1.940938	1.040337	-1.764583
H	-0.583970	-2.108475	-1.681375
H	-3.840512	1.493749	-2.641515
H	0.159244	0.434029	-2.063701
H	-1.740337	2.063586	-1.462305
O	-3.454536	-3.521223	-3.594543
H	-3.415595	-5.675374	-3.207333
C	-4.783125	-0.939567	-3.331695
H	-5.369950	-0.033869	-3.500750
H	-4.652526	-1.487497	-4.268017
H	-5.347737	-1.611321	-2.675573
Co	-0.026815	-0.123842	0.199125
C	2.127809	0.108492	-1.655778
O	1.722021	-0.182825	-0.479069
O	1.372894	0.645432	-2.522953
C	3.543660	-0.300854	-2.060490
C	3.367929	-1.638095	-2.824786
H	4.349043	-2.000466	-3.147018
H	2.914242	-2.401609	-2.184503
H	2.738780	-1.504366	-3.709279
C	4.150441	0.760195	-2.995915
H	4.286514	1.709434	-2.471112
H	5.129658	0.418368	-3.344982
H	3.511014	0.932357	-3.864361
C	4.433081	-0.509812	-0.826604
H	5.432275	-0.819691	-1.148192

H	4.526575	0.412637	-0.249174
H	4.025657	-1.283187	-0.170900

TS3-meta

Energy = -2172.34973847 ZPE = -2171.696575 H = -2171.652819 G = -2171.773929
Imaginary frequency: -1011.44

C	-4.181018	3.927381	0.648254
C	-5.199056	4.760502	0.153948
C	-5.614009	5.920046	0.839415
C	-5.042532	6.296911	2.036595
C	-4.011422	5.496548	2.593552
C	-3.568318	4.311218	1.914726
N	-2.580548	3.524704	2.432854
C	-2.029795	3.867734	3.584448
C	-2.394769	5.014304	4.328130
C	-3.386059	5.824462	3.824984
N	-3.694787	2.783952	0.063793
H	-6.405995	6.526860	0.406160
H	-5.365998	7.190909	2.562968
H	-3.704151	6.717974	4.356885
H	-1.898538	5.236857	5.267586
H	-1.247713	3.209033	3.962706
C	-4.187471	2.254409	-1.062738
C	-3.435110	0.969741	-1.375532
C	-4.083273	-0.229899	-1.760963
C	-2.055758	0.946738	-1.182393
C	-3.333332	-1.421258	-1.850780
C	-1.300920	-0.253720	-1.217761
C	-1.989167	-1.456764	-1.517730
H	-1.567397	1.890649	-0.948541
H	-3.844230	-2.341716	-2.119396
H	-0.190258	-0.064434	-1.869937
H	-1.472177	-2.410196	-1.489237
O	-5.125110	2.620258	-1.815372
H	-5.665730	4.484202	-0.781224
C	-5.565788	-0.265675	-2.005492
H	-6.106340	0.026980	-1.098167
H	-5.840599	0.472525	-2.762415
H	-5.897879	-1.261438	-2.307892
C	1.789903	-1.898162	-0.140761
C	1.619229	-2.499198	-1.365999
C	2.738747	-2.724935	-2.200808
C	4.004418	-2.345194	-1.808444
C	4.206660	-1.725691	-0.546586
C	3.084751	-1.503453	0.303689
N	3.180782	-0.926226	1.532286
C	4.376547	-0.546331	1.945732
C	5.556385	-0.709789	1.177896
C	5.471568	-1.302194	-0.062099
N	0.709577	-1.585875	0.755467
H	2.586028	-3.198023	-3.164760
H	4.859194	-2.514614	-2.456103
H	6.355058	-1.447573	-0.676619
H	6.505592	-0.369945	1.576749
H	4.429230	-0.088397	2.930565
C	-0.246017	-2.707327	1.133857
C	-1.450963	-2.130357	1.715214
C	-2.414661	-2.875573	2.434954
C	-1.609959	-0.758203	1.454328
C	-3.528552	-2.167731	2.896595
C	-2.742839	-0.078235	1.902669
C	-3.690039	-0.799071	2.639063
H	-4.291090	-2.697106	3.460979
H	-2.899418	0.973788	1.666256
H	-4.577348	-0.292566	3.010654
O	0.064647	-3.854468	0.922801
H	0.633514	-2.797292	-1.698214
C	-2.264048	-4.352262	2.690791
H	-3.071576	-4.720954	3.327615
H	-2.274452	-4.913040	1.750816
H	-1.306669	-4.577605	3.171562
Co	-0.255333	0.055677	0.424388
C	1.515496	1.081720	-1.608913
O	0.910137	0.375040	-2.476847
O	1.140029	1.154711	-0.395990
C	2.705334	1.935938	-2.059482
C	3.698541	2.121199	-0.900495
H	4.517245	2.773320	-1.220672
H	3.213056	2.571185	-0.032087
H	4.128744	1.164264	-0.593486
C	3.402005	1.287686	-3.266816
H	2.709280	1.161246	-4.101765
H	4.232484	1.920771	-3.594820
H	3.801688	0.303199	-3.005642
C	2.102522	3.303843	-2.463423
H	2.903089	3.971937	-2.796858
H	1.385436	3.190980	-3.282414
H	1.592696	3.773089	-1.616262
H	1.193212	-1.295542	1.630702

TS5-meta

Energy = -2171.90194126 ZPE = -2171.258857 H = -2171.216085 G = -2171.333429
Imaginary frequency: -94.45

C	-5.118055	0.402350	2.488977
C	-6.076393	0.994969	3.332888
C	-7.352506	0.433489	3.533622
C	-7.736379	-0.738670	2.916272
C	-6.817517	-1.396277	2.059041
C	-5.508250	-0.845575	1.837247
N	-4.612645	-1.474329	1.022010
C	-4.961177	-2.601493	0.426202
C	-6.224816	-3.217234	0.576196
C	-7.145898	-2.608149	1.396289
N	-3.865698	0.879903	2.198855
H	-8.047847	0.945371	4.195741
H	-8.721867	-1.168801	3.073589
H	-8.131689	-3.041159	1.549391
H	-6.447576	-4.143717	0.056266
H	-4.206626	-3.063652	-0.211109
C	-3.327078	1.949546	2.801035
C	-1.922284	2.237297	2.277515
C	-1.288735	3.506334	2.382339
C	-1.208860	1.192724	1.687784
C	0.019140	3.665498	1.875876
C	0.075311	1.358429	1.115974
C	0.682528	2.639286	1.227669
H	-1.705694	0.231164	1.669904
H	0.490825	4.641221	1.959065
H	0.860005	0.467988	1.148198
H	1.676795	2.760251	0.813182
O	-3.792200	2.698445	3.699430
H	-5.802892	1.912117	3.834457
C	-1.969016	4.702061	2.992685
H	-2.961391	4.849636	2.558853

H	-2.142289	4.538034	4.059291
H	-1.369961	5.605788	2.851617
C	1.452027	-1.035601	-1.566653
C	2.619250	-1.598132	-2.073150
C	2.904089	-2.966021	-1.848447
C	2.053560	-3.787959	-1.139012
C	0.850533	-3.250838	-0.607991
C	0.567461	-1.875405	-0.818001
N	-0.561975	-1.283633	-0.324255
C	-1.451973	-2.015111	0.340146
C	-1.253298	-3.389993	0.582183
C	-0.104673	-4.000560	0.121956
N	0.988429	0.263778	-1.720180
H	3.826164	-3.371227	-2.254904
H	2.283923	-4.837124	-0.982689
H	0.077120	-5.055558	0.307043
H	-2.007496	-3.941861	1.131771
H	-2.355113	-1.514480	0.687552
C	1.643358	1.302730	-2.374507
C	0.846628	2.557565	-2.260522
C	1.153069	3.763092	-2.921968
C	-0.301578	2.430303	-1.459647
C	0.253710	4.829139	-2.756998
C	-1.178213	3.503063	-1.312360
C	-0.897759	4.703874	-1.975455
H	0.461797	5.773461	-3.253817
H	-2.046526	3.422268	-0.663146
H	-1.569688	5.552349	-1.871074
O	2.688264	1.168083	-3.013012
H	3.301028	-0.981728	-2.639560
C	2.378897	3.932374	-3.786045
H	2.424027	4.943544	-4.200431
H	3.293002	3.741866	-3.216071
H	2.384334	3.211529	-4.608903
Co	-0.484382	0.695379	-0.722413
C	3.114638	-0.032259	1.099590
O	3.265253	1.039367	0.475964
O	1.994460	-0.523161	1.487585
C	4.391143	-0.826273	1.515119
C	4.062213	-2.268307	1.926483
H	4.973693	-2.791469	2.241910
H	3.347968	-2.285654	2.753395
H	3.621295	-2.822217	1.092186
C	5.392780	-0.826264	0.348148
H	5.586130	0.195561	0.014244
H	6.340696	-1.286741	0.652136
H	4.997062	-1.390491	-0.502527
C	4.996939	-0.064681	2.713786
H	5.926263	-0.542381	3.046885
H	5.219074	0.970433	2.436488
H	4.301228	-0.049899	3.560717

TS7-meta

Energy = -2171.92268291 ZPE = -2171.281509 H = -2171.238605 G = -2171.357043

Imaginary frequency: -1417.04

C	-5.074164	1.931895	1.194692
C	-6.457447	2.114870	1.387824
C	-6.974477	2.929741	2.412649
C	-6.150398	3.615955	3.280837
C	-4.745275	3.491629	3.135649
C	-4.189299	2.651797	2.108363
N	-2.838135	2.525783	1.958577
C	-2.036323	3.204221	2.761546
C	-2.485453	4.055549	3.797169
C	-3.841902	4.187967	3.980995
N	-4.477908	1.125307	0.260411
H	-8.054468	3.020495	2.510987
H	-6.552192	4.253232	4.064115
H	-4.241374	4.826854	4.765331
H	-1.770060	4.581149	4.422102
H	-0.966955	3.081971	2.593030
C	-5.143944	0.586822	-0.774552
C	-4.248671	-0.316663	-1.608651
C	-4.734492	-1.446661	-2.306718
C	-2.876319	-0.034442	-1.677551
C	-3.815842	-2.262833	-2.996245
C	-1.944898	-0.887568	-2.294015
C	-2.447915	-2.017383	-2.965185
H	-2.541612	0.864954	-1.160505
H	-4.191925	-3.139417	-3.519880
H	-0.844630	-0.274760	-2.924392
H	-1.760935	-2.720627	-3.430162
O	-6.343545	0.734410	-1.127874
H	-7.128565	1.607291	0.709519
C	-6.194061	-1.833319	-2.309937
H	-6.598744	-1.855342	-1.294299
H	-6.791500	-1.092604	-2.847383
H	-6.334867	-2.815232	-2.771923
C	2.034424	-1.172310	-0.538695
C	3.372095	-1.372793	-0.834193
C	4.370877	-0.820521	0.009561
C	4.058380	-0.089832	1.138405
C	2.695437	0.117386	1.484634
C	1.703624	-0.425996	0.629544
N	0.367778	-0.279071	0.876754
C	-0.041976	0.377220	1.949238
C	0.879273	0.930821	2.868331
C	2.233782	0.811481	2.633805
N	0.917376	-1.686041	-1.221565
H	5.413110	-0.983433	-0.248923
H	4.837589	0.324272	1.770578
H	2.954761	1.244490	3.321279
H	0.503467	1.453429	3.740350
H	-1.114047	0.504507	2.066236
C	0.797705	-3.091753	-1.210861
C	-0.509596	-3.505611	-0.647778
C	-0.923423	-4.843084	-0.463118
C	-1.286341	-2.426025	-0.193391
C	-2.131253	-5.050197	0.214960
C	-2.479427	-2.656737	0.490797
C	-2.893014	-3.977158	0.693540
H	-2.479544	-6.067508	0.375443
H	-3.099998	-1.826924	0.817840
H	-3.825252	-4.176950	1.217199
O	1.723389	-3.833701	-1.539997
H	3.642986	-1.962507	-1.700506
C	-0.110086	-6.015587	-0.953793
H	-0.631766	-6.957864	-0.762966
H	0.094042	-5.935912	-2.025910
H	0.868393	-6.046152	-0.465251
Co	-0.630568	-0.740855	-0.740025
C	0.438452	1.191905	-2.576104
O	-0.027525	0.431907	-3.500949
O	0.095567	1.085581	-1.369137
C	1.487306	2.230096	-2.985669
C	1.884972	3.092406	-1.779375
H	2.648338	3.817487	-2.080101

H	1.024647	3.640156	-1.384240
H	2.289145	2.474529	-0.972811
C	2.716449	1.446138	-3.500722
H	2.449622	0.822579	-4.357860
H	3.498467	2.148217	-3.808188
H	3.123869	0.799437	-2.716462
C	0.909828	3.106599	-4.114720
H	1.664116	3.826668	-4.448563
H	0.609866	2.494541	-4.968915
H	0.034733	3.667429	-3.768889

1a-1AQ-s

Energy = -1678.5196206 ZPE = -1677.982902 H = -1677.947497 G = -1678.048403

C	-1.534603	-0.635474	-1.632918
C	-2.400808	-1.303116	-2.489831
C	-3.445036	-0.586018	-3.123530
C	-3.639484	0.767860	-2.928262
C	-2.766934	1.483514	-2.066585
C	-1.722206	0.762335	-1.433796
N	-0.840446	1.378572	-0.590145
C	-0.938220	2.671226	-0.324478
C	-1.941798	3.459030	-0.925900
C	-2.849443	2.870791	-1.783803
N	-0.464169	-1.128641	-0.909693
H	-4.113065	-1.129443	-3.784911
H	-4.445639	1.296240	-3.426444
H	-3.635065	3.461781	-2.244855
H	-1.988096	4.516466	-0.693852
H	-0.221470	3.075208	0.379806
C	0.188395	-2.305461	-1.087219
C	1.451062	-2.276609	-0.262419
C	2.713037	-2.458822	-0.858194
C	1.343370	-1.856889	1.086164
C	3.841896	-2.194575	-0.074540
C	2.500351	-1.599218	1.843647
C	3.747815	-1.754334	1.253996
H	0.371083	-1.934646	1.571659
H	4.825732	-2.314902	-0.520612
H	2.406920	-1.287911	2.878852
H	4.653256	-1.555691	1.818833
O	-0.137903	-3.220888	-1.848781
H	-2.264252	-2.361643	-2.663327
C	2.853079	-2.852401	-2.307922
H	3.898628	-3.039221	-2.564206
H	2.261085	-3.741163	-2.534197
H	2.481649	-2.050724	-2.957368
Co	0.284522	0.116901	0.292114
C	-1.923638	-0.930678	1.827852
O	-1.080990	0.040008	1.577095
O	-1.728010	-2.126800	1.605555
C	-3.247953	-0.417804	2.439981
C	-4.134272	-1.606371	2.834701
H	-5.076545	-1.245883	3.261222
H	-4.361503	-2.231722	1.967242
H	-3.636901	-2.236070	3.578181
C	-2.945964	0.454841	3.673909
H	-2.312039	1.303333	3.405613
H	-3.879712	0.837429	4.100517
H	-2.433836	-0.125374	4.449580
C	-3.949797	0.433918	1.358724
H	-4.910829	0.801256	1.735147
H	-3.334945	1.294014	1.080805
H	-4.142506	-0.154598	0.454779
C	2.237764	1.385581	0.243768
O	1.420557	1.444185	1.229016
O	1.885226	0.624073	-0.720879
C	3.516964	2.196874	0.214775
C	3.103755	3.666762	-0.039698
H	3.998858	4.295395	-0.073939
H	2.576660	3.769783	-0.993839
H	2.453573	4.034267	0.759460
C	4.212122	2.076526	1.585262
H	4.499440	1.040324	1.787033
H	5.116498	2.692510	1.592787
H	3.553056	2.412803	2.389260
C	4.435752	1.694134	-0.909148
H	5.356104	2.285862	-0.921291
H	4.699255	0.643341	-0.758017
H	3.952551	1.784763	-1.885406

TS1-1AQ-s

Energy = -1678.50633533 ZPE = -1677.974366 H = -1677.939669 G = -1678.039478

Imaginary frequency: -977.79

C	0.005711	2.884425	-0.360236
C	0.142025	4.265105	-0.251482
C	0.619228	5.016638	-1.351875
C	0.956920	4.432132	-2.556248
C	0.823782	3.027303	-2.710264
C	0.349442	2.270566	-1.605282
N	0.194608	0.914600	-1.682607
C	0.485787	0.265570	-2.797097
C	0.950731	0.943120	-3.944623
C	1.122318	2.310959	-3.898309
N	-0.438348	1.980675	0.592256
H	0.718924	6.091765	-1.234339
H	1.317869	5.027642	-3.388657
H	1.486382	2.852158	-4.766811
H	1.173208	0.376124	-4.841202
H	0.357171	-0.810803	-2.772672
C	-1.143334	2.276456	1.726121
C	-1.629008	1.012768	2.375707
C	-2.741129	0.966185	3.234496
C	-0.930899	-0.165053	2.004900
C	-3.143401	-0.300856	3.689482
C	-1.372742	-1.410764	2.480458
C	-2.477681	-1.476163	3.325196
H	0.348485	-0.010009	2.202701
H	-4.006835	-0.366040	4.346789
H	-0.840983	-2.312966	2.193138
H	-2.826930	-2.431921	3.705281
O	-1.381058	3.417469	2.143932
H	-0.124437	4.750610	0.676459
C	-3.512960	2.195388	3.650132
H	-4.395141	1.918234	4.233529
H	-2.888990	2.865503	4.247420
H	-3.831385	2.775418	2.779655
Co	-0.259378	0.173088	0.079334
C	2.204906	0.349459	1.460512
O	1.641096	0.208005	0.328251
O	1.585650	0.245205	2.559983
C	3.689217	0.725269	1.444912
C	4.299741	0.595951	2.847275
H	5.353439	0.890485	2.817086
H	3.781047	1.236198	3.565025
H	4.241893	-0.435078	3.208938

C	4.434923	-0.176450	0.442819
H	4.003115	-0.090302	-0.556794
H	5.487779	0.119219	0.396333
H	4.390107	-1.226935	0.748947
C	3.741126	2.197180	0.967477
H	4.783006	2.529428	0.918737
H	3.292079	2.300836	-0.024189
H	3.204589	2.855332	1.658825
C	-1.717137	-1.428842	-0.774305
O	-0.486501	-1.694706	-0.552355
O	-2.085381	-0.233118	-0.505549
C	-2.704568	-2.449642	-1.304753
C	-3.310330	-1.892176	-2.611411
H	-4.054241	-2.594899	-2.999429
H	-3.798276	-0.929936	-2.436132
H	-2.539340	-1.754211	-3.376776
C	-1.999188	-3.788688	-1.562033
H	-1.557639	-4.184459	-0.643259
H	-2.723060	-4.517057	-1.940298
H	-1.200467	-3.679497	-2.301266
C	-3.813479	-2.616348	-0.240677
H	-4.556149	-3.336680	-0.597470
H	-3.400795	-2.984397	0.703895
H	-4.313572	-1.664139	-0.046566

1a-1AQ-t

Energy = -1678.51019423 ZPE = -1677.975514 H = -1677.939148 G = -1678.048208

C	-1.610887	-0.665658	-1.458343
C	-2.533767	-1.524356	-2.045381
C	-3.742264	-1.016624	-2.577659
C	-4.053363	0.326455	-2.535586
C	-3.141086	1.236589	-1.939803
C	-1.925766	0.730650	-1.404459
N	-1.018470	1.546449	-0.796981
C	-1.251650	2.844434	-0.692638
C	-2.426139	3.434548	-1.205489
C	-3.364451	2.632336	-1.822458
N	-0.381239	-1.006915	-0.887364
H	-4.440668	-1.716231	-3.026175
H	-4.987500	0.699134	-2.943649
H	-4.282555	3.057011	-2.217803
H	-2.578381	4.502510	-1.100098
H	-0.494032	3.426427	-0.176916
C	0.292187	-2.192744	-1.099329
C	1.608121	-2.272981	-0.374092
C	2.804737	-2.367287	-1.115666
C	1.636998	-2.215670	1.027111
C	4.011837	-2.386037	-0.410084
C	2.857506	-2.233987	1.708864
C	4.046348	-2.315230	0.986584
H	0.696169	-2.180220	1.568368
H	4.944300	-2.444662	-0.965428
H	2.871853	-2.191058	2.793758
H	5.001787	-2.326225	1.503007
O	-0.095865	-3.082191	-1.856284
H	-2.316636	-2.580916	-2.098209
C	2.793090	-2.394493	-2.624907
H	3.808775	-2.446388	-3.024374
H	2.221459	-3.247096	-3.000105
H	2.316638	-1.491195	-3.023846
Co	0.311445	0.298771	0.246165
C	-1.733584	-0.877902	1.892005
O	-0.958840	0.144473	1.603030
O	-1.472783	-2.057709	1.666362
C	-3.094415	-0.478118	2.511575
C	-3.376959	-1.400848	3.710316
H	-4.376545	-1.201550	4.111138
H	-3.321426	-2.449797	3.410347
H	-2.650754	-1.235021	4.513740
C	-3.130916	0.994470	2.944980
H	-2.958806	1.659340	2.094705
H	-4.110297	1.228546	3.376667
H	-2.365649	1.205582	3.698126
C	-4.143237	-0.720893	1.401449
H	-5.145118	-0.492440	1.780986
H	-3.954765	-0.081448	0.533079
H	-4.123203	-1.762372	1.069540
C	2.238829	1.635173	0.257988
O	1.286793	1.790756	1.101603
O	2.054716	0.702335	-0.598238
C	3.515306	2.443897	0.293738
C	3.929397	2.794700	-1.148736
H	4.878377	3.339184	-1.133384
H	4.056208	1.892167	-1.751401
H	3.178678	3.429091	-1.631088
C	3.313273	3.715249	1.132218
H	3.012152	3.471409	2.154073
H	4.249921	4.279564	1.171957
H	2.543488	4.358082	0.694105
C	4.587033	1.530847	0.941845
H	5.543061	2.062564	0.972208
H	4.308965	1.263241	1.966128
H	4.714203	0.608784	0.368463

TS1-1AQ-t

Energy = -1678.49134373 ZPE = -1677.961151 H = -1677.9256 G = -1678.02975

Imaginary frequency: -837.01

C	0.052637	2.961758	-0.275842
C	0.275005	4.322961	-0.115907
C	0.800107	5.080367	-1.192831
C	1.096846	4.514511	-2.415557
C	0.874102	3.125781	-2.617725
C	0.354963	2.368502	-1.536801
N	0.116596	1.027064	-1.649217
C	0.365933	0.393162	-2.783495
C	0.870694	1.074183	-3.910728
C	1.126148	2.428433	-3.826618
N	-0.438032	2.041784	0.652732
H	0.970364	6.141498	-1.039079
H	1.496241	5.112920	-3.228030
H	1.521479	2.970369	-4.680652
H	1.057094	0.521146	-4.823932
H	0.169737	-0.673330	-2.784806
C	-1.118781	2.349416	1.817357
C	-1.640785	1.093251	2.443223
C	-2.772080	1.057341	3.274259
C	-0.961725	-0.092279	2.062007
C	-3.218052	-0.211675	3.681386
C	-1.453017	-1.340951	2.479506
C	-2.579788	-1.396015	3.293612
H	0.301570	0.017158	2.188987
H	-4.099326	-0.272526	4.314592
H	-0.941055	-2.247522	2.172548
H	-2.968601	-2.351211	3.633685
O	-1.299510	3.487794	2.248138

H	0.045247	4.794346	0.828939
C	-3.516239	2.298484	3.701171
H	-4.425024	2.035510	4.248375
H	-2.890212	2.928802	4.338724
H	-3.788246	2.912260	2.838021
Co	-0.333371	0.251542	0.112822
C	2.254312	0.260374	1.411229
O	1.717662	-0.027126	0.296481
O	1.617534	0.261119	2.510824
C	3.725805	0.697652	1.391559
C	4.277175	0.858622	2.814347
H	5.320942	1.187049	2.772454
H	3.703583	1.598480	3.378567
H	4.236087	-0.087780	3.361803
C	4.548805	-0.341636	0.606282
H	4.148414	-0.472227	-0.401804
H	5.589577	-0.010061	0.529835
H	4.539226	-1.314295	1.110014
C	3.751165	2.054682	0.647985
H	4.780439	2.421792	0.579227
H	3.346718	1.949048	-0.362376
H	3.154748	2.805862	1.176992
C	-1.942275	-1.417365	-0.801169
O	-0.670939	-1.543926	-0.606900
O	-2.496994	-0.326207	-0.521938
C	-2.742596	-2.594195	-1.359562
C	-3.397572	-2.129832	-2.677558
H	-4.018882	-2.932314	-3.088502
H	-4.026055	-1.251723	-2.508683
H	-2.638397	-1.871387	-3.424088
C	-1.840008	-3.810549	-1.609390
H	-1.359878	-4.141080	-0.684044
H	-2.435680	-4.639663	-2.005404
H	-1.052466	-3.576057	-2.331210
C	-3.835560	-2.940564	-0.325059
H	-4.454222	-3.763027	-0.698759
H	-3.392245	-3.251439	0.627012
H	-4.477799	-2.076722	-0.136002

1a-1AQ-q

Energy = -1678.52204008 ZPE = -1677.989091 H = -1677.951977 G = -1678.061099

C	-1.058615	-1.955480	0.834599
C	-1.284121	-2.896893	1.876403
C	-2.471363	-3.628574	1.932643
C	-3.467386	-3.465432	0.975876
C	-3.296142	-2.542559	-0.097171
C	-2.095863	-1.793471	-0.174555
N	-1.862242	-0.915111	-1.174667
C	-2.793668	-0.720379	-2.105259
C	-4.020213	-1.407155	-2.103388
C	-4.269911	-2.323863	-1.099868
N	0.006392	-1.158205	0.716880
H	-2.620086	-4.331607	2.745213
H	-4.388818	-4.035649	1.037289
H	-5.203502	-2.876993	-1.069073
H	-4.746942	-1.210848	-2.882919
H	-2.558746	0.010669	-2.871792
C	1.205978	-1.382216	1.442905
C	1.886709	-0.144269	1.895692
C	3.282309	-0.118857	2.137534
C	1.107176	1.010948	2.089133
C	3.846910	1.097373	2.542518
C	1.693185	2.200233	2.511416
C	3.071497	2.243345	2.729622
H	0.035486	0.967048	1.912408
H	4.918832	1.144822	2.713106
H	1.080837	3.084266	2.659928
H	3.546448	3.167619	3.045891
O	1.642123	-2.517726	1.596026
H	-0.525757	-3.031462	2.636325
C	4.174082	-1.323070	1.957010
H	5.225364	-1.033780	2.032830
H	3.963044	-2.085303	2.712308
H	4.011244	-1.803351	0.988294
Co	-0.061520	0.222659	-0.899115
C	-2.049511	1.867171	0.372408
O	-1.088734	1.843224	-0.503567
O	-2.183170	1.043656	1.289611
C	-3.056739	3.023259	0.181664
C	-4.108449	3.006609	1.298745
H	-4.821528	3.827217	1.160817
H	-4.662562	2.063668	1.302347
H	-3.638881	3.118104	2.280480
C	-2.287907	4.359556	0.194679
H	-1.528014	4.375145	-0.590386
H	-2.976465	5.196771	0.033340
H	-1.788093	4.514622	1.157759
C	-3.737733	2.829362	-1.189936
H	-4.456922	3.634730	-1.376931
H	-2.994672	2.831160	-1.991870
H	-4.279521	1.877043	-1.227890
C	2.241424	-0.023206	-1.779517
O	1.751586	1.081825	-1.358073
O	1.507662	-1.058404	-1.783933
C	3.679164	-0.054702	-2.299423
C	4.188581	-1.500338	-2.394764
H	5.210403	-1.510088	-2.788301
H	4.196303	-1.981594	-1.411865
H	3.555205	-2.098247	-3.054610
C	3.654449	0.592495	-3.704258
H	3.278796	1.618537	-3.651868
H	4.666509	0.614001	-4.122153
H	3.015022	0.023811	-4.387969
C	4.579601	0.774675	-1.364066
H	5.605821	0.783518	-1.746320
H	4.222783	1.804661	-1.294054
H	4.593997	0.354963	-0.354096

TS1-1AQ-q

Energy = -1678.47620439 ZPE = -1677.948524 H = -1677.911923 G = -1678.020541

Imaginary frequency: -901.39

C	0.030050	2.960348	-0.415959
C	0.199038	4.362253	-0.251074
C	0.625701	5.156728	-1.318469
C	0.880396	4.615617	-2.573761
C	0.708642	3.220723	-2.808227
C	0.289259	2.392629	-1.737338
N	0.083525	1.065584	-1.899064
C	0.285121	0.509385	-3.089095
C	0.706740	1.249952	-4.208401
C	0.920098	2.607882	-4.066747
N	-0.360409	2.067386	0.505062
H	0.760711	6.221391	-1.159409
H	1.206410	5.250768	-3.391481
H	1.243434	3.212895	-4.908262

H	0.856881	0.751060	-5.158754
H	0.109595	-0.560771	-3.145311
C	-0.836890	2.368680	1.804171
C	-1.528450	1.188439	2.400481
C	-2.640196	1.369081	3.259018
C	-1.039226	-0.098487	2.040736
C	-3.282358	0.214784	3.723112
C	-1.715429	-1.213810	2.557058
C	-2.833106	-1.064683	3.378807
H	0.442942	-0.134301	2.130217
H	-4.152802	0.320645	4.365595
H	-1.365004	-2.211234	2.300168
H	-3.360381	-1.936565	3.758282
O	-0.715943	3.463759	2.346616
H	0.008998	4.792517	0.721468
C	-3.162189	2.727756	3.663968
H	-4.128588	2.634809	4.166759
H	-2.464310	3.229858	4.340479
H	-3.279667	3.390076	2.800969
Co	-0.312377	0.050341	-0.047566
C	2.268378	0.186499	1.364094
O	1.799405	0.077132	0.207874
O	1.558190	0.009607	2.430248
C	3.710483	0.656312	1.563773
C	4.299737	0.093476	2.867515
H	5.315875	0.475990	3.007839
H	3.697155	0.382943	3.731212
H	4.349005	-0.999906	2.836947
C	4.572757	0.247399	0.359053
H	4.163707	0.648609	-0.571004
H	5.590805	0.628763	0.486637
H	4.625905	-0.842165	0.265299
C	3.618198	2.201245	1.646195
H	4.618645	2.624133	1.783274
H	3.190484	2.615942	0.727503
H	2.993091	2.511821	2.489090
C	-1.761032	-1.750164	-0.940527
O	-0.529761	-1.945179	-0.655408
O	-2.253034	-0.586051	-0.833683
C	-2.659071	-2.913859	-1.372277
C	-3.334468	-2.540578	-2.707316
H	-4.019670	-3.336582	-3.018152
H	-3.900860	-1.611390	-2.607553
H	-2.590202	-2.405183	-3.500223
C	-1.847523	-4.207271	-1.528220
H	-1.360511	-4.481532	-0.588529
H	-2.506861	-5.028381	-1.829899
H	-1.068303	-4.094267	-2.287913
C	-3.733945	-3.088638	-0.276402
H	-4.413518	-3.904750	-0.544206
H	-3.275136	-3.327650	0.689090
H	-4.316597	-2.171486	-0.157348

2_anion_d

Energy = -1678.67331913 ZPE = -1678.139663 H = -1678.103172 G = -1678.208437

C	-1.593344	-0.731399	-1.429178
C	-2.497933	-1.604209	-2.037564
C	-3.720514	-1.132695	-2.565829
C	-4.078254	0.198729	-2.514421
C	-3.187127	1.130338	-1.922220
C	-1.947259	0.667548	-1.388696
N	-1.054833	1.526288	-0.816909
C	-1.334038	2.814907	-0.741855
C	-2.538253	3.363526	-1.237676
C	-3.457163	2.520793	-1.823539
N	-0.380914	-1.052794	-0.835321
H	-4.397747	-1.852399	-3.018327
H	-5.024353	0.546688	-2.918457
H	-4.395622	2.905459	-2.214049
H	-2.722795	4.428756	-1.148674
H	-0.584817	3.438061	-0.260174
C	0.242390	-2.248221	-0.975637
C	1.573887	-2.306685	-0.257373
C	2.763841	-2.511413	-0.986157
C	1.616562	-2.141343	1.134576
C	3.976261	-2.525585	-0.286977
C	2.839612	-2.161173	1.813203
C	4.022985	-2.347389	1.099365
H	0.677643	-2.018677	1.670728
H	4.901845	-2.667663	-0.840064
H	2.862231	-2.033052	2.892159
H	4.979996	-2.359078	1.613979
O	-0.148897	-3.227712	-1.638491
H	-2.247993	-2.653348	-2.092650
C	2.741046	-2.668675	-2.488114
H	3.747628	-2.824681	-2.885792
H	2.104904	-3.506821	-2.783146
H	2.322272	-1.774250	-2.965058
Co	0.385004	0.351661	0.274143
C	-1.769392	-0.724545	1.991663
O	-0.977168	0.239001	1.667536
O	-1.482113	-1.933663	2.024703
C	-3.216310	-0.302099	2.377612
C	-3.507380	-0.818976	3.799110
H	-4.546636	-0.612906	4.082019
H	-3.336339	-1.897484	3.853156
H	-2.856095	-0.333369	4.535676
C	-3.409003	1.219466	2.313896
H	-3.199193	1.597866	1.309845
H	-4.441358	1.481675	2.576785
H	-2.736973	1.732470	3.008285
C	-4.171047	-0.983956	1.375001
H	-5.214770	-0.766536	1.632523
H	-3.990345	-0.629235	0.355269
H	-4.025584	-2.067432	1.387168
C	2.360799	1.647565	0.187371
O	1.519863	1.768943	1.142241
O	2.090302	0.814768	-0.737826
C	3.662260	2.441274	0.149259
C	3.732432	3.188694	-1.198604
H	4.679234	3.733782	-1.275614
H	3.664210	2.487278	-2.033932
H	2.914674	3.912093	-1.289725
C	3.727722	3.434446	1.317628
H	3.674566	2.915472	2.278578
H	4.667794	3.995014	1.277758
H	2.898762	4.147190	1.275557
C	4.821986	1.424119	0.241454
H	5.782839	1.947326	0.189416
H	4.783479	0.868050	1.184114
H	4.769186	0.701524	-0.576708

TSch_anion_d

Energy = -1678.64561477 ZPE = -1678.116867 H = -1678.081091 G = -1678.185385

Imaginary frequency: -1341.42

C	0.208808	2.937463	-0.401618
C	0.626993	4.260564	-0.250158
C	1.177208	4.963170	-1.347308
C	1.317155	4.391968	-2.597270
C	0.898554	3.050084	-2.799517
C	0.352251	2.334363	-1.698968
N	-0.066299	1.035724	-1.818578
C	0.029504	0.416732	-2.984599
C	0.549116	1.055335	-4.131480
C	0.982686	2.360924	-4.038111
N	-0.351930	2.088184	0.529254
H	1.498181	5.989933	-1.192060
H	1.739740	4.949743	-3.427444
H	1.392490	2.873581	-4.904151
H	0.605397	0.508317	-5.066267
H	-0.298987	-0.617017	-2.996364
C	-0.824601	2.440664	1.759753
C	-1.525312	1.267664	2.396470
C	-2.526871	1.416396	3.376662
C	-1.161730	-0.007249	1.890234
C	-3.165106	0.250851	3.830862
C	-1.823435	-1.141050	2.383051
C	-2.826247	-1.015258	3.344370
H	0.205820	-0.144355	1.857544
H	-3.947464	0.341692	4.581243
H	-1.550456	-2.120255	1.997422
H	-3.347540	-1.892970	3.719136
O	-0.736027	3.565162	2.284676
H	0.518991	4.735138	0.714787
C	-2.946380	2.758955	3.930516
H	-3.811603	2.650977	4.591814
H	-2.131227	3.227037	4.489290
H	-3.199295	3.459485	3.129652
Co	-0.506134	0.265641	-0.056491
C	2.154437	0.181105	1.234930
O	1.761270	0.041665	0.058022
O	1.419775	-0.084901	2.263201
C	3.536628	0.789766	1.529915
C	4.234583	0.008585	2.657172
H	5.194003	0.477421	2.902750
H	3.615632	-0.011093	3.557237
H	4.431636	-1.026333	2.355605
C	4.402214	0.793740	0.262304
H	3.912754	1.349917	-0.540981
H	5.371947	1.258882	0.470926
H	4.580863	-0.225179	-0.096102
C	3.268388	2.244009	1.985230
H	4.215283	2.748101	2.209128
H	2.752620	2.810574	1.202489
H	2.644288	2.260082	2.883143
C	-2.089967	-1.582691	-0.971045
O	-0.836520	-1.551827	-0.676379
O	-2.827729	-0.575261	-0.904888
C	-2.689854	-2.934820	-1.410721
C	-3.312842	-2.746744	-2.808292
H	-3.804523	-3.669638	-3.136496
H	-4.052038	-1.941827	-2.791500
H	-2.546355	-2.491044	-3.549411
C	-1.627500	-4.041728	-1.450578
H	-1.170017	-4.182341	-0.467291
H	-2.081665	-4.990099	-1.760946
H	-0.828310	-3.795107	-2.155680
C	-3.794673	-3.299048	-0.397242
H	-4.284035	-4.236651	-0.684605
H	-3.377531	-3.426917	0.608007
H	-4.547468	-2.507857	-0.353223

2_anion_quar

Energy = -1678.69691404 ZPE = -1678.163495 H = -1678.12658 G = -1678.235421

C	-1.846325	1.704243	-1.072962
C	-2.413848	2.548980	-2.029957
C	-3.642985	3.206314	-1.795926
C	-4.342084	3.054033	-0.618394
C	-3.811572	2.211952	0.391974
C	-2.570649	1.542828	0.166382
N	-2.031188	0.728106	1.123327
C	-2.657741	0.542824	2.276579
C	-3.885463	1.164222	2.578672
C	-4.454565	1.994339	1.636699
N	-0.660221	0.984085	-1.175793
H	-4.039723	3.849320	-2.577001
H	-5.285457	3.563618	-0.447666
H	-5.400340	2.491322	1.834906
H	-4.359668	0.982786	3.536633
H	-2.171991	-0.121241	2.985492
C	0.228406	1.148825	-2.192026
C	1.434217	0.244225	-2.072898
C	2.735170	0.787831	-2.011611
C	1.245244	-1.143676	-2.030892
C	3.814725	-0.096417	-1.901010
C	2.337287	-2.009436	-1.928162
C	3.626085	-1.481843	-1.860502
H	0.234010	-1.539531	-2.063063
H	4.821946	0.308479	-1.838834
H	2.176158	-3.082481	-1.891769
H	4.485160	-2.141558	-1.774614
O	0.144716	1.938443	-3.149472
H	-1.888946	2.696743	-2.961684
C	2.955804	2.281568	-1.996774
H	4.022094	2.522960	-2.020122
H	2.461023	2.758763	-2.845414
H	2.528710	2.705591	-1.080616
Co	-0.278257	-0.168518	0.446948
C	-1.249399	-2.766290	-0.078633
O	-0.399924	-2.119449	0.653437
O	-2.000099	-2.235277	-0.914269
C	-1.239020	-4.300022	0.123346
C	-2.392190	-4.951641	-0.651767
H	-2.367508	-6.040038	-0.524136
H	-3.360483	-4.585779	-0.295982
H	-2.324279	-4.723799	-1.718682
C	0.112779	-4.827198	-0.404852
H	0.945392	-4.348729	0.117677
H	0.184027	-5.911260	-0.259128
H	0.218572	-4.623504	-1.476603
C	-1.364977	-4.617023	1.625930
H	-1.330249	-5.700086	1.791458
H	-0.552958	-4.150381	2.188328
H	-2.315279	-4.245582	2.026789
C	2.015908	1.200325	1.522314
O	1.407398	0.063890	1.408176
O	1.533926	2.301344	1.209330
C	3.428697	1.138944	2.159407
C	3.267459	1.607870	3.622336
H	4.237610	1.611610	4.132773
H	2.852791	2.619929	3.657645

H	2.595562	0.941790	4.175552
C	4.008083	-0.283144	2.125116
H	4.087283	-0.645961	1.095717
H	5.008910	-0.293499	2.573511
H	3.373456	-0.980525	2.677323
C	4.365462	2.102564	1.410632
H	5.339588	2.154201	1.910754
H	4.528382	1.763595	0.382876
H	3.933818	3.105112	1.371808

TSch_anion_quar

Energy = -1678.6451462 ZPE = -1678.116174 H = -1678.080007 G = -1678.186385

Imaginary frequency: -235.05

C	0.142447	2.954444	-0.344316
C	0.566804	4.260656	-0.077496
C	1.259722	5.014305	-1.051491
C	1.542629	4.513047	-2.305449
C	1.128500	3.195081	-2.632830
C	0.438156	2.416640	-1.655793
N	0.032488	1.140865	-1.920503
C	0.254685	0.611844	-3.110836
C	0.920303	1.309665	-4.142751
C	1.359820	2.592144	-3.897140
N	-0.532239	2.088283	0.486804
H	1.574296	6.023065	-0.795563
H	2.072328	5.105575	-3.045646
H	1.883412	3.157130	-4.664002
H	1.080578	0.830085	-5.102482
H	-0.101292	-0.404817	-3.255522
C	-0.963861	2.375320	1.747900
C	-1.645769	1.182736	2.389677
C	-2.701858	1.352177	3.313061
C	-1.180848	-0.101187	1.999863
C	-3.305059	0.195223	3.830082
C	-1.818436	-1.221473	2.559561
C	-2.875204	-1.082777	3.462235
H	0.414570	-0.105154	2.047483
H	-4.131217	0.301956	4.530387
H	-1.491233	-2.216781	2.262609
H	-3.369820	-1.957872	3.879609
O	-0.842870	3.463524	2.344457
H	0.349506	4.682057	0.893371
C	-3.219183	2.707744	3.743375
H	-4.137392	2.603264	4.330398
H	-2.476484	3.241836	4.342352
H	-3.425629	3.350634	2.882493
Co	-0.576834	0.107887	-0.085722
C	2.128808	0.263104	1.158793
O	1.651518	0.001713	0.042521
O	1.473409	0.088237	2.276192
C	3.521622	0.879153	1.311720
C	4.355589	0.025969	2.287803
H	5.339837	0.483625	2.432929
H	3.861542	-0.051156	3.259516
H	4.506613	-0.986121	1.896701
C	4.210394	0.964732	-0.057560
H	3.621171	1.568010	-0.753709
H	5.198539	1.423482	0.052585
H	4.337958	-0.028250	-0.498632
C	3.322043	2.300247	1.889462
H	4.295065	2.787753	2.012351
H	2.711046	2.913541	1.218870
H	2.826679	2.259896	2.862921
C	-1.802297	-1.917770	-0.955761
O	-0.659260	-2.112020	-0.451928
O	-2.238767	-0.730744	-1.136425
C	-2.720623	-3.095714	-1.316150
C	-3.196890	-2.929151	-2.772163
H	-3.899503	-3.727618	-3.036307
H	-3.695451	-1.965979	-2.905633
H	-2.352863	-2.977079	-3.469898
C	-1.987640	-4.433007	-1.144722
H	-1.641594	-4.560269	-0.115559
H	-2.657096	-5.264467	-1.392758
H	-1.112415	-4.488986	-1.799219
C	-3.933516	-3.030941	-0.361672
H	-4.620949	-3.859666	-0.565180
H	-3.612777	-3.098215	0.683698
H	-4.473661	-2.089101	-0.489932

D'-3

Energy = -1824.97699947 ZPE = -1824.476625 H = -1824.443825 G = -1824.538278

C	-2.642695	-0.822543	0.291622
C	-3.970465	-1.052065	0.671468
C	-4.755591	-2.006857	-0.011103
C	-4.267704	-2.751528	-1.068315
C	-2.927801	-2.555082	-1.491694
C	-2.126584	-1.593334	-0.810877
N	-0.830050	-1.353819	-1.171498
C	-0.289199	-2.025012	-2.174883
C	-1.007888	-2.998105	-2.903186
C	-2.317876	-3.259248	-2.563475
N	-1.728166	0.051317	0.829778
H	-5.782256	-2.155047	0.314658
H	-4.888478	-3.481203	-1.579575
H	-2.896460	-4.001228	-3.107279
H	-0.520792	-3.523430	-3.717744
H	0.742421	-1.779612	-2.406019
C	-1.955048	0.924165	1.859364
C	-0.720741	1.725225	2.132886
C	-0.629515	2.683945	3.169283
C	0.371210	1.454134	1.273766
C	0.586658	3.362973	3.324982
C	1.567462	2.154643	1.464095
C	1.674117	3.102067	2.485491
H	0.681426	4.103811	4.116033
H	2.415509	1.958642	0.813440
H	2.606282	3.644966	2.632218
O	-3.027929	1.039821	2.484703
H	-4.379839	-0.485436	1.495070
C	-1.774855	3.001814	4.104418
H	-2.650626	3.359461	3.555440
H	-2.110420	2.111181	4.643392
H	-1.476678	3.764443	4.831246
C	2.645989	-0.813839	-0.285495
C	3.974475	-1.041032	-0.664224
C	4.764090	-1.986446	0.026138
C	4.279940	-2.723976	1.090075
C	2.939370	-2.529775	1.512349
C	2.133662	-1.577404	0.823719
N	0.836222	-1.340620	1.182712
C	0.298621	-2.005688	2.191898
C	1.021856	-2.969370	2.928195
C	2.332915	-3.227525	2.590300
N	1.727861	0.052294	-0.830019

H	5.791224	-2.133045	-0.298856
H	4.904106	-3.446489	1.607344
H	2.914965	-3.962258	3.140208
H	0.537305	-3.489980	3.747287
H	-0.734013	-1.762833	2.421209
C	1.949491	0.914438	-1.869609
C	0.712567	1.709938	-2.147673
C	0.617567	2.660835	-3.190883
C	-0.377352	1.442967	-1.284665
C	-0.600168	3.336518	-3.349155
C	-1.575212	2.139897	-1.477725
C	-1.685511	3.079816	-2.505668
H	-0.697759	4.071463	-4.145345
H	-2.421669	1.947133	-0.824037
H	-2.618884	3.620083	-2.654422
O	3.020168	1.025822	-2.499560
H	4.380650	-0.479846	-1.493097
C	1.760561	2.974305	-4.130386
H	1.459405	3.730965	-4.862192
H	2.636458	3.337997	-3.585537
H	2.097212	2.080489	-4.663304
Co	-0.000228	0.081752	-0.000159

TS6c-s

Energy = -1824.9267333 ZPE = -1824.429127 H = -1824.396384 G = -1824.490945

Imaginary frequency: -110.90

C	0.913316	-1.907777	1.204156
C	1.611597	-2.703650	2.115410
C	2.732170	-3.453759	1.691521
C	3.178005	-3.441216	0.383331
C	2.487656	-2.659987	-0.581466
C	1.360326	-1.900965	-0.161644
N	0.619951	-1.143050	-1.033629
C	0.969655	-1.110812	-2.314362
C	2.081284	-1.822019	-2.815906
C	2.837410	-2.592335	-1.957055
N	-0.187975	-1.106448	1.418865
H	3.257806	-4.057316	2.427384
H	4.042834	-4.023271	0.078311
H	3.694502	-3.154456	-2.317925
H	2.321928	-1.756812	-3.872093
H	0.340672	-0.502120	-2.956966
C	-1.033326	-1.196462	2.478337
C	-2.266168	-0.374686	2.224390
C	-2.913808	0.286774	3.287043
C	-2.680601	-0.173456	0.853960
C	-3.968980	1.164670	3.004781
C	-3.763526	0.722436	0.636639
C	-4.380182	1.384194	1.684254
H	-4.465253	1.682635	3.821269
H	-4.128332	0.872460	-0.374048
H	-5.200701	2.068395	1.480377
O	-0.858178	-1.871174	3.515156
H	1.278519	-2.734858	3.143383
C	-2.478437	0.120289	4.727834
H	-2.676035	-0.892778	5.087329
H	-1.401699	0.273865	4.842837
H	-3.004709	0.832786	5.370440
C	-1.149026	2.171304	-1.704433
C	-1.468482	3.096634	-2.701399
C	-0.956774	4.412761	-2.641167
C	-0.139594	4.841662	-1.612336
C	0.195578	3.940756	-0.566555
C	-0.313853	2.613644	-0.621221
N	-0.062471	1.689949	0.361873
C	0.687355	2.043631	1.399058
C	1.245029	3.334155	1.528724
C	1.002338	4.278608	0.553219
N	-1.535332	0.852991	-1.590966
H	-1.218167	5.105298	-3.437522
H	0.245312	5.856987	-1.585302
H	1.414339	5.281138	0.630732
H	1.852913	3.566257	2.397231
H	0.845066	1.273968	2.148726
C	-2.581799	0.279151	-2.242454
C	-2.867070	-1.075376	-1.662498
C	-3.341712	-2.119835	-2.481252
C	-2.505880	-1.310457	-0.279584
C	-3.446877	-3.412272	-1.950071
C	-2.640592	-2.645854	0.197877
C	-3.084924	-3.668517	-0.620694
H	-3.804060	-4.221897	-2.581049
H	-2.409653	-2.859672	1.236149
H	-3.168205	-4.677754	-0.223572
O	-3.243393	0.785973	-3.174020
H	-2.111502	2.786791	-3.513142
C	-3.696606	-1.907065	-3.938004
H	-4.562059	-1.248347	-4.044447
H	-2.882760	-1.419601	-4.482825
H	-3.917069	-2.864063	-4.420894
Co	-0.825466	-0.116388	-0.095389

TS6c-t

Energy = -1824.91881755 ZPE = -1824.422593 H = -1824.389003 G = -1824.488389

Imaginary frequency: -232.91

C	0.695786	-2.939256	-0.171222
C	0.740196	-4.281289	-0.563243
C	-0.140108	-5.233632	-0.003276
C	-1.076112	-4.897208	0.954739
C	-1.151252	-3.553367	1.405473
C	-0.262499	-2.582234	0.853329
N	-0.271635	-1.284751	1.278519
C	-1.135009	-0.899814	2.203720
C	-2.064986	-1.785090	2.791835
C	-2.065991	-3.105171	2.394286
N	1.436519	-1.887309	-0.656891
H	-0.074371	-6.263126	-0.346959
H	-1.749434	-5.639710	1.373005
H	-2.762017	-3.816378	2.831751
H	-2.755642	-1.420444	3.544803
H	-1.087739	0.149262	2.485213
C	2.627769	-2.010181	-1.299031
C	3.222945	-0.654041	-1.580711
C	4.090314	-0.450722	-2.677582
C	2.817436	0.445297	-0.757525
C	4.512752	0.852416	-2.974515
C	3.259248	1.738419	-1.105576
C	4.086227	1.938227	-2.204350
H	5.167676	1.017231	-3.826471
H	2.964529	2.585748	-0.495997
H	4.411413	2.944342	-2.459578
O	3.203444	-3.074918	-1.612407
H	1.464327	-4.575518	-1.310239
C	4.547335	-1.579032	-3.577694
H	5.187588	-2.281740	-3.038539
H	3.702880	-2.169914	-3.943296

H	5.098941	-1.182670	-4.436022
C	-0.484292	2.542017	0.245566
C	-1.009043	3.789521	0.600040
C	-2.146026	4.314685	-0.053247
C	-2.790349	3.636675	-1.068995
C	-2.288720	2.375450	-1.484322
C	-1.134662	1.836722	-0.839382
N	-0.594733	0.643678	-1.226996
C	-1.159038	-0.050871	-2.200977
C	-2.314222	0.392667	-2.881459
C	-2.869147	1.603146	-2.524492
N	0.570751	1.870370	0.817151
H	-2.522339	5.284268	0.263947
H	-3.666684	4.050919	-1.558939
H	-3.752774	1.980645	-3.032710
H	-2.742190	-0.215076	-3.671647
H	-0.677815	-0.994146	-2.447212
C	1.536459	2.444108	1.581988
C	2.594117	1.434734	1.952892
C	3.348589	1.571843	3.140199
C	2.755563	0.284626	1.115687
C	4.228959	0.543777	3.505076
C	3.644618	-0.726489	1.532095
C	4.362533	-0.601721	2.715443
H	4.802097	0.636697	4.424158
H	3.783637	-1.604362	0.910242
H	5.039599	-1.395576	3.022945
O	1.596765	3.640840	1.937905
H	-0.525136	4.345076	1.391185
C	3.211486	2.763553	4.064125
H	3.554290	3.682211	3.581692
H	2.167305	2.943869	4.335159
H	3.790527	2.604657	4.979262
Co	1.041892	0.002597	0.083990

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