Supporting Information for

Accurate computed spin-state energetics for Co(III) complexes: implications for modelling homogeneous catalysis.

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S1. Overview of the CASSCF/NEVPT2 Procedure

Firstly, a single-point calculation was performed at the BP86/def2-TZVPP level, and the orbitals were then localized. The localized Kohn-Sham orbitals were then inspected, with the orbitals that correspond to M-L σ-bonds noted.

In the subsequent CASSCF/NEVPT2(10,7) calculations, the input localized BP86 orbitals were rotated prior to the CASSCF iterations, such that the σ-bonding M-L orbitals were situated behind the frontier non-bonding and σ* anti-bonding M-L orbitals. The CASSCF/NEVPT2 calculations were then performed, and the resulting active-space inspected to confirm the presence of 2 σ-bonding, 2 σ*-antibonding and 3 non-bonding d orbitals are present in the active space. If any of these were missing in the resulting active space in the final CAS orbitals, further orbital rotations were performed to ensure the correct selection of active space.

Once the correct (10,7) active space was achieved for each complex in both the singlet and triplet spin-states, this wavefunction was employed in a subsequent CASSCF/NEVPT2(10,12) calculation. The "extorbs doubleshell" keyword was invoked, a feature in the ORCA software package that automatically detects the double-shell (4d) orbitals and rotates them to be the first virtual orbitals of the (10,7) calculation, enabling their direct inclusion in the expanded (10,12) active space.

In some cases, the CASSCF calculation struggled to converge in the singlet or triplet states. This was typically resolved by performing a CASSCF calculation of the singlet/triplet geometry in the alternative triplet/singlet spin-state, and subsequently using the resulting orbitals to be read in the desired singlet/triplet spin-state, respectively. Smoother convergence was achieved with this strategy in some of the troublesome cases.

Additionally, convergence problems were encountered for **Co3** when the CPCM continuum approximation was used at the CASSCF level. For **^{1}Co3**, the energy convergence ("etol" keyword in the "%CASSCF" block) and gradient tolerance ("gtol") were both modified to 1 x 10^{-6} from the default values (2.5 x 10^{-8} and 1 x 10^{-4}, respectively), while the convergence algorithms were changed to the SuperCI algorithm for the "orbstep" selection (i.e. algorithm used when convergence is far from the required criteria) and GDIIS for the "switchstep" (when convergence is close to the criteria) instead of the default SuperCIPT algorithm. For **^{3}Co3**, "etol" and "gtol" were lowered to 1 x 10^{-8}, again with the "orbstep" and "switchstep" convergence algorithms modified to SupCI and GDIIS, respectively.

S2. Efforts to Improve the Spin-State Energetics of Species Co5

To assess whether any improvements can be made at this level of theory for **Co5**, the active spaces for both singlet (**^{1}Co5**) and triplet (**^{3}Co5**) species were initially inspected. For **^{1}Co5**, all M-L bonds are adequately covered in the two M-L σ-bonding orbitals (Figure S1a and S1b) which both feature in the active space. However, in **^{3}Co5** the Co-N σ-bond trans to the Co-S σ-bond is not included in the active space, while the remaining 5 M-L bonds are covered in the two σ-bonding molecular orbitals and are in the active space (see Figure S1c and S1d). This can be rationalized by the distortion from an ideal octahedral geometry seen in **^{3}Co5**. In **^{1}Co5** the N_6─Co_1─S_2 bond angle is 174.9 °, and so the near-linear L─Co─L relationship leads to both σ-bonds being captured in a single MO. In **^{3}Co5**, however, this bond angle is 155.7 °, and so this distortion results in the two σ-bonds being described as two separate MOs in the CASSCF wavefunction, where only the Co_1─S_2 is in the active space.

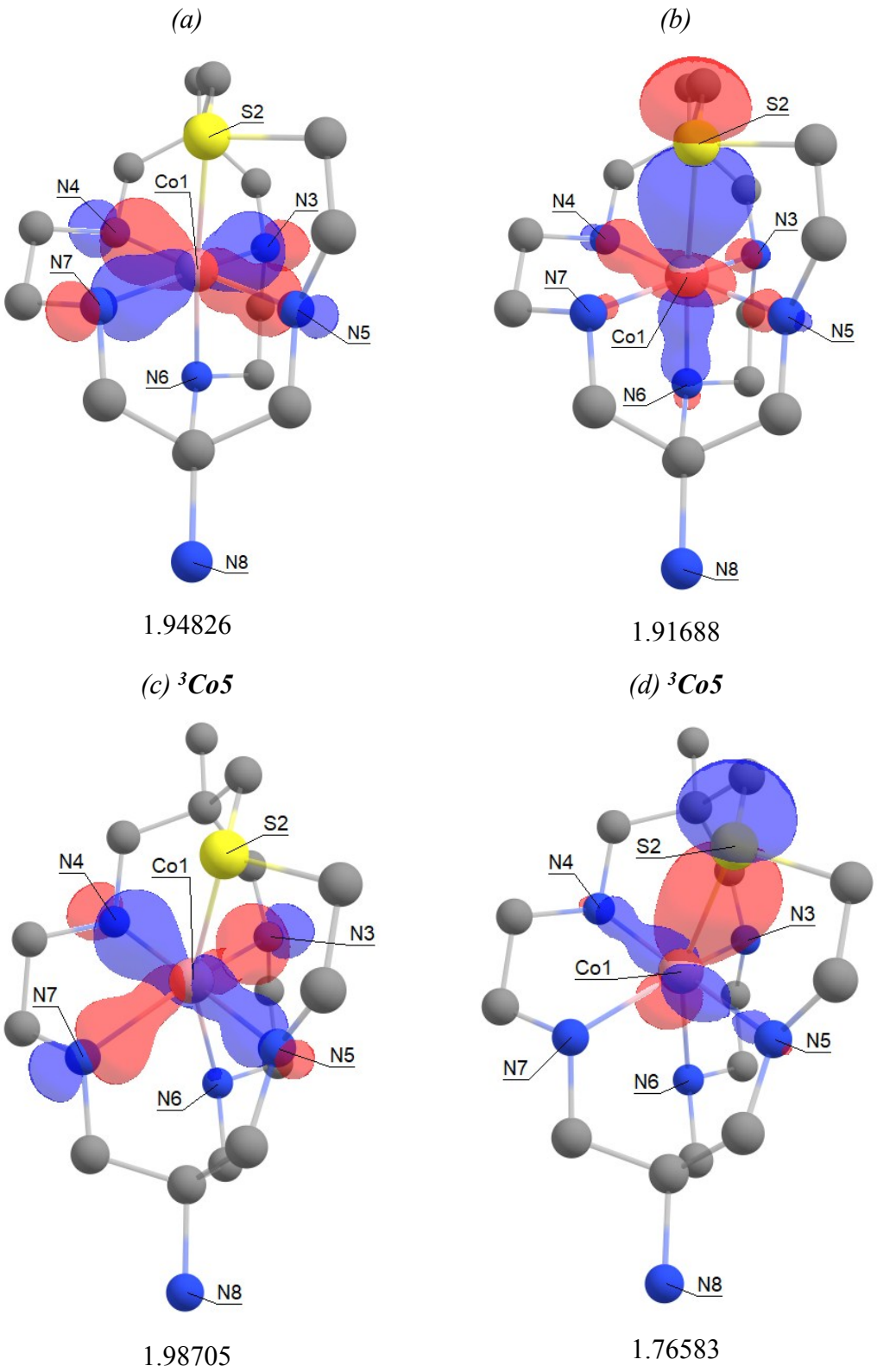

Figure S1. (*a, b*) The two M-L σ-bonding molecular orbitals of **^{1}Co5** in the active space, at the CASSCF(10,12)/def2-TZ level. (*c, d*) The two M-L σ-bonding molecular orbitals of **^{3}Co5** in the active space, at the same level. Occupancies of the MOs are quoted below the structures.

Therefore, **^{3}Co5** and **^{1}Co5** were recomputed with a larger (12,13) active space in order to try and incorporate all M-L bonds in the active space in both spin-states. Indeed, this approach resulted in a better active space for **^{3}Co5**, where the previously missing trans Co-N bond was incorporated. However, upon computation of **^{1}Co5** with the larger active space, the CASSCF wavefunction converged where, unusually, a low-energy MO with significant 3p character on Co, was incorporated into the active space. The inclusion of such a core orbital in the active space was proposed to be chemically inaccurate, as normally such core orbitals on metal atoms are likely to correlate minimally with more valence electrons. Therefore, this approach to enlarge the active space was deemed unsuccessful.

Another approach was a stepwise process to construct the **^{1}Co5** CAS(10,12) wavefunction, from the **^{3}Co5** CAS(10,12), and vice-versa, to attempt to yield a set of CASSCF wavefunctions in each spin-state that are most similar. While this was also unsuccessful, it should be noted that the state-averaged NEVPT2(10,12)/def2-TZ calculation with **^{3}Co5** afforded a lower energy root than that seen in the original approach. This improved the error of the **^{1}Co → ^{3}Co** splitting from +8.6 to +6.6, and in turn lowered the MAD to 2.5 kcal/mol, as reported below.

S3. Detailed Results at the NEVPT2 Level

Table S1. Computed deviation of ^{1}Co → ^{3}Co splitting energies and statistical data of the Co(III) complexes at the different tested NEVPT2 levels of theory, in kcal/mol. Experimental values in parentheses.

#	Theory	Co1 (30.3)	Co2 (32.3)	Co3 (26.2)	Co4 (33.6)	Co5 (32.5)	Co6 (34.7)	Co7 (32.6)	MAD	MSD	Max.
1	NEVPT2(10,7)/def2-QZ	-0.4	-0.9	-2.6	+7.8	+13.8	+10.4	-0.1	+4.8	+4.5	+13.8
2	NEVPT2(10,12)/def2-QZ	-1.3	-1.0	+4.9	+4.0	+9.1	+3.0	+0.9	+3.5	+2.8	+9.1
3	NEVPT2(10,12)/def2-QZ[a]	-0.8	-0.8	+3.1	+3.8	+9.6	+3.1	+0.1	+3.0	+2.6	+9.6
4	NEVPT2(10,12)/def2-TZ[a,b]	-2.1	-2.1	+1.7	+2.3	+6.6	+1.1	-1.2	+2.5	+0.9	+6.6

[a] Single-point CPCM solvation correction calculated at the BP86/def2-TZVP level. [b] The spin-splitting energy of **^{3}Co5** was obtained via identification of a lower energy root of **^{3}Co5** in a state-averaged (nroots = 10) calculation.

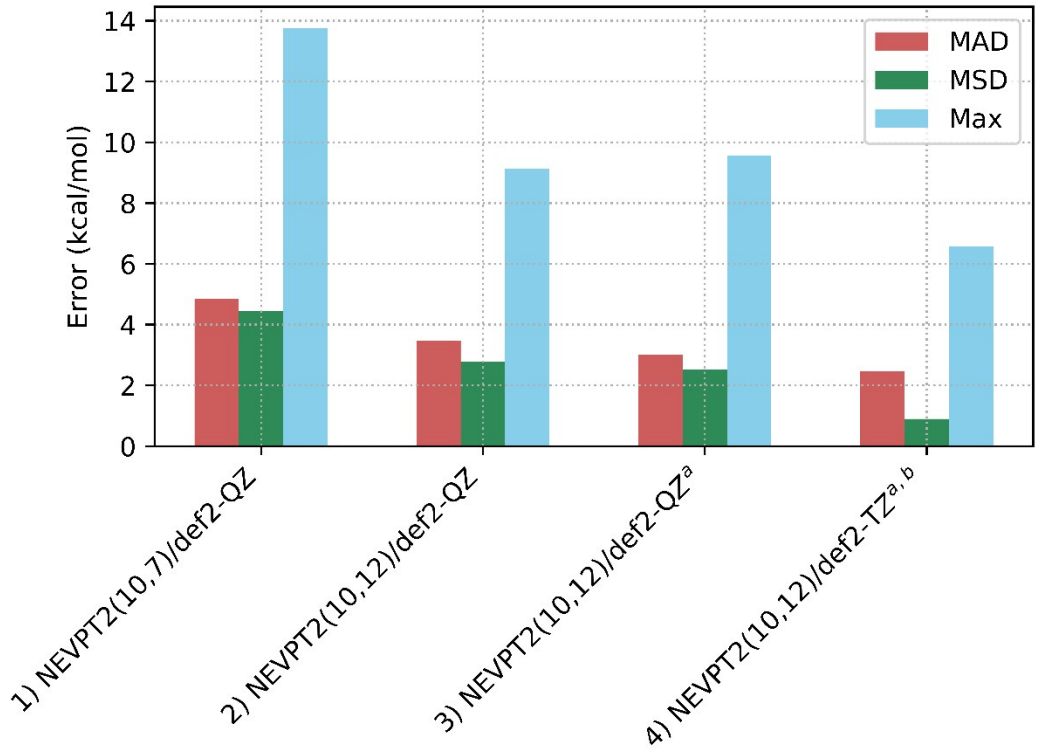

Figure S2. Mean absolute deviations (MAD, red), mean signed deviations (MSD, green) and Maximum deviations (Max, blue) for the different NEVPT2 protocols studied. [a] Single-point CPCM solvation correction calculated at the BP86/def2-TZVP level. [b] Revised splitting energy obtained via identification of a lower energy root of ^{3}Co5 via a state-averaged (nroots = 10) calculation.

An alternative approach employing the solvent correction from the BP86 level gave a small overall improvement (Entry 3, MAD = 3.0 kcal/mol) and this was most notable for **Co3** where the original convergence issues were most problematic (the error dropping from +4.9 to +3.1 kcal/mol). Moving to a def2-TZ basis set (Entry 4, MAD = +2.5 kcal/mol) stabilizes the triplet state in all cases and so has a detrimental effect for **Co1**, **Co2**, and **Co7**, while giving a slight improvement for the remaining complexes. This small change in spin-splitting energies between the def2-QZ and def2-TZ basis sets is associated with the NEVPT2 step as the uncorrected CASSCF results are much closer to when computed with both these basis-sets. As

discussed in *Section S2*, a further improvement to the spin-splitting energy of **Co5** was identified when species **^{3}Co5** was recomputed with a state-averaged (nroots=10) calculation at the NEVPT2(10,12)/def2-TZ Level, where the spin-splitting energy was reduced from +8.6 to +6.6 kcal/mol as a result of finding a lower energy root in this approach.

S4. Diagnostics for Multireference Character at the DLPNO-CCSD(T) Level

(a)	***T_1 diagnostics (approach #6)***	
	^{1}Co (S=0)	**^{3}Co (S=1)**
Co1	0.0184	0.0210
Co2	0.0225	0.0204
Co3	0.0196	0.0256
Co4	0.0170	0.0204
Co5	0.0166	0.0198
Co6	0.0176	0.0219
Co7	0.0175	0.0225

(b)	***$\|t_2,max\|$***	
	^{1}Co (S=0)	**^{3}Co (S=1)**
Co1	0.037737	0.044803
Co2	0.037751	0.044625
Co3	0.047685	0.049371
Co4	0.050396	0.059141
Co5	0.053500	0.050089
Co6	0.048924	0.057719
Co7	0.047279	0.057607

Table S2. (a) T_1 diagnostic values and (b) $|t_2,max|$ values for each complex at the T-PNO(BP)/cc-TZ level (*approach #6 in Table 1 in the main text*).

	DLPNO-CCSD amplitudes (approach #6)	
	^{1}Co (S=0)	**^{3}Co (S=1)**
Co1	0.038940, 0.038858, 0.038847	0.071909, 0.071888, 0.058677
Co2	0.037751, 0.037726, 0.037725	0.070119, 0.070114, 0.064052
Co3	0.049117, 0.046335, 0.042673	0.103508, 0.097636, 0.062905
Co4	0.050396, 0.050356, 0.050320	0.076192, 0.066730, 0.059141
Co5	0.053500, 0.047618, 0.045255	0.079797, 0.069509, 0.058220
Co6	0.048924, 0.048923, 0.048895	0.066587, 0.065612, 0.065162
Co7	0.047279, 0.047231, 0.046669	0.095850, 0.077537, 0.071780

Table S3. The three largest DLPNO-CCSD (singles *and* doubles) amplitudes for each complex at the T-PNO(BP)/cc-TZ level (*approach #6 in Table 1 in the main text*).

S5. Energies at Each Level of Theory (a.u)

	^{1}Co1	^{1}Co2	^{1}Co3	^{1}Co4	^{1}Co5	^{1}Co6	^{1}Co7
BP86 (SCF)	-1721.60522476	-1953.95504330	-2218.41316148	-3387.12239162	-2701.36176359	-3176.81106276	-2873.26220821
BP86 (G corr)	0.19490590	0.30300212	0.22912219	0.43716006	0.47324349	0.34169332	0.38554413
BP86 (CPCM SCF, ε=2)	N/A	N/A	N/A	-3387.57871014	-2701.82935541	-3177.08708305	-2873.53886627
BP86 (CPCM SCF, ε=20)	N/A	N/A	N/A	-3387.99682718	-2702.25714662	-3177.33863026	-2873.79284754
BP86 (CPCM SCF,ε=H_2O)	-1722.28500824	-1954.56849028	-2219.02709753	-3388.03190015	-2702.29313066	-3177.35979136	-2873.81431203
N-PNO(HF)/cc-TZ	-1719.99190806	-1951.82996286	-2216.07455605	-3382.90375881	-2697.97109728	-3173.02648146	-2869.81123245
N-PNO(HF)/cc-QZ	-1720.19235208	-1952.09660398	-2216.32971826	-3383.29497657	-2698.35458246	-3173.35851425	-2870.15020290
T-PNO(HF)/cc-TZ	-1720.00068778	-1951.84160500	-2216.08569438	-3382.92023588	-2697.98693043	-3173.04144975	-2869.82712632
N-PNO(BP)/cc-TZ	-1719.99314526	-1951.83437963	-2216.07371761	-3382.90776324	-2697.98004414	-3173.02784233	-2869.81266011
N-PNO(BP)/def2-TZ	-1719.95627271	-1951.80208701	-2216.03859301	-3382.86600753	-2697.95020963	-3172.98138519	-2869.77199649
T-PNO(BP)/cc-TZ (E[HF])	-1717.57565369	-1948.29377782	-2213.01790740	-3377.45076975	-2692.49488367	-3168.56031950	-2865.12700999
T-PNO(BP)/cc-TZ	-1719.99968042	-1951.83726687	-2216.07901202	-3382.90486069	-2697.97679957	-3173.02794461	-2869.81503993
T-PNO(BP)/def2-TZ	-1719.96307592	-1951.80535763	-2216.04395285	-3382.86403982	-2697.94779639	-3172.98232728	-2869.77505684
T-PNO(BP)/cc-DZ (E[HF])	-1717.49629452	-1948.17761333	-2212.88973622	-3377.25507174	-2692.30535066	-3168.40238780	-2864.96447498
T-PNO(BP)/cc-DZ	-1719.43785054	-1951.06557540	-2215.34133745	-3381.72914899	-2696.81977563	-3172.04566583	-2868.79893321
CCSD/def2-SVP	-1718.77562242	-1950.17350185	-2214.44573182	N/A	N/A	N/A	N/A
(T) def2-SVP	-0.06875659	-0.11111703	-0.08897507	N/A	N/A	N/A	N/A
T-PNO/def2-SVP (CCSD)	-1718.77470643	-1950.17269222	-2214.44509608	N/A	N/A	N/A	N/A
T-PNO/def2-SVP (T)	-0.05892765	-0.09655576	-0.07687255	N/A	N/A	N/A	N/A

Table S4a. Computed energetics of singlet (S=0,) species at each reported level of theory, in atomic units.

	^{1}Co1	^{1}Co2	^{1}Co3	^{1}Co4	^{1}Co5	^{1}Co6	^{1}Co7
TPSSh	-1722.16009389	-1954.51220522	-2218.91063062	-3388.00672669	-2702.30130863	-3177.20037828	-2873.68173154
ωB97X-D3	-1722.20140646	-1954.63833626	-2218.96741061	-3388.21701408	-2702.55936716	-3177.42450482	-2873.95304017
B3LYP	-1721.87114886	-1954.04842779	-2218.49934623	-3387.15591694	-2701.51822926	-3176.58268863	-2873.07231070
M06	-1721.81263516	-1953.94323881	-2218.44785560	-3387.05768163	-2701.36047778	-3176.52865510	-2872.98033278
B2PLYP	-1721.69021070	-1953.81308230	-2218.21784037	-3386.63544298	-2701.12573374	-3176.10833787	-2872.65082772
TPSS	-1722.23781031	-1954.61479448	-2219.00770477	-3388.15797100	-2702.44816052	-3177.41969597	-2873.90341441
BP86	-1722.39292136	-1954.72304242	-2219.16960063	-3388.29588718	-2702.52577975	-3177.58602540	-2874.03549338
OPBE	-1722.36388348	-1954.65305202	-2219.03731376	-3388.05187705	-2702.35193991	-3177.37905890	-2873.85955187
OPBE (D3BJ correction)	-0.110944918	-0.20610469	-0.145009752	-0.416987297	-0.404403237	-0.319507639	-0.334712247
M06L	-1722.02586313	-1954.29596818	-2218.72592169	-3387.61078094	-2701.93629334	-3176.96369957	-2873.45127605
CASSCF(10,7)/QZ	-1718.53908203	-1949.28203875	-2213.98786894	-3378.88754695	-2693.92500212	-3169.57852268	-2866.14501752
CASSCF(10,12)/QZ	-1718.65356788	-1949.40023792	-2214.10124972	-3379.02311371	-2694.05045127	-3169.71125244	-2866.27335827
CASSCF(10,12)/QZ(†)	-1717.97163376	-1948.78558300	-2213.48514356	-3378.14816884	-2693.15353810	-3169.18296643	-2865.74094791
CASSCF(10,12)/TZ(†)	-1717.92877015	-1948.73242293	-2213.42481523	-3378.05388816	-2693.07618960	-3169.09693750	-2865.66165534
NEVPT2(10,7)/QZ	-1720.70723127	-1952.47791906	-2216.74011423	-3383.82285494	-2698.90855431	-3173.59314789	-2870.37526786
NEVPT2(10,12)/QZ	-1720.67266977	-1952.43790190	-2216.70306222	-3383.75827167	-2698.85399891	-3173.53415623	-2870.31854950
NEVPT2(10,12)/QZ(†)	-1719.99172748	-1951.82342733	-2216.08859073	-3382.88271120	-2697.95573786	-3173.00608347	-2869.78542667
NEVPT2(10,12)/TZ	-1719.82094114	-1951.58240911	-2215.85821589	-3382.49158103	-2697.58629832	-3172.67573422	-2869.45412670

Table S4b. Computed energetics (continued) of singlet (S=0,) species at each reported level of theory, in atomic units. (†) CASSCF/NEVPT2 calculated without CPCM, where CPCM Solvation correction calculated at the BP86/def2-TZVP level and added to the resulting CASSCF/NEVPT2 energies.

	^{3}Co1	^{3}Co2	^{3}Co3	^{3}Co4	^{3}Co5	^{3}Co6	^{3}Co7
BP86 (SCF)	-1721.56077247	-1953.90757908	-2218.37898913	-3387.07851167	-2701.32068017	-3176.76375318	-2873.21454659
BP86 (G corr)	0.18722777	0.29568234	0.22175356	0.43223774	0.46792640	0.33597527	0.37925333
BP86 (CPCM SCF, ε=2)	N/A	N/A	N/A	-3387.53267019	-2701.82935541	-3177.08708305	-2873.53886627
BP86 (CPCM SCF, ε=20)	N/A	N/A	N/A	-3387.94687812	-2702.20926111	-3177.28550329	-2873.74101297
BP86 (CPCM SCF,ε=H_2O)	-1722.22849392	-1954.51299969	-2218.98124868	-3387.98175673	-2702.24502631	-3177.30642477	-2873.76232002
N-PNO(HF)/cc-TZ	-1719.94915108	-1951.78210629	-2216.03967896	-3382.86164409	-2697.91780813	-3172.98378320	-2869.77138337
N-PNO(HF)/cc-QZ	-1720.14811698	-1952.04648831	-2216.29243054	-3383.25173417	-2698.30078485	-3173.31490142	-2870.11007840
T-PNO(HF)/cc-TZ	-1719.95436894	-1951.78873799	-2216.04592056	-3382.86876216	-2697.92530270	-3172.98994362	-2869.77775370
N-PNO(BP)/cc-TZ	-1719.95362738	-1951.78849562	-2216.04488951	-3382.86499224	-2697.93325742	-3172.98348108	-2869.76764320
N-PNO(BP)/def2-TZ	-1719.91802373	-1951.75720489	-2216.00991112	-3382.82294532	-2697.90383104	-3172.93742569	-2869.72835969
T-PNO(BP)/cc-TZ (E[HF])	-1717.59315914	-1948.30087978	-2213.01940637	-3377.44782287	-2692.47964287	-3168.55972060	-2865.12135176
T-PNO(BP)/cc-TZ	-1719.95555083	-1951.78584137	-2216.04385779	-3382.85434888	-2697.92355737	-3172.97721888	-2869.76360892
T-PNO(BP)/def2-TZ	-1719.92025790	-1951.75437986	-2216.00885966	-3382.81272650	-2697.89405161	-3172.93154397	-2869.72438595
T-PNO(BP)/cc-DZ (E[HF])	-1717.51458111	-1948.18582843	-2212.89276280	-3377.25283131	-2692.29069323	-3168.40289571	-2864.95946843
T-PNO(BP)/cc-DZ	-1719.39827839	-1951.01803535	-2215.31219065	-3381.68036960	-2696.76768674	-3171.99801588	-2868.75084350
CCSD/def2-SVP	-1718.74734149	-1950.13822403	-2214.42307982	N/A	N/A	N/A	N/A
(T) def2-SVP	-0.05998264	-0.10243663	-0.08422259	N/A	N/A	N/A	N/A
T-PNO/def2-SVP (CCSD)	-1718.74447388	-1950.13522505	-2214.42050435	N/A	N/A	N/A	N/A
T-PNO/def2-SVP (T)	-0.05217592	-0.08981732	-0.07349756	N/A	N/A	N/A	N/A

Table S5a. Computed energetics of singlet (S=0,) species at each reported level of theory, in atomic units.

	^{3}Co1	^{3}Co2	^{3}Co3	^{3}Co4	^{3}Co5	^{3}Co6	^{3}Co7
TPSSh	-1722.10555905	-1954.45750492	-2218.86556897	-3387.95737999	-2702.25140567	-3177.15104775	-2873.63360526
ωB97X-D3	-1722.14174722	-1954.58842050	-2218.92662891	-3388.17073703	-2702.51035509	-3177.37237013	-2873.90781302
B3LYP	-1721.82354237	-1954.00138413	-2218.46048337	-3387.11368572	-2701.47394129	-3176.53932633	-2873.02970758
M06	-1721.76998963	-1953.90018068	-2218.41317062	-3387.01824114	-2701.31724417	-3176.48905543	-2872.94152289
B2PLYP	-1721.63515139	-1953.75523179	-2218.17138887	-3386.56106172	-2701.05788531	-3176.03526657	-2872.58695682
TPSS	-1722.17789023	-1954.55504391	-2218.95873826	-3388.10385882	-2702.39475207	-3177.36316121	-2873.84837766
BP86	-1722.33561167	-1954.66632504	-2219.12347905	-3388.24283860	-2702.47431303	-3177.53098617	-2873.98250443
OPBE	-1722.30991895	-1954.59947161	-2218.99573942	-3387.99807961	-2702.30259719	-3177.32260901	-2873.80729342
OPBE (D3BJ correction)	-0.10353384	-0.198951425	-0.139695128	-0.408674707	-0.395660979	-0.311889144	-0.327207481
M06L	-1721.97495663	-1954.24569980	-2218.68322891	-3387.56614263	-2701.88954731	-3176.91770018	-2873.40558328
CASSCF(10,7)/QZ	-1718.51816759	-1949.26082013	-2213.97200983	-3378.87792914	-2693.90803322	-3169.56161362	-2866.13377673
CASSCF(10,12)/QZ	-1718.62033838	-1949.36595500	-2214.07342509	-3378.99172435	-2694.01731982	-3169.68230872	-2866.24620468
CASSCF(10,12)/QZ(†)	-1717.95092143	-1948.75842734	-2213.46660950	-3378.12133384	-2693.12762906	-3169.15802269	-2865.71780203
CASSCF(10,12)/TZ(†)	-1717.90730076	-1948.70451939	-2213.40584773	-3378.02648527	-2693.04946956	-3169.07132154	-2865.63801487
NEVPT2(10,7)/QZ	-1720.65182319	-1952.42045879	-2216.68994979	-3383.75198998	-2698.82953701	-3173.51556501	-2870.31708102
NEVPT2(10,12)/QZ	-1720.61872255	-1952.38071099	-2216.64608072	-3383.69340776	-2698.78239340	-3173.46840457	-2870.25885160
NEVPT2(10,12)/QZ(†)	-1719.94897321	-1951.77383845	-2216.04622649	-3382.82421967	-2697.89023912	-3172.94591866	-2869.73116868
NEVPT2(10,12)/TZ(†)	-1719.78039139	-1951.53495710	-2215.81805025	-3382.43548485	-2697.52238196	-3172.61867322	-2869.40196368
NEVPT2(10,12)/TZ(†)(*)	N/A	N/A	N/A	N/A	-2697.52553164	N/A	N/A

Table S5b. Computed energetics (continued) of singlet (S=0,) species at each reported level of theory, in atomic units. (†) CASSCF/NEVPT2 calculated without CPCM, where CPCM Solvation correction calculated at the BP86/def2-TZVP level and added to the resulting CASSCF/NEVPT2 energies. (*) Resulting from taking the lowest energy root from a state-averaged (nroots=10) calculation.

S6. Computed Structures and Energies for the 7 Co(III) Complexes

^{1}Co1

```
SCF Energy (BP86/def2-TZVP): -1721.60522476
Free Energy (BP86/def2-TZVP): -1721.41031886
Enthalpy (BP86/def2-TZVP): -1721.35690978
Entropy Corr (BP86/def2-TZVP): -0.05340908
3 Lowest Freqs:
63.07
75.21
85.11
```

Co	-0.00003335708049	-0.00020318932169	-0.00019499953502
N	-1.11424549140414	-1.56903034800991	-0.65700258782748
H	-2.01355686708406	-1.68633613461009	-0.16688017447020
H	-0.65444002524113	-2.48826771104693	-0.57910268942430
H	-1.36774369757567	-1.49477335714064	-1.65358143589689
N	1.29482778131175	-1.23779122367280	0.96216035749579
H	1.52426842210737	-0.91897925005939	1.91539198373690
H	2.20792009802677	-1.34394616273581	0.49550443794520
H	0.95582663741702	-2.20265895357882	1.09113483016405
N	-1.29188689413177	1.28895865855088	-0.89683906346755
H	-2.18873021716143	0.86689626702800	-1.18018344698936
H	-0.93093783004699	1.73204570262008	-1.75469280798808
H	-1.55573454297174	2.08162940657499	-0.29272052181017
N	-1.11200586760988	0.06903431741229	1.70055781463099
H	-0.71050689172333	0.64473565511948	2.45548172723498
H	-1.24781555614559	-0.85773605183526	2.13137777425736
H	-2.06558489216082	0.43870467762097	1.57100147058688
N	1.11734641248123	-0.15577315341679	-1.69143082104407
H	0.65516842655810	0.18652333771866	-2.54686168552254
H	1.37785249554710	-1.12814815847125	-1.91408657914069
H	2.01321526600450	0.35326877478516	-1.65866394724344
N	1.10527515305062	1.60409152234382	0.58182500523795
H	0.68295581200823	2.16581289144687	1.33588091925389
H	1.26719117033265	2.28054049694940	-0.17916127745814
H	2.04765845549167	1.37054498572877	0.92840671727392

^{1}Co2

```
SCF Energy (BP86/def2-TZVP): -1953.95504330
Free Energy (BP86/def2-TZVP): -1953.65204118
Enthalpy (BP86/def2-TZVP): -1953.59705615
Entropy Corr (BP86/def2-TZVP): -0.05498503
3 Lowest Freqs:
83.07
83.90
89.03
```

Co	0.00005550787076	0.00047603183746	-0.00090487319586
C	1.84848460302163	-2.12533234910695	0.75211888482356
C	1.97028724685486	-2.01465004399292	-0.75115656204865
H	-0.20002398100284	-2.37162320018703	1.00742755923513
H	1.97915293330026	-3.16138468685980	1.09851699441728
H	0.46746611673898	-1.42715669241611	2.14338515001243
H	2.60147930864463	-1.51307254158562	1.26825937242351
H	2.37889633633270	0.00703966314809	-1.01138318699003
H	1.30168997154183	-2.71802019843320	-1.26753954709616
H	1.38304205410948	-0.58554864692546	-2.14505207001317
H	2.99332045356775	-2.22683570728840	-1.09586276446873
N	0.47910841756793	-1.60817005569856	1.13051179145688
N	1.56340287752874	-0.60899710164602	-1.13227678418556
N	-1.63258385514819	0.38907332882473	1.13090936649044
N	1.15409632463675	1.21915449105278	1.13027669957528
N	-1.30937201548487	-1.04973219976312	-1.13165528985094
N	-0.25510992332057	1.66016957159998	-1.13100057996687
C	-2.76487629738857	-0.53870161630722	0.75233727326873
H	-1.95465993915836	1.35878237824794	1.00801801114499

H	-1.47027459807735	0.30846373768353	2.14380493844363
C	0.91861221162977	2.66403839855122	0.75226985091320
H	2.15444226739715	1.01155251662362	1.00635277190242
H	1.00372653791859	1.11888925269060	2.14325860280361
C	-2.72996550860134	-0.69895911259961	-0.75100487251956
H	-1.18284199694475	-2.06360064866142	-1.00850343712267
H	-1.19876844641720	-0.90711247634747	-2.14468628732074
C	0.75927310730360	2.71489711071245	-0.75069130764899
H	-1.19634588670397	2.05736530499039	-1.00705744166476
H	-0.18762741742281	1.49349348899450	-2.14414498937505
H	-3.72751712109929	-0.13417648870887	1.09890139501142
H	-2.61049027099543	-1.49711989864041	1.26807518498039
H	1.75224316409493	3.29381254590367	1.09710219083332
H	0.01369673409487	3.01154907419262	1.27068565823155
H	-3.00425393208442	0.23206914730827	-1.26717442902046
H	-3.42545997985867	-1.47850241920569	-1.09607174887507
H	1.70190625668620	2.48801881511774	-1.26882116156361
H	0.43110973886722	3.70726922689430	-1.09415936304091

^{1}Co3

SCF Energy (BP86/def2-TZVP): -2218.41316148
Free Energy (BP86/def2-TZVP): -2218.18403929
Enthalpy (BP86/def2-TZVP): -2218.12071691
Entropy Corr (BP86/def2-TZVP): -0.06332238
3 Lowest Freqs:
17.96
63.24
82.73

Co	-1.05999333367460	0.00012539901932	0.00539529041332
O	0.86119608304269	-0.00005138730417	0.53703705730716
S	2.17181073279759	0.00009083433035	-0.38440312255298
C	3.15780841975560	1.38956481924583	0.19987178823280
C	3.15775934713381	-1.38958205698570	0.19946661236092
H	2.66308098811283	2.32199338225954	-0.09729156862459
H	4.12435855741489	1.32019019366059	-0.32489862536971
H	3.29970703756357	1.32196445876385	1.28642093680724
H	2.66303858449374	-2.32191028726997	-0.09803330422745
H	3.29963195221690	-1.32234417238265	1.28604187540844
H	4.12432751832340	-1.32004064376605	-0.32525151726500
N	-1.00755765977874	2.01066338300898	0.06780179241201
H	-0.23064931432571	2.28352155143034	0.68493998180194
H	-1.84793910763663	2.47041407944280	0.44576088304132
H	-0.82532462265808	2.48340604518811	-0.82779440103949
N	-0.72186609945010	-0.00081980771711	-1.97884918717922
H	0.29152663111690	-0.00199265288800	-2.17515121432754
H	-1.10014938764549	0.81257567134196	-2.48418195138589
H	-1.10206237331289	-0.81363319025191	-2.48368388350742
N	-3.05636503972749	0.00041401342565	-0.33313147764573
H	-3.38462898552479	-0.81773039278538	-0.86527817641041
H	-3.38284207430304	0.81398989063655	-0.87332462549851
H	-3.62335311318131	0.00525985299620	0.52633380403373
N	-1.00797569035063	-2.01034015661162	0.06941695595778
H	-0.82863694570073	-2.48419528883336	-0.82618037098107
H	-1.84731147879967	-2.46941166556521	0.45050835346253
H	-0.22929638109759	-2.28261449874846	0.68457872882513
N	-1.31446318063646	0.00085712708617	2.00740486742284
H	-1.79578123059698	0.81812841330452	2.40722472715901
H	-0.36442518940506	0.00008950218819	2.40870231768492
H	-1.79740064416595	-0.81523141621934	2.40768345368390

^{1}Co4

SCF Energy (BP86/def2-TZVP): -3387.12239162
Free Energy (BP86/def2-TZVP): -3386.68523156
Enthalpy (BP86/def2-TZVP): -3386.61277446
Entropy Corr (BP86/def2-TZVP): -0.07245709
3 Lowest Freqs:
49.89

78.47
78.90

Co	0.17671660525077	0.00037353784752	-0.00048044832666
S	-1.08760210513380	-0.28796090439860	-1.82040069679604
S	-1.08795613660167	-1.43215232613583	1.15735566524247
S	-1.08770176380711	1.71893024723262	0.66179060731247
N	1.36747100492190	-1.54614476182856	-0.71141251484353
N	1.36771084515557	0.15662334703484	1.69447810672440
N	1.36764353083115	1.39039090566463	-0.98317785860419
C	-2.88344688737470	-0.49187004365966	-1.39958776615115
C	-2.88371772593226	-0.96549161998082	1.12497462658200
C	-2.88335522881317	1.45780879064441	0.27296342513247
C	-0.49328459322500	-1.96073421990643	-2.31439726111528
C	-0.49229162844228	-1.02786775691429	2.85357815254463
C	-0.49200508403527	2.98638776091135	-0.53592868972824
C	1.01294713546898	-1.93383971106209	-2.13546666772612
C	1.01389463252074	-0.88509770975664	2.74016412841822
C	1.01412865668984	2.81682459824612	-0.60337529940351
C	2.85123762549228	-1.39941724030646	-0.52241763465857
C	2.85139579850642	0.24827075720571	1.47255651673870
C	2.85132937360659	1.15251036297399	-0.95156524425254
C	3.26970813765821	0.00033786271597	-0.00070888454020
C	-3.31838789384871	0.00025882097548	-0.00058757832303
C	-4.87658890069636	0.00057004385667	-0.00079413270754
H	1.07130152235100	-2.33998429224279	-0.12898717507423
H	1.07080898505958	1.05679350030689	2.09276092924150
H	1.07034929556924	1.28589024851322	-1.96183379989218
H	-3.12945724023375	-1.55381105669738	-1.54287594538089
H	-3.39878308759738	0.08484919859563	-2.18194212048676
H	-3.12924920228726	-0.55895885498741	2.11655304818815
H	-3.39907992153932	-1.93129518529809	1.01635291862065
H	-3.12877860657873	2.11276216354511	-0.57531900952826
H	-3.39923606053005	1.84714332992505	1.16321894274529
H	-0.76490065349621	-2.12012894905130	-3.36916074432712
H	-0.98443559865963	-2.72877546017277	-1.70000455858948
H	-0.76280775873480	-1.86362797174800	3.51691584510829
H	-0.98389404408353	-0.11319346175173	3.21458618448159
H	-0.76244069783769	3.97859316278264	-0.14337751682513
H	-0.98391441077425	2.84203945476180	-1.50844281240524
H	1.47871041130958	-1.20766173125439	-2.81756874777005
H	1.43533179026967	-2.92558825377961	-2.36732154375247
H	1.48023816048450	-1.83801562366033	2.45043471401856
H	1.43643803970011	-0.59201581944200	3.71553963967836
H	1.48085585248874	3.04220900916774	0.36658698444418
H	1.43629456703128	3.51512730861392	-1.34496569656775
H	3.20114017461914	-2.17581871469560	0.17570800138472
H	3.34673433561934	-1.59237192291874	-1.48739624042616
H	3.20088197525429	1.24119562686722	1.79612499570035
H	3.34778153028350	-0.49051004234039	2.12190129648395
H	3.20143894154697	0.93721731983068	-1.97316059538116
H	3.34736395636369	2.08396279992540	-0.63501042583789
H	-5.26890869863143	0.24882696741303	0.99544094243916
H	-5.26904122359851	-0.98613585959806	-0.28434233382351
H	-5.26865203332479	0.73952486091661	-0.71376853941256
N	4.81671897396520	0.00045711856234	-0.00075656693080
H	5.21268924817276	0.87806848024006	0.38548579609206
H	5.21294095404077	-0.10357611057864	-0.95383987538940
H	5.21287812558585	-0.77282998111003	0.56602845765548

^{1}Co5
SCF Energy (BP86/def2-TZVP): -2701.36176359
Free Energy (BP86/def2-TZVP): -2700.88852010
Enthalpy (BP86/def2-TZVP): -2700.81898003
Entropy Corr (BP86/def2-TZVP): -0.06954008
3 Lowest Freqs:
32.97
76.32

81.65

Co	0.03597145026716	-0.07021393445687	0.00034678015572
S	-1.18919114511016	1.64097733988034	0.75781866527322
N	-1.13203529425843	-0.38025602098095	-1.62940520269652
N	-1.14674937227607	-1.33076406832150	1.04865170559316
N	1.22662109731170	1.36181444722299	-0.92210365795114
N	1.26601954081573	-1.53337049517211	-0.80016808640028
N	1.21193152034447	-0.01348426336071	1.66804071353264
N	4.69517058665009	-0.01541427409420	0.04404346740649
C	-4.74637421594575	-0.35311295888457	-0.14065299474634
C	-3.20528270418423	-0.17543475029611	-0.07041924719326
C	-2.95731170683607	1.26294586340576	0.42938179795590
C	-2.65246607015391	-0.39694263758309	-1.48688876379295
C	-2.66697214080009	-1.23207277165850	0.91398481843389
C	-0.67097110599374	2.91331780106760	-0.45920097645945
C	-0.64326485108837	-1.63491802640563	-2.31201354401658
C	-0.70733052321256	-1.27771329156333	2.49052934962578
C	0.83720606159302	2.78526595218458	-0.54328278749782
C	0.86550530167353	-1.68673529765788	-2.24836129941626
C	0.80116744840924	-1.18240177346754	2.53405024598931
C	2.72219720675111	1.17570627567995	-0.84509392171409
C	2.75057941328791	-1.39370420033242	-0.61159677939646
C	2.69899027853119	0.09456254565932	1.49593759855129
C	3.14939541013936	-0.03681139883463	0.01887808167348
H	-0.93070833401232	0.39135246034416	-2.27700644748487
H	-0.90639504325424	-2.27189562277951	0.71286785616245
H	0.99182949445047	1.27560259483833	-1.91831656091149
H	1.00880639912355	-2.41880014664423	-0.34686649880478
H	0.90684430820346	0.83027373399650	2.17120924937263
H	5.09244344693943	-0.81500985853303	0.57278097902354
H	5.07285456761413	0.84300374428076	0.48810865344605
H	5.10976912688112	-0.05933816304722	-0.90609745689905
H	-5.20433695623669	-0.22806252355422	0.85024051986644
H	-5.01217223685364	-1.35302655965633	-0.51168017782073
H	-5.19920716601645	0.38752045372143	-0.81441240592236
H	-3.32708107136096	2.01219311461812	-0.28584926046758
H	-3.45961873412471	1.43857990243291	1.39253988205850
H	-3.06314060287645	0.36309700663082	-2.16699130808091
H	-3.00508904040314	-1.37193679922908	-1.85119348821514
H	-3.03334856637871	-2.22249605543102	0.60812386249396
H	-3.07468279819676	-1.03509765185644	1.91548785130596
H	-0.96243952434280	3.90051256025998	-0.06728185676185
H	-1.18075290239654	2.76129078923738	-1.42188304210504
H	-0.99809982087052	-1.66772165347941	-3.35447993645118
H	-1.09053271702742	-2.49931870052061	-1.79829172176480
H	-1.06506952963429	-2.16661748558720	3.03381188353326
H	-1.17294648961694	-0.39815470713554	2.95854448827020
H	1.24535521062380	3.49226802044017	-1.28380062094725
H	1.29972526482721	3.01537224194943	0.42723237670099
H	1.32647937428845	-0.87277446892380	-2.82829119627439
H	1.24546249238255	-2.63451229520136	-2.66208296157269
H	1.15896257183417	-1.04279129613673	3.56653063481588
H	1.27754751560871	-2.09323805192286	2.14081103966645
H	3.12279732609444	1.06791139997431	-1.86534279550751
H	3.16201082110311	2.09426648979697	-0.42641625428386
H	3.10841366843616	-2.21839962091535	0.02406432492061
H	3.24298424594887	-1.50978164182420	-1.59054476090221
H	3.03421441338717	1.06124723198370	1.90257991717527
H	3.18034009994064	-0.69072850415734	2.10071626945576

^{1}Co6

SCF Energy (BP86/def2-TZVP): -3176.81106276
Free Energy (BP86/def2-TZVP): -3176.46936944
Enthalpy (BP86/def2-TZVP): -3176.40329821
Entropy Corr (BP86/def2-TZVP): -0.06607123
3 Lowest Freqs:
58.18

79.56
79.80

Co	0.87838578360948	0.00152985049314	0.00055987656357
S	-0.38369302922156	0.48098464213791	1.78149601095033
S	-0.38332425951725	1.30226779733250	-1.30775568537659
S	-0.37811484197217	-1.78441526116934	-0.47280724548183
N	2.01837347685532	-1.13927842434015	1.29840444057603
N	2.01414043268196	1.69873593975774	0.34264056568994
N	2.01842809409218	-0.54921546229466	-1.63723019846875
C	-4.15626994778949	-0.00835580893405	-0.00199706496160
C	-2.60103189416224	-0.00485107983941	-0.00144559488044
C	-2.16361504350353	0.07277976286711	1.47920196345436
C	-2.16447485321429	1.23987860274817	-0.80752528115409
C	-2.15936124197134	-1.32419335925680	-0.67524819442534
C	0.21270711911223	-0.81418884783111	2.95289409585372
C	0.20727468759699	2.96515039897986	-0.76755934342934
C	0.21869773111163	-2.15160675197350	-2.18017623060973
C	1.71461825078898	-0.89557620001827	2.75512020563799
C	1.70928912220923	2.83847787747139	-0.59631872620793
C	1.71991256072173	-1.93452934652475	-2.15244236418164
H	3.03218996560439	-1.03492715681239	1.16221963335451
H	1.82650611949458	-2.13033086807821	1.09856301092681
H	3.02840902969422	1.53108625639129	0.32196913978928
H	1.81987591831339	2.02001676217116	1.30072895451528
H	3.03216893705130	-0.47861731737229	-1.48039327589356
H	1.82220021054821	0.11751610155382	-2.39607922789231
H	-4.54771288018832	-0.17371041722962	-1.01536640319904
H	-4.55092817041468	0.95040648479437	0.36205013544270
H	-4.54643830948716	-0.80464530141692	0.64697516283808
H	-2.70988914607864	0.87925610367417	1.98945317627600
H	-2.37902778854368	-0.86855958457858	2.00411144680034
H	-2.70857162580725	1.27835473353133	-1.76233774563980
H	-2.38281201955775	2.16434977627380	-0.25460788420439
H	-2.70281393090524	-2.17157213911066	-0.23282454393240
H	-2.37445049407989	-1.30785805418213	-1.75295187625777
H	-0.29597511854839	-1.76305053263659	2.73146020342431
H	-0.04854274083726	-0.49265395359416	3.97132001980601
H	-0.30319087243740	3.24372153016103	0.16514090828358
H	-0.05530079785061	3.68733396632086	-1.55387743681306
H	-0.29205572134807	-1.48762373986946	-2.89182749375149
H	-0.03941919022896	-3.19540475360391	-2.40966700154501
H	2.21164967851533	0.03416955250193	3.06385849139999
H	2.13256748870186	-1.70773179491314	3.37081727773158
H	2.12426205561432	3.77844524476201	-0.19932143424456
H	2.20821561271939	2.64300099305697	-1.55534369262456
H	2.13816878616134	-2.06153367059822	-3.16353153090513
H	2.21970285646714	-2.66401555080225	-1.50060124323407

^{1}Co7
SCF Energy (BP86/def2-TZVP): -2873.26220821
Free Energy (BP86/def2-TZVP): -2872.87666408
Enthalpy (BP86/def2-TZVP): -2872.80929589
Entropy Corr (BP86/def2-TZVP): -0.06736819
3 Lowest Freqs:
59.65
84.58
95.21

Co	0.00000188424527	-0.35248539284517	0.00000119064642
N	-1.21567217082308	-0.32975984211655	-1.62484153113545
H	-1.20258304249559	0.62829931667971	-1.99459233159457
H	-0.80907320533402	-0.87807848747640	-2.39408642214499
N	1.23216999485369	-1.79704167046432	-0.76956439762540
H	1.17249647015269	-2.60368643838479	-0.13583286248617
H	0.88473631039064	-2.15770858578748	-1.66712170492372
S	1.25932295640739	1.26350933066215	-0.93739669519792
C	0.75634650296256	2.81276200718249	-0.06152726890715

H	1.25860845774553	2.86565015296463	0.91492352792397
H	1.10229602972871	3.65759690788508	-0.67648041876855
C	2.99631634670706	0.97333784742667	-0.37957949130634
H	3.61575951311817	1.21487841982900	-1.25548307752210
H	3.22751314797210	1.70084283058378	0.41167797246252
C	2.70387748057721	-1.48914824673224	-0.95554922897658
H	2.84690137721258	-1.11647959631718	-1.97913166053123
H	3.25611592938169	-2.43704659702133	-0.87477119428367
C	-2.66036641802371	-0.75582640909648	-1.46947633923168
H	-2.72640242572317	-1.82912604197918	-1.69799212809805
H	-3.25090661116728	-0.23423322278050	-2.23747553540643
C	3.25581296144425	-0.48085749053492	0.07522243958570
C	4.78976542691436	-0.66196301130321	0.15959985198592
H	5.24725066388309	-0.61401567647962	-0.83826515746952
H	5.04377220419182	-1.63675503626386	0.59988125385885
H	5.25026956592588	0.11899319901505	0.78020997931035
C	-3.25580894075459	-0.48085526734450	-0.07522123913426
C	-2.99631057942318	0.97334690703054	0.37955738562765
S	-1.25931589232210	1.26352880929129	0.93736580432324
N	1.21567930407276	-0.32972959938467	1.62484342664235
H	1.20259411773799	0.62833786242785	1.99457282187943
H	0.80908113231229	-0.87802998919826	2.39410176052159
C	2.66037192261627	-0.75580339526462	1.46948331971459
H	2.72640521735338	-1.82909925088593	1.69801776567260
H	3.25091517605220	-0.23419879860968	2.23747243885471
N	-1.23216807138379	-1.79702372276235	0.76959825051857
H	-1.17248747956917	-2.60368669218038	0.13589069241624
H	-0.88473675211287	-2.15766197807072	1.66716783997469
C	-2.70387778462232	-1.48913033858957	0.95556784227355
H	-2.84690981298744	-1.11644765942703	1.97914401397515
H	-3.25611367020456	-2.43703090263601	0.87479906033163
C	-4.78976166669229	-0.66195935393671	-0.15959807160852
H	-5.24724858000098	-0.61399453175806	0.83826531283882
H	-5.04376952514100	-1.63675826931350	-0.59986359843622
H	-5.25026321899561	0.11898729229691	-0.78022213081358
C	-0.75634068963626	2.81276252926594	0.06146187504351
H	-1.25860270173333	2.86562831881960	-0.91499016255570
H	-1.10229114939676	3.65761081719625	0.67639606786601
H	-3.61575162985888	1.21490136017944	1.25545863746476
H	-3.22750907555760	1.70083958620884	-0.41171088355503

^{3}Co1

SCF Energy (BP86/def2-TZVP): -1721.56077247
Free Energy (BP86/def2-TZVP): -1721.37354470
Enthalpy (BP86/def2-TZVP): -1721.31517942
Entropy Corr (BP86/def2-TZVP): -0.05836528
3 Lowest Freqs:
44.23
58.27
88.91

Co	-0.01441563206038	-0.03077308894639	0.00020683609973
N	-0.07128053362444	-0.05230984411316	2.00979752166990
H	-0.61038383960514	0.72657690286915	2.41538020565727
H	0.85950868108665	-0.00222440863281	2.44884601470632
H	-0.50367250364050	-0.91032726567171	2.38349360364400
N	2.03300577756890	0.79774071045494	0.00689924020988
H	2.19896408608542	1.48597549431397	-0.74159114862824
H	2.76841470488004	0.08682324480013	-0.12074250087046
H	2.29394391950434	1.29228769562232	0.87210671347245
N	-2.10074817066485	-0.65352139640296	-0.04728378028556
H	-2.63758563546072	-0.42218160485206	0.80129466874225
H	-2.22506833969908	-1.67050887571787	-0.16526085365900
H	-2.63796491077341	-0.23592281678403	-0.82131674505296
N	-0.66077171136395	2.07628615131476	-0.01085959942406
H	-0.44935846888560	2.58673509986810	-0.88036088107556
H	-0.22464031823685	2.64268208358942	0.73107734296827
H	-1.67515952081763	2.19893018800328	0.12519651417558

N	0.81510341488751	-2.03992576039463	0.05102907783982
H	0.10340918555067	-2.77584290731045	0.17566952525064
H	1.48190675684774	-2.19151601523046	0.82206412449671
H	1.32808320603985	-2.31435077957836	-0.79944533045588
N	0.00314056920921	-0.09383107016591	-2.00942038083753
H	-0.53763823978388	0.66395608634828	-2.45096022385016
H	-0.39888723541840	-0.96770491397632	-2.38027465366551
H	0.94817475837449	-0.03144690940723	-2.41539929112790

^{3}Co2

SCF Energy (BP86/def2-TZVP): -1953.90757908
Free Energy (BP86/def2-TZVP): -1953.61189674
Enthalpy (BP86/def2-TZVP): -1953.55211776
Entropy Corr (BP86/def2-TZVP): -0.05977898
3 Lowest Freqs:
65.65
70.59
75.00

Co	-0.10082437282384	0.00017706383779	-0.00004459919604
C	-1.46890783600364	-2.57126662607357	0.67771109700798
C	-1.40190432853093	-2.48006346190582	-0.83077674779480
H	-2.36789880806212	-0.75776149581289	1.16247403455169
H	-2.38139850867525	-3.09007567657312	1.00826617358741
H	-1.21819496936299	-1.19244589425176	2.22598946504525
H	-0.61435798758467	-3.12651753082497	1.08966476903201
H	0.64226216232118	-2.17803967713807	-1.10558535562299
H	-2.30395674234020	-2.01202508926770	-1.25015813213184
H	-0.26970250153656	-1.37809565569774	-2.19331034670296
H	-1.30080047189023	-3.47167942807169	-1.29853626199384
N	-1.42293442104446	-1.16516011714512	1.21832404052551
N	-0.21499054807921	-1.61578024048003	-1.19381018410413
N	-0.20387336061164	1.61686974532080	1.19370918763555
N	1.63954196534826	-0.77632993159891	1.15147647008726
N	-1.41566169120198	1.17436725178622	-1.21795728857456
N	1.64394556751910	0.76553585357013	-1.15270481997054
C	-1.38525187883502	2.48893751087290	0.83126955062959
H	0.65699539395876	2.17351304295486	1.10501618202087
H	-0.25960745450656	1.37961261096228	2.19325693204534
C	2.91388278777806	-0.09489995075979	0.75340543067312
H	1.74886495036675	-1.78872192095401	1.00814807264958
H	1.50892633365497	-0.67343534887696	2.16577455435005
C	-1.45231455894668	2.58068094763065	-0.67717904428138
H	-2.36327100327400	0.77317374505023	-1.16202182121550
H	-1.21087533734640	1.20041507136058	-2.22564331935289
C	2.91452313697591	0.07726517029849	-0.75428180069612
H	1.75910461322915	1.77743957390988	-1.01050731052406
H	1.51243163999989	0.66230700959571	-2.16684669397923
H	-1.27741251163278	3.47984498411675	1.29903066981373
H	-2.29018582863499	2.02686281248938	1.25106292763911
H	3.78900329354215	-0.67773663832340	1.07957845872544
H	2.96540644297772	0.87516498165366	1.26868707433123
H	-0.59436710418917	3.13044186119624	-1.08943795611336
H	-2.36155326663846	3.10543874669844	-1.00730382190613
H	2.96101375521687	-0.89307904614131	-1.26951528164167
H	3.79283744886300	0.65538674659188	-1.08025030454868

^{3}Co3

SCF Energy (BP86/def2-TZVP): -2218.37898913
Free Energy (BP86/def2-TZVP): -2218.15723557
Enthalpy (BP86/def2-TZVP): -2218.08874345
Entropy Corr (BP86/def2-TZVP): -0.06849211
3 Lowest Freqs:
11.48
57.19
73.84

Co	-1.01491929679327	0.00561946960524	0.01052720377807

O	0.89050987190046	-0.01130509607885	0.48029272249625
S	2.23858117687696	-0.00086528760947	-0.41328553100430
C	3.17073383898000	1.41427104508435	0.20053625303806
C	3.20958888614066	-1.36971547843850	0.24099912390900
H	2.66100976681870	2.33135638224883	-0.11773780099894
H	4.15205296470553	1.36140666801039	-0.29961168369199
H	3.28322806096955	1.35187548848757	1.29057702629721
H	2.72221150390485	-2.30924633106638	-0.04533238122070
H	3.32356006899108	-1.27024948097558	1.32816717588040
H	4.18774927875722	-1.30799700515447	-0.26434993426663
N	-1.10364699949763	2.22012450931288	0.16371270073935
H	-0.38005516070517	2.53374008253006	0.82307026405751
H	-1.98636914000906	2.60596231342660	0.52513460297254
H	-0.92273066619875	2.74679320299258	-0.70078221328091
N	-0.73192846758255	0.08970345699274	-1.96671790823878
H	0.26934702021191	0.04049215875303	-2.20724343682444
H	-1.08495445000570	0.95356377668409	-2.39976076139663
H	-1.18478162183829	-0.67753554063743	-2.48139420640250
N	-3.15313387680145	0.01199763164072	-0.30826537932353
H	-3.48433465561269	-0.78131772346293	-0.87380850464113
H	-3.48518367576046	0.84829008365848	-0.80757255995563
H	-3.71315756765118	-0.02392892064160	0.55403505003673
N	-1.08485396408750	-2.21639895204264	-0.04483467797335
H	-0.87076526754547	-2.65264570504094	-0.95108008886995
H	-1.97386167479978	-2.64314237043991	0.24884565451760
H	-0.37879877578364	-2.58824400145927	0.60304011500877
N	-1.26360692634774	-0.08652038958738	1.99714611711216
H	-1.75699186656110	0.71303041770172	2.41573229697660
H	-0.31888278906129	-0.10107586159802	2.40886002096367
H	-1.74897459561422	-0.92672954289591	2.33828174030547

^{3}Co4

```
Co_AMN3S3sarH/Co_AMN3S3sarH_S1_BP86.out
SCF Energy (BP86/def2-TZVP): -3387.07851167
Free Energy (BP86/def2-TZVP): -3386.64627393
Enthalpy (BP86/def2-TZVP): -3386.57034017
Entropy Corr (BP86/def2-TZVP): -0.07593376
3 Lowest Freqs:
60.11
67.47
72.48
```

Co	-0.18585150330686	0.02632896660074	-0.20035748124957
S	1.17263704168692	0.59736611910709	1.77027773743984
S	1.10774817758656	-1.77525443602555	-0.31745727807910
S	1.26867106986522	1.31762364540354	-1.39137081993527
N	-1.53753467747970	-0.71352461281889	1.58037619884739
N	-1.54138841576931	-1.06652319024474	-1.41035251392014
N	-1.40897942170765	1.69480445865757	-0.16255338741177
C	2.93071581098188	0.08213424159944	1.49139917284152
C	2.87805185733747	-1.34828632117715	-0.64966898383296
C	3.02828180436743	1.20917467532321	-0.83079106152055
C	0.49952969512614	-0.56403197017389	3.01816659996146
C	0.45842391823712	-2.46911489743645	-1.89459424165185
C	0.60510911696717	2.97131902111431	-0.93491335099340
C	-1.01468069356697	-0.42891419173453	2.96108117419797
C	-1.05287937718514	-2.46641599769526	-1.74043310123265
C	-0.90494866983798	2.83885187709156	-1.02856752427769
C	-2.97307609796559	-0.35083454376489	1.44565781863377
C	-2.99386898905891	-1.05643038276405	-1.04573794317295
C	-2.86693703745562	1.45567195059190	-0.41464608464143
C	-3.36214929283244	0.04007657499306	-0.00612215391203
C	3.38118818065999	-0.04200032561103	0.01561299278523
C	4.93546880944401	-0.12131423659914	0.03204304340368
H	-1.44509123201643	-1.72521674558857	1.43424200311908
H	-1.43908974152051	-0.52212210544003	-2.27879786578684
H	-1.30579516732946	2.00701782246835	0.81203104540846
H	3.09262329014565	-0.86019683700110	2.03416602680624

H	3.51893201472443	0.86301791445644	1.99678342273201
H	3.02288796176399	-1.32875910896598	-1.73948960436038
H	3.42848136166762	-2.21121403157138	-0.24388273225882
H	3.24847442148115	2.14275387768670	-0.29187222915509
H	3.61069385084398	1.21276927806722	-1.76425754652890
H	0.87341952467263	-0.26028594666065	4.00796449508723
H	0.85167704929040	-1.58378400404905	2.80615007900653
H	0.84327656509519	-3.49557740612725	-2.00181289588270
H	0.81139457336200	-1.86799942133659	-2.74530631348216
H	0.97842829044300	3.71239125281887	-1.65809871832363
H	0.96000987658737	3.24186654372284	0.07039324651739
H	-1.31812586793711	0.59109131196364	3.24001238186350
H	-1.46496666505796	-1.11434264461249	3.69926216765545
H	-1.36120393444553	-3.13248947810867	-0.92155790423098
H	-1.53044137866445	-2.83185833756404	-2.66417044893697
H	-1.21101501310391	2.63415679676071	-2.06454555078477
H	-1.38162285924866	3.78413997026914	-0.72053274845433
H	-3.61087205394015	-1.18490168188539	1.78898716267591
H	-3.17993714632219	0.49722649108282	2.11752664350670
H	-3.59632267780096	-0.92808499961598	-1.96113370611813
H	-3.24818867104197	-2.04583937628557	-0.63568195585082
H	-3.44936162262859	2.22469864442188	0.12187870737184
H	-3.05026092521589	1.61139573060931	-1.48923247400112
H	5.32953221062379	-0.34373616990751	-0.96971686391136
H	5.27874506717382	-0.90986832240961	0.71690147732162
H	5.37292331834412	0.83044346718790	0.36610513564038
N	-4.90846877619417	0.11955894276119	-0.01729570002659
H	-5.28427000312719	0.46392705898708	-0.92039155689261
H	-5.27486235256033	0.75446816982089	0.71632613311005
H	-5.34864059415740	-0.80447708039197	0.15092587488431

^{3}Co5

SCF Energy (BP86/def2-TZVP): -2701.32068017
Free Energy (BP86/def2-TZVP): -2700.85275377
Enthalpy (BP86/def2-TZVP): -2700.77986277
Entropy Corr (BP86/def2-TZVP): -0.07289101
3 Lowest Freqs:
54.60
62.60
73.03

Co	-0.04251674958079	0.03073636252544	-0.17339596161852
S	1.38297967667006	1.59908376505134	-0.87424193206597
N	1.28938399869967	-0.21869974930819	1.73784555274976
N	1.19224536675168	-1.42439422553631	-0.84993462655905
N	-1.29791945446694	1.61407476722276	0.25888599040063
N	-1.40372332411371	-1.04403509409776	1.34813392511264
N	-1.42250805425575	-0.80007203602856	-1.57697492585106
N	-4.80156854856257	0.06915569428025	-0.01738566338373
C	4.82367804058468	-0.45309577392627	0.12977597946584
C	3.29128317210850	-0.21908792400927	0.10711505264953
C	3.08856964636406	1.26840173712627	-0.28345361779094
C	2.74365556612992	-0.53116984886620	1.51361222154634
C	2.68360621589380	-1.16453137253869	-0.95398430442295
C	0.69916749903677	3.08480264772428	-0.04246723610554
C	0.65094893764874	-1.17403772119308	2.68666013991804
C	0.64986162134796	-1.94745068621615	-2.15503353213287
C	-0.80051284648385	2.96684902544037	-0.23646563945827
C	-0.84206283094705	-0.93511227374929	2.73539982314879
C	-0.84873396299831	-2.11586007186261	-2.03799364412663
C	-2.74095785100408	1.44592701979208	-0.12416188060269
C	-2.85250662670635	-0.69218911352564	1.30807802523270
C	-2.88094530529111	-0.86712760208050	-1.26538417418198
C	-3.25783195225186	-0.01421839112617	-0.02400747889661
H	1.23536274715644	0.71324598202930	2.16433667082838
H	1.07601215014297	-2.17175362171336	-0.15206351167491
H	-1.25851015795697	1.65597904543976	1.28613927545022
H	-1.31984798901073	-2.03068266545205	1.07641301159892

H	-1.30234290780439	-0.14412514647508	-2.36179213392149
H	-5.24288906599713	-0.86938492589694	-0.04945807445369
H	-5.17692384467047	0.59486260759936	-0.82912768701942
H	-5.17114071462185	0.53536821105934	0.83225333248605
H	5.25314812312846	-0.37908300964867	-0.87910375107116
H	5.05991361189196	-1.45114288296211	0.52621788960935
H	5.32861155292874	0.28757465277547	0.76577971052365
H	3.30258639185533	1.95958160034613	0.54539186086865
H	3.73516725072612	1.53793101245708	-1.13283641359729
H	3.34224255362607	0.00906124985289	2.26452641971341
H	2.89359205503151	-1.60242287949575	1.71445037070004
H	3.18078702769312	-2.14537358541729	-0.88449804704611
H	2.87930793579972	-0.77659563066528	-1.96438506954809
H	1.09673756164907	3.98085025767686	-0.54465162161499
H	1.01323429718219	3.10772833575014	1.01137445265739
H	1.08133280159162	-1.07922830073482	3.69824959030895
H	0.87380471829252	-2.19965177978885	2.35164643050036
H	1.13568954606867	-2.90245030232026	-2.41320972354633
H	0.91275496931387	-1.22536996480649	-2.94269748781956
H	-1.32213978645792	3.77847472537151	0.29660296456237
H	-1.05755487256759	3.04636003201202	-1.30226496620885
H	-1.06969723096144	0.07146376317887	3.12212063154100
H	-1.32285911918635	-1.65500831553044	3.41810533085476
H	-1.28511169165278	-2.42697431986807	-3.00057549715396
H	-1.11197468830577	-2.88511027246011	-1.29543092430859
H	-3.34724849739469	2.10641564162487	0.52002802273811
H	-2.85633817847713	1.81400825277437	-1.15492657725540
H	-3.46307699011424	-1.59656966427511	1.47321258015115
H	-3.07035043742743	-0.01300959335457	2.14781128706967
H	-3.45882757550994	-0.53536706679795	-2.14434116990450
H	-3.15285978053501	-1.91899457738288	-1.08687926904554

^{3}Co6

SCF Energy (BP86/def2-TZVP): -3176.76375318
Free Energy (BP86/def2-TZVP): -3176.42777791
Enthalpy (BP86/def2-TZVP): -3176.35752196
Entropy Corr (BP86/def2-TZVP): -0.07025595
3 Lowest Freqs:
61.67
67.02
68.47

Co	0.94400657289594	0.06191253482104	0.13088345392997
S	-0.26984640628899	1.24609294812461	-1.31747213998572
S	-0.58474609552340	-1.85501259013980	-0.43266336997049
S	-0.49756284457867	0.48401317943321	1.84247491497845
N	2.29898946019011	1.74696677413208	0.05196874580682
N	2.05312773601119	-0.93318601487198	-1.54373399364961
N	1.98115329973890	-1.04023242117944	1.52292394121379
C	-4.17555128450847	0.29453755069445	-0.13622119349690
C	-2.62914852228308	0.15148476559255	-0.06262515136742
C	-2.04110233106650	1.37689694454657	-0.80311170305336
C	-2.27903697359170	-1.19043690863493	-0.75123928066966
C	-2.27278352490000	0.16558973238588	1.44700601661286
C	0.41990030815322	2.93245152347562	-1.03014714206061
C	0.07823402652277	-2.34648735365318	-2.07025560154629
C	0.05269047508637	-0.78198035007715	3.05960898173400
C	1.92973430438759	2.77054500900753	-0.98755987092741
C	1.59573625816062	-2.29462891372428	-1.96548567547179
C	1.56748060318156	-0.80615172743608	2.95456165761229
H	3.29573663841088	1.51901715995534	-0.05085142055652
H	2.22884676727773	2.18770131154538	0.97965859258493
H	3.06093858229254	-0.97828902219148	-1.35058609299229
H	1.96379641965463	-0.30129384053336	-2.34916241769542
H	2.99932647935183	-0.91421735450520	1.45926643593131
H	1.81875430191225	-2.03116638210604	1.29969876629006
H	-4.66919276557341	-0.46577883069757	0.48539395851763
H	-4.52972326747390	0.16806036986206	-1.16889463747362

H	-4.49883477718598	1.28389612274841	0.21644238860719
H	-2.57419057948135	1.52638554643502	-1.75409631288369
H	-2.14918567109092	2.29155527126622	-0.20287603284992
H	-2.95467512178846	-1.97781055443159	-0.38668891568590
H	-2.41239270367559	-1.11635984706312	-1.83969990036094
H	-2.81759874263446	0.97450156305339	1.95485771219068
H	-2.54102478020106	-0.78343240675121	1.93365332487903
H	0.00895266899409	3.33449436727545	-0.09283256872992
H	0.10018978057052	3.57086004346543	-1.86699937791565
H	-0.31598092926900	-1.66636278986893	-2.83867013193398
H	-0.26425541650582	-3.36791040855955	-2.28884858000896
H	-0.41169437952371	-1.74546206347982	2.80344335352791
H	-0.28182718656781	-0.47139241497297	4.05978747542148
H	2.32104905457994	2.43495087068701	-1.95767743491524
H	2.40158802074704	3.74051954624685	-0.76507626234018
H	2.03130593843638	-2.56238974358430	-2.94196334669072
H	1.96736472180292	-3.03008576372981	-1.23838280796341
H	1.97425159472013	-1.60053454981141	3.60064902324641
H	2.00521229063312	0.14452511724911	3.28802562011080

^{3}Co7

SCF Energy (BP86/def2-TZVP): -2873.21454659
Free Energy (BP86/def2-TZVP): -2872.83529326
Enthalpy (BP86/def2-TZVP): -2872.76384350
Entropy Corr (BP86/def2-TZVP): -0.07144975
3 Lowest Freqs:
56.32
66.80
84.71

Co	-0.01214503806704	-0.33354729225118	-0.11754246442290
N	-1.46756173767294	-0.49857451771885	-1.77549427952501
H	-1.45853559813103	0.42330679940751	-2.22678182283932
H	-1.14392108038959	-1.13099214218483	-2.51740578462040
N	1.27847784592147	-1.75167956299153	-0.83911853440535
H	1.21596856978661	-2.54281741535439	-0.18742030460084
H	0.95064996316155	-2.12659242273638	-1.73808595684221
S	1.31433950178726	1.32720929341791	-0.81386983936273
C	0.75183893252877	2.89188699315633	-0.01388420774153
H	1.19331286663956	2.95781883130821	0.99067764436272
H	1.12319926357040	3.73087794668347	-0.62181382884283
C	3.05575371213182	1.01874873091751	-0.30210182083938
H	3.66464921260003	1.32214470286042	-1.16655542833210
H	3.27683995407050	1.70055243323151	0.53247584934074
C	2.74588580402299	-1.41732530490740	-1.00838422945291
H	2.87755981775200	-0.99507660310799	-2.01457923862996
H	3.30258117854383	-2.36634567934128	-0.98220169409978
C	-2.89483233338576	-0.86082727140430	-1.44842824292260
H	-3.00931295895212	-1.94591285252700	-1.58494607432541
H	-3.56151815128540	-0.38445051653488	-2.18284335737555
C	3.32677101862728	-0.46396536250335	0.05991590178850
C	4.86665863260801	-0.62983644975289	0.04896703565487
H	5.27243329191622	-0.52882036813976	-0.96719699444499
H	5.15015167978834	-1.62162443579486	0.42936512654676
H	5.35238203590081	0.12343045193596	0.68464870033958
C	-3.34319208320850	-0.47398136242932	-0.02300671556969
C	-3.01494449640882	1.00857569057341	0.29280820026955
S	-1.27344574914104	1.27708134920651	0.83255178329709
N	1.38667607100168	-0.46636390420938	1.74605266933681
H	1.33995443068834	0.46327596459166	2.17655563104963
H	1.03953983559020	-1.08833932190730	2.48505407055282
C	2.82294205022699	-0.81822806942967	1.47684019272001
H	2.94685455832975	-1.89919449585077	1.63710601911812
H	3.46504857073301	-0.32263802593531	2.22122636019498
N	-1.28520264525321	-1.76828216358941	0.80834041406252
H	-1.25408570001278	-2.58529955236374	0.18626039198929
H	-0.90343651785139	-2.10531334703220	1.69940166606966
C	-2.73928547563704	-1.42148527407516	1.03673584574384

H	-2.82869876198722	-0.98365164555853	2.04080160130111
H	-3.31015009844127	-2.36249305899203	1.04670213695761
C	-4.88322998652547	-0.60899939892334	0.04259634905322
H	-5.24958390052109	-0.48038477576372	1.07058181928090
H	-5.20168816904264	-1.60145539781776	-0.30701349502278
H	-5.37539819699217	0.14312353589631	-0.58933888678876
C	-0.76665817341427	2.85022220926228	0.00848281863576
H	-1.20331038142536	2.89833155521165	-0.99862128978414
H	-1.17344049272596	3.67859920146481	0.60939757290927
H	-3.61805689881641	1.35441796406177	1.14573422273265
H	-3.21981435863892	1.66759834694129	-0.56314497251683