

Supporting Information for
**Co(salophen)-Catalyzed Aerobic Oxidation of *para*-Hydroquinone:
Mechanism and Implications for Aerobic Oxidation Catalysis**

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I. General Considerations.

All commercial reagents were purchased and used as obtained. Co(salophen) was synthesized as reported in the literature.¹ EPR spectra were recorded for frozen solutions in quartz tubes on a Bruker EleXsys E500 at 10 K. Methanol used in anaerobic experiments was deoxygenated by freeze-pump-thaw degassing. EPR simulations to obtain *g* and *A* values were performed using EasySpin.² UV-Vis spectra were recorded on an Agilent Cary 60 spectrometer using a 2 mm path length dip probe in a custom-designed 3-neck flask.

II. General Method for Analysis of Solvent Effects on the Reaction

Each set of data was collected using a 6-well gas uptake apparatus which holds individually calibrated 50 mL round bottom flasks, each connected to a pressure transducer designed to measure the gas pressure within the sealed reaction vessel. Solvents were investigated in sets of three, with three vessels used as a solvent control with just hydroquinone, and three vessels containing the complete reaction mixture. The apparatus was evacuated and filled with O₂ to 800 torr three times. The pressure was established at 500 torr and the flasks heated to 27 °C. A solution of catalyst was added via syringe through a septum, and the pressure and temperature allowed to equilibrate. When the pressure and temperature stabilized, a solution of hydroquinone was added via syringe through a septum. Data were acquired using custom software written within LabVIEW (National Instruments).

III. Comparison of Various Co-catalysts for Aerobic H₂Q oxidation in MeOH

To test the role the cobalt macrocycle catalyst is performing in the catalytic reaction, the catalytic activity of variety of cobalt precursors were measured using the single well gas uptake apparatus described in Section IV. The samples included a simple Co^{II} salt, Co(OAc)₂; a heterogeneous Co species, (Co₃O₄); a simple tetradeятate cobalt species, Co(acac)₂, and two metal macrocycles, Co(salen) and Co(salophen). Co(acac)₂ has been reported as a capable catalyst for the oxidation of 3,5-di-tert-butylcatechol in CHCl₃.³ Co(TPP) was not soluble in MeOH, but has also been reported as a catalyst for H₂Q oxidation by Bäckvall in AcOH.⁴ The only two catalysts which displayed activity for H₂Q oxidation were Co(salen) and Co(salophen) (Figure S1).

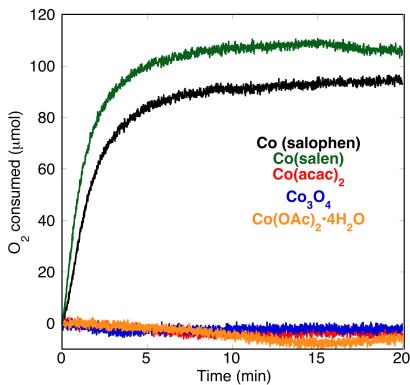


Figure S1. Time course data for the catalytic oxidation of H₂Q with a variety of Co sources measured by gas uptake as described. Reaction conditions: [Co(salophen)]: 1.7 mM (black), [Co(salen)]: 1.7 mM (green), [Co(acac)₂]: 1.7 mM (red), [Co₃O₄]: 1.7 mM (blue) but insoluble, [Co(OAc)₂•4H₂O]: 1.7 mM (orange); pO₂: 530 torr; [H₂Q]: 86 mM, 3.5 mL MeOH.

IV. General Method for Gas Uptake Kinetic Measurements

Each set of data was collected using a single-well gas uptake apparatus which holds a calibrated 50-mL round bottom flask connected to a pressure transducer designed to measure the gas pressure within the sealed reaction vessel. The apparatus was evacuated and filled with O₂ to 500 torr 4 times. The pressure was established at the desired pressure (500 torr for standard conditions) and the flasks were heated to 27 °C. A solution of catalyst was sonicated to make a homogeneous solution and added via syringe through a septum, and the pressure and temperature allowed to equilibrate. When the pressure and temperature equilibrated stabilized, a solution of hydroquinone was added via syringe through a septum. Data were acquired using custom software written within LabVIEW (National Instruments). The data in Figure 2 in the manuscript were obtained from linear fits to early reaction times of the time course traces below. Error bars are the standard deviation of the rate acquired from duplicated independent experiments.

A. [Co] dependence

Table S1. Reaction components for the catalytic oxidation of hydroquinone with varying concentrations of Co(salophen) measured by gas uptake.

Run	[H ₂ Q] (mM)	Solution volume (mL)	[Co(salophen)] (mM)
1	88.4	3.5	0.85
2	85.8	3.5	1.8
3	86.7	3.5	2.6
4	85.8	3.5	3.4
5	87.7	3.5	4.3
6	84.8	3.5	5.2

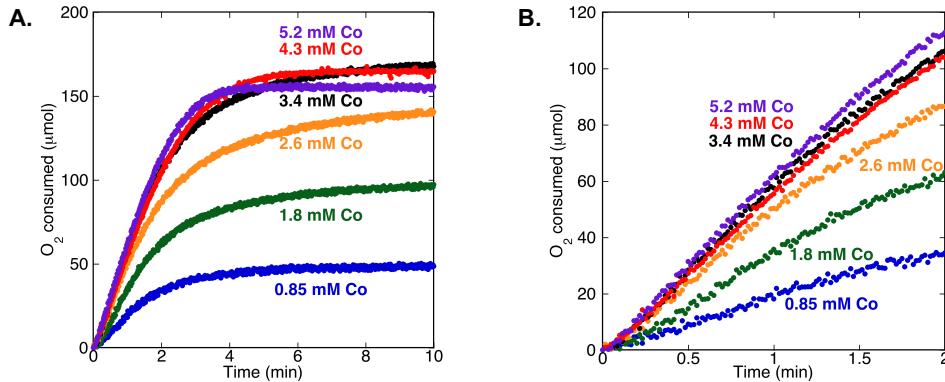


Figure S2. A) Overall and B) initial time course data for the catalytic oxidation of hydroquinone with varying quantities of Co(salophen) measured by gas uptake as described above. Reaction conditions: [Co(salophen)]: 0.85 mM (blue), 1.8 mM (green), 2.6 mM (orange), 3.4 mM (red), 4.3 mM (black), 5.2 mM (purple); pO_2 : 530 torr; $[H_2Q]$: 86 mM. The slope of the linear fit to the early time points yielded the initial rates used in Figure 2.

B. $[H_2Q]$ Dependence

Table S2. Reaction components for the catalytic oxidation of hydroquinone with varying concentrations of H_2Q measured by gas uptake.

Run	$[H_2Q]$ (mM)	Solution volume (mL)	[Co(salophen)] (mM)
1	13.1	3.5	1.6
2	22.5	3.5	1.8
3	43.2	3.5	1.7
4	85.8	3.5	1.8
5	129.9	3.5	1.8

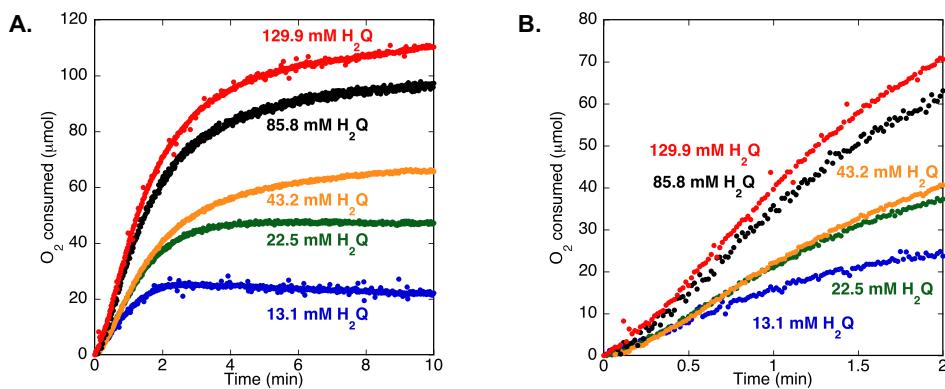


Figure S3. A) Overall and B) initial time course data for the catalytic oxidation of varying quantities of hydroquinone with Co(salophen) measured by gas uptake as described above. Reaction conditions: [Co(salophen)]: 1.7 mM; pO_2 : 530 torr; $[H_2Q]$: 13.1 mM (blue), 22.5 mM (green), 43.2 mM (orange), 85.8 mM (black), 129.9 mM (red). The slope of the linear fit to the early time points yielded the initial rates used in Figure 2.

C. $p\text{O}_2$ Dependence

Table S3. Reaction components for the catalytic oxidation of hydroquinone with varying $p\text{O}_2$ measured by gas uptake.

Run	[H ₂ Q] (mM)	Solution volume (mL)	[Co(salophen)] (mM)	$p\text{O}_2$ (torr)
1	86.4	3.5	1.7	225
2	85.0	3.5	1.8	321
3	84.0	3.5	1.7	428
4	85.8	3.5	1.8	537
5	86.5	3.5	1.8	644
6	84.8	3.5	1.7	746
7	87.7	3.5	1.7	829
8	86.2	3.5	1.8	907

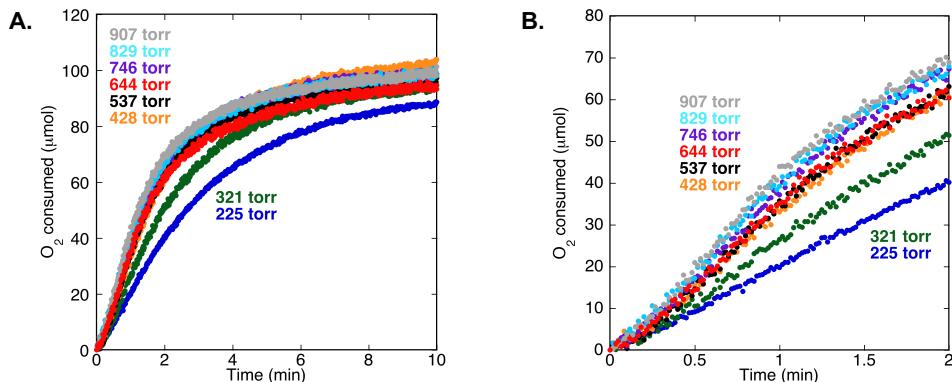


Figure S4. A) Overall and B) initial time course data for the catalytic oxidation of hydroquinone with Co(salophen) at various $p\text{O}_2$ measured by gas uptake as described above. Reaction conditions: [Co(salophen)]: 1.7 mM; $p\text{O}_2$: 225 torr (blue), 321 torr (green), 428 torr (orange), 537 torr (black), 644 torr (red), 746 torr (purple), 829 torr (teal), 907 torr (grey); [H₂Q]: 86 mM. The slope of the linear fit to the early time points yielded the initial rates used in Figure 2.

V. Investigation of Mass-transport Limitations

To test the hypothesis that the oxidation of H₂Q is mass-transport limited at high [Co], we investigated the influence of the stir rate upon the reaction at high (5 mol%) catalyst loadings using the single-well gas uptake apparatus as described above. A strobe (Extech digital StroboTach) was used to measure the stir rate of the reaction after injection of the Co(salophen) stock solution. A linear dependence upon stir rate was found for solutions at high [Co] (Figure S5).

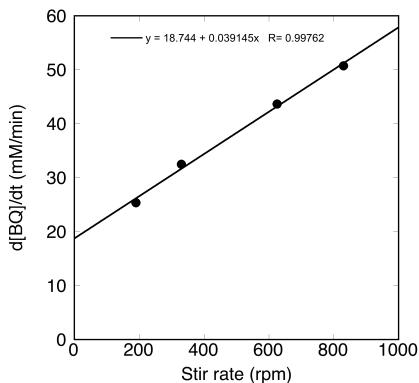


Figure S5. Stir rate dependence on the aerobic oxidation of H₂Q catalyzed by Co(salophen) at high catalyst loading, measured by initial rates at early time points. Conditions: 0.3 mmol H₂Q (86 mM), 5 mol% Co(salophen) (4.3 mM), 530 torr O₂, 3.5 mL MeOH, 27 °C.

To test whether mass-transport plays a role at lower Co(salophen) loadings, the stir rate dependence of the reaction at 1 mol% catalyst was examined under similar reaction conditions (86 mM H₂Q, 1 mol% Co(salophen), 530 torr O₂, 3.5 mL MeOH, 27 °C). The rate of the reaction was found to be independent of the stir rate (Fig S6).

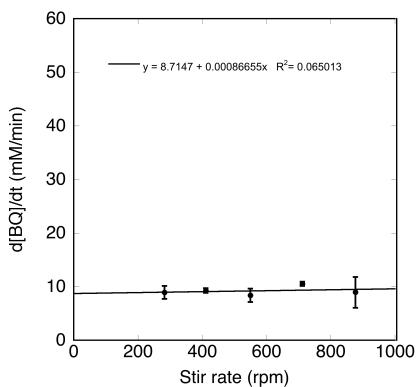


Figure S6. Stir rate dependence on the aerobic oxidation of H₂Q catalyzed by Co(salophen) at low catalyst loading, measured by initial rates at early time points. Conditions: 0.3 mmol H₂Q (86 mM), 1 mol% Co(salophen) (0.85 mM), 530 torr O₂, 3.5 mL MeOH, 27 °C.

VI. Methods for Determination of Kinetic Isotope Effect

Data were collected using the single-well gas uptake apparatus described previously. Hydroquinone-*d*2 (D₂Q) was generated *in situ* by dissolving H₂Q in MeOD prior to injection.⁵ Data was collected in duplicate, with the rates being determined from a linear fit to the early time points.

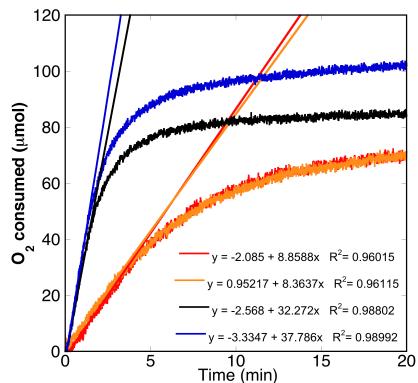


Figure S7. Time course data for the catalytic oxidation of H₂Q or D₂Q with Co(salophen) in MeOH or MeOD, respectively, measured by gas uptake as described above. Trial 1 (H₂Q): (blue); Trial 2 (H₂Q): (black); Trial 1 (D₂Q): (red); Trial 2 (D₂Q): (orange). Reaction conditions: [Co(salophen)]: 1.7 mM; pO_2 : 530 torr; [H₂Q] or [D₂Q]: 86 mM, 3.5 mL solvent. The slope of the linear fit to the early time points was used to determine k_H/k_D in Table S4.

Table S4. Independent rates measured by gas uptake for the oxidation of H₂Q or D₂Q with Co(salophen) in MeOH or MeOD, respectively.

Run	Initial Rate (μmol O ₂ /min)	
	H ₂ Q	D ₂ Q
1	32.3	8.86
2	37.8	8.36
Average	35.0	8.61
Std. dev.	3.9	0.4
k_H/k_D	4.0 ± 0.5	

VII. EPR Experiments and Simulations

EPR parameters for all experiments: microwave frequency 9.5 MHz, modulation amplitude 5 G, modulation frequency 100 kHz.

A. EPR spectra of Co(salophen) under N₂ or O₂

To generate the spectrum for Co(salophen) in MeOH or 50/50 DMF:MeOH under N₂, Co(salophen) was dissolved in the desired solvent (or solvent mixture) in a purge box, an aliquot transferred to a quart EPR tube and the tube capped with a septa. The sample was removed from the purge box and frozen in liquid nitrogen. The simulation values are given for the low-spin Co^{II} species in the two solvents under N₂ in Table S5 and compared to literature values. Microwave power = 1.002 mW in MeOH conditions, 0.100 mW in 1:1 DMF:MeOH conditions.

Table S5. Comparisons between literature values for low-spin Co^{II}(salen) or Co^{II}(salophen) species and the values obtained for Co(salophen) in the present work (bolded species).

Compound	solvent	<i>g</i> _x	<i>g</i> _y	<i>g</i> _z	<i>A</i> _x (MHz)	<i>A</i> _y (MHz)	<i>A</i> _z (MHz)
Co(salen)(py) ¹	pyridine	2.354	2.27	2.028	<60	<62	230
Co(salen) ²	CH ₂ Cl ₂	3.27	1.93	2.03	420	124	113
Co(salophen)(PPh ₃) ¹	CH ₂ Cl ₂	2.4	2.2	1.998			245
Co(salophen)(THF) ³	50/50 THF:toluene	2.514	2.256	2.017	175	97	336
Co(salophen)(MeOH)	MeOH	3.053	2.35	2.025	125	110	360
Co(salophen)(S)	50/50 DMF:MeOH	2.455	2.272	2.061	8	22	300

1: see ref. 6 2: see ref. 7. 3: see ref 8.

To generate the Co^{III}-superoxide species, a sample was prepared analogously in a purge box as described above. Before freezing in liquid nitrogen, the sample was purged with O₂ from a balloon for a brief period. The sample was then quickly capped with a septa and frozen in liquid N₂. The simulation values for the Co^{III}-superoxide species generated in the two solvent mixtures are given in Table S6 and compared to literature values. Microwave power = 0.6325 mW in MeOH conditions, 0.001 mW in 1:1 DMF:MeOH conditions.

Table S6. Comparisons between literature values for Co^{III}-superoxide species with salen- or salophen-based ligands and the values obtained for Co(salophen) in the present work (bolded species).

Compound	solvent	<i>g</i> _x	<i>g</i> _y	<i>g</i> _z	<i>A</i> _x (MHz)	<i>A</i> _y (MHz)	<i>A</i> _z (MHz)
Co(salchxtBu)(py)(O ₂ [·]) ¹	py	2.006	1.990	2.075	55	20	38
Na ₂ [Co(SO ₃ -sal-1,2-pn)(O ₂ [·])(S)] ²	DMF-H ₂ O	2.011	2.09	1.995	17	52	24
Co(salophen)(MeOH)(O₂[·])	MeOH	2.016	1.995	2.095	57	55	70
Co(salophen)(S)(O₂[·])	50/50 DMF:MeOH	2.023	2.023	2.115	48	33	72

1: see ref. 8. 2: see ref. 9.

B. EPR of quenched reaction mixture under 1 atm O₂

The reaction was run in MeOH at room temperature with [H₂Q] = 0.086 M and [Co(salophen)] = 1.7 mM in 3.5 mL MeOH under a balloon of O₂. The reaction was initiated by injection of a solution of H₂Q, an aliquot removed using a gas tight syringe, rapidly transferred to an EPR tube and immediately frozen in liquid nitrogen. Microwave power = 0.6325 mW.

C. Discussion of high-spin species

In many of the samples run in MeOH, there is a signal at ~1500 gauss that we have attribute to a high-spin Co^{II} species. Based on literature precedent,⁸ we believe that this structure is [Co^{II}(salophen)(OMe)]⁻. To probe this assignement, NaOMe (~12 equivalents) was added to a solution of Co^{II}(salophen) under N₂ in a purge box (Fig. S8). The most drastic difference is an increase in the signal attributed to the high-spin species. DFT studies (see Section XV) support that a methoxide-ligated Co^{II} species will be high-spin. Microwave power = 0.6325 mW.

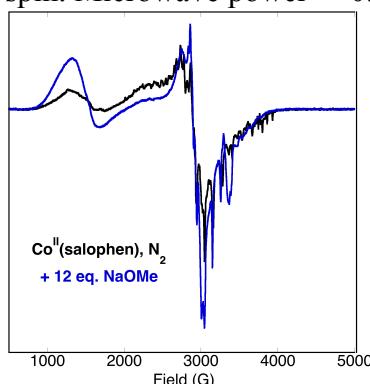


Figure S8. Effect of added base (in form of NaOMe) on EPR spectrum of Co(salophen) dissolved in MeOH under N₂.

VIII. Methods for Determination of the Fate of H₂O₂

Tests for the fate of H₂O₂ were based on modifications from literature precedent.¹⁰ Data was collected using a single-well gas uptake apparatus holding a custom designed 2-neck flask connected to a pressure transducer designed to measure the gas pressure within the sealed vessel. The pressure change due to the increase in solution volume was taken into account when determining the amount of O₂ evolved. Initial tests focused on comparing the rate of H₂O₂ disproportionation to the rate of catalytic H₂Q oxidation.

A. Determination of urea effect on aerobic H₂Q oxidation

To test whether urea has any effect on the rate of aerobic H₂Q oxidation by Co(salophen), reactions conducted in the presence of 1 eq. (relative to H₂Q) urea were conducted. Data were collected using the single-well gas uptake apparatus described previously. Data was collected in duplicate, with the rates being determined from a linear fit to the early time points (Fig. S9). 1 eq. of urea was added in the same stock solution as H₂Q. Comparing the rates here to the rates in the absence of urea, urea has a small effect on the rate of H₂Q oxidation (it proceeds at a rate of about 80% of the rate in the absence of urea).

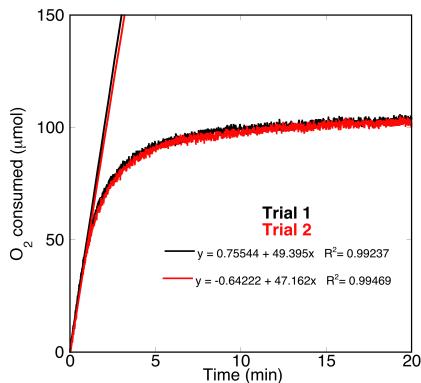


Figure S9. Time course data for the catalytic oxidation of H₂Q with Co(salophen) in the presence of 1 equivalent urea, measured by gas uptake as described above. Trial 1: red; Trial 2: black. Reaction conditions: [Co(salophen)]: 1.7 mM; pO₂: 530 torr; [H₂Q]: 86 mM, [urea]: 86 mM, 3.5 mL MeOH. The slope of the linear fit to the early time points was used to determine the rate.

B. Rate of H₂O₂ disproportionation in the presence of Co(salophen)

To compare the rates of O₂ uptake in the catalytic experiment in the presence of urea to the rate of O₂ evolution in the case of H₂O₂•urea disproportionation, a solution of H₂O₂•urea was added via syringe pump to a solution of Co(salophen) under N₂. A syringe pump was used to mimic catalytic conditions, where H₂O₂ would be formed during the course of the reaction, rather than generated entirely at the beginning of the reaction.

Experimental: A 3 mL anaerobic solution of Co(salophen) (3.0 mM) was added via syringe through a septum to the 2-neck flask under N₂. A second syringe containing an anaerobic sample of H₂O₂•urea (0.32 M in 2 mL) and attached to a syringe pump was added through a septum. The H₂O₂•urea had been titrated using by the KMnO₄ method.¹¹ When the pressure and temperature (27 °C) stabilized, data collection was started and 0.5 mL of the H₂O₂•urea solution was added over 5 minutes by syringe pump. Data were acquired every second using custom software written within LabVIEW (National Instruments). The results are shown in Fig. S10.

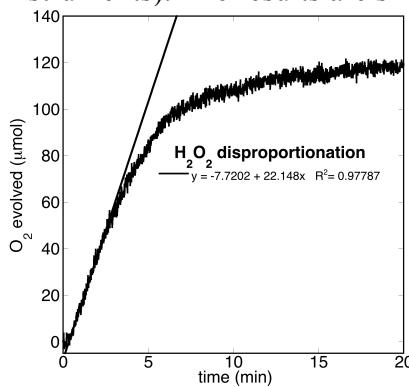


Figure S10. Time course data for the catalytic disproportionation of H₂O₂•urea by Co(salophen), measured by gas uptake as described above. The H₂O₂•urea solution was added via syringe pump as described above. Reaction conditions: 3 mL of 3.0 mM Co(salophen) in MeOH under N₂; 0.5 mL of an 0.32 M solution of H₂O₂•urea in MeOH under N₂ was added over 5 minutes. The slope of the linear fit to the early time points was used to determine the rate.

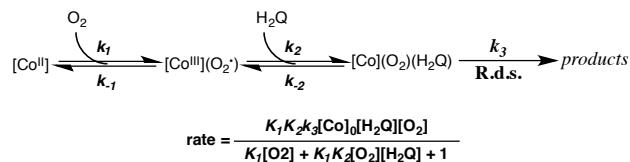
The results show that the catalytic oxidation of H₂Q in the presence of urea is faster than the rate of hydrogen peroxide disproportionation by a factor of ~2.2. A linear fit of the early time points of O₂ evolution gives a rate of 22.1 μmol O₂ evolved/minute, while the rate of O₂ reduction in the presence of urea is 48.3 ± 1.6 μmol O₂/min.

C. Detection of O₂ formation in the presence of substrate

Lastly, a solution of H₂O₂•urea was added to a solution of Co(salophen) and H₂Q under N₂. 3 mL of an anaerobic solution of Co(salophen) (3.0 mM) and 0.5 mL of an anaerobic solution of H₂Q (0.6 M) were added via syringe through a septum to the 2-neck flask under N₂. A second syringe containing an anaerobic sample of H₂O₂•urea (0.32 M in 2 mL) and attached to a syringe pump was added through a septum. The H₂O₂•urea had been titrated using the KMnO₄ method.¹¹ When the pressure and temperature (27 °C) stabilized, data collection was started and 0.5 mL of the H₂O₂•urea solution was added over 5 minutes by syringe pump. Data were acquired every second using custom software written within LabVIEW (National Instruments). The results are shown in the red trace in Fig. 7.

IX. Calculation of Standard State Barrier

Based on the observed kinetic dependencies, a rate law was derived:



To calculate the standard-state corrected barrier, a reaction was run in the regime where each reagent was in the first-order regime, and the observed rate was calculated. Conditions: 12 mM H₂Q, 1.8 mM Co(salophen), 217 torr O₂; initial rate = 11.2 umol O₂/min. Correcting for standard state (1 M Co(salophen), 1 atm O₂) gives rate = 27.6 M/min. Converting to ΔG[‡] gives value of 13.6 kcal/mol, which matches well with computed value.

X. Computational Details

All of the calculations were performed with density functional theory (DFT) utilizing the M06L functional¹² with the 6-31G**^{13,14,15} basis set for non-metal atoms and the LANL2DZ¹⁶ basis set for Co as implemented in Gaussian 09.¹⁷ All of the structures except O₂ and methanol were optimized in solution phase (solvent=methanol) with the SMD¹⁸ model that incorporates both electrostatic effects through the integral-equation-formalism polarizable continuum model (IEF-PCM) and non-electrostatic contributions to the solution phase free energy. Entropic and zero-point energy contributions to the total reaction free energies were included from vibrational frequency calculations at T=298.15. Vibrational frequency calculations also confirmed the presence of one imaginary frequency for each transition state and no imaginary frequency for each

minimum. The rotational contributions to the entropic portions of the free energies were excluded for all molecules except O₂ as suggested for association and dissociation reactions¹⁹ (Table S7). As the experiments were performed under 1 atm partial pressure of dioxygen and the solution phase concentration of methanol is 25 M, proper standard state corrections were included as follows:

- 1) The gas-phase free energy of O₂ was calculated at 1 atm partial pressure ($G(\text{gas})^0$). A correction was applied to account for the change in concentration from 1 atm partial pressure to 1 M in gas phase using the ideal gas law, $\Delta G^{0 \rightarrow *}=RT \ln(24.5)=1.89 \text{ kcal/mol}$.²⁰
- 2) The gas-phase free energy of methanol was calculated at 1 atm partial pressure ($G(\text{gas})^0$). A correction was applied to account for the change in concentration from 1 atm partial pressure to 25 M in gas phase using the ideal gas law, $\Delta G^{0 \rightarrow *}=RT \ln(24.5 \times 25)=3.79 \text{ kcal/mol}$. The solvation free energy of 4.84 kcal/mol, as obtained from the literature,²⁰ was added to the standard state corrected molar gas-phase free energy to obtain the molar solution phase free energy.
- 3) For all other species, the molar solution phase free energies were calculated directly with Gaussian 09.

XI. Full Computation Cycle

The absolute and relative solution phase free energies of each of the species from Scheme 4 are listed in Table S7. The full cycle with every species shown is in Scheme S1.

Table S7: Absolute and relative solution phase free energies of the species shown in the free energy diagram of the main article

Species	$G(\text{sol})^*\text{a}$	$S_{\text{rot}}\text{c}$	$E_{\text{rot}}\text{d}$	$G(\text{sol})^{*, \text{a,e}}$	$\Delta G(\text{sol})^*\text{g}$
³ O ₂	-150.320752 ^b			-150.320752 ^f	
MeOH	-115.676429 ^b	18.965	0.889	-115.668835	
<i>p</i> -hydroquinone	-382.591069	27.887	0.889	-382.579236	
H ₂ O	-76.420859	11.872	0.889	-76.416635	
<i>p</i> -quinone	-381.373042	27.764	0.889	-381.361267	
Products					-48.1 ^h
1	-1406.783338	35.853	0.889	-1406.767720	0.0
2	-1557.101812	36.098	0.889	-1557.086077	1.5
3	-1824.013046	36.887	0.889	-1823.996936	-0.3
3-TS	-1823.999839	36.844	0.889	-1823.983750	8.0
4	-1824.006284	37.082	0.889	-1823.990082	4.0
5	-1824.005260	37.136	0.889	-1823.989032	4.7
5-TS	-1823.993583	37.126	0.889	-1823.977360	12.0
6	-1824.001479	37.173	0.889	-1823.985234	7.1
5a	-1823.999384	37.050	0.889	-1823.983197	8.3
5a-TS	-1823.976912	37.090	0.889	-1823.960706	22.4
6a	-1366.245640	35.652	0.889	-1366.230117	-7.2

7	-1940.893744	37.418	0.889	-1940.877382	3.7
7-TS	-1940.885943	37.403	0.889	-1940.869588	8.6
8	-1940.905242	37.480	0.889	-1940.888851	-3.5
9	-1940.958071	37.459	0.889	-1940.941690	-36.7
10	-1864.546681	37.302	0.889	-1864.530374	-40.0
11	-1864.553455	37.275	0.889	-1864.537161	-44.2
12	-1864.554902	37.290	0.889	-1864.538601	-45.2

^a $G(\text{sol})^*$ is the solution phase free energy in hartrees for 1M concentration.

^b Standard state correction is included.

^c Rotational contribution to entropy in cal/K-mol.

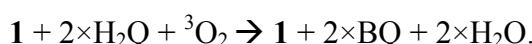
^d Rotational contribution to internal thermal energy = $(3/2) \times RT$ in kcal/mol.

^e $G(\text{sol})^{*'} = G(\text{sol})^* - (E_{\text{rot}} - S_{\text{rot}} \times 298.15/1000)/627.509$.

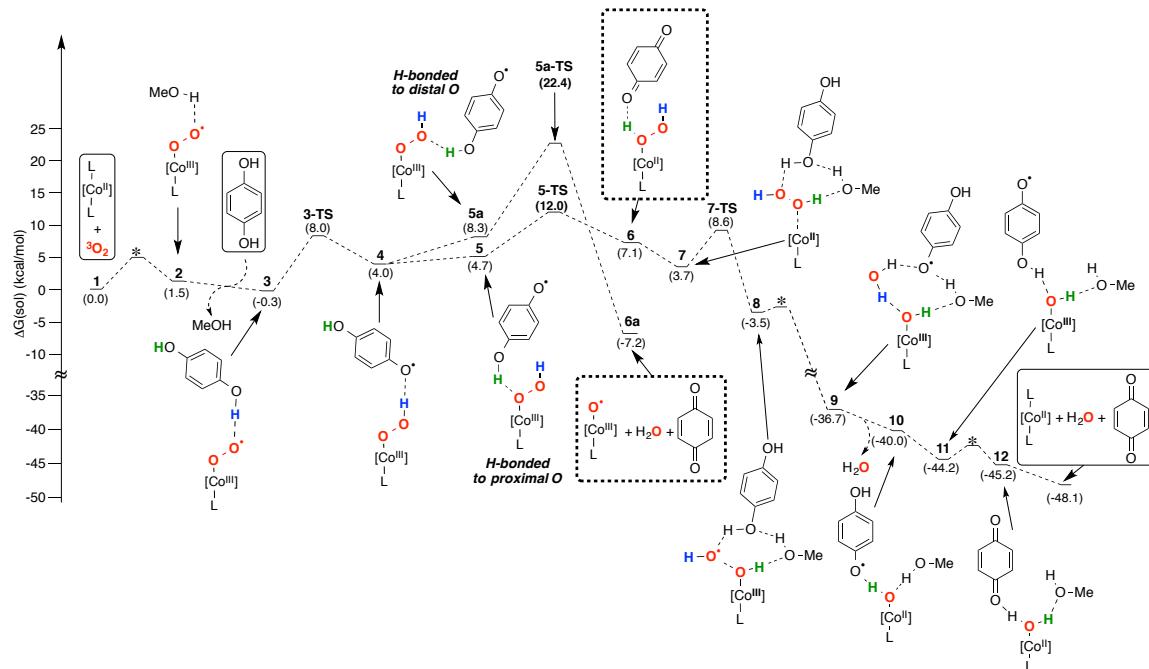
^f Since the solvation free energy is zero, no correction to the rotational contribution is made.

^g Relative free energy in kcal/mol. The reference is **1** + $2 \times \text{H}_2\text{Q} + {}^3\text{O}_2$. $\text{H}_2\text{O}/\text{MeOH}/p\text{-hydroquinone}/p\text{-quinone}$ is added to other species, as needed, to preserve the correct stoichiometry of each step.

^h The change in free energy corresponds to the following reaction:



Scheme S1. Free-energy diagram for H_2Q oxidation by Co(salophen) with all structures indicated. $[\text{Co}] = \text{Co}(\text{salophen})$, $L = \text{MeOH}$.



XII. Directionality in the PCET Step Resulting in H₂O₂ Formation

We investigated the activation free energies of the crucial PCET step between SQH[·] and the Co(salophen) complex for two different configurations of the hydrogen-bonding interaction between the two species. Species **5** is obtained if SQH[·] approaches the catalyst from the side of the phenoxide fragment of the salophen ligand. Alternatively, species **5b** is obtained if SQH[·] binds to the catalyst from the side of the phenyl fragment. Intuitively, **5b** is expected to be thermodynamically more stable than **5** due to a favorable π-π stacking interaction. As shown in Scheme S2, the free energy of species **5b** is lower than that of species **5** by 0.9 kcal mol⁻¹. However, the transition state associated with **5b** is significantly higher than that associated with species **5**.

Scheme S2. Comparison of activation free energies of the final PCET step for two different configurations of the SQH[·] and Co(salophen) hydrogen-bonded species, as depicted in Figures S11 and S12.

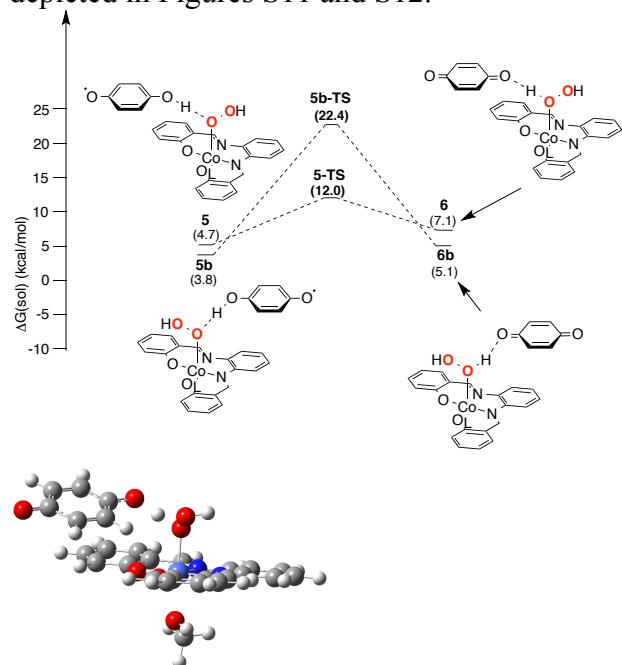


Figure S11. Structure of **5-TS**.

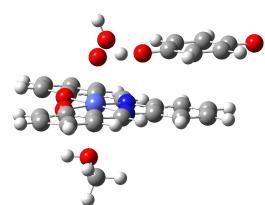


Figure S12. Structure of **5b-TS**.

Although the free energies of **5** and **5b** follow the expected ordering, the calculated free energies of the corresponding transition states, **5-TS** and **5b-TS**, are significantly different. Surprisingly, **5-TS** is *lower* in free energy than **5b-TS** by 10.4 kcal mol⁻¹. Both reactions, **5** → **6** and **5b** → **6b**, involve a proton-coupled electron transfer (PCET) from

SQH[•] to the Co^{III}(salophen)(OOH) complex, forming H₂O₂ bound to the Co^{II}(salophen)(MeOH) catalyst. A close inspection of the electronic structure reveals that the oxidation state of the Co-center remains +3 for both **5** and **5-TS**. In contrast, the Mulliken Spin Density distribution on the Co-center (+1.30e) and the *p*-quinone fragment (0.45e) reveals a much more complex electronic structure for **5b-TS**. Further analysis of the molecular orbitals indicates that the formal oxidation state of the metal center is reduced from +3 in **5b** to +2.5 in **5b-TS**. In short, the electron is transferred from the *p*-SHQ to the Co-center after the proton transfer transition state for **5-TS**, whereas partial transfer of electron density precedes the proton transfer transition state for **5b-TS**. Electrostatic potential (ESP) maps (Figures S13 and S14) show that the quinone fragment is much more negatively charged in **5-TS** than in **5b-TS**, thereby lending further support to this assignment. **5-TS** exhibits an unusual electronic structure in which the lone pairs of electrons on the oxygen atoms of the SQH[•], hydroperoxo, and salophen ligand strongly stabilize the transferring proton and Co^{III} center (Figure S15). Consequently, for **5** → **5-TS**, the change in the Co-O₂H bond length is small, changing from 1.894 Å to 1.922 Å. A much larger structural change is observed for **5b** → **5b-TS**, where the Co-O₂H bond length increases from 1.885 Å to 2.204 Å. This increase in metal-ligand bond length is consistent with the partial charge transfer to an anti-bonding Co *d*_{z²} orbital. Because a much smaller structural rearrangement is associated with the transfer of only a proton as compared to the transfer of both a proton and electron density, **5-TS** is significantly lower in free energy than **5b-TS**.

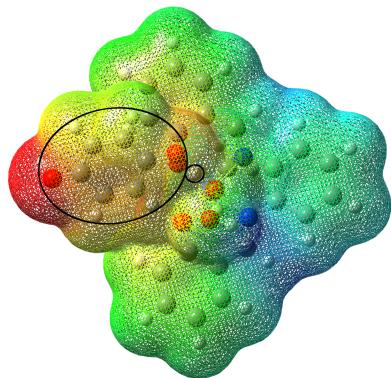


Figure S13. Electrostatic potential map of **5-TS** (top view). The encircled portion shows the position of SQH[•]. The SQH[•] is significantly more negatively charged than SQH[•] in **5b-TS** (Figure S14).

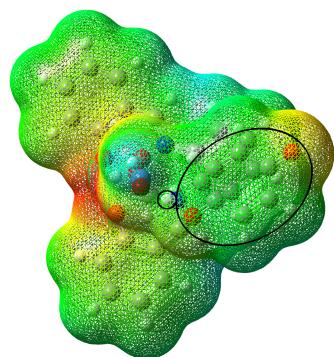


Figure S14. Electrostatic potential map of **5b-TS** (top view). The encircled portion shows the position of *p*-SHQ[•].

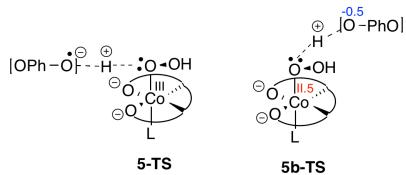


Figure S15. Schematic representation of charge distribution in **5-TS** and **5b-TS**.

XIII. Comparison of Disproportionation vs. Reduction Pathways for H₂O₂

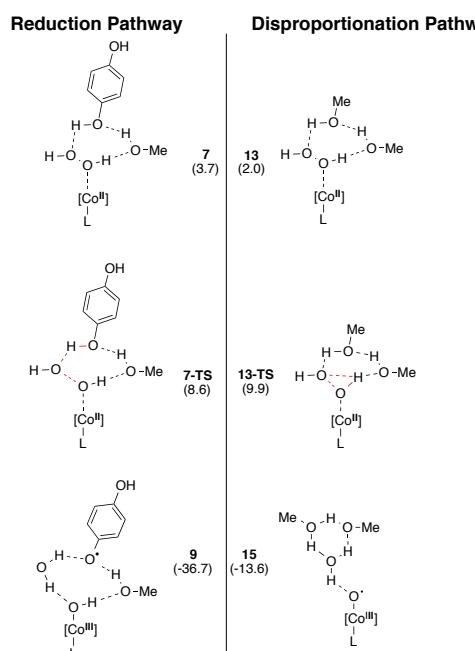
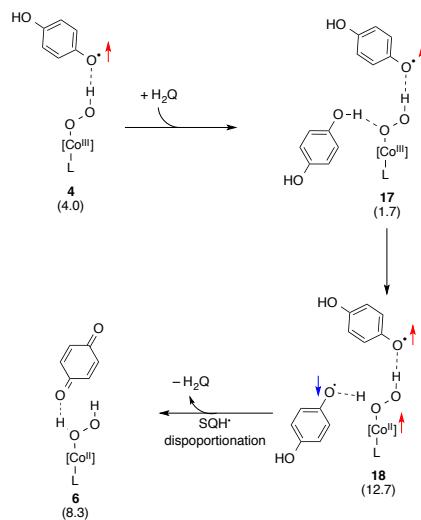


Figure S16. Comparison of solution phase free energies of key intermediates for H₂O₂ reduction and H₂O₂ disproportionation relative to species **1** with required number of reactant/solvent molecules added to make the overall reaction atom balanced. Note that structure **14**, similar to species **8** in Scheme S1, is not shown in the figure. Species **14** is a high-energy intermediate with a hydroxyl radical, and hence its existence under experimental conditions is questionable.

XIV. Alternative Studied Pathway for Second H-atom Transfer

Scheme S3. Thermodynamic outline of a possible pathway for formation of species **6** via disproportionation of 2 SQH[•] species.



XV. Calculations of Axial Ligand Effects on Spin State of Co^{II}

To further test the role of methoxide ligands to Co^{II} and the high-spin vs. low-spin behavior observed by EPR, computations using different functionals were performed on Co(salophen) with different axial ligands. The species considered were with two methanols ligated (Structure **1**, energies given in Table S8), one methanol ligated (Structure **19**, energies given in Table S9), and one methoxide ligated (structure **20**, energies given in Table S10). The functionals tested were MO6L, TPSSH,²¹ and OPBE.²²

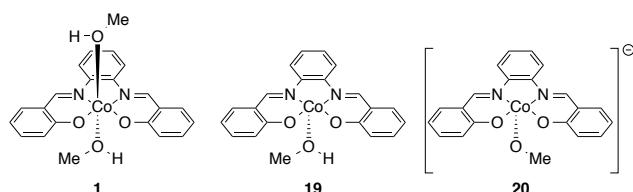


Table S8. Comparison of solution phase free energies of the low-spin and high-spin states of the 6-coordinate species **1** using different functionals.^a

Spin state	M06L		TPSSH	
	ΔG	$\langle S^2 \rangle$	ΔG	$\langle S^2 \rangle$
S = 1/2	0.00	0.77	0.00	0.76
S = 3/2	1.28	3.77	-2.34	3.76

^a With OPBE, one of the axial methanol molecules become uncoordinated and hence, the results are not considered here.

Table S9. Comparison of solution phase free energies of the low-spin and high-spin states of the 5-coordinate species **19** with one methanol axial ligand using different functionals.

Spin state	M06L		TPSSH		OPBE	
	ΔG	$\langle S^2 \rangle$	ΔG	$\langle S^2 \rangle$	ΔG	$\langle S^2 \rangle$
S = 1/2	0.00	0.77	0.00	0.76	0.00	0.77
S = 3/2	2.72	3.76	-3.31	3.76	7.95	3.77

Table S10. Comparison of solution phase free energies of the low-spin and high-spin states of the 5-coordinate species **20** with one methoxide axial ligand using different functionals.

Spin state	M06L		TPSSH		OPBE	
	ΔG	$\langle S^2 \rangle$	ΔG	$\langle S^2 \rangle$	ΔG	$\langle S^2 \rangle$
S = 1/2	0.00	0.77	0.00	0.77	0.00	0.78
S = 3/2	-6.22	3.77	-13.23	3.76	-7.24	3.81

With methoxide as a ligand (species **20**), the high-spin state for Co^{II} is highly favored with each functional examined, supporting the experimental evidence that addition of NaOMe to an anaerobic solution of Co^{II} increases the high-spin signal. For species **19**, the low-spin state for Co^{II} is favored with the M06L and OPBE functionals, but disfavored with the TPSSH functional. Given the error range of the computed relative energies, the results for species **1** are inconclusive but nevertheless indicate that the low-spin and high-spin species have similar free energies.

XVI. Coordinates of Computed Structures

Table S11: Coordinates of all species, **1-20**, mentioned in the main text and supporting information

1

Co	-0.17393100	0.13423600	1.47942400
O	-1.50947800	-1.22445800	1.24879300
O	1.08383000	-1.31604200	1.43822600
N	1.15393700	1.50403100	1.64878500
C	2.44577400	1.30740100	1.56023000
C	5.22161300	-1.11732800	1.17568300
C	4.52924800	-2.34250300	1.13591500
C	3.15376800	-2.38539000	1.22837200
C	2.37501700	-1.20424200	1.36200000
C	3.08500500	0.04725800	1.40732100
C	4.49913400	0.04714000	1.31145300
H	6.30431300	-1.09285300	1.10242800
H	5.08413300	-3.27203800	1.02951900

H	2.62212700	-3.33299700	1.19630000
H	5.01066500	1.00749700	1.35005500
C	-5.64023800	-0.82334800	1.29175700
C	-5.01362700	-2.07309100	1.12660800
C	-3.63882600	-2.18302200	1.11335900
C	-2.79573300	-1.04907500	1.26503600
C	-3.43807700	0.22882200	1.42741400
C	-4.85384400	0.29751500	1.43781800
H	-6.72289200	-0.74624100	1.30223300
H	-5.61971500	-2.96850400	1.00780100
H	-3.15776900	-3.14961100	0.98700300
H	-5.31358800	1.27647700	1.56345300
N	-1.42540600	1.58471000	1.57398600
C	-2.72805800	1.45146700	1.57245800
H	3.11550600	2.16997600	1.59625200
C	1.32858200	3.97116500	2.00651500
C	0.66189900	5.18322400	2.12804900
C	-0.73158900	5.23195300	2.04743100
C	-1.46356500	4.06740000	1.85789100
C	-0.80585300	2.83723500	1.74578900
C	0.60442600	2.79120500	1.80174400
H	2.41115200	3.94959700	2.07745500
H	1.23131500	6.09418100	2.28755100
H	-1.25061700	6.18160400	2.13830500
H	-2.54550900	4.12307100	1.79874900
H	-3.34933500	2.34150700	1.69740900
O	0.10815500	0.17842000	-0.94030400
O	-0.43359700	-0.15319500	3.86232200
C	0.79602200	0.06761300	4.54417800
H	-0.57428800	-1.10831300	3.82044000
H	1.64366400	-0.39910600	4.02593600
H	0.95949900	1.14725200	4.57681600
H	0.75781200	-0.31017100	5.57278100
C	-1.03761600	0.73897000	-1.57027900
H	-1.04379600	0.53608100	-2.64799700
H	-1.97295000	0.36535100	-1.13341200
H	-0.99266900	1.82043700	-1.42161100
H	0.05675000	-0.78090000	-1.04422900

³O₂

O	-1.90366100	0.00032000	1.46270000
O	-0.68723900	-0.05122000	1.46270000

H₂Q

O	-3.84587900	-0.07622900	2.03129200
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C	0.31793000	-0.13285600	2.03662800
C	-0.38796600	1.07067700	2.10622600
C	-1.77703700	1.06816000	2.10302300
C	-2.47810700	-0.13798800	2.03017600
C	-1.77438000	-1.34022900	1.96049100
C	-0.38103500	-1.33772300	1.96375400
O	1.68542200	-0.06566100	2.04394300
H	0.16235300	2.00554500	2.16235700
H	-2.33101100	2.00101800	2.15660300
H	-2.31717900	-2.28071100	1.90421200
H	0.16535600	-2.27627200	1.91012300
H	2.04238100	-0.96172200	1.99191500
H	-4.19874900	-0.97390800	1.97895500

MeOH

C	-1.69665900	0.30519000	1.38200000
O	-0.28644600	0.43717500	1.38200000
H	0.07914600	-0.45482100	1.38200000
H	-2.11869500	1.31331700	1.38200000
H	-2.07132300	-0.21973000	0.49211600
H	-2.07132300	-0.21973000	2.27188400

2

Co	0.17619200	-0.41261200	1.20345500
O	-1.24726600	-1.61279900	1.63168300
O	1.27800600	-1.96735700	1.37736600
N	1.62661400	0.81291400	0.88243300
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C	5.40247300	-2.24150300	1.02182800
C	4.59577800	-3.36607900	1.27672800
C	3.22556300	-3.25173500	1.38659700
C	2.57223700	-1.99978500	1.24933600
C	3.39453000	-0.85251200	0.98739800
C	4.79908600	-1.01258000	0.88251700
H	6.47953800	-2.34332500	0.93734400
H	5.05648700	-4.34469400	1.38967700
H	2.60530800	-4.12154100	1.58410500
H	5.39629400	-0.12465400	0.68468900
C	-5.32709100	-0.89968200	1.39988200
C	-4.80476600	-2.17736700	1.67465800
C	-3.44394600	-2.39391900	1.74152300
C	-2.51500500	-1.34051800	1.54054700
C	-3.04856800	-0.03486100	1.26702600
C	-4.45266900	0.14480200	1.20260500

H	-6.39944600	-0.74215300	1.34696700
H	-5.48254400	-3.01258300	1.83479200
H	-3.04406600	-3.38216100	1.95099400
H	-4.82706200	1.14456600	0.99160700
N	-0.93306900	1.14691300	1.07872600
C	-2.23976900	1.11452900	1.06990200
H	3.63353900	1.23908200	0.66335700
C	2.01396200	3.23417300	0.43180100
C	1.45591200	4.49529900	0.27943100
C	0.07757900	4.67993500	0.41669200
C	-0.75002300	3.60256400	0.69812500
C	-0.20179700	2.32266000	0.83992900
C	1.19153700	2.13903300	0.71992600
H	3.08573200	3.10736300	0.32174100
H	2.09915600	5.34078400	0.05511000
H	-0.35356700	5.66999000	0.30327600
H	-1.81820800	3.76109300	0.80308900
H	-2.78069500	2.04582600	0.89164200
O	0.07458200	-0.69788400	-0.67634000
O	-1.09556700	-0.84078800	-1.17705600
O	0.51936900	-0.18657200	3.27775600
C	-0.49762100	0.45729900	4.05582300
H	-0.28498100	0.32803500	5.12048600
H	-0.46599200	1.51969000	3.81144800
H	-1.49195800	0.05835200	3.82930200
H	0.54571500	-1.12097500	3.53552900
H	-1.99696100	0.92877100	-1.68747500
O	-1.97574200	1.86727800	-1.92346900
C	-0.73489400	2.09314400	-2.56535100
H	-0.69560300	3.15057000	-2.84185800
H	0.12667700	1.88233700	-1.91467000
H	-0.62424500	1.49643600	-3.48189100

3

Co	0.03591400	-0.29840100	1.40779500
O	-1.35095600	-1.49444000	1.95482000
O	1.26432700	-1.72360200	1.77197100
N	1.41997500	0.93388200	0.89510600
C	2.61106300	0.57839100	0.50180800
C	5.03993700	-2.18969700	0.10235700
C	4.37866500	-3.24038400	0.76295500
C	3.12528900	-3.06267900	1.31427100
C	2.44885200	-1.81981300	1.23223600
C	3.13479300	-0.74193600	0.57660000
C	4.41957200	-0.96234900	0.02440800
H	6.02324900	-2.34238600	-0.33078800

H	4.85743900	-4.21377900	0.83994400
H	2.61728100	-3.87878700	1.82047100
H	4.90961600	-0.12531600	-0.47095900
C	-5.43667800	-1.03643400	1.38193400
C	-4.87282600	-2.24549800	1.82831600
C	-3.51093500	-2.37476800	2.00928400
C	-2.62145300	-1.30099000	1.74880400
C	-3.19922200	-0.06305400	1.29986500
C	-4.60232400	0.02971200	1.13035400
H	-6.50904300	-0.94630900	1.24226600
H	-5.51733900	-3.09687200	2.03432200
H	-3.07927200	-3.31055400	2.35344600
H	-5.01079100	0.97986900	0.79176900
N	-1.13594800	1.19741500	1.12689800
C	-2.43677600	1.11057900	1.05633200
H	3.27486800	1.34243000	0.08636700
C	1.78323900	3.39048000	0.78084200
C	1.20647900	4.65340000	0.74960200
C	-0.18181200	4.79624200	0.81801900
C	-1.00183800	3.68083900	0.93681800
C	-0.43267900	2.40458200	0.97070300
C	0.96601900	2.26057700	0.87342800
H	2.86317400	3.28201600	0.74670500
H	1.84161900	5.53168900	0.68524600
H	-0.62725900	5.78639200	0.80566200
H	-2.07567400	3.80824000	1.02810000
H	-3.00515800	2.00875700	0.80098500
O	-0.04039000	-0.93465700	-0.37463100
O	-1.18477600	-0.93368900	-0.95298400
O	0.37310800	0.30450000	3.40402500
C	-0.74844100	0.64424700	4.22836300
H	-0.41811900	0.77701600	5.26207600
H	-1.14691000	1.58967900	3.85745200
H	-1.52600300	-0.12484600	4.18567200
H	0.77036100	-0.50666000	3.75654400
H	-0.93839900	0.67301400	-2.24759000
O	-0.52514600	1.54931200	-2.29785500
C	0.81546000	1.39289100	-2.51995600
C	1.39162900	0.16268300	-2.84439100
C	1.62596800	2.52570300	-2.41643400
C	2.76816000	0.06051000	-3.02721600
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C	3.00011000	2.42488300	-2.60012900
H	1.16891600	3.48082800	-2.17157200
C	3.57965100	1.18768900	-2.89386600
H	3.21569500	-0.90282700	-3.26170600
H	3.63598900	3.30104600	-2.50507500
O	4.94101300	1.13989900	-3.03098000

H	5.20214300	0.23389900	-3.24311400
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3-TS

Co	0.05520000	-0.18018400	1.38243100
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O	1.29752700	-1.50395000	1.99842300
N	1.42500000	1.06557400	0.86244500
C	2.67261700	0.74364200	0.66161600
C	5.28728200	-1.86716800	0.90521400
C	4.60179100	-2.89161300	1.58566300
C	3.27543400	-2.74799700	1.94148900
C	2.54875000	-1.57020500	1.63550900
C	3.25528200	-0.51901000	0.96125900
C	4.61600100	-0.70303600	0.61175900
H	6.33177000	-1.99296600	0.62836900
H	5.12092900	-3.81359800	1.83076800
H	2.74959300	-3.54307500	2.46408400
H	5.12159500	0.11372200	0.09757700
C	-5.38802800	-1.12404000	1.23698800
C	-4.79588600	-2.26679200	1.80488600
C	-3.43961300	-2.33046100	2.03842000
C	-2.57836400	-1.24985700	1.70978500
C	-3.18100200	-0.08095900	1.13442400
C	-4.58157400	-0.05352500	0.91712800
H	-6.45622200	-1.08680200	1.05986100
H	-5.41821200	-3.12182300	2.06571600
H	-2.98698600	-3.21631900	2.47568300
H	-5.01237100	0.84691800	0.48328400
N	-1.15316400	1.22779800	0.89146300
C	-2.44985500	1.08816100	0.79798200
H	3.34482500	1.49393400	0.23833800
C	1.68893000	3.49802400	0.40642400
C	1.06333800	4.70785500	0.14580300
C	-0.33371000	4.78782300	0.11210200
C	-1.11013900	3.66347000	0.35404000
C	-0.49154400	2.43435700	0.61110800
C	0.91516200	2.35023000	0.62227700
H	2.77148100	3.44738000	0.45098900
H	1.66196800	5.59628500	-0.01722900
H	-0.81768600	5.74213800	-0.07656600
H	-2.19211700	3.74432400	0.35616300
H	-3.03677600	1.93793300	0.44139600
O	0.12086500	-1.00192500	-0.29379900
O	-1.06075100	-1.01622900	-0.97888300
O	0.21663900	0.59355900	3.33939900
C	-0.96280300	1.06951100	3.99866000

H	-0.74020900	1.27491500	5.04789000
H	-1.25418700	1.99930200	3.50804800
H	-1.78042700	0.34360700	3.93173000
H	0.52746800	-0.19797400	3.80377700
H	-0.88147200	-0.25678700	-1.83733100
O	-0.56279100	0.66269800	-2.60355300
C	0.74225700	0.74507200	-2.63938900
C	1.56641900	-0.41286400	-2.74823900
C	1.38368900	2.01183200	-2.58744500
C	2.94016000	-0.31138200	-2.77640300
H	1.08434400	-1.38579500	-2.80200900
C	2.75763100	2.11700800	-2.63030400
H	0.76149200	2.90112300	-2.51602500
C	3.54772800	0.95499900	-2.71152600
H	3.56439900	-1.20074000	-2.84040700
H	3.24848800	3.08564800	-2.58931400
O	4.88692300	1.11929700	-2.71722300
H	5.32414600	0.25611200	-2.77985000

4

Co	0.44414600	-0.53529000	1.56162700
O	-1.15970700	-1.45250600	2.04743400
O	1.31523300	-1.94080200	2.53155200
N	2.05476900	0.44509500	1.18334900
C	3.25837800	-0.00846000	1.40798000
C	5.38521600	-2.70320800	2.79345500
C	4.42336100	-3.58021600	3.32861700
C	3.07515700	-3.30715400	3.22810100
C	2.59972300	-2.13658900	2.58161200
C	3.58212300	-1.23861200	2.03994300
C	4.95802800	-1.55524400	2.16591700
H	6.44358900	-2.92804500	2.87725700
H	4.74417300	-4.49083300	3.82921300
H	2.33454100	-3.98677300	3.64066000
H	5.68058100	-0.85597600	1.74951100
C	-4.98166700	-0.79857500	0.57029700
C	-4.67645500	-1.89502800	1.39846600
C	-3.39895900	-2.09367000	1.88049000
C	-2.33917700	-1.20506300	1.56248000
C	-2.65726800	-0.07527600	0.73374100
C	-3.97924400	0.09039100	0.25401700
H	-5.98890000	-0.65729600	0.19184200
H	-5.45794300	-2.60423700	1.66137800
H	-3.16575300	-2.94573300	2.51317600
H	-4.18393700	0.95107900	-0.38039900
N	-0.44393000	0.92065800	0.69275500

C	-1.71198300	0.92092100	0.37603000
H	4.11119000	0.59887700	1.09588600
C	2.76636600	2.63685000	0.23572200
C	2.38086200	3.82956400	-0.36071500
C	1.02937500	4.09763000	-0.59845400
C	0.05880500	3.16991700	-0.25036700
C	0.43517300	1.95108200	0.32690700
C	1.79934600	1.68729100	0.58380300
H	3.81752200	2.45304700	0.43196600
H	3.13649100	4.56133000	-0.63173300
H	0.73265300	5.03707200	-1.05640100
H	-0.98741800	3.39623800	-0.42918300
H	-2.10277200	1.75392800	-0.21293800
O	0.75572500	-1.41796000	-0.06354800
O	-0.43251700	-1.87887500	-0.70056000
O	0.38928700	0.43689000	3.43767400
C	-0.78420500	1.16897700	3.81176300
H	-0.72666600	1.44445500	4.86816800
H	-0.80510200	2.07731400	3.20804000
H	-1.69452000	0.58778000	3.63333000
H	0.46170900	-0.33186200	4.02391900
H	-0.64952100	-1.14970400	-1.31831300
O	-1.26499000	0.12053400	-2.40417300
C	-0.45238500	1.00101300	-2.82534200
C	0.97635200	0.85457100	-2.68017500
C	-0.93002200	2.20304200	-3.46490500
C	1.83801700	1.82775700	-3.11400800
H	1.34806600	-0.04496100	-2.19465200
C	-0.06456400	3.17495500	-3.88915600
H	-2.00381100	2.31682600	-3.58612900
C	1.32730600	3.00592600	-3.70266700
H	2.91324600	1.72282500	-2.99034800
H	-0.41743400	4.09005700	-4.35560300
O	2.11747500	4.01428400	-4.09482400
H	3.04570300	3.80333900	-3.91151300

5

Co	0.05193200	0.33089400	1.20163000
O	-1.22143900	-1.06396100	0.93792600
O	1.35092500	-1.01950200	0.81262700
N	1.35215600	1.70545800	1.54208000
C	2.61917600	1.61009500	1.24107800
C	5.37518300	-0.50648800	-0.04197300
C	4.73291200	-1.75016700	-0.18683700
C	3.39634900	-1.90323400	0.11958600
C	2.61407100	-0.81129700	0.57352000

C	3.27173700	0.45265700	0.73910800
C	4.64832300	0.56637500	0.42274200
H	6.42691600	-0.39835400	-0.28647900
H	5.29414200	-2.60763600	-0.55116100
H	2.89835100	-2.86178100	-0.00393100
H	5.12322400	1.53638700	0.55616700
C	-5.35380700	-0.75433000	0.78236600
C	-4.67939000	-1.94753300	0.46311400
C	-3.30292200	-2.02604700	0.51535500
C	-2.51136300	-0.91074700	0.89101600
C	-3.19977500	0.30706100	1.21658000
C	-4.61478400	0.34606800	1.15322400
H	-6.43695500	-0.70503200	0.73781600
H	-5.24932800	-2.82554300	0.16826600
H	-2.78461200	-2.94945600	0.27142400
H	-5.11011400	1.28110300	1.40737900
N	-1.23984800	1.65201300	1.71372900
C	-2.53413200	1.49148300	1.62646600
H	3.25466200	2.48715000	1.38363500
C	1.46978200	4.00104400	2.49993500
C	0.77760300	5.09047900	3.00941500
C	-0.61615800	5.06216400	3.10101000
C	-1.32382200	3.94410600	2.68339200
C	-0.63906700	2.84120100	2.16104100
C	0.76864500	2.86966700	2.06795500
H	2.55330300	4.02940700	2.45499800
H	1.32854100	5.96207200	3.34955300
H	-1.15271200	5.91169700	3.51243800
H	-2.40480900	3.92842600	2.77721700
H	-3.17882900	2.33299500	1.88975400
O	0.04550500	0.94678500	-0.58851200
O	-1.22930900	0.81174700	-1.22976000
O	0.29569900	-0.25868900	3.18693800
C	-0.85190500	-0.62608000	3.96683300
H	-0.52283600	-0.97807000	4.94807000
H	-1.45528100	0.27338800	4.09346200
H	-1.44140200	-1.40324100	3.47287200
H	0.84189100	-1.05145300	3.06370700
H	0.98639600	0.12122500	-1.61513800
O	1.64220000	-0.26668500	-2.27455400
C	1.41422300	-1.55831800	-2.48932300
C	0.29926200	-2.23921100	-1.93731400
C	2.34281900	-2.25797800	-3.30077200
C	0.12599500	-3.57538600	-2.18523500
H	-0.39745700	-1.68697500	-1.31090300
C	2.17296200	-3.59285300	-3.54868500
H	3.18870300	-1.70648700	-3.70285800
C	1.05229800	-4.32672000	-3.00290900

H	-0.72330300	-4.11188300	-1.76963900
H	2.88155000	-4.14081100	-4.16421200
O	0.89031200	-5.55985900	-3.22988100
H	-1.61887600	1.68926400	-1.08574000

5-TS

Co	0.19695600	0.57382800	1.29427800
O	-0.76974800	-1.06303300	1.32326000
O	1.69180400	-0.54853200	0.93850700
N	1.20252200	2.21538300	1.29154300
C	2.45042900	2.30665500	0.91684100
C	5.53630200	0.55910300	-0.14552400
C	5.13098300	-0.78839000	-0.09302200
C	3.85139300	-1.13560100	0.28302600
C	2.88949700	-0.14883400	0.61980300
C	3.30437000	1.22460200	0.57856300
C	4.63102600	1.53858000	0.19086900
H	6.54636800	0.81796400	-0.44293300
H	5.83464000	-1.57390200	-0.35895100
H	3.53638600	-2.17550600	0.31133600
H	4.91806400	2.58761000	0.16319300
C	-4.85538000	-1.61853000	1.76515900
C	-3.97843700	-2.68410300	1.47906200
C	-2.62440900	-2.47176200	1.32366800
C	-2.05797600	-1.17689400	1.45403600
C	-2.95293200	-0.09008500	1.73165800
C	-4.33800100	-0.35122400	1.88640300
H	-5.91852100	-1.79951800	1.88490200
H	-4.37156500	-3.69237400	1.37304600
H	-1.94800900	-3.29235500	1.09946600
H	-4.99328900	0.49329200	2.09882200
N	-1.30609700	1.69808400	1.72378700
C	-2.52969500	1.25753500	1.85875600
H	2.90130600	3.29953800	0.85490300
C	0.88118500	4.64718500	1.73146600
C	0.00097700	5.66618100	2.06535900
C	-1.34945200	5.38801500	2.29369800
C	-1.82562700	4.08920500	2.18884300
C	-0.94939000	3.05157300	1.85147500
C	0.41272500	3.33377200	1.61324800
H	1.92955900	4.87625900	1.57241400
H	0.37100000	6.68268700	2.15780300
H	-2.03342800	6.18793000	2.56018500
H	-2.87469900	3.88787300	2.38056100
H	-3.31621700	1.97940900	2.08175600
O	-0.09194700	0.92282600	-0.57429300

O	-1.36386300	0.44740600	-1.04853500
O	0.51833100	0.20557000	3.26601500
C	1.38201500	1.05296800	4.04027200
H	1.44602200	0.65468400	5.05555700
H	2.36596400	1.01623300	3.57296200
H	1.01792600	2.08448700	4.06971800
H	-0.34680100	0.17039200	3.70232400
H	0.67244400	0.35987600	-1.30818500
O	1.60071700	-0.08489000	-2.15286100
C	1.66770200	-1.38354500	-2.22989800
C	0.73387400	-2.25059100	-1.58232900
C	2.72330800	-1.98024600	-2.98625200
C	0.85384900	-3.61123800	-1.68187000
H	-0.06877000	-1.80542100	-0.99825100
C	2.84440400	-3.33953200	-3.08724300
H	3.43327400	-1.31340400	-3.47110000
C	1.91562200	-4.23584100	-2.43671500
H	0.14161900	-4.26658300	-1.18425400
H	3.65364300	-3.78688600	-3.66038600
O	2.02704300	-5.49551600	-2.52494000
H	-1.87653000	1.27286900	-1.04511800

6

Co	0.11103000	0.57779100	1.17743700
O	-0.87001500	-1.05730400	1.12647300
O	1.64097400	-0.51275400	0.82601600
N	1.07893400	2.22920300	1.14232600
C	2.29755800	2.36446400	0.68301200
C	5.37544400	0.68508600	-0.51602200
C	5.04584200	-0.67328600	-0.33871400
C	3.81085900	-1.04805700	0.14620700
C	2.81114600	-0.08821500	0.45582200
C	3.16287200	1.29890300	0.31629500
C	4.44658000	1.64278400	-0.17817800
H	6.35009100	0.96991600	-0.89923600
H	5.77248100	-1.44196600	-0.59285400
H	3.55172600	-2.09733000	0.26616500
H	4.68321000	2.69993900	-0.28390400
C	-4.92232700	-1.67273200	1.75256200
C	-4.05163900	-2.72462800	1.40945700
C	-2.70738000	-2.49621800	1.20243800
C	-2.14509400	-1.19814100	1.32610800
C	-3.03665700	-0.12247200	1.66771000
C	-4.41083700	-0.40012400	1.87469600
H	-5.97852800	-1.86290400	1.91455900
H	-4.44196900	-3.73435200	1.30483100

H	-2.03459400	-3.30817800	0.93747900
H	-5.06429000	0.43124000	2.13320800
N	-1.39894600	1.67194500	1.62607800
C	-2.61830800	1.22855500	1.80157500
H	2.70864500	3.37026100	0.56684200
C	0.76323900	4.63772000	1.70604400
C	-0.11383500	5.64027100	2.09946400
C	-1.45864600	5.34679200	2.33410000
C	-1.93116300	4.04900800	2.18578700
C	-1.05893900	3.02889300	1.79185400
C	0.29606600	3.33070300	1.53519500
H	1.81065700	4.87370900	1.54774700
H	0.25496800	6.65290600	2.23279500
H	-2.14124200	6.13158600	2.64628600
H	-2.97622300	3.83728600	2.38659200
H	-3.40386100	1.93800600	2.07067600
O	-0.28787800	1.09479800	-1.12684900
O	-1.44588900	0.37872400	-1.64127600
O	0.47590000	0.26008000	3.51886500
C	1.64749900	0.88467100	4.03009000
H	1.79682600	0.64702300	5.08990700
H	2.49519200	0.49298700	3.46343200
H	1.62235900	1.97546100	3.91227300
H	-0.28325800	0.62967000	3.98754600
H	0.45264400	0.65281200	-1.62126300
O	1.74858000	-0.08866900	-2.48234200
C	1.86059500	-1.32946100	-2.41538400
C	0.90876200	-2.15192100	-1.66702000
C	2.97361300	-2.00157000	-3.08706200
C	1.06109500	-3.49054700	-1.59480100
H	0.08790000	-1.64082700	-1.17114900
C	3.12488300	-3.33856000	-3.01215900
H	3.66771500	-1.36828600	-3.63353700
C	2.17820000	-4.17046500	-2.25780600
H	0.36611200	-4.11602400	-1.04052600
H	3.94834600	-3.85305700	-3.49996100
O	2.31999600	-5.40012900	-2.18720200
H	-1.76363600	1.00126900	-2.31379700

5a

Co	-0.00523500	0.18360000	1.28009700
O	-1.31831200	-1.17831900	1.05007700
O	1.26304000	-1.23206100	1.00878900
N	1.33972800	1.53166900	1.52987700
C	2.57393200	1.40801500	1.12245400
C	5.19422900	-0.82540300	-0.24946700

C	4.54879000	-2.07479500	-0.20774700
C	3.24815900	-2.19092300	0.23890700
C	2.50016100	-1.05652200	0.64308600
C	3.17159200	0.21261700	0.63870300
C	4.51160500	0.28925200	0.18499500
H	6.21656900	-0.74482000	-0.60446700
H	5.07475400	-2.96835300	-0.53818600
H	2.75514500	-3.15806100	0.27320900
H	4.99545300	1.26407700	0.18787900
C	-5.44263400	-0.76286700	0.96062600
C	-4.80584600	-1.98482300	0.67315100
C	-3.43128100	-2.09709500	0.70044300
C	-2.60313500	-0.98993900	1.01910900
C	-3.25276600	0.25935600	1.30613200
C	-4.66770000	0.33189200	1.26993800
H	-6.52492900	-0.68710100	0.93756700
H	-5.40418300	-2.85808400	0.42380000
H	-2.93999000	-3.04103000	0.47881000
H	-5.13361100	1.28922400	1.49574000
N	-1.25063100	1.57536400	1.70676900
C	-2.54970200	1.44463400	1.64759200
H	3.21957500	2.28932600	1.14617900
C	1.54179500	3.86766800	2.36022000
C	0.88921200	5.01460400	2.79052700
C	-0.50554100	5.04694000	2.86522500
C	-1.25406800	3.93164400	2.51588100
C	-0.60964800	2.76909800	2.07948000
C	0.79864700	2.74114500	1.99266400
H	2.62623900	3.84505700	2.32712500
H	1.47077400	5.88459700	3.08010200
H	-1.01193400	5.94314600	3.21074500
H	-2.33562300	3.96588100	2.59373400
H	-3.16978000	2.31314500	1.88243500
O	0.07111600	0.67093700	-0.52114800
O	-1.21235300	0.60849800	-1.17715000
O	0.18707500	-0.30173200	3.30985200
C	-0.97186500	-0.65073900	4.07928000
H	-0.66439000	-0.94847100	5.08526400
H	-1.59324600	0.24316500	4.14729200
H	-1.53729600	-1.46099600	3.61067700
H	0.75432800	-1.08617100	3.24638300
H	-0.42074200	0.16407800	-2.69421600
O	0.30526500	-0.05882600	-3.32679300
C	0.83719000	-1.24280500	-3.01382900
C	0.24401300	-2.11536500	-2.06860100
C	2.03226000	-1.61411100	-3.67553700
C	0.83643200	-3.31653300	-1.78401300
H	-0.67450700	-1.81283200	-1.57297400

C	2.63140100	-2.81148000	-3.38933500
H	2.45774200	-0.92192700	-4.39692400
C	2.07154600	-3.72462300	-2.41682200
H	0.39848300	-3.98918600	-1.05002900
H	3.55887300	-3.10281200	-3.87569100
O	2.64345100	-4.81165400	-2.12043500
H	-1.49147000	1.53920200	-1.17670000

5a-TS

Co	0.95100200	-0.12275000	1.90222700
O	0.15804800	-1.86805600	2.02105700
O	2.46132600	-0.94316100	2.75207900
N	1.72648200	1.62990500	1.85390900
C	2.99433300	1.87061500	2.04353700
C	6.32620100	0.54740400	2.96773200
C	6.01625700	-0.77982100	3.31517300
C	4.72411200	-1.25735500	3.23068300
C	3.65919400	-0.43202900	2.79132600
C	3.97350700	0.92332700	2.44312200
C	5.31185400	1.37654000	2.54484800
H	7.34644600	0.91065200	3.03561700
H	6.80592900	-1.44645600	3.65353600
H	4.48747600	-2.28308500	3.49877700
H	5.52153600	2.41018100	2.27725400
C	-3.27743600	-3.17093200	0.09220100
C	-2.35943800	-4.06607200	0.67256200
C	-1.21911500	-3.61257800	1.30463300
C	-0.91936300	-2.22913400	1.38589700
C	-1.85049400	-1.31674500	0.78405600
C	-3.01889600	-1.82085000	0.16065700
H	-4.16735000	-3.54056500	-0.40772400
H	-2.54696100	-5.13613900	0.62246900
H	-0.51521400	-4.30696100	1.75449300
H	-3.70658900	-1.10489800	-0.28513800
N	-0.60774400	0.73036600	1.18818300
C	-1.65683900	0.08781100	0.75032300
H	3.35502700	2.89016400	1.88982600
C	1.05338400	3.99105600	1.44003700
C	0.05500200	4.86391800	1.03088300
C	-1.19974500	4.37734700	0.65629300
C	-1.46529700	3.01560200	0.69328000
C	-0.46759800	2.12541200	1.10431600
C	0.80152700	2.61574000	1.47450900
H	2.01685400	4.38464600	1.74607800
H	0.25269700	5.93138400	1.01482600
H	-1.98020100	5.06509100	0.34542500

H	-2.45034500	2.65428600	0.41772200
H	-2.46512200	0.66446300	0.29494200
O	1.60532700	-0.62485200	0.30456700
O	1.57133400	0.66178900	-0.89501700
O	0.32333600	0.28363800	3.82972100
C	-1.05419000	0.08663700	4.18227400
H	-1.16323100	0.16283900	5.26654400
H	-1.62501300	0.88529400	3.70800700
H	-1.42023000	-0.88666400	3.84219500
H	0.86233800	-0.34381500	4.33770100
H	0.60970900	0.50797700	-1.38538200
O	-0.61185800	0.49131400	-2.00444900
C	-1.05827200	-0.64210900	-2.41012900
C	-0.37671700	-1.88091800	-2.13739700
C	-2.30066100	-0.69978800	-3.13319300
C	-0.91381200	-3.07360200	-2.51589000
H	0.55876200	-1.83375500	-1.58435700
C	-2.84394800	-1.89246600	-3.50546200
H	-2.79866900	0.24316300	-3.34697300
C	-2.19129500	-3.15421800	-3.20298100
H	-0.41276400	-4.01178500	-2.28778200
H	-3.79424700	-1.93804000	-4.03204700
O	-2.71075600	-4.25820700	-3.50854700
H	2.23695300	0.25338000	-1.47235300

6a

Co	0.04034900	0.17208200	1.63283600
O	-1.27121100	-1.21673600	1.76951200
O	1.30990000	-1.23758100	1.83300300
N	1.36258500	1.56982800	1.61165500
C	2.63290100	1.36543800	1.40308200
C	5.35361700	-1.10032100	0.91744000
C	4.68011300	-2.31251300	1.14978300
C	3.33229700	-2.33514000	1.44846300
C	2.57524700	-1.14096100	1.52798500
C	3.26159800	0.09576200	1.29526900
C	4.64579200	0.07824800	0.99781200
H	6.41295400	-1.09493400	0.68231600
H	5.22479900	-3.25179900	1.09081700
H	2.81371000	-3.27256500	1.62785700
H	5.14307300	1.03160800	0.83170400
C	-5.34148500	-0.90066100	1.03881600
C	-4.70211600	-2.14525400	1.19320000
C	-3.34601500	-2.22778700	1.42943600
C	-2.53787300	-1.06513800	1.52288000
C	-3.19151700	0.20536900	1.36933400

C	-4.58869500	0.24699800	1.13225600
H	-6.40921600	-0.84969400	0.85209500
H	-5.28377100	-3.06143400	1.12331800
H	-2.85606500	-3.18987800	1.54887000
H	-5.05713700	1.22312000	1.02399500
N	-1.23188700	1.60945000	1.65857400
C	-2.51705500	1.44687500	1.48805600
H	3.29175900	2.23161900	1.30582100
C	1.50839500	4.04069400	1.87470400
C	0.82688500	5.24048000	2.02164500
C	-0.56955100	5.25998300	2.05685600
C	-1.29147200	4.08057000	1.94151200
C	-0.61643300	2.86557600	1.78510300
C	0.79304400	2.84470000	1.75434400
H	2.59331500	4.03546300	1.87039500
H	1.38737900	6.16459500	2.12478100
H	-1.09835000	6.19906300	2.18862700
H	-2.37499200	4.10618300	1.98895300
H	-3.14682500	2.33788200	1.43163000
O	0.01984100	0.08802900	-0.10401600
O	0.15013700	0.29878200	3.75801100
C	-1.05438100	0.23045000	4.53206600
H	-0.80675000	0.20053100	5.59661200
H	-1.62216700	1.13889100	4.32541500
H	-1.65480100	-0.64562200	4.26850200
H	0.67520900	-0.49505800	3.94585700

H₂O

O	-2.20013400	-0.09151200	1.44730000
H	-2.96191100	0.49744300	1.44730000
H	-1.45815600	0.52226900	1.44730000

BQ

O	-3.74612800	-0.24399200	2.08140000
C	0.35179900	-0.24399200	2.08140000
C	-0.40940500	1.01843900	2.08140000
C	-1.75241200	1.01843900	2.08140000
C	-2.51361600	-0.24399200	2.08140000
C	-1.75241200	-1.50642300	2.08140000
C	-0.40940500	-1.50642300	2.08140000
O	1.58431200	-0.24399200	2.08140000
H	0.17141400	1.93664200	2.08140000
H	-2.33323000	1.93664200	2.08140000
H	-2.33323000	-2.42462500	2.08140000

H	0.17141400	-2.42462500	2.08140000
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7

Co	0.14510100	0.18603300	1.30612400
O	-1.16513300	-1.16462500	0.91968300
O	1.44174700	-1.12090100	0.77359200
N	1.43179600	1.56739200	1.62765100
C	2.70230600	1.49804800	1.31479200
C	5.44969800	-0.53396100	-0.11756600
C	4.81176800	-1.77230800	-0.32566700
C	3.48489700	-1.95331100	0.00236000
C	2.69865000	-0.89897200	0.54184000
C	3.35840000	0.35849900	0.77801200
C	4.72607700	0.49957600	0.43389500
H	6.49447300	-0.40065300	-0.38023300
H	5.37052700	-2.60120900	-0.75497600
H	2.99399200	-2.90963900	-0.16244900
H	5.19717400	1.46546200	0.61067100
C	-5.26828800	-0.70184200	0.48593600
C	-4.62069300	-1.91981900	0.20580200
C	-3.25648300	-2.05343800	0.36231400
C	-2.44447000	-0.97403600	0.80396700
C	-3.11023900	0.26836200	1.09628500
C	-4.51353000	0.36312100	0.92513300
H	-6.34202700	-0.60595700	0.35914400
H	-5.20168800	-2.77132100	-0.14146900
H	-2.76087000	-2.99610400	0.14362800
H	-4.98895100	1.31581000	1.15292400
N	-1.14381900	1.52579800	1.76571900
C	-2.43460800	1.42470100	1.57221100
H	3.32986300	2.38182500	1.45780400
C	1.56014500	3.83881200	2.65824900
C	0.86839400	4.91670300	3.19676500
C	-0.52556400	4.89146400	3.27729600
C	-1.23451400	3.78878900	2.81726400
C	-0.55150600	2.70258400	2.26058500
C	0.85847900	2.72603600	2.18298500
H	2.64473200	3.86051700	2.62873900
H	1.42039400	5.77346300	3.57195900
H	-1.06154200	5.72792700	3.71603600
H	-2.31562200	3.77011800	2.91098300
H	-3.06864700	2.29071200	1.77881600
O	0.09379300	1.22250100	-1.05016700
O	-0.94045600	0.75822200	-1.96562700
O	0.34587400	-0.63603500	3.52738800
C	-0.86096800	-0.57377500	4.28112200

H	-0.78372500	-1.15834900	5.20505100
H	-1.02440600	0.47323600	4.54569600
H	-1.72456100	-0.93042400	3.70548100
H	0.49312200	-1.56051700	3.28705800
H	-0.11666200	-0.30269800	-3.25922200
O	0.48124500	-0.84508000	-3.81591700
C	0.73884200	-2.02266800	-3.16002200
C	0.09827600	-2.37115700	-1.97183200
C	1.69171000	-2.88308500	-3.71018700
C	0.41025900	-3.57016400	-1.33590300
H	-0.63182600	-1.69948100	-1.52885300
C	1.99947400	-4.08177200	-3.07781900
H	2.19159500	-2.60199800	-4.63311800
C	1.36191600	-4.42959200	-1.88421100
H	-0.07408100	-3.82587500	-0.39573000
H	2.74408900	-4.75279400	-3.49692700
O	1.72679400	-5.60824100	-1.29076100
H	-1.18980800	1.58654700	-2.40686400
H	0.92498700	0.91822800	-1.50981800
H	1.22236700	-5.71625900	-0.47405700
O	2.39420800	0.58695500	-2.32825000
H	2.06295000	0.23307100	-3.16983200
C	3.02175600	1.83874200	-2.57293400
H	3.99368300	1.71033400	-3.06492200
H	2.39758400	2.49938400	-3.18699900
H	3.18395600	2.32074300	-1.60458400

7-TS

Co	-0.13129700	0.34974200	1.06316300
O	-1.54041100	-0.88514500	0.63457900
O	1.05458200	-1.07739400	0.58931200
N	1.27477300	1.55680400	1.58897600
C	2.53357300	1.21808700	1.71761700
C	5.15689600	-1.32745700	1.13319400
C	4.41589600	-2.36687800	0.53742500
C	3.05327700	-2.25894100	0.35609600
C	2.33846900	-1.10049800	0.76336100
C	3.09982200	-0.03007400	1.35082800
C	4.49788500	-0.18416900	1.52510000
H	6.22873000	-1.42515400	1.27324500
H	4.92384200	-3.27273000	0.21366300
H	2.48191400	-3.06299100	-0.10260800
H	5.04701300	0.64111400	1.97505100
C	-5.60251000	-0.10958300	0.30014300
C	-5.04910900	-1.35720100	-0.04494500
C	-3.69530700	-1.59269000	0.07189400

C	-2.80097500	-0.59332200	0.54176800
C	-3.36766000	0.68218900	0.89009600
C	-4.76485500	0.88178100	0.75870100
H	-6.66917700	0.06632600	0.20423100
H	-5.69667300	-2.15053500	-0.41151900
H	-3.27197000	-2.55756500	-0.19475000
H	-5.16558900	1.85637200	1.03158300
N	-1.30376400	1.80020600	1.52368200
C	-2.60146900	1.78065000	1.36351600
H	3.23205700	1.94698300	2.13537200
C	1.58636800	3.92631900	2.30060300
C	0.98777600	5.12565900	2.66141400
C	-0.40414900	5.24277500	2.67470800
C	-1.20205400	4.16578900	2.31392000
C	-0.61295600	2.95202200	1.94135500
C	0.79334300	2.82614700	1.95464100
H	2.66899900	3.85466800	2.28041700
H	1.60922000	5.97496300	2.92932600
H	-0.86971800	6.18137400	2.96021700
H	-2.28137300	4.27611600	2.32205600
H	-3.17260500	2.68228000	1.59700100
O	-0.02242800	1.16336800	-0.82897200
O	-0.80948200	0.92901200	-2.28486200
O	-0.21472200	-0.39583100	3.22407700
C	0.11429900	-1.76799900	3.43633100
H	-0.48266900	-2.35221500	2.73399400
H	1.17514500	-1.97094700	3.25162900
H	-0.13800000	-2.07259600	4.45805600
H	0.37272900	0.13805000	3.77520400
H	0.29465900	-0.06131100	-3.20438100
O	1.02059200	-0.60541700	-3.60036200
C	0.97923500	-1.86973100	-3.07253900
C	-0.05316200	-2.30537900	-2.24054100
C	2.02203300	-2.74412100	-3.38989900
C	-0.03739000	-3.59911300	-1.72455600
H	-0.86235800	-1.62853500	-1.97823500
C	2.03266900	-4.03814900	-2.88316500
H	2.82482300	-2.39924900	-4.03600600
C	1.00327500	-4.47176900	-2.04356500
H	-0.83563700	-3.92745200	-1.06222000
H	2.84325400	-4.72018000	-3.12440700
O	1.07484300	-5.75107600	-1.56198300
H	-0.78739200	1.85557700	-2.57140500
H	0.89353000	0.92319000	-1.13793800
H	0.32021900	-5.90916000	-0.98002500
O	2.51551500	0.87750700	-1.76667400
H	2.30402400	0.33800200	-2.55071400
C	2.66554600	2.22422900	-2.19625100

H	3.56748400	2.35570100	-2.80577800
H	1.79869500	2.57338800	-2.77275300
H	2.75798300	2.84596600	-1.30087500

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Co	-0.14100800	0.61873300	0.96829200
O	-1.54230500	-0.51962800	0.34544400
O	1.00045900	-0.75353100	0.31024800
N	1.27506900	1.68710700	1.71469900
C	2.51662700	1.29160200	1.81571800
C	5.00705200	-1.37275600	1.18381300
C	4.23563900	-2.31889000	0.48271100
C	2.90174300	-2.09502100	0.21183700
C	2.25466400	-0.90138300	0.62196000
C	3.03564700	0.05562800	1.35302400
C	4.40447400	-0.21032700	1.60757000
H	6.05618300	-1.55951700	1.38867300
H	4.69283400	-3.24743100	0.14697300
H	2.30540400	-2.83014700	-0.32249200
H	4.97354100	0.53880200	2.15439200
C	-5.63437800	0.02444800	0.71955800
C	-5.08195700	-1.10441200	0.08590000
C	-3.71686800	-1.25849700	-0.03496500
C	-2.81389500	-0.29238000	0.48042000
C	-3.37690700	0.86298800	1.12059100
C	-4.78565200	0.98456000	1.22073100
H	-6.71023500	0.13571100	0.80698100
H	-5.73939600	-1.87100900	-0.31747300
H	-3.29160800	-2.13202200	-0.52214000
H	-5.18500100	1.87075800	1.70986800
N	-1.29534000	1.99529600	1.65798000
C	-2.59860800	1.92576700	1.64920000
H	3.23201400	1.95509100	2.30709700
C	1.64034000	3.99190800	2.58171000
C	1.06759000	5.18436900	3.00099500
C	-0.32019400	5.34437200	2.98851400
C	-1.14278000	4.31505100	2.55322200
C	-0.57954300	3.10462900	2.13425300
C	0.82142400	2.94137400	2.15470500
H	2.72024800	3.88765200	2.57497800
H	1.70714200	5.99895500	3.32700300
H	-0.76278700	6.28358500	3.30609400
H	-2.21717500	4.46346300	2.52859300
H	-3.16526100	2.75368300	2.08147700
O	-0.02707700	1.58052900	-0.60590200
O	-0.82657300	0.43129900	-2.41836300

O	-0.35319300	-0.35843200	2.77624800
C	-0.19775600	-1.78787500	2.79887800
H	-0.72921800	-2.17807200	1.93125200
H	0.85478700	-2.07946300	2.74766200
H	-0.64681000	-2.17783000	3.71625800
H	0.24667600	0.02100100	3.43504000
H	0.46689000	-0.35992600	-2.92230700
O	1.30702800	-0.83110900	-3.23782200
C	1.28107800	-2.14278400	-2.87229200
C	0.18975000	-2.71958700	-2.21517700
C	2.39835800	-2.93378700	-3.16031500
C	0.22502300	-4.05969900	-1.83668500
H	-0.68098700	-2.11172000	-1.98437800
C	2.43331800	-4.27178000	-2.78503900
H	3.24667600	-2.48395700	-3.66940000
C	1.34700200	-4.84172900	-2.11650300
H	-0.62496600	-4.50055000	-1.31979400
H	3.30295100	-4.88551500	-3.00380100
O	1.43546300	-6.16338300	-1.76925900
H	-0.78532600	1.33016300	-2.77394800
H	0.84855900	1.33260200	-0.98079100
H	0.62115100	-6.42053700	-1.31813000
O	2.49908000	1.21901300	-1.78325800
H	2.33257900	0.35059900	-2.19768600
C	2.33341500	2.18485200	-2.81148100
H	3.09365900	2.08176500	-3.59646100
H	1.34189700	2.12321400	-3.28042300
H	2.43749300	3.17391500	-2.35866400

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Co	0.34816100	0.34865100	1.38134700
O	-0.87238400	-1.02068100	0.81559800
O	1.73119500	-0.90495900	0.97353800
N	1.56280900	1.69920700	1.99869900
C	2.83045500	1.73342200	1.69427300
C	5.68016600	-0.00218400	0.08041700
C	5.12603300	-1.26706000	-0.18510900
C	3.81444800	-1.55429100	0.13620100
C	2.97145700	-0.58219300	0.72955300
C	3.54565200	0.69838100	1.03091400
C	4.89548800	0.95217500	0.68958900
H	6.71077100	0.21386100	-0.18190700
H	5.73585700	-2.03348600	-0.65774100
H	3.38558100	-2.52948400	-0.07870800
H	5.30343900	1.93343000	0.92356300
C	-4.84252000	-0.48572700	-0.26765600

C	-4.14562600	-1.67671600	-0.54293100
C	-2.82672200	-1.83516800	-0.17102800
C	-2.11342600	-0.80375200	0.49318400
C	-2.83053400	0.40707600	0.78738300
C	-4.18599000	0.52780600	0.39302200
H	-5.87958000	-0.37214600	-0.56645200
H	-4.65078500	-2.48831900	-1.06149300
H	-2.29121000	-2.75479500	-0.39143500
H	-4.70322700	1.45595200	0.62882900
N	-1.02055800	1.58461500	1.89062700
C	-2.26315500	1.49648400	1.50103200
H	3.40698200	2.62357700	1.96005100
C	1.52317700	3.77337500	3.37125000
C	0.75078300	4.74317800	3.99692400
C	-0.64370100	4.68235500	3.93864200
C	-1.27508900	3.65205700	3.25412000
C	-0.50873000	2.67536500	2.61114700
C	0.89957000	2.73634600	2.67145300
H	2.60538600	3.81052200	3.44582400
H	1.23818400	5.54086500	4.54928600
H	-1.24253400	5.43292700	4.44568900
H	-2.35897700	3.59763400	3.23725700
H	-2.93939000	2.32372600	1.73213200
O	0.35060100	1.10356100	-0.32814900
O	-1.08086400	0.26055700	-2.52027100
O	0.38937000	-0.46264600	3.29414400
C	-0.84965600	-0.76183700	3.95322400
H	-0.64795500	-1.32398300	4.86835700
H	-1.31472900	0.18943000	4.21381800
H	-1.51831600	-1.33628400	3.30505800
H	0.84848100	-1.29993900	3.12447800
H	-0.36202400	-0.15440800	-3.01855500
O	1.07605600	-1.39003800	-3.83738400
C	0.90384500	-2.45493800	-3.16214600
C	0.70446700	-2.41308100	-1.73422700
C	0.90716200	-3.75050400	-3.79588100
C	0.53582300	-3.56218800	-1.00754600
H	0.68515900	-1.44143100	-1.24464800
C	0.73559900	-4.89432400	-3.06567700
H	1.05526700	-3.78866300	-4.87104400
C	0.54861500	-4.81410400	-1.66436100
H	0.38910700	-3.52601200	0.06982600
H	0.73914100	-5.87562700	-3.53048300
O	0.38682800	-5.97043900	-1.01322400
H	-0.64116800	0.52988000	-1.68188600
H	1.16031300	0.76981700	-0.75655300
H	0.26544300	-5.81028000	-0.06474600
O	2.41192900	0.52398700	-2.26877700

H	1.98959300	-0.18371800	-2.79539500
C	2.08871900	1.74164500	-2.91836500
H	2.56991200	1.82216800	-3.90321500
H	1.00458800	1.86397800	-3.05171400
H	2.45390700	2.56171600	-2.29287400

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Co	0.28311000	0.30228400	1.22337300
O	-0.98889900	-0.95131500	0.54839400
O	1.57972300	-1.02896500	0.76491100
N	1.56258500	1.53076300	1.95413500
C	2.84733100	1.45440200	1.74238500
C	5.65808100	-0.45963400	0.27340900
C	5.01208400	-1.63718000	-0.14522100
C	3.65520700	-1.80915600	0.03617800
C	2.85644900	-0.80530000	0.63959900
C	3.51786900	0.38895500	1.08291900
C	4.91299500	0.52552800	0.88192300
H	6.72527900	-0.33319500	0.12248200
H	5.58711200	-2.42534800	-0.62567800
H	3.15516000	-2.71513600	-0.29621200
H	5.38879000	1.44240400	1.22407500
C	-4.99673600	-0.28199700	-0.27976100
C	-4.35624500	-1.49151900	-0.60777000
C	-3.02814700	-1.70159900	-0.29985700
C	-2.24791300	-0.70103900	0.33426300
C	-2.90996600	0.51879000	0.70254400
C	-4.27758800	0.69285900	0.37415000
H	-6.04138200	-0.12615000	-0.52883600
H	-4.91162400	-2.27508600	-1.11862900
H	-2.53088400	-2.63085100	-0.56699300
H	-4.75305500	1.62952600	0.65835000
N	-1.02320200	1.58520000	1.79419700
C	-2.27652800	1.56282200	1.42871500
H	3.48240400	2.27148800	2.09393500
C	1.62314000	3.56467400	3.38761200
C	0.90079400	4.56379600	4.02546500
C	-0.49297900	4.59665000	3.93433900
C	-1.17211800	3.63035200	3.20502200
C	-0.45579200	2.62369300	2.54916200
C	0.95199100	2.59091600	2.64044700
H	2.70307800	3.53288900	3.48892600
H	1.42571500	5.31198100	4.61166000
H	-1.05413400	5.37021000	4.44978100
H	-2.25634400	3.64939800	3.16371800
H	-2.91310800	2.40781400	1.70307100

O	0.47071600	1.17925300	-0.41686500
O	0.23499100	-0.64858100	3.06605300
C	-1.02791100	-0.87867000	3.70721900
H	-0.88533700	-1.54634400	4.56021400
H	-1.38833700	0.08634200	4.06492400
H	-1.75591700	-1.31299500	3.01497100
H	0.61801000	-1.50882300	2.83289400
O	-1.37563400	0.32262000	-2.48624700
C	-1.18741800	-0.87772100	-2.84481800
C	0.01054600	-1.60292500	-2.48501100
C	-2.17282200	-1.58548000	-3.63002500
C	0.19407100	-2.90588900	-2.86850000
H	0.77058800	-1.07779100	-1.90979500
C	-1.98288800	-2.88659300	-4.00885900
H	-3.07752700	-1.04857800	-3.90237600
C	-0.79844800	-3.56160800	-3.63122100
H	1.09761800	-3.44913500	-2.60197500
H	-2.72052600	-3.42549500	-4.59622300
O	-0.67292300	-4.83176600	-4.03773000
H	-0.22474900	0.81321700	-0.99577800
O	2.56047200	0.68728600	-2.05395000
H	1.84297400	0.82084700	-1.38282100
C	2.05334400	1.17052200	-3.27782200
H	2.87492500	1.21229000	-4.00043600
H	1.27153200	0.52102500	-3.70490800
H	1.63192600	2.18338500	-3.19193900
H	0.16884300	-5.20235400	-3.73180100

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Co	0.13473800	0.35544800	1.24531400
O	-1.20572200	-0.89045400	0.68969200
O	1.36427000	-0.98363700	0.66463700
N	1.47865500	1.56109300	1.89896300
C	2.75783600	1.41731100	1.68795900
C	5.46996800	-0.62328600	0.20329500
C	4.76317800	-1.75256400	-0.24734900
C	3.39733400	-1.85531500	-0.07383100
C	2.65335900	-0.82484500	0.55404300
C	3.37512800	0.32202100	1.02506800
C	4.77669900	0.38666600	0.83243600
H	6.54320800	-0.55211000	0.05997000
H	5.29654500	-2.55964700	-0.74392600
H	2.85008700	-2.72569000	-0.42682800
H	5.29999400	1.26882600	1.19570000
C	-5.22282500	-0.12423600	0.01223000
C	-4.62359400	-1.34666400	-0.34530600

C	-3.28946300	-1.58957800	-0.09206500
C	-2.46388600	-0.61066500	0.51836900
C	-3.08047200	0.62673400	0.90733900
C	-4.45564800	0.83355600	0.63595800
H	-6.27275800	0.05559500	-0.19478700
H	-5.21701500	-2.11402300	-0.83741100
H	-2.82510100	-2.52833300	-0.38389900
H	-4.89557400	1.78239100	0.93632600
N	-1.11279600	1.66661800	1.87734500
C	-2.38527100	1.66442400	1.58186600
H	3.43402700	2.19897300	2.04184600
C	1.65315000	3.63625600	3.26581300
C	0.98431300	4.65873100	3.92418900
C	-0.41202500	4.70665000	3.92323700
C	-1.14681300	3.73453400	3.25924100
C	-0.48454400	2.70732200	2.57857300
C	0.92520100	2.65219700	2.58813900
H	2.73708300	3.59937300	3.29588100
H	1.55452000	5.41455900	4.45565100
H	-0.93028300	5.49803400	4.45612500
H	-2.23118000	3.76521300	3.28739700
H	-2.98677600	2.52926200	1.87255900
O	0.14969400	1.23213700	-0.42023800
O	0.19416300	-0.60351100	3.06665600
C	-0.99546400	-0.64332600	3.87061300
H	-0.84665100	-1.33943600	4.69924500
H	-1.15087400	0.35993300	4.26793200
H	-1.86569500	-0.94926000	3.28149800
H	0.40146100	-1.51183200	2.79581100
O	-1.59235500	0.56318200	-2.12610500
C	-1.43396100	-0.64589400	-2.63696600
C	-0.29725500	-1.45211900	-2.35614300
C	-2.44997900	-1.14417100	-3.49490700
C	-0.18759900	-2.70245600	-2.90455300
H	0.47360400	-1.05371800	-1.70070700
C	-2.34487100	-2.39405600	-4.04150700
H	-3.31099100	-0.50874200	-3.68713600
C	-1.20599500	-3.24530000	-3.77554800
H	0.67998900	-3.32500600	-2.69774800
H	-3.12237100	-2.78517100	-4.69280000
O	-1.10588800	-4.40022600	-4.28121900
H	0.99729300	0.98761100	-0.83939500
O	2.40503900	0.73366300	-2.12664300
H	2.63931900	-0.19204200	-2.26972800
C	1.84776400	1.22754500	-3.33686000
H	2.59230400	1.26065700	-4.14213900
H	0.99202400	0.63039100	-3.67920900
H	1.50182200	2.24558300	-3.14321100

H	-0.85753600	0.79014700	-1.41943800
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Co	0.08850200	0.31030200	1.10570900
O	-1.24722700	-0.95871400	0.61715500
O	1.30351200	-1.02827400	0.51026500
N	1.44138000	1.55289900	1.67347500
C	2.71669600	1.39722300	1.44399600
C	5.38561200	-0.64775700	-0.10460400
C	4.66773200	-1.78419100	-0.52040600
C	3.31095600	-1.89383300	-0.29488700
C	2.58819600	-0.86357600	0.35499300
C	3.31937600	0.28856600	0.79274500
C	4.71265100	0.36171300	0.54540800
H	6.45169500	-0.57140800	-0.29186500
H	5.18589000	-2.59008600	-1.03456300
H	2.75419100	-2.76662100	-0.62539300
H	5.24282500	1.25205100	0.87790200
C	-5.30440800	-0.28496200	0.10622900
C	-4.69473800	-1.49979300	-0.26033000
C	-3.34584300	-1.71088000	-0.06445900
C	-2.51840400	-0.70458300	0.49383100
C	-3.14152300	0.52528500	0.89102600
C	-4.53210900	0.69954300	0.67881400
H	-6.36611400	-0.13115300	-0.05673000
H	-5.29204000	-2.28658700	-0.71544200
H	-2.87307900	-2.64202900	-0.36610600
H	-4.97845200	1.64407700	0.98269800
N	-1.15237400	1.62598600	1.74823500
C	-2.43735700	1.58925000	1.51117600
H	3.39984700	2.18702300	1.76539100
C	1.63945200	3.67706700	2.95714000
C	0.98293800	4.71605600	3.60128100
C	-0.41289700	4.74926400	3.64954600
C	-1.16001600	3.74524200	3.05035100
C	-0.51067000	2.69867100	2.38700400
C	0.89869900	2.66013000	2.34515800
H	2.72388500	3.65424400	2.94607600
H	1.56307200	5.49775200	4.08204600
H	-0.92119600	5.55545500	4.16953100
H	-2.24268800	3.76947500	3.11516400
H	-3.04226800	2.44821800	1.81064800
O	0.05353200	1.19635600	-0.60949200
O	0.24513100	-0.56278000	2.90424500
C	-0.91854300	-0.66422300	3.74652600
H	-0.68594000	-1.32618900	4.58291700

H	-1.13214100	0.33581300	4.12288400
H	-1.77762600	-1.05050900	3.19119500
H	0.52657900	-1.46213000	2.66689300
O	-1.77162100	0.40051500	-2.23573200
C	-1.62714200	-0.77551100	-2.73817600
C	-0.44990200	-1.57230200	-2.52580100
C	-2.66632200	-1.35752400	-3.54076500
C	-0.32881300	-2.82696900	-3.06165500
H	0.34783500	-1.15482700	-1.91395100
C	-2.54675600	-2.61188700	-4.07453800
H	-3.56425500	-0.76229100	-3.69904800
C	-1.36869200	-3.42199500	-3.86791000
H	0.57015300	-3.41762300	-2.89182400
H	-3.34662800	-3.03978700	-4.67610700
O	-1.25483100	-4.58425300	-4.36693000
H	0.89078100	1.00423400	-1.10753500
O	2.26965300	0.90739100	-2.14198500
H	1.95291500	0.70717700	-3.03231300
C	2.83360500	2.21458200	-2.16817900
H	3.75672200	2.24044000	-2.75902700
H	2.13235100	2.95689700	-2.56743000
H	3.07497000	2.48629200	-1.13725100
H	-0.68627800	0.83000900	-1.21881100

5b

Co	0.36860300	-0.60552800	1.34427800
O	-1.18035800	-1.65270600	0.91812000
O	1.07162400	-2.25986000	2.00117800
N	1.87346700	0.46851300	1.87010100
C	2.95483600	-0.00988000	2.42211800
C	4.81910800	-2.97046200	3.63357500
C	3.89284900	-4.00442100	3.40644500
C	2.65408500	-3.74410200	2.85700000
C	2.26242500	-2.42853300	2.50131500
C	3.20874000	-1.37356000	2.72807600
C	4.46973400	-1.68230800	3.29606200
H	5.79107500	-3.18558600	4.06554000
H	4.15314400	-5.02802700	3.66546100
H	1.94010200	-4.54414600	2.68230000
H	5.16755100	-0.86351200	3.45962300
C	-4.49075600	-0.52085500	-1.31143600
C	-4.29962600	-1.84495700	-0.87383100
C	-3.19021300	-2.20151600	-0.13583300
C	-2.19614600	-1.25090900	0.21288700
C	-2.39466600	0.10129100	-0.22782700
C	-3.54775700	0.42648900	-0.98516200

H	-5.36713100	-0.25379100	-1.89291900
H	-5.03676700	-2.60498000	-1.12186700
H	-3.04604200	-3.22500300	0.19861800
H	-3.67020600	1.45987600	-1.30345800
N	-0.38452700	1.05893800	0.74766400
C	-1.50176200	1.16033000	0.07642500
H	3.75449000	0.68609000	2.68543800
C	2.59835400	2.85134200	1.91304100
C	2.30442900	4.16512300	1.57871700
C	1.09060000	4.48345800	0.96225100
C	0.16445700	3.48985400	0.68233900
C	0.45346000	2.15762300	1.00292700
C	1.67997800	1.83653300	1.62148500
H	3.54526500	2.62047600	2.38958800
H	3.02517000	4.94738100	1.79778500
H	0.86594900	5.51324000	0.69999500
H	-0.77556000	3.75679900	0.21093100
H	-1.79337600	2.14344700	-0.30046700
O	0.99997300	-0.92391400	-0.40336500
O	2.38020200	-1.30245500	-0.42207200
O	-0.36111600	-0.36430000	3.27893300
C	-1.63658100	0.26815100	3.45931300
H	-1.95979400	0.14336200	4.49579200
H	-1.50105800	1.32972900	3.25060900
H	-2.39164100	-0.14893800	2.78553500
H	-0.44986400	-1.29654200	3.53324400
H	2.32295800	-2.26270700	-0.28970600
O	0.45436300	0.88315200	-2.23964400
C	1.20271200	1.98387800	-2.23318900
C	2.46098700	2.04220300	-1.58353000
C	0.69653700	3.12376000	-2.90558600
C	3.17603200	3.21014100	-1.58300500
H	2.83595900	1.15088600	-1.08530500
C	1.40450200	4.29556200	-2.90026500
H	-0.26793100	3.04173200	-3.39990500
C	2.67856000	4.40767700	-2.22380600
H	4.13888500	3.27235000	-1.08220900
H	1.01873200	5.18257000	-3.39609500
O	3.31908100	5.49649600	-2.18739100
H	0.79344900	0.20626400	-1.57927700

5b-TS

Co	0.37309300	-0.63722000	1.27355300
O	-1.19418600	-1.70448600	1.08671100
O	1.13148300	-2.19312600	2.07274900
N	1.88008000	0.48785900	1.62865700

C	2.95089900	0.12085200	2.28780500
C	4.78286600	-2.60775600	3.99518600
C	3.88552600	-3.68278600	3.85855200
C	2.67633800	-3.52360500	3.21321100
C	2.28916000	-2.27566200	2.66058500
C	3.20751200	-1.17955700	2.79653700
C	4.43710700	-1.38272400	3.46931600
H	5.73080100	-2.74332600	4.50588500
H	4.14513200	-4.65650700	4.26732400
H	1.98385100	-4.35443400	3.10949000
H	5.11343400	-0.53483200	3.55987900
C	-4.77285400	-0.75939800	-0.76805400
C	-4.54550400	-2.02256800	-0.18475200
C	-3.35178900	-2.31448500	0.43746900
C	-2.30162900	-1.36040400	0.50851700
C	-2.54156700	-0.06349300	-0.06937400
C	-3.78417900	0.19451100	-0.70197700
H	-5.71687900	-0.54372100	-1.25806400
H	-5.32306100	-2.78152800	-0.22658200
H	-3.17369700	-3.28887700	0.88350300
H	-3.93999000	1.18008800	-1.13587900
N	-0.41896300	0.94565500	0.54796700
C	-1.60647200	0.99763400	-0.01322500
H	3.72908400	0.86266000	2.47871400
C	2.66279400	2.81672800	1.20086600
C	2.37110000	4.06789100	0.66558700
C	1.12126600	4.32060700	0.09820100
C	0.16030400	3.32032900	0.04751900
C	0.44521300	2.05088800	0.56699300
C	1.70675000	1.80197300	1.15478100
H	3.64445000	2.63604200	1.62613200
H	3.12679600	4.84804400	0.68775700
H	0.90032700	5.29780100	-0.32150700
H	-0.80296800	3.53162300	-0.40475800
H	-1.92761600	1.93285200	-0.47611800
O	0.99116300	-1.25479200	-0.74888600
O	2.45146100	-1.33235200	-0.77478700
O	-0.42198900	-0.11061700	3.55210700
C	-1.61404700	0.66580800	3.56799100
H	-2.07954600	0.66509400	4.56063100
H	-1.33684100	1.69223300	3.31648400
H	-2.34866900	0.31118700	2.83360900
H	-0.66711500	-1.02594800	3.74113400
H	2.58953200	-1.96760300	-1.49326600
O	0.22326300	0.77933000	-2.41713600
C	1.03143800	1.76134200	-2.55969200
C	2.38458500	1.72521400	-2.06768500
C	0.56166200	2.94516800	-3.24429600

C	3.18993600	2.80869100	-2.20231000
H	2.72265300	0.80867400	-1.58567300
C	1.36955000	4.02220300	-3.39329500
H	-0.45902200	2.93272800	-3.61701800
C	2.72784200	4.03214700	-2.85403300
H	4.20972400	2.80630100	-1.82661800
H	1.02859700	4.92321800	-3.89570200
O	3.45777400	5.03907300	-2.94517000
H	0.69018200	-0.22425800	-1.60986100

6b

Co	0.32108600	-0.65452800	1.38127800
O	-1.25488800	-1.72334400	1.15808800
O	1.07786600	-2.21614100	2.18533800
N	1.87274200	0.44315400	1.64750700
C	2.99198100	0.03996300	2.19736400
C	4.87315400	-2.72667900	3.78407600
C	3.92473900	-3.76750800	3.76163200
C	2.66830500	-3.57469900	3.22740400
C	2.27399800	-2.32586300	2.67571300
C	3.24375300	-1.26223000	2.70159100
C	4.52433200	-1.50236900	3.26097400
H	5.85936100	-2.88831400	4.20751000
H	4.18451900	-4.74133100	4.17070000
H	1.93898700	-4.38035000	3.21069700
H	5.23746400	-0.67978500	3.26692400
C	-4.65089900	-0.86400900	-1.06156600
C	-4.48720800	-2.09292200	-0.39104800
C	-3.35487200	-2.35474300	0.34913700
C	-2.30237500	-1.40598500	0.46428300
C	-2.47819000	-0.14392300	-0.20850000
C	-3.65927300	0.08382200	-0.96101000
H	-5.54698700	-0.66920900	-1.64214600
H	-5.26524300	-2.85003100	-0.45791000
H	-3.22879200	-3.30445500	0.86215900
H	-3.76530200	1.04478700	-1.46126300
N	-0.40584900	0.89341000	0.52363100
C	-1.54199700	0.91729200	-0.13694700
H	3.81983700	0.74678200	2.29042700
C	2.61970800	2.80203000	1.31754700
C	2.32262000	4.05833600	0.80024000
C	1.08601100	4.30262800	0.19670200
C	0.14556700	3.28779800	0.09438200
C	0.44246000	2.00672500	0.57918200
C	1.69336100	1.76406600	1.20125800
H	3.57986600	2.63878900	1.79517000

H	3.05652700	4.85576500	0.87703400
H	0.85565900	5.28999300	-0.19374100
H	-0.81704500	3.49794500	-0.36031500
H	-1.81433700	1.82279200	-0.68396900
O	0.99634900	-1.47453300	-0.78749300
O	2.44687700	-1.57123400	-0.80258700
O	-0.47944600	-0.06815800	3.57996100
C	-1.66804900	0.71371400	3.53382000
H	-2.17686500	0.72710100	4.50460500
H	-1.37546500	1.73530600	3.28055500
H	-2.36944000	0.35173500	2.77067700
H	-0.73450600	-0.97294800	3.80387100
H	2.58318200	-2.24427400	-1.48827700
O	0.34702400	0.63870500	-2.42673300
C	1.06364600	1.65510200	-2.50435700
C	2.41673000	1.68440000	-1.95118000
C	0.56285800	2.86339300	-3.17023800
C	3.16963200	2.80091800	-2.02389300
H	2.77719300	0.76845500	-1.48613800
C	1.31788400	3.97497000	-3.24968300
H	-0.44130800	2.81287500	-3.58338500
C	2.66353300	4.02573000	-2.65683300
H	4.17563100	2.84340400	-1.61523300
H	0.96086000	4.88120700	-3.73155700
O	3.33998500	5.06182200	-2.69182700
H	0.83489400	-0.71285300	-1.40261100

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Co	0.09182500	0.04084200	0.98611100
O	-1.22430100	-1.34071500	0.82985700
O	1.34162100	-1.29857500	0.41707500
N	1.41287500	1.40756900	1.21802800
C	2.70568100	1.19569800	1.23283800
C	5.48426500	-1.18653700	0.66587900
C	4.79196100	-2.33902100	0.24820700
C	3.41497800	-2.35226900	0.16716300
C	2.63400900	-1.21480400	0.50661100
C	3.34499400	-0.03489600	0.92568600
C	4.76006500	-0.06117500	0.99060000
H	6.56814500	-1.18489200	0.72450400
H	5.34869900	-3.23574700	-0.01500300
H	2.88389900	-3.24367200	-0.15673700
H	5.27051800	0.84780600	1.30507200
C	-5.35025000	-1.01946000	1.14252000
C	-4.71689900	-2.24032800	0.84134400
C	-3.34378700	-2.32393800	0.74476100

C	-2.50809700	-1.19138300	0.94339000
C	-3.15728800	0.05508200	1.25713300
C	-4.57162500	0.09803600	1.34414800
H	-6.43178700	-0.96217400	1.21483300
H	-5.31667500	-3.13330500	0.67974000
H	-2.85751900	-3.26733200	0.50994300
H	-5.03666500	1.05367300	1.58071600
N	-1.15535400	1.41581100	1.47645500
C	-2.45620400	1.26793000	1.49748700
H	3.37192700	2.01835100	1.50512800
C	1.57618200	3.86150100	1.64084600
C	0.91178400	5.03757200	1.96333200
C	-0.47040400	5.03237600	2.16466600
C	-1.19581300	3.85601400	2.02587100
C	-0.54224900	2.66628100	1.68536700
C	0.86029700	2.66556000	1.51847400
H	2.64863200	3.88024200	1.47479300
H	1.47299900	5.96279000	2.05533300
H	-0.98756600	5.95194300	2.42253500
H	-2.26940100	3.87232300	2.18273900
H	-3.08398900	2.13674500	1.70996100
O	-0.25230900	0.79431600	-1.27066100
O	-0.79776200	-0.24363300	-2.14415700
O	0.52172900	-0.74759600	3.24795300
C	-0.53637300	-0.39099400	4.12960100
H	-0.46893600	-0.93512200	5.07922700
H	-0.44079100	0.67806300	4.33421000
H	-1.52353400	-0.57415900	3.68502000
H	0.41826200	-1.68428100	3.03405600
H	0.40083000	-0.27821700	-3.69712500
O	1.03170800	0.10919700	-4.33126600
H	-1.49734500	0.25730400	-2.59467700
H	0.70984300	0.78110900	-1.53817400
O	2.32445900	0.88466400	-2.06131100
H	2.07574600	0.62157900	-2.97543900
C	2.66035000	2.26586000	-2.06696000
H	3.20399700	2.54528100	-2.97601300
H	1.77076900	2.90659300	-1.98114000
H	3.30896700	2.46588000	-1.20808500
C	0.43914800	1.31448900	-4.79709100
H	1.16224900	1.80600000	-5.45200000
H	-0.47465100	1.12084300	-5.37275200
H	0.19337400	2.00145200	-3.97589300

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Co	0.29628600	-0.26203400	1.14186900
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O	-1.09527300	-1.58388000	1.00475200
O	1.50161300	-1.74979100	1.21894600
N	1.66058100	1.07172600	1.30174100
C	2.93999600	0.82733600	1.14631400
C	5.60932700	-1.67953500	0.61789800
C	4.88410000	-2.89134200	0.68743500
C	3.51712700	-2.89184200	0.89075300
C	2.78695900	-1.67661500	1.03140100
C	3.53153400	-0.45342100	0.97868700
C	4.93601700	-0.49676800	0.76394100
H	6.68467500	-1.69072000	0.45781700
H	5.40033400	-3.83328700	0.57996100
H	2.96100300	-3.81694800	0.94351200
H	5.47204700	0.45663900	0.72890300
C	-5.10081600	-0.97773200	0.06622900
C	-4.54242100	-2.26442500	0.19346000
C	-3.21166000	-2.44374500	0.50517400
C	-2.33924800	-1.33851500	0.71451600
C	-2.90635100	-0.02396300	0.59992000
C	-4.28627800	0.11639100	0.27254300
H	-6.14330200	-0.85252200	-0.17328800
H	-5.17341900	-3.14006900	0.03699800
H	-2.78827200	-3.43842800	0.59562800
H	-4.69418100	1.12338400	0.18480400
N	-0.90679100	1.25485300	1.07688500
C	-2.18438200	1.17608000	0.80223700
H	3.63058400	1.67461400	1.12842600
C	1.90974400	3.50687100	1.76439700
C	1.28818000	4.74036200	1.86252500
C	-0.09558200	4.85114300	1.69084200
C	-0.85984100	3.72711200	1.42194600
C	-0.24587000	2.47828900	1.30688200
C	1.15472800	2.37090600	1.46047000
H	2.98244100	3.42711800	1.92076600
H	1.87750700	5.62436900	2.10104800
H	-0.57707700	5.82355700	1.77632900
H	-1.93724300	3.82356600	1.30741600
H	-2.75755100	2.10178200	0.73231100
O	0.33574800	-0.13894800	-0.87009100
O	0.84238900	-1.15092000	-2.15226900
O	-0.04134700	-0.46721500	3.38612200
C	-0.25706500	0.72953100	4.18893300
H	-0.42679600	0.44882100	5.23055900
H	0.67458500	1.34672800	4.13290200
H	-1.12707800	1.34702800	3.83847300
H	-0.91200400	-0.98463800	3.36718900
H	0.10049900	0.14401400	-3.23807000
O	-0.09645900	1.00435900	-3.67385900

H	0.12089700	-1.80024500	-2.02763400
H	0.96930800	0.60240600	-1.11223100
O	2.03002900	1.70303600	-2.04300000
H	1.42003300	1.61243000	-2.81481500
C	2.12136900	3.08435100	-1.73469700
H	2.46508300	3.67763300	-2.58880000
H	1.16250100	3.51026100	-1.39473800
H	2.85233800	3.20120000	-0.92368800
C	-1.13000200	1.64991300	-2.93687500
H	-1.48519100	2.49656100	-3.53009400
H	-1.97803500	0.97523400	-2.75228300
H	-0.77282100	2.03068000	-1.96437300

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Co	0.17047000	0.04733700	1.03032500
O	-1.14181300	-1.33090700	0.88635200
O	1.40510500	-1.34070900	0.60230800
N	1.50832600	1.39917800	1.31424600
C	2.79345600	1.16699900	1.32786600
C	5.54956000	-1.23152000	0.74628400
C	4.84203000	-2.39018500	0.37603700
C	3.46326900	-2.40198300	0.32893300
C	2.70285500	-1.25040400	0.65524700
C	3.42405000	-0.06729600	1.02705300
C	4.84024800	-0.09513300	1.06161700
H	6.63429000	-1.23436800	0.77655200
H	5.38780500	-3.29552000	0.12074700
H	2.91987100	-3.29745300	0.04131200
H	5.36041500	0.81880700	1.34191700
C	-5.26171100	-0.90470100	0.69144300
C	-4.62269700	-2.13269500	0.43706100
C	-3.24951500	-2.24972100	0.49644700
C	-2.42607100	-1.14102600	0.82150800
C	-3.07726200	0.11389600	1.07361600
C	-4.49072400	0.19196500	1.00221300
H	-6.34276500	-0.82544200	0.64066200
H	-5.21822500	-3.00713800	0.18549700
H	-2.75782300	-3.19811100	0.29897500
H	-4.95745600	1.15474000	1.20103900
N	-1.08129400	1.43739200	1.48597200
C	-2.37755700	1.30477900	1.39888100
H	3.46405400	1.98648200	1.59649400
C	1.67703100	3.84128900	1.76121600
C	1.01468600	5.01688600	2.08329600
C	-0.37287300	5.02317300	2.24852800
C	-1.10613500	3.85867300	2.07171100

C	-0.45215500	2.66881700	1.73318100
C	0.95225900	2.65378300	1.60754100
H	2.75320300	3.85160200	1.62387800
H	1.58229200	5.93427200	2.20612500
H	-0.88680600	5.94340700	2.50918100
H	-2.18321100	3.87922900	2.19861800
H	-3.00093100	2.18441000	1.57521300
O	-0.04573500	0.56229200	-0.73606500
O	-0.38861700	-1.21375200	-2.09927800
O	0.45976800	-0.52769700	2.99461400
C	-0.59369600	-0.28721000	3.93995400
H	-0.36098100	-0.80030400	4.87613500
H	-0.62732700	0.78777700	4.11815200
H	-1.56037400	-0.63294500	3.56002500
H	0.55542800	-1.48805800	2.89343600
H	0.27610000	-0.36308000	-3.38895200
O	0.70609500	0.26882900	-4.03127600
H	-1.28553500	-0.85132300	-2.06117700
H	0.85417300	0.51039700	-1.12847700
O	2.46474900	0.75851800	-2.00495100
H	1.97701100	0.58097300	-2.84248800
C	2.68065600	2.15676300	-1.93158700
H	3.08992900	2.55718600	-2.86801800
H	1.76050300	2.71251300	-1.69391300
H	3.40912400	2.35177100	-1.13730000
C	-0.09987800	1.43368500	-4.02585200
H	0.40760800	2.20862200	-4.60789300
H	-1.08224700	1.25202600	-4.48454000
H	-0.26750800	1.82113500	-3.01081800

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Co	0.35216500	-0.65368800	1.41019000
O	-1.35070400	-1.51076900	1.54062100
O	0.92015400	-1.88904200	2.74188000
N	2.02188200	0.29210100	1.38019100
C	3.15192700	-0.23599900	1.75653700
C	4.83503600	-3.08909600	3.41389300
C	3.73599600	-3.81615400	3.90338300
C	2.44056300	-3.39855000	3.66933400
C	2.16981800	-2.22953000	2.91926600
C	3.29053700	-1.47900200	2.43153900
C	4.60350800	-1.93499900	2.69869400
H	5.84815100	-3.42848500	3.60328000
H	3.90321900	-4.72705000	4.47307000
H	1.59273800	-3.96182100	4.04811000
H	5.43491500	-1.34355500	2.32123000

C	-4.45663900	-1.20587400	-1.19277500
C	-4.41605200	-2.21724000	-0.21512700
C	-3.37213900	-2.30303400	0.68270600
C	-2.29382800	-1.38285100	0.65262800
C	-2.34114100	-0.34331000	-0.33893300
C	-3.43474000	-0.28552800	-1.23824900
H	-5.28231100	-1.15149600	-1.89475300
H	-5.21824900	-2.94973200	-0.16539100
H	-3.34451200	-3.08436900	1.43680100
H	-3.44458600	0.51355600	-1.97663300
N	-0.26370400	0.75133700	0.26062000
C	-1.36889600	0.68576200	-0.43136200
H	4.07562200	0.31236100	1.55624500
C	2.91920200	2.51453900	0.71300400
C	2.67057200	3.73057900	0.08958600
C	1.42401100	3.99148500	-0.48444200
C	0.41882100	3.03403000	-0.45004400
C	0.66168100	1.80254700	0.16408700
C	1.91238800	1.54629400	0.76173000
H	3.87988000	2.33362800	1.18456100
H	3.44796700	4.48856900	0.06902300
H	1.23027100	4.95289400	-0.95043800
H	-0.55342600	3.25260800	-0.87974600
H	-1.57769000	1.48569400	-1.14585600
O	0.81542700	-1.65254300	0.06183800
O	2.87454900	-0.64957400	-1.44990100
O	-0.17213600	0.57571500	3.07173700
C	-1.46735500	1.18977900	3.10546500
H	-1.62996500	1.64547700	4.08563100
H	-1.47359300	1.97099200	2.34407400
H	-2.26211300	0.46686000	2.89804300
H	-0.12886100	-0.07426300	3.79027800
H	2.13021000	-1.00093100	-0.90087300
H	2.63496300	0.27863600	-1.60611100
O	2.49078000	1.82746400	-2.94821900
H	2.40272000	1.04656900	-3.53252100
C	3.85340100	2.21292700	-2.99266300
H	4.23215400	2.28006400	-4.02116300
H	3.94220900	3.20398300	-2.53760100
H	4.50372100	1.52626400	-2.42924400
O	2.51702300	-0.69804900	-4.16225800
H	2.55701800	-0.94948600	-3.21280900
C	3.81166900	-0.92333000	-4.69505300
H	3.88150400	-0.40085500	-5.65319600
H	4.60582800	-0.54267400	-4.03867500
H	3.99993300	-1.99123300	-4.87269100

Co	0.28907200	-0.06689300	1.15663000
O	-1.03200100	-1.44602400	1.06881500
O	1.53938100	-1.50492900	1.09291100
N	1.61088000	1.31934200	1.29924700
C	2.89474100	1.12352500	1.16472300
C	5.64900400	-1.27579300	0.56391100
C	4.95929500	-2.50197700	0.55134100
C	3.59177800	-2.55487700	0.72769000
C	2.82614100	-1.37863500	0.92553800
C	3.52963500	-0.12819700	0.94622400
C	4.93468700	-0.11615900	0.76249800
H	6.72416300	-1.24696900	0.42020600
H	5.50892000	-3.42746600	0.39666300
H	3.06207200	-3.50309900	0.71501700
H	5.44180400	0.84658400	0.78157700
C	-5.03238300	-1.01536200	0.06322500
C	-4.41468300	-2.27730600	0.15750000
C	-3.08518800	-2.39867100	0.50173900
C	-2.28271600	-1.25906600	0.76619100
C	-2.91912200	0.02720200	0.69607700
C	-4.28846500	0.10896500	0.33763000
H	-6.07833500	-0.93396600	-0.21396800
H	-4.99165100	-3.17521200	-0.05086800
H	-2.60853900	-3.37288800	0.56249800
H	-4.74208400	1.09670400	0.28493300
N	-0.98064000	1.36567800	1.27850000
C	-2.24845200	1.24278800	0.98561000
H	3.56126100	1.98754100	1.22069500
C	1.75043600	3.77116700	1.72811100
C	1.06340800	4.95610100	1.95204700
C	-0.33355800	4.97062100	1.98026000
C	-1.05132900	3.80139000	1.77234200
C	-0.37014700	2.60394600	1.53102500
C	1.03980200	2.58287100	1.52457800
H	2.83553300	3.77331700	1.72389900
H	1.62076400	5.87284700	2.11878600
H	-0.86506400	5.89735400	2.17413400
H	-2.13577000	3.81718100	1.81302100
H	-2.85728200	2.14929200	0.94269100
O	0.26021900	0.09622400	-0.72023400
O	-1.57207600	-1.17327600	-2.38582100
O	0.36730700	-0.27154600	3.18669200
C	-0.85035200	-0.20974300	3.94887100
H	-0.63389900	-0.48003000	4.98487400
H	-1.20141500	0.82157100	3.91208300
H	-1.61129500	-0.88014100	3.53956500

H	0.73801100	-1.16413000	3.28037800
H	-2.28278600	-0.54020700	-2.24088700
O	-0.29432300	2.13377100	-2.94476400
H	-0.86501100	-0.84183900	-1.79823800
H	1.17538500	0.18970100	-1.04477500
O	2.29510100	1.06248000	-2.41075700
H	1.41958200	1.21633100	-2.81389800
C	2.72576800	2.32922800	-1.94284700
H	2.79093400	3.06415600	-2.75646900
H	2.06302600	2.74121800	-1.16668200
H	3.72483100	2.20844700	-1.51459100
O	-0.84973000	2.08833000	-1.74055900
H	-0.37209400	1.26664400	-1.24511100

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Co	0.43157000	-0.45003700	1.67824300
O	-1.14406200	-1.43983100	2.11473200
O	1.32321300	-1.78505800	2.71435600
N	2.00571300	0.60809700	1.35509100
C	3.21719100	0.23589400	1.67305400
C	5.40714400	-2.34617200	3.16830200
C	4.46481500	-3.27186900	3.65613500
C	3.11102000	-3.05680800	3.50749700
C	2.61176100	-1.90865600	2.84003300
C	3.57168800	-0.95918600	2.35150500
C	4.95474900	-1.21067100	2.53654000
H	6.47043400	-2.52836000	3.28753100
H	4.80695100	-4.17664500	4.15358800
H	2.38498500	-3.77985600	3.86948300
H	5.66051800	-0.47784500	2.14987300
C	-4.94025400	-0.98704500	0.50329900
C	-4.61466600	-2.04982900	1.36681800
C	-3.34571100	-2.18169500	1.89179800
C	-2.31594500	-1.25463100	1.58546300
C	-2.65446300	-0.16014800	0.71821700
C	-3.96722300	-0.06345400	0.19506000
H	-5.94046200	-0.89779400	0.09185100
H	-5.37289900	-2.78597000	1.62346600
H	-3.09629000	-3.00793400	2.55180400
H	-4.18955800	0.77246700	-0.46569700
N	-0.48689300	0.93431300	0.72467000
C	-1.74224900	0.86802400	0.36582300
H	4.05129600	0.88628100	1.39961900
C	2.64975700	2.80425600	0.36871100
C	2.23430700	3.95436900	-0.28794100
C	0.88553800	4.13986800	-0.60618900

C	-0.05176700	3.17237500	-0.27626200
C	0.35651700	1.99575800	0.36400100
C	1.71717700	1.81478200	0.69994000
H	3.69765600	2.68528900	0.62332300
H	2.96382100	4.71687100	-0.54542100
H	0.56480300	5.04592300	-1.11256700
H	-1.09701300	3.33512700	-0.51878600
H	-2.14937500	1.66813800	-0.25631400
O	0.85090800	-1.35432400	0.07758900
O	-0.29845500	-1.85552200	-0.60724900
O	0.22394100	0.52554000	3.52380200
C	-0.92280900	1.35894400	3.74020700
H	-0.98033100	1.63486800	4.79625600
H	-0.78267300	2.26000600	3.14200900
H	-1.84849400	0.85765500	3.43899900
H	0.15340800	-0.24274500	4.11170100
H	-0.50379900	-1.13232700	-1.25407100
O	-1.09346600	0.06781100	-2.38669600
C	-0.28813200	0.95970700	-2.79893800
C	1.13499400	0.86726700	-2.57642200
C	-0.77080400	2.12128600	-3.50571800
C	1.98524800	1.85623700	-2.99634100
H	1.51164700	-0.00500400	-2.04669000
C	0.08279700	3.10927000	-3.91627500
H	-1.83966900	2.19273300	-3.68719600
C	1.46736500	2.99677100	-3.64983500
H	3.05509800	1.79321200	-2.81324300
H	-0.27489300	3.99601000	-4.43124400
O	2.24185400	4.02043600	-4.03249900
H	3.16547300	3.85240600	-3.79066400
O	1.77506400	-3.96722100	0.59547100
H	1.50106600	-3.03324300	0.45860400
C	3.08817000	-4.10980800	0.26324100
C	3.71294600	-5.32410000	0.56669200
C	3.82954300	-3.10028400	-0.35667100
C	5.05370100	-5.52404000	0.26168600
H	3.13599500	-6.10532100	1.05459900
C	5.17520200	-3.29926100	-0.65947900
H	3.35286300	-2.15189600	-0.59511100
C	5.79441900	-4.51007800	-0.35045800
H	5.54068700	-6.46548400	0.50060000
H	5.74696700	-2.50613700	-1.13648100
O	7.11410900	-4.76180000	-0.62106800
H	7.50191300	-3.97954200	-1.03363100

Co	0.54633700	-0.56082200	1.50301400
O	-0.98872500	-1.63252300	1.89217300
O	1.53920900	-1.97976700	2.33299600
N	2.07649500	0.55314200	1.18419900
C	3.29953000	0.27091500	1.55573400
C	5.61183900	-2.20357400	3.05958800
C	4.73600000	-3.25121700	3.40209300
C	3.38301800	-3.15124400	3.15867500
C	2.81579900	-1.99966800	2.54485600
C	3.71532600	-0.92799500	2.19659400
C	5.09491400	-1.06530600	2.47630800
H	6.67664100	-2.29057400	3.25386100
H	5.13082600	-4.15595700	3.85934700
H	2.70515400	-3.96114100	3.41644300
H	5.75310900	-0.24243800	2.20320200
C	-4.93559100	-0.98388500	0.78832700
C	-4.53890000	-2.12966200	1.50444500
C	-3.22246300	-2.32328300	1.86662500
C	-2.21064700	-1.38300200	1.53396600
C	-2.62011700	-0.20637900	0.81291200
C	-3.98233600	-0.04760200	0.45624500
H	-5.97401100	-0.84251900	0.50578400
H	-5.28007800	-2.87784700	1.77622200
H	-2.91917400	-3.21138800	2.41476400
H	-4.26079400	0.84941600	-0.09443000
N	-0.44170800	0.86281800	0.69301800
C	-1.72887900	0.83456500	0.44398200
H	4.09224800	0.99922300	1.37136300
C	2.64863400	2.77896800	0.20420300
C	2.18661300	3.94835000	-0.38726300
C	0.81969900	4.13487900	-0.60674300
C	-0.08802500	3.14531500	-0.25574400
C	0.36478500	1.95038100	0.31802000
C	1.74522700	1.77583500	0.56936100
H	3.71355600	2.65330900	0.36955800
H	2.89514000	4.71956800	-0.67627400
H	0.46120500	5.05322000	-1.06357900
H	-1.14627400	3.30824100	-0.43235100
H	-2.18385200	1.67408800	-0.08609800
O	0.83398400	-1.52781900	-0.60558900
O	-0.44052000	-1.89693200	-1.22844900
O	0.37121800	0.41815100	3.74583400
C	-0.79993900	1.21501200	3.88019100
H	-1.01583100	1.43687000	4.93223700
H	-0.61313800	2.15680100	3.35869200
H	-1.67935400	0.73473100	3.43185500
H	0.19736500	-0.42821800	4.17864700
H	-0.63591100	-1.06234300	-1.73166300

O	-1.21468200	0.34566900	-2.52181600
C	-0.40428000	1.23597100	-2.93428200
C	1.02417000	1.08582200	-2.81708400
C	-0.88968900	2.45278700	-3.53567200
C	1.87921300	2.07544800	-3.22998800
H	1.40539900	0.16892600	-2.37339400
C	-0.03039700	3.43874200	-3.94472600
H	-1.96489200	2.56901000	-3.64118500
C	1.36168700	3.27006400	-3.77606400
H	2.95621000	1.96789000	-3.12328100
H	-0.39220600	4.36509200	-4.38134800
O	2.14816100	4.29415200	-4.14314500
H	3.07777600	4.07681700	-3.97692800
O	1.62161400	-3.97983700	0.05726700
H	1.16990400	-2.44232800	-0.37168000
C	2.87423800	-4.18853000	0.15524100
C	3.37990500	-5.44457600	0.64884700
C	3.84634200	-3.19159800	-0.21444400
C	4.72526900	-5.66808000	0.78470500
H	2.65623200	-6.20764200	0.92155000
C	5.19205300	-3.42226500	-0.07909000
H	3.48369900	-2.24311400	-0.60445700
C	5.64538100	-4.65356600	0.43927100
H	5.10981400	-6.60866300	1.16821700
H	5.92024600	-2.66127700	-0.34947000
O	6.94771500	-4.92308500	0.62857600
H	7.48876100	-4.16643200	0.35730700

1, M06L functional, spin 3/2

Co	-0.16705800	-0.15728900	1.44059600
O	-1.72798900	-1.25968600	0.81283700
O	1.33403200	-1.44113200	1.76559600
N	1.20321500	1.43723400	1.59330900
C	2.47317800	1.28908500	1.33378900
C	5.35024000	-0.98455400	0.79758800
C	4.78133300	-2.24853200	1.03168500
C	3.44567800	-2.37529800	1.35663500
C	2.58154700	-1.25149500	1.46017200
C	3.17046500	0.04601400	1.22603000
C	4.54657700	0.13056000	0.90240200
H	6.40161300	-0.88909300	0.54489300
H	5.39889200	-3.14092800	0.95546400
H	3.00852500	-3.35468100	1.53605200
H	4.96558100	1.12211000	0.73614200
C	-5.74070700	-0.77878000	1.78303600
C	-5.23806700	-1.99038200	1.27756200

C	-3.90199700	-2.12460400	0.95773000
C	-2.97128500	-1.06368000	1.12908500
C	-3.49280200	0.18302800	1.63898600
C	-4.87156200	0.27824700	1.94898500
H	-6.79244600	-0.67659400	2.03156500
H	-5.90849100	-2.83532100	1.13562500
H	-3.51587000	-3.06316100	0.56700700
H	-5.23964000	1.23066500	2.32826000
N	-1.44476100	1.50703200	1.61599900
C	-2.72696000	1.37656100	1.81952300
H	3.10014000	2.17605300	1.17612900
C	1.34169900	3.89372500	1.92589400
C	0.67993900	5.10738300	2.05267400
C	-0.71471100	5.15246100	2.00157000
C	-1.44463400	3.98115900	1.85248800
C	-0.79678500	2.74213400	1.74997600
C	0.62391000	2.70308100	1.74744900
H	2.42590600	3.86906600	1.98093100
H	1.25177800	6.02069900	2.19004000
H	-1.23440400	6.10299800	2.08157300
H	-2.52787000	4.03430400	1.80180300
H	-3.31212200	2.24128500	2.15698400
O	0.42179800	-0.15380500	-0.80752300
O	-0.81801900	-0.60341700	3.59813900
C	-0.13399800	0.20164100	4.55610200
H	-0.49870900	-1.50997700	3.70094900
H	0.95216100	0.19030200	4.39883700
H	-0.49690300	1.22484400	4.43398400
H	-0.35258600	-0.12888700	5.57722800
C	-0.23025400	0.89087300	-1.52560500
H	-0.05580100	0.79932000	-2.60338700
H	-1.31128400	0.90409000	-1.33623500
H	0.19863900	1.83470100	-1.18066400
H	0.02165000	-0.98899300	-1.08467600

1, TPSSH functional, spin 1/2

Co	-0.16722200	0.26981500	1.47894000
O	-1.48866000	-1.09185100	1.34814200
O	1.07873400	-1.15304100	1.23837800
N	1.16202600	1.63094100	1.64194400
C	2.45901200	1.43065000	1.61580500
C	5.24133300	-1.01482000	1.27321900
C	4.53579300	-2.22508100	1.08789800
C	3.15150200	-2.25085900	1.07767000
C	2.38456300	-1.06415100	1.25548000
C	3.10278300	0.16784700	1.44292900
C	4.52516600	0.15443100	1.44503000

H	6.32679000	-1.00583300	1.27869800
H	5.08579900	-3.15296900	0.95088000
H	2.61177000	-3.18323800	0.93509400
H	5.04582800	1.09914300	1.58691800
C	-5.63723100	-0.73170800	1.38341300
C	-4.99748100	-1.98511200	1.25332500
C	-3.61665400	-2.08514500	1.24343700
C	-2.78726800	-0.93345000	1.36341800
C	-3.43862200	0.34250700	1.49463100
C	-4.85972700	0.40451100	1.50164600
H	-6.72064200	-0.66515100	1.39032500
H	-5.59639600	-2.88765500	1.15886600
H	-3.12729200	-3.05021600	1.14261300
H	-5.32891500	1.38083800	1.60332600
N	-1.42008400	1.70220400	1.63579900
C	-2.72635200	1.57287900	1.62499400
H	3.12726500	2.28363800	1.72754800
C	1.34129000	4.12220500	1.92868600
C	0.67035200	5.33661300	2.05542400
C	-0.73033900	5.37585200	2.04047800
C	-1.46471400	4.20014400	1.90249600
C	-0.80055000	2.96879100	1.77949700
C	0.61270000	2.92946700	1.78902900
H	2.42561600	4.11593300	1.93802600
H	1.24089900	6.25414400	2.16329500
H	-1.25123800	6.32383200	2.13554000
H	-2.54776900	4.25234000	1.88921700
H	-3.34418200	2.46438500	1.72723000
O	0.06397100	0.37694100	-1.01060700
O	-0.35661900	-0.12909600	3.83888500
C	0.76625600	-0.55372800	4.63032900
H	-0.91529800	-0.90668200	3.66961500
H	1.31780200	-1.36517400	4.14412400
H	1.41992500	0.31318600	4.74241900
H	0.43614400	-0.88309100	5.62249200
C	-1.08781400	0.25952800	-1.86015700
H	-0.79353500	0.00311400	-2.88517000
H	-1.79000300	-0.49407200	-1.48831700
H	-1.57811100	1.23513800	-1.86571600
H	0.45017900	-0.50852600	-0.89596800

1, TPSSH functional, spin 3/2

Co	-0.14072800	-0.12316200	1.67155800
O	-1.65343900	-1.24859800	0.95211400
O	1.36817400	-1.40390700	1.89721400
N	1.19741800	1.46784500	1.64695200
C	2.44751000	1.32488600	1.28460500

C	5.30269500	-0.95232600	0.58545000
C	4.76326600	-2.21667000	0.90627100
C	3.45487800	-2.34253000	1.34303500
C	2.59376700	-1.21532200	1.48086300
C	3.14979500	0.07939200	1.15831900
C	4.49965100	0.16535800	0.71887900
H	6.32940900	-0.86028400	0.24524500
H	5.38064600	-3.10645400	0.80859500
H	3.04220800	-3.31771900	1.58870900
H	4.89678100	1.15138000	0.48583900
C	-5.75015700	-0.79302400	1.60115300
C	-5.19527000	-2.02064700	1.18653800
C	-3.83087300	-2.14786900	0.97238500
C	-2.93579600	-1.06160200	1.17162600
C	-3.50348000	0.19591700	1.58890700
C	-4.90721000	0.28924500	1.78702900
H	-6.81881400	-0.69722900	1.76587200
H	-5.84216300	-2.88051800	1.03042300
H	-3.40430100	-3.09411500	0.64951700
H	-5.31644400	1.24894800	2.09637200
N	-1.45565900	1.52789900	1.70203400
C	-2.75479000	1.41115300	1.77364400
H	3.03946400	2.21304400	1.04638100
C	1.34074700	3.92951700	1.99318900
C	0.67907400	5.14526200	2.14973900
C	-0.72123500	5.18872000	2.13666400
C	-1.45732200	4.01548700	1.98704700
C	-0.80876400	2.77611700	1.84165900
C	0.61368500	2.73939400	1.81395100
H	2.42521500	3.90348900	2.03059300
H	1.25328800	6.05647200	2.28895000
H	-1.23996400	6.13579800	2.25247600
H	-2.54077200	4.07159100	1.98225800
H	-3.36759400	2.29249100	1.98038200
O	0.13729500	-0.36442800	-0.85560600
O	-0.78769400	-0.53195100	3.79546000
C	-0.04942500	0.15081100	4.82956800
H	-0.60922400	-1.48304400	3.88516300
H	1.02739800	-0.01770800	4.72433900
H	-0.26606100	1.21423600	4.72095000
H	-0.38139700	-0.18832700	5.81612100
C	-0.08584700	0.72990100	-1.75335400
H	-0.45341500	0.37321800	-2.72374600
H	-0.80073900	1.45453000	-1.34551900
H	0.87564500	1.22653200	-1.90287100
H	-0.72865200	-0.76083200	-0.62173100

19, M06L functional, spin 3/2

Co	0.13646200	-0.08188000	1.93369400
O	-1.32023200	-1.24562200	1.24635700
O	1.65972900	-1.32610200	2.18009700
N	1.43440200	1.47654900	1.52403500
C	2.66559900	1.28662200	1.12880500
C	5.48400500	-1.05014300	0.57331500
C	4.97980400	-2.25536800	1.09409800
C	3.70795700	-2.32175500	1.62499900
C	2.84470100	-1.19313700	1.66408500
C	3.36611500	0.04373700	1.13067600
C	4.68137000	0.06878400	0.60350900
H	6.48685100	-1.00251800	0.16070400
H	5.59889300	-3.14973000	1.08004200
H	3.32235800	-3.25526100	2.02747700
H	5.05161200	1.01661600	0.21579600
C	-5.44469400	-0.77119700	1.44503000
C	-4.84983100	-2.03106500	1.26382700
C	-3.47660200	-2.16496800	1.20005800
C	-2.60339700	-1.05228800	1.32926000
C	-3.21686900	0.23827700	1.51659200
C	-4.62780300	0.33462900	1.55755700
H	-6.52462400	-0.66999800	1.48763200
H	-5.47647800	-2.91511800	1.16723600
H	-3.01957200	-3.14027900	1.05076500
H	-5.06467800	1.32411500	1.68612400
N	-1.19445500	1.57416100	1.66600000
C	-2.49000900	1.46740300	1.60217400
H	3.24170200	2.14056600	0.75121100
C	1.61644700	3.94302000	1.66949900
C	0.97717800	5.16885200	1.79841000
C	-0.41554200	5.22670800	1.88168400
C	-1.16716000	4.06026500	1.83890400
C	-0.54284500	2.81336900	1.70102000
C	0.87324900	2.75748200	1.60737300
H	2.70157000	3.90273600	1.64727900
H	1.56583600	6.08001200	1.85450700
H	-0.91619300	6.18367400	1.99828800
H	-2.24720000	4.12331100	1.92955600
H	-3.11665000	2.36827600	1.58872800
O	-0.52423400	-0.02582600	4.06235600
C	0.15188000	0.95818100	4.85117400
H	-0.07316100	0.82598300	5.91378400
H	1.23816200	0.91977900	4.70256500
H	-0.21630000	1.93481400	4.53014500
H	-0.25825500	-0.89476500	4.39257100

19, TPSSH functional, spin 1/2

Co	0.01767100	0.26762100	1.72708100
O	-1.28406000	-1.11092100	1.78507800
O	1.27968500	-1.14804100	1.71287500
N	1.32073800	1.64575100	1.52014900
C	2.60778800	1.45777600	1.33551000
C	5.38774100	-0.99686300	1.05009700
C	4.70544100	-2.22019600	1.24116500
C	3.33947200	-2.25022800	1.46313100
C	2.56735700	-1.05400200	1.50601700
C	3.26247800	0.19079600	1.31248900
C	4.66722600	0.18122400	1.08745300
H	6.45913200	-0.98608800	0.87626800
H	5.26013900	-3.15493100	1.21324800
H	2.81710100	-3.19194200	1.60874000
H	5.16929300	1.13576500	0.94394400
C	-5.40312800	-0.85937100	1.22818400
C	-4.75012100	-2.09651400	1.43047300
C	-3.37991900	-2.15957600	1.61728800
C	-2.57444700	-0.98512300	1.61086900
C	-3.23983900	0.27415300	1.40781200
C	-4.64972800	0.29871600	1.21979400
H	-6.47809500	-0.82240000	1.08230200
H	-5.33050100	-3.01590900	1.43902800
H	-2.87971000	-3.11204800	1.77068500
H	-5.12945800	1.26344900	1.06862900
N	-1.25601900	1.67889900	1.54794500
C	-2.55103800	1.52344400	1.39475900
H	3.24814100	2.32408500	1.17325400
C	1.46932000	4.15370000	1.58357100
C	0.78107900	5.36499400	1.62580900
C	-0.61979100	5.38276200	1.64328500
C	-1.33930100	4.18937000	1.61769200
C	-0.65759500	2.96323700	1.56509300
C	0.75565500	2.94526700	1.54935300
H	2.55396000	4.15954100	1.59706800
H	1.33897900	6.29582700	1.66141100
H	-1.15299900	6.32732000	1.69309300
H	-2.42269800	4.22293500	1.65883000
H	-3.17200900	2.40485600	1.23736800
O	-0.07499900	0.44766400	4.02282700
C	1.05861300	0.05219200	4.81776600
H	0.81382300	0.10574900	5.88428200
H	1.38648100	-0.96208900	4.56834600
H	1.86135000	0.75777300	4.59843400
H	-0.78410900	-0.19772300	4.18050100

19, TPSSH functional, spin 3/2

Co	0.23283200	0.17025000	2.13755200
O	-1.15127600	-1.11554600	1.52270500
O	1.79420600	-1.01823300	2.42472200
N	1.47098400	1.69702900	1.48157900
C	2.67848800	1.48327700	1.02048400
C	5.51015900	-0.87667600	0.53378800
C	5.06698000	-2.02400000	1.22718100
C	3.83178800	-2.04485200	1.85236200
C	2.94932200	-0.92544500	1.81887300
C	3.40829400	0.25179600	1.11498900
C	4.68764600	0.23336100	0.49261200
H	6.47997300	-0.86663200	0.04634400
H	5.70211000	-2.90550900	1.27169500
H	3.49264900	-2.92963300	2.38511900
H	5.01275600	1.13166000	-0.02821300
C	-5.31305500	-0.80538800	1.52594800
C	-4.65952500	-2.05476600	1.53105500
C	-3.27518000	-2.13541800	1.52956700
C	-2.45383600	-0.97257600	1.54349800
C	-3.12554800	0.30390200	1.54581500
C	-4.54418800	0.34616700	1.52012300
H	-6.39713100	-0.74856800	1.51992000
H	-5.24617900	-2.97044400	1.53128900
H	-2.77478700	-3.10043200	1.52207300
H	-5.02604300	1.32196200	1.50486800
N	-1.15599700	1.72999600	1.66724800
C	-2.44041600	1.56893300	1.50543200
H	3.20136600	2.29618800	0.50847700
C	1.58546000	4.18042500	1.36179600
C	0.90646600	5.39778300	1.37690300
C	-0.48910500	5.42336500	1.49709500
C	-1.20758000	4.23293400	1.59931500
C	-0.54210800	2.99578900	1.56728800
C	0.87411300	2.97204200	1.44572300
H	2.67007800	4.16955800	1.31559300
H	1.46659300	6.32639200	1.31884900
H	-1.01646600	6.37213400	1.53140600
H	-2.28502800	4.27251800	1.72377900
H	-3.07748500	2.43415900	1.29978200
O	-0.33825800	0.48665900	4.22121000
C	-0.11063500	-0.62834500	5.11126400
H	-0.40045800	-0.35561000	6.13031100
H	-0.67093200	-1.51093600	4.78650600
H	0.95813000	-0.83941400	5.07712700
H	-1.28007500	0.72104300	4.25794500

19, OPBE functional, spin 1/2

Co	0.02254700	0.35204700	1.46422500
O	-1.27104500	-1.02350900	1.61648800
O	1.25096400	-1.08771400	1.54613300
N	1.33056300	1.69179600	1.28701800
C	2.62196300	1.47381000	1.12953900
C	5.37212000	-1.02954800	0.99669500
C	4.66687900	-2.23293300	1.22720300
C	3.29446800	-2.23306400	1.41607000
C	2.53889400	-1.02365800	1.37969600
C	3.26087300	0.20346900	1.15336600
C	4.67147600	0.16220100	0.96446400
H	6.45150800	-1.04187900	0.84836900
H	5.20887900	-3.18002400	1.25594200
H	2.75365700	-3.16397000	1.59032500
H	5.19827800	1.10294300	0.79333000
C	-5.40341400	-0.76946000	1.23073900
C	-4.75057700	-2.00034800	1.46965300
C	-3.37333500	-2.06519300	1.60422100
C	-2.56040000	-0.89762400	1.50200100
C	-3.22898200	0.35856100	1.27160100
C	-4.64624100	0.38387700	1.13713200
H	-6.48730800	-0.73079600	1.12619200
H	-5.33725800	-2.91750100	1.54860500
H	-2.87314800	-3.01733900	1.78481400
H	-5.13259400	1.34517600	0.96143700
N	-1.22536300	1.75178100	1.32060600
C	-2.52975000	1.59511300	1.20314700
H	3.27897200	2.32914600	0.96144800
C	1.51590600	4.19827600	1.30400500
C	0.84007700	5.41787100	1.32364000
C	-0.56052700	5.45055300	1.34349800
C	-1.29278400	4.26388500	1.34286000
C	-0.62488000	3.02751800	1.31086000
C	0.79046900	2.99445700	1.29248300
H	2.60372200	4.20012300	1.31686900
H	1.41128200	6.34618200	1.33989700
H	-1.08741400	6.40429600	1.37599600
H	-2.37842400	4.31702600	1.38716300
H	-3.14876600	2.47986200	1.04238300
O	-0.15087900	0.00365400	4.90448000
C	0.86314200	-0.19895900	5.87662400
H	0.55959800	-0.92098200	6.65383200
H	1.81183700	-0.54584300	5.43283400
H	1.04767500	0.76749500	6.36347000
H	-0.30356200	-0.84987100	4.47764600

19, OPBE functional, spin 3/2

Co	0.12957200	0.04622100	2.18763500
O	-1.33747400	-1.22497800	1.74084100
O	1.71477700	-1.13031500	2.48229500
N	1.37474000	1.55886400	1.55090700
C	2.54764600	1.32872200	1.00823300
C	5.26186500	-1.11609400	0.29319400
C	4.84095100	-2.24952000	1.02251900
C	3.66055200	-2.23110500	1.74859500
C	2.81052600	-1.08356400	1.78378500
C	3.24912100	0.08025200	1.03580900
C	4.47417700	0.02177600	0.31423000
H	6.19283900	-1.13589800	-0.27277100
H	5.45116100	-3.15481200	1.01634000
H	3.34041100	-3.10958000	2.31081300
H	4.78876700	0.90989100	-0.23762200
C	-5.39854800	-0.80424000	0.91296600
C	-4.80685800	-2.06991700	1.10485600
C	-3.45287700	-2.18947900	1.38338800
C	-2.60318600	-1.04881400	1.50175700
C	-3.21614500	0.24697400	1.31297800
C	-4.60163700	0.32565100	1.00981800
H	-6.46126700	-0.71646600	0.68855700
H	-5.41816700	-2.97134700	1.02883500
H	-2.99842100	-3.17188500	1.52006100
H	-5.04093300	1.31406900	0.85895500
N	-1.23406800	1.61585200	1.70651900
C	-2.49011200	1.48410100	1.36656800
H	3.05300100	2.14443300	0.47609000
C	1.54240400	4.03506200	1.66919300
C	0.88106300	5.25526800	1.81634100
C	-0.51447200	5.28981200	1.93814900
C	-1.25427300	4.10645800	1.90421700
C	-0.60892500	2.86888500	1.73172300
C	0.81127800	2.83492400	1.62108800
H	2.63081400	4.01024600	1.63046900
H	1.45886200	6.17860200	1.86679500
H	-1.02821500	6.24021500	2.08591600
H	-2.33365900	4.14738100	2.04455800
H	-3.06007100	2.37142400	1.06357400
O	-0.33549600	0.40049000	4.49464900
C	0.72158400	0.62318000	5.42698900
H	0.32864500	0.71013900	6.45159800
H	1.47730900	-0.17584500	5.40008500
H	1.19919200	1.57044400	5.15301400
H	-0.74735600	-0.44457700	4.72449100

20, M06L functional, spin 1/2

Co	-0.17597700	0.14057800	1.36052700
O	-1.53097900	-1.22659800	1.33616700
O	1.06682900	-1.32885600	1.39758600
N	1.16131500	1.48360400	1.62172200
C	2.45377400	1.27747200	1.54630200
C	5.20823000	-1.17613600	1.17799700
C	4.50453400	-2.39529400	1.15131800
C	3.12811100	-2.42280400	1.23732100
C	2.35803900	-1.23199700	1.34233700
C	3.08115600	0.01307700	1.37997500
C	4.49550000	-0.00305900	1.29654400
H	6.29166600	-1.16243200	1.11094000
H	5.05104700	-3.33146100	1.05923900
H	2.58652700	-3.36528000	1.21418300
H	5.01668700	0.95253400	1.33003000
C	-5.64188300	-0.75118100	1.02400800
C	-5.03447700	-2.02090500	1.00129700
C	-3.66644400	-2.15573700	1.11612700
C	-2.80917600	-1.02908600	1.24830900
C	-3.43412000	0.26800700	1.28262200
C	-4.84334500	0.36212200	1.16808000
H	-6.71922400	-0.65281100	0.93373000
H	-5.64971200	-2.91109700	0.88935300
H	-3.19922600	-3.13718500	1.09568300
H	-5.28900800	1.35530100	1.19850300
N	-1.41359300	1.58479200	1.58578800
C	-2.71511900	1.47953200	1.47217100
H	3.13292600	2.12952800	1.62502000
C	1.36142700	3.94253300	2.02976500
C	0.70527100	5.15212600	2.21759500
C	-0.69009900	5.20567800	2.20394700
C	-1.43286600	4.05012600	2.00038500
C	-0.78524900	2.82580400	1.79928700
C	0.62602800	2.77077700	1.81693300
H	2.44599100	3.91763700	2.05706800
H	1.28459500	6.05589400	2.38306500
H	-1.20205100	6.15101000	2.35904100
H	-2.51655300	4.10756600	2.00606400
H	-3.32829900	2.38174800	1.53364400
O	-0.19414600	0.35074500	-0.75667500
C	0.18923100	-0.76516400	-1.45383200
H	-0.09326100	-0.71847700	-2.53039700
H	1.29001500	-0.96254800	-1.46285500
H	-0.26049000	-1.71837100	-1.08486100

20, M06L functional, spin 3/2

Co	-0.14677100	-0.00484000	1.20541800
O	-1.67113400	-1.29883400	1.60282800
O	1.26864300	-1.41236600	1.63329200
N	1.22690900	1.49757600	1.65488600
C	2.51300800	1.32724100	1.50704800
C	5.36119100	-0.99171300	1.02145600
C	4.74501900	-2.25317900	1.10966700
C	3.38561500	-2.36280900	1.31560600
C	2.53520600	-1.22635500	1.44082200
C	3.17556900	0.07019500	1.35220200
C	4.57678300	0.13402400	1.14855800
H	6.43169600	-0.90775000	0.86119800
H	5.34547500	-3.15562900	1.01406100
H	2.91231000	-3.33967000	1.38471500
H	5.03169100	1.12250600	1.09286400
C	-5.68199700	-0.60146600	0.75036500
C	-5.15807300	-1.90207400	0.86284900
C	-3.82344800	-2.10443800	1.14734000
C	-2.90868200	-1.02843200	1.33226000
C	-3.45267000	0.30834500	1.21176300
C	-4.83220900	0.46851400	0.93016200
H	-6.73328300	-0.44442700	0.52940000
H	-5.81128900	-2.76117200	0.72393700
H	-3.42073400	-3.11105200	1.23569600
H	-5.21472900	1.48588100	0.85458600
N	-1.42391000	1.59289300	1.60355700
C	-2.71125700	1.51570300	1.40026600
H	3.18216100	2.19752100	1.49393400
C	1.37014700	3.92165900	2.17771200
C	0.71205500	5.11986000	2.41574300
C	-0.68377200	5.16954900	2.38807800
C	-1.41494900	4.02066700	2.12257600
C	-0.77027500	2.80372800	1.85844200
C	0.65219400	2.75275600	1.88642100
H	2.45430600	3.89127000	2.23159300
H	1.28660600	6.01447300	2.63921000
H	-1.20205800	6.10292000	2.58953000
H	-2.49988000	4.06625100	2.13329600
H	-3.31447800	2.43192600	1.35753400
O	-0.13024000	0.09058700	-0.74592000
C	-0.09466500	-1.13963300	-1.38411800
H	-0.49464400	-1.08621100	-2.41567100
H	0.92982200	-1.55684700	-1.48346200
H	-0.68765600	-1.92544000	-0.87064400

20, TPSSH functional, spin 1/2

Co	-0.15025600	0.16928600	1.09158800
O	-1.49214400	-1.17976400	0.93466300
O	1.08213800	-1.29197800	1.05319400
N	1.17857800	1.46648000	1.54874000
C	2.45917100	1.23111300	1.71971100
C	5.20229700	-1.28321600	1.65673400
C	4.49524300	-2.46732400	1.34687100
C	3.12458300	-2.45072400	1.15429800
C	2.37087100	-1.24383800	1.25059800
C	3.09292300	-0.03926200	1.56959800
C	4.49983800	-0.09799800	1.76745900
H	6.27735200	-1.30642500	1.80590700
H	5.03404100	-3.40764800	1.25673700
H	2.58325800	-3.36264400	0.91628900
H	5.02122900	0.82643600	2.00788100
C	-5.61236000	-0.87751800	1.45480100
C	-4.98718000	-2.10483600	1.13671700
C	-3.61567300	-2.18445000	0.96843400
C	-2.77816600	-1.03807600	1.10298600
C	-3.41727400	0.21158400	1.42577400
C	-4.82866300	0.25221800	1.59575800
H	-6.68876400	-0.82569400	1.58599200
H	-5.59043200	-3.00232200	1.02175800
H	-3.13702400	-3.12921500	0.72421800
H	-5.28664400	1.20826000	1.84121600
N	-1.39610600	1.56881000	1.47705700
C	-2.69578700	1.43031500	1.60500300
H	3.11438000	2.05221400	2.01043800
C	1.38086800	3.95176700	1.86896500
C	0.71966500	5.17202900	2.00134100
C	-0.67972800	5.22628600	1.96152200
C	-1.42342400	4.05993900	1.78924500
C	-0.76929500	2.82422500	1.66350700
C	0.64297100	2.76876400	1.70335500
H	2.46526000	3.93445900	1.87829000
H	1.29778800	6.08347100	2.12123300
H	-1.19215600	6.17959700	2.05067600
H	-2.50498900	4.12242000	1.73661400
H	-3.29418100	2.29844400	1.88201600
O	-0.08816000	0.59513200	-0.98751200
C	0.06605400	-0.46493900	-1.87708200
H	-0.17157800	-0.16938700	-2.92206600
H	1.09872500	-0.88009500	-1.91921300
H	-0.59364400	-1.33418900	-1.66025500

20, TPSSH functional, spin 3/2

Co	-0.15195200	0.08764700	0.57512100
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O	-1.65753200	-1.28616500	0.68740000
O	1.22567300	-1.38926900	0.89584200
N	1.21969500	1.46104100	1.41788600
C	2.44554500	1.20805400	1.79068100
C	5.25749900	-1.22497400	1.96174500
C	4.64621200	-2.42131000	1.52860500
C	3.30673600	-2.44854100	1.17867400
C	2.48321600	-1.28143400	1.21884200
C	3.11827300	-0.05527300	1.65398800
C	4.48990900	-0.07557000	2.02569100
H	6.30646100	-1.20854200	2.24127700
H	5.23129900	-3.33658800	1.47213800
H	2.83660400	-3.37379600	0.85424400
H	4.93897000	0.85721700	2.36239600
C	-5.64976600	-0.85837200	1.82282100
C	-5.13529900	-2.08070600	1.33782700
C	-3.80694400	-2.19410100	0.96620300
C	-2.89654800	-1.09433000	1.03842600
C	-3.43110100	0.15917700	1.53020400
C	-4.79821400	0.22721100	1.91694200
H	-6.69123900	-0.77464700	2.11783700
H	-5.78839900	-2.94678500	1.25764400
H	-3.41097400	-3.13830300	0.59993700
H	-5.17295100	1.17789600	2.29228200
N	-1.42265000	1.54511600	1.35794500
C	-2.67147000	1.36639300	1.70289600
H	3.03598400	1.99587600	2.26990100
C	1.36988400	3.93582300	1.71106800
C	0.70361800	5.15556700	1.82833100
C	-0.69592600	5.19860000	1.79762700
C	-1.42974500	4.02174900	1.64980600
C	-0.77530000	2.78279000	1.54799800
C	0.64654900	2.73843000	1.57901400
H	2.45542300	3.91851000	1.69225700
H	1.27622800	6.07419800	1.91808000
H	-1.21507900	6.15041800	1.86352800
H	-2.51226900	4.07008100	1.58208200
H	-3.21263900	2.18463000	2.18823000
O	-0.04560800	0.66471100	-1.27423600
C	0.07282700	-0.35150000	-2.23905100
H	-0.24969500	0.00320900	-3.23565600
H	1.11285200	-0.71174900	-2.35660900
H	-0.54455300	-1.24068100	-2.00681100

20, OPBE functional, spin 1/2

Co -0.14587600 0.20408000 1.07033400
O -1.47699100 -1.16484300 0.89387300

O	1.07813900	-1.27342600	0.99136500
N	1.16540200	1.45843400	1.53454100
C	2.43918900	1.20531700	1.76899300
C	5.16087600	-1.33942900	1.78614300
C	4.45887100	-2.50374100	1.40042400
C	3.09850200	-2.46290100	1.13779500
C	2.35174200	-1.24981800	1.24003500
C	3.07361000	-0.06216300	1.62982100
C	4.46813800	-0.14602100	1.89788600
H	6.23058300	-1.38036800	1.99050100
H	4.99268600	-3.45152400	1.30634100
H	2.56017800	-3.36445500	0.84208100
H	4.99338800	0.76477900	2.19277800
C	-5.57598400	-0.93723800	1.56513600
C	-4.95142500	-2.14278700	1.17281600
C	-3.58483100	-2.19833900	0.94889700
C	-2.75266100	-1.04766300	1.10134300
C	-3.39590600	0.18374700	1.49366300
C	-4.80025300	0.19880000	1.72081800
H	-6.65105900	-0.90290700	1.74042600
H	-5.55060100	-3.04631100	1.04335600
H	-3.10650700	-3.13148900	0.64802700
H	-5.26514400	1.14008800	2.02074900
N	-1.37859900	1.55811800	1.47892000
C	-2.67444400	1.39913900	1.67011800
H	3.07904700	2.02038800	2.11457400
C	1.38692800	3.95035500	1.79293900
C	0.72577100	5.17584200	1.89661100
C	-0.67321500	5.23002100	1.86149700
C	-1.42031200	4.05862900	1.72425100
C	-0.76751200	2.81804200	1.63448900
C	0.64669100	2.76311200	1.66697800
H	2.47501300	3.93690400	1.78490300
H	1.30838900	6.09335800	1.98284000
H	-1.18749900	6.18961000	1.92005800
H	-2.50451100	4.12717800	1.66134000
H	-3.26214100	2.25697500	2.00529500
O	-0.11692900	0.69367800	-1.05278500
C	0.05255500	-0.29815000	-1.99693400
H	-0.15375600	0.07600000	-3.02894900
H	1.08514100	-0.72573400	-2.05557300
H	-0.62107800	-1.18158100	-1.87766300

20, OPBE functional, spin 3/2

Co	-0.14703600	0.18882600	0.41170900
O	-1.66608800	-1.22325700	0.50343300
O	1.27576200	-1.33996400	0.60069500

N	1.20952800	1.47379800	1.32197100
C	2.38483300	1.17185100	1.82069800
C	5.11536600	-1.32688500	2.22908800
C	4.54933600	-2.48845000	1.65901100
C	3.26837100	-2.46779000	1.13152900
C	2.46213400	-1.28218300	1.11019800
C	3.05424000	-0.09074400	1.69872200
C	4.36431600	-0.16343400	2.24943000
H	6.12163100	-1.34612000	2.64733600
H	5.12452900	-3.41664400	1.63529800
H	2.83289000	-3.37001400	0.69808100
H	4.78499900	0.74205100	2.69295100
C	-5.52777000	-0.96699500	2.05664600
C	-5.02729900	-2.16086000	1.49231600
C	-3.73799400	-2.22059900	0.98863800
C	-2.85709600	-1.08987000	0.99045900
C	-3.38078100	0.13523200	1.57368400
C	-4.70451000	0.14592300	2.09634500
H	-6.54095900	-0.92310800	2.45590100
H	-5.66001100	-3.05026200	1.45459000
H	-3.35298700	-3.14774600	0.56010700
H	-5.07504600	1.07486500	2.53595000
N	-1.41952600	1.56777800	1.26242200
C	-2.63042800	1.34863300	1.72010500
H	2.91479400	1.92413200	2.42017700
C	1.37727900	3.94320200	1.60840200
C	0.71492500	5.16917100	1.71385400
C	-0.68397700	5.21848700	1.68164100
C	-1.42484400	4.04170500	1.54441300
C	-0.77667200	2.79784300	1.45042500
C	0.64896800	2.74698700	1.48323300
H	2.46648800	3.91905700	1.58976400
H	1.29469000	6.08928000	1.79531500
H	-1.20153900	6.17675800	1.73830300
H	-2.51101700	4.09280600	1.47580800
H	-3.12491100	2.13618300	2.30395900
O	-0.05377400	0.81508400	-1.40790300
C	0.06226000	-0.12962800	-2.42875300
H	-0.24278400	0.30116200	-3.40506200
H	1.10221800	-0.49513500	-2.56407200
H	-0.56890500	-1.02941800	-2.27576600

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