

Supporting Information

Unprecedented HAT Rate Acceleration in Water by a Non-heme Manganese Oxo Complex

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1. Materials and Methods

Aqueous sodium hypochlorite solution (4% Chlorine), Merck, was used directly without any purification, Iodosobenzene was prepared from (diacetoxy) iodobenzene following the literature method.¹ Aqueous sodium hypochlorite (4 % available chlorine, Merck) (NaOCl) was used as purchased. Acetonitrile (LC-MS and HPLC grade, Sigma Aldrich) was passed through an activated neutral alumina column and distilled and used thereafter.² All the other solvents required were purchased and used after distillation over drying agents. All the substrates required for hydroxylation and OAT reactivity were bought from TCI, Sigma Aldrich or Thermo-fischer scientific. Unless mentioned separately, the reactions were performed at room temperature under air. All indicated solvents were purified prior to use as per standard literature protocols. All the organic chemicals required for ligand synthesis (Sigma Aldrich, TCI India, Spectrochem) were used as received unless synthesized or mentioned; their purity was checked by GC. H₂O¹⁸ was purchased from Icon isotopes. For electrochemical experiments, Glassy Carbon, Platinum (wire and mesh), Ag/AgNO₃ (Non-aqueous), and Ag/AgCl (sat. KCl), Saturated Calomel electrodes were purchased from CH Instruments.

2. General Instrumentations and Techniques

¹H and ¹³C NMR spectra were recorded on Bruker AV 400 or JEOL 400 instruments in solvents as indicated. Chemical shifts (δ) are given in ppm.

All the cyclic voltammetry studies were carried out in CHI-660 potentiostat. UV–vis spectral studies were carried out using an Agilent diode array Cary-8454 spectrophotometer with an attached electrically controlled thermostat. GC-MS was performed on a Thermo Scientific ISQ QD Mass Spectrometer attached with Thermo Scientific TRACE 1300 gas chromatograph using an HP-5 ms capillary column (30 m $\times$ 0.25 mm $\times$ 0.25 μ m, J&W Scientific) with helium as the carrier gas. Water HRMS was performed in a Bruker microTOF-Q II Spectrometer.

2A. EPR Measurements

Electron Paramagnetic Resonance (EPR) spectroscopy was studied by a Bruker spectrometer (Bruker, EMXmicro) operating at X-band frequency (Microwave frequency 9.31 GHz) and magnetic field modulation of 100 kHz, with a microwave power of 48.83 mW and modulation amplitude of 10 G at 100 K.

2B. Electrochemical Measurements

Cyclic voltammetry and differential pulse voltammetry experiment were carried out in CHI-660 potentiostat instrument. Solution of **1** was placed in simple undivided three electrode cells. Glassy Carbon (GC) or gold electrode (3 mm of diameter) was used as working, Saturated Calomel electrode as reference and Pt wire as counter electrode. Before each measurement, working electrode was polished with 0.05 μ m alumina paste and rinsing with water/acetone and finally blow-drying.

2C. Single Crystal X-ray Diffraction (SCXRD) Measurements

X-ray diffraction data for (Et₄N)₂[Mn^{III}(Cl)(Ph,Me-bTAML)], **1** and (Et₄N)[Mn^V(O)(Ph,Me-bTAML)], **2** crystal was collected at 100 K on a SuperNova, Eos diffractometer using monochromatic Mo-K α radiation (λ = 0.71073 Å) and graphite monochromated Cu-K α radiation (λ = 1.54184 Å) having a 300 μ m beam size. Using Olex2 (1.2.9 version)³ the structure was solved using the SHELXT⁴ structure solution program following an intrinsic phasing solution method and refined with the ShelXL⁵ refinement package using Least Squares minimization. All the non-hydrogen atoms were refined anisotropically. All the crystal packing diagrams were prepared using Mercury (3.10.1 version) software.

2D. Resonance Raman Measurements

rRaman spectra were obtained on a Trivista 555 triple spectrophotometer (gratings used in the three stages were 900, 900, and 1800 grooves/mm) fitted with an electronically cooled Pixis CCD (camera) detector (Princeton Instruments) at 78 K. The 413.1 nm excitation beam from a Kr ion laser (Coherent, Santa Clara, CA) was focused on the EPR tube with complex **2** (10 mM in CH₃CN or H₂O) by a cylindrical lens. Power at the sample was kept less than 3-5 mW to prevent photodegradation and the acquisition time was 10 min. The Raman shift was calibrated by using naphthalene as the reference. The data were processed using WinSpec/32 (Princeton Photonics, Inc., Princeton, NJ).

The comparative Raman spectra for complex **2** (6 mM) both in H₂O and H₂O¹⁸ was obtained on micro-Raman spectrometer LABRAM HR from Horiba Jobin Yvon with an 1800 grooves mm⁻¹ grating. All the experiments were performed at RT using the excitation wavelength λ = 488.0 nm (blue) of an Ar-ion laser in the back scattering geometry and the spectral resolution was 2 cm⁻¹.

2E. Rate Measurements from UV-vis Kinetics

Second-order rate constant (k_2) determination in CH₃CN and Water: The higher room temperature stability of **2** in both solvents has prompted us to study the oxidation of C–H bonds at single turnover condition. The reactions follow second order and the rates of these reactions were found to be around twenty-six thousand times faster in water than in CH₃CN solvent. Kinetics were monitored in kinetic mode using a 1.0 cm quartz cell at 442 nm in CH₃CN over the temperature range 333-303 K and 432 nm in water at 293 K. All of the kinetic experiments were carried out in H₂O/CH₃CN mixtures where the percentage of water present varied as required per experiment at 293 K. During kinetic measurements, the concentration of the **2** (5 $\times 10^{-5}$ M) was kept constant while the substrate concentration was varied. A pseudo-first-order rate constant (k_{obs}) was calculated at the 442 or 432 nm wavelength by nonlinear curve fitting [$A_t = A_\infty - (A_\infty - A_0) e^{(-k_{\text{obs}}t)}$] and was in good agreement with the rate constant value. The resulting k_{obs} values correlated linearly with the substrate concentration to give the second-order rate constant k_2 .

3. Computational Details

Calculations related to the figures provided in the main text were carried out with the Gaussian 16 program (G16)⁶, employing the ω B97X functional⁷, which already includes long-range and damped atom-atom dispersion corrections. 6-31G(d, p) Pople basis sets⁸ were employed for H,

C, N and O while Mn was modelled with the SDD basis⁹ set that employs Stuttgart effective core potential.¹⁰ The functional and the basis set was chosen by comparing the results from different combinations of functionals (B3LYP-D3¹¹, M06 and M06L¹²) and basis sets (6-31G(d, p) and 6-311G(d, p)) with the experimental data. The effect of the solvent environment (CH₃CN and H₂O) is incorporated with the self-consistent reaction field method SMD that employs IEFPCM method¹³ to compute the electrostatic component along with other non-electrostatic terms. All optimised stationary points were subsequently characterized by frequency analyses, to ensure that stationary points are found at minima and 1st order saddle points respectively on the potential energy hyper-surfaces. Unless otherwise mentioned, all reported free energies, as obtained from standard thermochemical considerations in G16, are in kcal/mol. Transition states were obtained by scanning the relevant reaction coordinate followed by QST3 calculations.¹⁴ The same level of theory was used to determine the minimum energy crossing points (MECP) using a python adaptation of the original Jeremy Harvey's method,¹⁵ EasyMECP.

3A. Benchmarking of functionals

Benchmarking was performed via comparing (1) the deviation of the computed structure from the experimental crystal structure and (2) IR and Raman spectra.

3A.1. Structural comparison

Two comprehensive sets of calculations were performed: Set-1 calculations were carried out by optimising by keeping Mn, O, and N (of counter cation) fixed, and Set-2 calculations were performed by optimising the whole metal complex alone. Initially, 6-31G (d,p) with SDD/SDD (ecp) on Mn and the RMSD deviation values from the real experimental structure were meticulously analysed, providing detailed insights into the structural comparison.

DFT Functional	Set-1	Set-2
B3LYP-D3	0.444	0.245
M06	0.643	0.206
M06L	0.517	0.252
ω B97X	0.429	0.244

Table S1: RMSD of the computed structures and the experimental crystal structures for various DFT functionals with 6-31G (d,p) basis set for H, C, N, O and SSD ECP for Mn.

The RMSD is calculated by overlaying the computed structure with the experimental one in the presence (Set-1) or absence (Set-2) of the counter ion. It can be clearly seen from the table that M06 and M06L results deviate much more from the crystal structure as compared to the other functionals and hence, were not considered for any subsequent calculations.

Furthermore, the variation of structure with basis sets was also computed employing B3LYP-D3 and ω B97X functionals.

Basis Set	Functional	Set-1	Set-2
6-31G(d,p) + ECP (SDD/SDD) for Mn	B3LYP-D3 ω B97X	0.444 0.429	0.245 0.244
6-31G(d,p) (For all elements)	B3LYP-D3 ω B97X	0.682 0.426	0.255 0.252
6-311G(d,p) (For all elements)	B3LYP-D3 ω B97X	0.946 0.699	0.246 0.222

Table S2: RMSD values of computed structures with different basis sets and functionals for the two sets mentioned above.

From the above table two things are apparent: (1) entry 1 seems to work better than the other options (2) ω B97X shows less deviation than B3LYP-D3.

3A.2. Comparing the IR Spectra

Due to similar values of RMSD for B3LYP-D3 and ω B97X, we compared the (scaled) vibrational frequencies¹⁶ to see whether we can distinguish between the two functionals. For 6-31G(d,p) basis set, scaling factors of 0.9633 and 0.9508 are used for B3LYP-D3 and ω B97X, respectively.

The IR spectrum obtained corresponds to a solid-state KBr pellet, prompting comparison with gas-phase calculations.

Data Type	IR Frequencies
Experimental (KBr pellet)	973, 1365, 1638, 1738
ω B97X	973.424, 1366.91, 1660.13, 1730.04
B3LYP-D3	973.068, 1366.3, 1660.61, 1717.34

Table S3: Important IR frequencies (in cm^{-1}). The frequency that is different is highlighted either in black (ω B97X) or in gray (B3LYP-D3).

3A.3. Comparing Raman Data

Data Type	100% CH ₃ CN	100% H ₂ O	$\Delta\nu$ (cm^{-1})
Experimental	972.000	978.000	6.000

ω B97X	972.047	974.730	2.683
B3LYP-D3	975.800	976.385	0.585

Table S4: Raman frequencies in different solvents (in cm^{-1}), where ΔE is the difference in Raman frequencies from water to acetonitrile.

The ω B97X functional seems to perform better than B3LYP-D3 across multiple benchmark studies: in predicting the key vibrational frequencies and less deviation of the optimized structures from the crystal structure.

3B. Minimum Energy Crossing Pathway

In some situations, we have a spin crossover in the rate-determining step, which requires advanced computational methods to find the lowest energy points where PESs of different spins intersect.¹⁷ These points are called the MECPs - Minimum Energy Crossing Points. We efficiently locate the minimum energy crossing points using a gradient-based optimisation method.¹⁸ In this method, one finds and calculates the energies of both PESs near MECP. Mathematically, MECP is where both the PESs intersect at their lowest possible energy. It is a minimum in a subspace of the complete PES. The PESs depend on $(3N-6)$ degrees of freedom, while the intersection between them has $3N-7$ degrees of freedom.¹⁹ Thus, at MECP the following criteria are fulfilled:

1. when approaching from both surfaces, energies should be the same ($E_1 = E_2$).
2. the gradients (1st derivatives of energy with respect to nuclear coordinates 'q') are parallel (not necessarily equal).

There can be multiple minima within the intersection domain; thus, one might find various MECP points. Therefore, Harvey et al. have adopted a method to start geometry optimizations from several starting points and check out MECPs by spanning the space along the potential energy surfaces.¹⁵ To efficiently locate MECPs, **f** and **g** vectors are constructed, which are as follows:

$$\text{Gradient difference vector } (\mathbf{x}_1) = \left(\frac{\partial E_1}{\partial q} \right) - \left(\frac{\partial E_2}{\partial q} \right)$$

Further, we define the **f** vector as:

$$\mathbf{f} = (E_1 - E_2) \cdot \mathbf{x}_1$$

We define the **g** vector as:

$$\mathbf{g} = \left(\frac{\partial E_1}{\partial q} \right) - \frac{\mathbf{x}_1}{|\mathbf{x}_1|} \left(\frac{\partial E_1}{\partial q} \cdot \frac{\mathbf{x}_1}{|\mathbf{x}_1|} \right)$$

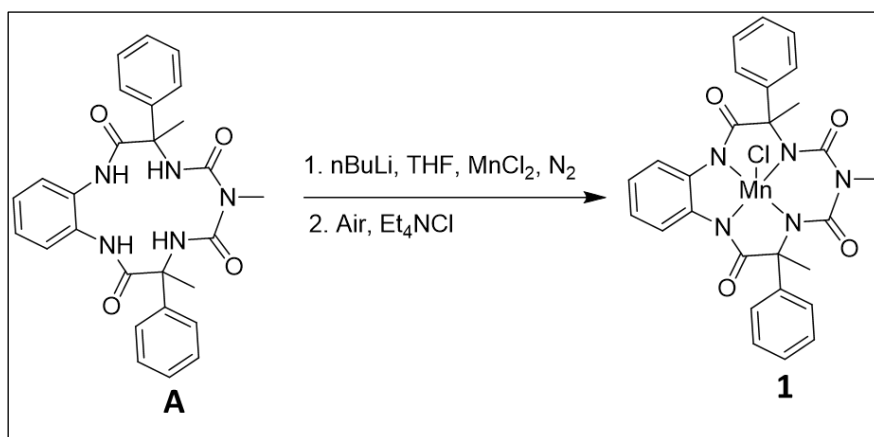
At MECP, since there is no energy difference and since the gradients are becoming parallel to the **g** vector, both **f** and **g** turn zero. This means a particular geometry is on a crossing hyperline, a special constraint surface in multidimensional space, which indicates that on this hyperline

the energy difference vanishes and additionally, the forces acting on the nuclei from both the states are aligned such that the system doesn't favour one state over another at the crossing.

In this study, we used the same level of theory to calculate the gradients and energies during optimization. We also ensured that the spin density distribution in the triplet state, during MECP optimization, is similar to the one found in the transition state.

4. Experimental Results

4A. Synthesis of 1



Macrocycle **A** was prepared following the previous literature method.²⁰

Macrocycle **A** (75 mg, 0.15 mmol) was dissolved in dry, deoxygenated THF under an argon atmosphere. To this solution, a stoichiometric amount of *n*-butyllithium (1.6 M in THF) was added dropwise at 0 °C and the mixture was stirred for 5 min. Subsequently, anhydrous MnCl_2 (0.3 mmol) was added, and the reaction mixture was stirred for 3 h, to yield a brownish solution. After completion, the solvent was removed under reduced pressure, and the residue was dissolved in methanol. The resulting methanolic solution was passed through an ion-exchange resin to replace the lithium counterion with $[\text{Et}_4\text{N}]^+$. The product was purified by alumina column chromatography to afford the pure Mn(III) complex (**1**), which was further recrystallized from a $\text{CH}_3\text{CN}/\text{Et}_2\text{O}$ mixture via slow vapor diffusion technique.

$[\text{Et}_4\text{N}]_2[\text{Mn}^{\text{III}}(\text{Cl})(\text{Ph}, \text{Me-bTAML})]$ (complex **1**)

NMR inactive (paramagnetic)

HRMS: 537.1138 (m/z) [calc'd 537.1130 (m/z)]

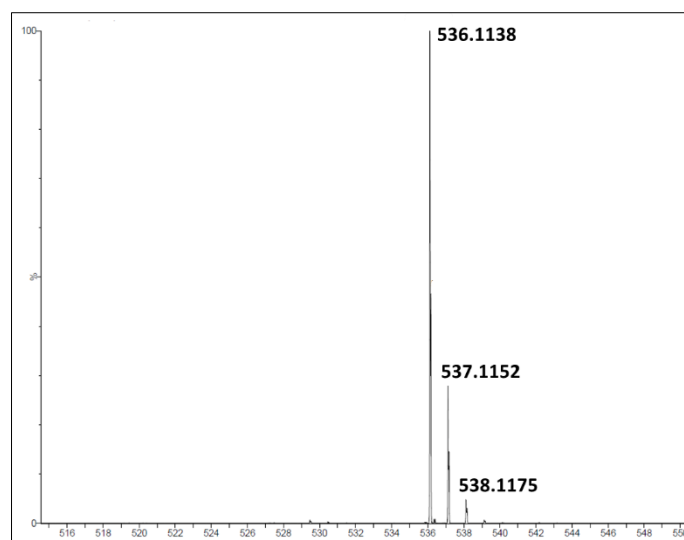


Figure S1: HRMS of Complex **1**.

Single Crystal X-ray Diffraction (SCXRD) of **1**:

CCDC number: 2378349

The X-ray crystal structure of **1** indicates a square-pyramidal Mn(III) with an axial Chlorine atom (Fig. SXX), resulting from an orthorhombic crystal system (space group, *Pbca* (no. 61)). All the four Mn–N bond lengths are around 1.92045 Å and the Mn (III) lies 0.463 Å above the plane formed by the four donor nitrogens (N1, N2, N3, N5). The N4 atom of the Me-biuret ring is 3.135 Å away from the Mn (III) indicating that this N-atom is not involved in bonding with the Mn (III) centre.

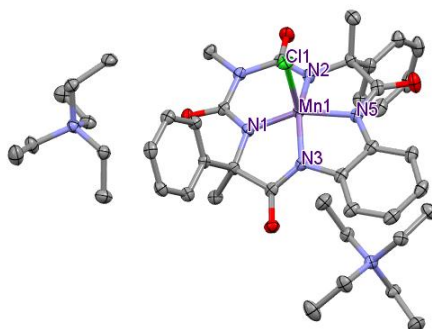


Figure S2. Thermal ellipsoid structure of [Et₄N]₂[Mn^{III}(Cl)(Ph,Me-bTAML)] (**1**) with 50% probability, omitted hydrogen atoms for clarity.

Table S5. Data collection and structure refinement parameters of **1**:

Identification number	2378349
Empirical formula	C ₄₃ H ₆₃ MnN ₇ O ₄
Formula weight	832.39
Temperature [K]	100.15
Crystal system	orthorhombic
Space group (number)	<i>Pbca</i> (61)
<i>a</i> [Å]	13.99310(10)
<i>b</i> [Å]	16.36970(10)

<i>c</i> [Å]	37.9318(2)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å ³]	8688.77(9)
<i>Z</i>	97
ρ_{calc} [gcm ⁻³]	1.273
μ [mm ⁻¹]	3.423
<i>F</i> (000)	3552.0
Crystal size [mm ³]	0.05 × 0.04 × 0.02
Crystal colour	Deep brown
Crystal shape	Block
Radiation	CuK α (λ = 1.54184)
2 θ range [°]	7.852 to 136.29
Index ranges	-16 ≤ <i>h</i> ≤ 16, -19 ≤ <i>k</i> ≤ 19, -45 ≤ <i>l</i> ≤ 32
Reflections collected	70282
Independent reflections	7899 <i>R</i> _{int} = 0.0403 <i>R</i> _{sigma} = 0.0215
Completeness to θ = 25.242°	99.6
Data / Restraints / Parameters	7899/0/516
Goodness-of-fit on <i>F</i> ²	1.053
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0293, <i>wR</i> ₂ = 0.0755
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0331, <i>wR</i> ₂ = 0.0773
Largest peak/hole [eÅ ⁻³]	0.41/-0.29

Table S6. Some important bond lengths and bond angles of the crystal structure of **1**

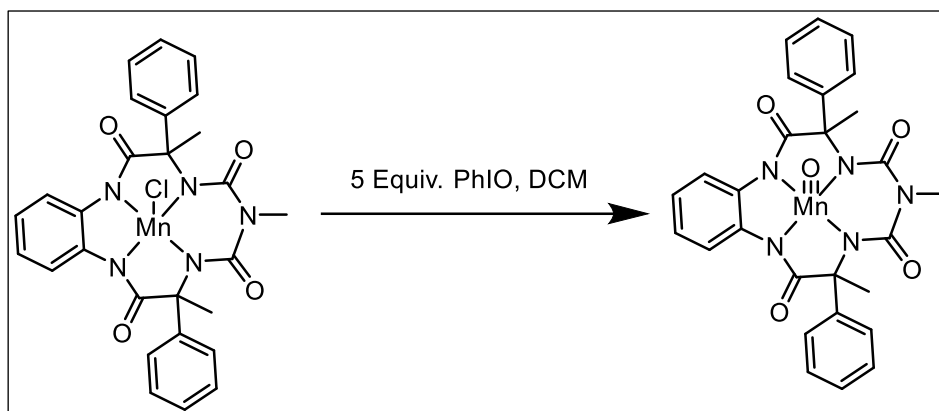
Bond length (Å)	
Mn1–Cl1	2.4269(4)
Mn1–N1	1.9129(12)
Mn1–N2	1.9110(12)
Mn1–N3	1.9335(12)
Mn1–N5	1.9244(12)

Bond angles (°)			
N1–Mn1–N3	84.57(5)	N1–Mn1–N2	95.19(5)
N2–Mn1–N3	151.68(5)	Cl1–Mn1–N2	100.22(4)
N1–Mn1–N5	150.97(5)	Cl1–Mn1–N3	106.82(4)

N2–Mn1–N5	84.06(5)	Cl1–Mn1–N5	100.83(4)
N3–Mn1–N5	82.77(5)	Cl1–Mn1–N1	107.83(4)

4B. Preparation of (Et₄N)[Mn^V(O)(Ph,Me-bTAML)], **2**

25 mg of complex **1** and its 5 equiv. iodosobenzene were taken in 5 mL DCM and the mixture was stirred for 3-4 hr to yield a dark greenish solution. After that the solution was filtered by passing through celite 545 pad. The whole filtered solution was evaporated in rota vapour and the obtained solid part was put for crystallization in DCM/ Benzene solvent mixture.



Single Crystal X-ray Diffraction (SCXRD) of **2**:

CCDC number: 2377771

The X-ray crystal structure of **2** indicates a square-pyramidal Mn(V) with an axial Oxygen atom (Fig. SXX), resulting from an orthorhombic crystal system (space group, *Pban* (no. 50)). All the four Mn–N bond lengths are around 1.864 Å and the Mn (V) lies 0.603 Å above the plane formed by the four donor nitrogen's (N1, N2, N3, N5). The N4 atom of the Me-biuret ring is 3.090 Å away from the Mn (V) indicating that this N-atom is not involved in bonding with the Mn (V) centre.

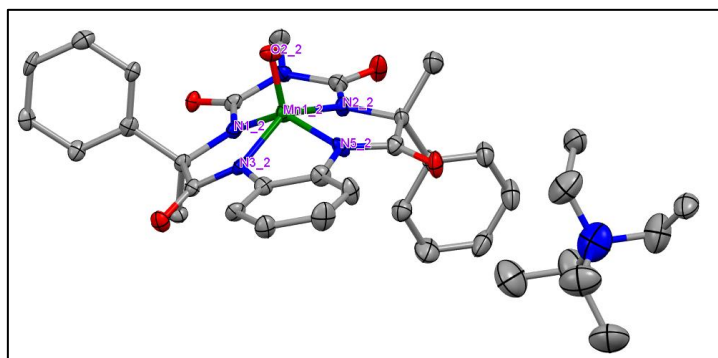


Figure S3. Thermal ellipsoid structure of [Et₄N][Mn^V(O)(Ph, Me-bTAML)], **2** with 35% probability, omitted hydrogen atoms, solvent molecules for clarity.

Table S7. Some important bond lengths and bond angles of the crystal structure of **2**

Bond length (Å)	
Mn1_2–O2_2	1.556(7)
Mn1_2–N1_2	1.857(7)
Mn1_2–N2_2	1.861(7)
Mn1_2–N3_2	1.866(7)
Mn1_2–N5_2	1.874(7)

Bond angles (°)			
N1_2–Mn1_2–N3_2	82.9(3)	N1_2–Mn1_2–N2_2	90.3(3)
N2_2–Mn1_2–N3_2	142.9(3)	O2_2–Mn1_2–N2_2	107.8(3)
N1_2–Mn1_2–N5_2	140.9(3)	O2_2–Mn1_2–N3_2	108.8(3)
N2_2–Mn1_2–N5_2	82.2(3)	O2_2–Mn1_2–N5_2	109.4(3)
N3_2–Mn1_2–N5_2	80.5(3)	O2_2–Mn1_2–N1_2	109.4(3)

Table S8. Data collection and structure refinement parameters of **2**.

Identification number	2377771
Empirical formula	C ₃₅ H ₄₃ MnN ₆ O ₅
Formula weight	682.69
Temperature [K]	100(2)
Crystal system	orthorhombic
Space group (number)	<i>Pban</i> (50)
<i>a</i> [Å]	27.554(2)
<i>b</i> [Å]	28.710(2)
<i>c</i> [Å]	17.7286(16)
α [°]	90
β [°]	90
γ [°]	90
Volume [Å ³]	14025(2)
<i>Z</i>	16
ρ_{calc} [gcm ⁻³]	1.293
μ [mm ⁻¹]	0.425
<i>F</i> (000)	5760
Crystal size [mm ³]	0.043×0.074×0.241
Crystal colour	Deep green
Crystal shape	Needle
Radiation	MoK α (λ =0.71073 Å)
2 θ range [°]	3.94 to 52.01 (0.81 Å)
Index ranges	–33 ≤ <i>h</i> ≤ 33 –35 ≤ <i>k</i> ≤ 35 –21 ≤ <i>l</i> ≤ 21
Reflections collected	668403
Independent reflections	52117

	$R_{\text{int}} = 0.0522$ $R_{\text{sigma}} = 0.1529$
Completeness to $\theta = 25.242^\circ$	99.9
Data / Restraints / Parameters	52117 / 26 / 864
Goodness-of-fit on F^2	1.029
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.1098$ $wR_2 = 0.2247$
Final R indexes [all data]	$R_1 = 0.1900$ $wR_2 = 0.2633$
Largest peak/hole [$\text{e}\text{\AA}^{-3}$]	1.38/−0.57

4C. Characterization Data

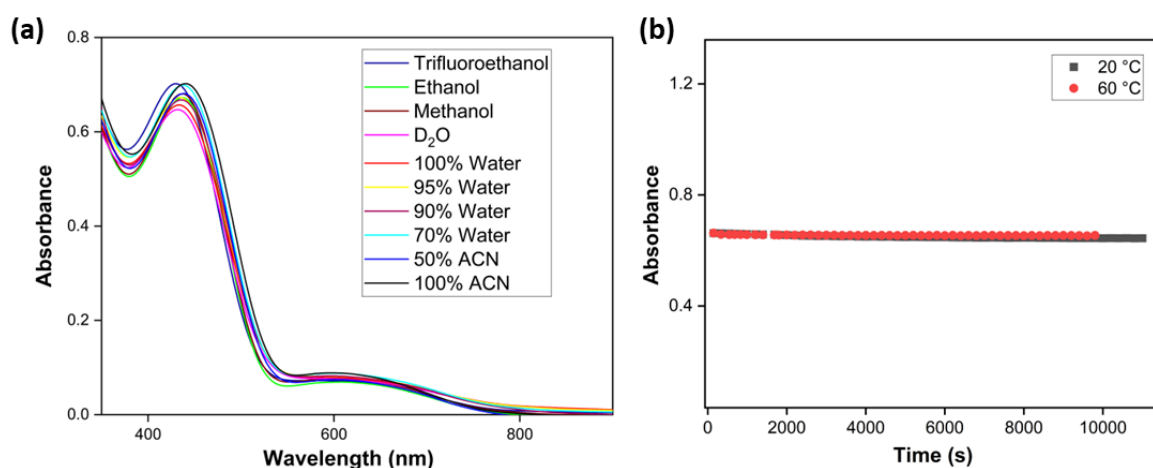


Figure S4. (a) UV-vis spectra of **2** at different solvents at RT and (b) stability of **2** (0.15 mM) in CH_3CN both at 20 °C and 60 °C, data collected at λ_{max} : 442 nm.

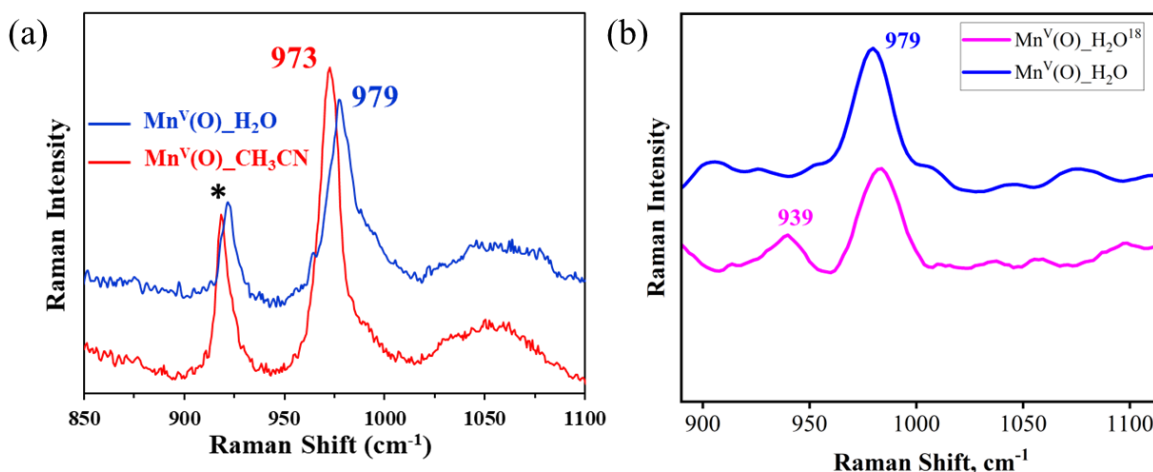


Figure S5. Resonance raman spectra of (a) ^{16}O labeled complex **2** (10mM) recorded in CH_3CN and water at 77 K with 413.1 nm laser excitation. The * marked peak originates from solvent CH_3CN . The residual CH_3CN peak in blue spectra for complex **2** in water originates from slight (3%) CH_3CN used for dissolving the 10 mM complex **2**. and (b) comparative Raman spectra

of **2** (6 mM) both in H₂O¹⁶ and H₂¹⁸O at RT with 488 nm laser excitation. The peak at 979 cm⁻¹ for Mn–O stretch in H₂O¹⁶ shifted at 939 cm⁻¹ in H₂¹⁸O.

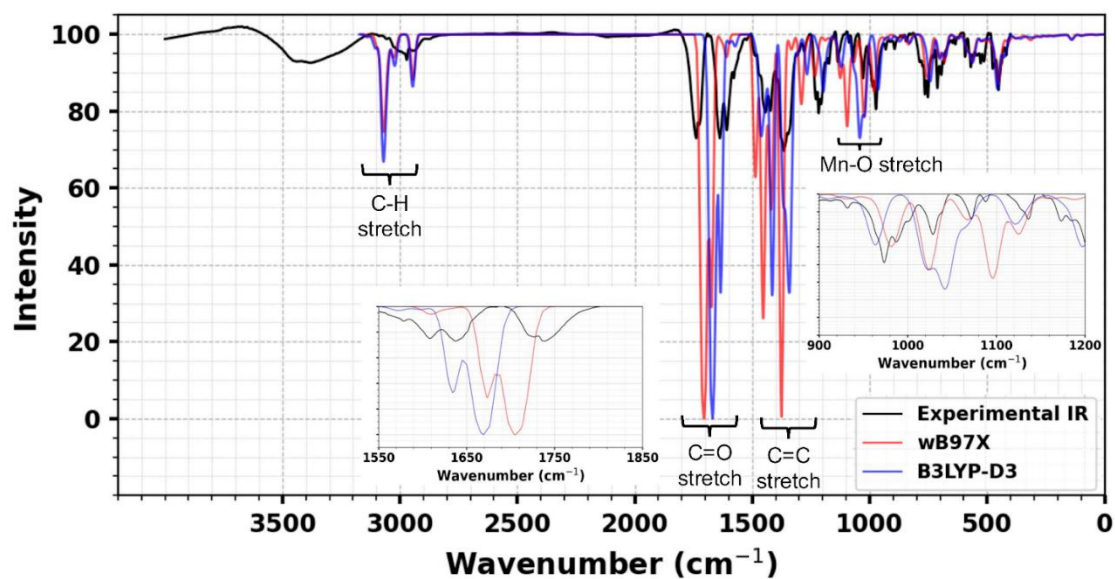


Figure S6: IR spectrum of Mn(V) oxo compound with ω B97X and B3LYP-D3 in 6-31G(d,p) with Mn (SDD/SDD).

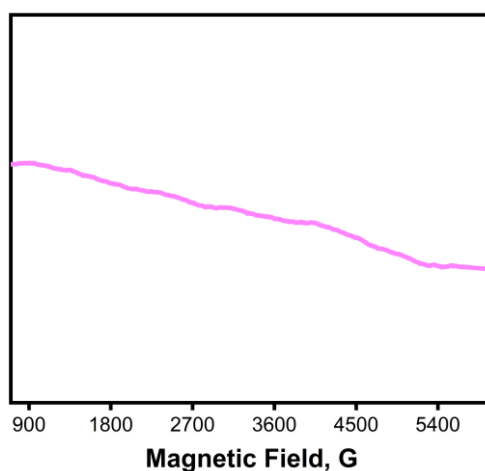


Figure S7. EPR data of **2** (5 mM) at 100 K.

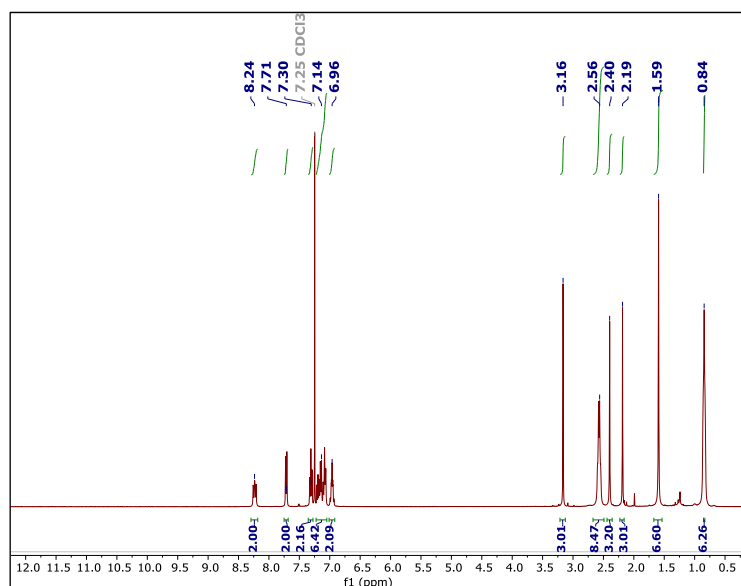


Figure S8. NMR data of **2** (10 mM) at RT.

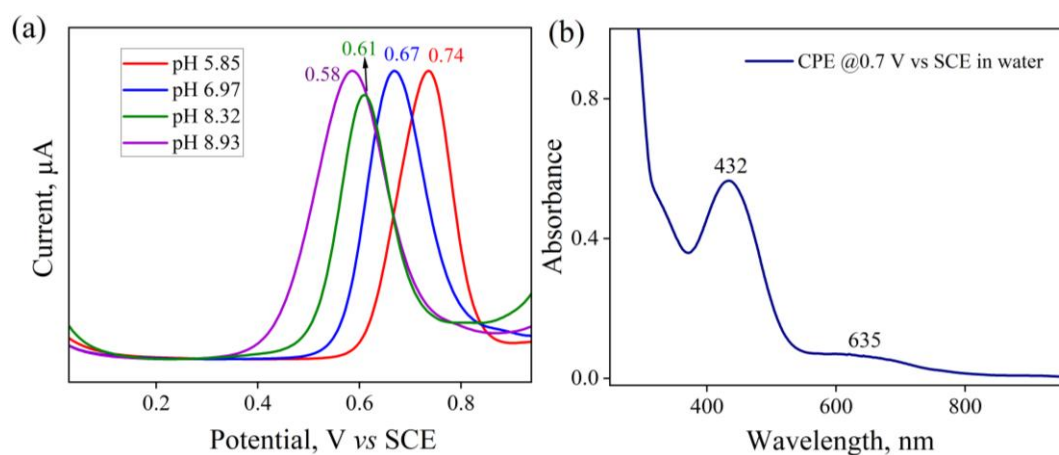


Figure S9. (a) DPV data of **1** (0.5 mM) (Potential for $\text{Mn}^{\text{IV/V}}$ redox couple) in water with varying pH using Glassy Carbon as working and Pt wire as counter electrode at RT. (b) Formation of **2** via controlled-potential electrolysis (CPE) of **1** @0.8 V vs. SCE in water at RT.

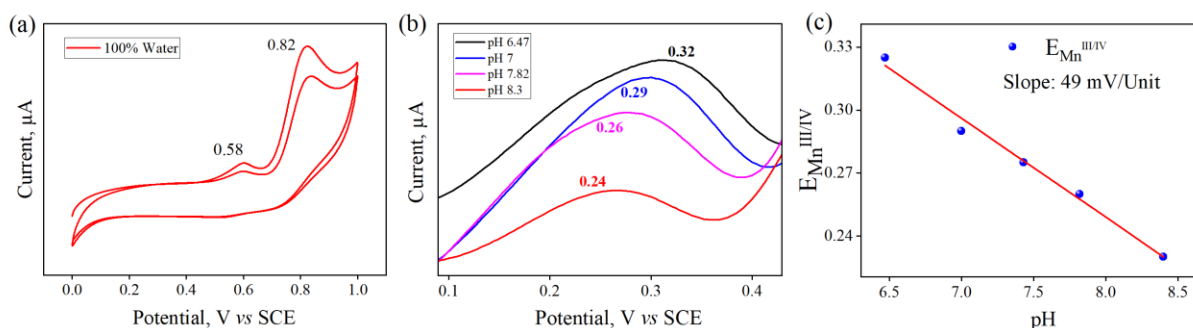


Figure S10. (a) CV and (b) DPV of **1** (0.5 mM) at varying pH in water using a gold working and Pt wire counter electrode at RT. (c) Plot of $\text{Mn}^{\text{III}}/\text{Mn}^{\text{IV}}$ redox potential vs. pH shows a slope of 49 mV/unit, indicating a $1\text{e}^-/1\text{H}^+$ PCET process.

4D. Reactivity and Kinetic Studies

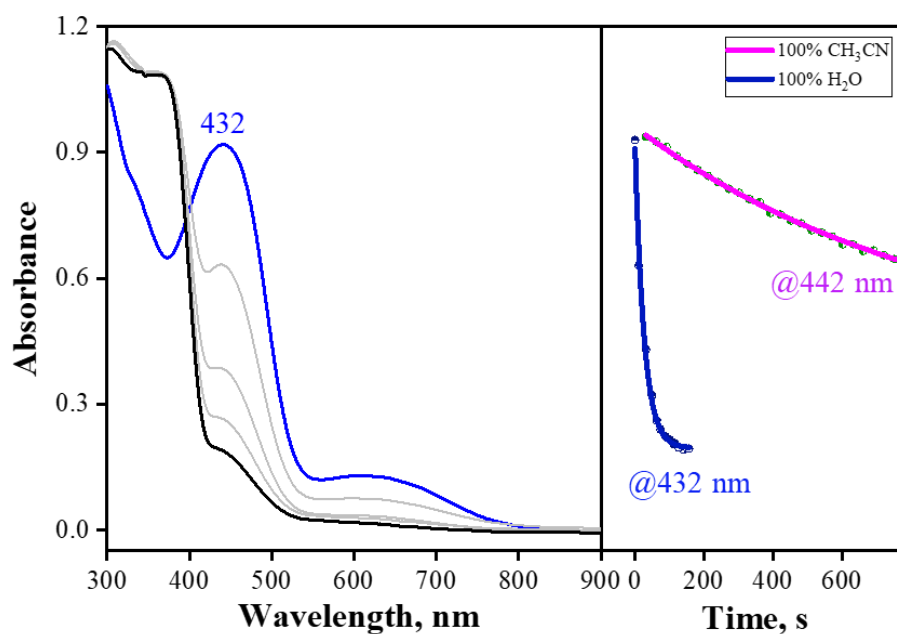


Figure S11. Left: UV-vis kinetic spectra for the reaction of **2** (0.2 mM) with BNAH in water. Right: Decay profiles of **2** in both water and CH₃CN at 293 K, monitored at 432 nm and 442 nm, respectively.

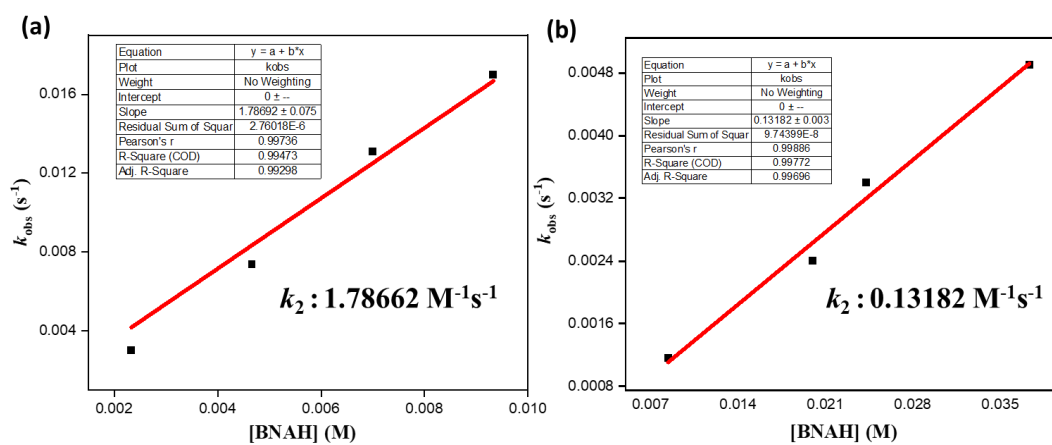


Figure S12. Determination of second-order rate constant values for the reaction of **2** (0.05 mM) in the presence of different BNAH concentrations at 293 K in 80% water (a) and 50% water (b).

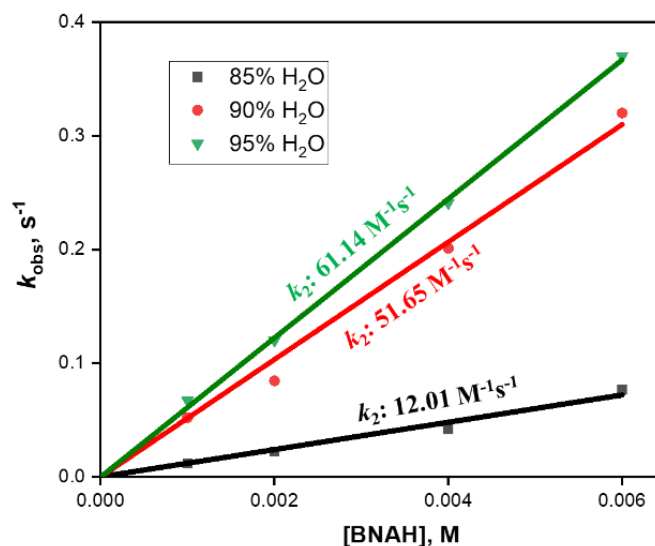


Figure S13. Determination of second-order rate constant values for the reaction of **2** (0.05 mM) in the presence of different BNAH concentrations at 293 K in 85%, 90% and 95% water.

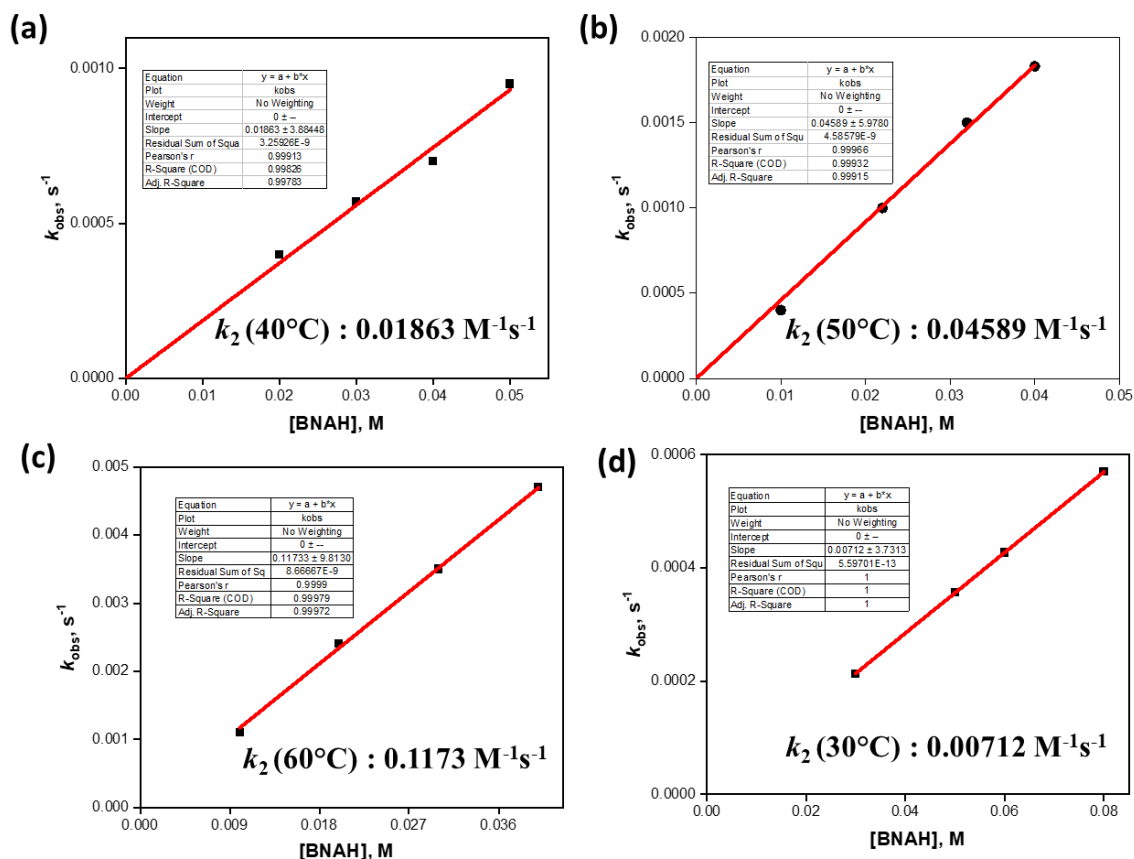


Figure S14. Determination of second-order rate constant values for the reaction of **2** (0.05 mM) in the presence of different BNAH concentrations at different temperatures in CH₃CN.

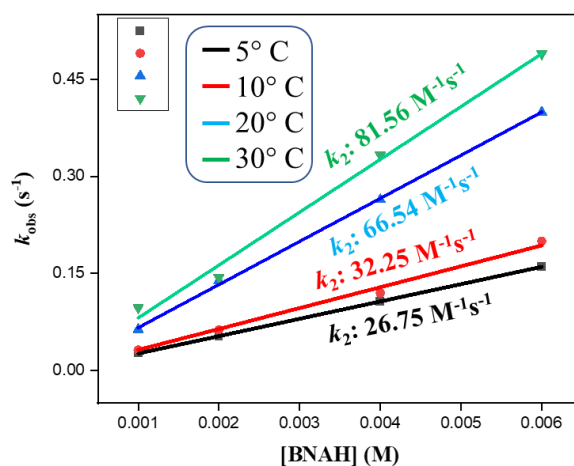


Figure S15. Determination of second-order rate constant values for the reaction of **2** (0.05 mM) in the presence of different BNAH concentrations at different temperatures in 100% water.

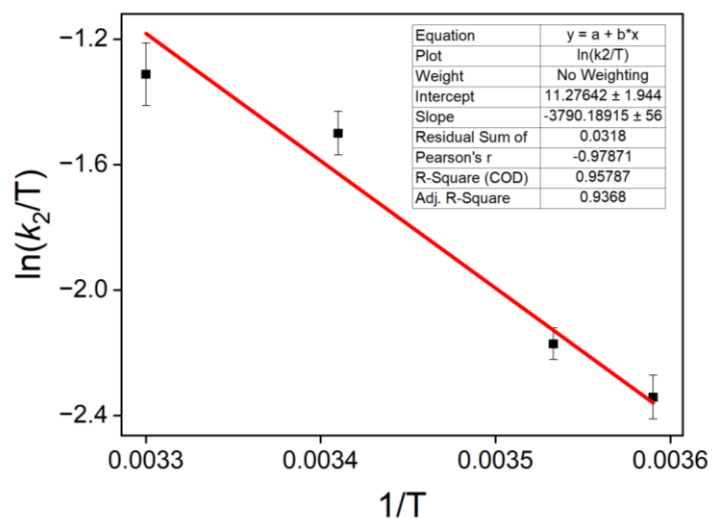


Figure S16. Plot of $\ln(k_2/T)$ vs. $1/T$ for the variable temperature range of BNAH oxidation by **2** in 100% water.

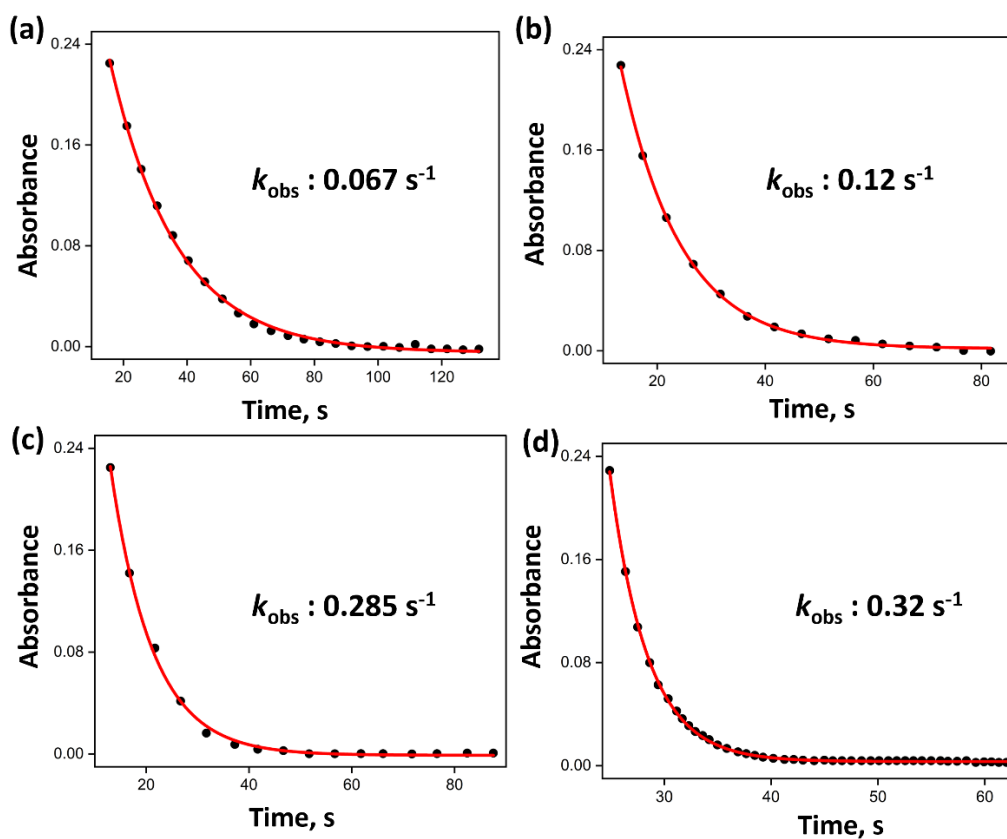


Figure S17. Plot of k_{obs} values for the reaction of **2** (0.05 mM) in the presence of 0.001 M (a), 0.002 M (b), 0.004 M (c), 0.005 M (d) BNAH concentration at 20° C in 100% water.

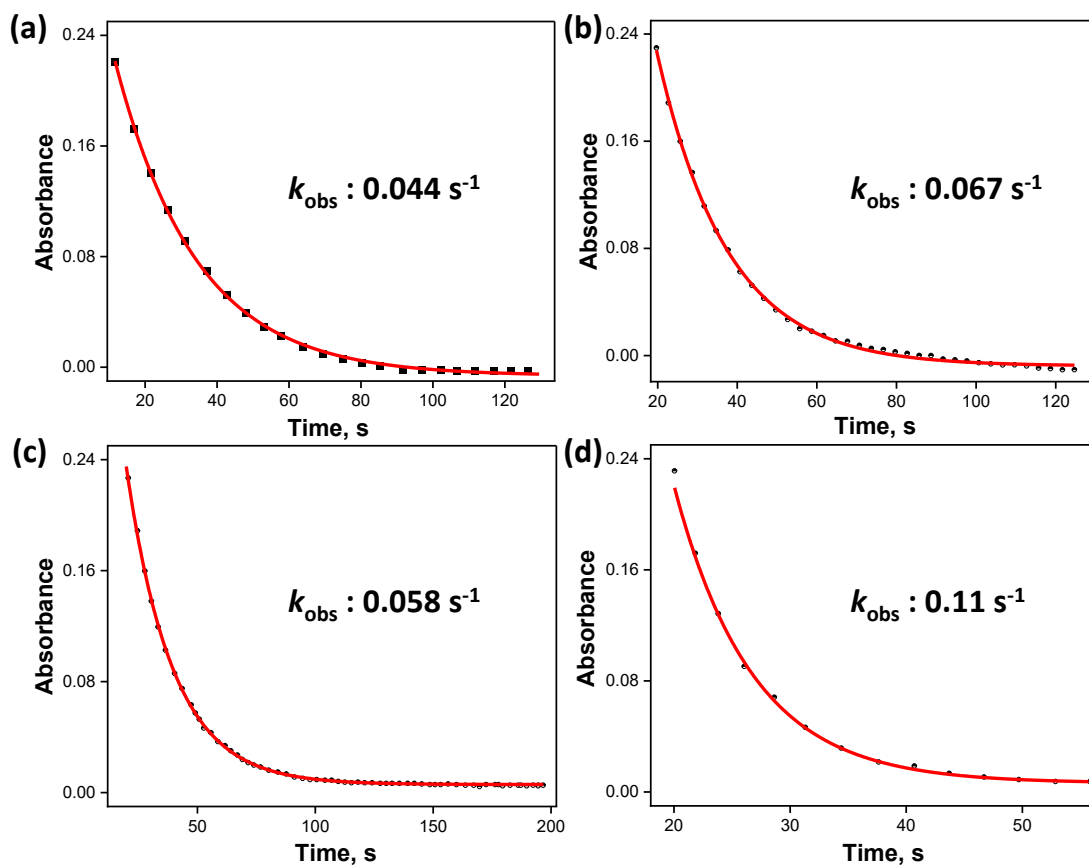


Figure S18. Plot of k_{obs} values for the reaction of **2** (0.05 mM) in presence of 0.003 M (a), 0.004 M (b) BNAH concentration at 5° C and 0.002 M (c), 0.004 M (d) BNAH concentration at 10° C in 100% water.

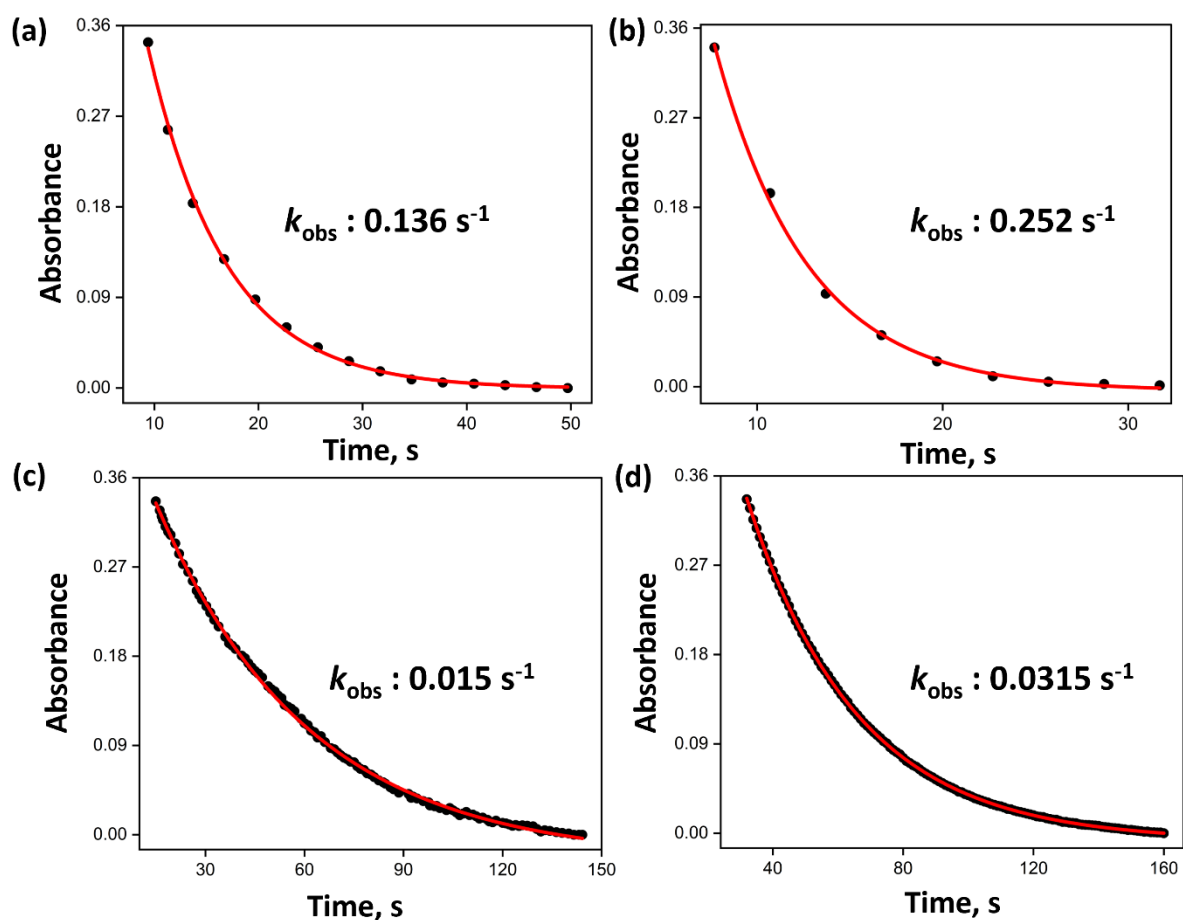


Figure S19. Plot of k_{obs} values for the reaction of **2** (0.075 mM) with (a) 0.001 M BNAH in 2M aq. LiCl (b) 0.002 M BNAH in 2M aq. LiCl (c) 0.001 M BNAH in 2M aq. Guanidinium chloride, and (d) 0.002 M BNAH in 2M aq. Guanidinium chloride at 20° C.

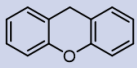
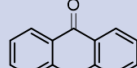
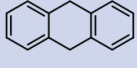
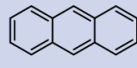
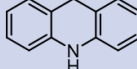
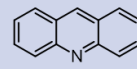
Substrate	Solvent	Product	STON Yield%
	100% ACN		69%
	100% Water		75%
	100% ACN		67%
	100% Water		74.2 %
	100% ACN		95%
	100% Water		96%

Table S9. Reported GC-MS yield for the reaction of several substrates containing C–H bond (0.1 M) with **2** (0.4 mM) under a single turnover condition at room temperature.

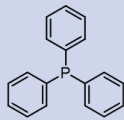
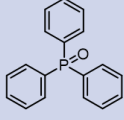
Substrate	Product	Solvent	STON Yield%
		ACN	98%
		Water	96%
		ACN	85%
		Water	72%
	NOT	ACN	NOT
		Water	

Table S10. Reported GC-MS yield for the OAT reaction of several substrates (0.1 M) with **2** (0.4 mM) under a single turnover condition at room temperature.

Solvent	k_{initial} (s^{-1})		
	9,10 AcrH ₂	Xanthene	9,10 DHA
100% CH ₃ CN	1.1×10^{-5}	0.17×10^{-5}	0.08×10^{-5}
100% H ₂ O	3.8×10^{-2}	0.8×10^{-2}	0.4×10^{-2}

Table S11. Determination of the initial rate constant for **2** (0.4 mM) with various C–H bond substrates in both solvents at RT.

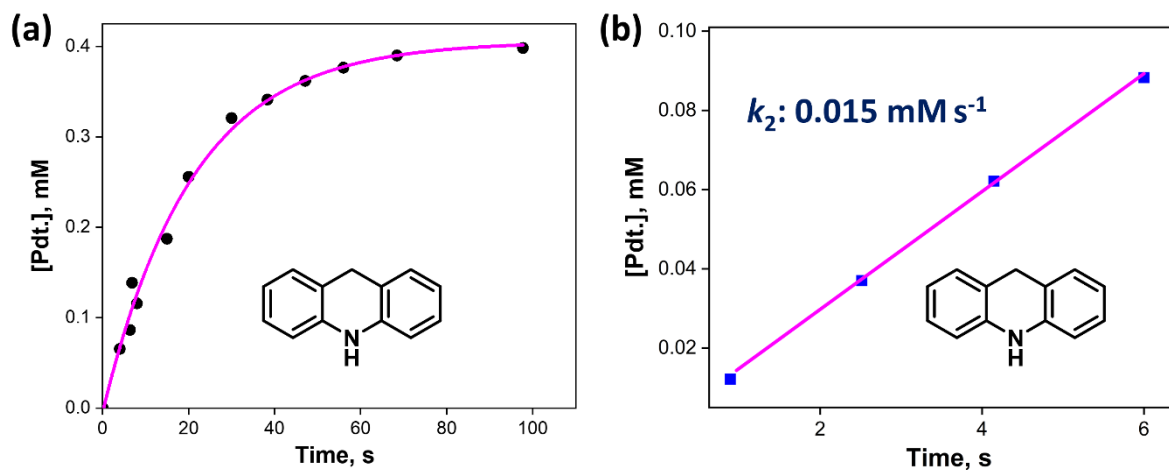


Figure S20. (a) A plot of time-dependent product analysis for 9, 10 dihydroacridine oxidation with **2** (0.4 mM) under single turnover conditions in water at RT. (b) Determination of the initial rate in water by estimating the product concentration during the early phase of the reaction.

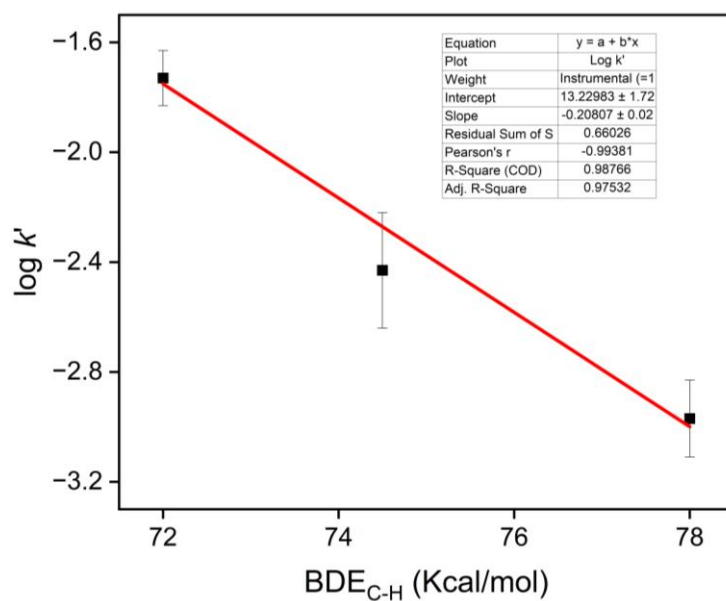


Figure S21. Plot of $\log k'$ (k' : k /number of equivalent hydrogen atoms, k : Initial rate constant) vs BDE_{C-H} of various hydrocarbons for the reaction of **2** (0.4 mM) in water at RT.

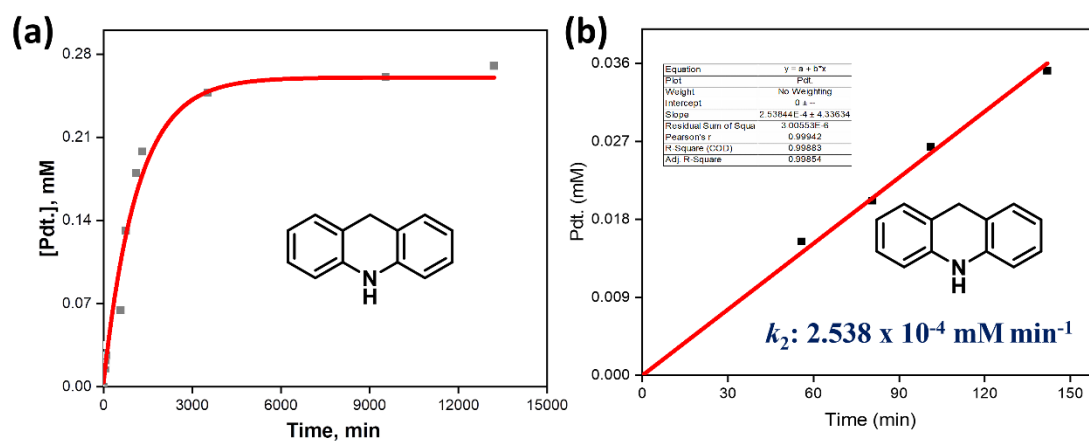


Figure S22. (a) A plot of time-dependent product analysis for 9, 10 dihydroacridine oxidation with **2** (0.4 mM) under single turnover condition in CH_3CN at RT. (b) Determination of the initial rate in CH_3CN by estimating the product concentration during the early phase of the reaction.

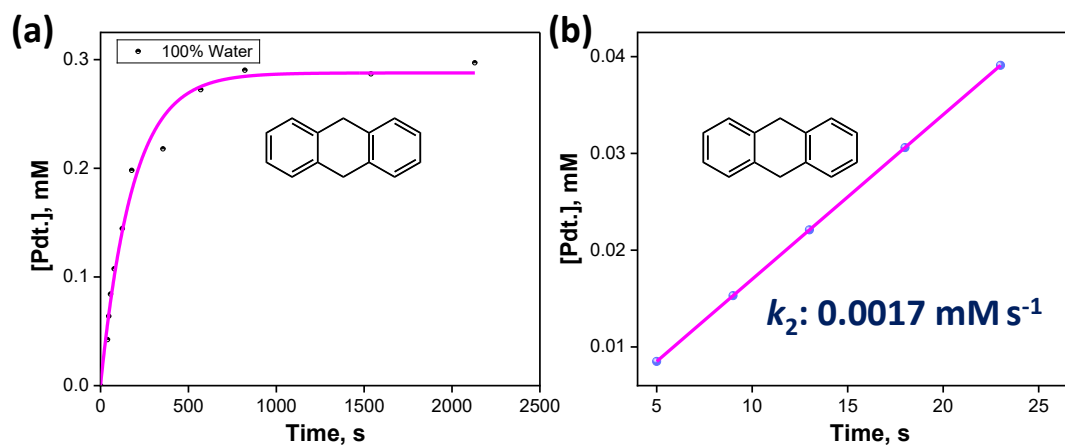


Figure S23. (a) A plot of time-dependent product analysis for 9, 10-dihydroanthracene oxidation with **2** (0.4 mM) under single turnover condition in water at RT. (b) Determination of initial rate by estimating the product concentration during the early phase of the reaction.

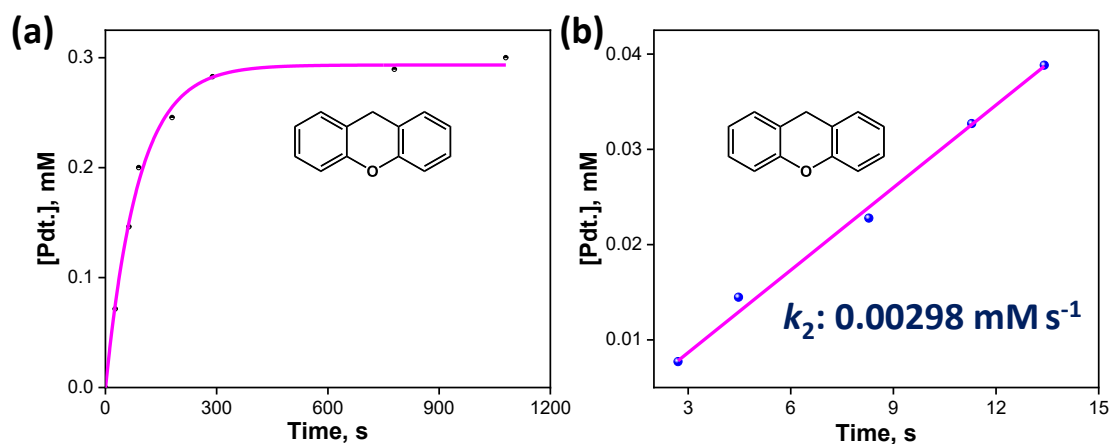


Figure S24. (a) A plot of time dependent product analysis for xanthene oxidation with **2** (0.4 mM) under single turnover condition in water at RT. (b) Determination of initial rate by estimating the product concentration during the early phase of the reaction.

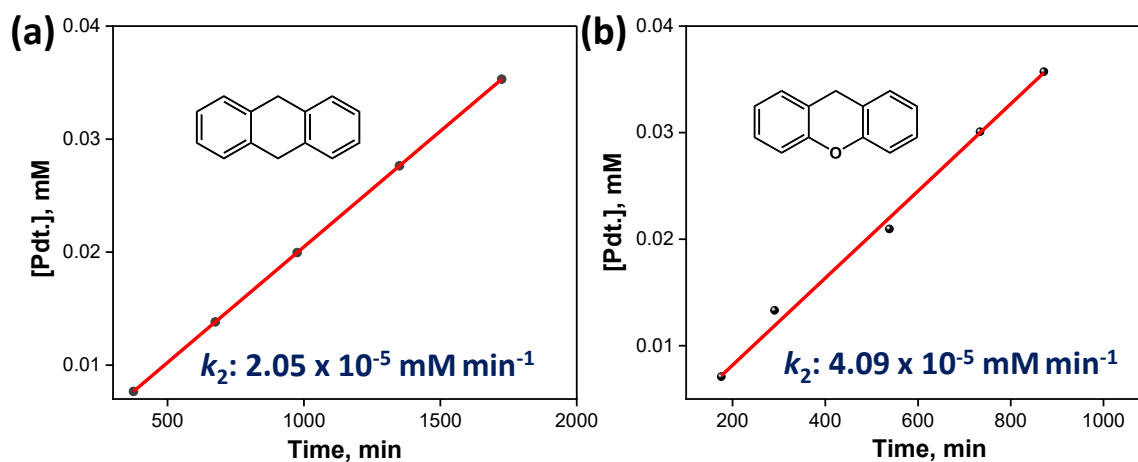


Figure S25. Determination of initial rate by estimating the product concentration during the early phase of the reaction for (a) 9, 10-dihydroanthracene and (b) Xanthene with **2** (0.4 mM) in CH₃CN at RT.

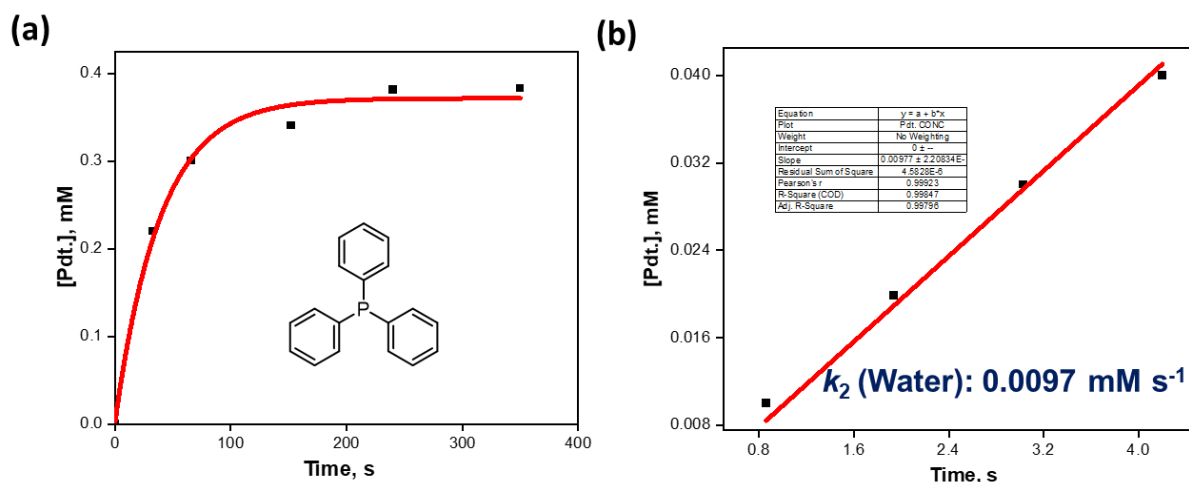


Figure S26. (a) A plot of time dependent product analysis for Triphenylphosphine oxidation with **2** (0.4 mM) in water at single turnover condition at RT. (b) Determination of initial rate by estimating the product concentration during the early phase of the reaction.

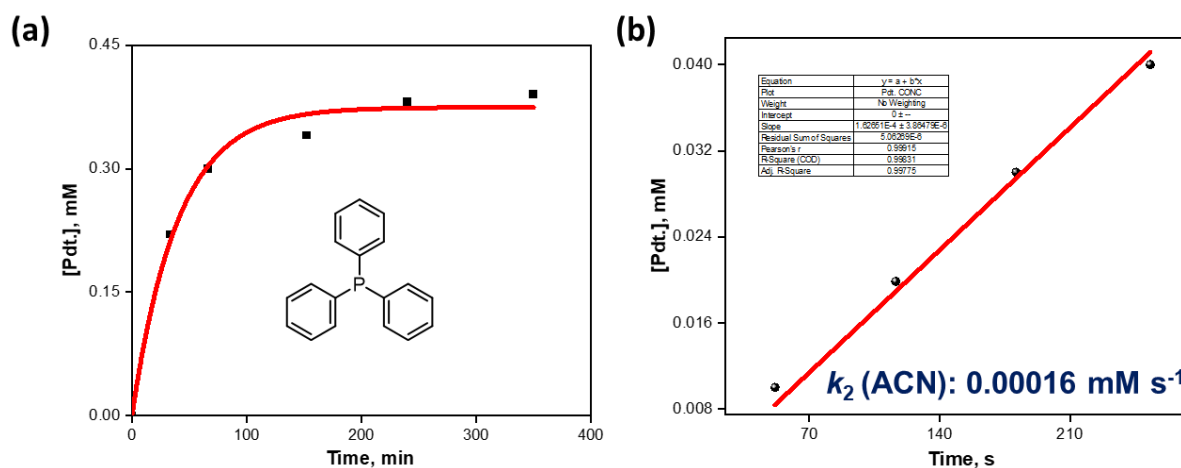


Figure S27. (a) A plot of time dependent product analysis for Triphenylphosphine oxidation with **2** (0.4 mM) in CH₃CN at RT at single turnover condition at RT. (b) Determination of initial rate by estimating the product concentration during the early phase of the reaction.

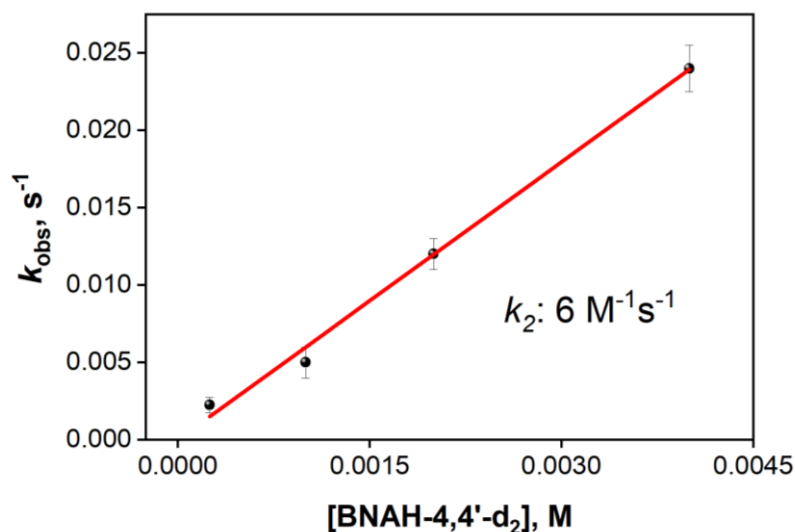


Figure S28. Plot of the pseudo-first-order rate constants, k_{obs} vs $[\text{BNAH-4,4'-d}^2]$ for the reaction with **2** (0.05 mM) in water at 293 K.

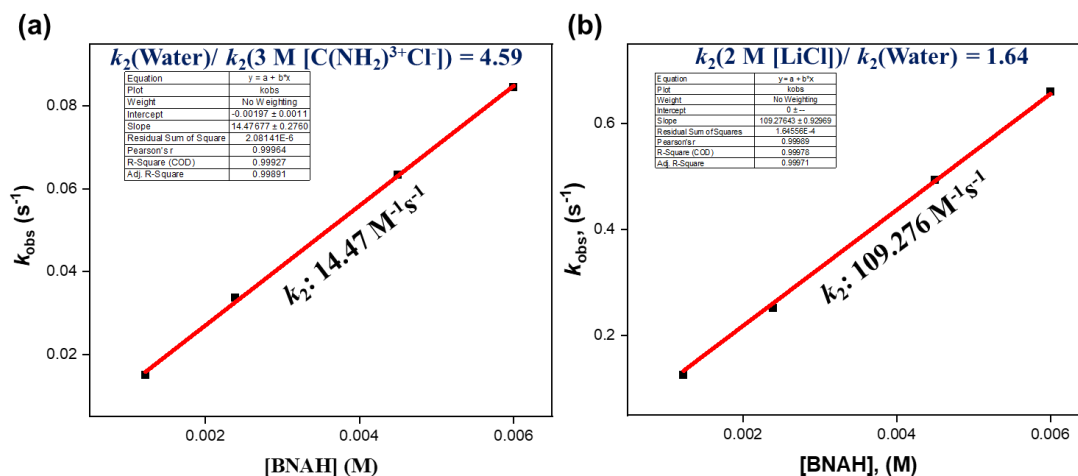


Figure S29. Determination of second-order rate constant values for BNAH oxidation with **2** (a) in 3M guanidinium chloride, and (b) 2M lithium chloride aqueous solution at 20°C.

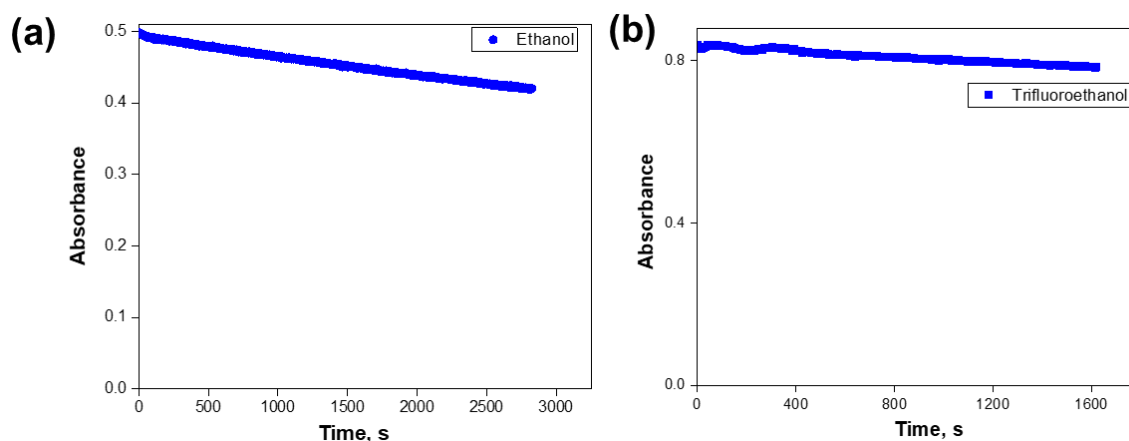


Figure S30. (a) UV-vis absorption study for the reaction of BNAH with **2** in Ethanol (a) and trifluoroethanol (b), showing no significant change in the absorption spectra.

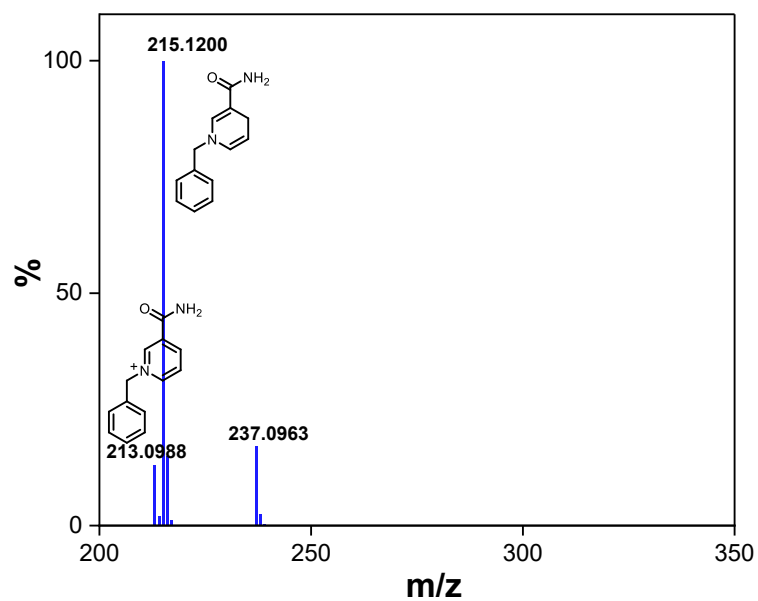


Figure S31. HRMS data for the reaction of BNAH with **2** (0.05 mM) in water showing the formation of BNA⁺.

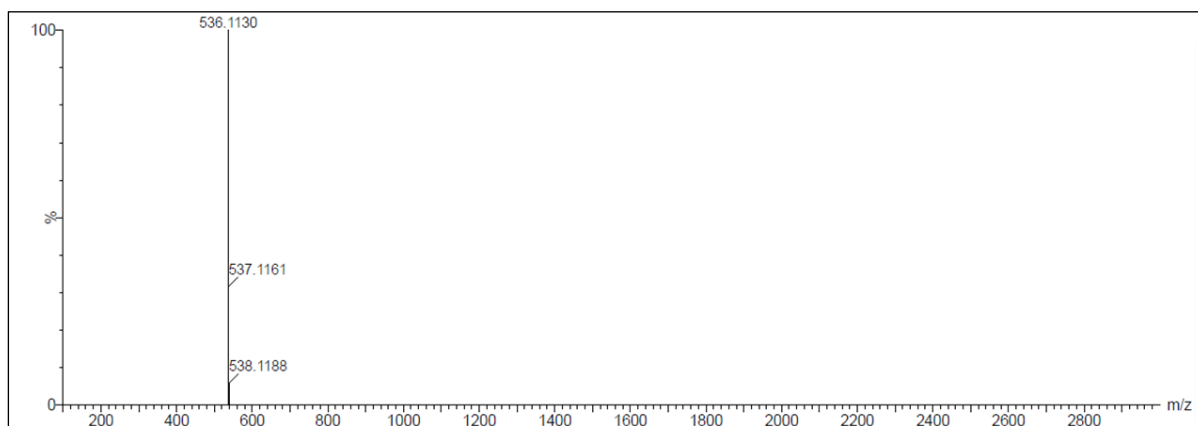
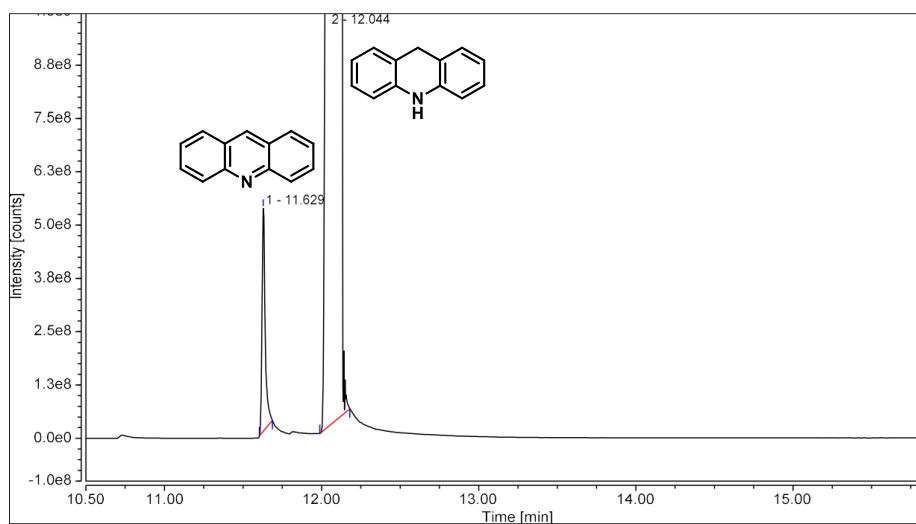


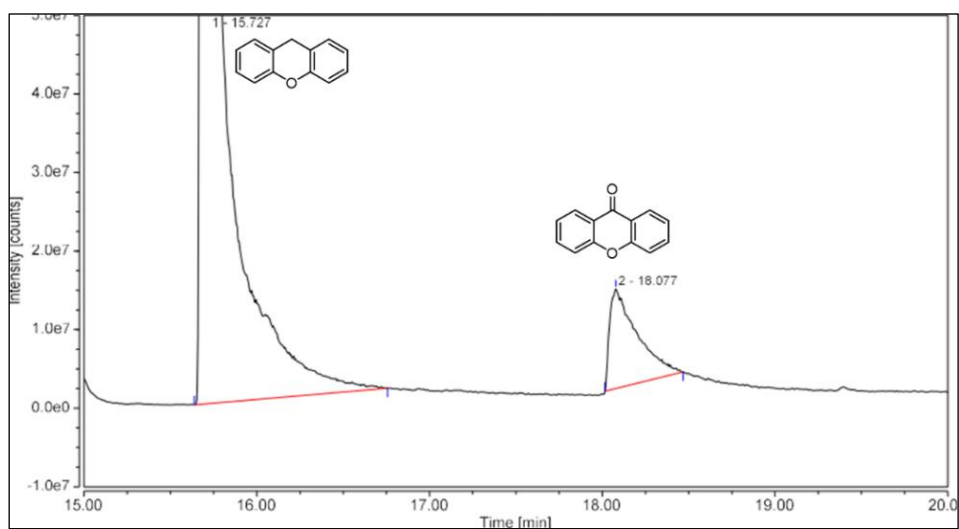
Figure S32. HRMS (-ve mode) data for the reaction of BNAH with **2** (0.05 mM) in water showing the formation of complex **1** [Calculated m/z = 536.1131].

5. GC-MS datas

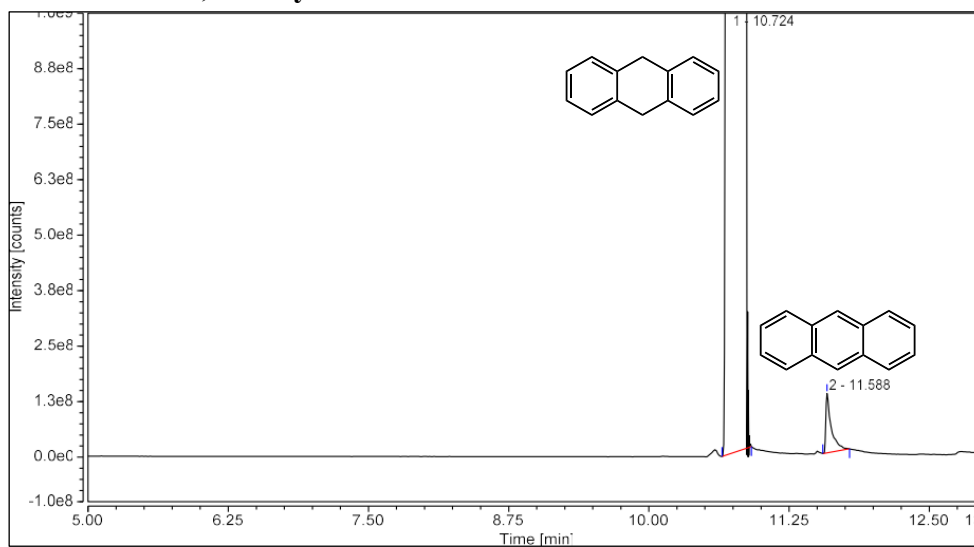
GC-MS trace for 9, 10 dihydroacridine



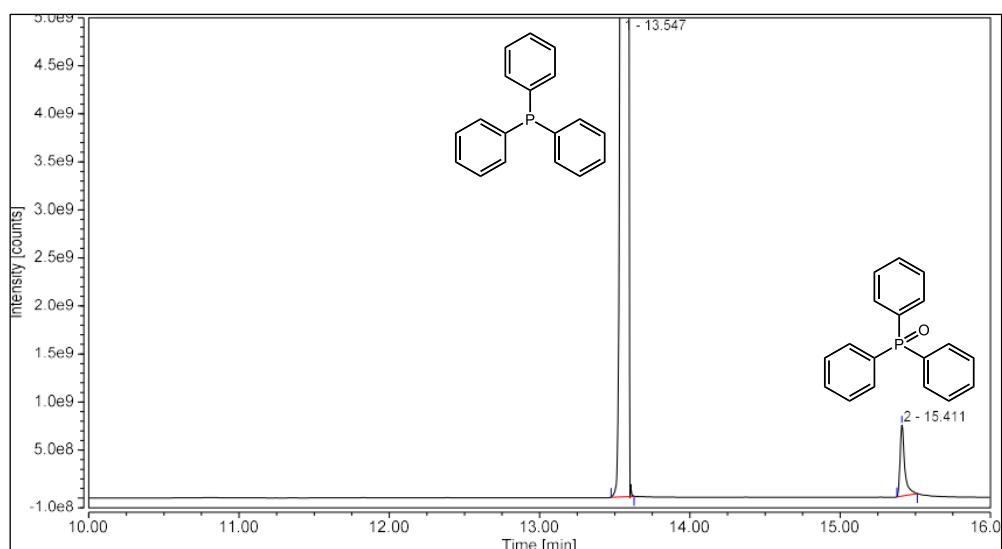
(a) GC-MS trace for xanthene



(b) GC-MS trace for 9,10 dihydroanthracene



(c) GC-MS trace for Triphenylphosphine



(d) GC-MS trace for Thioanisole

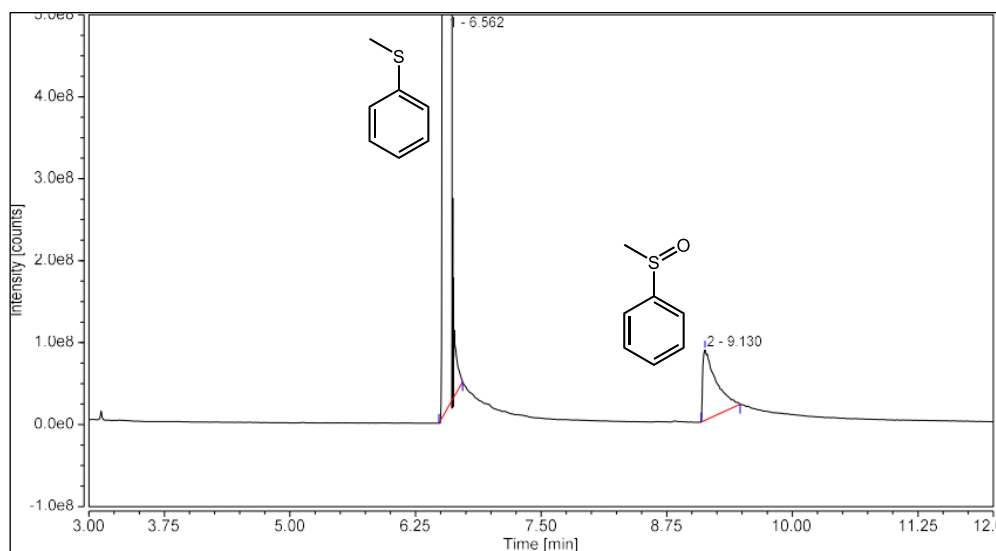


Figure S33. (a) – (e). GC-MS traces for reactivity studies of **2** (0.4 mM) at Single turnover condition in water at RT.

6. Coordinates of the reactants and complexes involved in the reaction pathway

Acetonitrile:

Mn-oxo

Mn	0.030940000	-0.048374000	-0.009407000
O	1.085533000	-0.653909000	3.816359000
O	3.968639000	0.515506000	-0.232571000
O	-1.751259000	-1.886307000	-3.052006000
O	-2.591363000	-2.369920000	1.956470000
N	-0.277361000	-0.693766000	-1.742225000

N	1.006193000	-0.386545000	1.547903000
N	-1.193539000	-1.380701000	0.443359000
N	-0.867098000	-1.153449000	2.780749000
N	1.741487000	0.209472000	-0.732132000
C	0.467943000	-0.727805000	2.755746000
C	-1.603031000	-1.681054000	1.710307000
C	2.429645000	-0.012323000	1.558476000
C	1.712384000	2.254861000	2.476474000
H	0.722328000	2.076725000	2.065637000
C	4.229385000	2.736066000	3.542017000
H	5.219078000	2.913876000	3.955994000
C	2.814520000	0.280311000	0.100671000
C	-1.340632000	-1.512995000	-1.960915000
C	2.702950000	1.275577000	2.348686000
C	1.815983000	0.231085000	-2.137895000
C	0.647398000	-0.288740000	-2.721896000
C	3.234689000	3.700812000	3.671117000
H	3.439345000	4.636078000	4.186105000
C	3.967158000	1.536310000	2.882802000
H	4.761397000	0.801534000	2.794074000
C	-2.008870000	-1.941345000	-0.647376000
C	2.868002000	0.673692000	-2.936121000
H	3.767347000	1.062376000	-2.475557000
C	-0.764387000	-4.126427000	-0.373631000
H	0.119561000	-3.538048000	-0.134379000
C	-1.974549000	-3.475248000	-0.633899000
C	1.973690000	3.454165000	3.133145000
H	1.185716000	4.197959000	3.225239000
C	-3.094359000	-4.246069000	-0.945210000
H	-4.046769000	-3.769119000	-1.156880000

C	-1.423704000	-1.402590000	4.108620000
H	-1.158511000	-2.398807000	4.478310000
H	-2.507967000	-1.326848000	4.051382000
H	-1.029524000	-0.656584000	4.796023000
C	1.581814000	0.076766000	-4.901687000
H	1.493993000	0.019933000	-5.983701000
C	0.524403000	-0.369990000	-4.107033000
H	-0.376901000	-0.781295000	-4.543707000
C	2.738218000	0.592250000	-4.323890000
H	3.553296000	0.937759000	-4.954696000
C	3.308740000	-1.194345000	1.996870000
H	3.214049000	-1.369968000	3.068405000
H	4.352823000	-1.002468000	1.741445000
H	2.989760000	-2.092766000	1.457489000
C	-0.679709000	-5.514835000	-0.406100000
H	0.269580000	-6.001782000	-0.195836000
C	-3.011848000	-5.637542000	-0.977189000
H	-3.898204000	-6.221182000	-1.214387000
C	-3.422615000	-1.344853000	-0.671825000
H	-3.350763000	-0.252582000	-0.624265000
H	-4.006812000	-1.698253000	0.178063000
H	-3.927023000	-1.609273000	-1.604679000
C	-1.806491000	-6.278155000	-0.706423000
O	-0.647239000	1.296737000	0.126463000
H	-1.743935000	-7.363206000	-0.729969000

BNAH

O	0.023956000	-0.012824000	0.035163000
N	-2.611256000	3.086399000	0.754250000
N	1.454984000	0.690399000	1.636263000
C	-3.906558000	3.064323000	0.103210000

C	-0.176288000	2.931060000	2.361301000
C	-0.566266000	1.944589000	1.277089000
C	-1.711550000	2.070953000	0.574530000
C	-5.011105000	2.388647000	0.898988000
C	-2.356088000	4.012816000	1.771388000
C	-1.253902000	3.975773000	2.523602000
C	-4.753512000	1.656414000	2.056872000
C	-6.328776000	2.492003000	0.442598000
C	0.301832000	0.797326000	0.924276000
C	-5.795237000	1.034944000	2.745949000
C	-7.367340000	1.870607000	1.126663000
C	-7.102987000	1.138445000	2.284025000
H	-3.789579000	2.557844000	-0.860741000
H	-4.199677000	4.096149000	-0.119961000
H	0.785403000	3.413728000	2.123585000
H	-0.008282000	2.415111000	3.320335000
H	-1.957357000	1.342832000	-0.193654000
H	-3.121982000	4.772865000	1.896299000
H	-1.120819000	4.741017000	3.282852000
H	-3.735641000	1.569175000	2.429296000
H	-6.539736000	3.065717000	-0.458422000
H	-5.579236000	0.468385000	3.648346000
H	-8.386478000	1.959745000	0.758793000
H	-7.913847000	0.653928000	2.821668000
H	2.037328000	-0.116890000	1.474565000
H	1.660336000	1.272844000	2.432065000
R (Singlet)			
Mn	-0.014423000	-0.032486000	-0.028287000
O	2.094985000	-1.995604000	2.765163000
O	3.603643000	-0.032523000	-1.696902000

O	-3.183171000	-0.416298000	-2.378596000
O	-2.320689000	-2.414732000	2.236351000
N	-1.056107000	-0.033372000	-1.579119000
N	1.309703000	-0.998388000	0.865975000
N	-1.321861000	-1.219310000	0.565471000
N	-0.153284000	-1.826727000	2.537844000
N	1.344576000	0.183445000	-1.301309000
C	1.151785000	-1.625027000	2.069217000
C	-1.330125000	-1.850182000	1.776343000
C	2.694178000	-0.887856000	0.373037000
C	3.053287000	1.180469000	1.799503000
H	2.011302000	1.438180000	1.625982000
C	5.715209000	0.549859000	2.264122000
H	6.757025000	0.292956000	2.440448000
C	2.617258000	-0.187601000	-0.989629000
C	-2.325904000	-0.519113000	-1.511735000
C	3.574931000	-0.005028000	1.268508000
C	0.934091000	0.630361000	-2.572220000
C	-0.456836000	0.510236000	-2.730889000
C	5.186187000	1.722395000	2.794262000
H	5.809113000	2.387895000	3.386528000
C	4.917306000	-0.304309000	1.503933000
H	5.354393000	-1.213839000	1.103100000
C	-2.590101000	-1.238704000	-0.182445000
C	1.723686000	1.132436000	-3.604257000
H	2.794854000	1.216054000	-3.471819000
C	-2.017813000	-3.567665000	-0.985858000
H	-0.975345000	-3.254941000	-1.000837000
C	-2.999233000	-2.670189000	-0.552813000
C	3.849083000	2.034885000	2.556948000

H	3.421123000	2.948385000	2.963053000
C	-4.330354000	-3.086424000	-0.548409000
H	-5.115366000	-2.410691000	-0.222176000
C	-0.258271000	-2.408013000	3.874603000
H	-0.157269000	-3.498259000	3.850303000
H	-1.232255000	-2.154812000	4.289034000
H	0.534432000	-1.995880000	4.496003000
C	-0.272310000	1.390036000	-4.955636000
H	-0.740965000	1.690944000	-5.889251000
C	-1.068793000	0.890233000	-3.923453000
H	-2.140981000	0.790210000	-4.034249000
C	1.105913000	1.508382000	-4.798817000
H	1.713719000	1.901742000	-5.610244000
C	3.288908000	-2.275226000	0.093067000
H	3.490128000	-2.806570000	1.023387000
H	4.209755000	-2.178468000	-0.486266000
H	2.573434000	-2.854073000	-0.500827000
C	-2.356411000	-4.855976000	-1.387703000
H	-1.577558000	-5.539676000	-1.716840000
C	-4.671436000	-4.377537000	-0.949317000
H	-5.714024000	-4.685922000	-0.931271000
C	-3.684685000	-0.434988000	0.532149000
H	-3.287157000	0.550510000	0.800526000
H	-4.008419000	-0.945018000	1.439813000
H	-4.537890000	-0.284198000	-0.133949000
C	-3.687724000	-5.267862000	-1.369099000
O	-0.221098000	1.285705000	0.696323000
H	-3.955112000	-6.274507000	-1.680442000
O	-2.265693000	4.290397000	-2.938142000
N	1.732178000	4.842205000	-3.801401000

N	-1.827138000	3.467696000	-0.877281000
C	2.096690000	5.405426000	-5.086021000
C	1.007840000	3.928745000	-1.124087000
C	0.021536000	4.198360000	-2.245953000
C	0.425018000	4.630845000	-3.459905000
C	2.312152000	6.909739000	-5.081369000
C	2.709514000	4.628961000	-2.823887000
C	2.416121000	4.208586000	-1.590236000
C	1.904672000	7.713386000	-4.017214000
C	2.919934000	7.509151000	-6.188751000
C	-1.434533000	3.989619000	-2.077378000
C	2.098206000	9.094258000	-4.060318000
C	3.110191000	8.886105000	-6.234754000
C	2.699312000	9.684803000	-5.167499000
H	1.304752000	5.151581000	-5.799209000
H	3.007449000	4.909651000	-5.441324000
H	0.942525000	2.884925000	-0.780323000
H	0.769983000	4.539256000	-0.237836000
H	-0.310325000	4.819175000	-4.237551000
H	3.728138000	4.822804000	-3.148196000
H	3.230762000	4.048217000	-0.888855000
H	1.435777000	7.261687000	-3.146038000
H	3.246893000	6.887976000	-7.021182000
H	1.777271000	9.708303000	-3.222327000
H	3.584428000	9.337662000	-7.102752000
H	2.850798000	10.760765000	-5.199711000
H	-2.796065000	3.192641000	-0.801482000
H	-1.174114000	3.000202000	-0.265057000

R (Triplet)

Mn	0.113132000	-0.171388000	0.030299000
O	2.647832000	-1.581629000	2.736088000
O	3.513345000	0.034328000	-2.065132000
O	-3.134099000	-1.115300000	-2.032254000
O	-1.691502000	-2.612897000	2.704688000
N	-1.041842000	-0.375804000	-1.428197000
N	1.613897000	-0.906959000	0.817626000
N	-1.065229000	-1.390366000	0.876757000
N	0.381648000	-1.665903000	2.720254000
N	1.333882000	0.306919000	-1.370775000
C	1.611944000	-1.396067000	2.105958000
C	-0.867410000	-1.928447000	2.101432000
C	2.922704000	-0.602368000	0.199326000
C	3.011537000	1.457565000	1.716066000
H	1.940121000	1.370367000	1.872887000
C	5.747088000	1.730117000	1.327223000
H	6.818387000	1.826642000	1.168227000
C	2.634258000	-0.047046000	-1.216589000
C	-2.222958000	-1.036804000	-1.222481000
C	3.683446000	0.515086000	0.930383000
C	0.727232000	0.617163000	-2.600340000
C	-0.632106000	0.249979000	-2.629042000
C	5.070690000	2.658280000	2.114095000
H	5.607363000	3.483492000	2.575195000
C	5.059144000	0.670736000	0.738029000
H	5.608624000	-0.035638000	0.123338000
C	-2.306519000	-1.712269000	0.162096000
C	1.320475000	1.222241000	-3.704496000
H	2.369477000	1.493715000	-3.667435000
C	-1.266868000	-3.919005000	-0.518280000

H	-0.312965000	-3.398055000	-0.579330000
C	-2.410040000	-3.219990000	-0.115720000
C	3.698094000	2.516410000	2.305023000
H	3.154213000	3.233160000	2.915828000
C	-3.623338000	-3.904515000	-0.049155000
H	-4.528815000	-3.387863000	0.254767000
C	0.481813000	-2.091713000	4.116102000
H	0.783732000	-3.140897000	4.198984000
H	-0.492341000	-1.967245000	4.584412000
H	1.222744000	-1.473084000	4.620223000
C	-0.805294000	1.119822000	-4.859301000
H	-1.403648000	1.324002000	-5.743469000
C	-1.406316000	0.505452000	-3.759013000
H	-2.450360000	0.219620000	-3.774023000
C	0.541678000	1.471548000	-4.835133000
H	0.994157000	1.951482000	-5.699329000
C	3.744159000	-1.884899000	0.021946000
H	4.146827000	-2.223166000	0.976552000
H	4.555700000	-1.709805000	-0.686565000
H	3.099479000	-2.666867000	-0.392808000
C	-1.332187000	-5.272902000	-0.831200000
H	-0.431319000	-5.798915000	-1.137860000
C	-3.690117000	-5.262110000	-0.360767000
H	-4.643858000	-5.780161000	-0.295370000
C	-3.533557000	-1.122095000	0.867029000
H	-3.354447000	-0.060250000	1.066864000
H	-3.711366000	-1.634721000	1.813123000
H	-4.415799000	-1.202698000	0.227549000
C	-2.546824000	-5.951901000	-0.751783000
O	-0.213493000	1.205482000	0.743988000

H	-2.600234000	-7.010409000	-0.993477000
O	-1.400901000	4.979369000	-2.496316000
N	2.615425000	4.741466000	-3.449291000
N	-1.119102000	3.792307000	-0.588396000
C	3.089281000	5.379825000	-4.661686000
C	1.741603000	3.767209000	-0.836846000
C	0.824996000	4.336190000	-1.904163000
C	1.296965000	4.786204000	-3.086425000
C	3.640589000	6.782107000	-4.464265000
C	3.534904000	4.236864000	-2.521713000
C	3.171958000	3.776511000	-1.321484000
C	3.338989000	7.541747000	-3.333781000
C	4.454308000	7.337865000	-5.455646000
C	-0.642040000	4.399375000	-1.715128000
C	3.837977000	8.837018000	-3.199252000
C	4.949863000	8.631243000	-5.324648000
C	4.642763000	9.386207000	-4.193125000
H	2.253896000	5.410656000	-5.369806000
H	3.861650000	4.747571000	-5.114224000
H	1.453940000	2.738168000	-0.574563000
H	1.652208000	4.339676000	0.101250000
H	0.610822000	5.194206000	-3.823938000
H	4.567232000	4.236900000	-2.860082000
H	3.941949000	3.379540000	-0.663493000
H	2.713821000	7.121299000	-2.549198000
H	4.702233000	6.748572000	-6.337033000
H	3.595947000	9.416800000	-2.311815000
H	5.582445000	9.049270000	-6.103978000
H	5.032416000	10.39543800	-4.086644000
H	-2.123492000	3.710696000	-0.517922000

H -0.574413000 3.096293000 -0.095065000

MECP

Mn 0.161303000 0.166582000 -0.406020000

O 3.454609000 -0.582832000 1.818799000

O 2.955760000 1.917888000 -2.676634000

O -2.844779000 -1.683542000 -2.285616000

O -0.220491000 -3.138089000 1.890959000

N -1.083829000 -0.278097000 -1.781923000

N 1.952467000 0.014201000 0.196043000

N -0.314115000 -1.532129000 0.266400000

N 1.397512000 -1.538811000 1.908615000

N 0.951338000 1.153493000 -1.841261000

C 2.340526000 -0.678238000 1.298698000

C 0.237031000 -2.126949000 1.352271000

C 2.943118000 0.860360000 -0.488920000

C 2.733369000 2.428280000 1.535364000

H 1.933989000 1.800094000 1.916156000

C 4.738541000 4.083821000 0.556795000

H 5.516244000 4.729346000 0.154339000

C 2.284026000 1.382714000 -1.794449000

C -1.902704000 -1.339196000 -1.577190000

C 3.353422000 2.098837000 0.328002000

C 0.138651000 1.321584000 -2.979914000

C -1.021944000 0.512948000 -2.941868000

C 4.132892000 4.387496000 1.773677000

H 4.437143000 5.266995000 2.336125000

C 4.357135000 2.948291000 -0.153166000

H 4.836185000 2.731063000 -1.102508000

C -1.525530000 -2.141383000 -0.305575000

C 0.371454000 2.159248000 -4.069248000

H	1.271257000	2.762661000	-4.097898000
C	-0.067709000	-3.842636000	-1.482072000
H	0.671263000	-3.052830000	-1.606032000
C	-1.255367000	-3.571569000	-0.794096000
C	3.127580000	3.553851000	2.257330000
H	2.640138000	3.779481000	3.203161000
C	-2.190790000	-4.597521000	-0.653292000
H	-3.125220000	-4.420751000	-0.128466000
C	1.847878000	-2.147466000	3.159112000
H	2.429048000	-1.415441000	3.716067000
H	2.473044000	-3.030643000	2.984059000
H	0.974615000	-2.449043000	3.734693000
C	-1.689407000	1.389746000	-5.081894000
H	-2.400944000	1.420230000	-5.903419000
C	-1.934508000	0.546745000	-3.995264000
H	-2.812826000	-0.086754000	-3.957645000
C	-0.550695000	2.187995000	-5.118718000
H	-0.370097000	2.840880000	-5.969336000
C	4.171581000	0.043946000	-0.928169000
H	4.764561000	-0.246471000	-0.061865000
H	4.780637000	0.627214000	-1.620986000
H	3.836202000	-0.859591000	-1.449673000
C	0.184353000	-5.107352000	-2.004204000
H	1.114831000	-5.295581000	-2.534836000
C	-1.939768000	-5.866364000	-1.173705000
H	-2.680238000	-6.653385000	-1.048968000
C	-2.715314000	-2.029383000	0.656161000
H	-2.809290000	-0.989466000	0.988406000
H	-2.560759000	-2.666102000	1.528698000
H	-3.644849000	-2.309519000	0.154150000

C	-0.752629000	-6.127818000	-1.850859000
O	-0.564296000	1.246353000	0.539977000
H	-0.558223000	-7.116806000	-2.257572000
O	-2.803501000	4.192693000	-2.651021000
N	0.734439000	6.096084000	-1.747749000
N	-2.578601000	2.743558000	-0.912047000
C	1.405093000	6.928538000	-2.747961000
C	-0.457273000	4.373147000	0.224500000
C	-0.969556000	4.526241000	-1.174118000
C	-0.357992000	5.349250000	-2.068011000
C	2.827701000	6.481840000	-3.018607000
C	1.229384000	6.074557000	-0.453153000
C	0.682246000	5.295123000	0.496899000
C	3.811358000	7.436545000	-3.282082000
C	3.166494000	5.127672000	-3.036706000
C	-2.186776000	3.804862000	-1.659292000
C	5.114698000	7.041659000	-3.576256000
C	4.469057000	4.733105000	-3.329616000
C	5.446404000	5.688671000	-3.601988000
H	1.396304000	7.965991000	-2.397398000
H	0.807446000	6.880091000	-3.662099000
H	-0.145453000	3.323630000	0.407215000
H	-1.265939000	4.533431000	0.956118000
H	-0.731665000	5.442648000	-3.082548000
H	2.075561000	6.728590000	-0.269527000
H	1.097252000	5.329787000	1.498867000
H	3.555467000	8.494145000	-3.255166000
H	2.422445000	4.365165000	-2.813434000
H	5.873641000	7.793784000	-3.776549000
H	4.704518000	3.671907000	-3.336465000

H	6.464955000	5.381480000	-3.826201000
H	-3.326816000	2.189551000	-1.307666000
H	-1.909340000	2.241400000	-0.322716000

TS (Singlet)

Mn	-0.083715000	0.035247000	0.002897000
O	3.014646000	-1.297840000	2.202974000
O	3.009973000	0.721893000	-2.489863000
O	-3.503466000	-1.231078000	-1.517605000
O	-1.173842000	-2.726271000	2.806787000
N	-1.354581000	-0.408967000	-1.298695000
N	1.606991000	-0.540787000	0.560722000
N	-0.943723000	-1.352757000	0.985390000
N	0.806512000	-1.639520000	2.530786000
N	0.896511000	0.585187000	-1.569233000
C	1.875933000	-1.164400000	1.749010000
C	-0.507682000	-1.949340000	2.115809000
C	2.775062000	-0.069711000	-0.209594000
C	3.073202000	1.690844000	1.639427000
H	2.148383000	1.350216000	2.094912000
C	5.418948000	2.620803000	0.481049000
H	6.334770000	2.978903000	0.015672000
C	2.239528000	0.479155000	-1.555280000
C	-2.454509000	-1.100189000	-0.893283000
C	3.539964000	1.075599000	0.475583000
C	0.139768000	0.657560000	-2.748912000
C	-1.159394000	0.125290000	-2.586291000
C	4.950272000	3.215139000	1.651055000
H	5.497105000	4.035331000	2.109566000
C	4.721262000	1.562970000	-0.098592000
H	5.091420000	1.122649000	-1.019419000

C	-2.261761000	-1.761658000	0.488627000
C	0.540077000	1.145623000	-3.993377000
H	1.549265000	1.519521000	-4.117446000
C	-1.229004000	-3.896286000	-0.400480000
H	-0.334121000	-3.314950000	-0.615038000
C	-2.323093000	-3.272155000	0.209184000
C	3.772745000	2.744002000	2.225570000
H	3.390031000	3.199177000	3.136398000
C	-3.463087000	-4.034195000	0.466233000
H	-4.331645000	-3.579090000	0.933066000
C	1.195062000	-2.176492000	3.832395000
H	1.623536000	-3.181632000	3.749160000
H	0.308875000	-2.226066000	4.461455000
H	1.940443000	-1.520383000	4.279786000
C	-1.647415000	0.627546000	-4.890552000
H	-2.344785000	0.622300000	-5.724800000
C	-2.056732000	0.122709000	-3.654218000
H	-3.049243000	-0.286425000	-3.513479000
C	-0.359968000	1.125908000	-5.061394000
H	-0.047165000	1.508391000	-6.030057000
C	3.710427000	-1.235117000	-0.583570000
H	4.250984000	-1.591749000	0.291696000
H	4.413176000	-0.917296000	-1.355582000
H	3.111841000	-2.057469000	-0.992211000
C	-1.266073000	-5.248510000	-0.726195000
H	-0.402032000	-5.713374000	-1.195265000
C	-3.502367000	-5.390127000	0.142774000
H	-4.398388000	-5.966905000	0.360243000
C	-3.389428000	-1.256064000	1.394878000
H	-3.245174000	-0.185479000	1.578776000

H	-3.373024000	-1.782389000	2.350657000
H	-4.361180000	-1.387764000	0.912254000
C	-2.405083000	-6.004225000	-0.453274000
O	-0.490406000	1.445241000	0.669240000
H	-2.436202000	-7.061482000	-0.704539000
O	-2.125150000	4.134589000	-3.261588000
N	1.872689000	4.070585000	-2.120348000
N	-2.724732000	3.204121000	-1.278665000
C	2.953842000	3.943176000	-3.106843000
C	-0.139937000	3.824237000	-0.164643000
C	-0.442991000	3.904729000	-1.588879000
C	0.571243000	3.988706000	-2.496253000
C	3.978899000	5.048635000	-3.003988000
C	2.182918000	4.236125000	-0.783660000
C	1.228275000	4.195353000	0.169136000
C	3.603364000	6.383476000	-3.182460000
C	5.313277000	4.745950000	-2.734934000
C	-1.821986000	3.763826000	-2.129543000
C	4.550341000	7.398031000	-3.094391000
C	6.265335000	5.761575000	-2.650573000
C	5.884760000	7.088129000	-2.829035000
H	2.481265000	3.949486000	-4.093096000
H	3.420516000	2.960300000	-2.965271000
H	-0.242995000	2.569916000	0.195851000
H	-0.913738000	4.196374000	0.514210000
H	0.369822000	3.985644000	-3.562195000
H	3.229266000	4.421831000	-0.563176000
H	1.507562000	4.367370000	1.202873000
H	2.562253000	6.625283000	-3.389601000
H	5.607532000	3.707946000	-2.590403000

H	4.249514000	8.433106000	-3.235398000
H	7.302947000	5.514063000	-2.441167000
H	6.624483000	7.881794000	-2.760858000
H	-3.634373000	2.980143000	-1.656741000
H	-2.427032000	2.686064000	-0.463592000

TS (Triplet)

Mn	0.221333000	0.218628000	-0.443673000
O	3.471820000	-0.584118000	1.846841000
O	3.056868000	1.867851000	-2.720196000
O	-2.896890000	-1.529123000	-2.258293000
O	-0.270302000	-3.026036000	1.941660000
N	-1.083067000	-0.175167000	-1.798188000
N	2.001572000	0.069841000	0.213643000
N	-0.353907000	-1.430756000	0.304181000
N	1.367639000	-1.440865000	1.939607000
N	1.016099000	1.225638000	-1.870366000
C	2.356210000	-0.627782000	1.320455000
C	0.191421000	-2.022626000	1.389821000
C	3.002304000	0.887934000	-0.491900000
C	2.885792000	2.439814000	1.554912000
H	2.119861000	1.798729000	1.978407000
C	4.802444000	4.135359000	0.474201000
H	5.544751000	4.797165000	0.033011000
C	2.356553000	1.394190000	-1.822930000
C	-1.931955000	-1.203683000	-1.568706000
C	3.433356000	2.132159000	0.307457000
C	0.196825000	1.387292000	-3.008929000
C	-0.990488000	0.610580000	-2.959354000
C	4.266376000	4.418619000	1.728827000
H	4.591370000	5.296807000	2.281421000

C	4.396053000	3.000310000	-0.222635000
H	4.816953000	2.797172000	-1.202300000
C	-1.562972000	-2.021484000	-0.293800000
C	0.445613000	2.204045000	-4.110092000
H	1.364778000	2.777069000	-4.151698000
C	-0.095445000	-3.706074000	-1.483513000
H	0.633162000	-2.907105000	-1.608222000
C	-1.286058000	-3.447064000	-0.795106000
C	3.306875000	3.563743000	2.264450000
H	2.873807000	3.773047000	3.240239000
C	-2.208021000	-4.484020000	-0.652100000
H	-3.143545000	-4.315667000	-0.126824000
C	1.790613000	-2.031817000	3.207848000
H	2.387871000	-1.303264000	3.753347000
H	2.394135000	-2.935104000	3.061621000
H	0.904920000	-2.297742000	3.781858000
C	-1.642548000	1.492396000	-5.106602000
H	-2.357417000	1.535509000	-5.924860000
C	-1.905529000	0.667962000	-4.009551000
H	-2.802803000	0.062231000	-3.959146000
C	-0.479991000	2.253594000	-5.156557000
H	-0.281355000	2.891236000	-6.014548000
C	4.224996000	0.050303000	-0.904934000
H	4.797302000	-0.242481000	-0.025502000
H	4.854301000	0.620818000	-1.590420000
H	3.886819000	-0.852452000	-1.426455000
C	0.173046000	-4.969390000	-2.000638000
H	1.106741000	-5.148176000	-2.528887000
C	-1.940870000	-5.752328000	-1.167104000
H	-2.670711000	-6.548065000	-1.036890000

C	-2.762605000	-1.926355000	0.655582000
H	-2.867081000	-0.889978000	0.995150000
H	-2.613307000	-2.568261000	1.525481000
H	-3.683881000	-2.207334000	0.138835000
C	-0.750269000	-6.001830000	-1.842541000
O	-0.538802000	1.414137000	0.479255000
H	-0.542350000	-6.990884000	-2.243153000
O	-2.968609000	4.173910000	-2.596636000
N	0.720382000	5.813929000	-1.711951000
N	-2.726616000	2.604710000	-0.959244000
C	1.365128000	6.738573000	-2.655272000
C	-0.533038000	4.097221000	0.169650000
C	-1.071211000	4.342377000	-1.174058000
C	-0.421906000	5.159203000	-2.053281000
C	2.801176000	6.371439000	-2.959491000
C	1.240390000	5.693540000	-0.441488000
C	0.642127000	4.907664000	0.484477000
C	3.731949000	7.387639000	-3.182399000
C	3.204292000	5.039855000	-3.062099000
C	-2.338836000	3.696317000	-1.654843000
C	5.046600000	7.075594000	-3.520349000
C	4.519102000	4.727767000	-3.397677000
C	5.443386000	5.744184000	-3.629941000
H	1.313632000	7.744011000	-2.225978000
H	0.765290000	6.735011000	-3.568687000
H	-0.281107000	2.930987000	0.252595000
H	-1.298165000	4.123654000	0.959458000
H	-0.805791000	5.329861000	-3.053378000
H	2.128513000	6.281895000	-0.238430000
H	1.060761000	4.874720000	1.484315000

H	3.425245000	8.427662000	-3.090195000
H	2.505326000	4.229001000	-2.869480000
H	5.763570000	7.874806000	-3.690503000
H	4.806359000	3.681804000	-3.469465000
H	6.470316000	5.500797000	-3.890511000
H	-3.51113700	2.094644000	-1.342501000
H	-2.046603000	2.075809000	-0.398116000

P-1

Mn	0.168755000	-0.023677000	-0.047742000
O	2.058995000	-2.230397000	2.799490000
O	3.833043000	-0.320659000	-1.694943000
O	-3.079694000	0.025820000	-2.395809000
O	-2.378880000	-2.296184000	2.189589000
N	-0.892992000	0.147194000	-1.637970000
N	1.451329000	-1.060612000	0.918464000
N	-1.341676000	-0.995489000	0.609503000
N	-0.162131000	-1.839013000	2.488037000
N	1.622910000	0.234529000	-1.295788000
C	1.197050000	-1.729242000	2.065335000
C	-1.374593000	-1.729005000	1.738447000
C	2.834688000	-0.992223000	0.422274000
C	3.209056000	0.736005000	2.273043000
H	2.133302000	0.764103000	2.421828000
C	5.959193000	0.676766000	1.907471000
H	7.035631000	0.646032000	1.754173000
C	2.819390000	-0.304075000	-0.990015000
C	-2.199657000	-0.180425000	-1.555992000
C	3.743244000	-0.127196000	1.311346000
C	1.213801000	0.694120000	-2.560516000
C	-0.203268000	0.662095000	-2.746773000

C	5.414613000	1.526308000	2.867404000
H	6.059600000	2.159984000	3.471236000
C	5.132174000	-0.137163000	1.136586000
H	5.575361000	-0.776994000	0.379930000
C	-2.553570000	-0.920228000	-0.220621000
C	2.033893000	1.143411000	-3.594114000
H	3.108485000	1.139666000	-3.447408000
C	-2.085507000	-3.237797000	-1.124166000
H	-1.030870000	-2.968179000	-1.118796000
C	-3.029434000	-2.314429000	-0.659025000
C	4.033534000	1.553694000	3.043332000
H	3.591582000	2.211627000	3.788405000
C	-4.375569000	-2.681496000	-0.681348000
H	-5.135928000	-1.989124000	-0.331627000
C	-0.326044000	-2.466194000	3.796629000
H	-0.277883000	-3.560968000	3.743514000
H	-1.298013000	-2.186631000	4.199171000
H	0.469259000	-2.122623000	4.456274000
C	0.088507000	1.539865000	-4.980895000
H	-0.346114000	1.867233000	-5.923100000
C	-0.751512000	1.089948000	-3.955415000
H	-1.828009000	1.054306000	-4.080706000
C	1.467351000	1.562830000	-4.803738000
H	2.115437000	1.904474000	-5.608276000
C	3.421617000	-2.396150000	0.198211000
H	3.602652000	-2.890544000	1.152886000
H	4.345795000	-2.339206000	-0.379745000
H	2.704204000	-2.993587000	-0.376697000
C	-2.472235000	-4.492797000	-1.583430000
H	-1.718846000	-5.193002000	-1.937226000

C	-4.767641000	-3.939670000	-1.138468000
H	-5.822574000	-4.204720000	-1.139190000
C	-3.646173000	-0.098358000	0.471941000
H	-3.222757000	0.862738000	0.786937000
H	-4.011201000	-0.623584000	1.357437000
H	-4.475853000	0.104634000	-0.210575000
C	-3.819388000	-4.851935000	-1.590892000
O	0.128628000	1.686265000	0.715877000
H	-4.125308000	-5.832518000	-1.947223000
O	-2.404721000	4.249136000	-2.540326000
N	1.537762000	4.767141000	-3.582880000
N	-1.821733000	3.216205000	-0.589948000
C	1.906670000	5.063110000	-4.993854000
C	0.857953000	4.317700000	-0.965565000
C	-0.105969000	4.215713000	-1.965734000
C	0.267015000	4.466733000	-3.274628000
C	1.981581000	6.551795000	-5.232569000
C	2.489438000	4.844793000	-2.629459000
C	2.171353000	4.631511000	-1.306438000
C	0.811078000	7.291596000	-5.418583000
C	3.216271000	7.201389000	-5.251768000
C	-1.560961000	3.885048000	-1.725422000
C	0.875664000	8.667249000	-5.614803000
C	3.281310000	8.578902000	-5.450860000
C	2.111685000	9.312471000	-5.630405000
H	1.149391000	4.590054000	-5.621075000
H	2.867876000	4.579267000	-5.178256000
H	0.587957000	4.167920000	0.075038000
H	-0.449650000	4.429085000	-4.087455000
H	3.490172000	5.090303000	-2.968561000

H	2.946437000	4.714188000	-0.553274000
H	-0.152850000	6.786112000	-5.411626000
H	4.129470000	6.625515000	-5.116037000
H	-0.038715000	9.236368000	-5.760511000
H	4.246807000	9.077624000	-5.467557000
H	2.161864000	10.38693800	-5.787018000
H	-2.781446000	2.921434000	-0.464299000
H	-1.087931000	2.685330000	-0.088539000
H	1.027054000	2.037043000	0.709386000

P-2

Mn	-0.04211100	0.009477000	-0.206985000
O	3.089599000	-0.993507000	2.204635000
O	3.002857000	1.469909000	-2.379649000
O	-3.199475000	-1.579168000	-2.132547000
O	-0.748883000	-3.291001000	2.093623000
N	-1.356130000	-0.285337000	-1.585074000
N	1.713221000	-0.240029000	0.522129000
N	-0.747260000	-1.610953000	0.529932000
N	0.954279000	-1.774940000	2.177158000
N	0.889949000	0.915186000	-1.629903000
C	1.998821000	-0.977848000	1.617869000
C	-0.243152000	-2.281934000	1.583435000
C	2.775431000	0.540382000	-0.132681000
C	2.612893000	2.097264000	1.913001000
H	1.875859000	1.428425000	2.346360000
C	4.522485000	3.815315000	0.860097000
H	5.268022000	4.482276000	0.431355000
C	2.224055000	1.039488000	-1.517845000
C	-2.246298000	-1.285526000	-1.406201000
C	3.177598000	1.794546000	0.670484000

C	0.123567000	1.110874000	-2.795984000
C	-1.141610000	0.449468000	-2.763877000
C	3.961616000	4.096425000	2.104815000
H	4.267254000	4.979245000	2.661241000
C	4.138456000	2.676101000	0.157374000
H	4.575064000	2.475448000	-0.815678000
C	-1.951858000	-2.141394000	-0.127324000
C	0.481859000	1.854274000	-3.920002000
H	1.456644000	2.328835000	-3.948321000
C	-0.519547000	-3.848586000	-1.327542000
H	0.236836000	-3.070817000	-1.416613000
C	-1.715396000	-3.565307000	-0.656930000
C	3.003266000	3.231286000	2.625547000
H	2.554731000	3.433926000	3.595638000
C	-2.669422000	-4.578646000	-0.557369000
H	-3.610048000	-4.394290000	-0.046438000
C	1.316175000	-2.425781000	3.433562000
H	1.904942000	-3.338179000	3.277011000
H	0.404079000	-2.695007000	3.963010000
H	1.910694000	-1.736834000	4.031656000
C	-1.628747000	1.309891000	-4.971244000
H	-2.308802000	1.387879000	-5.816576000
C	-2.005198000	0.558212000	-3.852780000
H	-2.956743000	0.039680000	-3.815986000
C	-0.397288000	1.951904000	-5.005130000
H	-0.106962000	2.532308000	-5.878019000
C	4.018277000	-0.308969000	-0.453608000
H	4.535675000	-0.589337000	0.462891000
H	4.688676000	0.245433000	-1.113371000
H	3.708469000	-1.221584000	-0.976639000

C	-0.279089000	-5.106931000	-1.870190000
H	0.659415000	-5.301866000	-2.384370000
C	-2.431163000	-5.842952000	-1.096325000
H	-3.187521000	-6.618527000	-0.998366000
C	-3.182436000	-2.028938000	0.779231000
H	-3.264095000	-0.997465000	1.140741000
H	-3.083587000	-2.694008000	1.639689000
H	-4.096178000	-2.266454000	0.227518000
C	-1.235865000	-6.114427000	-1.754987000
O	-0.741606000	1.433779000	0.755535000
H	-1.050367000	-7.099896000	-2.175176000
O	-2.469148000	4.378273000	-2.688012000
N	1.303152000	5.785450000	-1.831777000
N	-2.395761000	2.933654000	-0.920359000
C	2.117155000	6.470828000	-2.866796000
C	-0.203282000	4.569490000	0.111948000
C	-0.621990000	4.543478000	-1.215639000
C	0.156570000	5.174739000	-2.170632000
C	3.501225000	5.879789000	-2.996258000
C	1.728493000	5.811317000	-0.549926000
C	0.985201000	5.215560000	0.443977000
C	4.594091000	6.731321000	-3.162151000
C	3.699762000	4.498088000	-2.991431000
C	-1.919906000	3.928974000	-1.685859000
C	5.872749000	6.206453000	-3.337079000
C	4.978403000	3.975136000	-3.160824000
C	6.067349000	4.827100000	-3.337224000
H	2.166840000	7.526853000	-2.591812000
H	1.562387000	6.387565000	-3.803581000
H	-0.017378000	1.870558000	1.219703000

H	-0.807006000	4.109989000	0.888692000
H	-0.133557000	5.202626000	-3.215426000
H	2.664037000	6.327508000	-0.362553000
H	1.337495000	5.258825000	1.467739000
H	4.442871000	7.808752000	-3.154456000
H	2.871457000	3.808834000	-2.837741000
H	6.717936000	6.877859000	-3.464874000
H	5.106965000	2.895751000	-3.147484000
H	7.065670000	4.417663000	-3.468996000
H	-3.220029000	2.464006000	-1.271016000
H	-1.784590000	2.408198000	-0.271356000

P-3

Mn	-0.690836000	0.258005000	-0.448243000
O	2.351492000	-0.700868000	2.103216000
O	2.487770000	1.220519000	-2.743814000
O	-3.901933000	-1.458996000	-2.174147000
O	-1.696597000	-2.472833000	2.420261000
N	-2.011875000	-0.182938000	-1.796229000
N	1.046347000	0.005943000	0.354591000
N	-1.548067000	-1.148894000	0.555771000
N	0.109705000	-1.084955000	2.252152000
N	0.346533000	0.767857000	-2.015581000
C	1.251808000	-0.592295000	1.547676000
C	-1.111702000	-1.623873000	1.736144000
C	2.198022000	0.426225000	-0.460556000
C	2.484435000	2.289778000	1.276151000
H	1.541909000	1.985352000	1.721293000
C	4.896366000	3.090013000	0.161244000
H	5.842263000	3.392727000	-0.283221000
C	1.680436000	0.874647000	-1.872696000

C	-2.958879000	-1.093326000	-1.471575000
C	2.970793000	1.601486000	0.161688000
C	-0.384903000	0.794722000	-3.220162000
C	-1.709233000	0.282740000	-3.091456000
C	4.404446000	3.759247000	1.280347000
H	4.961294000	4.584049000	1.718209000
C	4.187333000	2.024597000	-0.390700000
H	4.582272000	1.523133000	-1.268295000
C	-2.751446000	-1.731146000	-0.056116000
C	0.069274000	1.225434000	-4.465916000
H	1.089783000	1.580144000	-4.556991000
C	-1.330021000	-3.691035000	-0.805526000
H	-0.507752000	-2.986443000	-0.915973000
C	-2.564439000	-3.232526000	-0.330835000
C	3.192912000	3.353040000	1.833267000
H	2.793801000	3.863115000	2.707289000
C	-3.603943000	-4.154653000	-0.198445000
H	-4.576708000	-3.833383000	0.162054000
C	0.397151000	-1.487370000	3.626435000
H	0.856030000	-2.481471000	3.686049000
H	-0.536113000	-1.506495000	4.187236000
H	1.083870000	-0.766895000	4.068892000
C	-2.082215000	0.702910000	-5.441621000
H	-2.743939000	0.673600000	-6.304119000
C	-2.548331000	0.249588000	-4.202870000
H	-3.549932000	-0.148885000	-4.089512000
C	-0.784195000	1.178556000	-5.574045000
H	-0.422910000	1.520715000	-6.541025000
C	3.133033000	-0.765700000	-0.747449000
H	3.609049000	-1.099123000	0.174997000

H	3.893310000	-0.494610000	-1.482569000
H	2.542055000	-1.591852000	-1.160141000
C	-1.136032000	-5.031348000	-1.125263000
H	-0.166380000	-5.363434000	-1.489208000
C	-3.411961000	-5.499606000	-0.513602000
H	-4.234840000	-6.200749000	-0.394214000
C	-4.006207000	-1.416779000	0.766621000
H	-4.042149000	-0.338908000	0.960723000
H	-3.975526000	-1.943387000	1.722425000
H	-4.909920000	-1.691404000	0.216339000
C	-2.178304000	-5.945156000	-0.978348000
O	-1.412939000	2.012509000	0.312099000
H	-2.029063000	-6.993662000	-1.224162000
O	-2.216263000	4.340368000	-3.695900000
N	1.828003000	4.455447000	-2.624348000
N	-2.644621000	3.421985000	-1.639316000
C	2.931867000	4.211751000	-3.595309000
C	-0.181338000	4.725917000	-0.775421000
C	-0.476251000	4.336123000	-2.079461000
C	0.555591000	4.233701000	-2.993817000
C	3.906272000	5.359891000	-3.652137000
C	2.131414000	4.830525000	-1.364820000
C	1.137759000	4.994864000	-0.424418000
C	3.506845000	6.599631000	-4.160139000
C	5.216162000	5.191063000	-3.203979000
C	-1.875096000	4.026271000	-2.557928000
C	4.407853000	7.657023000	-4.214773000
C	6.121763000	6.249398000	-3.264110000
C	5.717819000	7.482288000	-3.767414000
H	2.455104000	4.049120000	-4.563968000

H	3.407436000	3.277973000	-3.283976000
H	-0.976616000	4.832533000	-0.044062000
H	0.381181000	3.953621000	-4.026347000
H	3.181915000	4.986971000	-1.145159000
H	1.404936000	5.311356000	0.576872000
H	2.485705000	6.733173000	-4.512944000
H	5.527178000	4.225939000	-2.808421000
H	4.090894000	8.618286000	-4.610735000
H	7.141412000	6.108924000	-2.915095000
H	6.422142000	8.308971000	-3.813214000
H	-3.565108000	3.140424000	-1.950750000
H	-2.206663000	2.922383000	-0.823246000
H	-0.770908000	2.463656000	0.869305000

Water:

Mn-oxo

Mn	0.014543000	-0.036411000	-0.013858000
O	1.038545000	-0.619193000	3.818798000
O	3.959843000	0.478293000	-0.230799000
O	-1.693597000	-1.957955000	-3.056277000
O	-2.589566000	-2.392005000	1.945499000
N	-0.289474000	-0.680821000	-1.751241000
N	0.988058000	-0.397511000	1.543446000
N	-1.208596000	-1.374766000	0.435141000
N	-0.903637000	-1.121211000	2.768446000
N	1.728037000	0.222873000	-0.731513000
C	0.432062000	-0.706346000	2.745585000
C	-1.613371000	-1.675896000	1.696652000
C	2.411546000	-0.023634000	1.556770000
C	1.679470000	2.227214000	2.511117000
H	0.674050000	2.027733000	2.150740000

C	4.234728000	2.764072000	3.455340000
H	5.238273000	2.963801000	3.822060000
C	2.794819000	0.262877000	0.101051000
C	-1.316408000	-1.536509000	-1.963310000
C	2.686018000	1.272497000	2.334021000
C	1.798402000	0.263911000	-2.140037000
C	0.635033000	-0.257694000	-2.727917000
C	3.225775000	3.705952000	3.631987000
H	3.433797000	4.645186000	4.137492000
C	3.968583000	1.559041000	2.808331000
H	4.773537000	0.841562000	2.682147000
C	-2.007554000	-1.947138000	-0.660755000
C	2.838903000	0.738861000	-2.933203000
H	3.733876000	1.141489000	-2.477062000
C	-0.814046000	-4.148713000	-0.275567000
H	0.059560000	-3.576454000	0.028557000
C	-1.990155000	-3.480688000	-0.630908000
C	1.946054000	3.431441000	3.156320000
H	1.147223000	4.156749000	3.288229000
C	-3.097463000	-4.233930000	-1.020728000
H	-4.023271000	-3.743336000	-1.305415000
C	-1.468524000	-1.364758000	4.096175000
H	-1.184346000	-2.348107000	4.482885000
H	-2.552828000	-1.308696000	4.029174000
H	-1.105027000	-0.597379000	4.776190000
C	1.552359000	0.162327000	-4.903142000
H	1.458912000	0.126557000	-5.985013000
C	0.504711000	-0.311703000	-4.112718000
H	-0.393315000	-0.716276000	-4.560986000
C	2.704182000	0.681722000	-4.320925000

H	3.510585000	1.051988000	-4.947849000
C	3.288339000	-1.203879000	2.005384000
H	3.200091000	-1.372858000	3.078235000
H	4.333578000	-1.016055000	1.753520000
H	2.971400000	-2.106596000	1.473819000
C	-0.751809000	-5.538175000	-0.294589000
H	0.169748000	-6.039293000	-0.009819000
C	-3.036025000	-5.626640000	-1.039020000
H	-3.911662000	-6.196877000	-1.338330000
C	-3.413629000	-1.331684000	-0.713153000
H	-3.326983000	-0.240901000	-0.673101000
H	-4.020098000	-1.669900000	0.127428000
H	-3.911186000	-1.596891000	-1.649068000
C	-1.865365000	-6.284340000	-0.675519000
O	-0.660787000	1.309938000	0.120464000
H	-1.819423000	-7.370009000	-0.688342000

BNAH

O	0.022051000	0.019806000	-0.036542000
N	-2.580565000	3.204868000	-0.473211000
N	1.274667000	1.118877000	1.483083000
C	-3.876434000	2.926523000	-1.094029000
C	-0.377296000	3.457480000	1.431757000
C	-0.652097000	2.233272000	0.580842000
C	-1.698144000	2.177415000	-0.270596000
C	-4.897434000	2.383553000	-0.117091000
C	-2.470939000	4.321312000	0.371281000
C	-1.475984000	4.473863000	1.245679000
C	-4.894160000	1.029199000	0.227244000
C	-5.827077000	3.232628000	0.485077000
C	0.221966000	1.047029000	0.639444000

C	-5.801010000	0.534026000	1.159233000
C	-6.737125000	2.739690000	1.417887000
C	-6.724481000	1.389659000	1.757441000
H	-3.705276000	2.211709000	-1.903393000
H	-4.240163000	3.856399000	-1.540411000
H	0.597502000	3.902868000	1.176571000
H	-0.300190000	3.184898000	2.495510000
H	-1.871202000	1.285264000	-0.865643000
H	-3.251480000	5.065040000	0.241497000
H	-1.447266000	5.379067000	1.844745000
H	-4.177749000	0.357893000	-0.242806000
H	-5.841044000	4.287198000	0.216663000
H	-5.790968000	-0.521906000	1.416055000
H	-7.457903000	3.410802000	1.877395000
H	-7.434781000	1.002997000	2.483300000
H	1.892725000	0.324428000	1.545312000
H	1.476739000	1.935594000	2.036703000

R (Singlet)

Mn	0.010193000	-0.062705000	-0.004723000
O	2.843142000	-1.556381000	2.434501000
O	3.264391000	0.779733000	-2.091068000
O	-3.340209000	-1.170723000	-1.836309000
O	-1.446618000	-2.758421000	2.610956000
N	-1.253491000	-0.313201000	-1.368592000
N	1.609784000	-0.742584000	0.690441000
N	-0.962460000	-1.427204000	0.820565000
N	0.596096000	-1.778695000	2.568084000
N	1.095673000	0.293818000	-1.488929000
C	1.749351000	-1.363436000	1.892687000
C	-0.659389000	-2.024971000	2.002134000

C	2.852669000	-0.298058000	0.036079000
C	2.947442000	1.528584000	1.823927000
H	1.900983000	1.339305000	2.046688000
C	5.624012000	2.038211000	1.290367000
H	6.672064000	2.228113000	1.073675000
C	2.435900000	0.336575000	-1.297214000
C	-2.364709000	-1.037898000	-1.098071000
C	3.601844000	0.771687000	0.846189000
C	0.428475000	0.584805000	-2.696398000
C	-0.932590000	0.249277000	-2.620857000
C	4.968193000	2.775205000	2.272022000
H	5.498591000	3.542413000	2.829714000
C	4.945956000	1.048524000	0.581117000
H	5.481685000	0.486792000	-0.177789000
C	-2.298392000	-1.715189000	0.272913000
C	0.962078000	1.103020000	-3.874308000
H	2.013500000	1.350118000	-3.933995000
C	-1.417182000	-3.970175000	-0.478797000
H	-0.442470000	-3.504185000	-0.605451000
C	-2.489502000	-3.214096000	0.005281000
C	3.623914000	2.518041000	2.532135000
H	3.096699000	3.085978000	3.294426000
C	-3.730827000	-3.831837000	0.156928000
H	-4.582728000	-3.269650000	0.527110000
C	0.817077000	-2.355467000	3.895400000
H	1.130674000	-3.401962000	3.833998000
H	-0.110294000	-2.294950000	4.460223000
H	1.590767000	-1.782538000	4.401832000
C	-1.241532000	1.003580000	-4.876173000
H	-1.893798000	1.180193000	-5.726946000

C	-1.777982000	0.466076000	-3.706095000
H	-2.828097000	0.214429000	-3.637951000
C	0.113140000	1.310395000	-4.961278000
H	0.520205000	1.724592000	-5.879705000
C	3.739646000	-1.496339000	-0.349116000
H	4.214331000	-1.929193000	0.530400000
H	4.507595000	-1.186226000	-1.060215000
H	3.120655000	-2.258153000	-0.833489000
C	-1.578880000	-5.316669000	-0.788620000
H	-0.731783000	-5.888690000	-1.158385000
C	-3.893220000	-5.181409000	-0.152733000
H	-4.866533000	-5.647109000	-0.021222000
C	-3.404153000	-1.079200000	1.126652000
H	-3.152904000	-0.029424000	1.310757000
H	-3.502234000	-1.593450000	2.083222000
H	-4.359595000	-1.109959000	0.597649000
C	-2.819687000	-5.929352000	-0.625336000
O	-0.299620000	1.239307000	0.701671000
H	-2.947293000	-6.981603000	-0.865006000
O	-0.931304000	4.163503000	-3.420143000
N	3.186196000	4.470458000	-3.198362000
N	-1.118026000	3.675251000	-1.222862000
C	3.889079000	5.069851000	-4.318729000
C	1.699690000	3.895391000	-0.747971000
C	1.074205000	4.112283000	-2.112313000
C	1.821522000	4.385974000	-3.204724000
C	4.026328000	6.580551000	-4.251791000
C	3.838825000	4.359648000	-1.961021000
C	3.193541000	4.092922000	-0.824099000
C	3.339709000	7.352536000	-3.315223000

C	4.858861000	7.219225000	-5.176093000
C	-0.378603000	3.980957000	-2.319708000
C	3.480991000	8.740580000	-3.305215000
C	4.997838000	8.602516000	-5.168867000
C	4.307533000	9.369558000	-4.230307000
H	3.357906000	4.791126000	-5.235030000
H	4.884089000	4.617080000	-4.383315000
H	1.478538000	2.883591000	-0.370733000
H	1.265936000	4.580591000	-0.002951000
H	1.345853000	4.536167000	-4.170202000
H	4.915614000	4.494708000	-2.003702000
H	3.771923000	4.001345000	0.091304000
H	2.690921000	6.875640000	-2.584366000
H	5.401758000	6.622768000	-5.907315000
H	2.940749000	9.329510000	-2.568404000
H	5.648444000	9.084169000	-5.894335000
H	4.416830000	10.450744000	-4.220935000
H	-2.092611000	3.457565000	-1.373598000
H	-0.688682000	3.324168000	-0.379603000

R (Triplet)

Mn	0.028668000	-0.214415000	-0.020929000
O	2.738279000	-1.513774000	2.585841000
O	3.364215000	0.386311000	-2.148497000
O	-3.253822000	-1.387589000	-1.917328000
O	-1.566400000	-2.639174000	2.802899000
N	-1.199246000	-0.488204000	-1.412986000
N	1.593895000	-0.875867000	0.718720000
N	-1.068430000	-1.443362000	0.919520000
N	0.478289000	-1.641753000	2.689168000
N	1.161881000	0.231152000	-1.496884000

C	1.664052000	-1.350744000	2.003841000
C	-0.788937000	-1.944906000	2.138372000
C	2.859968000	-0.479683000	0.058256000
C	2.911688000	1.514538000	1.658459000
H	1.845909000	1.387401000	1.827712000
C	5.635263000	1.877213000	1.259029000
H	6.701852000	2.008698000	1.096472000
C	2.492576000	0.106215000	-1.323851000
C	-2.324058000	-1.203996000	-1.136543000
C	3.600029000	0.632746000	0.817571000
C	0.487433000	0.514840000	-2.698738000
C	-0.863233000	0.120862000	-2.647009000
C	4.944665000	2.742096000	2.102531000
H	5.465825000	3.552501000	2.604977000
C	4.968112000	0.834387000	0.618384000
H	5.531447000	0.174589000	-0.034087000
C	-2.348122000	-1.790848000	0.286819000
C	1.004769000	1.111012000	-3.844758000
H	2.046161000	1.406029000	-3.877899000
C	-1.390867000	-4.084296000	-0.221818000
H	-0.413035000	-3.616400000	-0.310282000
C	-2.504260000	-3.308638000	0.117183000
C	3.577459000	2.557225000	2.296480000
H	3.023037000	3.224871000	2.951008000
C	-3.747959000	-3.931240000	0.223044000
H	-4.630966000	-3.355250000	0.481972000
C	0.661571000	-2.048465000	4.084713000
H	0.978442000	-3.092504000	4.164514000
H	-0.283078000	-1.921591000	4.608246000
H	1.417832000	-1.412046000	4.540192000

C	-1.185811000	0.970633000	-4.866507000
H	-1.840173000	1.160792000	-5.712613000
C	-1.708670000	0.357068000	-3.727198000
H	-2.749347000	0.063955000	-3.680561000
C	0.155396000	1.336555000	-4.927952000
H	0.548839000	1.812406000	-5.822042000
C	3.724921000	-1.718729000	-0.213806000
H	4.154057000	-2.104630000	0.710694000
H	4.526871000	-1.472963000	-0.911992000
H	3.104943000	-2.494420000	-0.673335000
C	-1.516398000	-5.452865000	-0.436188000
H	-0.638273000	-6.039265000	-0.693916000
C	-3.874084000	-5.303161000	0.009269000
H	-4.850357000	-5.771588000	0.103147000
C	-3.520647000	-1.118376000	1.013902000
H	-3.302902000	-0.052087000	1.131635000
H	-3.665083000	-1.561699000	2.000250000
H	-4.441659000	-1.214791000	0.434584000
C	-2.760736000	-6.069178000	-0.320099000
O	-0.299977000	1.194400000	0.634832000
H	-2.860065000	-7.138660000	-0.485197000
O	-0.951252000	4.334262000	-3.464956000
N	3.166696000	4.672509000	-3.491316000
N	-0.977658000	3.498381000	-1.365994000
C	3.791528000	5.428640000	-4.561567000
C	1.865639000	3.729931000	-1.049896000
C	1.141201000	4.133285000	-2.319932000
C	1.804988000	4.578890000	-3.409560000
C	3.963706000	6.910431000	-4.279698000
C	3.912427000	4.362204000	-2.343822000

C	3.354101000	3.913593000	-1.218091000
C	3.336510000	7.543054000	-3.206938000
C	4.764138000	7.668667000	-5.139555000
C	-0.320091000	3.994512000	-2.446837000
C	3.503804000	8.912470000	-2.999550000
C	4.928900000	9.034103000	-4.935618000
C	4.297696000	9.661722000	-3.861718000
H	3.184833000	5.295698000	-5.463654000
H	4.769354000	4.982899000	-4.772857000
H	1.651148000	2.681537000	-0.793581000
H	1.506905000	4.314689000	-0.187817000
H	1.260064000	4.863283000	-4.305605000
H	4.985124000	4.493017000	-2.453001000
H	4.001161000	3.666901000	-0.379996000
H	2.714064000	6.969565000	-2.524066000
H	5.261693000	7.180309000	-5.975624000
H	3.009881000	9.392346000	-2.158543000
H	5.554036000	9.610305000	-5.612967000
H	4.427491000	10.728293000	-3.698613000
H	-1.948735000	3.258633000	-1.510018000
H	-0.488895000	2.982581000	-0.645469000

MECP

Mn	-0.021801000	0.023695000	-0.287386000
O	3.166625000	-0.797157000	2.036708000
O	2.904213000	1.416336000	-2.621413000
O	-3.020962000	-1.800415000	-2.212574000
O	-0.617869000	-3.174600000	2.106527000
N	-1.290809000	-0.382176000	-1.649374000
N	1.747170000	-0.245358000	0.325569000
N	-0.592848000	-1.627693000	0.424160000

N	1.066344000	-1.648393000	2.114734000
N	0.844782000	0.877699000	-1.747745000
C	2.061020000	-0.875449000	1.483714000
C	-0.096733000	-2.201682000	1.542812000
C	2.797650000	0.521946000	-0.365720000
C	2.560349000	2.210895000	1.557452000
H	1.725122000	1.636420000	1.946128000
C	4.669978000	3.732688000	0.581347000
H	5.489021000	4.325729000	0.180448000
C	2.190188000	0.996752000	-1.706712000
C	-2.115617000	-1.434093000	-1.457904000
C	3.220518000	1.791143000	0.398991000
C	0.040774000	1.090268000	-2.888559000
C	-1.177431000	0.381851000	-2.828572000
C	4.023698000	4.125897000	1.750064000
H	4.335586000	5.024798000	2.275543000
C	4.276417000	2.573308000	-0.082823000
H	4.797953000	2.285750000	-0.990558000
C	-1.832635000	-2.185159000	-0.140347000
C	0.328293000	1.898356000	-3.985996000
H	1.264959000	2.440814000	-4.028038000
C	-0.463291000	-4.107033000	-1.062378000
H	0.368112000	-3.412219000	-1.157703000
C	-1.672023000	-3.663353000	-0.517272000
C	2.966325000	3.359996000	2.232432000
H	2.444625000	3.658804000	3.138475000
C	-2.725388000	-4.570402000	-0.399950000
H	-3.676140000	-4.256498000	0.020006000
C	1.453848000	-2.220920000	3.405394000
H	2.045899000	-3.133660000	3.284992000

H	0.552753000	-2.457672000	3.966521000
H	2.043533000	-1.488778000	3.953106000
C	-1.805399000	1.301705000	-4.959393000
H	-2.526480000	1.389896000	-5.767672000
C	-2.102888000	0.488449000	-3.864314000
H	-3.035787000	-0.059062000	-3.815101000
C	-0.602289000	1.996882000	-5.021510000
H	-0.381915000	2.629906000	-5.876721000
C	4.003782000	-0.362504000	-0.721808000
H	4.580609000	-0.610870000	0.167509000
H	4.646495000	0.151206000	-1.438298000
H	3.649212000	-1.287494000	-1.188142000
C	-0.307479000	-5.428174000	-1.469754000
H	0.642442000	-5.753972000	-1.885631000
C	-2.570672000	-5.894877000	-0.807379000
H	-3.401859000	-6.587128000	-0.701992000
C	-3.030206000	-1.899413000	0.777758000
H	-3.031377000	-0.835589000	1.037280000
H	-2.965185000	-2.486464000	1.695068000
H	-3.970175000	-2.124092000	0.267693000
C	-1.362816000	-6.329525000	-1.343864000
O	-0.663073000	1.157594000	0.621512000
H	-1.243973000	-7.362184000	-1.661554000
O	-2.272356000	4.068592000	-3.008739000
N	1.280945000	5.781372000	-1.785886000
N	-2.503180000	2.936416000	-1.056335000
C	2.168447000	6.431872000	-2.758225000
C	-0.371913000	4.456601000	0.171997000
C	-0.651742000	4.464384000	-1.304731000
C	0.171891000	5.098829000	-2.181413000

C	3.560441000	5.840626000	-2.755507000
C	1.586958000	5.872457000	-0.433939000
C	0.826075000	5.286498000	0.503648000
C	4.637816000	6.564968000	-2.244390000
C	3.777279000	4.557918000	-3.264459000
C	-1.855315000	3.803608000	-1.872097000
C	5.920355000	6.018158000	-2.249450000
C	5.055623000	4.009092000	-3.268092000
C	6.130610000	4.740336000	-2.761694000
H	2.211888000	7.499261000	-2.519389000
H	1.703234000	6.321636000	-3.739996000
H	-0.208674000	3.425905000	0.535074000
H	-1.249162000	4.811411000	0.734781000
H	-0.034798000	5.094314000	-3.246861000
H	2.470972000	6.454792000	-0.195890000
H	1.105914000	5.404520000	1.545283000
H	4.471751000	7.564457000	-1.847517000
H	2.937771000	3.991318000	-3.663269000
H	6.754452000	6.592896000	-1.854856000
H	5.212331000	3.009452000	-3.666300000
H	7.130489000	4.314543000	-2.768777000
H	-3.227241000	2.388005000	-1.502518000
H	-1.991293000	2.469826000	-0.312532000
TS (Singlet)			
Mn	-0.074433000	-0.011048000	0.000644000
O	3.044680000	-1.356649000	2.165528000
O	2.978669000	0.628920000	-2.551498000
O	-3.519443000	-1.291191000	-1.475296000
O	-1.122029000	-2.785584000	2.813387000
N	-1.384379000	-0.431965000	-1.274431000

N	1.621546000	-0.617763000	0.528023000
N	-0.934324000	-1.387731000	1.004680000
N	0.835662000	-1.663956000	2.526179000
N	0.884120000	0.503729000	-1.591578000
C	1.896039000	-1.214638000	1.720801000
C	-0.473104000	-1.988542000	2.115519000
C	2.780709000	-0.173347000	-0.271516000
C	3.123552000	1.616262000	1.538669000
H	2.179060000	1.325699000	1.989614000
C	5.528471000	2.415373000	0.405972000
H	6.470637000	2.716906000	-0.045789000
C	2.220694000	0.387500000	-1.599053000
C	-2.462282000	-1.134852000	-0.856319000
C	3.585033000	0.953869000	0.398140000
C	0.095217000	0.624598000	-2.748763000
C	-1.212220000	0.127273000	-2.558452000
C	5.063775000	3.057730000	1.551531000
H	5.637673000	3.863287000	2.001827000
C	4.797499000	1.374482000	-0.162798000
H	5.180183000	0.890932000	-1.056261000
C	-2.265270000	-1.781022000	0.528628000
C	0.470337000	1.136482000	-3.991143000
H	1.481645000	1.492095000	-4.144930000
C	-1.280896000	-3.981946000	-0.264283000
H	-0.345427000	-3.455117000	-0.438620000
C	-2.373182000	-3.293158000	0.274167000
C	3.857144000	2.651547000	2.114050000
H	3.477907000	3.143025000	3.006704000
C	-3.562237000	-3.991674000	0.486951000
H	-4.429271000	-3.485177000	0.900085000

C	1.232566000	-2.192384000	3.831552000
H	1.624338000	-3.212147000	3.759694000
H	0.362798000	-2.194375000	4.484341000
H	2.002714000	-1.550196000	4.254356000
C	-1.766011000	0.733116000	-4.820643000
H	-2.493904000	0.786079000	-5.625875000
C	-2.145948000	0.191527000	-3.591723000
H	-3.148162000	-0.186444000	-3.439250000
C	-0.468233000	1.190494000	-5.022305000
H	-0.177648000	1.600217000	-5.986052000
C	3.670801000	-1.365192000	-0.671368000
H	4.222120000	-1.747336000	0.186277000
H	4.374087000	-1.069682000	-1.451216000
H	3.039907000	-2.164810000	-1.073932000
C	-1.370693000	-5.336536000	-0.567666000
H	-0.508140000	-5.853195000	-0.980915000
C	-3.652986000	-5.349995000	0.185364000
H	-4.586487000	-5.877009000	0.365881000
C	-3.365469000	-1.226856000	1.442540000
H	-3.189416000	-0.157984000	1.602874000
H	-3.356770000	-1.734369000	2.408648000
H	-4.349850000	-1.341094000	0.982718000
C	-2.559319000	-6.028360000	-0.342634000
O	-0.457292000	1.407816000	0.647175000
H	-2.630840000	-7.087101000	-0.577142000
O	-1.795491000	3.915771000	-3.552679000
N	2.044121000	3.986249000	-2.039586000
N	-2.665750000	3.377867000	-1.534946000
C	3.203918000	3.914138000	-2.939619000
C	-0.117154000	3.783453000	-0.243795000

C	-0.308197000	3.852408000	-1.689831000
C	0.778694000	3.912171000	-2.514484000
C	4.050777000	5.164539000	-2.899945000
C	2.255495000	4.151307000	-0.682888000
C	1.230795000	4.128327000	0.192668000
C	3.545902000	6.372163000	-3.390389000
C	5.341764000	5.126648000	-2.374465000
C	-1.634355000	3.718083000	-2.338659000
C	4.323433000	7.524332000	-3.355484000
C	6.123899000	6.280535000	-2.341222000
C	5.615603000	7.479635000	-2.831026000
H	2.816164000	3.741446000	-3.946835000
H	3.794998000	3.037152000	-2.654025000
H	-0.265421000	2.554443000	0.118425000
H	-0.924281000	4.190096000	0.373656000
H	0.664759000	3.902220000	-3.592738000
H	3.285188000	4.322627000	-0.384523000
H	1.432687000	4.292222000	1.245608000
H	2.538286000	6.404812000	-3.801315000
H	5.734574000	4.187802000	-1.987787000
H	3.924453000	8.458850000	-3.740842000
H	7.129326000	6.240593000	-1.930729000
H	6.223609000	8.380062000	-2.806010000
H	-3.558356000	3.197454000	-1.970897000
H	-2.527767000	3.063682000	-0.586147000

TS (Triplet)

Mn	0.039375000	0.101379000	-0.325257000
O	3.185771000	-0.809588000	2.060897000
O	2.998494000	1.426550000	-2.637178000
O	-3.067019000	-1.624862000	-2.189820000

O	-0.684265000	-2.997377000	2.192765000
N	-1.281951000	-0.256022000	-1.673514000
N	1.795393000	-0.140093000	0.364258000
N	-0.661015000	-1.465338000	0.493247000
N	1.018210000	-1.482453000	2.165322000
N	0.911913000	0.994708000	-1.771356000
C	2.072350000	-0.792298000	1.514338000
C	-0.164528000	-2.033546000	1.608171000
C	2.858895000	0.580211000	-0.359305000
C	2.804116000	2.218877000	1.622189000
H	1.992434000	1.649265000	2.063450000
C	4.850764000	3.738191000	0.521156000
H	5.647424000	4.328206000	0.074240000
C	2.258818000	1.059998000	-1.716980000
C	-2.142989000	-1.267655000	-1.449086000
C	3.350934000	1.829507000	0.397150000
C	0.108507000	1.178234000	-2.921959000
C	-1.124719000	0.485172000	-2.862401000
C	4.313557000	4.102607000	1.754125000
H	4.690340000	4.974615000	2.282248000
C	4.378736000	2.611066000	-0.145866000
H	4.813556000	2.343795000	-1.104171000
C	-1.882935000	-2.019454000	-0.114636000
C	0.411233000	1.960402000	-4.033916000
H	1.355470000	2.489650000	-4.078797000
C	-0.473946000	-3.916405000	-1.032587000
H	0.346989000	-3.208099000	-1.120538000
C	-1.696311000	-3.494353000	-0.498488000
C	3.288723000	3.336668000	2.299876000
H	2.853748000	3.609228000	3.258438000

C	-2.733738000	-4.421299000	-0.394259000
H	-3.695240000	-4.125657000	0.014494000
C	1.371103000	-2.016066000	3.482487000
H	1.925571000	-2.957459000	3.412238000
H	0.456620000	-2.188542000	4.045993000
H	1.985493000	-1.286097000	4.005759000
C	-1.718228000	1.373130000	-5.020604000
H	-2.429817000	1.453386000	-5.838018000
C	-2.035191000	0.586521000	-3.912147000
H	-2.976906000	0.054308000	-3.857143000
C	-0.506572000	2.053217000	-5.081704000
H	-0.267399000	2.665913000	-5.946721000
C	4.029506000	-0.352174000	-0.714655000
H	4.583150000	-0.634810000	0.179289000
H	4.703850000	0.142221000	-1.415425000
H	3.642152000	-1.256773000	-1.195250000
C	-0.290149000	-5.233473000	-1.440294000
H	0.669293000	-5.541423000	-1.848146000
C	-2.550302000	-5.742607000	-0.800528000
H	-3.369360000	-6.450771000	-0.703996000
C	-3.105662000	-1.758776000	0.775234000
H	-3.133968000	-0.696147000	1.037816000
H	-3.052437000	-2.347172000	1.692869000
H	-4.030063000	-2.000560000	0.244970000
C	-1.329371000	-6.154841000	-1.324092000
O	-0.623550000	1.394441000	0.565284000
H	-1.186804000	-7.185166000	-1.638975000
O	-2.471134000	4.030961000	-3.037144000
N	1.203225000	5.417447000	-1.727852000
N	-2.718449000	2.746966000	-1.176243000

C	2.047855000	6.224369000	-2.631158000
C	-0.464847000	3.993311000	0.066780000
C	-0.803778000	4.198308000	-1.342116000
C	0.043847000	4.867692000	-2.176639000
C	3.479460000	5.748394000	-2.683274000
C	1.542952000	5.331943000	-0.394982000
C	0.741757000	4.689118000	0.488187000
C	4.500791000	6.516437000	-2.123529000
C	3.794734000	4.542377000	-3.312290000
C	-2.058044000	3.646988000	-1.936458000
C	5.824980000	6.086964000	-2.197060000
C	5.114172000	4.107228000	-3.378699000
C	6.132678000	4.881427000	-2.822702000
H	2.004124000	7.260694000	-2.283872000
H	1.587617000	6.175707000	-3.619728000
H	-0.334291000	2.771663000	0.242146000
H	-1.307587000	4.108030000	0.761704000
H	-0.183380000	5.005005000	-3.228148000
H	2.458064000	5.837693000	-0.106701000
H	1.021005000	4.688576000	1.535886000
H	4.258032000	7.458289000	-1.636004000
H	3.000331000	3.947730000	-3.757500000
H	6.615123000	6.694875000	-1.764551000
H	5.347521000	3.164898000	-3.867630000
H	7.164641000	4.545670000	-2.880606000
H	-3.481408000	2.265873000	-1.634446000
H	-2.205308000	2.220051000	-0.470156000

P-1

Mn	0.221785000	-0.036916000	0.012997000
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O	2.073745000	-2.198879000	2.909273000
O	3.930736000	-0.241804000	-1.534882000
O	-2.976985000	0.063688000	-2.373136000
O	-2.321019000	-2.419747000	2.150615000
N	-0.788503000	0.086091000	-1.616683000
N	1.491892000	-1.056778000	1.003783000
N	-1.299803000	-1.019394000	0.644938000
N	-0.143728000	-1.846898000	2.538880000
N	1.708862000	0.290808000	-1.180228000
C	1.216469000	-1.713772000	2.145956000
C	-1.328552000	-1.782235000	1.744038000
C	2.885694000	-0.976633000	0.534285000
C	3.222733000	0.798513000	2.339120000
H	2.142217000	0.896428000	2.403114000
C	5.984426000	0.561694000	2.201956000
H	7.065046000	0.459326000	2.140630000
C	2.891652000	-0.248470000	-0.852431000
C	-2.097306000	-0.194616000	-1.534147000
C	3.779189000	-0.137963000	1.461557000
C	1.321524000	0.744800000	-2.458935000
C	-0.081085000	0.643639000	-2.699073000
C	5.418746000	1.486722000	3.074690000
H	6.051656000	2.110505000	3.700345000
C	5.173011000	-0.239694000	1.401712000
H	5.640559000	-0.949426000	0.726086000
C	-2.487489000	-0.946616000	-0.219308000
C	2.157357000	1.246739000	-3.453834000
H	3.222854000	1.318800000	-3.267961000
C	-2.015321000	-3.332699000	-0.958879000
H	-0.962561000	-3.144267000	-0.761178000

C	-2.956646000	-2.331185000	-0.694583000
C	4.032426000	1.601804000	3.138133000
H	3.575005000	2.318083000	3.816198000
C	-4.301729000	-2.603163000	-0.952378000
H	-5.059570000	-1.849122000	-0.762245000
C	-0.328819000	-2.477772000	3.845991000
H	-0.229768000	-3.568082000	3.801360000
H	-1.322480000	-2.234474000	4.215749000
H	0.417620000	-2.091562000	4.537599000
C	0.254174000	1.530306000	-4.921069000
H	-0.158680000	1.834465000	-5.879897000
C	-0.601619000	1.039779000	-3.929952000
H	-1.667612000	0.961224000	-4.106331000
C	1.620309000	1.632710000	-4.686041000
H	2.280426000	2.017370000	-5.460143000
C	3.457534000	-2.380235000	0.274946000
H	3.617320000	-2.912788000	1.212948000
H	4.397632000	-2.325606000	-0.275947000
H	2.745866000	-2.947297000	-0.334688000
C	-2.407921000	-4.572249000	-1.453297000
H	-1.658656000	-5.336419000	-1.644573000
C	-4.697849000	-3.845676000	-1.446090000
H	-5.751870000	-4.036220000	-1.632272000
C	-3.595674000	-0.129858000	0.458270000
H	-3.172433000	0.813655000	0.819725000
H	-4.011307000	-0.672862000	1.310043000
H	-4.399336000	0.108511000	-0.242241000
C	-3.754223000	-4.835877000	-1.698917000
O	0.043192000	1.662847000	0.789162000
H	-4.063340000	-5.804625000	-2.082470000

O	-2.426822000	3.881338000	-2.833913000
N	1.471094000	4.821487000	-3.682537000
N	-1.885906000	3.054842000	-0.785216000
C	1.866043000	5.136799000	-5.082264000
C	0.748326000	4.281639000	-1.094872000
C	-0.175380000	4.125126000	-2.125713000
C	0.218189000	4.422489000	-3.419173000
C	1.860749000	6.624751000	-5.329128000
C	2.387601000	4.946443000	-2.700398000
C	2.045703000	4.691361000	-1.391247000
C	0.656389000	7.292056000	-5.564587000
C	3.054938000	7.345332000	-5.308461000
C	-1.598844000	3.663575000	-1.943240000
C	0.647377000	8.667504000	-5.771662000
C	3.046333000	8.722534000	-5.518621000
C	1.843180000	9.384082000	-5.748860000
H	1.159897000	4.616758000	-5.731713000
H	2.859776000	4.711005000	-5.233539000
H	0.465606000	4.098198000	-0.063157000
H	-0.466912000	4.345585000	-4.255581000
H	3.378443000	5.264836000	-3.005722000
H	2.790010000	4.814221000	-0.613554000
H	-0.275188000	6.729801000	-5.586796000
H	3.993759000	6.824595000	-5.132346000
H	-0.292419000	9.180814000	-5.955933000
H	3.980350000	9.277482000	-5.504568000
H	1.836076000	10.458055000	-5.914473000
H	-2.813205000	2.652563000	-0.723266000
H	-1.153552000	2.624471000	-0.201392000
H	0.909200000	2.088856000	0.795155000

P-2

Mn	-0.084600000	0.044379000	-0.220949000
O	3.127668000	-0.834226000	2.125708000
O	2.848700000	1.430780000	-2.567180000
O	-3.185473000	-1.715542000	-2.097634000
O	-0.572816000	-3.292922000	2.091053000
N	-1.437218000	-0.298020000	-1.553314000
N	1.703836000	-0.175609000	0.440558000
N	-0.739192000	-1.581822000	0.567881000
N	1.003092000	-1.643457000	2.170295000
N	0.772131000	0.976513000	-1.668756000
C	2.018479000	-0.856120000	1.557053000
C	-0.158403000	-2.230596000	1.585331000
C	2.733325000	0.595678000	-0.276282000
C	2.586944000	2.234822000	1.701953000
H	1.828274000	1.603033000	2.154711000
C	4.537828000	3.872687000	0.597992000
H	5.301146000	4.506140000	0.150919000
C	2.110806000	1.058612000	-1.638634000
C	-2.250840000	-1.348452000	-1.364905000
C	3.155927000	1.873594000	0.477002000
C	-0.056346000	1.171047000	-2.796525000
C	-1.295884000	0.473088000	-2.725982000
C	3.974972000	4.210736000	1.827150000
H	4.295262000	5.107184000	2.351790000
C	4.135862000	2.715899000	-0.064970000
H	4.591375000	2.470808000	-1.019394000
C	-1.918927000	-2.175287000	-0.081519000
C	0.219736000	1.974026000	-3.900947000
H	1.164885000	2.502839000	-3.952428000

C	-0.399927000	-3.871139000	-1.198938000
H	0.359533000	-3.093524000	-1.244945000
C	-1.632706000	-3.595543000	-0.595978000
C	2.997309000	3.385568000	2.374205000
H	2.546303000	3.634057000	3.331922000
C	-2.587137000	-4.612512000	-0.547174000
H	-3.554612000	-4.434078000	-0.087474000
C	1.393466000	-2.235163000	3.449590000
H	2.010537000	-3.132312000	3.327195000
H	0.494860000	-2.505511000	4.000879000
H	1.959697000	-1.502551000	4.021963000
C	-1.929941000	1.418660000	-4.856941000
H	-2.659915000	1.518466000	-5.656171000
C	-2.222340000	0.605699000	-3.757821000
H	-3.163772000	0.072320000	-3.698077000
C	-0.718991000	2.095467000	-4.929401000
H	-0.495851000	2.727775000	-5.784989000
C	3.958616000	-0.263675000	-0.631956000
H	4.524638000	-0.524125000	0.261092000
H	4.608084000	0.269888000	-1.327621000
H	3.625813000	-1.186496000	-1.119792000
C	-0.125839000	-5.128054000	-1.727810000
H	0.840278000	-5.318999000	-2.188448000
C	-2.313518000	-5.874967000	-1.073020000
H	-3.070040000	-6.653751000	-1.016492000
C	-3.149803000	-2.093557000	0.830226000
H	-3.263337000	-1.063081000	1.182890000
H	-3.038502000	-2.748900000	1.696890000
H	-4.059475000	-2.365746000	0.288734000
C	-1.083233000	-6.139224000	-1.665657000

O	-0.830558000	1.433915000	0.770096000
H	-0.870358000	-7.123086000	-2.075360000
O	-2.381605000	4.240108000	-2.888600000
N	1.358176000	5.669816000	-1.879250000
N	-2.474034000	2.984753000	-0.988869000
C	2.245516000	6.291511000	-2.905304000
C	-0.291532000	4.609574000	0.037408000
C	-0.629803000	4.510572000	-1.309928000
C	0.219731000	5.064268000	-2.253046000
C	3.632873000	5.704289000	-2.888655000
C	1.709820000	5.757969000	-0.578181000
C	0.893398000	5.241774000	0.402314000
C	4.698683000	6.426625000	-2.350462000
C	3.858904000	4.431065000	-3.415388000
C	-1.906053000	3.883232000	-1.806801000
C	5.980172000	5.879051000	-2.335657000
C	5.136197000	3.880968000	-3.394925000
C	6.198685000	4.604849000	-2.853966000
H	2.267088000	7.362111000	-2.692102000
H	1.757395000	6.135259000	-3.867831000
H	-0.113808000	1.987807000	1.105008000
H	-0.952861000	4.215280000	0.803126000
H	-0.004581000	5.041154000	-3.313967000
H	2.643228000	6.266479000	-0.362052000
H	1.183080000	5.342406000	1.441037000
H	4.524174000	7.422064000	-1.947656000
H	3.029890000	3.871882000	-3.844111000
H	6.806729000	6.448621000	-1.919693000
H	5.301552000	2.886201000	-3.800187000
H	7.197483000	4.176897000	-2.842024000

H	-3.270798000	2.493862000	-1.374372000
H	-1.906439000	2.479356000	-0.292855000

P-3

Mn	-0.727571000	0.220995000	-0.457616000
O	2.387794000	-0.882171000	1.948080000
O	2.378114000	1.146528000	-2.861190000
O	-3.978171000	-1.476513000	-2.134172000
O	-1.653988000	-2.587276000	2.369579000
N	-2.123983000	-0.152785000	-1.751793000
N	1.035964000	-0.118455000	0.260474000
N	-1.591367000	-1.171720000	0.568738000
N	0.140877000	-1.184811000	2.185504000
N	0.260703000	0.713140000	-2.057266000
C	1.264417000	-0.726233000	1.435763000
C	-1.096708000	-1.700784000	1.695359000
C	2.165163000	0.284360000	-0.595031000
C	2.522556000	2.147135000	1.125576000
H	1.546170000	1.916353000	1.543734000
C	5.019198000	2.766761000	0.082456000
H	5.997776000	2.996569000	-0.333034000
C	1.596330000	0.787864000	-1.964665000
C	-3.034620000	-1.088170000	-1.428898000
C	2.997156000	1.415395000	0.032805000
C	-0.536004000	0.835362000	-3.217579000
C	-1.869782000	0.371512000	-3.040766000
C	4.542026000	3.474447000	1.183633000
H	5.142416000	4.259948000	1.634950000

C	4.256351000	1.746966000	-0.483459000
H	4.657851000	1.203423000	-1.332941000
C	-2.818328000	-1.730650000	-0.022658000
C	-0.137894000	1.330328000	-4.457488000
H	0.886293000	1.655554000	-4.596934000
C	-1.469060000	-3.738227000	-0.785510000
H	-0.622443000	-3.066933000	-0.912806000
C	-2.680218000	-3.237186000	-0.294770000
C	3.288513000	3.159364000	1.700558000
H	2.900032000	3.702189000	2.558862000
C	-3.748597000	-4.121169000	-0.137868000
H	-4.703184000	-3.766753000	0.239082000
C	0.472935000	-1.622280000	3.541515000
H	0.905795000	-2.628164000	3.565426000
H	-0.433913000	-1.619359000	4.143678000
H	1.189967000	-0.925420000	3.971891000
C	-2.370736000	0.985551000	-5.320599000
H	-3.087544000	1.056231000	-6.134467000
C	-2.778970000	0.461514000	-4.090202000
H	-3.795917000	0.116458000	-3.945637000
C	-1.060711000	1.406484000	-5.504875000
H	-0.744342000	1.804750000	-6.465349000
C	3.038371000	-0.932477000	-0.959808000
H	3.575026000	-1.297481000	-0.084025000
H	3.755378000	-0.677822000	-1.742326000
H	2.394359000	-1.732998000	-1.339753000
C	-1.327615000	-5.085386000	-1.101799000
H	-0.376388000	-5.452411000	-1.478967000
C	-3.608037000	-5.472844000	-0.451000000
H	-4.451984000	-6.144400000	-0.314683000

C	-4.045724000	-1.372660000	0.824689000
H	-4.051407000	-0.292821000	1.005026000
H	-4.014311000	-1.888617000	1.786559000
H	-4.971307000	-1.632845000	0.305168000
C	-2.398758000	-5.961249000	-0.934497000
O	-1.399294000	2.009752000	0.345597000
H	-2.289911000	-7.014636000	-1.178705000
O	-1.866455000	4.272895000	-3.808613000
N	2.078473000	4.466924000	-2.440965000
N	-2.471735000	3.470837000	-1.755609000
C	3.255230000	4.251182000	-3.330696000
C	-0.055739000	4.740230000	-0.739939000
C	-0.256430000	4.339896000	-2.059520000
C	0.837513000	4.232903000	-2.899086000
C	4.076291000	5.503264000	-3.499023000
C	2.291684000	4.844285000	-1.163880000
C	1.234541000	5.007935000	-0.296013000
C	3.596803000	6.558019000	-4.280279000
C	5.323437000	5.613455000	-2.883891000
C	-1.613847000	4.016884000	-2.626492000
C	4.355871000	7.711944000	-4.438999000
C	6.086145000	6.768512000	-3.046146000
C	5.602590000	7.817563000	-3.822279000
H	2.862093000	3.899906000	-4.285792000
H	3.840834000	3.447166000	-2.878998000
H	-0.899171000	4.850965000	-0.065298000
H	0.740158000	3.949158000	-3.940833000
H	3.323623000	5.003491000	-0.870115000
H	1.429185000	5.323136000	0.722246000
H	2.626197000	6.469460000	-4.764734000

H	5.696272000	4.790473000	-2.276511000
H	3.978621000	8.528570000	-5.048410000
H	7.057602000	6.846799000	-2.565895000
H	6.196705000	8.718462000	-3.950006000
H	-3.350532000	3.156543000	-2.147633000
H	-2.109677000	2.986076000	-0.905971000
H	-0.654438000	2.477070000	0.741325000

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