

Supplementary Information

Hafnium Catalysts for Direct Alkene Epoxidation using Molecular Oxygen as Oxidant

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DFT calculations were performed using the B3LYP functional and LANL2DZ basis sets. All energies in the table beneath each conformation are in Hartrees. **E** is the electronic energy without zero point vibrations or thermal contributions. **E_{zp}** includes zero-point vibrations but no thermal contributions (i.e., the energy at 0 Kelvin). **H** and **G** are the computed enthalpy and Gibbs free energy at 298.15 Kelvin and 1 atmosphere pressure. For each conformation, the Cartesian coordinates (Å) of each atom are listed. For transition states, the imaginary frequency f (cm⁻¹) along the reaction coordinate is listed.

1.1 Hf_NCCN system

Fig. S2 shows the computed chemical potential diagram for the Hf_NCCN catalyst. The bare complex (M'') and the bisozone complexes ($M''(\eta^2-O_3)_2$ and $M''(\eta^2-O_3) \cdot (\eta^2-O_3)$) have the highest relative energies on the oxygen-rich and oxygen-starved ends, respectively. Accordingly, these structures will not be stable within the catalytic system. On the oxygen-rich end, all the major

catalyst forms containing one to six adsorbed oxygen atoms settle within a ~ 50 kcal/mol window. This energy range is not narrow enough for Hf_NCCN to work as a good oxygen transfer catalyst.

Notably, singlet oxo η^3 -ozone and singlet peroxo η^3 -ozone ground states do not exist within the Hf_NCCN system. Constrained geometry optimizations were performed to verify the nonexistence of these states. In these calculations, the distance between the Hf atom and the μ -O atom (the center oxygen atom in the ozone group) were frozen at a series of different lengths. All of the other geometric parameters were fully relaxed to minimize the energy. The energy was plotted against the Hf to μ -O distance, as shown in Fig. S3. Within the energy-distance plot, a local or global minimum represents a ground state and a peak on the curve represents a transition state. As we can see in both panels of Fig. S3, only one minimum (which represents a stable η^2 -ozone conformation) was achieved in each case and no other ground state or transition state was observed. On the oxo ozone energy curve, as illustrated in the upper panel, there is a nearly flat region around 2.4 Å which demonstrates that an oxo- η^3 -ozone-like region exists as a non-stationary state that would spontaneously revert to the oxo η^2 -ozone complex without an energy barrier. The peroxo ozone energy curve in the lower panel shows a similar nearly flat region around 2.3 Å. While a singlet peroxo η^3 -ozone complex did not exist for Hf_NCCN, the triplet peroxo η^3 -ozone complex exists for this system (Fig. S35).

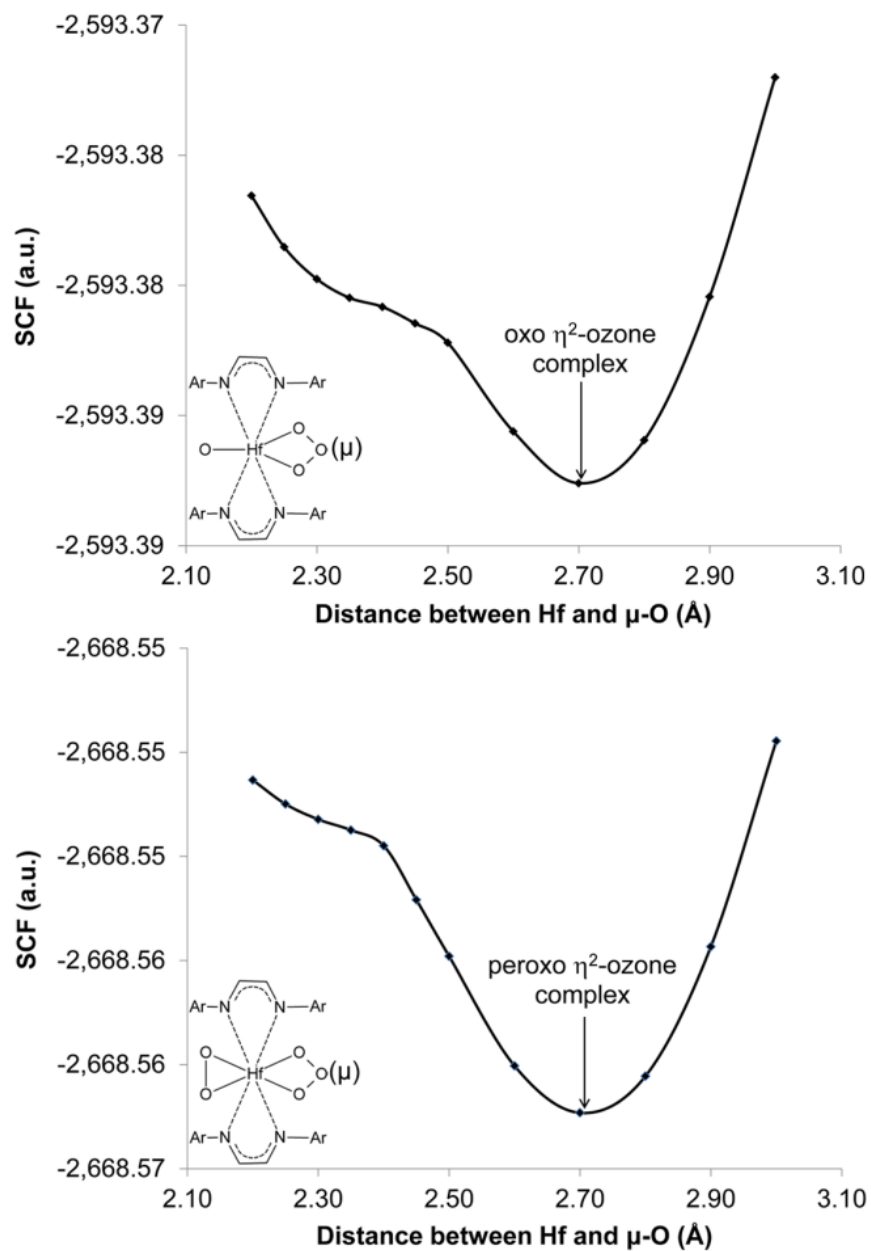


Fig. S3: Hf_NCCN constrained geometry optimizations that show the singlet oxo η^3 -ozone state (upper panel) and the singlet peroxo η^3 -ozone state (lower panel) do not exist. The single minimum corresponds to the singlet oxo η^2 -ozone complex (upper panel) and the singlet peroxo η^2 -ozone complex (lower panel).

Table S1: Assigned Spin Magnetic Moments for Hf_NCCN catalyst

Species	Hafnium	Non-ligand Oxygens		Nitrogens		Other Atoms
		Strongly Ads.	Weakly Ads.	Ligand 1	Ligand 2	
M''^T	0.8916	—	—	0.5176	-0.0124	0.6032
$M''O^T$	0.0188	0.0678	—	0.5513	0.5511	0.8110
$M''(O)_2^T$	-0.1030	1.1246	—	0.5372	0.0149	0.4263
$M''(O_2)^T$	0.0889	0.0191	—	0.5261	0.5259	0.8400
$M''(O_2) \cdot O^T$	-0.0160	0.0635	0.9056	0.5786	0.0170	0.4513
$M''O \cdot (O_2)_{(planar)}^T$	-0.0052	0.0296	1.0074	0.5605	0.0037	0.4040
$M''O \cdot (O_2)_{(butterfly)}^T$	-0.0157	0.0494	0.9972	0.5569	0.0054	0.4068
$M''(\eta^2-O_3)^T$	0.1062	0.0451	—	0.5088	0.5087	0.8312
$M''(O_2) \cdot (O_2)_{(spiro)}^T$	-0.0068	0.0266	1.0078	0.5700	-0.0006	0.4030
$M''(O_2) \cdot (O_2)_{(butterfly)}^T$	0.0269	0.0440	0.9872	0.5162	0.0148	0.4109
$M''O \cdot (\eta^2-O_3)^T$	-0.0003	0.0533	0.9889	0.5566	0.0035	0.3980
$M''(O_2) \cdot (\eta^2-O_3)^T$	0.0057	0.0324	0.9876	0.5680	0.0051	0.4012
$M''(\eta^3-O_3) \cdot (O_2)^T$	0.0125	0.0163	1.0006	0.5378	0.0061	0.4267
$M''(\eta^2-O_3) \cdot (\eta^2-O_3)^T$	0.0056	0.0450	0.5643	0.5642	0.0094	0.8115

Examining Fig. S2, the singlet spiro bisperoxo form is the low energy form for oxygen chemical potentials > -13 kcal/mol. Therefore, under normal reaction conditions, the catalyst resting state is the singlet spiro bisperoxo complex. For the reaction $M''(O_2)_{2(spiro)}^S + P \rightarrow M''O(O_2)^S + PO$, the transition state energy relative to the reactants is 39.5 (E), 38.6 (E_{zp}), 39.2 (H), and 47.8 (G) kcal/mol. Since $M''(O_2)_{2(spiro)}^S$ is the catalyst resting state, it immediately follows that the SCF energetic span for this catalyst is at least 39.5 kcal/mol. Therefore, even without computing a complete reaction cycle, we can already determine that the SCF energetic span is ≥ 40 kcal/mol. Based on these results, we predict that Hf_NCCN would not make a good direct propene epoxidation catalyst.

1.2 Zr_NCCN system

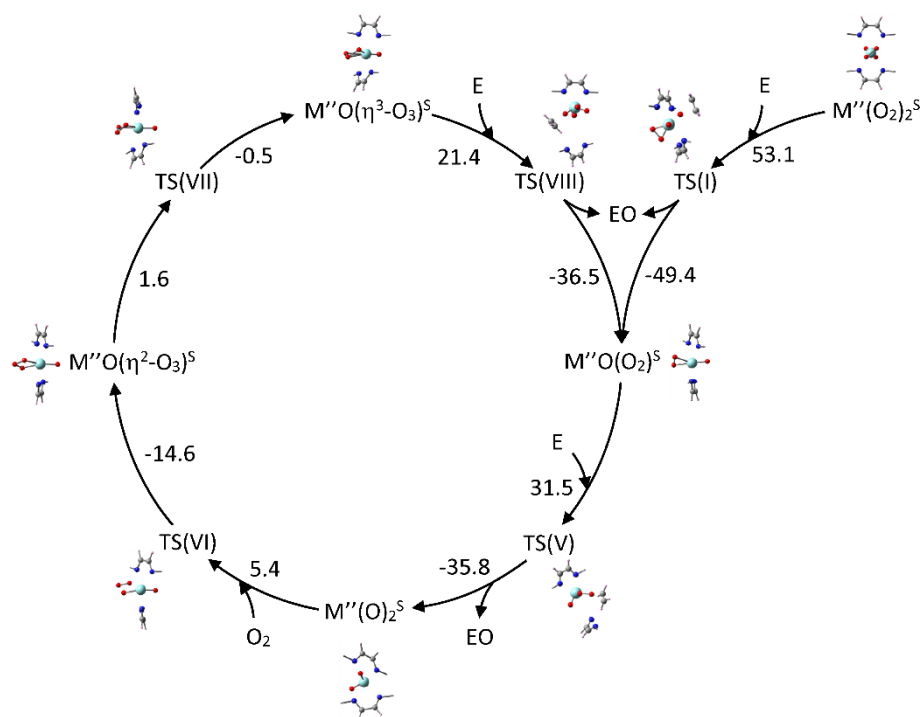


Fig. S4: Catalytic cycle for direct ethylene epoxidation using Zr_NCCN catalyst. Energy differences are presented in kcal/mol. E and EO represent ethylene and ethylene oxide, respectively. In the displayed chemical structures, portions of the ligands are unillustrated for display purposes.

Table S2: Computed reaction energies and energetic spans (kcal/mol) for direct ethylene epoxidation using Zr_NCCN catalyst

reactant	product	activation barrier (kcal/mol)				net rxn energy (kcal/mol)			
		E _{EL}	E _{ZP}	H	G	E _{EL}	E _{ZP}	H	G
$M''(O)_2^S + E$	$M''O(O_2)^S + EO$	53.1	52.6	52.7	62.0	3.7	4.8	4.4	3.8
$M''O(O_2)^S + E$	$M''(O)_2^S + EO$	31.5	30.2	30.9	34.4	-4.4	-3.7	-4.0	-6.7
$M''(O)_2^S + O_2$	$M''O(\eta^2-O_3)^S$	5.4	6.5	5.8	18.5	-9.2	-6.8	-8.1	6.6
$M''O(\eta^2-O_3)^S$	$M''O(\eta^3-O_3)^S$	1.6	1.6	1.6	1.1	1.1	1.3	1.8	-0.5
$M''O(\eta^3-O_3)^S + E$	$M''O(O_2)^S + EO$	21.4	20.0	20.7	24.8	-15.1	-13.3	-14.1	-11.9
energetic span		53.1	52.6	52.7	62.0				

2. Additional Figures and Tables for NCCNO catalysts

2.1 Hf_NCCNO system

Table S3: Assigned Spin Magnetic Moments for Hf_NCCNO catalyst

Species	Hafnium	Non-ligand Oxygens		Nitrogens		Other Atoms
		Strongly Ads.	Weakly Ads.	Ligand 1	Ligand 2	
M'^T	0.8818	—	—	0.3140	0.2845	0.5197
$M'O^T$	-0.0093	0.0477	—	0.5815	0.5814	0.7987
$M'(O)_2^T$	-0.1071	1.1234	—	0.5226	0.0354	0.4257
$M'(O_2)^T$	0.0048	0.0136	—	0.5820	0.5820	0.8176
$M'O \cdot (O_2)_{(planar)}^T$	-0.0161	0.0100	0.9997	0.5756	-0.0020	0.4328
$M'O \cdot (O_2)_{(butterfly)}^T$	-0.0214	0.0314	0.9965	0.5857	0.0052	0.4026
$M'O^*(O_2)^T$	-0.0066	0.0189	1.2890	0.5820	-0.1903	0.3070
$M'(\eta^2-O_3)^T$	0.0079	0.0238	—	0.5687	0.5684	0.8312
$M'(O_2) \cdot (O_2)_{(spiro)}^T$	-0.0196	0.0069	0.9962	0.5773	0.0026	0.4366
$M'(O_2) \cdot (O_2)_{(planar)}^T$	-0.0088	0.0148	1.0014	0.5658	-0.0013	0.4281
$M'(O_2) \cdot (O_2)_{(butterfly)}^T$	-0.0290	0.1374	0.9409	0.5808	-0.0310	0.4009
$M'O \cdot (\eta^2-O_3)^T$	-0.0050	0.0245	0.9904	0.5795	0.0012	0.4094
$M'(\eta^2-O_3) \cdot (O_2)^T$	-0.0103	-0.0185	0.9908	0.5530	0.0275	0.4575
$M'(O_2) \cdot (\eta^2-O_3)^T$	0.0044	0.0199	0.9782	0.5709	0.0047	0.4219
$M'(\eta^3-O_3) \cdot (O_2)^T$	-0.0131	0.0102	0.9731	0.5779	0.0057	0.4462

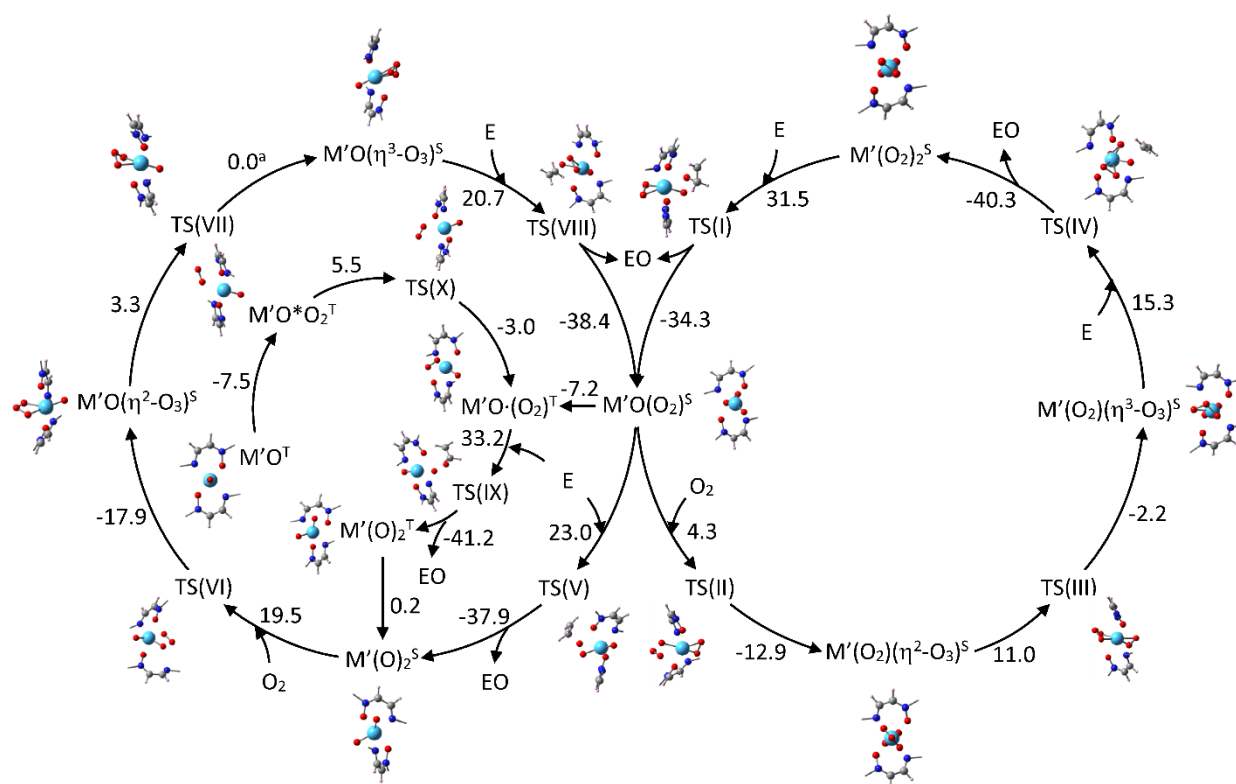


Fig. S5: Master catalytic cycle for direct ethylene epoxidation using Hf_NCCNO catalyst. Energy differences are presented in kcal/mol. E and EO represent ethylene and ethylene oxide, respectively. ^aWithin a computational precision of ~0.1 kcal/mol, the energy difference between M'O(η^3 -O₃)^S and TS(VII) is negligible. In the displayed chemical structures, portions of the ligands are unillustrated for display purposes.

Table S4: Computed reaction energies and energetic spans (kcal/mol) for direct ethylene epoxidation using Hf_NCCNO catalyst

reactant	product	activation barrier				net rxn energy			
		E	E _{zp}	H	G	E	E _{zp}	H	G
M'(O ₂) ₂ (spiro) ^S +E	M'O(O ₂) _(planar) ^S +EO	31.5	32.7	32.0	45.3	-2.8	-1.3	-1.9	-2.1
M'O(O ₂) _(planar) ^S +O ₂	M'(O ₂)(η ² -O ₃) ^S	4.3	5.8	4.9	17.8	-8.6	-6.4	-7.0	4.5
M'(O ₂)(η ² -O ₃) ^S	M'(O ₂)(η ³ -O ₃) ^S	11.0	10.3	9.9	10.9	8.8	8.5	8.3	8.9
M'(O ₂)(η ³ -O ₃) ^S +E	M'(O ₂) ₂ (spiro) ^S +EO	15.3	16.7	16.1	30.1	-25.0	-23.4	-23.8	-23.9
M'O(O ₂) _(planar) ^S +E	M'(O) ₂ ^S +EO	23.0	23.7	23.2	36.5	-15.0	-4.8	-5.2	-5.3
M'(O) ₂ ^S +O ₂	M'O(η ² -O ₃) ^S	19.5	11.4	10.9	21.4	1.7	-5.3	-5.8	4.3
M'O(η ² -O ₃) ^S	M'O(η ³ -O ₃) ^S	3.3 ^a	3.5 ^a	2.7 ^a	6.7	3.3 ^a	3.5 ^a	2.7 ^a	5.8
M'O(η ³ -O ₃) ^S +E	M'O(O ₂) _(planar) ^S +EO	20.7	22.5	21.6	36.2	-17.6	-16.1	-16.8	-17.3
M'O ^T +O ₂	M'O*(O ₂) ^T	0.0	0.0	0.0	4.5	-7.5	-6.1	-6.3	4.5
M'O*(O ₂) ^T	M'O·(O ₂) _(planar) ^T	5.5	5.1	4.8	5.7	2.5	3.1	2.8	4.0
M'O·(O ₂) _(planar) ^T +E	M'(O) ₂ ^T +EO	26.5	27.0	26.3	39.4	-10.2	-10.4	-10.6	-12.3
M'(O) ₂ ^T	M'(O) ₂ ^S	—	—	—	—	0.2	10.7	10.2	12.5
M'O(O ₂) _(planar) ^S	M'O·(O ₂) _(planar) ^T	—	—	—	—	-7.2	-7.4	-7.2	-7.6
E _{span}		25.8	26.1	25.0	45.3				

^a For this reaction, the potential energy surface between the transition state and reaction product is nearly flat — the transition state and reaction product have the same energy within the resolution of the calculation.

The SCF energetic span for direct ethylene epoxidation using the Hf_NCCNO catalyst was computed as follows. The singlet cycle, which passes through M'O(η³-O₃)^S complex, exhibits the lowest forward barrier in this system. This barrier is maximized at 19.5 – 17.9 + 3.3 + 0.1 + 20.7 = 25.8 kcal/mol with M'(O)₂^S as TDI and TS(VIII) as TDTs. Since other junior cycles in this system exhibits higher energetic spans, 25.8 kcal/mol is accordingly determined as the overall SCF energetic span for Hf_NCCNO catalyzed direct ethylene epoxidation. The E_{zp}, H, and G based energetic spans were computed in a similar manner with the TDI and TDTs determined independently for each energy type.

[illegible]

Fig. S6: Master catalytic cycle for direct ethylene epoxidation using Zr_NCCNO catalyst. Energy differences are presented in kcal/mol. E and EO represent ethylene and ethylene oxide, respectively. In the displayed chemical structures, portions of the ligands are unillustrated for display purposes.

Table S5: Computed reaction energies and energetic spans (kcal/mol) for direct ethylene epoxidation using Zr_NCCNO catalyst

reactant	product	activation barrier				net rxn energy			
		E	E _{zp}	H	G	E	E _{zp}	H	G
M'(O ₂) ₂ (spiro) ^S +E	M'O(O ₂) _(planar) ^S +EO	30.2	30.5	30.2	41.5	-4.6	-3.3	-3.8	-3.5
M'O(O ₂) _(planar) ^S +O ₂	M'(O ₂)(η ² -O ₃) ^S	14.7	16.3	15.4	26.7	-5.6	-3.3	-3.9	6.2
M'(O ₂)(η ² -O ₃) ^S	M'(O ₂)(η ³ -O ₃) ^S	9.4	9.1	8.6	10.9	8.1	7.9	7.7	9.3
M'(O ₂)(η ³ -O ₃) ^S +E	M'(O ₂) ₂ (spiro) ^S +EO	14.4	15.8	15.2	29.2	-25.5	-23.8	-24.3	-24.5
M'O(O ₂) _(planar) ^S +E	M'(O) ₂ ^S +EO	37.8	39.3	38.6	51.2	-16.2	-14.6	-15.1	-15.5
M'(O ₂) ₂ ^S +O ₂	M'O(η ² -O ₃) ^S	22.1	22.6	22.1	32.3	4.3	5.1	4.4	14.6
M'O(η ² -O ₃) ^S	M'O(η ³ -O ₃) ^S	2.4	3.5	3.0	6.2	2.4	3.6	3.6	5.3
M'O(η ³ -O ₃) ^S +E	M'O(O ₂) _(planar) ^S +EO	20.5	21.8	21.3	34.1	-18.0	-16.6	-17.2	-16.9
M'O ^T +O ₂	M'O*(O ₂) ^T	0.0	0.0	0.0	6.4	-7.8	-6.0	-6.4	6.4
M'O*(O ₂) ^T	M'O·(O ₂) _(planar) ^T	7.5	7.3	6.3	9.6	1.2	1.8	1.5	2.1
M'O·(O ₂) _(planar) ^T +E	M'(O) ₂ ^T +EO	34.1	34.9	34.0	47.3	-5.0	-4.8	-5.0	-6.6
M'(O) ₂ ^T	M'(O) ₂ ^S	—	—	—	—	-3.8	-2.4	-2.8	-0.4
M'O(O ₂) _(planar) ^S	M'O·(O ₂) _(planar) ^T	—	—	—	—	-7.4	-7.4	-7.3	-8.5
E _{span}		30.2	30.5	30.2	44.7				

The SCF energetic span for direct ethylene epoxidation using the Zr_NCCNO catalyst was computed as follows. The singlet cycle, which passes through M'(O₂)(η³-O₃)^S complex, exhibits the lowest forward barrier in this system. This barrier is maximized at 30.2 kcal/mol with M'(O₂)₂(spiro)^S as TDI and TS(I) as TDTS. Since other junior cycles in this system exhibits higher energetic spans, 30.2 kcal/mol is accordingly determined as the overall SCF energetic span for Zr_NCCNO catalyzed direct ethylene epoxidation. The E_{zp}, H, and G based energetic spans were computed in a similar manner with the TDI and TDTS determined independently for each energy type.

Figure 1 is a plot showing the singlet energy (SCF in a.u.) versus the distance between the marked oxygen atoms (Å) for the singlet ground state (S.G.) and singlet excited state (S.E.) of the [2+2] photocycloaddition of 1,2-diphenyl-1,2-dicyanoethene. The plot displays four curves: S.G.(S.E.) (blue line with diamond markers), S.G.(T.E.) (red line with square markers), T.G.(S.E.) (green dashed line with triangle markers), and T.G.(T.E.) (purple dashed line with cross markers). A red circle highlights the crossing point of the S.G.(S.E.) and S.G.(T.E.) curves at approximately 2.0 Å. An inset shows the chemical structure of the molecule with the two oxygen atoms marked.

Distance between marked O atoms (Å)	S.G.(S.E.) (a.u.)	S.G.(T.E.) (a.u.)	T.G.(S.E.) (a.u.)	T.G.(T.E.) (a.u.)
1.6	-2894.078	-2894.052	-2894.050	-2894.085
1.7	-2894.072	-2894.042	-2894.038	-2894.078
1.8	-2894.065	-2894.038	-2894.032	-2894.072
1.9	-2894.058	-2894.045	-2894.042	-2894.065
2.0	-2894.052	-2894.052	-2894.048	-2894.062
2.1	-2894.045	-2894.060	-2894.052	-2894.065
2.2	-2894.042	-2894.065	-2894.050	-2894.070

Figure 1 consists of two panels, (a) and (b), showing relative energy diagrams. The y-axis for both panels is 'Relative Energy (kcal/mol)' ranging from -60 to 60. The x-axis for both panels is 'Singlet Geometry O Atom Chemical Potential (kcal/mol)' for (a) and 'Triplet Geometry O Atom Chemical Potential (kcal/mol)' for (b), ranging from -16 to 0.

Panel (a) shows singlet geometries. The y-axis is labeled 'Relative Energy (kcal/mol)' and the x-axis is labeled 'Singlet Geometry O Atom Chemical Potential (kcal/mol)'. The diagram includes a horizontal line for 'PO Chemical Potential' at approximately 55 kcal/mol and a horizontal line for 'O₂ Chemical Potential' at approximately -55 kcal/mol. Various chemical species are plotted as lines with different slopes, including $M(\eta^2-O_3)_2$, $MO(\eta^2-O_3)$, $M(O_2)_2(\text{planar})$, $M(\eta^2-O_3)$, $M(O_2)_2(\text{spiro})$, M , MO , $M(O_2)$, $MO(O_2)(\text{planar})$, $MO(O_2)(\text{butterfly})$, $M(O_2)_2(\text{butterfly})$, $M(O_2)_2(\text{oct})$, and $MO(O_2)(\text{oct})$.

Panel (b) shows triplet geometries. The y-axis is labeled 'Relative Energy (kcal/mol)' and the x-axis is labeled 'Triplet Geometry O Atom Chemical Potential (kcal/mol)'. The diagram includes a horizontal line for 'PO Chemical Potential' at approximately 55 kcal/mol and a horizontal line for 'O₂ Chemical Potential' at approximately -55 kcal/mol. Various chemical species are plotted as lines with different slopes, including $M(\eta^2-O_3)_2$, $M(\eta^2-O_3) \cdot (\eta^2-O_3)$, $M(\eta^2-O_3)_2$, $M(O_2)(\eta^2-O_3)$, M , $MO(O_2)(\text{planar})$, $M(\eta^2-O_3) \cdot (O_2)$, $M(O_2) \cdot (O_2)(\text{planar})$, $M(O_2)_2(\text{butterfly})$, $M(O_2)_2(\text{oct})$, $M(O_2)_2(\text{spiro})$, $M(O_2)$, MO , $MO^*(O_2)$, $MO(O_2) \cdot (O_2)$, $MO(O_2)(\text{butterfly})$, $MO(O_2)(\text{oct})$, $MO(O_2)_2(\text{butterfly})$, and $MO(O_2)_2(\text{oct})$.

Fig. S8 shows the computed chemical potential diagram for Hf_ONCCNO. On both singlet and triplet panels, the octahedral complex, $M(O)_{2(\text{oct})}$, is the preferred structure among all catalyst forms across the entire oxygen chemical potential range. With additional energy, $M(O)_{2(\text{oct})}$ could transform into the dioxo complex, $M(O)_2$. The bare complex, M , has the highest relative energy on the oxygen-rich end, indicating that M easily adsorbs O_2 to form oxygenated forms. Bis- η^2 -ozone complexes (i.e., $M(\eta^2-O_3)_2$, $M \cdot (\eta^2-O_3)_2$, and $M(\eta^2-O_3) \cdot (\eta^2-O_3)$) have the highest relative

energy on the oxygen-starved end and demonstrate accordingly that bis- η^2 -ozone complexes will not be stable and would easily react with propene to form propylene oxide. On the oxygen-rich end, all the major oxidation states that range from one adsorbed oxygen atom to six adsorbed oxygen atoms settle within a ~ 40 kcal/mol window.

Table S6: Assigned Spin Magnetic Moments for Hf_ONCCNO catalyst

Species	Hafnium	Non-ligand Oxygens		Nitrogens		Other Atoms
		Strongly Ads.	Weakly Ads.	Ligand 1	Ligand 2	
M^T	0.9895	—	—	0.2826	0.2824	0.4455
MO^T	0.0112	0.0164	—	0.5538	0.5354	0.8832
$M(O)_2^T$	-0.0987	1.1234	—	0.5044	0.0309	0.4400
$M(O)_{2(oct.)}^T$	0.0087	0.0172	—	0.5494	0.4685	0.9562
$M(O_2)^T$	0.0330	0.0039	—	0.5544	0.5543	0.8544
$MO \cdot (O_2)_{(planar)}^T$	0.0004	-0.0014	1.0114	0.5196	0.0030	0.4670
$MO \cdot (O_2)_{(butterfly)}^T$	-0.0119	0.0236	1.0027	0.5338	0.0027	0.4491
$MO^*(O_2)^T$	-0.0049	0.0076	1.9033	0.5315	-0.5054	0.0679
$M(\eta^2-O_3)^T$	0.0385	0.0175	—	0.5479	0.5479	0.8482
$M \cdot (O_2)_2^T$	0.0223	—	0.0354	0.5343	0.5406	0.8674
$M(O_2) \cdot (O_2)_{(planar)}^T$	-0.0050	0.0032	1.0038	0.5302	-0.0028	0.4706
$M(O_2) \cdot (O_2)_{(butterfly)}^T$	-0.0021	0.0603	0.9798	0.5076	0.0244	0.4300
$MO \cdot (\eta^2-O_3)^T$	0.0123	0.0136	0.9747	0.5354	0.0026	0.4614
$M(\eta^2-O_3) \cdot (O_2)^T$	0.0102	-0.1086	1.0258	0.4880	0.1138	0.4708
$M \cdot (O_2)(\eta^2-O_3)^T$	-0.0251	—	1.7606	0.5334	-0.4204	0.1514
$M(\eta^3-O_3) \cdot (O_2)^T$	-0.0027	0.0056	1.0151	0.4834	0.0462	0.4524
$M(\eta^2-O_3) \cdot (\eta^2-O_3)^T$	0.0215	-0.0434	0.9932	0.5211	0.0518	0.4558
$M \cdot (\eta^2-O_3)_2^T$	-0.0197	—	1.8543	0.5427	-0.4874	0.1101

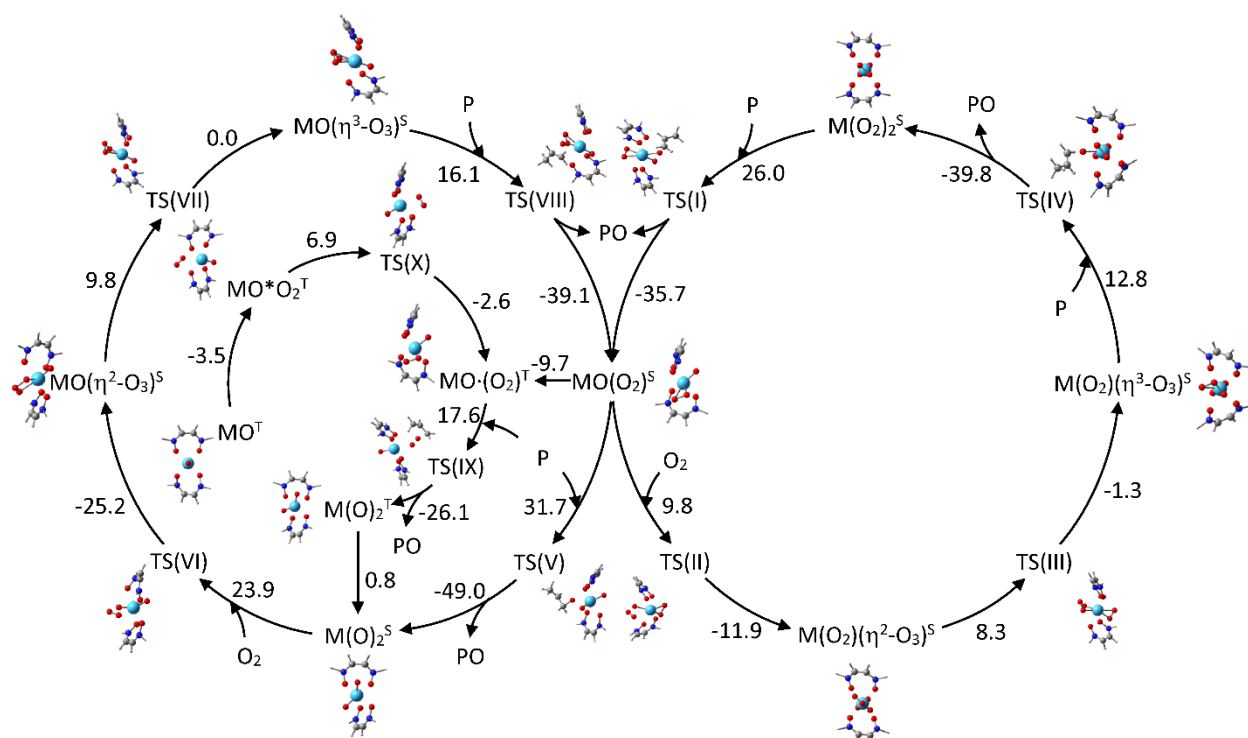


Fig. S9: Master catalytic cycle for direct propene epoxidation using Hf_ONCCNO catalyst. Energy differences are presented in kcal/mol. P represents propene and PO represents propylene oxide. In the displayed chemical structures, portions of the ligands are unillustrated for display purposes.

The Hf_ONCCNO system contains several bisperoxo complexes. The planar complex has a higher energy than the spiro bisperoxo complex. Although the butterfly bisperoxo complex is lower in energy than the spiro bisperoxo complex, we expect the spiro bisperoxo complex to play a more important role in the reaction kinetics. For all structures within the master catalytic cycle, the two ONCCNO ligands sit on opposite sides of the metal atom. In contrast, the two ligands sit on the same side in the butterfly complexes. A movement which makes the ligands shift from one side to the other would involve molecule stretching and ligand rotation. A certain amount of energy would be required to perform this transformation, and we think it would be a rare occasion. However, for the sake of completeness, we also computed energy barriers for the butterfly forms. There is an energy barrier of 27.2 kcal/mol and net reaction energy of -14.4 kcal/mol for the $M(O_2)_2(\text{butterfly})^S$ complex reacting with propene to form the $MO(O_2)(\text{butterfly})^S$ complex plus propylene oxide. The $MO(O_2)(\text{butterfly})^S$ complex would then react with propene to form propylene oxide and the $M(O_2)_2^S$ complex, bringing the reaction back into the main cycle. The energy barrier for this step is 29.4 kcal/mol and the net reaction energy is -5.5 kcal/mol. Therefore, the butterfly and spiro bisperoxo pathways have similar energetics.

Table S7: Computed reaction energies and energetic spans (kcal/mol) for direct propene epoxidation using Hf_ONCCNO catalyst

reactant	product	activation barrier				net rxn energy			
		E	E _{ZP}	H	G	E	E _{ZP}	H	G
M(O ₂) ₂ (spiro) ^S +P	MO(O ₂) _(planar) ^S +PO	26.0	27.1	26.5	41.3	-9.7	-8.1	-8.7	-8.4
MO(O ₂) _(planar) ^S +O ₂	M(O ₂)(η ² -O ₃) ^S	9.8	11.2	10.3	24.0	-2.2	-0.5	-1.1	11.2
M(O ₂)(η ² -O ₃) ^S	M(O ₂)(η ³ -O ₃) ^S	8.3	7.9	7.5	8.3	7.0	6.8	6.7	6.8
M(O ₂)(η ³ -O ₃) ^S +P	M(O ₂) ₂ (spiro) ^S +PO	12.8	14.0	13.6	26.5	-26.9	-25.5	-25.9	-26.2
MO(O ₂) _(planar) ^S +P	M(O) ₂ ^S +PO	31.7	31.8	31.7	44.3	-17.3	-16.3	-16.4	-17.6
M(O ₂) ₂ ^S +O ₂	MO(O ₃) ^S	23.9	25.0	24.0	37.6	-1.4	0.9	-0.1	13.3
MO(O ₃) ^S	MO(η ³ -O ₃) ^S	9.8	9.3	9.0	10.3	9.8	9.4	9.6	8.9
MO(η ³ -O ₃) ^S +P	MO(O ₂) _(planar) ^S +PO	16.1	17.0	16.4	31.2	-23.0	-21.3	-22.0	-21.1
MO ^T +O ₂	MO*(O ₂) ^T	0.0	0.0	0.0	6.3	-3.5	-2.7	-2.3	6.3
MO*(O ₂) ^T	MO·(O ₂) _(planar) ^T	6.9	7.9	6.8	12.1	4.3	5.8	4.8	9.6
MO·(O ₂) _(planar) ^T	M(O) ₂ ^T	17.6	19.1	18.1	34.1	-8.4	-8.1	-8.1	-9.6
M(O) ₂ ^T	M(O) ₂ ^S	—	—	—	—	0.8	2.8	2.2	5.0
MO(O ₂) _(planar) ^S	MO·(O ₂) _(planar) ^T	—	—	—	—	-9.7	-11.0	-10.4	-13.1
E _{span}		57.2	60.6	60.4	87.1				
with allylic H transfer		70.1	73.7	71.4	88.7				
E _{span} (Zr)		55.8	59.3	57.9	89.2				
with allylic H transfer (Zr)		63.4	66.7	64.8	80.3				

The chemical potential diagram in Fig. S8 shows that the triplet octahedral complex ($M(O)_{2(oct)}^T$) has the lowest relative energy among all singlet and triplet intermediates over the entire oxygen chemical potential range. Therefore, the highest energy barrier will result if this complex is included in the complete forward reaction cycle. Since $M(O)_{2(oct)}^T$ is a reversible state of the catalyst and does not contribute to the forward motion of the cycle, we computed the energetic span for this catalyst with and without including this $M(O)_{2(oct)}^T$. When $M(O)_{2(oct)}^T$ was neglected, the forward barrier is maximized at 26.0 kcal/mol within the peroxo η^3 -ozone cycle with $M(O_2)_{2(spiro)}^S$ as TDI and TS(I) as TDTS. A slightly lower forward barrier (25.9 kcal/mol with $MO(\eta^2-O_3)^S$ as TDI and TS(VIII) as TDTS) is achieved using the oxo η^3 -ozone cycle incorporating $MO \cdot (O_2)_{(planar)}^T$ and $M(O)_2^T$ intermediates as a detour. $M(O)_{2(oct)}^T$ can be included in the energetic span calculation as follows. The SCF reaction energy for forming $M(O)_2^S$ from $M(O)_{2(oct)}^T$ is 32.7 kcal/mol. The $M(O)_2^S$ would then follow the oxo η^3 -ozone cycle and generate $MO(O_2)_{(planar)}^S$, as shown in Fig. S9. $MO(O_2)_{(planar)}^S$ could keep following the oxo η^3 -ozone cycle or switch to the peroxo η^3 -ozone cycle based on different reaction conditions. Although different pathways might be chosen through the reaction, the forward barrier for both pathways would be the same at $32.7+23.9-25.2+9.8-0.0+16.1=57.2$ kcal/mol with $M(O)_{2(oct)}^T$ as TDI and TS(VIII) as TDTS. Since $M(O)_{2(oct)}^T$ is the resting state of this catalyst, we think the computed energetic span corresponds most closely to the real reaction by including $M(O)_{2(oct)}^T$. Accordingly, the SCF energetic span for Hf_ONCCNO is 57.2 kcal/mol. Many activation barriers for reactions involved in the oxo η^3 -ozone junior cycle are slightly higher for Hf_ONCCNO than for Zr_ONCCNO: 5.2, 1.3, 6.1, 0.5 and 1.1 kcal/mol higher for steps involving TS(V), TS(VI), TS(VII), TS(VIII) and TS(X), respectively. The enthalpic energetic span for direct propene epoxidation over Hf_ONCCNO is 60.4 kcal/mol, which is 2.5 kcal/mol higher than for the Zr_ONCCNO catalyst. When the allylic H transfer deformation route is included, the SCF energy required to generate $M(O)^T$ is 51.7 kcal/mol (Table 2). In this case, the transferred allylic H product (Fig. S103) is the TDI and TS(IX) is the TDTS leading to an SCF energetic span of $51.7-3.5+6.9-2.6+17.6=70.1$ kcal/mol. This clearly demonstrates the key role of allylic H transfer in increasing the energetic span. As shown in Table S7, allylic H transfer also increases the E, E_{ZP} , and H energetic spans for the Zr_ONCCNO catalyst. In summary, formation of an inert octahedral complex makes Hf_ONCCNO infeasible for direct propene epoxidation.

4. Singlet Ground States for NCCN Complex

4.1 Zero Oxygen Atoms

Bare Complex

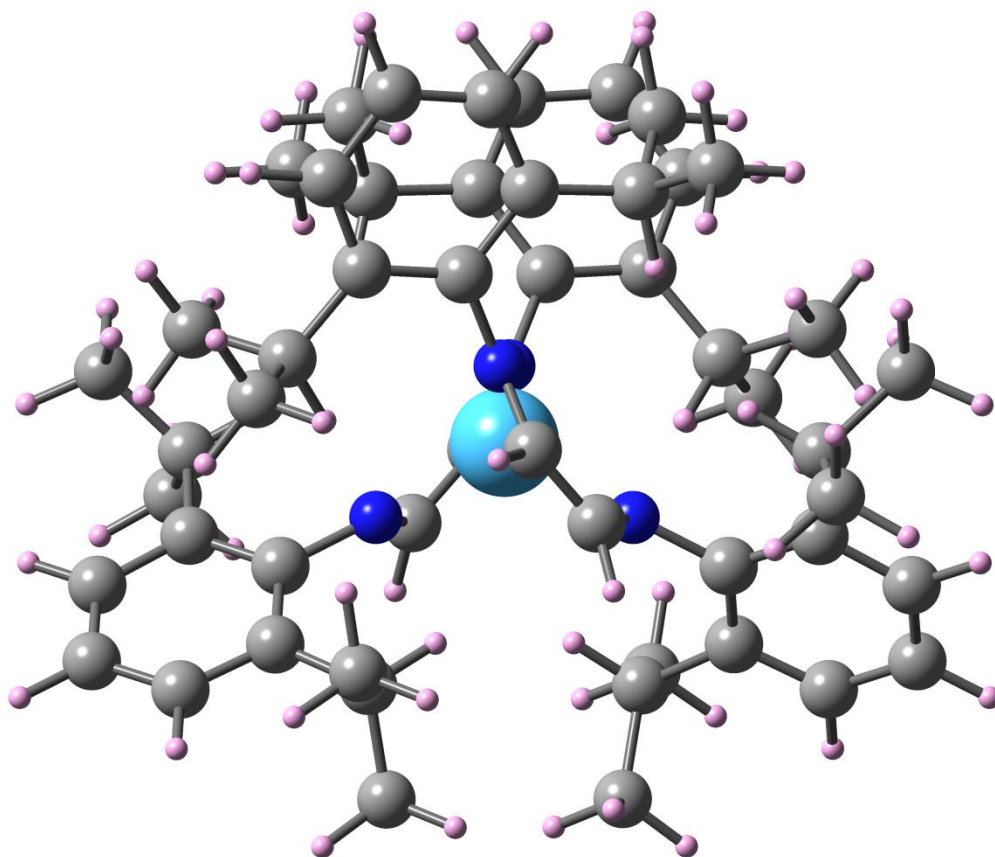


Fig. S10: NCCN Bare Complex

E	E_{zp}	H	G
-2292.6257	-2291.4921	-2291.4284	-2291.5912

N	-1.69333690	-1.26557505	-0.72321967
N	0.05792811	0.72422745	-1.78083138
N	-0.05820091	0.72735999	1.78007735
N	1.69304959	-1.26448440	0.72805888
C	-1.21337204	-1.34216526	-2.07133169
C	-0.37100597	-0.37836753	-2.59114614
C	0.37165578	-0.37235067	2.59387619
C	1.21423911	-1.33734634	2.07667863
C	-2.95034879	-1.90369263	-0.41011294
C	-4.14467288	-1.50716530	-1.09772722
C	-5.35843485	-2.15561584	-0.79142392
C	-5.43293814	-3.15257668	0.19089770
C	-4.26778031	-3.52288551	0.87249751
C	-3.01938475	-2.92913130	0.58464547
C	-4.36033257	-0.98616027	-3.58304194

C	-4.17438733	-0.39730367	-2.15790158
C	-5.28306139	0.65062981	-1.87544027
C	0.53927147	1.93035286	-2.41664339
C	1.87779517	1.99636933	-2.90630183
C	2.32113123	3.19417778	-3.50571382
C	1.47745341	4.30853659	-3.61752078
C	0.16352441	4.23202951	-3.13404484
C	-0.33146752	3.05179905	-2.53934759
C	-1.55506726	-4.96428779	0.98913325
C	-1.79811122	-3.47083458	1.33499395
C	-1.93266873	-3.29762370	2.87018012
C	-0.53974365	1.93582580	2.41132227
C	0.33281260	3.05572926	2.53528017
C	-0.16268235	4.23904053	3.12336431
C	-1.47899547	4.32000606	3.59957539
C	-2.32422424	3.20685928	3.48763395
C	-1.88034920	2.00606074	2.89457318
C	2.02393699	4.00536671	0.88142806
C	1.78677697	3.02172979	2.05767180
C	2.76740955	3.31558453	3.22277618
C	2.94981253	-1.90319873	0.41490748
C	3.01736404	-2.93201851	-0.57643389
C	4.26554388	-3.52592892	-0.86498804
C	5.43195160	-3.15249940	-0.18726088
C	5.35893117	-2.15225142	0.79182325
C	4.14539156	-1.50360829	1.09856372
C	-4.11716285	1.21476935	1.96514583
C	-2.86112622	0.83431737	2.79008039
C	-3.27107517	0.30854534	4.19102881
C	3.26499387	0.29294472	-4.19985419
C	2.85750844	0.82383386	-2.80021075
C	4.11491038	1.20630796	-1.97819194
C	1.92561035	-3.30819891	-2.85832695
C	1.79486682	-3.47712093	-1.32233280
C	1.55413888	-4.96982051	-0.97153284
C	4.36847383	-0.97413627	3.58130975
C	4.17674018	-0.39021411	2.15492847
C	5.28247331	0.65876241	1.86495054
C	-2.77047771	3.32056410	-3.21036543
C	-1.78250903	3.02309571	-2.05250501
C	-2.00768690	4.00814078	-0.87497318
H	-6.26238241	-1.86419549	-1.32035826
H	-6.38174745	-3.63214197	0.41897988
H	-4.32038482	-4.30122943	1.63019873
H	-3.21500206	0.12614402	-2.13721250
H	-3.55825456	-1.69037365	-3.83302161
H	-4.35687779	-0.18444508	-4.33395404
H	-5.31565442	-1.52229976	-3.66325019
H	-6.28650623	0.21256525	-1.94938217
H	-5.22604252	1.46314412	-2.61077722
H	-5.17886489	1.08355056	-0.87373607
H	3.33995335	3.25596405	-3.88131140

H	1.83985236	5.22562309	-4.07607693
H	-0.48909478	5.09728592	-3.22361854
H	-0.91227443	-2.91429925	1.01194455
H	-2.39642211	-5.58748277	1.31815825
H	-0.64882092	-5.33293422	1.48772864
H	-1.43514303	-5.10711926	-0.09112783
H	-2.09170760	-2.24861818	3.14259050
H	-1.02362933	-3.64997980	3.37612328
H	-2.77830429	-3.87777198	3.26198341
H	0.49135156	5.10318266	3.21343183
H	-1.84194348	5.23949344	4.05286296
H	-3.34466394	3.27185687	3.85826392
H	1.99700841	2.01149585	1.69186794
H	1.83050850	5.04301901	1.18495731
H	1.37206998	3.77807958	0.02943680
H	3.06492571	3.94535109	0.53619427
H	3.80516779	3.26130424	2.87004672
H	2.64152498	2.59232864	4.03875870
H	2.61007633	4.31995154	3.63711587
H	4.31704830	-4.30685488	-1.62009118
H	6.38057897	-3.63220364	-0.41580453
H	6.26382670	-1.85846660	1.31781885
H	-2.36544162	0.01436476	2.25974881
H	-4.71466177	1.98113010	2.47631104
H	-4.75306609	0.33394871	1.81042695
H	-3.83377526	1.60957653	0.98192914
H	-2.39564438	-0.00344025	4.77570508
H	-3.94562817	-0.55246007	4.09398761
H	-3.79449779	1.08307087	4.76682929
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H	3.78896864	1.06465530	-4.77891958
H	4.71206650	1.97062411	-2.49280626
H	4.75057226	0.32572592	-1.82109685
H	3.83288911	1.60480995	-0.99606773
H	0.90919706	-2.92060354	-0.99877473
H	2.08360230	-2.25988308	-3.13409084
H	1.01548885	-3.66229272	-3.36111517
H	2.77048675	-3.88915708	-3.25054472
H	2.39556066	-5.59311464	-1.30019322
H	0.64738405	-5.34095883	-1.46734378
H	1.43634179	-5.10950699	0.10937628
H	3.21635550	0.13139560	2.13580386
H	3.56864231	-1.67927640	3.83590483
H	4.36565832	-0.17010555	4.32973538
H	5.32514653	-1.50805072	3.66022698
H	6.28698016	0.22268544	1.93616971
H	5.22711361	1.47348958	2.59798670
H	5.17353050	1.08843737	0.86234924
H	-1.99398341	2.01367242	-1.68500524
H	-2.61243595	4.32421861	-3.62614962

H	-3.80569442	3.27045347	-2.84964092
H	-2.65374655	2.59666052	-4.02713222
H	-1.35038933	3.77929668	-0.02766029
H	-3.04623566	3.95180473	-0.52187774
H	-1.81305923	5.04490908	-1.18079301
H	-0.07268780	-0.50172507	3.57802694
H	1.43893582	-2.22737274	2.66126673
H	-1.43694243	-2.23421964	-2.65325262
H	0.07380455	-0.51090145	-3.57467040
Hf	0.00028081	-0.27554633	0.00055573

4.2 One Oxygen Atom

Oxo Complex

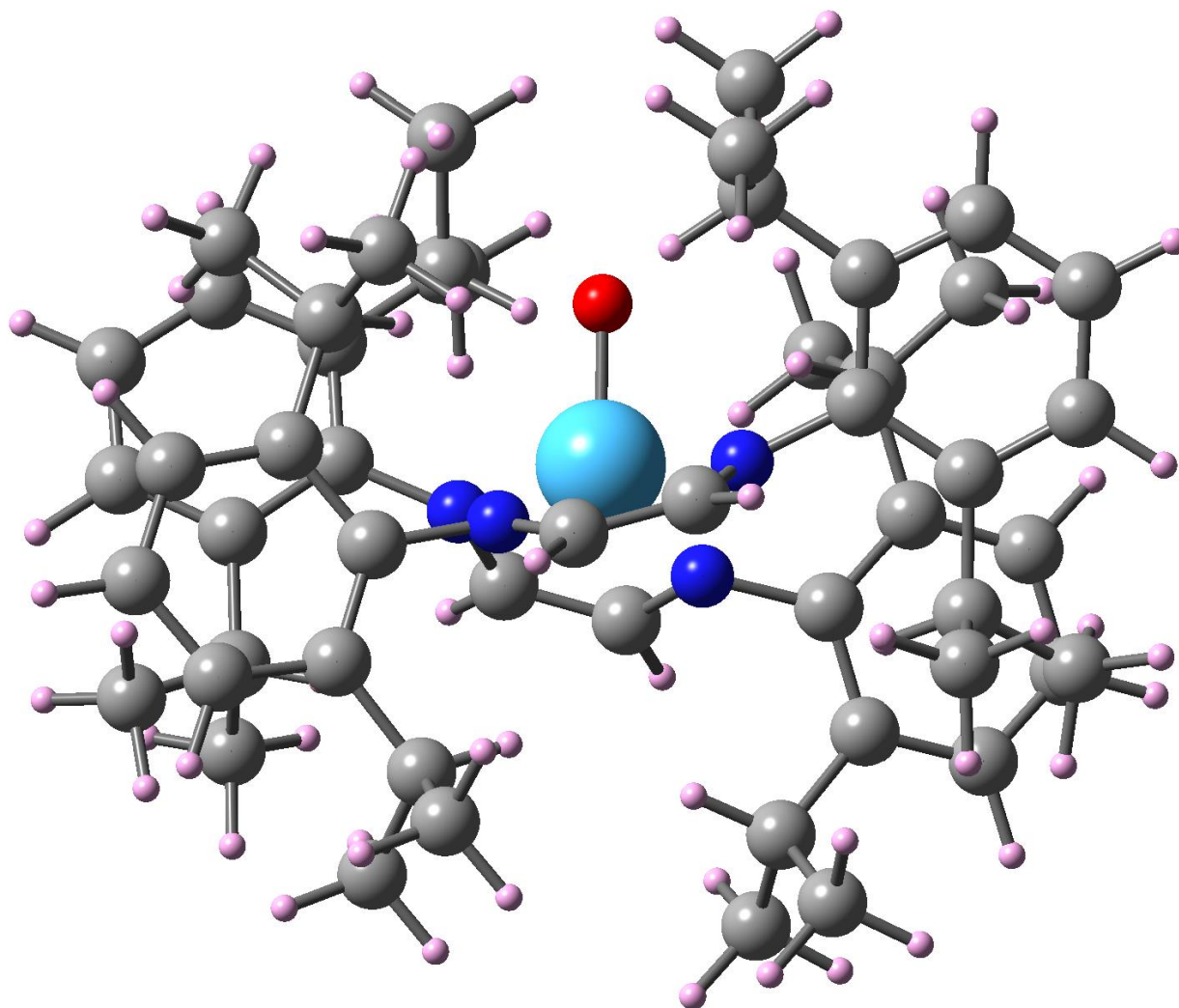


Fig. S11: NCCN Oxo Complex

E	E_{zp}	H	G
-2367.8607	-2366.7234	-2366.6581	-2366.8237

O	0.02826328	2.10895754	-0.37077351
N	-1.12571969	-0.29890899	1.80428416
N	1.57038420	0.36967438	1.60011809
N	1.13065694	-0.89820387	-1.58991757
N	-1.56564462	-0.18536317	-1.62914414
C	-0.29090622	-0.42309042	2.87742147
C	1.06112389	-0.05440203	2.78325414
C	0.28985924	-1.38556224	-2.54999183
C	-1.06073527	-1.00349543	-2.58676884
C	-2.52118743	-0.55022879	2.14051581

C	-3.44051625	0.53977770	2.13875767
C	-4.74378276	0.31078632	2.62706369
C	-5.13248692	-0.94654334	3.11577701
C	-4.22301726	-2.01262752	3.09007690
C	-2.91109237	-1.84474247	2.59991756
C	-4.14334619	2.79503263	1.10767426
C	-3.00838975	1.95420522	1.73589992
C	-2.40640805	2.69851682	2.96037330
C	1.65886971	4.53044051	1.06890241
C	1.67985023	3.32140738	2.03560310
C	1.57045675	3.79103495	3.51290811
C	2.87736897	1.02707579	1.70265917
C	2.92636896	2.44505267	1.85944604
C	4.19250172	3.06154205	1.96347975
C	5.37567476	2.31272057	1.94925334
C	5.30714038	0.91548400	1.85696904
C	4.07054175	0.24456728	1.74358818
C	-2.51730949	-4.19603240	1.67723274
C	-1.97224771	-3.06199503	2.58495781
C	-1.71159740	-3.60676939	4.01505409
C	5.27130870	-1.90519480	1.00813273
C	4.05676180	-1.29003596	1.74406798
C	4.02596927	-1.85582146	3.19394815
C	2.52620684	-1.24180797	-1.83290674
C	2.92428081	-2.61312403	-1.81915886
C	4.23213579	-2.93387189	-2.23883749
C	5.12952927	-1.93834130	-2.64876166
C	4.73470605	-0.59167905	-2.61835248
C	3.43623185	-0.21365061	-2.21736654
C	2.56639777	-4.50376400	-0.13567283
C	1.99751574	-3.75471753	-1.36977752
C	1.72361640	-4.76165045	-2.51918493
C	-1.75097347	3.94633727	-2.42885748
C	-1.72892827	2.48963263	-2.95153666
C	-1.59913672	2.45941082	-4.49996322
C	-2.88212234	0.37979961	-1.94131248
C	-2.95928658	1.68303859	-2.51936167
C	-4.23594445	2.20811716	-2.81600108
C	-5.40428124	1.47032220	-2.58791929
C	-5.30756795	0.16694534	-2.08153999
C	-4.05928385	-0.40824838	-1.76069448
C	4.13238264	2.25642344	-1.98973983
C	3.00119047	1.25293372	-2.31287590
C	2.40932385	1.54518718	-3.72004035
C	-5.17702181	-2.24368222	-0.35258344
C	-4.02059668	-1.87586906	-1.31328032
C	-4.07713882	-2.83418923	-2.53841186
H	-5.45623422	1.12984942	2.64265722
H	-6.13707520	-1.09385095	3.50483688
H	-4.53512069	-2.98962561	3.45196598
H	-2.21330104	1.88507165	0.98475109
H	0.79444977	2.73057986	1.79858251

H	-4.91434045	3.05969711	1.84411405
H	-4.62340535	2.26880649	0.27514985
H	-3.72888430	3.73366282	0.71852585
H	-3.16328139	2.82350384	3.74706484
H	-2.05336726	3.69369912	2.66046351
H	-1.55694767	2.15269873	3.38756034
H	2.52485635	5.19151563	1.21021351
H	0.75203943	5.12587440	1.23949259
H	1.63332502	4.18080354	0.03244783
H	1.54866352	2.93864279	4.20542295
H	0.64917099	4.37130439	3.65775019
H	2.41963751	4.42846716	3.79423377
H	4.24534108	4.14128092	2.07583205
H	6.34013469	2.80866718	2.03059993
H	6.22611049	0.33778632	1.87707888
H	-1.00661965	-2.75678219	2.16835647
H	3.14454752	-1.61821842	1.23080769
H	-3.48678620	-4.56671711	2.03432460
H	-1.81776599	-5.04298878	1.66901021
H	-2.64750508	-3.85043982	0.64514792
H	-2.63921526	-3.96703380	4.47827591
H	-1.29168506	-2.83571327	4.67326654
H	-1.00515393	-4.44692611	3.98184009
H	5.42028604	-1.45399633	0.02409252
H	5.11777554	-2.98184959	0.86755809
H	6.19478267	-1.78296587	1.58999794
H	4.89537301	-1.49780418	3.76150753
H	4.06565896	-2.95373967	3.17169904
H	3.12348359	-1.56486957	3.74087287
H	4.54966057	-3.97410015	-2.24270913
H	6.13004132	-2.20638325	-2.97958969
H	5.43835459	0.17539205	-2.92747370
H	1.03490512	-3.32821634	-1.06860581
H	-0.83696847	2.03175675	-2.52420057
H	3.53558330	-4.96810698	-0.35899098
H	1.87724438	-5.30112697	0.17433289
H	2.70520768	-3.82442516	0.71328607
H	1.29137646	-4.26773184	-3.39845723
H	1.02314948	-5.53958641	-2.18728779
H	2.64835190	-5.25834229	-2.84036759
H	-2.61700466	4.51133762	-2.80058469
H	-0.84395145	4.47102527	-2.75679015
H	-1.75751945	3.95477575	-1.33448633
H	-1.54469897	1.42958006	-4.87819117
H	-0.68713225	2.98553804	-4.81294980
H	-2.45561917	2.94864964	-4.98366955
H	-4.30821334	3.20177472	-3.25016148
H	-6.37715567	1.89522499	-2.82379576
H	-6.21315819	-0.41502868	-1.93793163
H	2.20048709	1.43744070	-1.58846705
H	-3.07312543	-2.04648522	-0.78727385
H	4.90985758	2.26359592	-2.76579832

H	4.60493843	2.03540522	-1.02600701
H	3.71570015	3.27013049	-1.93586000
H	2.05786203	2.58377000	-3.77296202
H	1.56015038	0.88877414	-3.94462198
H	3.17054425	1.39833043	-4.49876998
H	-5.25381326	-1.53784786	0.47739540
H	-5.01391726	-3.24485882	0.06527376
H	-6.14143340	-2.26593401	-0.87732697
H	-3.23824646	-2.68854698	-3.22706364
H	-5.00513076	-2.67359986	-3.10322963
H	-4.06162247	-3.88038571	-2.20305835
Hf	0.00720886	0.33460114	-0.05963249
H	-0.69227365	-0.73345008	3.83854814
H	1.66648998	-0.02222205	3.68519502
H	0.68702418	-2.01159553	-3.34446224
H	-1.66982392	-1.29417795	-3.43826463

4.3 Two Oxygen Atoms

Dioxo Complex (lower energy conformation)

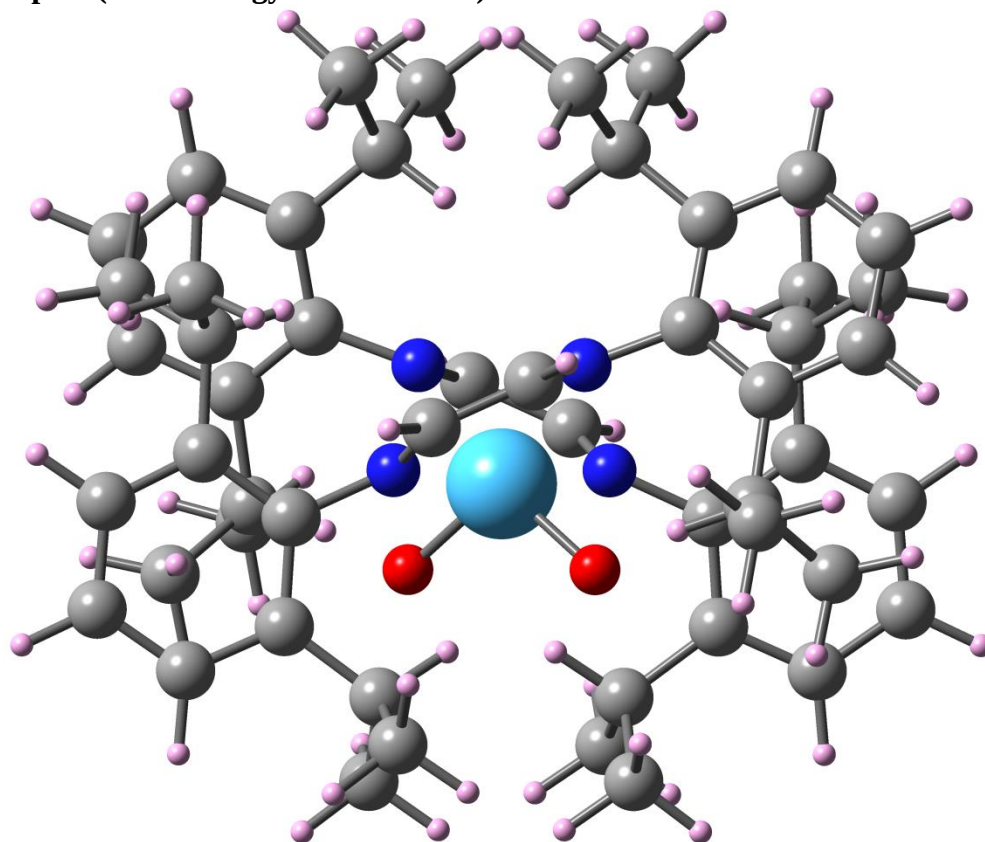


Fig. S12: NCCN Dioxo Complex (lower energy conformation)

E	E_{zp}	H	G
-2443.0564	-2441.9168	-2441.8493	-2442.0208

N	-1.40177400	-0.46228800	1.92969400
N	1.07938800	0.90073400	1.91203800
N	1.40207600	-0.46576500	-1.92740900
N	-1.07875600	0.89810900	-1.91548500
C	-0.91155300	0.09088700	3.00714700
C	0.41559200	0.69426300	3.01875400
C	0.91156800	0.08258900	-3.00718000
C	-0.41528400	0.68657600	-3.02139800
C	-2.72935500	-1.07294900	2.04877300
C	-3.87716900	-0.24041800	2.17452800
C	-5.13218100	-0.86944700	2.31986200
C	-5.24760700	-2.26606400	2.34631300
C	-4.09892800	-3.06166600	2.23020500
C	-2.81822100	-2.49089500	2.07951400
C	-4.88104400	1.91580800	1.23046900
C	-3.81771300	1.29427600	2.16909000
C	-3.98652900	1.86962100	3.60322100

C	1.99759100	4.64727200	0.15820900
C	1.55307600	3.69795300	1.29624900
C	0.98526000	4.50677600	2.49610700
C	2.43891200	1.40691900	2.07801100
C	2.67867400	2.77561900	1.77233400
C	3.95969800	3.30444600	2.02413700
C	4.98358200	2.49984000	2.54611800
C	4.73319900	1.14830400	2.81948200
C	3.46380100	0.56551300	2.60505800
C	-1.72091000	-4.49988100	0.95853000
C	-1.59075000	-3.40584000	2.04534100
C	-1.34472600	-4.02624400	3.44850200
C	4.29859800	-1.81190600	2.22925300
C	3.26210400	-0.91423500	2.95154400
C	3.32071800	-1.13957600	4.48643100
C	2.72921700	-1.07823900	-2.04535300
C	2.81622800	-2.49611200	-2.07790500
C	4.09641800	-3.06822200	-2.22874300
C	5.24610800	-2.27382600	-2.34265900
C	5.13238200	-0.87705500	-2.31391000
C	3.87797900	-0.24686400	-2.16867100
C	1.71560000	-4.50134800	-0.95397900
C	1.58781500	-3.40987500	-2.04383200
C	1.34308800	-4.03364200	-3.44565700
C	-1.99207400	4.65282400	-0.17455400
C	-1.54957900	3.69635800	-1.30734900
C	-0.97965600	4.49761900	-2.51128800
C	-2.43792300	1.40430000	-2.08228600
C	-2.67679200	2.77382500	-1.77920400
C	-3.95789300	3.30268100	-2.03042400
C	-4.98276600	2.49740300	-2.54949200
C	-4.73327400	1.14521700	-2.82041100
C	-3.46390500	0.56226200	-2.60634000
C	4.88814800	1.90948100	-1.23078300
C	3.81889900	1.28776100	-2.16241600
C	3.97873800	1.86323400	-3.59758500
C	-4.30036500	-1.81311800	-2.22236800
C	-3.26404500	-0.91867200	-2.94892000
C	-3.32537900	-1.14837200	-4.48304700
H	-1.45807100	0.06131200	3.95096000
H	0.84808100	0.92144000	3.99569800
H	1.45793600	0.04853500	-3.95094400
H	-0.84764600	0.90972600	-3.99933900
H	-6.02660700	-0.25906400	2.40897400
H	-6.22457300	-2.72998400	2.46009700
H	-4.19244000	-4.14358600	2.26104700
H	-2.83564700	1.60835200	1.79290300
H	0.73967600	3.07008100	0.91001200
H	-5.89800300	1.75070900	1.60871000
H	-4.81878200	1.49410200	0.22288600
H	-4.73185100	3.00076700	1.15553800
H	-4.95769400	1.57641700	4.02252300

H	-3.94257100	2.96716800	3.58579000
H	-3.21011900	1.50837900	4.28961400
H	2.76943000	5.35194500	0.49207100
H	1.14684500	5.24248800	-0.19498400
H	2.40005800	4.08489800	-0.69375500
H	0.62051900	3.84020900	3.28832500
H	0.15161000	5.14642500	2.17853600
H	1.76168500	5.14883700	2.93250200
H	4.15644800	4.35287900	1.81811800
H	5.96692900	2.92267800	2.73740200
H	5.53224600	0.52787200	3.21608600
H	-0.70393800	-2.82117200	1.78453500
H	2.29241000	-1.24557500	2.56532100
H	-2.58742200	-5.15481900	1.12673100
H	-0.82090900	-5.12815600	0.95978100
H	-1.80712300	-4.02007300	-0.02221000
H	-2.18308900	-4.66523500	3.75933100
H	-1.21212300	-3.25101800	4.21682700
H	-0.43611700	-4.64194500	3.42888300
H	4.21606700	-1.69086000	1.14434000
H	4.09097600	-2.86491100	2.45805800
H	5.33153900	-1.59502200	2.53723900
H	4.30487700	-0.87411600	4.89761500
H	3.13518800	-2.19719700	4.71563900
H	2.56821200	-0.54148000	5.01964700
H	4.18862900	-4.15021800	-2.26120400
H	6.22262000	-2.73870600	-2.45643000
H	6.02764200	-0.26766700	-2.40121800
H	0.70116300	-2.82382900	-1.78542100
H	-0.73783700	3.06842600	-0.91751900
H	2.58231500	-5.15685300	-1.11892400
H	0.81542500	-5.12939600	-0.95544000
H	1.80024800	-4.01900600	0.02565900
H	1.21216700	-3.26035500	-4.21622200
H	0.43397300	-4.64860200	-3.42560000
H	2.18123000	-4.67423000	-3.75376200
H	-2.76221800	5.35757700	-0.51219500
H	-1.14016600	5.24824600	0.17563900
H	-2.39595900	4.09592200	0.68031800
H	-0.61576200	3.82616500	-3.29970300
H	-0.14510500	5.13751000	-2.19659300
H	-1.75477300	5.13871600	-2.95140200
H	-4.15404600	4.35156300	-1.82627700
H	-5.96623000	2.92019900	-2.74027700
H	-5.53314000	0.52429700	-3.21458800
H	2.83906100	1.60151800	-1.78004600
H	-2.29425000	-1.25008400	-2.56303500
H	5.90263600	1.74513100	-1.61597500
H	4.83280300	1.48758600	-0.22285400
H	4.73886100	2.99430000	-1.15458000
H	3.93556800	2.96081900	-3.57980800
H	3.19766600	1.50259200	-4.27893100

H	4.94702400	1.56937100	-4.02306900
H	-4.21588200	-1.68899100	-1.13794800
H	-4.09424000	-2.86701000	-2.44842400
H	-5.33358700	-1.59603300	-2.52927900
H	-2.57303300	-0.55266500	-5.01914000
H	-4.30987300	-0.88291800	-4.89343000
H	-3.14144000	-2.20685700	-4.70951700
O	1.21337000	-1.75487400	0.84311800
O	-1.21469300	-1.75273800	-0.84041200
Hf	0.00044900	-0.63962700	0.00123100

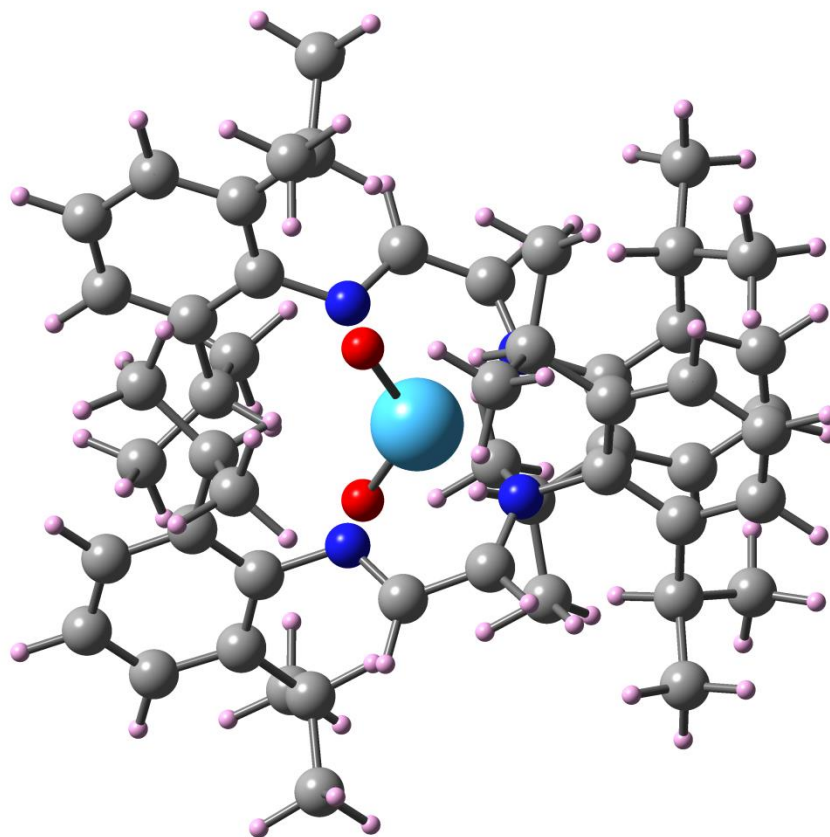
Dioxo Complex (higher energy conformation)

Fig. S13: NCCN Dioxo Complex (higher energy conformation)

E	E_{zp}	H	G
-2443.0530	-2441.9131	-2441.8461	-2442.0155

O	1.01221401	-1.16877600	1.22275580
O	1.01130329	1.16930665	-1.22298644
N	-1.42438663	1.11084832	1.44138607
N	1.24247129	1.86464175	1.17924161
N	1.24407278	-1.86455035	-1.17945105
N	-1.42247543	-1.11275097	-1.44233578
C	-0.95220279	2.20336100	2.00130955
C	0.38848523	2.68445674	1.74005573
C	0.39125936	-2.68459286	-1.74180326
C	-0.94941460	-2.20388015	-2.00401984
C	-2.74484141	0.70391922	1.94390130
C	-3.89286861	1.47498995	1.60261363
C	-5.11757599	1.13976337	2.21963636
C	-5.20447945	0.09043502	3.14518836
C	-4.06165804	-0.66060456	3.45678797
C	-2.81126603	-0.37845082	2.86697462
C	-4.98172758	2.58274177	-0.43017845
C	-3.85419821	2.66270139	0.62891030

C	-3.95194218	4.01956934	1.38139255
C	2.11492599	4.09398216	-2.18793378
C	1.81560818	4.18371091	-0.67028586
C	1.67654840	5.65941320	-0.21038620
C	2.60445581	2.31792998	0.97798886
C	2.88094676	3.43963782	0.14420086
C	4.22637054	3.84572535	0.02290470
C	5.25746213	3.17535704	0.69646341
C	4.95933965	2.06922494	1.50780563
C	3.63481655	1.61508902	1.66697336
C	-1.82214941	-2.68323773	3.41698158
C	-1.56987190	-1.15974988	3.31033489
C	-1.04322033	-0.60389101	4.66215930
C	4.41799150	-0.59664836	2.71839075
C	3.30438636	0.47059745	2.62722338
C	2.98950925	1.03728673	4.04066205
C	2.60614406	-2.31723527	-0.97721755
C	2.88267359	-3.43888704	-0.14340858
C	4.22812304	-3.84471911	-0.02171028
C	5.25928495	-3.17407245	-0.69491977
C	4.96116146	-2.06784559	-1.50611880
C	3.63657254	-1.61395117	-1.66558071
C	2.11616082	-4.09193330	2.18874457
C	1.81726502	-4.18287176	0.67107854
C	1.67873947	-5.65891852	0.21215550
C	-1.81885069	2.68094479	-3.41441131
C	-1.56800081	1.15674279	-3.31415743
C	-1.04699726	0.60471069	-4.66969026
C	-2.74285527	-0.70531537	-1.94489585
C	-2.80916690	0.37596774	-2.86914755
C	-4.05981779	0.65839922	-3.45838726
C	-5.20292940	-0.09147678	-3.14524555
C	-5.11609152	-1.13996393	-2.21868185
C	-3.89118987	-1.47535407	-1.60218084
C	4.41995835	0.59844147	-2.71533997
C	3.30643594	-0.46903573	-2.62542738
C	2.99235133	-1.03500229	-4.03934080
C	-4.98176680	-2.58453062	0.42920662
C	-3.85212073	-2.66242619	-0.62775679
C	-3.94630700	-4.01995408	-1.37968799
H	-6.00851180	1.71262894	1.97735204
H	-6.15539585	-0.14053863	3.61917685
H	-4.13517353	-1.47155157	4.17557655
H	-2.89962938	2.64221908	0.08908554
H	0.85417602	3.68000822	-0.53597047
H	-5.97121629	2.72686512	0.02304998
H	-4.97897469	1.61919425	-0.94633079
H	-4.84727769	3.37214223	-1.18143684
H	-4.89402116	4.08400982	1.94145429
H	-3.92633113	4.85250104	0.66647375
H	-3.13306500	4.16434606	2.09687132
H	3.08419776	4.54216055	-2.44456134

H	1.33845322	4.62614515	-2.75651991
H	2.10589550	3.04029970	-2.48246716
H	1.42608227	5.73425373	0.85740672
H	0.88671608	6.16429386	-0.78327834
H	2.60993300	6.21628785	-0.36697347
H	4.46835760	4.68848644	-0.61997212
H	6.28680109	3.50964718	0.58713241
H	5.76266399	1.55300704	2.02413010
H	-0.76396711	-1.03340533	2.57874902
H	2.40905025	-0.04411501	2.25177334
H	-2.50395242	-2.94053310	4.23930579
H	-0.86921580	-3.19433783	3.60001491
H	-2.24445193	-3.08329178	2.48569630
H	-1.78801881	-0.72592877	5.46116827
H	-0.79736073	0.46383648	4.58948524
H	-0.13003187	-1.13712162	4.95479513
H	4.68443976	-0.97747267	1.72532439
H	4.05863999	-1.44586584	3.31375179
H	5.32802658	-0.21647223	3.20484257
H	3.86710827	1.54382013	4.46753181
H	2.70090714	0.22275855	4.71875294
H	2.16354530	1.76062861	4.01355493
H	4.47006700	-4.68744446	0.62123171
H	6.28866136	-3.50817182	-0.58536718
H	5.76453479	-1.55129835	-2.02204792
H	0.85567468	-3.67967094	0.53599077
H	-0.75992675	1.02720598	-2.58557632
H	3.08545103	-4.53983988	2.44581504
H	1.33965262	-4.62376839	2.75759196
H	2.10704180	-3.03801391	2.48245705
H	1.42853271	-5.73453806	-0.85564420
H	0.88888620	-6.16357777	0.78521361
H	2.61219334	-6.21550906	0.36935032
H	-2.50454124	2.94188813	-4.23233031
H	-0.86621406	3.19157013	-3.60026723
H	-2.23590212	3.07812232	-2.47952776
H	-0.80290632	-0.46374750	-4.60152933
H	-0.13392395	1.13736198	-4.96378009
H	-1.79426946	0.73073198	-5.46577481
H	-4.13317334	1.46861322	-4.17804584
H	-6.15400887	0.13966320	-3.61882472
H	-6.00722489	-1.71197121	-1.97517531
H	2.41083447	0.04538953	-2.25030805
H	-2.89841733	-2.63991841	-0.08644283
H	5.33032305	0.21867262	-3.20147946
H	4.68577491	0.97869172	-1.72189307
H	4.06080585	1.44795717	-3.31038993
H	2.70416856	-0.22010113	-4.71715994
H	2.16631928	-1.75829895	-4.01297927
H	3.87013033	-1.54137462	-4.46601933
H	-4.98366448	-1.62001652	0.94357498
H	-4.84563291	-3.37199833	1.18216413

H	-5.96990678	-2.73341981	-0.02546866
H	-3.12513569	-4.16450267	-2.09251643
H	-4.88670097	-4.08545770	-1.94243559
H	-3.92200444	-4.85236691	-0.66411796
Hf	0.17563412	-0.00007799	-0.00013308
H	-1.55654144	2.75700043	2.72102354
H	0.65958510	3.68917511	2.06427849
H	0.66345224	-3.68892699	-2.06626490
H	-1.55275655	-2.75626935	-2.72551255

Peroxo Complex

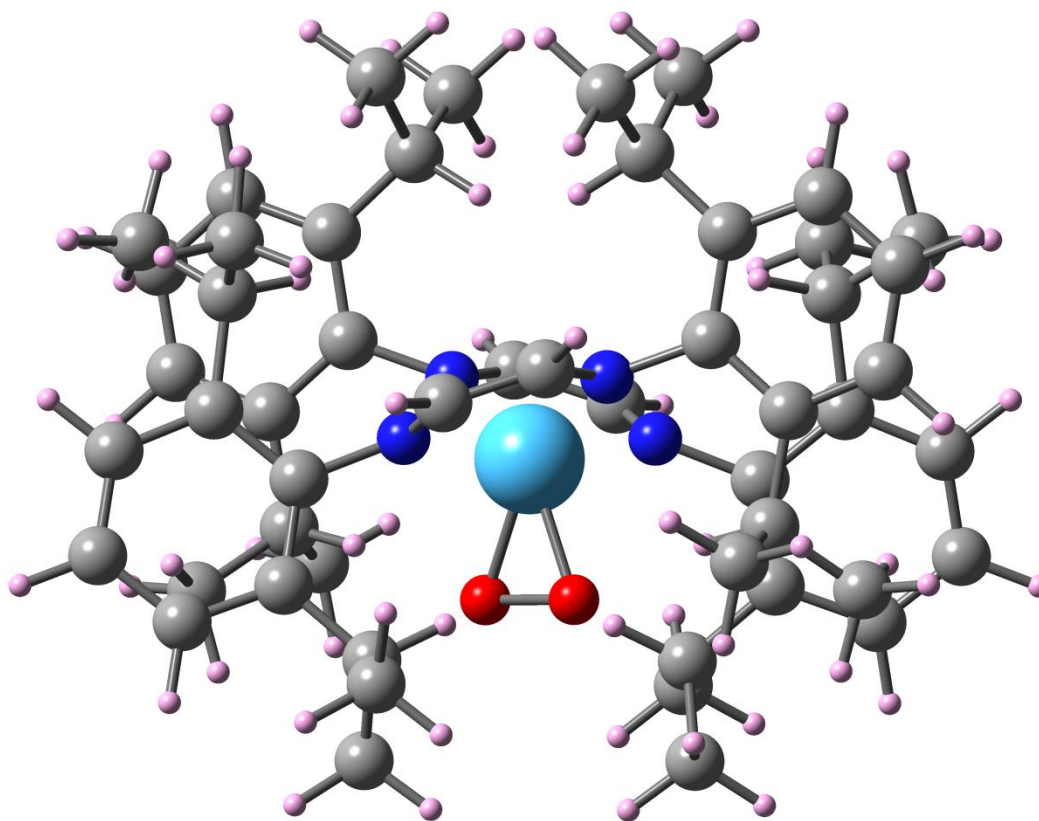


Fig. S14: NCCN Peroxo Complex

E	E_{zp}	H	G
-2443.0194	-2441.8785	-2441.8124	-2441.9777
O	0.57465516	-2.33674038	0.53876905
O	-0.57857697	-2.33375572	-0.54891315
N	1.63915656	-0.22958450	-1.58004155
N	-1.00879544	0.56632538	-1.70881300
N	-1.63844784	-0.23887436	1.58150669
N	1.00861627	0.55578319	1.71233151
C	1.12882951	0.23037745	-2.74613139
C	-0.20315582	0.67400874	-2.80503155
C	-1.12749084	0.21319665	2.75013866
C	0.20465345	0.65656210	2.81028786
C	3.00412612	-0.76245059	-1.69262373
C	4.11110145	0.13694779	-1.62485979
C	5.41182693	-0.39256003	-1.76194461
C	5.62471838	-1.76076967	-1.98354243
C	4.52530605	-2.61908406	-2.10350698
C	3.20039404	-2.14536703	-1.97897288
C	5.07864148	2.33037871	-0.69520268
C	3.93572246	1.65574443	-1.49089080

C	3.84446523	2.33810382	-2.88700927
C	-1.99989349	4.47861383	-0.59621232
C	-1.50125906	3.48605429	-1.67841808
C	-0.99434735	4.26524522	-2.92193308
C	-2.36212780	1.05389283	-1.99283096
C	-2.57850711	2.46086816	-2.06143607
C	-3.82322392	2.92199044	-2.53797863
C	-4.82924197	2.02560009	-2.92618657
C	-4.60794507	0.64409466	-2.82437030
C	-3.37594215	0.12785529	-2.36712695
C	2.15451424	-4.42916481	-1.44853281
C	2.05376664	-3.12036398	-2.26923024
C	1.99860865	-3.43039160	-3.79174416
C	-4.33884541	-2.20597694	-1.88047333
C	-3.13070478	-1.38498550	-2.39086323
C	-2.73347381	-1.84375064	-3.82171298
C	-3.00356055	-0.77205143	1.68963260
C	-3.20092929	-2.15634025	1.96831105
C	-4.52635926	-2.63001664	2.08764310
C	-5.62511283	-1.77053623	1.97005601
C	-5.41118515	-0.40123658	1.75616746
C	-4.10995053	0.12828191	1.62440655
C	-2.15472257	-4.43773783	1.42779777
C	-2.05534860	-3.13338775	2.25578219
C	-2.00387352	-3.45172414	3.77673715
C	2.00057103	4.47401322	0.62099016
C	1.50230632	3.47517993	1.69758240
C	0.99619266	4.24716261	2.94590451
C	2.36248725	1.04110963	1.99756118
C	2.57963427	2.44754429	2.07386574
C	3.82487536	2.90537454	2.55217891
C	4.83069433	2.00628776	2.93465001
C	4.60855311	0.62548779	2.82545854
C	3.37591389	0.11244243	2.36628176
C	-5.07446665	2.32807756	0.70640385
C	-3.93293100	1.64763537	1.49907120
C	-3.84167429	2.32205461	2.89904353
C	4.33675970	-2.21911297	1.86564894
C	3.12981855	-1.40037438	2.38245467
C	2.73483650	-1.86643764	3.81155923
H	6.26664970	0.27345103	-1.69910875
H	6.63643321	-2.14761421	-2.08110808
H	4.68997306	-3.67259292	-2.31298005
H	2.99377676	1.83895930	-0.95915725
H	-0.64679899	2.94611348	-1.25544720
H	6.01040832	2.35364616	-1.27628674
H	5.27258191	1.81789262	0.25026583
H	4.81318102	3.37040933	-0.46909523
H	4.74724848	2.12569084	-3.47528379
H	3.76572310	3.42791340	-2.77037788
H	2.97814039	2.00005619	-3.46429231
H	-2.84826367	5.07571486	-0.95475919

H	-1.19552347	5.17550455	-0.32513980
H	-2.31694653	3.95317553	0.31213284
H	-0.58546283	3.58803192	-3.68169778
H	-0.20390733	4.97194300	-2.63537767
H	-1.80721026	4.83816505	-3.38729078
H	-4.00390582	3.99187607	-2.60980623
H	-5.77897217	2.39981074	-3.30095987
H	-5.39258314	-0.04491173	-3.12353746
H	1.10476654	-2.66103928	-1.99283106
H	-2.28747134	-1.61676278	-1.73334103
H	3.05879642	-5.00553731	-1.68894181
H	1.28558997	-5.06458074	-1.66340505
H	2.14439397	-4.20570033	-0.37731274
H	2.91636332	-3.92853081	-4.13300513
H	1.87465851	-2.51457734	-4.38578459
H	1.15102897	-4.09403692	-4.00918290
H	-4.65957432	-1.87448368	-0.88706913
H	-4.05770008	-3.26431450	-1.80866780
H	-5.19849776	-2.14046293	-2.56142193
H	-3.54366195	-1.64319049	-4.53632844
H	-2.52803765	-2.92192371	-3.82799695
H	-1.83289903	-1.32613240	-4.17449433
H	-4.69198217	-3.68456767	2.29098792
H	-6.63719146	-2.15743655	2.06353939
H	-6.26553187	0.26555280	1.69528217
H	-1.10551707	-2.67294023	1.98394947
H	0.64755532	2.93777894	1.27195764
H	-3.06038943	-5.01439654	1.66219391
H	-1.28720045	-5.07521012	1.64227131
H	-2.14077016	-4.20853337	0.35784479
H	-1.88131070	-2.53919552	4.37609968
H	-1.15687415	-4.11661955	3.99264680
H	-2.92245646	-3.95164783	4.11313729
H	2.85063659	5.06716927	0.98193308
H	1.19695290	5.17407642	0.35586323
H	2.31503209	3.95394725	-0.29132720
H	0.58709755	3.56563955	3.70166838
H	0.20613090	4.95601387	2.66369300
H	1.80951478	4.81678041	3.41448394
H	4.00613018	3.97475174	2.62993921
H	5.78089996	2.37790349	3.31079570
H	5.39304908	-0.06557212	3.12029726
H	-2.99035728	1.83263147	0.96899281
H	2.28525336	-1.62829877	1.72530208
H	-6.00665857	2.34917145	1.28690759
H	-5.26830693	1.82111446	-0.24206187
H	-4.80761463	3.36901524	0.48627599
H	-3.76088900	3.41235062	2.78851523
H	-2.97643627	1.97926182	3.47510239
H	-4.74532904	2.10802148	3.48539823
H	4.65634482	-1.88192840	0.87379415
H	4.05498332	-3.27688499	1.78798690

H	5.19734762	-2.15800827	2.54581541
H	1.83454262	-1.35089534	4.16813546
H	3.54591703	-1.66910526	4.52603913
H	2.52985191	-2.94471209	3.81272607
Hf	-0.00097500	-0.50134277	-0.00129976
H	1.73253330	0.21847868	-3.64987069
H	-0.60179255	1.07455988	-3.73322393
H	-1.73033275	0.19522077	3.65435870
H	0.60446924	1.05145847	3.74039423

4.4 Three Oxygen Atoms

Oxo Peroxo Complex (planar conformation)

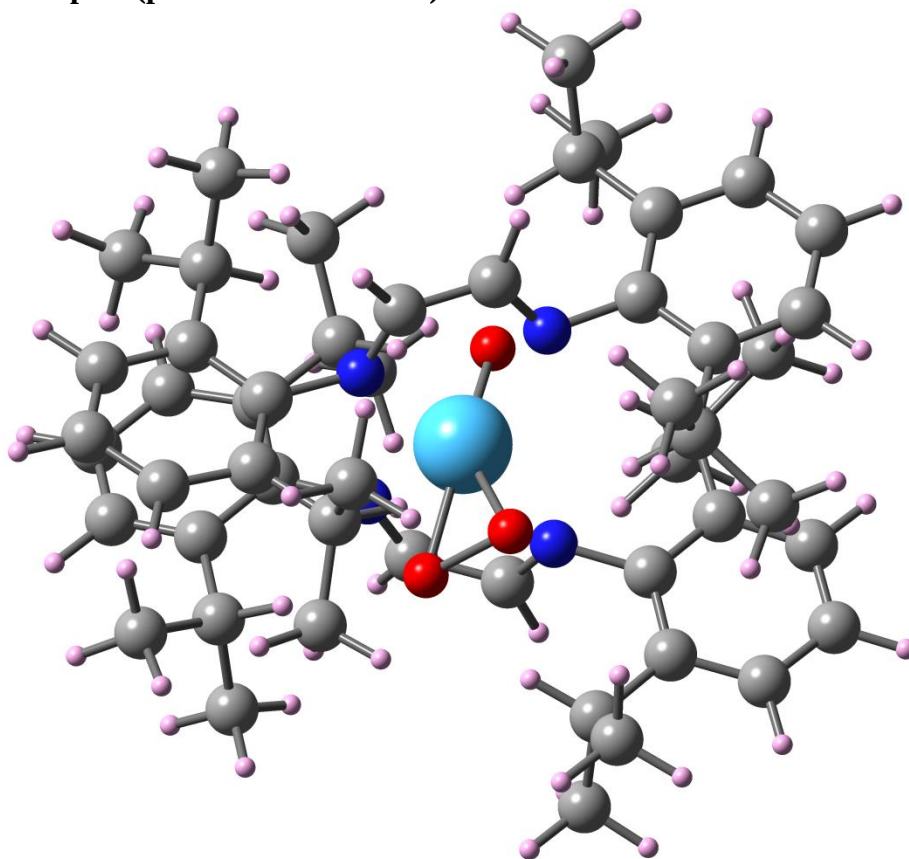


Fig. S15: NCCN Oxo Peroxo Complex (planar conformation)

E	E_{zp}	H	G
-2518.2303	-2517.0860	-2517.0181	-2517.1870

O	0.48240791	-1.30966881	1.15242307
O	-0.48668097	1.97473559	-0.80656121
O	0.73768533	1.33471663	-1.54372527
N	1.27178580	-1.57520078	-1.36072599
N	-1.43393898	-0.96232107	-1.63430432
N	-1.32989465	0.89492006	1.72898125
N	1.36652266	1.52229252	1.33576328
C	0.51022815	-2.28657906	-2.14887728
C	-0.86369909	-1.87197759	-2.38132245
C	-0.70137557	1.70712058	2.52923233
C	0.69433288	2.07792411	2.29584964
C	2.63034432	-2.05930358	-1.15675400
C	3.68938778	-1.32199196	-1.75764948
C	4.99767540	-1.82821008	-1.62279607
C	5.24737394	-3.02096068	-0.92490862
C	4.18537993	-3.72646202	-0.34203556
C	2.85325328	-3.26999185	-0.44193000

C	4.53909101	0.96486761	-2.57528683
C	3.40951906	-0.08849037	-2.62251381
C	3.14823931	-0.51783754	-4.09451578
C	-2.01716130	2.69264330	-3.67314808
C	-1.80487057	1.15933256	-3.66959746
C	-1.56608586	0.63456338	-5.11273573
C	-2.80087414	-0.60017692	-2.03869284
C	-2.97575074	0.41000265	-3.02258923
C	-4.29422757	0.67013203	-3.45642351
C	-5.38744155	-0.03958490	-2.94077688
C	-5.18294917	-1.03672194	-1.97428915
C	-3.88848118	-1.34601862	-1.50673961
C	1.97138911	-4.23164353	1.74793154
C	1.73668565	-4.08498493	0.22344992
C	1.58085313	-5.47445734	-0.45105438
C	-4.84253520	-2.64816372	0.49271349
C	-3.67914491	-2.49969717	-0.51597755
C	-3.48456447	-3.85065400	-1.26273123
C	-2.70327412	0.57320745	2.13277444
C	-2.90790518	-0.50767526	3.03169377
C	-4.21879562	-0.70088675	3.51743788
C	-5.27557949	0.13052609	3.11487785
C	-5.04402660	1.17240031	2.20240862
C	-3.75208548	1.42316259	1.69284147
C	-2.12330721	-2.90428302	3.49614592
C	-1.75473776	-1.40053585	3.50962812
C	-1.29244178	-0.97936108	4.93155169
C	2.27957701	4.34711215	-1.62391600
C	1.97846309	4.02438923	-0.13952801
C	1.80853286	5.33076873	0.68319250
C	2.76293768	1.92944592	1.17782389
C	3.05865440	3.13266374	0.48462882
C	4.41601413	3.51468906	0.40813895
C	5.42819735	2.73574548	0.98678030
C	5.10170894	1.54953692	1.66444038
C	3.76367922	1.12002447	1.78154372
C	-4.61894021	2.80955848	-0.28506506
C	-3.49160726	2.61016313	0.75560167
C	-3.29591578	3.92139469	1.56784175
C	4.47582975	-1.23133502	2.53445405
C	3.39874032	-0.12447273	2.60098070
C	3.14957259	0.26083786	4.08756838
H	5.82491756	-1.28943828	-2.07424527
H	6.26412505	-3.39666267	-0.83645453
H	4.38920277	-4.64395067	0.20404788
H	2.49818286	0.39755480	-2.25617825
H	-0.89629619	0.98992778	-3.08636167
H	5.45550670	0.61054061	-3.06763837
H	4.78415695	1.24518578	-1.54514773
H	4.21472573	1.87130939	-3.10162676
H	4.03492780	-1.00642964	-4.52191274
H	2.91147611	0.36243864	-4.70607978

H	2.30573340	-1.21693389	-4.17259630
H	-2.89981700	2.99601529	-4.25367978
H	-1.13930872	3.18076865	-4.11547457
H	-2.11142790	3.05660699	-2.64556649
H	-1.36472380	-0.44609751	-5.12759715
H	-0.70237256	1.14465033	-5.55880681
H	-2.43857114	0.81783802	-5.75514194
H	-4.45991797	1.43448750	-4.21046964
H	-6.39331896	0.17810256	-3.29207797
H	-6.03583264	-1.58331972	-1.58431478
H	0.79756321	-3.53237669	0.13378460
H	-2.76364919	-2.29813830	0.05674271
H	2.93286639	-4.71078452	1.97773779
H	1.17482604	-4.84711840	2.18900435
H	1.93062505	-3.24182842	2.21163678
H	2.48837703	-6.08121049	-0.33165559
H	1.38274114	-5.38817811	-1.52872848
H	0.74789644	-6.02576705	0.00563749
H	-5.07489802	-1.69915896	0.98392809
H	-4.57135990	-3.37455781	1.26896504
H	-5.75353965	-3.01955880	0.00469911
H	-4.36436430	-4.07835256	-1.87928082
H	-3.35350892	-4.66671984	-0.53993280
H	-2.60806084	-3.84440160	-1.92094671
H	-4.41112531	-1.51095109	4.21562419
H	-6.27652055	-0.03498180	3.50659869
H	-5.87085205	1.80286386	1.88867664
H	-0.90745773	-1.29018329	2.81923384
H	1.02663124	3.48480088	-0.14465088
H	-2.91442852	-3.15176140	4.21765627
H	-1.23743351	-3.49809243	3.75478475
H	-2.45506464	-3.21813962	2.49920675
H	-0.95802650	0.06654585	4.95828795
H	-0.45229447	-1.60701305	5.25652716
H	-2.10465408	-1.08800627	5.66401889
H	3.22375788	4.89492596	-1.75193392
H	1.47233361	4.96716954	-2.03585676
H	2.31508167	3.41909374	-2.20246158
H	1.54180387	5.12280526	1.72924196
H	1.01295263	5.94971259	0.24748913
H	2.73341812	5.92415830	0.69067425
H	4.67771576	4.43033055	-0.11557319
H	6.46671781	3.05018816	0.91207363
H	5.89255716	0.95415653	2.11016142
H	-2.56450115	2.42070668	0.20003801
H	2.46691204	-0.54600441	2.19874300
H	-5.55414296	3.14535742	0.18366397
H	-4.82179017	1.88757626	-0.83879665
H	-4.31925966	3.57911503	-1.00768257
H	-3.10585850	4.76033403	0.88613150
H	-2.44753467	3.85634698	2.26064657
H	-4.19339154	4.15356264	2.15746493

H	4.72356008	-1.48892481	1.49976322
H	4.10190609	-2.13789235	3.02631766
H	5.40061123	-0.93683000	3.05022627
H	2.34295351	0.99698949	4.19565151
H	4.05635351	0.68942700	4.53660238
H	2.86860165	-0.62969396	4.66528011
Hf	0.04952523	0.07813462	-0.07005793
H	0.87230720	-3.18699105	-2.64548719
H	-1.40493922	-2.33359930	-3.20811695
H	-1.19176100	2.11349890	3.41485929
H	1.14624504	2.81463208	2.96166269

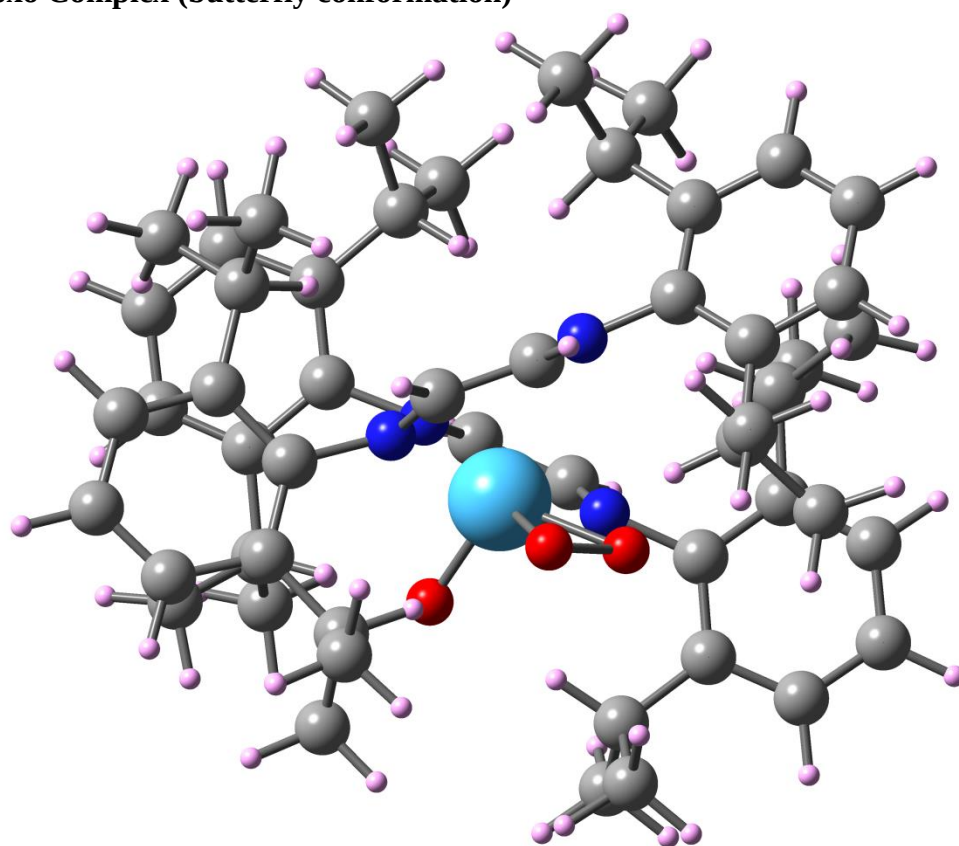
Oxo Peroxo Complex (butterfly conformation)

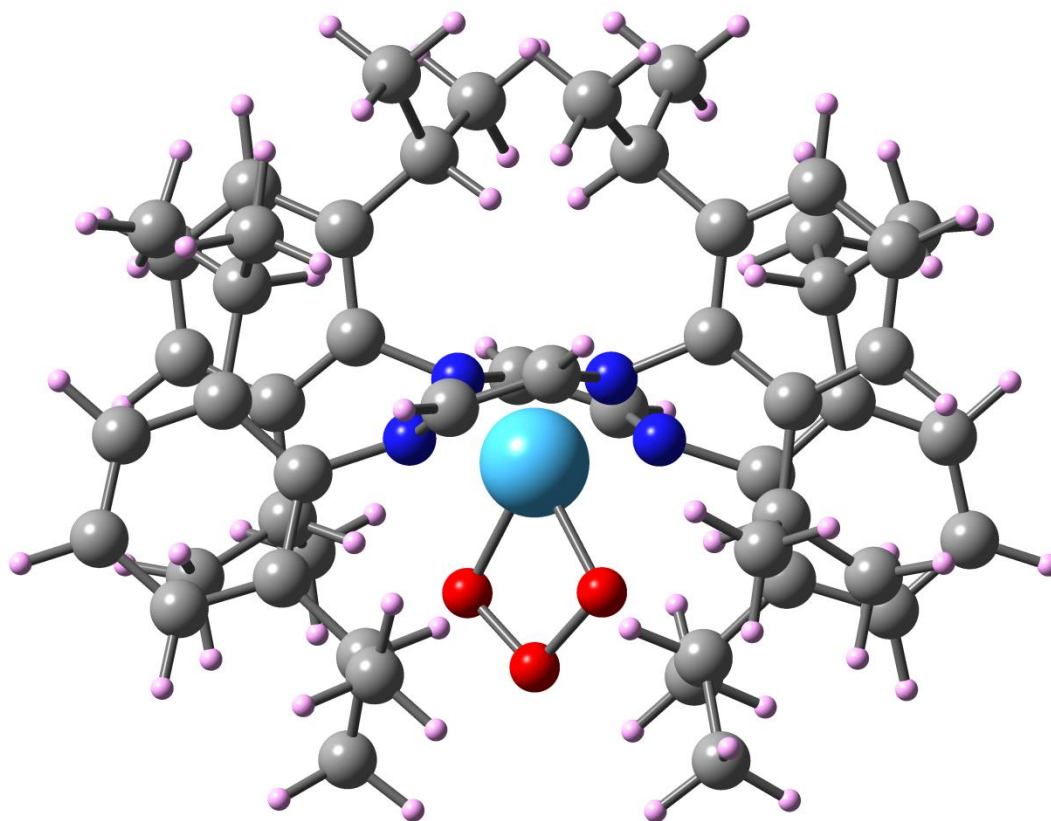
Fig. S16: NCCN Oxo Peroxo Complex (butterfly conformation)

E	E_{zp}	H	G
-2518.2226	-2517.0789	-2517.0107	-2517.1820
O	1.72831600	-1.53765700	0.93978800
N	-1.07674300	0.26397600	-1.92771200
N	1.43427000	-1.01942100	-1.75913600
N	-1.53629500	0.05250300	1.76038100
N	1.12487100	1.40576300	1.59696000
C	-0.36297400	0.00231600	-2.98761800
C	0.96841300	-0.59812900	-2.89890700
C	-0.89188500	0.60671100	2.75124300
C	0.49245000	1.09843900	2.69855300
C	-2.42286900	0.79204900	-2.23471500
C	-3.50373700	-0.11348800	-2.43227000
C	-4.73831400	0.43087600	-2.85221300
C	-4.89777000	1.80195100	-3.09098000
C	-3.81544300	2.67020700	-2.89291300
C	-2.56370700	2.19041200	-2.45579300
C	-4.53181800	-2.25538700	-1.48150700
C	-3.37093200	-1.63312600	-2.29581300
C	-3.28193400	-2.29351100	-3.69957700

C	1.78824600	-4.77544000	-0.00001300
C	1.66388200	-3.93729100	-1.29582600
C	1.45934500	-4.84926400	-2.53694800
C	2.76621100	-1.62845500	-1.75620400
C	2.87446000	-3.02376200	-1.50247700
C	4.16344800	-3.59437100	-1.53213200
C	5.30188400	-2.82238700	-1.79970400
C	5.16840500	-1.44965500	-2.04961100
C	3.90635000	-0.81973300	-2.03678500
C	-1.79637800	4.45396300	-1.53700300
C	-1.39585300	3.17485400	-2.31318100
C	-0.82527300	3.55166300	-3.70885700
C	4.85737000	1.47658700	-1.43612800
C	3.84410200	0.69137800	-2.30615900
C	4.08348100	1.00774500	-3.80884500
C	-2.94164300	-0.30467800	2.00827600
C	-3.26200300	-1.61702700	2.45605000
C	-4.62321400	-1.91024100	2.69553700
C	-5.62674300	-0.95147600	2.51321300
C	-5.28277100	0.34223900	2.09437900
C	-3.94180700	0.69625200	1.83865500
C	-2.48647900	-3.99886600	1.95499800
C	-2.22395500	-2.70232300	2.76253300
C	-2.18242900	-2.99199700	4.28824300
C	2.06062800	4.59991200	-0.99833000
C	1.56010400	3.94771900	0.31356400
C	0.88740300	5.00532800	1.23340900
C	2.45078600	1.97737400	1.72256900
C	2.67547200	3.23061900	1.07695300
C	3.92109900	3.86612200	1.23890500
C	4.94073100	3.27763600	2.00089200
C	4.71851100	2.03409200	2.60621000
C	3.48515900	1.35509900	2.49389400
C	-4.71084200	2.80257600	0.58545800
C	-3.60437400	2.14094100	1.44162900
C	-3.34322500	3.02568900	2.69402400
C	4.43384400	-1.00349800	2.66951900
C	3.36089300	-0.01031600	3.18640200
C	3.45657800	0.13608800	4.72971100
H	-0.75631600	0.18288000	-3.99001900
H	1.52607700	-0.72845400	-3.82700800
H	-1.38515800	0.72472600	3.71970300
H	0.93403200	1.29060300	3.67984700
H	-5.57733300	-0.24063900	-3.00965100
H	-5.85436000	2.19070600	-3.43148100
H	-3.94371800	3.73180900	-3.08394300
H	-2.45476500	-1.87311600	-1.74720800
H	0.75937400	-3.33439900	-1.18313100
H	-5.49973200	-2.17673500	-1.99682000
H	-4.62335600	-1.78097800	-0.49787600
H	-4.32762900	-3.32109100	-1.31861500
H	-4.19313400	-2.11622800	-4.28855000

H	-3.15011400	-3.37777700	-3.59169800
H	-2.43005400	-1.90912100	-4.27802400
H	2.63413800	-5.47695200	-0.03585400
H	0.87169000	-5.36160100	0.14607700
H	1.91106800	-4.10998700	0.86019600
H	1.32618800	-4.25931000	-3.45512000
H	0.56230900	-5.46682900	-2.39930700
H	2.31515400	-5.52111500	-2.69223100
H	4.27006100	-4.65928600	-1.34572100
H	6.28569500	-3.28535200	-1.81459900
H	6.05643000	-0.85653600	-2.24930600
H	-0.59329600	2.68630400	-1.74651600
H	2.84657100	1.06180300	-2.03894300
H	-2.58769800	5.01167500	-2.05198600
H	-0.93520500	5.12481900	-1.44311600
H	-2.15287500	4.21231600	-0.52911300
H	-1.59256700	4.04060400	-4.32300100
H	-0.47875900	2.66637800	-4.25724200
H	0.02217300	4.24190600	-3.60750100
H	4.72096900	1.26003200	-0.37214400
H	4.72394900	2.55589700	-1.58197700
H	5.89325500	1.23439100	-1.70469900
H	5.07781700	0.66517400	-4.12304000
H	4.02811900	2.09025900	-3.98692400
H	3.34837100	0.51619500	-4.45984600
H	-4.89031400	-2.90637900	3.03766500
H	-6.66715600	-1.20471400	2.70294100
H	-6.06521700	1.08315200	1.96491100
H	-1.22980100	-2.35814500	2.47304800
H	0.79818700	3.20215400	0.05771500
H	-3.47946000	-4.42301800	2.16091500
H	-1.73568600	-4.75451900	2.22253600
H	-2.38777400	-3.79206000	0.88450500
H	-1.96998000	-2.08242500	4.86723100
H	-1.39125700	-3.72131600	4.50429000
H	-3.13432200	-3.40528900	4.64957100
H	2.76826600	5.41576800	-0.80551800
H	1.22068200	5.02917500	-1.55763000
H	2.56107300	3.86520900	-1.64216200
H	0.48623300	4.53836200	2.14199300
H	0.06168600	5.51037500	0.71564000
H	1.61442300	5.76806000	1.54227200
H	4.09460200	4.83218800	0.77295900
H	5.89757200	3.78077200	2.11842100
H	5.51638300	1.57428300	3.18309700
H	-2.68453100	2.12259400	0.84136200
H	2.40023600	-0.46527800	2.94379000
H	-5.61014900	3.00740000	1.18089500
H	-4.99355500	2.17454800	-0.26444300
H	-4.35786200	3.76484300	0.19454900
H	-3.13192200	4.06091800	2.39292200
H	-2.49473900	2.66983000	3.28928800

H	-4.22658900	3.03496900	3.34615700
H	4.32048100	-1.15807400	1.59225000
H	4.29480800	-1.97749800	3.15598300
H	5.45646900	-0.66047400	2.88080100
H	2.68788300	0.81342700	5.12865700
H	4.43375200	0.53095500	5.03962400
H	3.32325600	-0.84412800	5.20552800
O	-0.99461900	-2.25499700	-0.43474200
O	0.65980800	-1.49044600	2.02002800
Hf	-0.02498700	-0.83233500	0.14659300

η^2 -ozone ComplexFig. S17: NCCN η^2 -ozone Complex

E	E_{zp}	H	G
-2518.1678	-2517.0237	-2516.9565	-2517.1251

O	0.88400583	-2.26540091	0.75606127
O	-0.88015206	-2.27448342	-0.73623928
N	1.63797585	-0.26529156	-1.57748494
N	-1.00443425	0.52631590	-1.69958222
N	-1.63742441	-0.25468505	1.57878425
N	1.00401105	0.53892056	1.69736983
C	1.11074332	0.13828106	-2.75624008
C	-0.22283687	0.57448382	-2.81612263
C	-1.11096732	0.15548958	2.75565906
C	0.22244456	0.59251524	2.81364728
C	3.03285169	-0.72412397	-1.68302948
C	4.08764858	0.23585414	-1.62537644
C	5.41557081	-0.22225775	-1.76209814
C	5.70440782	-1.57700976	-1.97615651
C	4.65426599	-2.49565595	-2.08866771
C	3.30646097	-2.09478190	-1.96154583
C	4.95629557	2.48667842	-0.73952709
C	3.83251245	1.74402970	-1.50149655

C	3.67214028	2.40467454	-2.90197227
C	-1.87360944	4.52274849	-0.57521603
C	-1.37671124	3.46483342	-1.59437644
C	-0.75825164	4.17090702	-2.83216292
C	-2.34241868	1.07809980	-1.98380313
C	-2.49282442	2.49645261	-2.01146153
C	-3.70271118	3.03220862	-2.49896510
C	-4.74434427	2.20174904	-2.93494515
C	-4.58762307	0.81070875	-2.88005359
C	-3.38951652	0.21869768	-2.42193989
C	2.44642008	-4.47102048	-1.51075526
C	2.21234765	-3.12855635	-2.24478281
C	2.09167338	-3.36491517	-3.77707463
C	-4.44963370	-2.06448432	-1.92995214
C	-3.23718224	-1.30179990	-2.51742067
C	-2.99158263	-1.72763454	-3.99165099
C	-3.03269756	-0.71183942	1.68603239
C	-3.30764948	-2.08087115	1.97076006
C	-4.65585142	-2.47961605	2.10076572
C	-5.70504278	-1.56039551	1.98453765
C	-5.41488981	-0.20701643	1.76345875
C	-4.08655570	0.24901518	1.62399955
C	-2.44994079	-4.45834933	1.52472162
C	-2.21474216	-3.11508309	2.25700538
C	-2.09533188	-3.34858079	3.78976078
C	1.86893536	4.52804924	0.54596691
C	1.37533698	3.47574870	1.57247257
C	0.75788771	4.18852829	2.80688296
C	2.34197752	1.09222215	1.97822314
C	2.49251417	2.51076578	1.99438141
C	3.70303881	3.05026599	2.47603283
C	4.74494170	2.22307914	2.91762190
C	4.58752394	0.83170469	2.87509771
C	3.38869116	0.23606791	2.42341620
C	-4.95240131	2.49593177	0.72547521
C	-3.82992194	1.75625900	1.49236752
C	-3.66990389	2.42442284	2.88931382
C	4.44441293	-2.05191674	1.94564804
C	3.23586690	-1.28339059	2.53377730
C	2.99954828	-1.69516394	4.01353279
H	6.23223603	0.48995927	-1.70417729
H	6.73588932	-1.90749700	-2.07313012
H	4.87687042	-3.53936897	-2.29083039
H	2.89468239	1.88186477	-0.94967016
H	-0.58037584	2.88807462	-1.11064020
H	5.87162164	2.55347538	-1.34290179
H	5.19926378	1.99478446	0.20581729
H	4.64173100	3.51313404	-0.51622453
H	4.56837920	2.22892248	-3.51180381
H	3.54336843	3.49078889	-2.79552916
H	2.80776957	2.01803687	-3.45081734
H	-2.67559602	5.14337448	-0.99398228

H	-1.05277747	5.19530804	-0.29752502
H	-2.25317210	4.05162468	0.33856419
H	-0.34938435	3.44499508	-3.54510379
H	0.05545938	4.84129954	-2.52453117
H	-1.51164734	4.77128468	-3.35890786
H	-3.82837300	4.11093719	-2.54386482
H	-5.66675305	2.63477499	-3.31446361
H	-5.39393799	0.16807029	-3.22242022
H	1.25312742	-2.74301511	-1.90017788
H	-2.36263088	-1.61458911	-1.94445564
H	3.34143917	-4.99154342	-1.87824126
H	1.58589425	-5.13216769	-1.66929609
H	2.54941645	-4.31042292	-0.43247631
H	3.02579996	-3.76887464	-4.19044884
H	1.86243523	-2.43455837	-4.31366451
H	1.28699902	-4.08261142	-3.98457123
H	-4.64826633	-1.76264265	-0.89586983
H	-4.24010256	-3.14192071	-1.93239037
H	-5.36421717	-1.90467599	-2.51752876
H	-3.84517884	-1.46135835	-4.63048605
H	-2.84694943	-2.81431213	-4.04899729
H	-2.09601611	-1.24601060	-4.40516950
H	-4.87946936	-3.52209789	2.30816299
H	-6.73682236	-1.88923234	2.08390184
H	-6.23088838	0.50571521	1.70226442
H	-1.25478172	-2.73135722	1.91242154
H	0.57884831	2.89532469	1.09339161
H	-3.34730418	-4.97598110	1.89050270
H	-1.59140722	-5.12121020	1.68670986
H	-2.54944055	-4.29890005	0.44593900
H	-1.86548217	-2.41730269	4.32453911
H	-1.29146078	-4.06661275	3.99916822
H	-3.03000997	-3.75078428	4.20360058
H	2.67021949	5.15317762	0.95937767
H	1.04568807	5.19652975	0.26553099
H	2.24784148	4.05189591	-0.36546290
H	0.35262623	3.46630010	3.52559188
H	-0.05828293	4.85475468	2.49666976
H	1.51084205	4.79443552	3.32792159
H	3.82890184	4.12931969	2.51198405
H	5.66804371	2.65890885	3.29221944
H	5.39392248	0.19180162	3.22241270
H	-2.89155048	1.89022829	0.94059009
H	2.35774351	-1.60182991	1.96942886
H	-5.86767154	2.56795019	1.32833137
H	-5.19612000	1.99856783	-0.21681193
H	-4.63616097	3.52047866	0.49575857
H	-3.54058036	3.50987605	2.77690746
H	-2.80590958	2.04037508	3.44056808
H	-4.56648236	2.25240778	3.49968218
H	4.63540382	-1.76076907	0.90707085
H	4.23534221	-3.12934700	1.96079539

H	5.36319030	-1.88558993	2.52481484
H	2.10724198	-1.20846467	4.42819538
H	3.85741856	-1.42409577	4.64452610
H	2.85398239	-2.78108471	4.08196863
O	0.00308822	-3.24728757	0.01484496
H	-0.63578073	0.93643266	-3.75353582
H	1.70746180	0.10005931	-3.66378607
H	-1.70822495	0.12197832	3.66304618
H	0.63512096	0.95944725	3.74924372
Hf	0.00017574	-0.56488815	0.00206580

4.5 Four Oxygen Atoms

Bisperoxo Complex (spiro conformation)

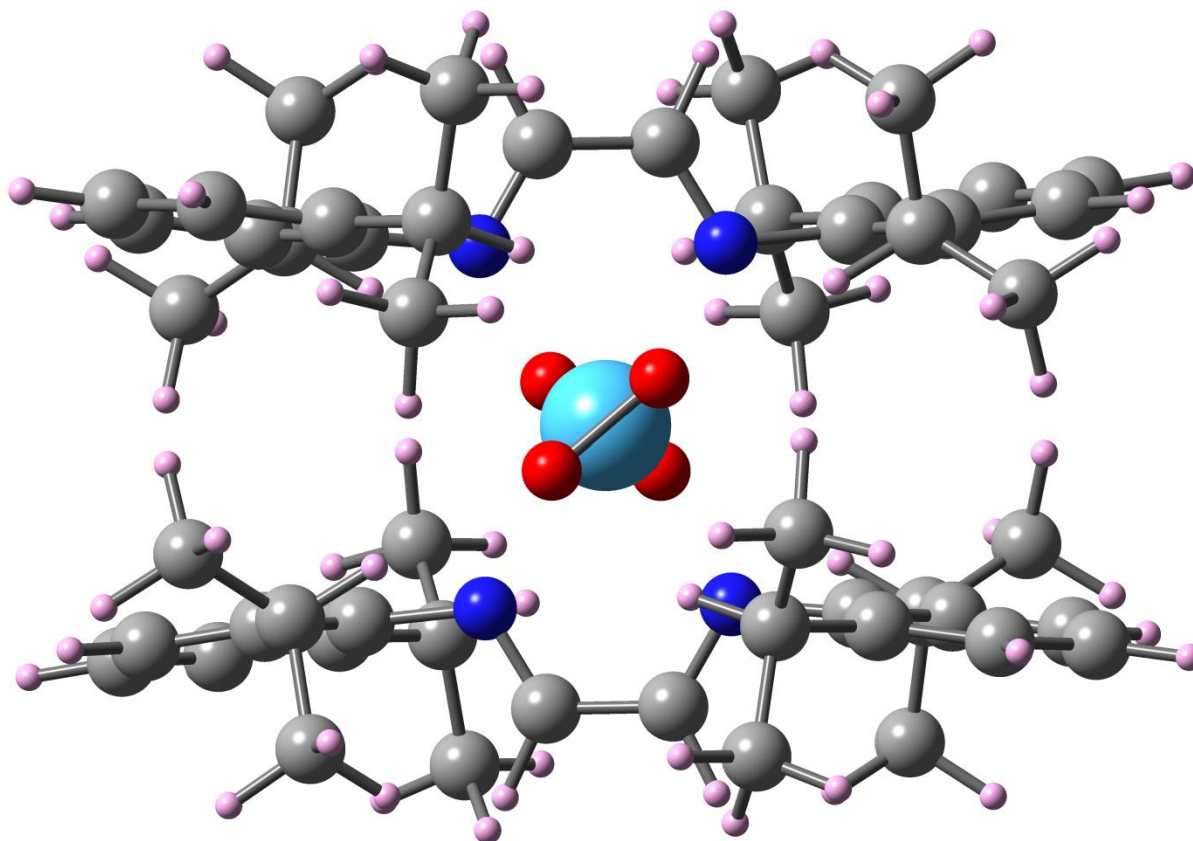


Fig. S18: NCCN Bisperoxo Complex (spiro conformation)

E	E _{zp}	H	G
-2593.4173	-2592.2690	-2592.2003	-2592.3697
O	-0.59819998	1.92607263	0.43339967
O	0.59818865	1.89283963	-0.56017619
O	0.59812715	-1.89314054	0.56039655
O	-0.59800879	-1.92644719	-0.43348101
N	-1.35047630	0.31603748	-1.99763684
N	1.35143301	-0.44567256	-1.97209000
N	1.35106759	0.44543925	1.97247497
N	-1.35089560	-0.31632185	1.99760804
C	-0.69652024	0.12552009	-3.10192487
C	0.69885294	-0.32461933	-3.08695179
C	0.69829294	0.32438261	3.08721603
C	-0.69706976	-0.12577176	3.10197122
C	-2.72917915	0.79337156	-2.13802934
C	-3.77554328	-0.16818374	-2.14890163
C	-5.08820788	0.30399368	-2.35646513
C	-5.34670945	1.66974300	-2.55589825
C	-4.29092823	2.59258374	-2.54387088

C	-2.95684187	2.18155178	-2.33199638
C	-4.59912364	-2.44195311	-1.27889751
C	-3.49052122	-1.67087358	-2.03214993
C	-3.28862636	-2.29616809	-3.44181165
C	2.08917932	-4.47574452	-1.09902751
C	1.82418069	-3.36476246	-2.14491553
C	1.59914987	-3.97927056	-3.55359771
C	2.72980010	-0.93237075	-2.08097906
C	2.95603398	-2.33041817	-2.18436438
C	4.28971324	-2.75567349	-2.36902851
C	5.34637887	-1.83660242	-2.44132816
C	5.08923898	-0.46050261	-2.33130128
C	3.77706929	0.02545518	-2.15463889
C	-2.09502850	4.39526901	-1.38992222
C	-1.82611070	3.21752453	-2.35882496
C	-1.59830536	3.73710478	-3.80481133
C	4.60264870	2.34937110	-1.43193477
C	3.49373693	1.53290046	-2.13518547
C	3.29417466	2.06669217	-3.58232211
C	2.72928480	0.93249064	2.08164789
C	2.95501409	2.33060204	2.18517156
C	4.28853898	2.75633794	2.36985987
C	5.34553547	1.83764302	2.44206428
C	5.08888923	0.46146494	2.33187458
C	3.77689493	-0.02497024	2.15520024
C	2.08715409	4.47531042	1.09939727
C	1.82277570	3.36453575	2.14565154
C	1.59776138	3.97932008	3.55421240
C	-2.09569649	-4.39483814	1.38809255
C	-1.82703025	-3.21780521	2.35791801
C	-1.59984226	-3.73841492	3.80362575
C	-2.72968096	-0.79345179	2.13795260
C	-2.95761844	-2.18165100	2.33133857
C	-4.29184014	-2.59252461	2.54268243
C	-5.34745220	-1.66947906	2.55476501
C	-5.08865017	-0.30369285	2.35593553
C	-3.77582881	0.16831137	2.14893054
C	4.60307177	-2.34839629	1.43157117
C	3.49413021	-1.53253336	2.13548952
C	3.29532461	-2.06686851	3.58253041
C	-4.59798406	2.44238935	1.27825698
C	-3.49043050	1.67097931	2.03271228
C	-3.29007811	2.29599498	3.44271908
H	-5.91191478	-0.40327792	-2.36891523
H	-6.36599146	2.01095363	-2.72134688
H	-4.49996405	3.64769265	-2.69908160
H	-2.55853806	-1.80927020	-1.47062850
H	0.89997360	-2.87422613	-1.82600294
H	-5.53328449	-2.48489959	-1.85574592
H	-4.81400150	-1.98855402	-0.30602641
H	-4.27459911	-3.47557652	-1.10486932
H	-4.19410078	-2.17937867	-4.05288988

H	-3.07085544	-3.36818870	-3.35045271
H	-2.45584596	-1.83146294	-3.98482820
H	3.00298878	-5.04673127	-1.31483368
H	1.24698490	-5.18017246	-1.09038238
H	2.16434684	-4.03506482	-0.10015201
H	1.35914824	-3.20995952	-4.30122626
H	0.76615499	-4.69409554	-3.52441739
H	2.49205323	-4.51410052	-3.90557684
H	4.49768564	-3.81888128	-2.45507522
H	6.36531088	-2.18888326	-2.58418979
H	5.91365016	0.24363520	-2.38980425
H	-0.90220538	2.75037109	-2.00573545
H	2.56146033	1.70825597	-1.58460020
H	-3.00800926	4.95051639	-1.64648536
H	-1.25287991	5.09893255	-1.42471705
H	-2.17418773	4.02177882	-0.36430674
H	-2.49085415	4.24652595	-4.19349392
H	-1.35620616	2.91986903	-4.49903360
H	-0.76587699	4.45299298	-3.82158466
H	4.81587306	1.95912818	-0.43172152
H	4.27942019	3.39247537	-1.32499294
H	5.53736963	2.35391762	-2.00943171
H	4.19980117	1.90898767	-4.18391686
H	3.07870727	3.14285093	-3.56025637
H	2.46079461	1.56988918	-4.09518617
H	4.49613412	3.81961394	2.45598151
H	6.36434365	2.19027512	2.58493840
H	5.91355994	-0.24236670	2.39029926
H	0.89871038	2.87355923	1.82700431
H	-0.90291781	-2.75051687	2.00554912
H	3.00090897	5.04656164	1.31472547
H	1.24478856	5.17953392	1.09089964
H	2.16204182	4.03436258	0.10062183
H	1.35799935	3.21014017	4.30205626
H	0.76461844	4.69397019	3.52494796
H	2.49059221	4.51441903	3.90596319
H	-3.00890900	-4.95008721	1.64382508
H	-1.25369675	-5.09868658	1.42280318
H	-2.17428223	-4.02067692	0.36267748
H	-1.35783485	-2.92169119	4.49848118
H	-0.76753739	-4.45444941	3.82018563
H	-2.49261119	-4.24794945	4.19165396
H	-4.50112148	-3.64765649	2.69741251
H	-6.36684195	-2.01056735	2.71980191
H	-5.91223530	0.40372315	2.36838300
H	2.56169908	-1.70810143	1.58522703
H	-2.55776936	1.80929025	1.47230044
H	5.53791394	-2.35310431	2.00887643
H	4.81603863	-1.95751606	0.43155143
H	4.28002529	-3.39149777	1.32407545
H	3.08034379	-3.14311647	3.56017779
H	2.46189028	-1.57064188	4.09585051

H	4.20109734	-1.90895740	4.18385290
H	-4.81181156	1.98914953	0.30508844
H	-4.27300960	3.47596592	1.10474831
H	-5.53281601	2.48547460	1.85400614
H	-2.45803832	1.83100450	3.98662930
H	-4.19628970	2.17924720	4.05270631
H	-3.07199568	3.36799210	3.35183571
Hf	-0.00043285	-0.00018411	0.00006355
H	-1.16047070	0.29962157	-4.07428794
H	1.16376175	-0.55997369	-4.04585760
H	1.16301320	0.55981936	4.04619499
H	-1.16115863	-0.29975125	4.07429239

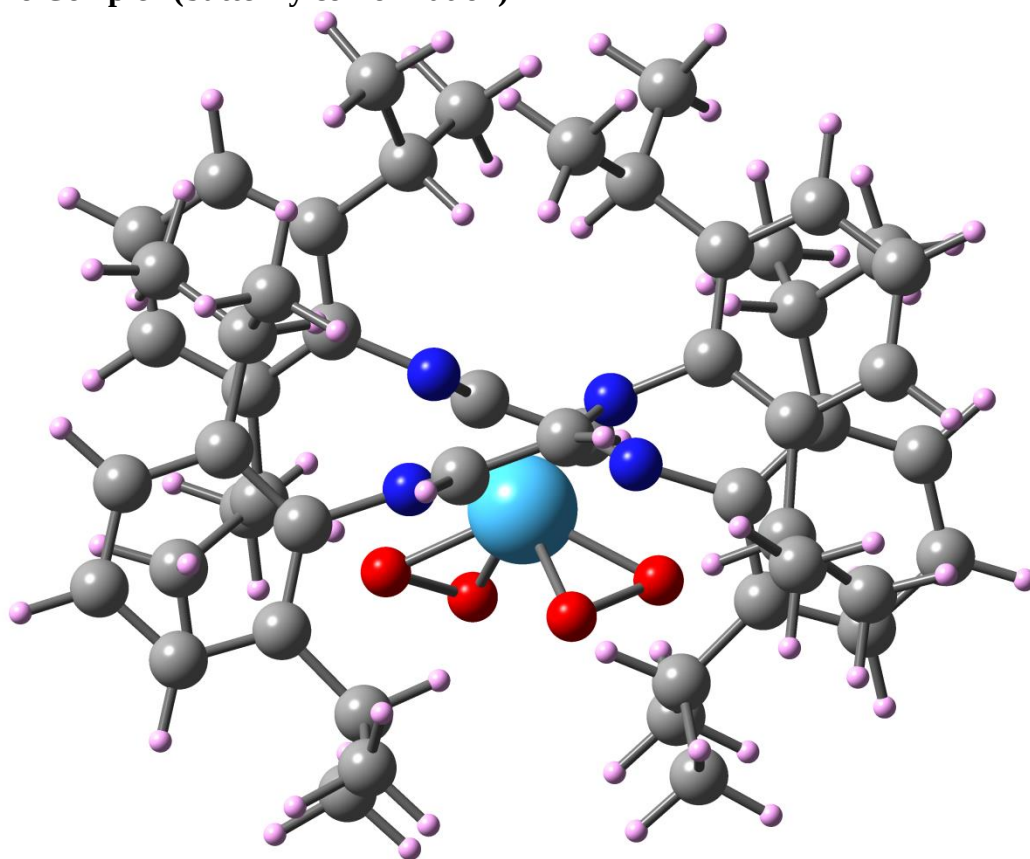
Bisperoxo Complex (butterfly conformation)

Fig. S19: NCCN Bisperoxo Complex (butterfly conformation)

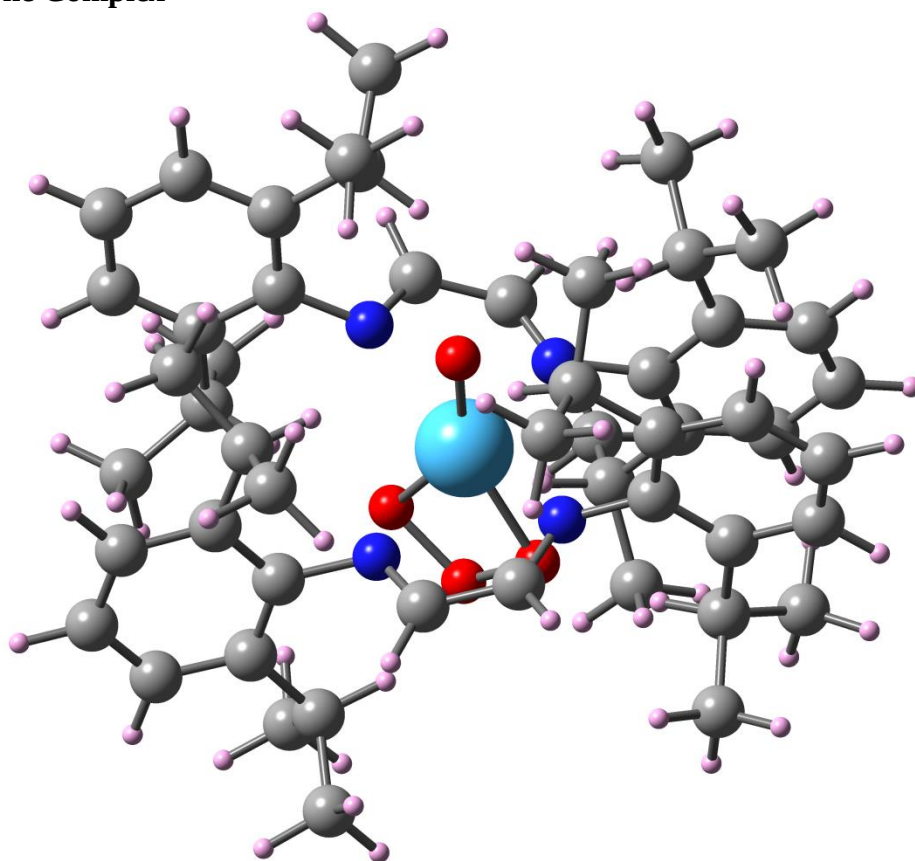
E	E_{zp}	H	G
-2593.3698	-2592.2235	-2592.1541	-2592.3281

O	1.78225500	-1.75341000	0.33517100
N	-1.15783600	0.94240500	-1.81518700
N	1.48496800	-0.23611200	-1.91570300
N	-1.47949900	-0.56407900	1.87712400
N	1.15680900	0.61111900	1.93806700
C	-0.55636200	0.61744600	-2.92497300
C	0.82618700	0.12140500	-2.97517500
C	-0.81399800	-0.38563200	2.97669600
C	0.56696600	0.11775700	2.99150100
C	-2.49510200	1.50974000	-1.97070800
C	-3.55359000	0.75924600	-2.56620300
C	-4.78890700	1.41796500	-2.75996800
C	-4.97275700	2.76233100	-2.41525100
C	-3.91352800	3.48385500	-1.84476000
C	-2.66652700	2.87637200	-1.60370000
C	-4.49788300	-1.59303700	-2.31163500
C	-3.44192300	-0.70393300	-3.01650700
C	-3.57832300	-0.82069000	-4.55964700

C	2.30984000	-4.30954100	-1.71196200
C	2.07938100	-3.09332300	-2.64387000
C	2.01102900	-3.53389300	-4.13162100
C	2.87798500	-0.66430600	-2.11734400
C	3.15342700	-2.01869100	-2.44820400
C	4.50447800	-2.37845000	-2.64884400
C	5.53892800	-1.44269300	-2.53624500
C	5.23750800	-0.10707600	-2.23027300
C	3.90812300	0.31255800	-2.02037700
C	-1.92488700	4.77314100	-0.03882100
C	-1.49571100	3.71485000	-1.08216700
C	-0.76044500	4.40079700	-2.26881500
C	4.76008100	2.52706700	-1.03692100
C	3.60529300	1.79437300	-1.75900200
C	3.28482200	2.54412400	-3.08409400
C	-2.87119300	-1.02001600	2.00378500
C	-3.14808200	-2.40962300	2.11169300
C	-4.50054500	-2.79635600	2.23929300
C	-5.53503000	-1.85430500	2.26702900
C	-5.23229500	-0.48709100	2.18018900
C	-3.90168900	-0.04023700	2.05141900
C	-2.29029500	-4.53127800	0.99180400
C	-2.07571200	-3.50344900	2.13180300
C	-2.03074500	-4.20576900	3.51598000
C	1.89774700	4.69203800	0.79159000
C	1.47276200	3.46427500	1.63119400
C	0.70551900	3.92607100	2.90289000
C	2.49193000	1.15847600	2.17222500
C	2.65078200	2.56697500	2.02272800
C	3.89228700	3.14032100	2.35654400
C	4.95778600	2.34807900	2.80966500
C	4.78684000	0.96449900	2.93774100
C	3.55781600	0.33293800	2.64079100
C	-4.74453400	2.29982000	1.41423800
C	-3.59679200	1.46365500	2.02654700
C	-3.28997700	1.99771800	3.45530900
C	4.51910500	-1.93673800	2.00267700
C	3.46039200	-1.18458800	2.84893700
C	3.60694900	-1.55137400	4.35121800
H	-1.04082500	0.76206300	-3.89323300
H	1.28372100	0.07303500	-3.96597700
H	-1.26279900	-0.59569500	3.95019900
H	1.06089700	0.11826100	3.96557700
H	-5.61347700	0.86307000	-3.19917700
H	-5.93021500	3.24635000	-2.59228200
H	-4.06068800	4.52890300	-1.59018300
H	-2.47208800	-1.10786200	-2.72331700
H	1.10037300	-2.69249400	-2.37744800
H	-5.52548000	-1.29859200	-2.56738400
H	-4.37006200	-1.54738000	-1.22632000
H	-4.35943700	-2.63809800	-2.61730000
H	-4.56463300	-0.48341600	-4.90640500

H	-3.45467200	-1.86786600	-4.86459700
H	-2.82192800	-0.22319300	-5.08863000
H	3.25375300	-4.82758100	-1.93352700
H	1.49208800	-5.03127500	-1.83851000
H	2.31869200	-3.97735400	-0.66939800
H	1.80765100	-2.68361900	-4.79823200
H	1.20659100	-4.26867900	-4.26534600
H	2.95130200	-3.99726200	-4.46069600
H	4.74003300	-3.40996400	-2.89617600
H	6.57155100	-1.74665300	-2.69068600
H	6.04504400	0.61336000	-2.15261600
H	-0.77970000	3.03447000	-0.60270200
H	2.71743200	1.84995600	-1.11271900
H	-2.57364500	5.54054100	-0.47943400
H	-1.04593900	5.29070700	0.36093300
H	-2.46187200	4.31598700	0.80041400
H	-1.43476300	5.09333300	-2.78949400
H	-0.40541200	3.66493700	-3.00103200
H	0.10703500	4.97074300	-1.91111100
H	5.06964000	1.99756700	-0.13071500
H	4.44353600	3.53591700	-0.74682500
H	5.63423700	2.63978600	-1.69151500
H	4.14031500	2.48692100	-3.76997900
H	3.07848100	3.60464400	-2.88453200
H	2.41492100	2.12489200	-3.60252300
H	-4.73723200	-3.85422300	2.31441300
H	-6.56876500	-2.17876500	2.36002900
H	-6.03982500	0.23684300	2.20970400
H	-1.09273500	-3.06308500	1.95821500
H	0.77785000	2.86410000	1.02889600
H	-3.23835600	-5.07661000	1.10226800
H	-1.47487500	-5.26639600	1.00034900
H	-2.28245000	-4.01715900	0.02589300
H	-1.83723900	-3.49097400	4.32852300
H	-1.22859200	-4.95508300	3.52598300
H	-2.97550100	-4.71885700	3.74195000
H	2.52470300	5.38287500	1.36886100
H	1.01546500	5.25595300	0.46958100
H	2.45564400	4.39329900	-0.10345100
H	0.34660300	3.07146200	3.48966000
H	-0.16359000	4.53895500	2.63102300
H	1.35937900	4.52615100	3.54935200
H	4.02991800	4.21323000	2.26664400
H	5.91060600	2.80725100	3.06186200
H	5.61659800	0.35518100	3.28514600
H	-2.70181400	1.61746200	1.40623700
H	2.49195700	-1.54358300	2.49803400
H	-5.62604300	2.30919000	2.06861000
H	-5.04321700	1.91691800	0.43354200
H	-4.42718600	3.34147400	1.28724400
H	-3.08581000	3.07683400	3.42563200
H	-2.42276600	1.50456100	3.90983000

H	-4.15081000	1.83230100	4.11645700
H	4.38477100	-1.71441400	0.94017900
H	4.39069600	-3.01894200	2.13313500
H	5.54592100	-1.67889700	2.29820300
H	2.84712600	-1.05794100	4.97409900
H	4.59152000	-1.26502100	4.74524800
H	3.49593800	-2.63574200	4.48003700
O	-0.65105600	-1.97028700	-1.59919600
O	-1.78645200	-1.64397000	-0.60131300
O	0.64453800	-2.22726400	1.26795500
Hf	0.00256000	-0.82327100	-0.05402700

Oxo η^2 -Ozone ComplexFig. S20: NCCN Oxo η^2 -Ozone Complex

E	E_{zp}	H	G
-2593.3881	-2592.2412	-2592.1717	-2592.3457

O	1.07807543	-1.00120077	1.78017956
O	-1.04580798	-1.79928498	0.98633249
O	0.10815419	1.16531923	-1.18892421
N	1.29277280	-1.71834137	-1.10809254
N	-1.40333162	-1.17940680	-1.62921541
N	-1.30834892	1.11617974	1.68686507
N	1.39445294	1.65031707	1.21349411
C	0.61681283	-2.43607057	-1.95784537
C	-0.77398531	-2.11478041	-2.27568532
C	-0.65836046	1.99181873	2.40147251
C	0.72699728	2.33590568	2.09449153
C	2.71798491	-2.04475650	-0.97663205
C	3.63745211	-1.26946874	-1.73644701
C	5.00002984	-1.62594704	-1.66809361
C	5.42970016	-2.71278495	-0.88990278
C	4.49776806	-3.46249250	-0.15943095
C	3.12126339	-3.14860587	-0.18190230
C	4.19976105	0.99502464	-2.81503052

C	3.16728766	-0.14664130	-2.67121201
C	2.83718072	-0.71917195	-4.07960388
C	-1.79655399	2.26643692	-4.09425978
C	-1.58920094	0.75260800	-3.84565672
C	-1.19293418	0.04447763	-5.17022793
C	-2.73424891	-0.83422237	-2.14002485
C	-2.82255602	0.08242495	-3.22555381
C	-4.10462374	0.32910748	-3.76128709
C	-5.24782432	-0.29455904	-3.23972337
C	-5.12860576	-1.18841507	-2.16454197
C	-3.87264865	-1.48655853	-1.59396792
C	2.55720942	-4.15162632	2.09577618
C	2.13739808	-4.01484120	0.61140034
C	1.98061377	-5.41293545	-0.04668756
C	-4.91070192	-2.48805662	0.53145674
C	-3.75218070	-2.54493562	-0.49167272
C	-3.67105580	-3.96659489	-1.11650796
C	-2.72796649	0.94971336	2.02695328
C	-3.09850904	0.13163287	3.12543185
C	-4.46879242	0.07960199	3.46180015
C	-5.42617822	0.80455179	2.73934084
C	-5.02901433	1.60689110	1.65793155
C	-3.67381879	1.70513221	1.28021009
C	-2.48341359	-2.13598389	4.12547014
C	-2.08427357	-0.64822845	3.96856588
C	-1.89775840	0.01940610	5.35877464
C	1.65712165	4.04814062	-2.19052344
C	1.55117650	3.95878676	-0.64814560
C	1.31498603	5.36344034	-0.03032792
C	2.71253533	2.17407121	0.85336547
C	2.78495183	3.29234029	-0.02458239
C	4.06595027	3.81734693	-0.30103249
C	5.22231184	3.26203787	0.26452054
C	5.11868265	2.16182310	1.13019837
C	3.86682399	1.59683961	1.45088818
C	-4.30263823	2.80719886	-0.95457977
C	-3.24273478	2.66499993	0.16214845
C	-2.92384343	4.07202481	0.74450871
C	4.93449373	-0.52578114	2.43357779
C	3.76046467	0.47820249	2.49221483
C	3.65667011	1.08727168	3.91960546
H	5.72897196	-1.05275053	-2.23218630
H	6.48501887	-2.97316622	-0.85598085
H	4.83793031	-4.30203571	0.44076753
H	2.24655793	0.28992737	-2.26149817
H	-0.76300194	0.68607307	-3.12911426
H	5.09280052	0.67063434	-3.36694740
H	4.51554628	1.37889130	-1.83999151
H	3.75474209	1.82609920	-3.37586188
H	3.73116723	-1.16689351	-4.53472352
H	2.48087653	0.08286407	-4.73932070
H	2.05835935	-1.49104179	-4.04323466

H	-2.57651922	2.47062157	-4.84085580
H	-0.86080168	2.70817649	-4.46049178
H	-2.06131459	2.77596866	-3.16171101
H	-0.98087178	-1.02247590	-5.01767764
H	-0.29310053	0.50885129	-5.59573561
H	-1.99763740	0.11764774	-5.91509175
H	-4.20532477	1.02037860	-4.59351043
H	-6.22505817	-0.08763421	-3.66981881
H	-6.01762122	-1.66966147	-1.76786324
H	1.15991850	-3.52749632	0.62431418
H	-2.82292085	-2.37570389	0.06402933
H	3.51832792	-4.67193490	2.20866466
H	1.79747303	-4.72406632	2.64283889
H	2.62866713	-3.16206607	2.55813679
H	2.93463499	-5.95720785	-0.06022541
H	1.62747161	-5.33943003	-1.08502140
H	1.25475065	-6.01501893	0.51541247
H	-5.02762522	-1.48177855	0.94725517
H	-4.69940260	-3.17368937	1.36220944
H	-5.86920785	-2.79435284	0.08950993
H	-4.57626222	-4.19418320	-1.69647381
H	-3.57149429	-4.72024130	-0.32448769
H	-2.80807489	-4.07043467	-1.78690657
H	-4.78392601	-0.53834411	4.29806331
H	-6.47611345	0.74781679	3.01679482
H	-5.77815322	2.16597594	1.10640469
H	-1.11964338	-0.65274003	3.45653141
H	0.67921541	3.32659440	-0.46055674
H	-3.42543564	-2.25744932	4.67790062
H	-1.69899616	-2.67140068	4.67489990
H	-2.58126537	-2.60413078	3.14094226
H	-1.55346832	1.05964015	5.27110720
H	-1.15286943	-0.53410801	5.94527819
H	-2.83820138	0.02929155	5.92640307
H	2.53103246	4.62721650	-2.51901580
H	0.75980301	4.53527379	-2.59530984
H	1.70891676	3.04044674	-2.61350621
H	1.20288257	5.31594996	1.06187298
H	0.40329232	5.81329450	-0.44624596
H	2.15253312	6.04091115	-0.24564428
H	4.15349734	4.67071257	-0.96842629
H	6.19770949	3.68552867	0.03655387
H	6.01757317	1.74211145	1.57146777
H	-2.32339299	2.27800974	-0.29792654
H	2.84016149	-0.08862990	2.31173504
H	-5.19489097	3.34155360	-0.60113209
H	-4.61350586	1.83291631	-1.34390496
H	-3.88712305	3.38711481	-1.78782962
H	-2.60833640	4.75117966	-0.05839789
H	-2.12043770	4.04217572	1.49060379
H	-3.81286848	4.50022068	1.22685660
H	5.06832515	-0.92638656	1.42300200

H	4.72841382	-1.36883210	3.10554147
H	5.88294116	-0.07411410	2.75684985
H	2.78479817	1.74672279	4.01938316
H	4.55328809	1.67418151	4.16312435
H	3.55667273	0.28625346	4.66359669
O	0.02596655	-2.07432249	2.03051688
Hf	0.01780241	-0.13567555	0.14484046
H	-1.23425436	-2.64475358	-3.11116705
H	1.08701111	-3.25710477	-2.50100052
H	-1.15001166	2.52810538	3.21425283
H	1.15092047	3.21444021	2.58369333

4.6 Five Oxygen Atoms

Peroxo η^2 -Ozone Complex

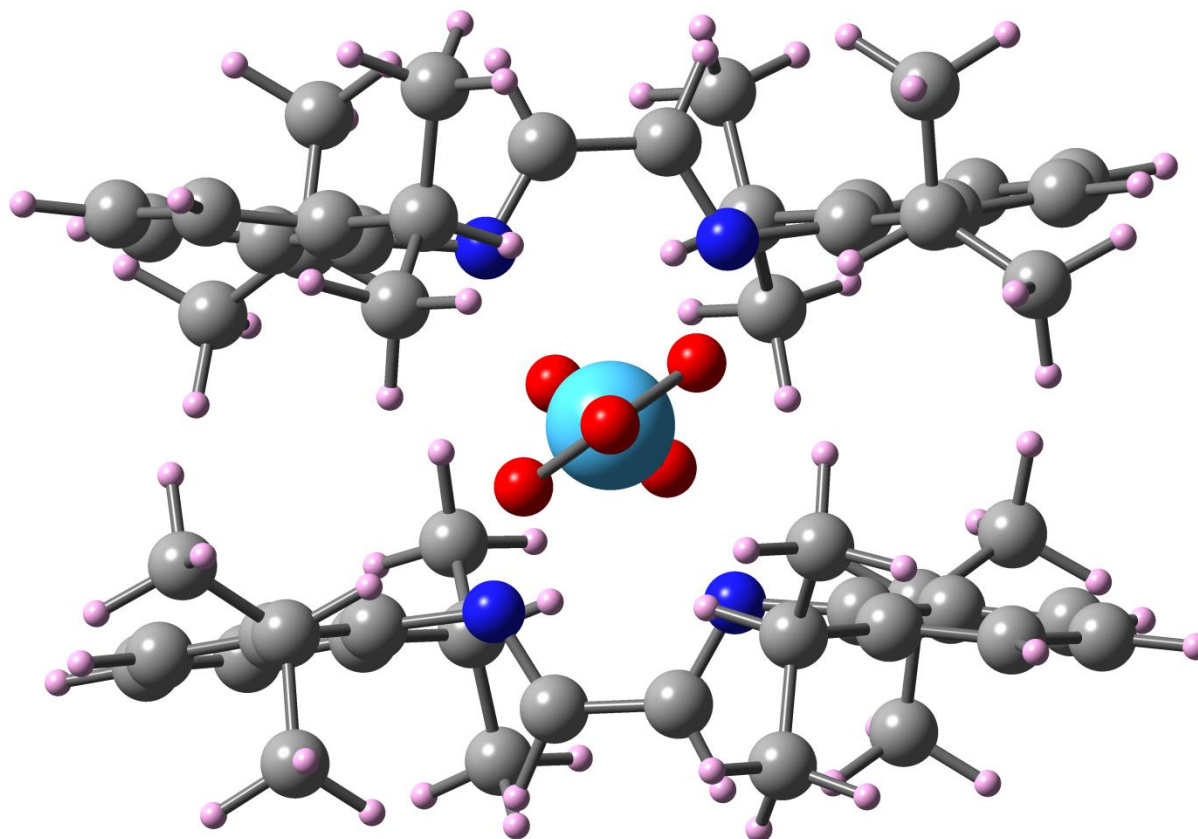


Fig. S21: NCCN Peroxo η^2 -Ozone Complex

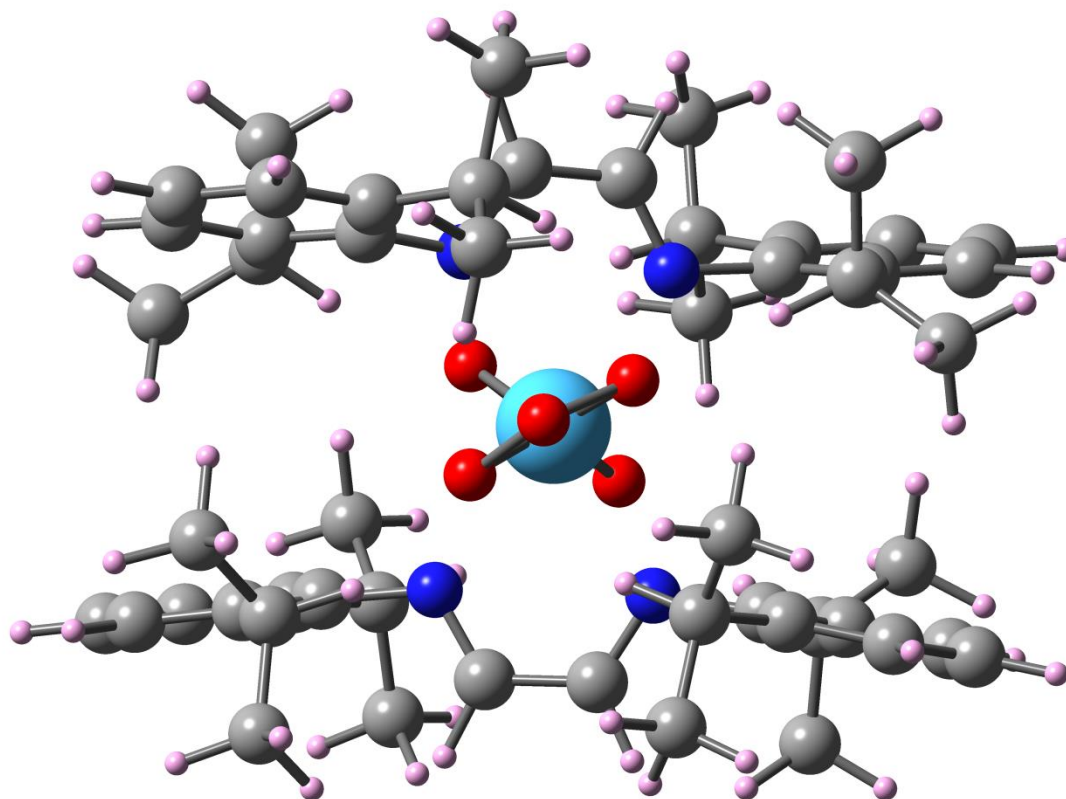
E	E_{zp}	H	G
-2668.5639	-2517.0860	-2517.0181	-2517.1870
O	-0.97690244	1.91577787	-0.49257472
O	0.99042868	1.17070487	-1.58457882
O	0.60568064	-1.21131219	1.40361529
O	-0.61121096	-1.75143936	0.59881171
N	-1.32575209	-0.73424692	-1.92987230
N	1.36174012	-1.46323322	-1.46492976
N	1.32912569	1.51335032	1.41095436
N	-1.36118438	0.81346394	1.90457796
C	-0.66488378	-1.47241886	-2.77005553
C	0.72113801	-1.88100404	-2.51151670
C	0.66766242	2.01245303	2.41142994
C	-0.71850677	1.61885460	2.69100400
C	-2.73309754	-0.47299805	-2.26645636
C	-3.72092520	-1.33606279	-1.71530209
C	-5.06306926	-1.10707770	-2.08284096
C	-5.41063168	-0.07639683	-2.96993560

C	-4.41265295	0.74494734	-3.51145531
C	-3.05243351	0.56865831	-3.17617082
C	-4.40155738	-2.83328600	0.26240510
C	-3.35440632	-2.53844690	-0.83632647
C	-3.15013928	-3.80441810	-1.71665539
C	1.80946289	-4.43406148	1.46579915
C	1.61889755	-4.02096893	-0.01425898
C	1.32315168	-5.26447608	-0.89725760
C	2.70601381	-2.01623027	-1.25507340
C	2.82643474	-3.25165833	-0.56243239
C	4.12084391	-3.79903495	-0.43234746
C	5.24602526	-3.14936315	-0.95984123
C	5.09479815	-1.93119000	-1.63955808
C	3.82571890	-1.33788104	-1.80932265
C	-2.32593172	2.96476253	-3.67911402
C	-1.99428845	1.46045192	-3.83339236
C	-1.81848583	1.08720298	-5.33072766
C	4.80191415	0.97197180	-2.36619488
C	3.67711597	-0.05547068	-2.63538409
C	3.62197989	-0.39370061	-4.15186430
C	2.73446240	1.92921467	1.29397620
C	3.04850960	3.17371298	0.68775719
C	4.40771361	3.55469291	0.65096816
C	5.41028089	2.73875194	1.19167432
C	5.06845943	1.51823105	1.79469029
C	3.72779149	1.08712440	1.86753095
C	2.31358989	4.54683218	-1.33391323
C	1.98873686	4.12318239	0.11954744
C	1.82329961	5.36902829	1.03189366
C	-1.80835354	-3.01820450	3.52895802
C	-1.62988178	-1.49351253	3.73245596
C	-1.36674581	-1.16480997	5.22774043
C	-2.70695278	0.41116185	2.33217100
C	-2.83290436	-0.69611522	3.21453802
C	-4.13083690	-1.02592879	3.66071080
C	-5.25385238	-0.29422433	3.24900728
C	-5.09698799	0.79616256	2.37986876
C	-3.82467331	1.17943515	1.90525479
C	4.42381161	-1.31136722	2.48507572
C	3.36653992	-0.19275332	2.63134379
C	3.14862487	0.12415268	4.13836113
C	-4.79499969	2.58193559	-0.01689037
C	-3.67061635	2.43184395	1.03492297
C	-3.60876985	3.70320964	1.92782814
H	-5.84063450	-1.74596448	-1.67568126
H	-6.45205526	0.07969053	-3.24129264
H	-4.68706437	1.53544283	-4.20462471
H	-2.40653495	-2.33126418	-0.32788795
H	0.74297327	-3.36717998	-0.02894859
H	-5.34679131	-3.20311700	-0.15812565
H	-4.61455413	-1.94333734	0.86328570
H	-4.01804721	-3.60964309	0.93641955

H	-4.07491962	-4.06091499	-2.25132000
H	-2.86798504	-4.65925760	-1.08827568
H	-2.35987211	-3.66431890	-2.46575834
H	2.66010529	-5.11528855	1.60648553
H	0.90708031	-4.94759250	1.82318710
H	1.95541290	-3.54402648	2.08628127
H	1.13372341	-4.98547658	-1.94350811
H	0.43664369	-5.79284222	-0.52182613
H	2.16575882	-5.96950837	-0.89115718
H	4.24367290	-4.74495510	0.08812871
H	6.23350876	-3.59063298	-0.84629238
H	5.96944042	-1.43592512	-2.05108734
H	-1.03817024	1.31292862	-3.32713349
H	2.73293101	0.43097214	-2.36834338
H	-3.25356106	3.24093921	-4.19913775
H	-1.51144399	3.56753380	-4.10036389
H	-2.42122936	3.22393450	-2.61978118
H	-2.75042240	1.23883911	-5.89205682
H	-1.52396694	0.03588964	-5.45762484
H	-1.04129305	1.71387945	-5.78755521
H	4.89638482	1.19034199	-1.29723180
H	4.56967215	1.91261558	-2.88224960
H	5.77714471	0.62675780	-2.73676198
H	4.54758924	-0.88723941	-4.47905410
H	3.49699438	0.52563059	-4.73891879
H	2.78451075	-1.06184341	-4.39348292
H	4.67762102	4.50168011	0.19144599
H	6.45066998	3.05234335	1.14937960
H	5.84950245	0.89562575	2.21996879
H	1.03003334	3.60267176	0.07106709
H	-0.74336073	-1.22010765	3.15429209
H	3.24429548	5.12710914	-1.39851244
H	1.50020686	5.16878996	-1.72856636
H	2.40054382	3.66309628	-1.97408590
H	1.53747723	5.09037943	2.05597289
H	1.04387047	6.03017944	0.63080474
H	2.75665144	5.94483093	1.09504097
H	-2.67860653	-3.41475511	4.06991491
H	-0.91725202	-3.54526055	3.89505966
H	-1.91427182	-3.24056336	2.46251757
H	-1.19321448	-0.09058551	5.38365332
H	-0.48052502	-1.70660837	5.58426103
H	-2.21800818	-1.45613237	5.85823832
H	-4.25781507	-1.86585160	4.33852004
H	-6.24393276	-0.56803936	3.60602775
H	-5.97000336	1.36303872	2.07001157
H	2.42464456	-0.58809438	2.23504941
H	-2.72694228	2.36759370	0.48290127
H	5.36295318	-1.06016994	2.99700639
H	4.64749149	-1.51886365	1.43374127
H	4.04346165	-2.23635812	2.93633035
H	2.86839553	-0.78925411	4.67903708

H	2.35201017	0.86294936	4.29479046
H	4.06737342	0.52308106	4.58965950
H	-4.89793120	1.67609050	-0.62365917
H	-4.55572072	3.41379119	-0.69194465
H	-5.76792359	2.80295830	0.44361722
H	-2.77053890	3.66630679	2.63628808
H	-4.53314927	3.82055855	2.51017992
H	-3.48039946	4.59698316	1.30321289
O	0.01262449	2.33400248	-1.56726339
Hf	-0.00012800	0.08810372	-0.05782503
H	1.17338714	-2.58272533	-3.21510843
H	-1.13259099	-1.84215543	-3.68422595
H	1.13467628	2.71946593	3.09943040
H	-1.16969162	2.00077328	3.60883412

4.7 Six Oxygen Atoms

Bis- η^2 -ozone ComplexFig. S22: NCCN Bis- η^2 -ozone Complex

E	E_{zp}	H	G
-2743.7037	-2742.5503	-2742.4787	-2742.6581

O	0.81575367	1.52248869	1.10646436
O	-1.20182754	0.42535331	1.61012332
O	-0.93669111	-0.44240962	-1.90029640
O	0.92549607	-1.60775327	-1.06491248
N	1.18204063	-1.44678796	1.58485715
N	-1.46909186	-2.00515947	0.70524813
N	-1.19322070	2.04180616	-0.90178303
N	1.47459092	1.29294125	-1.54363660
C	0.50312215	-2.46244879	2.02675883
C	-0.86164520	-2.75266507	1.57414227
C	-0.46199250	2.73583332	-1.71907332
C	0.89483107	2.32134936	-2.08644372
C	2.53776274	-1.29985291	2.14500086
C	3.61790853	-1.97651554	1.51249715
C	4.89208747	-1.87027054	2.11024387
C	5.08755130	-1.13934340	3.29116180

C	3.99999618	-0.50042188	3.90259144
C	2.70321323	-0.56437301	3.34938576
C	4.54706323	-2.68888012	-0.77329530
C	3.42944339	-2.87075334	0.28128478
C	3.33955623	-4.36238341	0.70990547
C	-2.19873607	-3.71616269	-3.08343917
C	-1.94820532	-3.84264671	-1.56197608
C	-1.71600415	-5.32659389	-1.16412825
C	-2.85398978	-2.38534514	0.38000003
C	-3.08467398	-3.24472301	-0.72855027
C	-4.41535822	-3.62731979	-0.99860616
C	-5.47850009	-3.18907420	-0.19702979
C	-5.22028614	-2.36582828	0.90756832
C	-3.91022800	-1.94877444	1.22961199
C	1.81842237	1.56923850	4.44371809
C	1.53600791	0.08710720	4.09780117
C	1.19444085	-0.72248121	5.37869472
C	-4.62677556	0.11050728	2.57528788
C	-3.68792807	-1.11854102	2.50002370
C	-3.85571813	-2.00861065	3.76230237
C	-2.48088375	2.62269073	-0.50857893
C	-2.49870032	3.71621587	0.40411788
C	-3.76006469	4.23749757	0.76728351
C	-4.94945115	3.71526999	0.24294547
C	-4.89937303	2.66339561	-0.68438965
C	-3.67190934	2.09945597	-1.08575375
C	-1.31283239	4.58767916	2.50424851
C	-1.23649413	4.38327634	0.97062373
C	-0.97961017	5.74606962	0.26732402
C	2.17717403	-1.55184364	-4.58741682
C	1.99762548	-0.07558133	-4.15560892
C	1.92720076	0.85118475	-5.40044671
C	2.86102392	1.03987456	-1.96843992
C	3.10836358	0.38486442	-3.20490818
C	4.45517937	0.19962169	-3.58753715
C	5.51243755	0.65088752	-2.78698666
C	5.23871133	1.32037750	-1.58461969
C	3.91475160	1.53913028	-1.15125701
C	-4.85211315	0.10715309	-2.21452112
C	-3.62976794	1.05151544	-2.20099166
C	-3.49254833	1.75503485	-3.58169334
C	4.69478426	2.18599977	1.21453318
C	3.64561160	2.38673649	0.09704185
C	3.57314627	3.89250306	-0.28656248
H	5.73536241	-2.37516067	1.64787937
H	6.07792038	-1.07649122	3.73586339
H	4.15328513	0.05238964	4.82529046
H	2.49059432	-2.60466724	-0.21274122
H	-1.03006677	-3.28941525	-1.35909492
H	5.52058662	-3.05144390	-0.41549028
H	4.65490939	-1.63812424	-1.06127918
H	4.29554781	-3.26053367	-1.67607524

H	4.26382903	-4.68678637	1.20751387
H	3.18343324	-4.99954058	-0.17058300
H	2.50820048	-4.54084520	1.40548339
H	-3.07227242	-4.29600287	-3.41190167
H	-1.32473791	-4.08715777	-3.63368337
H	-2.34731402	-2.66692365	-3.36004192
H	-1.47636208	-5.42730796	-0.09623147
H	-0.88061783	-5.74635771	-1.73996187
H	-2.60761951	-5.93690983	-1.36243626
H	-4.61420075	-4.28540553	-1.83996541
H	-6.49680381	-3.49645101	-0.42306312
H	-6.04397191	-2.04430380	1.53913151
H	0.65464071	0.09127029	3.45393957
H	-2.67211104	-0.71789782	2.49165584
H	2.67419713	1.68199977	5.12341279
H	0.94008042	2.00856060	4.93334302
H	2.01276420	2.13864158	3.52899214
H	2.04072164	-0.73712913	6.07866964
H	0.94016285	-1.76580167	5.14479577
H	0.33571964	-0.27140577	5.89303739
H	-4.50388512	0.75175016	1.69602857
H	-4.38033339	0.70866299	3.46229010
H	-5.68451038	-0.17701984	2.65146493
H	-4.87189023	-2.42063200	3.82892215
H	-3.66942700	-1.41783319	4.66913961
H	-3.15567490	-2.85598355	3.76021611
H	-3.80556462	5.06398032	1.47081393
H	-5.90762649	4.13283258	0.54320814
H	-5.82219685	2.27978327	-1.10817227
H	-0.37730190	3.73228943	0.79103853
H	1.03917734	-0.02798841	-3.63554861
H	-2.09325886	5.30670878	2.78700857
H	-0.35495816	4.97821070	2.87318780
H	-1.50732803	3.63633485	3.00784028
H	-0.86728895	5.63643309	-0.82009129
H	-0.06303353	6.20783228	0.65848027
H	-1.81037284	6.44280318	0.44187952
H	3.08648062	-1.69951663	-5.18598019
H	1.31996590	-1.86660202	-5.19620895
H	2.22284218	-2.20404697	-3.70926329
H	1.74511619	1.89844632	-5.12119071
H	1.11326856	0.53163159	-6.06464094
H	2.86396477	0.82090144	-5.97301972
H	4.67143210	-0.30374010	-4.52584040
H	6.54144097	0.49323700	-3.10129572
H	6.06107207	1.68610500	-0.97762615
H	-2.73882783	0.42861380	-2.07136163
H	2.67205894	2.10986028	0.51471495
H	-5.77312106	0.62574725	-2.51553426
H	-5.01762574	-0.35250346	-1.23430149
H	-4.68168168	-0.70078094	-2.93708065
H	-3.43266984	1.00514065	-4.38107424

H	-2.58812155	2.37464598	-3.63740711
H	-4.35823920	2.40255733	-3.77899526
H	4.82915024	1.12629472	1.45428481
H	4.36079267	2.69689366	2.12645280
H	5.67289626	2.60734318	0.94363201
H	2.77905908	4.09422846	-1.01724004
H	4.52299946	4.23144214	-0.72246236
H	3.36826226	4.49876166	0.60553095
O	-0.36515981	1.60271890	2.06077318
Hf	-0.03093940	-0.02918874	-0.05405162
H	-1.34969567	-3.62646456	2.01114452
H	0.92786859	-3.13845029	2.77136552
H	-0.81828311	3.67800310	-2.13900760
H	1.41659581	2.93692747	-2.82153465
O	0.01595853	-1.55988124	-2.27769908

5. Triplet Ground States for NCCN Complex

5.1 Zero Oxygen Atoms

Bare Complex

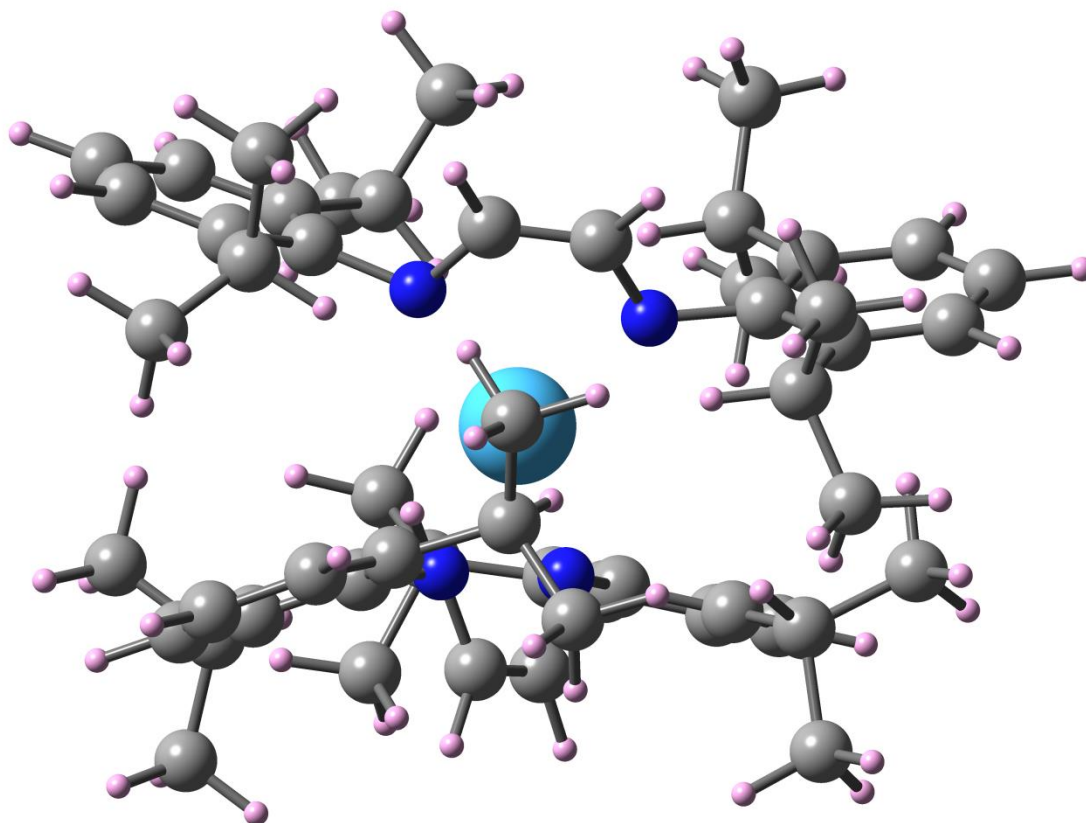


Fig. S23: NCCN Bare Complex

E	E_{zp}	H	G
-2292.5637	-2291.4302	-2291.3662	-2291.5307
N	1.40719536	-0.38045742	1.55360458
N	-1.15106178	0.89577337	1.49217636
N	1.00929453	-0.04510254	-1.92590860
N	-1.40445596	-1.22798926	-1.39799176
C	0.47912713	-0.52634821	2.63116154
C	-0.75829523	0.07682458	2.60173819
C	0.42820490	-0.82611075	-2.87696656
C	-0.81519154	-1.43331930	-2.60504098
C	2.75776445	-0.82174101	1.82893785
C	3.77837452	0.14740609	2.05945538
C	5.08400371	-0.29547629	2.36337541
C	5.38747345	-1.66011554	2.46645587
C	4.37662974	-2.60730389	2.25144498
C	3.06059615	-2.21634802	1.92725433
C	3.81582796	2.30536844	3.39676034

C	3.50079011	1.65210380	2.02499843
C	4.29262863	2.35689798	0.89285495
C	-2.15322766	1.91765621	1.70968646
C	-3.51309067	1.57399417	1.98800125
C	-4.45875602	2.61162394	2.14626685
C	-4.09340437	3.95861961	2.03698208
C	-2.74964233	4.28945100	1.80619661
C	-1.76276256	3.29282779	1.66168144
C	1.74518374	-4.10801762	3.01994062
C	2.01050129	-3.31402196	1.71252172
C	2.40995843	-4.28571427	0.57154912
C	2.18742966	0.69900506	-2.36236204
C	2.02909030	2.06281348	-2.75161645
C	3.16222243	2.76465497	-3.21106618
C	4.41571208	2.14076900	-3.30678509
C	4.55006465	0.79454588	-2.94324420
C	3.44979941	0.04812334	-2.46728716
C	0.70974070	4.26051782	-2.48892896
C	0.65368364	2.74020983	-2.76206335
C	-0.07302773	2.48023612	-4.11185930
C	-2.76947981	-1.72316891	-1.29495777
C	-3.04474570	-2.90884083	-0.55791213
C	-4.36210429	-3.41374860	-0.56550471
C	-5.38291560	-2.77328297	-1.28351209
C	-5.10041882	-1.59562449	-1.99047950
C	-3.80224889	-1.04354582	-2.00736090
C	4.93358047	-1.69376814	-1.30862501
C	3.64712332	-1.43439841	-2.12972716
C	3.67059754	-2.30176415	-3.41955664
C	-4.20675850	-0.16429497	3.70519378
C	-3.99030980	0.12996172	2.19257438
C	-5.29657684	-0.19314093	1.42686422
C	-2.32256298	-4.03696742	1.62692838
C	-1.94320985	-3.68725488	0.16689912
C	-1.56584483	-4.96615073	-0.62797089
C	-3.79016512	0.06296895	-4.30600439
C	-3.56103923	0.25951896	-2.78371144
C	-4.43947854	1.42038656	-2.24732635
C	0.33693517	3.58491008	3.00872673
C	-0.28679463	3.69492855	1.58885082
C	-0.04224852	5.11300620	1.02480784
H	5.86712643	0.43895385	2.53716069
H	6.39688229	-1.98117154	2.71291294
H	4.61275912	-3.66601875	2.33472279
H	2.43395849	1.78573827	1.82249853
H	3.21444267	1.85629607	4.19710555
H	3.59843721	3.38124624	3.36880219
H	4.87450715	2.18820197	3.66334247
H	5.37676397	2.26442580	1.04568316
H	4.05004994	3.42837308	0.86841809
H	4.05345018	1.93158852	-0.08843915
H	-5.49478436	2.35767772	2.35542884

H	-4.84015031	4.74154969	2.14841027
H	-2.46443980	5.33567944	1.75632374
H	1.06937455	-2.83627369	1.41731107
H	2.64895314	-4.63511044	3.35288897
H	0.95778487	-4.85811905	2.86331474
H	1.42867205	-3.44594659	3.83557020
H	2.56546411	-3.74880529	-0.37191036
H	1.62091506	-5.03317939	0.41200291
H	3.33627697	-4.82534397	0.80765214
H	3.06379716	3.80533400	-3.50441774
H	5.27722435	2.69854335	-3.66614930
H	5.52150241	0.31529964	-3.02606641
H	0.04945241	2.28284228	-1.96565322
H	1.16123541	4.80802801	-3.32678283
H	1.28248521	4.48679172	-1.58290621
H	-0.30727966	4.65136976	-2.35685562
H	-1.06659939	2.94885671	-4.10650757
H	-0.20326554	1.40940480	-4.30400894
H	0.50083586	2.90732810	-4.94547203
H	-4.58618505	-4.32616948	-0.01839789
H	-6.38925372	-3.18516470	-1.28817897
H	-5.89830566	-1.09546286	-2.53448857
H	2.79472399	-1.75925450	-1.52094308
H	5.83695227	-1.51059486	-1.90542092
H	4.96520851	-2.74045436	-0.98165785
H	4.97643247	-1.06242104	-0.41623625
H	2.74300144	-2.20825107	-3.99644619
H	3.80660391	-3.36137765	-3.16399975
H	4.50207807	-2.00140854	-4.07113232
H	-3.21647270	-0.54763541	1.81517025
H	-3.31704658	0.05944771	4.30605693
H	-4.47012883	-1.22001630	3.85852257
H	-5.02784618	0.44939559	4.09941373
H	-6.15037639	0.36900417	1.82715219
H	-5.53141993	-1.26084201	1.51934247
H	-5.20522806	0.03629882	0.36167963
H	-1.05225092	-3.04771039	0.20733009
H	-2.57358444	-3.13359256	2.19639291
H	-1.47999641	-4.53101439	2.12862923
H	-3.18136430	-4.71906655	1.67484488
H	-2.42502087	-5.64521431	-0.70993484
H	-0.75239691	-5.50710223	-0.12612452
H	-1.23475438	-4.71839798	-1.64465029
H	-2.51737626	0.56005637	-2.64529734
H	-3.13932557	-0.72190198	-4.71248766
H	-3.58096521	0.99501149	-4.84779603
H	-4.82871177	-0.22293572	-4.51832333
H	-5.50978225	1.20125519	-2.35579792
H	-4.22999203	2.34127138	-2.80826948
H	-4.23875237	1.61740009	-1.18765661
H	0.23377727	2.97416328	0.94518948
H	-0.20275265	4.23346890	3.71251957

H	1.38779615	3.89891272	2.99305932
H	0.29241903	2.55641462	3.38249234
H	-0.55365324	5.26788231	0.06743394
H	1.03324198	5.26802282	0.86661512
H	-0.38059337	5.89119992	1.72211932
H	0.88293049	-0.93037580	-3.85908014
H	-1.31155965	-2.02897142	-3.36867920
H	0.71580563	-1.22276653	3.43294925
H	-1.46994775	-0.13696769	3.39210138
Hf	-0.03973647	-0.12522828	0.07354172

5.2 One Oxygen Atom

Oxo Complex

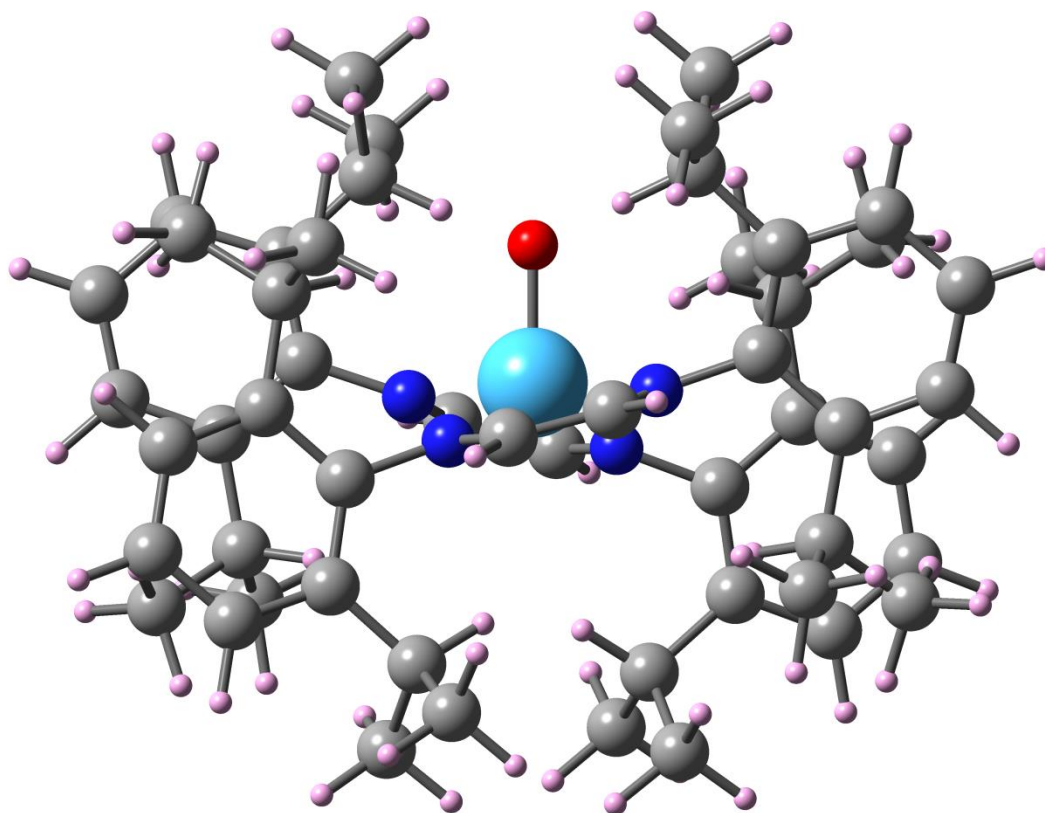


Fig. S24: NCCN Oxo Complex

E	E_{zp}	H	G
-2367.8813	-2366.7439	-2366.6785	-2366.8456

O	0.00403823	2.19619102	-0.05304111
N	-1.09799606	-0.35755139	1.80812681
N	1.61632871	0.30119826	1.64223454
N	1.09770284	-0.45284912	-1.78752437
N	-1.61572712	0.21790222	-1.65275981
C	-0.31464849	-0.31100389	2.92780973
C	1.04038244	0.04836854	2.84533002
C	0.31125865	-0.46977724	-2.90586131
C	-1.04329466	-0.10477589	-2.84065990
C	-2.44364619	-0.85344893	2.07314953
C	-3.50162595	0.07487166	2.28713812
C	-4.75479531	-0.43056779	2.69389259
C	-4.95557188	-1.80489754	2.89929555
C	-3.90520305	-2.70572112	2.67175292
C	-2.63752068	-2.25359256	2.24950973
C	-4.51058123	2.35332808	1.64773407
C	-3.27552501	1.58742209	2.17623097

C	-2.83985785	2.17469529	3.54832188
C	2.31008017	4.40117608	1.12402344
C	2.13671665	3.20370835	2.09047527
C	2.05640020	3.69229080	3.56265663
C	2.99837255	0.77528912	1.72685891
C	3.25126829	2.16251893	1.93405729
C	4.59315209	2.58214558	2.07031082
C	5.65361929	1.66858834	2.02030980
C	5.38485466	0.30240016	1.84558217
C	4.06390649	-0.17264623	1.70673045
C	-1.90572961	-4.38233984	1.02694019
C	-1.50988193	-3.27181729	2.03404138
C	-1.05632960	-3.90216111	3.37840226
C	4.93497903	-2.45701651	0.90420974
C	3.80516398	-1.68222859	1.62227547
C	3.59818502	-2.29351240	3.03814621
C	2.44520274	-0.95535035	-2.02974223
C	2.64678821	-2.36149060	-2.13512713
C	3.91698947	-2.82704102	-2.53460632
C	4.96185398	-1.93290748	-2.80918125
C	4.75285258	-0.55103785	-2.67567080
C	3.49691440	-0.03295035	-2.29411794
C	1.92069425	-4.41385642	-0.78615112
C	1.52580385	-3.37471790	-1.86695047
C	1.09293248	-4.09608042	-3.17166524
C	-2.33001767	4.33818418	-1.30824377
C	-2.14907728	3.09790330	-2.21775550
C	-2.06604948	3.51913694	-3.71049729
C	-2.99992542	0.68163040	-1.75976231
C	-3.25911736	2.05903121	-2.01927900
C	-4.60251376	2.46654082	-2.17502838
C	-5.65883052	1.55032647	-2.09402336
C	-5.38389992	0.19285151	-1.86942614
C	-4.06091010	-0.27050030	-1.70999051
C	4.48380128	2.28216044	-1.76121152
C	3.26079616	1.48180732	-2.26657382
C	2.84154698	1.99136936	-3.67443986
C	-4.90812568	-2.52181045	-0.79744407
C	-3.79825010	-1.77587397	-1.57523050
C	-3.62995229	-2.43849576	-2.97295441
H	-5.57644244	0.25830160	2.86612429
H	-5.92492196	-2.16970071	3.23083410
H	-4.07034212	-3.76961026	2.82511568
H	-2.45216387	1.76306785	1.47297696
H	1.18207458	2.74539084	1.82805410
H	-5.33104279	2.35713945	2.37830473
H	-4.88203343	1.92520675	0.71108811
H	-4.24084370	3.39985126	1.45681888
H	-3.62196843	2.01527105	4.30344203
H	-2.66540925	3.25492916	3.45817379
H	-1.91430530	1.71386391	3.91154694
H	3.24070827	4.95573741	1.30883342

H	1.47142976	5.09902642	1.24506329
H	2.30294506	4.05668627	0.08446279
H	1.88885850	2.85588727	4.25453114
H	1.22649358	4.40201855	3.68026462
H	2.98141968	4.19945307	3.86981584
H	4.80307525	3.63718254	2.22654490
H	6.67953930	2.01330565	2.12771026
H	6.21052516	-0.40203846	1.82361409
H	-0.64709421	-2.74291805	1.61253993
H	2.87704431	-1.82916846	1.05431038
H	-2.75076899	-4.97936566	1.39325885
H	-1.06076842	-5.06571203	0.86755532
H	-2.18989287	-3.95712430	0.05675245
H	-1.87699249	-4.45988380	3.84861356
H	-0.72441254	-3.13420902	4.08773731
H	-0.22307667	-4.59897315	3.21597932
H	5.18616582	-2.00476271	-0.05903518
H	4.62049183	-3.49226614	0.72143383
H	5.84516706	-2.49923585	1.51758524
H	4.48518097	-2.12043546	3.66225889
H	3.44231676	-3.37884751	2.96445929
H	2.73243968	-1.86303261	3.55138277
H	4.08828015	-3.89646472	-2.63353959
H	5.93311341	-2.30867180	-3.12239967
H	5.56979232	0.13323619	-2.88510362
H	0.65363163	-2.82783654	-1.49034803
H	-1.19311141	2.65732684	-1.93128804
H	2.77526427	-5.02475339	-1.10490492
H	1.08057961	-5.09418860	-0.59151941
H	2.19050916	-3.92490209	0.15760883
H	0.75880244	-3.37996932	-3.93227415
H	0.26675723	-4.79126757	-2.97083251
H	1.92427041	-4.67313169	-3.59772633
H	-3.26145408	4.88134701	-1.52094400
H	-1.49296802	5.03198161	-1.45930614
H	-2.32541884	4.04298240	-0.25352111
H	-1.89220774	2.65299328	-4.36306017
H	-1.23912350	4.22686471	-3.85778890
H	-2.99255642	4.00724305	-4.04309278
H	-4.81707633	3.51381997	-2.37196307
H	-6.68604315	1.88589055	-2.21690101
H	-6.20624608	-0.51463258	-1.82487190
H	2.42572078	1.69001660	-1.58669426
H	-2.85504609	-1.90356397	-1.02822626
H	5.31600219	2.25088406	-2.47776557
H	4.84266872	1.90695197	-0.79734511
H	4.20612878	3.33601734	-1.63143611
H	2.65865148	3.07353564	-3.64506408
H	1.92441958	1.50410552	-4.02467297
H	3.63501089	1.79716467	-4.40921156
H	-5.13210312	-2.03370126	0.15482857
H	-4.58945308	-3.55033456	-0.58540090

H	-5.83542803	-2.58510957	-1.38259724
H	-2.77907801	-2.02612798	-3.52484940
H	-4.53361364	-2.28756729	-3.57853597
H	-3.47099926	-3.52038267	-2.86453283
Hf	0.00143739	0.40319398	-0.00984444
H	-0.74639796	-0.56014092	3.89447408
H	1.62122712	0.15119012	3.75933846
H	0.74045457	-0.77358555	-3.85797299
H	-1.62612206	-0.05340010	-3.75766884

5.3 Two Oxygen Atoms

Dioxo Complex

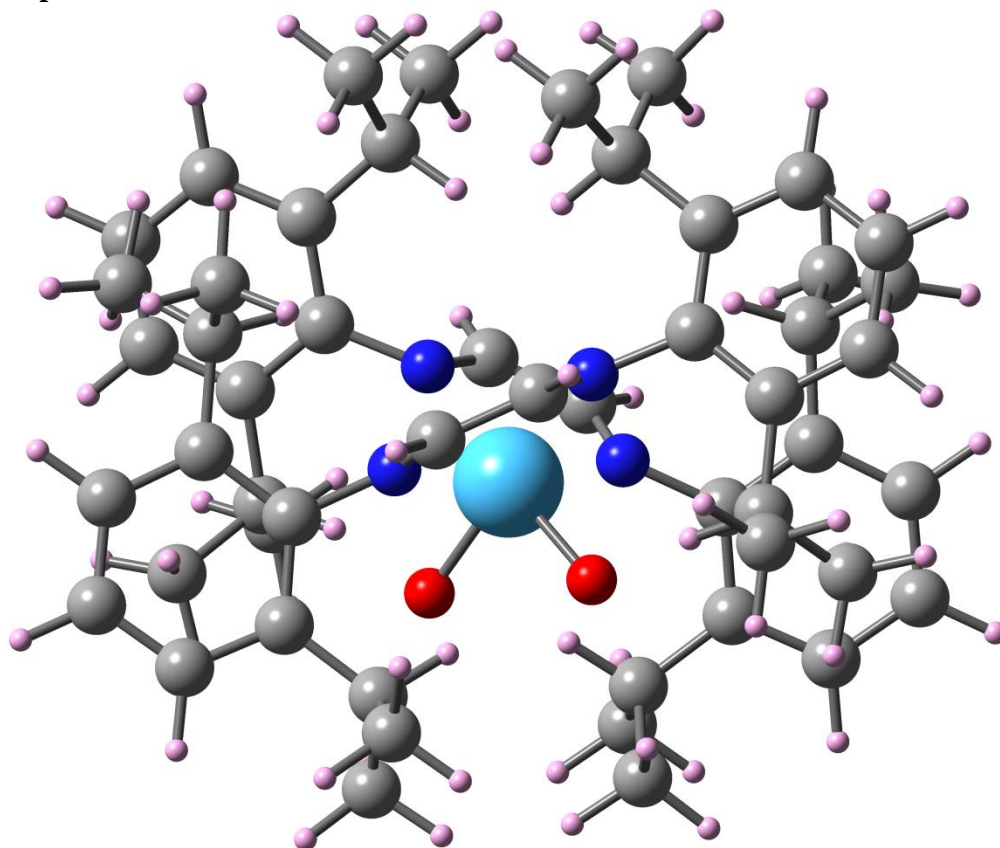


Fig. S25: NCCN Dioxo Complex

E	E_{zp}	H	G
-2443.0446	-2441.9064	-2441.8388	-2442.0107

N	-1.49450500	-0.47971300	1.80212700
N	1.06884800	0.75198700	1.90158200
N	1.47248600	-0.36172600	-1.81427900
N	-1.06218500	0.85698000	-1.71341500
C	-0.95611100	-0.09578000	2.92094300
C	0.37745800	0.51500900	2.97659100
C	1.00450300	0.36713300	-2.86110200
C	-0.26619800	0.97201700	-2.81051600
C	-2.82873300	-1.09526600	1.90647600
C	-3.96917900	-0.24629900	1.89765100
C	-5.23591600	-0.85437500	2.01880000
C	-5.36435900	-2.24477600	2.15509700
C	-4.21972600	-3.05242300	2.18386000
C	-2.92494200	-2.50295100	2.06357900
C	-5.02901700	1.93597000	1.05139400
C	-3.85434800	1.28230700	1.81540100
C	-3.75759000	1.91574800	3.23282300

C	1.91503300	4.62133900	0.38301000
C	1.45058200	3.60402800	1.45327000
C	0.79451300	4.33382800	2.65838500
C	2.40556600	1.30767700	2.13219500
C	2.58899000	2.70280000	1.93784300
C	3.83076300	3.26416400	2.29476900
C	4.86473500	2.46696500	2.80820100
C	4.67213600	1.08656000	2.95562400
C	3.44451000	0.46959300	2.62754900
C	-1.79304700	-4.63097500	1.21405500
C	-1.70659200	-3.42527000	2.18156600
C	-1.53379700	-3.90039700	3.65102000
C	4.39382500	-1.81934100	2.03462700
C	3.29964300	-1.04562100	2.81475200
C	3.32712800	-1.42909600	4.31857700
C	2.78861800	-0.96753400	-1.98937300
C	2.89276100	-2.37689800	-2.17955300
C	4.17639100	-2.94052000	-2.33967600
C	5.33143600	-2.14705600	-2.34072700
C	5.21229800	-0.75845000	-2.19342900
C	3.95433300	-0.14230100	-2.01819200
C	1.72937800	-4.48374300	-1.31633200
C	1.67437700	-3.29543600	-2.30835800
C	1.52992900	-3.79570800	-3.77178700
C	-2.02866000	4.63172100	-0.08175300
C	-1.54583300	3.75723600	-1.26685000
C	-1.04180600	4.65455300	-2.43009900
C	-2.40243700	1.40158500	-1.92481200
C	-2.63629500	2.79667100	-1.75322200
C	-3.89941500	3.32258900	-2.09903100
C	-4.91797500	2.49889400	-2.59751400
C	-4.68133600	1.12507900	-2.74869000
C	-3.43217700	0.55026000	-2.42737800
C	4.94280800	1.93444600	-0.89113100
C	3.90725600	1.38805000	-1.90423400
C	4.13779200	2.05923800	-3.28748200
C	-4.31957000	-1.83292500	-2.11160200
C	-3.20714300	-0.93800300	-2.71110900
C	-3.07088500	-1.18454000	-4.23870600
H	-1.46971700	-0.24632300	3.87198200
H	0.77158200	0.74215300	3.97013100
H	1.59652500	0.45532300	-3.76919700
H	-0.62936500	1.49902700	-3.69232900
H	-6.12800800	-0.23634400	2.00308400
H	-6.35090000	-2.69342700	2.24318100
H	-4.32585400	-4.12716100	2.30126500
H	-2.93334900	1.52634500	1.26775400
H	0.68335100	2.96842300	0.99206800
H	-5.96508000	1.87208400	1.62185900
H	-5.18241100	1.46870900	0.07463200
H	-4.81995500	2.99914900	0.88442700
H	-4.64877100	1.66705800	3.82391900

H	-3.69502400	3.00971600	3.15703700
H	-2.88161700	1.56646800	3.79296000
H	2.63426600	5.34294200	0.79054600
H	1.05785100	5.19236500	0.00756500
H	2.38724500	4.11478500	-0.46755800
H	0.41445100	3.62011500	3.40145700
H	-0.04416400	4.95837200	2.32668100
H	1.52416900	4.98073400	3.16271000
H	3.98870100	4.33228500	2.17481600
H	5.81564200	2.91713400	3.08203800
H	5.48334200	0.47106000	3.33471400
H	-0.80569600	-2.87593600	1.89829900
H	2.34674100	-1.37889800	2.39065200
H	-2.65045100	-5.28143700	1.43588000
H	-0.88179800	-5.23731900	1.29927200
H	-1.86649600	-4.26937300	0.18389300
H	-2.39797800	-4.49036700	3.98549500
H	-1.42254700	-3.05362800	4.34383200
H	-0.63848500	-4.52950700	3.73864100
H	4.36660100	-1.57001000	0.96832600
H	4.21621800	-2.89797200	2.12735500
H	5.40205100	-1.60799400	2.41707000
H	4.28010700	-1.14775100	4.78705900
H	3.20305800	-2.51382600	4.43097000
H	2.52315600	-0.93578700	4.88296400
H	4.26599800	-4.01467600	-2.48092300
H	6.31086000	-2.60237500	-2.46900300
H	6.10812400	-0.14311000	-2.21397700
H	0.77213200	-2.73135900	-2.06932800
H	-0.69582700	3.15777500	-0.92091700
H	2.58883100	-5.14130500	-1.50907300
H	0.81631200	-5.08672100	-1.40870400
H	1.78854600	-4.10892100	-0.28904200
H	1.44745400	-2.95550000	-4.47465500
H	0.62639800	-4.41231000	-3.87054500
H	2.39216400	-4.40496700	-4.07624900
H	-2.87090500	5.27322400	-0.37020700
H	-1.22112500	5.29060000	0.26198300
H	-2.35267100	4.01293900	0.76510100
H	-0.64880500	4.04879500	-3.25556600
H	-0.24074800	5.32418200	-2.08885800
H	-1.85587400	5.27478100	-2.82781200
H	-4.08282200	4.38898000	-1.98908300
H	-5.88229900	2.92261100	-2.86836800
H	-5.46880400	0.48729700	-3.14186500
H	2.91137200	1.67923000	-1.54963800
H	-2.27193700	-1.25337800	-2.24147000
H	5.97086600	1.78284700	-1.24491400
H	4.84475300	1.44716000	0.08337400
H	4.80227800	3.01404200	-0.74902000
H	4.09038900	3.15349400	-3.19762200
H	3.39162400	1.74600900	-4.02712300

H	5.12744800	1.79456400	-3.68269200
H	-4.42291400	-1.66493000	-1.03330500
H	-4.06023800	-2.88870400	-2.26040600
H	-5.29574200	-1.65717100	-2.58518600
H	-2.24266100	-0.60364800	-4.66492700
H	-3.99016000	-0.90419300	-4.77213400
H	-2.87411300	-2.24730400	-4.43241500
O	1.06718200	-1.91363700	0.81103500
O	-1.04000700	-2.08691300	-0.73221200
Hf	-0.01371200	-0.64605700	-0.13841600

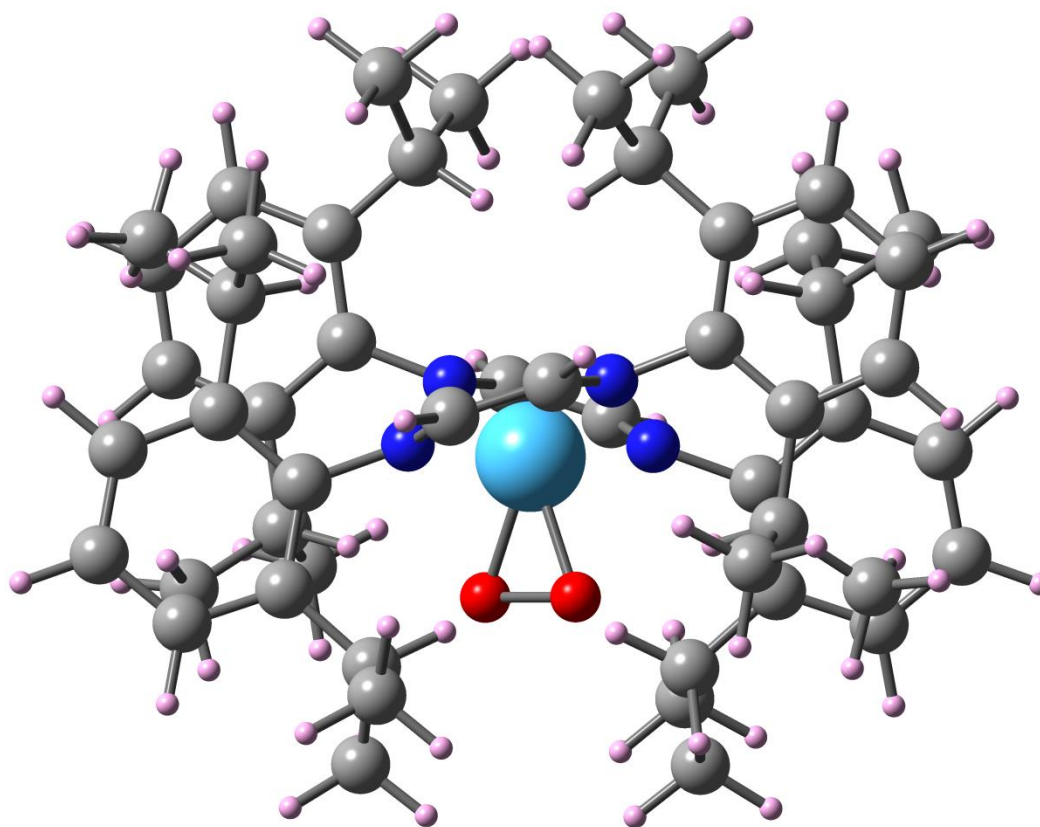
Peroxo Complex

Fig. S26: NCCN Peroxo Complex

E	E_{zp}	H	G
-2443.0381	-2441.8974	-2441.8311	-2441.9989
O	-0.58738775	-2.27659169	-0.51876606
O	0.58627885	-2.27104463	0.54176691
N	-1.59548166	-0.28972480	1.63564112
N	1.05311038	0.54499642	1.74875569
N	1.59529401	-0.30731029	-1.63425121
N	-1.05246898	0.52602329	-1.75559854
C	-1.04941342	0.08210092	2.82088852
C	0.28328007	0.52348297	2.87573562
C	1.04858039	0.04952460	-2.82377485
C	-0.28421872	0.49017055	-2.88323048
C	-2.97231853	-0.78570418	1.73668634
C	-4.05518945	0.14186159	1.68695472
C	-5.36798703	-0.35607499	1.82746614
C	-5.61233711	-1.72195629	2.03304144
C	-4.53452146	-2.61132049	2.12456803
C	-3.19968560	-2.16903231	1.99272224
C	-4.97244389	2.38103976	0.81300241
C	-3.83416309	1.65602638	1.56962265

C	-3.67710743	2.31006557	2.97304482
C	1.92051664	4.51266971	0.65412606
C	1.46724086	3.47413365	1.71201065
C	0.93775791	4.19493885	2.98102185
C	2.39512171	1.06979916	2.00465325
C	2.58259739	2.48008117	2.06166444
C	3.83021123	2.97207415	2.49941997
C	4.86771052	2.09970382	2.85799859
C	4.67479363	0.71266412	2.76836609
C	3.44154012	0.16796724	2.35044832
C	-2.21003847	-4.44955224	1.35993540
C	-2.06961142	-3.17690749	2.23050249
C	-2.00013169	-3.55028679	3.73798538
C	4.44681432	-2.13728501	1.82077302
C	3.23304650	-1.35072991	2.37078446
C	2.89242344	-1.83335019	3.80868585
C	2.97254811	-0.80317403	-1.72955755
C	3.20151720	-2.18866593	-1.97167881
C	4.53695051	-2.63097039	-2.09745005
C	5.61377161	-1.73964950	-2.01348760
C	5.36781881	-0.37197785	-1.82175202
C	4.05439495	0.12590919	-1.68766696
C	2.21066795	-4.46069745	-1.31193626
C	2.07260934	-3.19998237	-2.20002933
C	2.00821213	-3.59355886	-3.70261668
C	-1.92335421	4.50262738	-0.69053679
C	-1.46707657	3.45381016	-1.73686904
C	-0.93095712	4.16149588	-3.01046944
C	-2.39455615	1.04836046	-2.01597325
C	-2.58231308	2.45818664	-2.08207932
C	-3.82917900	2.94704404	-2.52512106
C	-4.86587699	2.07199333	-2.87993109
C	-4.67279361	0.68567028	-2.78103373
C	-3.43997071	0.14404641	-2.35759105
C	4.96819213	2.37615870	-0.83801017
C	3.83084400	1.64076852	-1.58584563
C	3.67106560	2.27974790	-2.99591731
C	-4.44189160	-2.15522571	-1.79904902
C	-3.23202239	-1.37495250	-2.36653108
C	-2.90351974	-1.87040457	-3.80270497
H	-6.20688088	0.33110995	1.78057615
H	-6.63259027	-2.08423067	2.13621477
H	-4.72476442	-3.66450909	2.31349334
H	-2.90064351	1.81733593	1.01486098
H	0.63004131	2.91177391	1.28185716
H	-5.89327377	2.41342402	1.41076131
H	-5.19619560	1.89870307	-0.14212450
H	-4.68358400	3.41967906	0.60958531
H	-4.56980895	2.12115235	3.58413257
H	-3.55897139	3.39804427	2.87345633
H	-2.80760510	1.92607860	3.51577519
H	2.74770988	5.13272107	1.02267181

H	1.08988042	5.18575795	0.40444421
H	2.25279857	4.02193296	-0.26842069
H	0.55379048	3.47802439	3.71696691
H	0.12425554	4.88511915	2.71998338
H	1.73398322	4.77661295	3.46388950
H	3.98886449	4.04579328	2.56472926
H	5.82018799	2.49652062	3.20135906
H	5.48472586	0.04295504	3.04312344
H	-1.11625317	-2.72323292	1.95782789
H	2.37550723	-1.59565460	1.73627571
H	-3.12693973	-5.01181600	1.58579126
H	-1.35616742	-5.11515098	1.54184622
H	-2.20379501	-4.18457922	0.29805567
H	-2.92188045	-4.04654715	4.07137081
H	-1.85252643	-2.66208777	4.36731652
H	-1.16151394	-4.23646377	3.91697869
H	4.73673500	-1.78647322	0.82482823
H	4.18893809	-3.20104889	1.74158777
H	5.32020841	-2.06008526	2.48282496
H	3.71562017	-1.61088792	4.50164851
H	2.72494353	-2.91816291	3.81113938
H	1.98483630	-1.35194040	4.19246525
H	4.72834883	-3.68584134	-2.27557128
H	6.63450472	-2.10189872	-2.11187462
H	6.20590148	0.31657097	-1.78080405
H	1.11830117	-2.74236858	-1.93729960
H	-0.63264533	2.89395754	-1.29807543
H	3.12958005	-5.02414291	-1.52637131
H	1.35871833	-5.13011326	-1.48881828
H	2.19913553	-4.18167221	-0.25373496
H	1.86288918	-2.71373835	-4.34414417
H	1.17006698	-4.28193620	-3.87519183
H	2.93090935	-4.09436134	-4.02641047
H	-2.74709173	5.12135121	-1.06887535
H	-1.09247697	5.17594589	-0.44230036
H	-2.26162269	4.02053726	0.23441598
H	-0.54437793	3.43664257	-3.73721070
H	-0.11789022	4.85337687	-2.75265126
H	-1.72442448	4.73899465	-3.50276868
H	-3.98811707	4.02025990	-2.59750521
H	-5.81779240	2.46639546	-3.22760302
H	-5.48208770	0.01388026	-3.05273747
H	2.89740491	1.80578331	-1.03204251
H	-2.36950882	-1.61482094	-1.73687109
H	5.88867612	2.40347284	-1.43658325
H	5.19324032	1.90494728	0.12234949
H	4.67754634	3.41649776	-0.64609544
H	3.54986163	3.36836085	-2.90753649
H	2.80232406	1.88773639	-3.53409579
H	4.56393398	2.08707137	-3.60560780
H	-4.72082604	-1.79662743	-0.80274904
H	-4.18556937	-3.21901479	-1.71487560

H	-5.32176250	-2.08053540	-2.45269829
H	-1.99875748	-1.39293647	-4.19814483
H	-3.73198478	-1.65356394	-4.49115838
H	-2.73673645	-2.95533229	-3.79719893
Hf	-0.00046528	-0.44424253	0.00168856
H	-1.63250700	0.01514724	3.73597362
H	0.70519859	0.84949506	3.82353016
H	1.63119954	-0.02857346	-3.73830635
H	-0.70729081	0.80386137	-3.83465377

5.4 Three Oxygen Atoms

Peroxo Complex with One Adsorbed Oxygen Atom

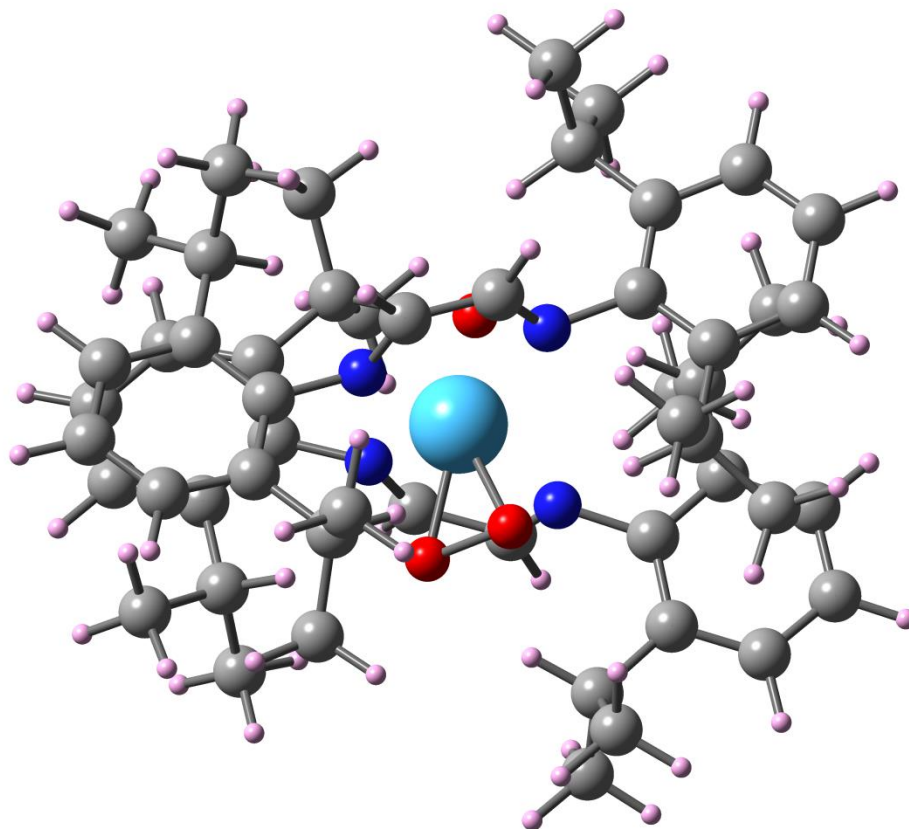


Fig. S27: NCCN Peroxo Complex with One Adsorbed Oxygen Atom

E	E_{zp}	H	G
-2518.2123	-2517.0696	-2517.0014	-2517.1733
O	0.22711756	1.51344541	-1.13620950
O	0.73861979	-1.56166153	1.32734834
O	-0.46823899	-2.03519943	0.47021854
N	-1.32420589	-0.61426125	-1.82512944
N	1.43049921	-1.24868907	-1.50674955
N	1.27754457	1.33303892	1.45336999
N	-1.41633055	0.68192705	1.72714269
C	-0.65901156	-1.29786337	-2.70850300
C	0.74572949	-1.67955207	-2.51838888
C	0.56078203	1.81721906	2.49821601
C	-0.79263465	1.47333951	2.64955765
C	-2.70755006	-0.28867551	-2.20497522
C	-3.73864582	-1.19153866	-1.83105161
C	-5.03936390	-0.91771876	-2.30374123
C	-5.29954314	0.19500465	-3.11892944
C	-4.25983258	1.06989335	-3.46619962
C	-2.93995767	0.85395467	-3.01634478

C	-4.58549991	-2.80534424	-0.02254034
C	-3.45385305	-2.46176776	-1.01924968
C	-3.20534586	-3.67030268	-1.96557134
C	2.28483500	-4.52071395	0.95348028
C	2.00848038	-3.99241266	-0.47648525
C	1.86597658	-5.16916267	-1.48006040
C	2.81957526	-1.70350718	-1.41683706
C	3.09439540	-3.01359365	-0.94143802
C	4.44633298	-3.42171860	-0.92425464
C	5.47346973	-2.57221179	-1.35679716
C	5.16792806	-1.28488064	-1.82724114
C	3.83741632	-0.82251190	-1.87426942
C	-2.19168746	3.29517870	-3.24176904
C	-1.81760385	1.80685607	-3.44631000
C	-1.41191456	1.55006716	-4.92313233
C	4.60721997	1.59606094	-2.27908088
C	3.49873967	0.54018936	-2.49086991
C	3.21572893	0.39068187	-4.01372245
C	2.63874519	1.83916257	1.35140062
C	2.85903442	3.12700256	0.78248467
C	4.17200461	3.64422917	0.79193422
C	5.23777892	2.91359965	1.33732012
C	5.00324925	1.64342288	1.88678580
C	3.70771135	1.08433118	1.91396712
C	2.01965641	4.50204249	-1.21194314
C	1.71799898	3.98071307	0.21469028
C	1.39121399	5.16463767	1.16567689
C	-2.07019680	-3.15892215	3.26957149
C	-1.85526348	-1.64413267	3.51214650
C	-1.66056971	-1.35465270	5.02579974
C	-2.78419039	0.31387908	2.08116288
C	-3.00146563	-0.79455952	2.94920589
C	-4.32555053	-1.07542868	3.35178975
C	-5.40192460	-0.28877083	2.91917651
C	-5.16845947	0.80596484	2.07202509
C	-3.86461525	1.13502670	1.64418155
C	4.58916584	-1.28552652	2.38632730
C	3.46126595	-0.25323714	2.62019419
C	3.25893104	-0.02768190	4.14527864
C	-4.79435287	2.69918042	-0.17453590
C	-3.63154712	2.39454226	0.79912545
C	-3.38894263	3.63398469	1.70691007
H	-5.85236932	-1.58562308	-2.03623805
H	-6.30852667	0.37949707	-3.47963214
H	-4.47219690	1.93220403	-4.09212250
H	-2.54007407	-2.30898185	-0.43274217
H	1.05068569	-3.46856220	-0.41693956
H	-5.50039670	-3.12946018	-0.53720393
H	-4.83027112	-1.95220458	0.61752261
H	-4.26536039	-3.63032931	0.62590981
H	-4.08820746	-3.86599467	-2.58921923
H	-2.99461704	-4.57108960	-1.37536592

H	-2.35167817	-3.50397458	-2.63523666
H	3.23250586	-5.07270177	1.01851571
H	1.47806032	-5.20045667	1.25779401
H	2.30364270	-3.68598734	1.66055088
H	1.62846978	-4.81634732	-2.49389434
H	1.06124823	-5.84347438	-1.15839208
H	2.79192077	-5.75663602	-1.54481687
H	4.69161361	-4.41651210	-0.56217035
H	6.50685696	-2.90956404	-1.32968045
H	5.96956393	-0.63526123	-2.16366884
H	-0.93708697	1.63255575	-2.81497534
H	2.58084740	0.91643017	-2.01955384
H	-3.02264954	3.60889078	-3.88775727
H	-1.32684382	3.92759428	-3.47911894
H	-2.47203417	3.48760005	-2.20022581
H	-2.25761629	1.72785077	-5.60130017
H	-1.07290287	0.51719452	-5.08172156
H	-0.59403236	2.22190206	-5.21424598
H	4.88468907	1.68332156	-1.22436535
H	4.25268613	2.57795888	-2.61570277
H	5.50945098	1.35980574	-2.85965916
H	4.10262539	0.00645731	-4.53553916
H	2.95846524	1.36615955	-4.44685706
H	2.38428315	-0.29571690	-4.21768773
H	4.35964596	4.62871989	0.36990667
H	6.24212900	3.33129088	1.33826097
H	5.83229350	1.08518818	2.31234357
H	0.82517805	3.35351799	0.13149051
H	-0.92929299	-1.38025338	2.99730889
H	2.89517970	5.16487350	-1.23471938
H	1.15962634	5.07209741	-1.58860190
H	2.19422326	3.66641505	-1.89808644
H	1.10973014	4.81099360	2.16567778
H	0.55625365	5.75644499	0.76660467
H	2.25700211	5.83147063	1.27795405
H	-2.98261846	-3.53360961	3.75419325
H	-1.21905522	-3.72159272	3.67532131
H	-2.12240708	-3.36645291	2.19577358
H	-1.46004386	-0.29063134	5.20826247
H	-0.81036981	-1.93128550	5.41398979
H	-2.55182157	-1.63210475	5.60547527
H	-4.50972984	-1.91492175	4.01752702
H	-6.41387036	-0.51995307	3.24428962
H	-6.00733337	1.41532606	1.74914062
H	2.53461337	-0.68493139	2.22942111
H	-2.72149423	2.24007152	0.20529868
H	5.52584881	-0.99006642	2.87910812
H	4.79207950	-1.42555270	1.31901050
H	4.29206652	-2.25593058	2.80484273
H	3.06235331	-0.98512611	4.64586088
H	2.40984670	0.63671801	4.34494156
H	4.15557351	0.41901995	4.59727340

H	-5.06200245	1.82360972	-0.77401345
H	-4.50510050	3.50646220	-0.85971930
H	-5.69112658	3.03777834	0.36156505
H	-2.50454919	3.50832841	2.33987058
H	-4.25554625	3.80891082	2.35901629
H	-3.23831439	4.53174128	1.09184148
Hf	-0.01417108	-0.07064452	0.16824626
H	-1.13187290	-1.60742473	-3.64214357
H	1.18727027	-2.33509361	-3.27167414
H	1.03322190	2.47869903	3.22160048
H	-1.34361757	1.81767022	3.52150079

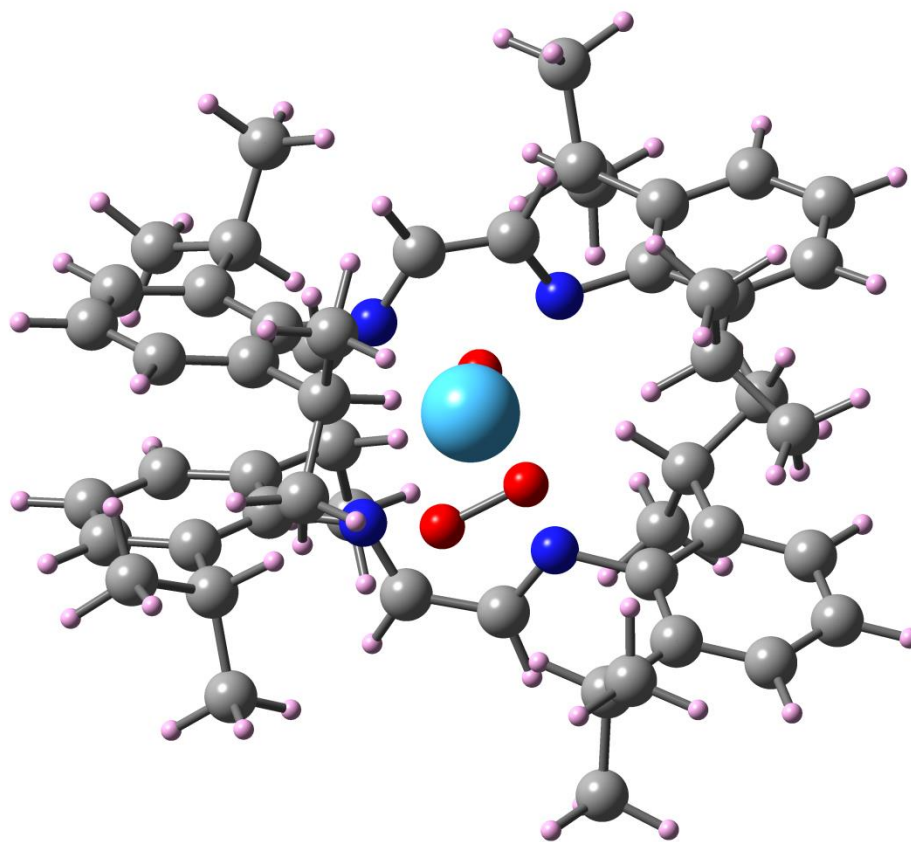
Oxo Complex with Adsorbed Oxygen Molecule (planar conformation)

Fig. S28: NCCN Oxo Complex with Adsorbed Oxygen Molecule (planar conformation)

E	E_{zp}	H	G
-2518.2254	-2517.0822	-2517.0138	-2517.1868
O	0.21891897	0.70757520	-1.67699653
O	0.89435142	-0.93202662	1.95139815
O	-0.32228850	-1.54161662	1.64112898
N	-1.47475975	-1.48669192	-1.11521567
N	1.31424123	-1.88727476	-0.70761196
N	1.38275382	1.81157146	0.78894974
N	-1.32657011	1.42557746	1.23147975
C	-0.84598874	-2.53234860	-1.56836668
C	0.56672573	-2.78158670	-1.28177939
C	0.70689962	2.66366362	1.59693221
C	-0.65913165	2.45084671	1.84090177
C	-2.84472041	-1.33609711	-1.62324318
C	-3.91801473	-1.81441489	-0.82355429
C	-5.21791069	-1.73476551	-1.36290912
C	-5.44019231	-1.22063051	-2.65043779
C	-4.35957239	-0.77194213	-3.42223452
C	-3.03539658	-0.81595034	-2.93356957
C	-4.83672848	-2.31489710	1.52629215

C	-3.67027670	-2.49491821	0.52841556
C	-3.39654703	-4.01450692	0.33422473
C	2.41422503	-3.78068429	2.86188571
C	2.07752941	-3.94648733	1.35809736
C	2.00145622	-5.45059964	0.97704801
C	2.72199676	-2.23452990	-0.51077286
C	3.08270636	-3.20875337	0.46191213
C	4.45430511	-3.52194702	0.58616194
C	5.42074405	-2.90924874	-0.22159941
C	5.03217442	-1.96917723	-1.18952648
C	3.67955539	-1.61545676	-1.36396777
C	-2.11636162	1.06053888	-4.41562037
C	-1.87959332	-0.35473528	-3.83278967
C	-1.64305627	-1.37396626	-4.98093404
C	4.32285908	0.34178702	-2.90372981
C	3.24900553	-0.69816317	-2.51445724
C	2.88274083	-1.55248672	-3.76299723
C	2.72376978	2.23237136	0.40792649
C	2.87946124	3.13806940	-0.68127392
C	4.18021256	3.59154048	-0.98843497
C	5.29380988	3.17014189	-0.24691734
C	5.12011086	2.28699203	0.82989260
C	3.84051163	1.80871252	1.18424247
C	1.85184456	3.47152305	-3.00426592
C	1.68742110	3.68111422	-1.47899062
C	1.45090402	5.18011179	-1.14932786
C	-2.35203551	-1.12406372	4.36504273
C	-2.04026791	0.32313163	3.90701226
C	-1.92457023	1.26445369	5.13670130
C	-2.73104468	1.34449499	1.61487360
C	-3.07815699	0.85090632	2.90677550
C	-4.43444652	0.89299692	3.29650946
C	-5.42186209	1.40044143	2.44170818
C	-5.06304029	1.88671872	1.17434839
C	-3.72048935	1.88480215	0.74130326
C	4.77450666	-0.12878593	2.59571311
C	3.66851565	0.94164682	2.43660046
C	3.60809360	1.83505020	3.70739145
C	-4.46717480	2.51138472	-1.64223148
C	-3.33620478	2.54700143	-0.58850848
C	-2.90316561	4.02327283	-0.35628385
H	-6.06066534	-2.08533043	-0.77586187
H	-6.45052890	-1.17485796	-3.04996002
H	-4.54102726	-0.37992838	-4.41951074
H	-2.77245784	-2.05023046	0.97696656
H	1.08183522	-3.51540823	1.22263720
H	-5.72624744	-2.87818130	1.21306402
H	-5.11151400	-1.26243035	1.63855225
H	-4.54192440	-2.69508924	2.51221402
H	-4.26343660	-4.50550753	-0.12805898
H	-3.21072922	-4.49024127	1.30589106
H	-2.52428957	-4.20385861	-0.30262838

H	3.39506905	-4.20644654	3.11098717
H	1.66038810	-4.29611983	3.47155156
H	2.40646412	-2.72170632	3.13894410
H	1.71846783	-5.59225066	-0.07533598
H	1.25778081	-5.96256233	1.60186544
H	2.96774206	-5.94966253	1.12684645
H	4.76336025	-4.25481702	1.32659523
H	6.47066790	-3.16640760	-0.10425335
H	5.78622687	-1.51092764	-1.82079472
H	-0.96956832	-0.26855363	-3.23029758
H	2.34316643	-0.15298807	-2.21746879
H	-3.00816240	1.10913337	-5.05551529
H	-1.25061944	1.35579841	-5.02211023
H	-2.22179256	1.79443068	-3.61031169
H	-2.52159040	-1.44798887	-5.63652311
H	-1.43176320	-2.38241582	-4.59894290
H	-0.78854147	-1.05984669	-5.59489686
H	4.66171950	0.91809222	-2.03702296
H	3.90303607	1.04748755	-3.63069606
H	5.19745031	-0.12907839	-3.37429370
H	3.75630806	-2.11648769	-4.11812265
H	2.54086371	-0.89889682	-4.57562498
H	2.07995771	-2.27070393	-3.55375554
H	4.31894956	4.28602260	-1.81348737
H	6.28739144	3.53403069	-0.49916269
H	5.98484879	1.97661510	1.41017531
H	0.79640600	3.11857476	-1.19239828
H	-1.06401293	0.29651804	3.41746817
H	2.75076144	3.96505947	-3.39885834
H	0.98248122	3.88656260	-3.53226009
H	1.89823869	2.40169337	-3.23019125
H	1.28981525	5.33353055	-0.07409018
H	0.56516137	5.55139955	-1.68255780
H	2.30940545	5.79623642	-1.45001266
H	-3.32310291	-1.19131399	4.87410940
H	-1.58003862	-1.46884114	5.06565188
H	-2.35582658	-1.80896150	3.51046081
H	-1.66149848	2.28722905	4.83805191
H	-1.14761550	0.90012417	5.82208276
H	-2.87020298	1.31228388	5.69327991
H	-4.71601103	0.52691987	4.28094186
H	-6.46139222	1.42565160	2.76075976
H	-5.83355628	2.28770766	0.52348682
H	2.71263074	0.41572908	2.36277239
H	-2.46843936	2.01495660	-0.99966837
H	5.75183295	0.32128930	2.81702991
H	4.87543739	-0.73837141	1.69142251
H	4.52600437	-0.79679221	3.43106488
H	3.46907103	1.21430620	4.60290437
H	2.77673566	2.54836341	3.65822999
H	4.53881186	2.40640575	3.82736247
H	-4.85872470	1.49922721	-1.78625772

H	-4.08617509	2.86799894	-2.60725622
H	-5.30068320	3.16988813	-1.36187445
H	-2.03666898	4.09405286	0.30888711
H	-3.72658092	4.60041280	0.08658017
H	-2.63230930	4.49207382	-1.31199477
Hf	0.08768952	0.10824779	0.04083516
H	-1.34343571	-3.24398736	-2.22951272
H	0.98242160	-3.73362481	-1.61666686
H	1.20466799	3.53571646	2.01556966
H	-1.19841372	3.11629341	2.51110623

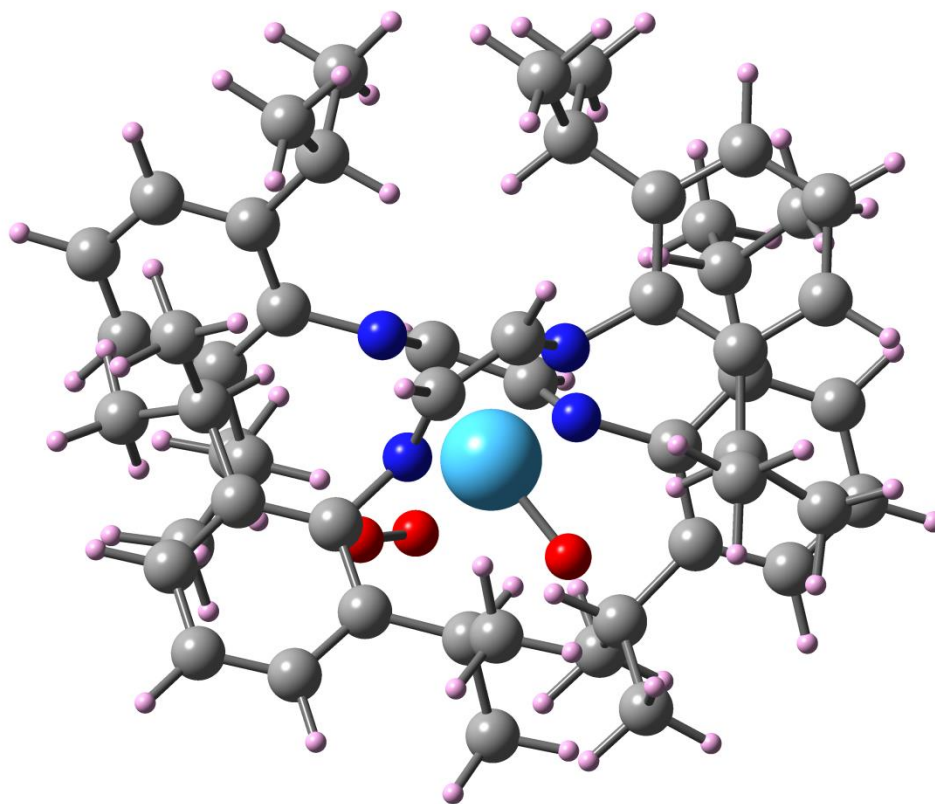
Oxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

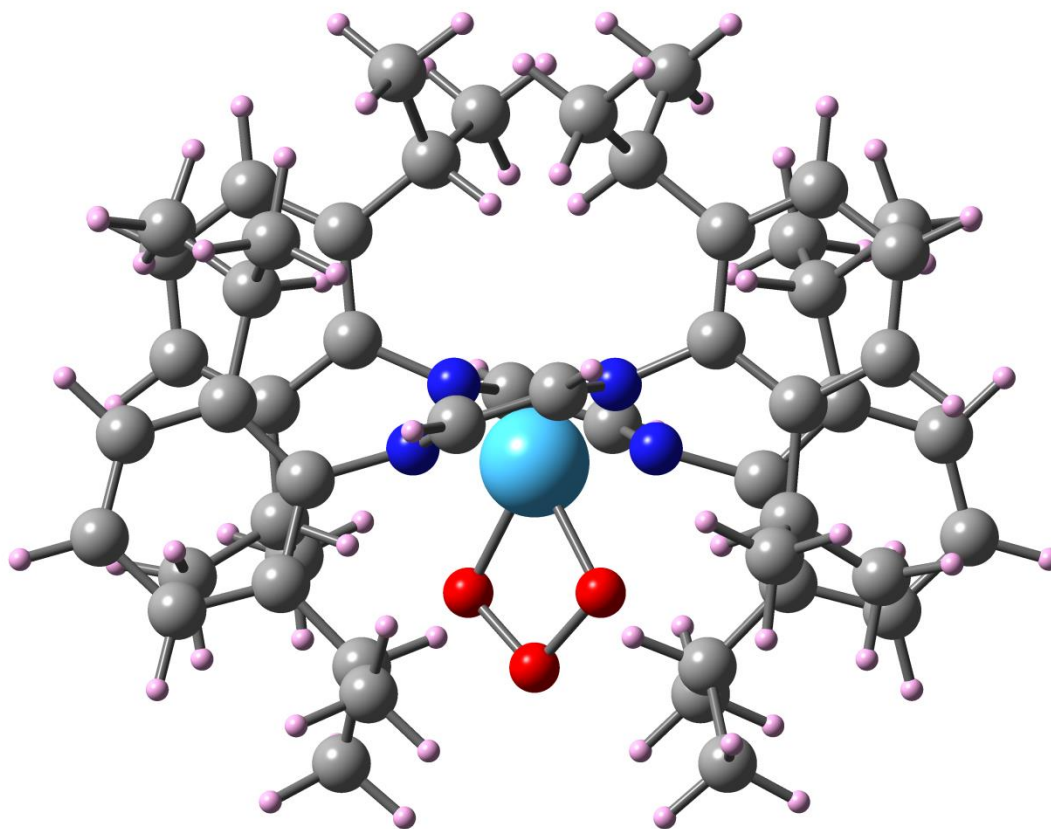
Fig. S29: NCCN Oxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

E	E_{zp}	H	G
-2518.2209	-2517.0778	-2517.0103	-2517.1805
O	-1.90011100	0.92601800	1.49924600
N	1.09730300	0.55554500	-1.69052200
N	-1.26964300	1.85285200	-1.06270100
N	1.34864900	-1.12267100	1.48106000
N	-1.29880000	-2.15205600	0.57837000
C	0.38730300	1.22301100	-2.65139200
C	-0.81093700	1.88550600	-2.33517000
C	0.78961100	-2.23892100	1.85665900
C	-0.55468800	-2.70720400	1.48577900
C	2.43408100	0.18351900	-2.17255600
C	3.54829500	1.01911700	-1.85439000
C	4.79080600	0.74710000	-2.46805900
C	4.94276100	-0.29590800	-3.39186800
C	3.84201000	-1.10529900	-3.69915500
C	2.58161500	-0.88936600	-3.10146700
C	4.58199500	2.41978500	0.03582100
C	3.42065500	2.26684300	-0.97644700
C	3.31217200	3.53368100	-1.87075400

C	-0.39710300	5.17804200	1.28038200
C	-0.65419300	4.59910000	-0.13352700
C	-0.34328700	5.65485700	-1.22876300
C	-2.37394800	2.74843600	-0.73885200
C	-2.08372400	4.06740800	-0.28543900
C	-3.16519500	4.92980700	-0.00459500
C	-4.49370100	4.51424000	-0.16952500
C	-4.76112300	3.21456400	-0.62342100
C	-3.71602200	2.31226000	-0.91234800
C	1.74693600	-3.29263500	-3.28866400
C	1.42031500	-1.79608600	-3.52755000
C	1.04790500	-1.56562600	-5.01818000
C	-5.19016400	0.23773100	-0.63995000
C	-4.05452600	0.91635700	-1.44224300
C	-4.42407700	0.97648100	-2.95020400
C	2.71702600	-0.91325800	2.00237400
C	2.91155500	-0.02273500	3.09575100
C	4.22781800	0.15102900	3.57230300
C	5.30953100	-0.53809100	3.00939400
C	5.08558400	-1.44581400	1.96592200
C	3.79243000	-1.66674700	1.44551600
C	1.99674300	2.15156700	4.10552600
C	1.76387500	0.64202200	3.86277000
C	1.52277300	-0.11227400	5.20097100
C	-2.52081400	-2.67902400	-3.36007400
C	-2.00744600	-3.24684700	-2.01519100
C	-1.60959900	-4.74322500	-2.16161100
C	-2.65075800	-2.64089600	0.40853600
C	-3.02693900	-3.10993300	-0.88346100
C	-4.33738400	-3.58737400	-1.07243200
C	-5.26361200	-3.59787400	-0.01893600
C	-4.88103200	-3.12934600	1.24433500
C	-3.57902900	-2.64792100	1.49972100
C	4.76825900	-2.72027300	-0.68233800
C	3.61479900	-2.72957000	0.34950800
C	3.51069200	-4.15884400	0.95765300
C	-4.22381400	-0.98487900	3.32959800
C	-3.27466600	-2.14069800	2.91812000
C	-3.34052400	-3.29894900	3.95042300
H	0.79388400	1.30993600	-3.65677100
H	-1.32725100	2.46830500	-3.09563700
H	1.32015800	-2.89737500	2.54706400
H	-0.89807700	-3.58088600	2.04940000
H	5.64061500	1.38389300	-2.23813900
H	5.90394400	-0.47177600	-3.86924500
H	3.95898100	-1.91137900	-4.41968300
H	2.50344300	2.20036500	-0.39039500
H	0.04462300	3.76893400	-0.25144800
H	5.54376000	2.62468300	-0.45529500
H	4.69470700	1.51980100	0.65177400
H	4.36877600	3.26069200	0.70806500
H	4.21838500	3.67327600	-2.47723100

H	3.17908900	4.42541900	-1.24365800
H	2.45397200	3.46953800	-2.55201100
H	-1.04245700	6.03999900	1.49891200
H	0.64680300	5.50792700	1.36359500
H	-0.56542900	4.41065700	2.04370200
H	-0.48103600	5.23925000	-2.23605500
H	0.69678400	5.99733600	-1.14138500
H	-0.99786300	6.53254400	-1.13629200
H	-2.95995700	5.93956000	0.34216900
H	-5.31216500	5.19626400	0.04982600
H	-5.79249000	2.89701100	-0.75298400
H	0.54283900	-1.54263300	-2.92251200
H	-3.15924200	0.29065800	-1.34080200
H	2.63927100	-3.60351600	-3.84609500
H	0.91513600	-3.92368700	-3.62395600
H	1.92635300	-3.49762100	-2.22581400
H	1.89560000	-1.79573400	-5.67662100
H	0.75556200	-0.52491300	-5.20291500
H	0.20916900	-2.21061700	-5.31279600
H	-4.96600700	0.23628000	0.43238400
H	-5.31412000	-0.80204100	-0.96447600
H	-6.15153400	0.74745800	-0.78664200
H	-5.29540200	1.62604900	-3.10834700
H	-4.67484400	-0.02399900	-3.32901500
H	-3.59716300	1.37401500	-3.55228900
H	4.39907800	0.82838300	4.40371000
H	6.31600500	-0.38182200	3.38980600
H	5.92534300	-1.99087600	1.54672800
H	0.84921600	0.56665800	3.27509600
H	-1.10751600	-2.68596300	-1.73574200
H	2.89019700	2.34510000	4.71488500
H	1.13485800	2.57500500	4.63837500
H	2.08579700	2.66582400	3.14427200
H	1.30539300	-1.17706000	5.03458700
H	0.66806800	0.32941600	5.72943200
H	2.40029600	-0.05025600	5.85892400
H	-3.39382100	-3.23194400	-3.72969600
H	-1.73821900	-2.75312700	-4.12519700
H	-2.80249300	-1.62421400	-3.26348500
H	-1.18546300	-5.13623300	-1.22810600
H	-0.86532700	-4.87530700	-2.95543100
H	-2.48607300	-5.35431500	-2.41319500
H	-4.63111700	-3.96803500	-2.04676400
H	-6.27231000	-3.96972400	-0.18031400
H	-5.60626800	-3.13254800	2.05346300
H	2.68754300	-2.51812700	-0.19736100
H	-2.26933600	-1.71618300	2.95202800
H	5.69743200	-3.11336400	-0.24888300
H	4.96065100	-1.71407300	-1.06150400
H	4.51098000	-3.35995900	-1.53511900
H	3.42657100	-4.90518300	0.15624400
H	2.64778200	-4.28152900	1.62295100

H	4.41126000	-4.39027200	1.54135800
H	-4.11171000	-0.13261800	2.65125500
H	-3.97099600	-0.64036900	4.34078600
H	-5.27634100	-1.29703100	3.33393500
H	-2.65124300	-4.11600000	3.69515200
H	-4.34960400	-3.72745500	4.00763200
H	-3.07722200	-2.92843000	4.94969900
O	0.96315100	1.98158600	1.07572600
O	-1.06252300	0.13471900	2.27722300
Hf	0.00055100	0.65045300	0.36736200

η^2 -ozone ComplexFig. S30: NCCN η^2 -ozone Complex

E	E_{zp}	H	G
-2518.1819	-2517.0374	-2516.9703	-2517.1388
O	-0.86808500	-2.21634700	-0.75846300
O	0.86748700	-2.21683300	0.75675400
N	-1.59267100	-0.33115300	1.62817700
N	1.05615000	0.51111700	1.73035300
N	1.59241900	-0.33052100	-1.62847300
N	-1.05629900	0.51191700	-1.73041600
C	-1.02414000	-0.01508000	2.81890300
C	0.31073000	0.41839600	2.87103400
C	1.02389300	-0.01417800	-2.81915000
C	-0.31096100	0.41936700	-2.87115100
C	-3.00100300	-0.73601500	1.73184400
C	-4.01897600	0.26274700	1.68469800
C	-5.36150200	-0.14567100	1.83307700
C	-5.69749900	-1.49017400	2.04745600
C	-4.68213600	-2.44941300	2.13808600
C	-3.32186700	-2.09853400	1.99426100
C	-4.81853100	2.56046200	0.85011300
C	-3.70206700	1.75957300	1.56144900

C	-3.45185600	2.39558100	2.95988200
C	1.79730400	4.59058800	0.71579300
C	1.35283300	3.45324500	1.66973900
C	0.70639400	4.05208900	2.94949700
C	2.38070200	1.09104200	1.99830300
C	2.50767800	2.51042200	2.03218800
C	3.72348900	3.06548400	2.48268600
C	4.79323100	2.25004000	2.87747300
C	4.65831600	0.85642300	2.82143100
C	3.45672600	0.24713600	2.39725700
C	-2.52881600	-4.45277800	1.37397900
C	-2.26324800	-3.18235300	2.21804500
C	-2.17417900	-3.54192300	3.72764800
C	4.54470900	-2.00695200	1.83949800
C	3.33487000	-1.27786800	2.47366300
C	3.14660400	-1.73541700	3.94709300
C	3.00088900	-0.73490700	-1.73217600
C	3.32227500	-2.09727000	-1.99480000
C	4.68268100	-2.44762700	-2.13854700
C	5.69769200	-1.48803400	-2.04764600
C	5.36118900	-0.14368700	-1.83310500
C	4.01849300	0.26422200	-1.68479700
C	2.52993500	-4.45169900	-1.37447000
C	2.26410300	-3.18148400	-2.21876000
C	2.17555100	-3.54123800	-3.72834900
C	-1.79730400	4.59033200	-0.71197400
C	-1.35245800	3.45370900	-1.66656900
C	-0.70449500	4.05343300	-2.94512700
C	-2.38068800	1.09227800	-1.99815300
C	-2.50734400	2.51168300	-2.03081500
C	-3.72280300	3.06741200	-2.48143300
C	-4.79248100	2.25249500	-2.87750100
C	-4.65795000	0.85878200	-2.82243800
C	-3.45673800	0.24889400	-2.39807400
C	4.81728700	2.56209700	-0.84989400
C	3.70107200	1.76092700	-1.56131800
C	3.45066900	2.39708900	-2.95964500
C	-4.54515600	-2.00495800	-1.84072400
C	-3.33520400	-1.27609900	-2.47497500
C	-3.14729300	-1.73344200	-3.94849100
H	-6.15277200	0.59534100	1.78541100
H	-6.73941900	-1.78169800	2.15714200
H	-4.94195800	-3.48628600	2.33258800
H	-2.78123300	1.86288600	0.97267200
H	0.58009800	2.87017500	1.15415900
H	-5.70922000	2.65478000	1.48565600
H	-5.11347800	2.09568700	-0.09465000
H	-4.46950600	3.57700900	0.63227600
H	-4.33179500	2.26008300	3.60285000
H	-3.26917700	3.47452800	2.85895200
H	-2.58857500	1.95585500	3.46911000
H	2.56981600	5.22284000	1.17026100

H	0.94563500	5.23900000	0.47841600
H	2.19741400	4.19117600	-0.22361000
H	0.33689600	3.26453900	3.61708000
H	-0.13989700	4.70096900	2.68682600
H	1.43540700	4.65273200	3.50942600
H	3.83301900	4.14559000	2.53161700
H	5.72075000	2.69676800	3.22766000
H	5.48733700	0.22665500	3.13209400
H	-1.28862800	-2.79970200	1.91519900
H	2.44792400	-1.59656600	1.92225000
H	-3.45954000	-4.95622700	1.66951000
H	-1.70458700	-5.16435000	1.50678800
H	-2.58620100	-4.20295600	0.30942400
H	-3.12165000	-3.96004400	4.09406600
H	-1.93804700	-2.66135400	4.34000000
H	-1.38645300	-4.28931600	3.89061900
H	4.71326300	-1.68016400	0.80806100
H	4.35434000	-3.08792700	1.82447000
H	5.47059600	-1.84330600	2.40805200
H	4.01156500	-1.45514600	4.56421900
H	3.03589300	-2.82682300	3.98897100
H	2.25053900	-1.29021700	4.39806000
H	4.94289900	-3.48437900	-2.33318200
H	6.73972500	-1.77917500	-2.15726900
H	6.15217900	0.59761500	-1.78523700
H	1.28926400	-2.79915800	-1.91622300
H	-0.58048300	2.86979500	-1.15078600
H	3.46107800	-4.95467300	-1.66949900
H	1.70614900	-5.16372600	-1.50759600
H	2.58668300	-4.20174800	-0.30991100
H	1.93931400	-2.66079100	-4.34083600
H	1.38809200	-4.28888200	-3.89144500
H	3.12323800	-3.95911400	-4.09448800
H	-2.56738900	5.22481700	-1.16748100
H	-0.94494600	5.23657000	-0.47126500
H	-2.20062500	4.19020400	0.22573800
H	-0.33407700	3.26632700	-3.61271700
H	0.14137500	4.70225100	-2.68095200
H	-1.43287000	4.65436100	-3.50558300
H	-3.83209800	4.14758800	-2.52940300
H	-5.71970700	2.69970000	-3.22785700
H	-5.48698900	0.22944800	-3.13395200
H	2.78021400	1.86386100	-0.97250900
H	-2.44823800	-1.59508100	-1.92371800
H	5.70790800	2.65680100	-1.48546900
H	5.11242400	2.09728500	0.09478500
H	4.46789100	3.57849100	-0.63192300
H	3.26764900	3.47595900	-2.85852000
H	2.58753700	1.95719300	-3.46897900
H	4.33066200	2.26197900	-3.60262100
H	-4.71325400	-1.67850100	-0.80910900
H	-4.35522800	-3.08601700	-1.82618100

H	-5.47113400	-1.84065700	-2.40894100
H	-2.25120900	-1.28835800	-4.39954400
H	-4.01228900	-1.45292000	-4.56545300
H	-3.03680800	-2.82486200	-3.99055200
O	-0.00029500	-3.19717200	-0.00116100
H	0.75009100	0.69650800	3.82576900
H	-1.59823700	-0.10353700	3.73770200
H	1.59802300	-0.10242500	-3.73794400
H	-0.75033200	0.69779400	-3.82579100
Hf	-0.00014700	-0.51009300	-0.00029600

5.5 Four Oxygen Atoms

Peroxo Complex with Adsorbed Oxygen Molecule (spiro conformation)

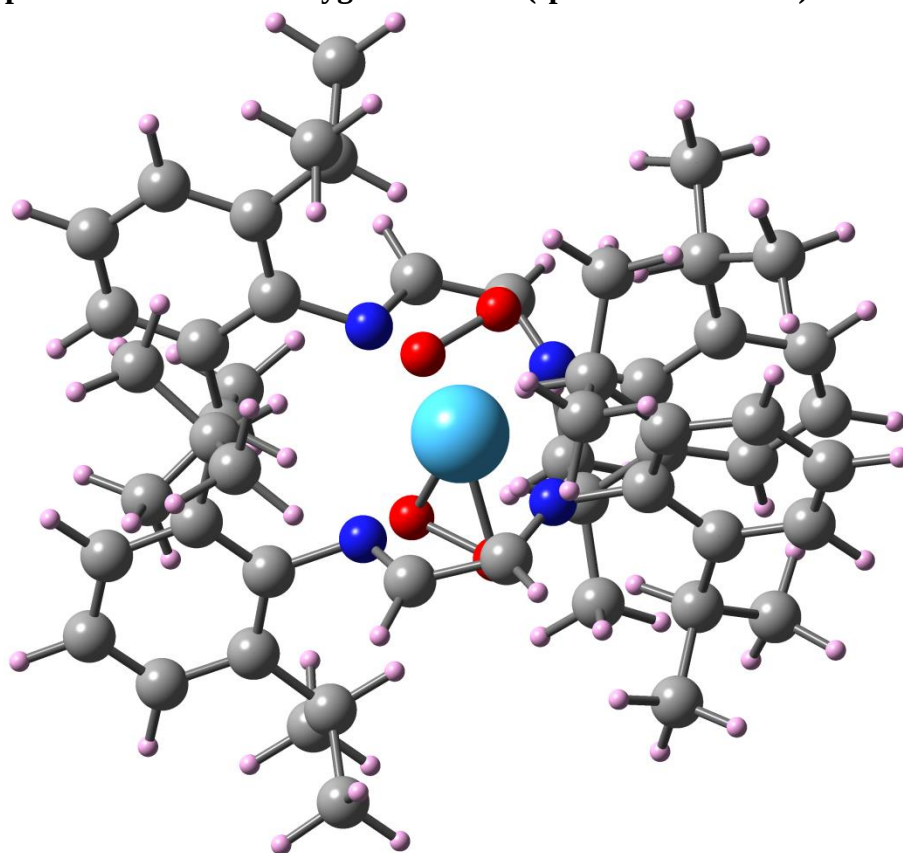


Fig. S31: NCCN Peroxo Complex with Adsorbed Oxygen Molecule (spiro conformation)

E	E _{zp}	H	G
-2593.3954	-2592.2487	-2592.1795	-2592.3523
O	0.57276410	1.82512101	1.14182439
O	-0.53233523	1.16863497	1.67973794
O	-0.69637373	-1.21413008	-1.59659742
O	0.52437299	-1.81851646	-0.84730505
N	1.36607144	-0.98613849	1.69636992
N	-1.40856281	-1.52725781	1.24492449
N	-1.31985204	1.58006716	-1.17008517
N	1.36369283	1.01095834	-1.64604376
C	0.68309886	-1.81250681	2.43047855
C	-0.72194756	-2.14040567	2.15833545
C	-0.62792496	2.26853575	-2.11532505
C	0.72168784	1.97089935	-2.36671678
C	2.75428485	-0.76379122	2.12544982
C	3.78399950	-1.48584854	1.45891291
C	5.10533426	-1.30474052	1.91473391
C	5.39449294	-0.45841926	2.99691493
C	4.35757002	0.22031808	3.64950297

C	3.01345017	0.08282571	3.23824809
C	4.60195181	-2.66071358	-0.67882347
C	3.47117664	-2.51292864	0.36416100
C	3.17171322	-3.90105804	1.00010384
C	-2.13452901	-4.25559709	-1.83967866
C	-1.88321386	-4.01650115	-0.32962659
C	-1.69830964	-5.36654598	0.41636803
C	-2.78386587	-1.99911125	1.05068306
C	-3.00691862	-3.19415908	0.31450749
C	-4.34089226	-3.64475794	0.20563844
C	-5.40126154	-2.94543807	0.79740159
C	-5.14774664	-1.77065743	1.52333603
C	-3.83726539	-1.27440591	1.67264536
C	2.16734313	2.35104717	4.05496275
C	1.92362734	0.82043337	4.02888893
C	1.81462866	0.25844222	5.47283779
C	-4.69783531	0.98898782	2.54387124
C	-3.55806593	-0.05465568	2.55838169
C	-3.27986604	-0.49787505	4.02338077
C	-2.69893716	2.01168648	-0.98020550
C	-2.96986138	3.19206650	-0.22768727
C	-4.30972378	3.62470673	-0.11965554
C	-5.35394685	2.92414164	-0.73811977
C	-5.06850625	1.77570272	-1.49318203
C	-3.74693359	1.30463631	-1.64166544
C	-2.08923477	4.21822286	1.94450198
C	-1.86960982	4.04254406	0.42046157
C	-1.75766718	5.42525189	-0.27735315
C	2.02526732	-2.46304769	-3.87057887
C	1.79889265	-0.93106745	-3.83883166
C	1.58557752	-0.37868348	-5.27472879
C	2.72855572	0.73423019	-2.08087653
C	2.94569966	-0.18754588	-3.14473460
C	4.26609629	-0.36675583	-3.61133931
C	5.34045214	0.33907331	-3.05099991
C	5.10702753	1.25149640	-2.01029258
C	3.80543790	1.47533403	-1.51300728
C	-4.55483345	-0.95193570	-2.58534521
C	-3.45404738	0.13411951	-2.58696838
C	-3.23929122	0.65977396	-4.03505145
C	4.66170958	2.60147709	0.63697806
C	3.56899855	2.56224897	-0.45738916
C	3.45466074	3.95881063	-1.13171467
H	5.91302049	-1.83667963	1.42269976
H	6.42156719	-0.33522904	3.33154576
H	4.58844481	0.86637178	4.49225357
H	2.56886383	-2.19592780	-0.17195525
H	-0.94638827	-3.45657903	-0.27186633
H	5.48987439	-3.14809734	-0.25282756
H	4.89930954	-1.69234394	-1.09232103
H	4.25374075	-3.28618165	-1.50967505
H	4.04602571	-4.27163690	1.55253244

H	2.92715291	-4.62687517	0.21435184
H	2.32378658	-3.86702472	1.69567361
H	-3.06084438	-4.81636807	-2.02485291
H	-1.30208128	-4.83167113	-2.26483414
H	-2.18129475	-3.29788912	-2.36657274
H	-1.47528862	-5.21867942	1.48269269
H	-0.86913723	-5.93245247	-0.02837105
H	-2.60240712	-5.98691544	0.35230112
H	-4.54555028	-4.55363762	-0.35363982
H	-6.41975110	-3.31247563	0.69605873
H	-5.97420503	-1.23699720	1.98184544
H	0.95659771	0.67139908	3.54170940
H	-2.65512902	0.44241974	2.18542082
H	3.11690316	2.60508218	4.54407170
H	1.36020528	2.84812954	4.60883749
H	2.17690562	2.75575845	3.03781533
H	2.74581826	0.41391834	6.03266149
H	1.60397417	-0.81995246	5.47567317
H	1.00654308	0.76529149	6.01640072
H	-4.97174426	1.27117185	1.52294462
H	-4.37326466	1.89637842	3.06847404
H	-5.59547451	0.61854675	3.05751909
H	-4.15462142	-1.01277615	4.44281393
H	-3.06539886	0.37867243	4.64849750
H	-2.42344271	-1.18004722	4.09649998
H	-4.53298395	4.52427992	0.44907344
H	-6.37918617	3.27516816	-0.64434849
H	-5.87938419	1.24840450	-1.98713541
H	-0.91163682	3.53262321	0.29536375
H	0.87933611	-0.76702922	-3.27360085
H	-3.03672863	4.72820805	2.16480569
H	-1.27679765	4.81952321	2.37442100
H	-2.09171536	3.24518407	2.44845683
H	-1.55917808	5.31665054	-1.35148853
H	-0.93822459	6.00876517	0.16359762
H	-2.68344276	6.00535325	-0.16603449
H	2.93957315	-2.73774349	-4.41505545
H	1.17780879	-2.95244820	-4.36879140
H	2.08438895	-2.85699712	-2.85063791
H	1.37989709	0.69984483	-5.26244012
H	0.73259934	-0.88115179	-5.75045126
H	2.47082412	-0.54427975	-5.90432648
H	4.44997576	-1.06207158	-4.42680374
H	6.34970460	0.18782068	-3.42759561
H	5.94160242	1.80605217	-1.59002692
H	-2.51983794	-0.34206178	-2.27445268
H	2.61225916	2.35774063	0.03346158
H	-5.48452255	-0.59535611	-3.05027580
H	-4.78610726	-1.29250150	-1.57041373
H	-4.21453249	-1.82029031	-3.16410238
H	-3.01478338	-0.17668796	-4.71027502
H	-2.40336404	1.36671038	-4.08716199

H	-4.14150901	1.16738789	-4.40411482
H	4.81548365	1.61646285	1.08890996
H	4.36727099	3.29952433	1.43196615
H	5.62448787	2.94960091	0.23899886
H	2.62777457	3.99406480	-1.85012613
H	4.38111758	4.20819802	-1.66690173
H	3.27773456	4.73433560	-0.37408317
Hf	0.01068542	0.00882415	-0.15830060
H	1.14171820	-2.30692679	3.28927424
H	-1.16246308	-2.93993379	2.75758064
H	-1.11932704	3.05855556	-2.67950480
H	1.25024007	2.49354021	-3.16066428

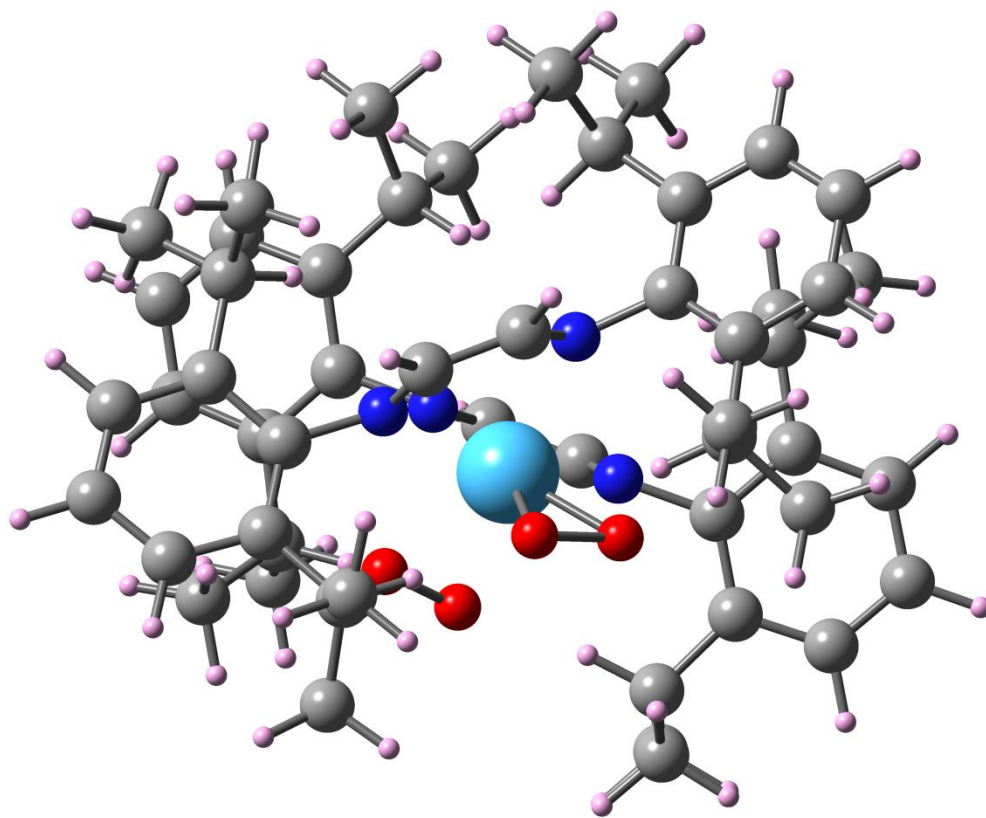
Peroxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

Fig. S32: NCCN Peroxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

E	E_{zp}	H	G
-2593.3588	-2592.2122	-2592.1430	-2592.3166
O	-1.66240580	-2.11325121	0.03236082
N	1.00874004	1.17029927	1.55525880
N	-1.68321450	0.12591694	1.74090247
N	1.60626435	-0.81513273	-1.61687081
N	-0.98630563	0.17796987	-1.87268891
C	0.28129918	1.23689495	2.63410204
C	-1.08780684	0.71469146	2.73181591
C	1.09238428	-0.56628511	-2.84339621
C	-0.21233592	-0.05755427	-2.96966635
C	2.34126280	1.78987035	1.71719756
C	3.33340601	1.14424807	2.51140480
C	4.54354657	1.84039518	2.73189599
C	4.75508118	3.13110752	2.23294324
C	3.75083178	3.75478437	1.48026144
C	2.53495651	3.10011426	1.20071734
C	4.25574567	-1.22116661	2.71793425
C	3.16108250	-0.22592575	3.17947209
C	3.16487168	-0.08765007	4.72687081

C	-2.46643539	-3.98367799	2.63793406
C	-2.24335566	-2.51888444	3.08903306
C	-2.14963417	-2.43843723	4.63843890
C	-3.07420814	-0.30271798	1.98434187
C	-3.33318959	-1.56965926	2.57952908
C	-4.68330411	-1.93084054	2.78384589
C	-5.73511883	-1.07623367	2.43590282
C	-5.45160931	0.18675235	1.89671480
C	-4.12509831	0.60625942	1.66920841
C	1.94670253	4.62479001	-0.77235581
C	1.42612988	3.86399890	0.47131602
C	0.72702992	4.84178398	1.45762053
C	-5.01075856	2.61102534	0.32454721
C	-3.85562605	2.03394568	1.17515720
C	-3.59429745	2.99880730	2.36838889
C	2.98676609	-1.31401259	-1.60698047
C	3.24404567	-2.71290587	-1.51882632
C	4.58494635	-3.15410162	-1.51128181
C	5.65242753	-2.25590138	-1.62060018
C	5.38518561	-0.88742564	-1.76169234
C	4.06452414	-0.39018354	-1.76291734
C	2.21512442	-4.68205118	-0.25533298
C	2.14602378	-3.77904352	-1.51196154
C	2.19899191	-4.62818887	-2.81155373
C	-1.85318801	4.34718936	-1.35545043
C	-1.37832136	3.09968278	-2.14043260
C	-0.73132151	3.53109779	-3.48690708
C	-2.31298941	0.68549099	-2.25991205
C	-2.50448907	2.09336600	-2.39707782
C	-3.73414218	2.57089678	-2.89492429
C	-4.76862066	1.69366678	-3.24626421
C	-4.56387835	0.31409061	-3.13032844
C	-3.33820896	-0.21885820	-2.67098411
C	4.92079999	1.98019395	-1.28811809
C	3.85035619	1.11232505	-1.99259476
C	3.85135076	1.45381105	-3.51046721
C	-4.20763290	-2.48223601	-1.86510735
C	-3.16272315	-1.74029444	-2.73638547
C	-3.22745327	-2.23802710	-4.20719942
H	0.66915339	1.71915449	3.53390907
H	-1.58804687	0.85552025	3.69187327
H	1.67714306	-0.77123243	-3.73687570
H	-0.61232231	0.13037599	-3.96433111
H	5.31965897	1.36273679	3.32315917
H	5.68932108	3.64950626	2.43390737
H	3.91196535	4.76389119	1.11239939
H	2.20798217	-0.66381027	2.88343088
H	-1.27396568	-2.22085192	2.68692234
H	5.26347799	-0.88981412	3.00563532
H	4.22123809	-1.35339470	1.63253079
H	4.07776847	-2.20205149	3.17683979
H	4.12256151	0.29951258	5.10018605

H	2.99753533	-1.07031204	5.18644110
H	2.37402861	0.58943583	5.08046039
H	-3.35968984	-4.43039065	3.09587974
H	-1.60239740	-4.59223374	2.93419340
H	-2.56462627	-4.04139662	1.54890673
H	-1.93263416	-1.41700278	4.98112485
H	-1.34501434	-3.09242590	4.99842924
H	-3.08824226	-2.75635395	5.11306428
H	-4.90429787	-2.89754151	3.22694178
H	-6.76599839	-1.38259251	2.59603014
H	-6.27086306	0.85377621	1.65128748
H	0.67387350	3.14199530	0.13097602
H	-2.95611581	2.01136790	0.54548483
H	2.67352660	5.39973195	-0.49992145
H	1.12001797	5.12629387	-1.28825278
H	2.42832880	3.94290800	-1.48263988
H	1.44416772	5.57640714	1.84631030
H	0.30088145	4.30796078	2.31745460
H	-0.08453484	5.38606870	0.95936175
H	-5.29955690	1.92878005	-0.47985668
H	-4.70012129	3.55726867	-0.13329376
H	-5.89418470	2.82338728	0.94130273
H	-4.45950685	3.01104896	3.04418682
H	-3.43562210	4.02233248	2.00250188
H	-2.71559801	2.71569963	2.95913192
H	4.78688804	-4.21927238	-1.43183457
H	6.67860583	-2.61614023	-1.61268510
H	6.21470466	-0.19573750	-1.87206313
H	1.17771757	-3.28399246	-1.49566106
H	-0.60328431	2.59747161	-1.54996033
H	3.14771679	-5.26263077	-0.22264974
H	1.37755278	-5.39267527	-0.25834717
H	2.14849571	-4.06916769	0.64884545
H	2.10930852	-3.99745865	-3.70652368
H	1.37353348	-5.35258057	-2.82012099
H	3.14056459	-5.18813534	-2.88958549
H	-2.61171206	4.91275144	-1.91038671
H	-1.01335831	5.02803474	-1.17774672
H	-2.28122433	4.07279181	-0.38423846
H	-0.33521736	2.66666229	-4.03234031
H	0.09612177	4.23181838	-3.31530705
H	-1.47034292	4.02573250	-4.13106727
H	-3.88157858	3.64014206	-3.02028296
H	-5.71220413	2.08043250	-3.62383794
H	-5.35260226	-0.36976417	-3.43322763
H	2.86853939	1.38374674	-1.58382599
H	-2.17565915	-2.00184028	-2.35913769
H	5.90136849	1.87700198	-1.77100117
H	5.02787941	1.71085400	-0.23342429
H	4.64528902	3.04026304	-1.34276595
H	3.72158464	2.53495731	-3.66036544
H	3.05053056	0.93962671	-4.05189695

H	4.80691044	1.16100102	-3.96574372
H	-4.15159614	-2.15616952	-0.82137551
H	-4.01751584	-3.56324401	-1.89062935
H	-5.23067408	-2.31162079	-2.22794460
H	-2.46787868	-1.74790175	-4.83068731
H	-4.20888197	-2.04204293	-4.65899100
H	-3.04971208	-3.32101936	-4.24376555
O	0.43636087	-1.60957980	1.88962092
O	1.63275280	-1.64224679	0.92527561
O	-0.64118418	-2.61076289	-0.78257052
Hf	0.06352090	-0.72786670	0.07047949

Oxo Complex with Adsorbed Ozone Group

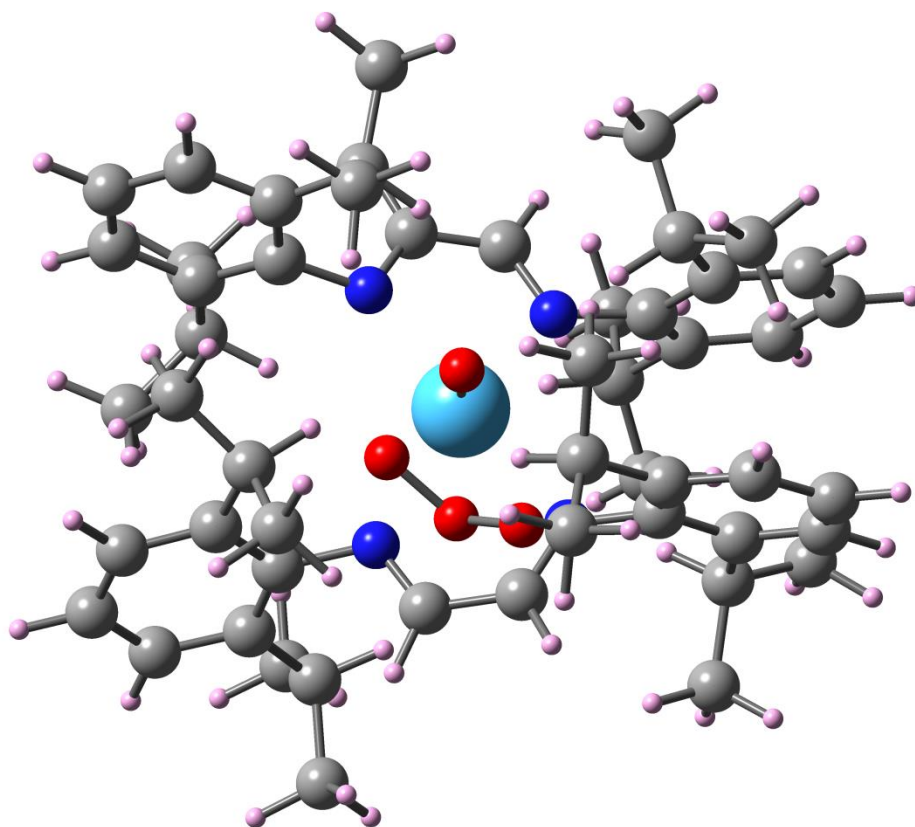


Fig. S33: NCCN Oxo Complex with Adsorbed Ozone Group

E	E_{zp}	H	G
-2593.3696	-2592.2229	-2592.1536	-2592.3271
O	-1.14588956	-0.62811428	-2.19675908
O	0.81935792	-1.61161959	-1.52668169
O	-0.05189382	0.64497810	1.62370930
N	-1.30527746	-1.90219147	0.56272552
N	1.49544909	-1.58553801	1.09405181
N	1.28356825	1.46048511	-1.28708154
N	-1.40830800	1.81050305	-0.71794710
C	-0.58530481	-2.82277563	1.13744124
C	0.81953410	-2.62114001	1.49386852
C	0.56892196	2.44940572	-1.89972005
C	-0.78936401	2.64116042	-1.59502437
C	-2.73154954	-2.22007491	0.40419793
C	-3.63865868	-1.63446008	1.33261076
C	-5.00057159	-1.97949657	1.21804165
C	-5.44507149	-2.88111361	0.23832878
C	-4.52598813	-3.46267509	-0.64413069
C	-3.14943496	-3.15378614	-0.58239392
C	-4.20236801	0.27612791	2.95973649

C	-3.15277672	-0.75795758	2.49417864
C	-2.74153153	-1.65199056	3.69998379
C	1.80324871	0.78884742	4.50397145
C	1.70898530	-0.64285490	3.92014827
C	1.54151615	-1.68792973	5.05612232
C	2.82286634	-1.42920219	1.69193410
C	2.92089257	-0.98688262	3.04238466
C	4.21564702	-0.88894501	3.59820299
C	5.35820281	-1.22057376	2.85838539
C	5.22862375	-1.67217433	1.53517022
C	3.96442051	-1.79478080	0.92501737
C	-2.61771318	-3.66286853	-3.02925532
C	-2.19300316	-3.86042106	-1.55173292
C	-2.08526732	-5.37363589	-1.21630205
C	5.02616646	-2.13724387	-1.39500424
C	3.82413914	-2.42073757	-0.46638714
C	3.61382017	-3.95768637	-0.34425111
C	2.70754563	1.46104731	-1.59609698
C	3.15977406	1.04071089	-2.88039986
C	4.53690510	1.14718392	-3.17273006
C	5.44473615	1.64755145	-2.23016045
C	4.98283790	2.06182514	-0.97065141
C	3.61546345	1.99317641	-0.63241382
C	2.61939698	-0.90659403	-4.44456580
C	2.21643817	0.51235315	-3.96837315
C	2.14997297	1.48754116	-5.17506370
C	-1.57682440	3.32944017	3.17698670
C	-1.49895210	3.57503408	1.65047194
C	-1.22349632	5.07352926	1.34793741
C	-2.70909656	2.26506053	-0.23713847
C	-2.75939796	3.10970104	0.91113903
C	-4.01719777	3.59665807	1.32592058
C	-5.19175320	3.27242330	0.63119175
C	-5.12136114	2.46010710	-0.50992620
C	-3.88850487	1.95093276	-0.97264629
C	4.15965445	2.50915546	1.83288678
C	3.11720842	2.58145132	0.69382429
C	2.67670144	4.05938107	0.48930038
C	-4.93062477	0.06540010	-2.37208126
C	-3.84761718	1.16798569	-2.28901626
C	-3.98115950	2.13587117	-3.49796264
H	-5.71770773	-1.54394912	1.90583323
H	-6.50068442	-3.13200845	0.16905376
H	-4.87629984	-4.16675721	-1.39396737
H	-2.25776806	-0.20621391	2.17913611
H	0.80845023	-0.63569927	3.30056384
H	-5.05551532	-0.20405446	3.45895083
H	-4.57856135	0.87568084	2.12517448
H	-3.74553905	0.96177984	3.68329158
H	-3.60168791	-2.22863183	4.06681431
H	-2.37183613	-1.02496414	4.52137691
H	-1.94643925	-2.36234336	3.44055767

H	2.70101045	0.93148506	5.12066279
H	0.92613050	0.98995596	5.13310192
H	1.80465443	1.52349832	3.69319240
H	1.44061230	-2.70898617	4.66213009
H	0.64482471	-1.46197966	5.64857803
H	2.40358659	-1.68272932	5.73677193
H	4.32326499	-0.54764702	4.62445828
H	6.34366404	-1.13591634	3.31025740
H	6.11796470	-1.94158543	0.97452838
H	-1.19346549	-3.42982940	-1.44987630
H	2.92877492	-2.00751910	-0.94420056
H	-3.58631888	-4.13527721	-3.23905378
H	-1.87310301	-4.11642591	-3.69617222
H	-2.69040021	-2.59824536	-3.27393045
H	-3.05703107	-5.87385106	-1.31920049
H	-1.73601949	-5.54079695	-0.18806456
H	-1.37910086	-5.86376933	-1.89918871
H	5.24677953	-1.06693869	-1.45133223
H	4.79811133	-2.48824201	-2.40937604
H	5.93156980	-2.66461162	-1.06460041
H	4.48081455	-4.43100986	0.13652890
H	3.48886536	-4.40067046	-1.34087600
H	2.72317908	-4.20650117	0.24569059
H	4.89802041	0.83414541	-4.14948241
H	6.50193773	1.72184825	-2.47473366
H	5.69162586	2.45797696	-0.25014428
H	1.20937061	0.43794941	-3.55075627
H	-0.65199811	2.98664135	1.29293896
H	3.61546932	-0.91098606	-4.90716080
H	1.90115865	-1.27133548	-5.19088817
H	2.62302036	-1.61016816	-3.60538059
H	1.82982686	2.49106811	-4.86637466
H	1.43616308	1.11798061	-5.92342190
H	3.12902230	1.58590387	-5.66276273
H	-2.42105774	3.85651417	3.64249287
H	-0.65532911	3.68484430	3.65771316
H	-1.66552725	2.25772694	3.38199030
H	-1.12203694	5.25244871	0.26940642
H	-0.29290813	5.39535470	1.83471528
H	-2.03775159	5.71150144	1.71819395
H	-4.07417925	4.24519183	2.19665906
H	-6.15053742	3.66098256	0.96728291
H	-6.03078667	2.23023618	-1.05917675
H	2.23167818	2.01927598	1.01363473
H	-2.87534787	0.67676144	-2.37124481
H	5.00376048	3.18987474	1.65629807
H	4.55358839	1.49526202	1.95999335
H	3.69369793	2.81170383	2.77907478
H	2.30274203	4.47761960	1.43358897
H	1.87868131	4.14507386	-0.25602065
H	3.52597100	4.67183538	0.15609078
H	-4.87596119	-0.61506858	-1.51612523

H	-4.78924368	-0.52577354	-3.28684861
H	-5.94411813	0.48799960	-2.40758316
H	-3.18314941	2.88883583	-3.50174975
H	-4.94322946	2.66568301	-3.47355679
H	-3.92304289	1.57607648	-4.44118805
O	-0.13191798	-1.51916566	-2.58080217
Hf	-0.06757539	0.08842678	-0.10624763
H	1.25451502	-3.35387791	2.17700592
H	-1.03973983	-3.76545004	1.44838236
H	1.06824060	3.12404355	-2.59160227
H	-1.32135737	3.49451869	-2.00994885

5.6 Five Oxygen Atoms

Peroxo Complex with Adsorbed Ozone Group

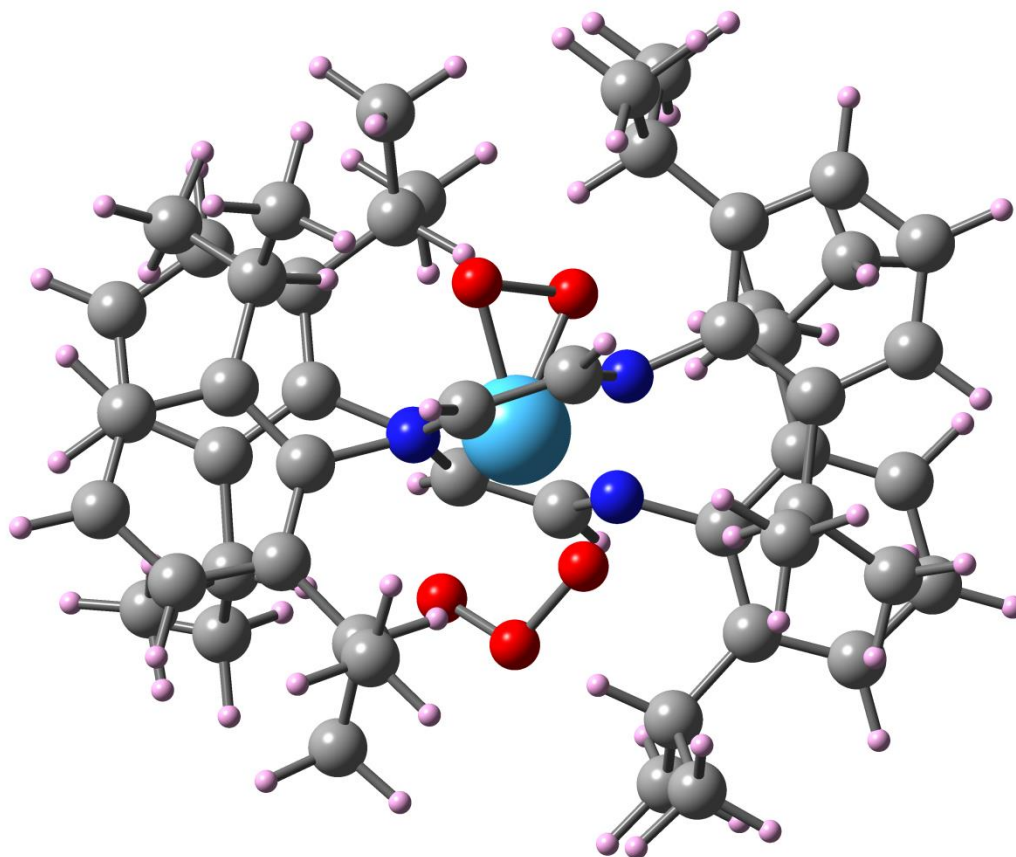


Fig. S34: NCCN Peroxo Complex with Adsorbed Ozone Group

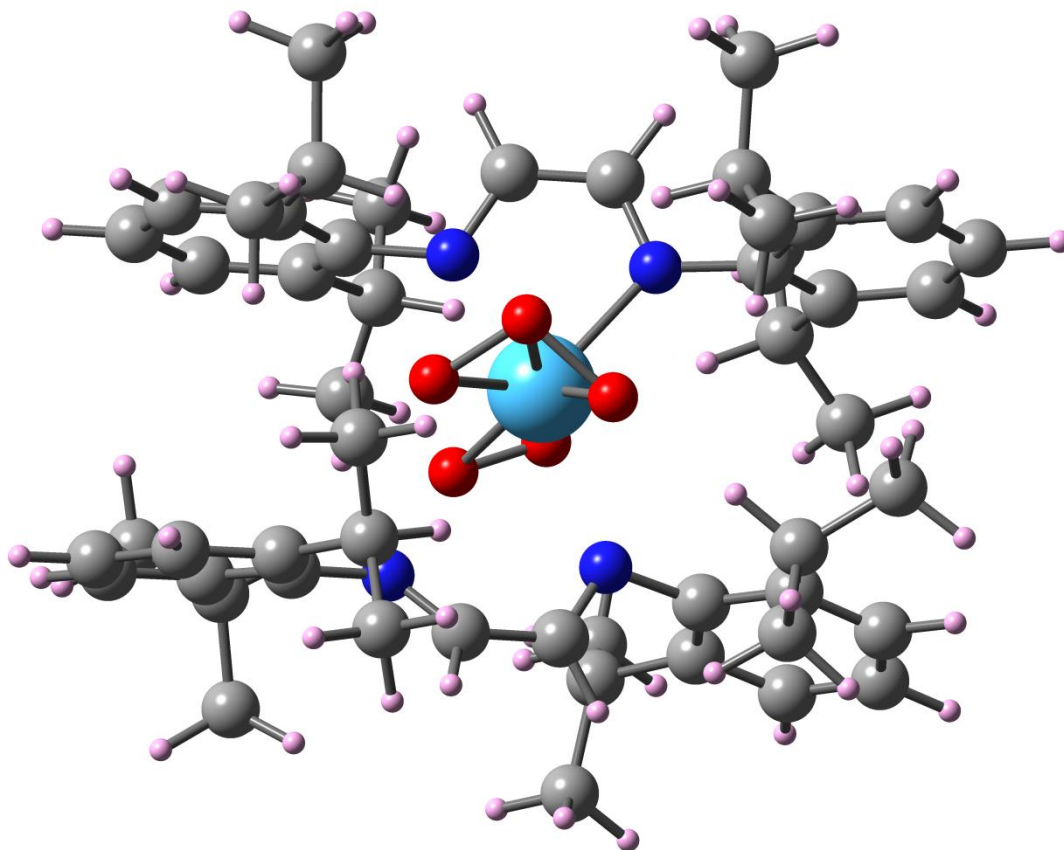
E	E_{zp}	H	G
-2668.5337	-2667.3839	-2667.3136	-2667.4897

O	-0.98521184	-2.18998003	-0.21621430
O	0.85864998	-1.77098984	1.05209430
O	0.72174170	1.77993556	-0.72614990
O	-0.52579596	1.92439356	0.19478280
N	-1.35453114	-0.07725882	1.97369012
N	1.42309809	0.70445857	1.87580612
N	1.29697165	-0.86721153	-1.80043629
N	-1.36164186	-0.03944133	-1.94689010
C	-0.66911628	0.26732747	3.02376191
C	0.72689138	0.72533988	2.96812848
C	0.58588836	-1.02739493	-2.94917949
C	-0.75207838	-0.60590413	-3.02519056
C	-2.76103298	-0.43419095	2.23501179
C	-3.75296452	0.56357037	2.01390007
C	-5.09056357	0.22946388	2.30852129
C	-5.43396776	-1.03150796	2.81941085
C	-4.43356754	-1.98146738	3.05910250

C	-3.07606731	-1.70758004	2.78246662
C	-4.48920451	2.67914874	0.74535515
C	-3.39197693	1.99208020	1.58964448
C	-3.08481748	2.86042557	2.84362974
C	1.87532626	4.66014575	0.58522063
C	1.69783165	3.67392236	1.76682587
C	1.46969130	4.44500321	3.09580402
C	2.76387954	1.30008248	1.94450090
C	2.88919101	2.71634221	1.89691548
C	4.18984230	3.25563377	2.00480197
C	5.31490362	2.43424574	2.15388346
C	5.15881259	1.04079342	2.21045887
C	3.88613577	0.44250643	2.11467109
C	-2.34094113	-4.13075564	2.44103665
C	-2.03051509	-2.77577513	3.12712019
C	-1.91705054	-2.95988708	4.66560834
C	4.89904550	-1.88984668	1.71588144
C	3.72622450	-1.06948123	2.29977205
C	3.54467353	-1.40937376	3.80680729
C	2.70161971	-1.26026422	-1.88260380
C	3.05972321	-2.63887312	-1.82461587
C	4.42095524	-2.98760208	-1.96157525
C	5.40698226	-2.01259268	-2.16059442
C	5.03680708	-0.66207613	-2.24625750
C	3.68996870	-0.25911619	-2.12465736
C	2.34063904	-4.68372385	-0.46699693
C	2.03092130	-3.76568137	-1.67685460
C	1.93736957	-4.60509149	-2.98043738
C	-1.71925691	4.13567440	-2.09128202
C	-1.57660882	2.78036161	-2.82640921
C	-1.31287237	3.00228284	-4.34141541
C	-2.68823200	0.51499863	-2.21519821
C	-2.79713973	1.87464145	-2.63066620
C	-4.07657657	2.37433112	-2.95519123
C	-5.21786988	1.56257759	-2.88733036
C	-5.08995717	0.21928329	-2.50605338
C	-3.83344708	-0.33385968	-2.17565265
C	4.34808387	2.21209959	-1.81223308
C	3.31644367	1.20606001	-2.37318984
C	3.11418166	1.44793158	-3.89612771
C	-4.80011754	-2.32440991	-0.86983915
C	-3.73866526	-1.83589017	-1.88484886
C	-3.85228794	-2.64978183	-3.20439945
H	-5.86855421	0.96716888	2.14186119
H	-6.47293178	-1.26651314	3.03679749
H	-4.70360480	-2.95077524	3.46920040
H	-2.48272263	1.96498742	0.97963348
H	0.79682979	3.10046635	1.53755630
H	-5.37880209	2.91753443	1.34474925
H	-4.79535159	2.05858431	-0.10220060
H	-4.10297237	3.62399417	0.34421297
H	-3.96566712	2.92501760	3.49694279

H	-2.80915058	3.87688932	2.53541237
H	-2.25495881	2.45696090	3.43788892
H	2.74951541	5.31279242	0.71417758
H	0.98756170	5.30106341	0.50265517
H	1.97664271	4.10438694	-0.35180729
H	1.29520921	3.76292830	3.94018741
H	0.59582450	5.10383733	3.00516942
H	2.33700380	5.06873569	3.35107456
H	4.31646452	4.33419947	1.96699230
H	6.30600101	2.87496917	2.23039132
H	6.03307838	0.40984995	2.33654217
H	-1.05152857	-2.45256321	2.76585490
H	2.81719509	-1.38914668	1.78145962
H	-3.27415634	-4.56956326	2.81728691
H	-1.53195135	-4.84573789	2.63877005
H	-2.43091224	-4.00878759	1.35649104
H	-2.86608795	-3.30497647	5.09564917
H	-1.64797606	-2.02153811	5.16967029
H	-1.14762774	-3.70636028	4.90244678
H	5.08880885	-1.62956905	0.66973231
H	4.65633741	-2.95948169	1.75781287
H	5.82696019	-1.74394108	2.28573662
H	4.42948637	-1.10678379	4.38316785
H	3.40382251	-2.49047769	3.93655598
H	2.67313270	-0.90258104	4.24134770
H	4.70716263	-4.03574802	-1.91808730
H	6.45052668	-2.30154181	-2.26313139
H	5.80087572	0.08862012	-2.42601272
H	1.04845395	-3.32015443	-1.50879944
H	-0.69974834	2.28951651	-2.40174353
H	3.28974249	-5.22008985	-0.59935592
H	1.54709840	-5.43360094	-0.34895005
H	2.40176059	-4.10297648	0.46015185
H	1.66885173	-3.97977833	-3.84167352
H	1.17309850	-5.38708297	-2.87601211
H	2.89335033	-5.09462383	-3.20893055
H	-2.56857223	4.72544978	-2.46371289
H	-0.80888072	4.73272759	-2.23531049
H	-1.84308781	3.97033142	-1.01582530
H	-1.16171954	2.04858623	-4.86438989
H	-0.41116618	3.61344722	-4.48303765
H	-2.15327708	3.52008780	-4.82415947
H	-4.17472238	3.40817781	-3.27675472
H	-6.19402012	1.96761939	-3.14480386
H	-5.97236868	-0.41498695	-2.47996338
H	2.36214646	1.41380756	-1.88298942
H	-2.75739358	-2.04677477	-1.45496395
H	5.29581191	2.18472850	-2.36768793
H	4.56297819	2.02179043	-0.75507508
H	3.95004880	3.23151041	-1.89777299
H	2.82247908	2.49102181	-4.07801474
H	2.32770208	0.80193899	-4.30437996

H	4.04189772	1.24853599	-4.45046449
H	-4.75903595	-1.74855921	0.06024012
H	-4.62332751	-3.38060840	-0.62525196
H	-5.81887065	-2.24729514	-1.27334254
H	-3.06800417	-2.37095635	-3.91901774
H	-4.82351429	-2.48002587	-3.68887945
H	-3.75683583	-3.72454092	-2.99838410
O	-0.03517824	-2.79182699	0.61823480
Hf	-0.02169272	0.00522635	-0.13992296
H	1.13855087	1.12650670	3.89713284
H	-1.13503781	0.26702495	4.01151157
H	1.06320903	-1.46183413	-3.82516840
H	-1.29095076	-0.69308009	-3.96577376

Peroxo η^3 -Ozone ComplexFig. S35: NCCN Peroxo η^3 -Ozone Complex

E	E_{zp}	H	G
-2668.5250	-2667.376602	-2667.305945	-2667.484171

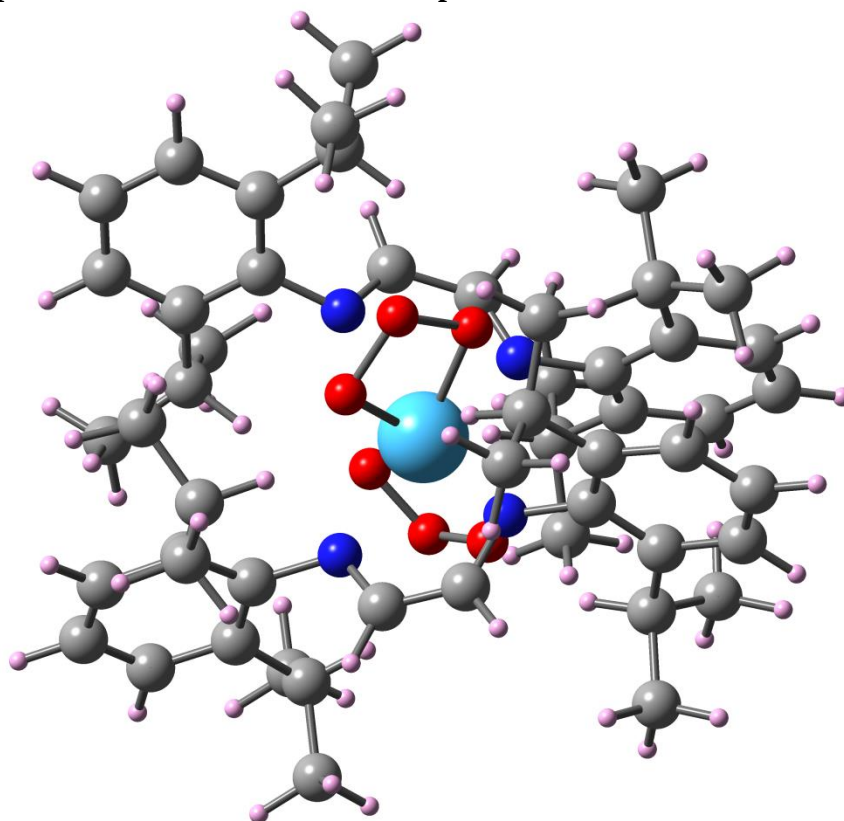
O	-1.41861300	-0.22968800	-1.42931400
N	0.86387100	2.10488600	0.12150600
N	-2.10889700	2.12121600	-0.32608200
N	-0.69326600	-2.31588300	0.46748600
N	1.87309400	-1.82050700	-0.19927100
C	0.10276900	3.10135400	-0.24243100
C	-1.28426800	3.04128600	-0.71346800
C	0.16457600	-3.36034500	0.42087400
C	1.49856900	-3.10275500	0.06385200
C	2.17180300	2.54304000	0.65724800
C	2.25052100	2.94073400	2.02168200
C	3.49046300	3.42589200	2.49145500
C	4.60190200	3.52929100	1.64485800
C	4.48834600	3.16104700	0.29604100
C	3.27485300	2.67363900	-0.23362000
C	1.34013500	2.19921900	4.29837300
C	1.04765200	2.95066000	2.97593300
C	0.60002900	4.41083200	3.26400700

C	-4.95392400	0.87055200	2.55995100
C	-4.02901300	1.76603000	1.70605300
C	-3.94120300	3.19165300	2.32161500
C	-3.45664300	2.06397300	-0.77742300
C	-4.44328400	1.84674700	0.23550800
C	-5.79399200	1.79214100	-0.14937600
C	-6.16518500	1.91715200	-1.49902900
C	-5.18215900	2.08304300	-2.48562800
C	-3.81172100	2.16132600	-2.16131300
C	4.44175000	1.84364700	-2.37110000
C	3.15207200	2.41794600	-1.74117100
C	2.75832500	3.72835900	-2.48232900
C	-2.97594600	1.14468300	-4.35158100
C	-2.79395500	2.27444500	-3.30586100
C	-2.86923900	3.66632100	-3.99033300
C	-2.05497500	-2.60546300	0.90248600
C	-3.04714700	-2.93419200	-0.06565200
C	-4.35812600	-3.19811300	0.38446500
C	-4.68245700	-3.16471300	1.74851500
C	-3.68128100	-2.89638500	2.69228900
C	-2.35401200	-2.62446700	2.29689900
C	-3.74177400	-2.42588500	-2.48102800
C	-2.71829000	-3.11769800	-1.55055600
C	-2.60876500	-4.63085800	-1.88896800
C	4.65602400	-0.20982900	2.68293300
C	3.83798600	-1.26914300	1.90922400
C	3.95734100	-2.64620700	2.62147300
C	3.27501400	-1.66897100	-0.57966700
C	4.23890100	-1.39431500	0.43431400
C	5.59913900	-1.33474700	0.06522800
C	6.00232100	-1.56261600	-1.25987700
C	5.04320800	-1.85848900	-2.23888400
C	3.66821300	-1.92022100	-1.92501700
C	-1.66254800	-1.41192900	4.45297400
C	-1.28140200	-2.46311500	3.38137000
C	-0.98333500	-3.83493500	4.04837200
C	2.76497500	-1.40474200	-4.26524400
C	2.67199500	-2.32021600	-3.01929400
C	2.86772700	-3.80861800	-3.41910000
H	0.51468200	4.11440800	-0.19612100
H	-1.58667900	3.88419500	-1.34512600
H	-0.16738400	-4.36706700	0.66245700
H	2.22424500	-3.90836400	-0.01038200
H	3.57874900	3.73518600	3.52935300
H	5.54687700	3.90605400	2.02867600
H	5.34814100	3.26367900	-0.35835500
H	0.20761400	2.43777800	2.50196000
H	-3.02087200	1.33668200	1.73488800
H	2.15033800	2.67238800	4.86840400
H	1.61344500	1.15872100	4.09560000
H	0.44408900	2.19712300	4.93293600
H	1.39347600	4.97857900	3.76750200

H	-0.28461300	4.41502700	3.91424800
H	0.34429900	4.94693700	2.33988400
H	-5.95496900	1.30724700	2.68050400
H	-4.52684500	0.75291300	3.56450300
H	-5.05857100	-0.12829500	2.12116900
H	-3.24023600	3.82762900	1.76624500
H	-3.59765700	3.13630000	3.36341500
H	-4.92454100	3.68159400	2.31195800
H	-6.56131700	1.64246000	0.60369200
H	-7.21455400	1.87185000	-1.78123200
H	-5.48334600	2.14360300	-3.52836400
H	2.35154500	1.69122800	-1.91766700
H	-1.78522600	2.14239900	-2.90390700
H	5.24672000	2.59056300	-2.40572000
H	4.23906200	1.53519700	-3.40409100
H	4.80405400	0.96874300	-1.82403100
H	3.52105400	4.50446800	-2.33144000
H	1.79772100	4.13047000	-2.13795100
H	2.67174700	3.53644100	-3.55953300
H	-2.87663300	0.16547500	-3.87425200
H	-2.20004800	1.22669200	-5.12436100
H	-3.95229800	1.19727100	-4.85077700
H	-3.85490000	3.82721600	-4.44671600
H	-2.11426100	3.74187000	-4.78423100
H	-2.70169100	4.48638600	-3.27825800
H	-5.12914500	-3.44281600	-0.34131500
H	-5.70000700	-3.36933300	2.07386700
H	-3.92846600	-2.90933600	3.75090200
H	-1.74587600	-2.66186600	-1.74612200
H	2.78452300	-0.97331900	1.94636200
H	-4.73655000	-2.88727300	-2.41499800
H	-3.41076700	-2.50569600	-3.52533200
H	-3.83191200	-1.36432800	-2.22970800
H	-1.83892100	-5.12414600	-1.28108700
H	-2.34477600	-4.76579200	-2.94676000
H	-3.56119400	-5.14724500	-1.70733800
H	5.70001800	-0.52306200	2.81938400
H	4.22647300	-0.06664300	3.68315900
H	4.65222100	0.75707900	2.17065100
H	3.32211200	-3.40357000	2.14823800
H	3.65309800	-2.55777200	3.67314700
H	4.99453400	-3.00716000	2.59503500
H	6.34935400	-1.12302900	0.82183600
H	7.05659900	-1.52046100	-1.52389100
H	5.36399700	-2.05062200	-3.25983900
H	-0.35580200	-2.12165500	2.91115500
H	1.66003800	-2.21332100	-2.62204300
H	-2.55613200	-1.70924800	5.01793000
H	-1.85342200	-0.43849900	3.98860100
H	-0.84059900	-1.29363400	5.17192500
H	-0.18287800	-3.73198900	4.79369800
H	-0.66594200	-4.58009100	3.30730500

H	-1.87289000	-4.22898900	4.55774000
H	2.54387800	-0.36789800	-3.99264500
H	2.02834500	-1.72065200	-5.01597500
H	3.75821900	-1.44721500	-4.73252100
H	2.75361100	-4.47639600	-2.55511500
H	3.86599200	-3.97937900	-3.84406800
H	2.12450000	-4.09904200	-4.17364700
O	-0.76263300	0.31918700	1.75894600
O	0.55427400	-0.06713500	2.03727900
O	-0.24685100	-0.76803300	-2.26989200
O	0.83293100	0.30438300	-2.04079200
Hf	0.20914300	-0.30903700	-0.13081900

5.7 Six Oxygen Atoms

 η^2 -ozone Complex with Adsorbed Ozone GroupFig. S36: NCCN η^2 -ozone Complex with Adsorbed Ozone Group

E	E_{zp}	H	G
-2743.6693	-2742.5161	-2742.4449	-2742.6223

O	0.71357802	1.64191647	1.05391368
O	-1.26757761	0.59629231	1.66977531
O	-0.88569856	-0.57047758	-1.91946719
O	0.95718892	-1.71259383	-1.23344501
N	1.23987349	-1.29621784	1.53163705
N	-1.35703378	-1.92261799	0.71453503
N	-1.30786235	1.90713552	-0.97023920
N	1.44032763	1.16827163	-1.54055484
C	0.61409393	-2.41880499	1.98807489
C	-0.69286691	-2.72861853	1.58388690
C	-0.55152595	2.55983290	-1.79869380
C	0.81409625	2.14430456	-2.13070488
C	2.58413363	-1.10707446	2.08471630
C	3.68302522	-1.81702493	1.51553403
C	4.95279062	-1.68226603	2.11847827
C	5.13678535	-0.89564834	3.26405550

C	4.03801496	-0.23848966	3.83504135
C	2.74816382	-0.33311836	3.27015327
C	4.56765316	-2.56673191	-0.77710205
C	3.52609929	-2.79494904	0.34488158
C	3.60474157	-4.26229483	0.85182925
C	-2.12577033	-3.76914505	-2.97387935
C	-1.88347803	-3.90907561	-1.45042641
C	-1.71347715	-5.40481353	-1.06446310
C	-2.73690809	-2.34276004	0.44113441
C	-2.99522962	-3.26551389	-0.61614098
C	-4.32363224	-3.68599605	-0.83985694
C	-5.37580176	-3.24389692	-0.02719797
C	-5.09954333	-2.38924652	1.04784194
C	-3.78925348	-1.93364623	1.31499289
C	1.81687411	1.79979825	4.34061998
C	1.57047861	0.30780491	4.01043146
C	1.24967774	-0.49325048	5.30261359
C	-4.46020269	0.15090162	2.64360248
C	-3.55836989	-1.10606901	2.58426276
C	-3.76472573	-1.98846578	3.84613384
C	-2.59170918	2.52220510	-0.63129186
C	-2.61403664	3.71632414	0.14842158
C	-3.87872067	4.25884781	0.46676444
C	-5.06690520	3.66410129	0.02551540
C	-5.01467639	2.51227836	-0.77439514
C	-3.78556796	1.92272969	-1.12638666
C	-1.43040135	4.80747685	2.14371941
C	-1.36095845	4.46096273	0.63478489
C	-1.13985795	5.75897483	-0.19246506
C	2.17937004	-1.59838632	-4.62533325
C	1.99597720	-0.11232766	-4.22322915
C	1.96223190	0.78789000	-5.48933918
C	2.83078404	0.96571507	-1.99038548
C	3.08672933	0.35754678	-3.25122564
C	4.43475763	0.21799622	-3.64973099
C	5.48626312	0.67983005	-2.84947967
C	5.20457861	1.31827578	-1.63240111
C	3.88055521	1.48722520	-1.17951178
C	-5.00519420	-0.12623178	-2.10763472
C	-3.74081275	0.75952823	-2.12078210
C	-3.50016382	1.29916845	-3.56010608
C	4.72172555	2.23931390	1.13583171
C	3.60010255	2.31884512	0.07638233
C	3.36492902	3.80698025	-0.31212971
H	5.79997717	-2.21571890	1.69488562
H	6.12171202	-0.81124238	3.71778068
H	4.17702391	0.34478646	4.74162956
H	2.53944628	-2.65436257	-0.09988975
H	-0.94236029	-3.41244208	-1.21339469
H	5.59049442	-2.77621991	-0.43572980
H	4.53733893	-1.53734552	-1.14712162
H	4.35853605	-3.23832918	-1.62073960

H	4.58306576	-4.47165467	1.30520195
H	3.46066550	-4.96079767	0.01639054
H	2.83512011	-4.47158269	1.60529800
H	-3.01666762	-4.32529971	-3.29484634
H	-1.26746615	-4.16711882	-3.53141499
H	-2.25832742	-2.71862293	-3.25619503
H	-1.48187928	-5.51645078	0.00268749
H	-0.89370271	-5.85577399	-1.64000459
H	-2.62792987	-5.97677196	-1.27005651
H	-4.52918734	-4.38535405	-1.64657138
H	-6.39300982	-3.58037786	-0.21418028
H	-5.90778974	-2.08004361	1.70576918
H	0.68790359	0.26770181	3.37184246
H	-2.52918366	-0.74731359	2.59012457
H	2.66702301	1.93842887	5.02297033
H	0.92738131	2.22482298	4.82288071
H	2.00470522	2.36852213	3.42350211
H	2.09694233	-0.48013677	6.00184559
H	1.01714175	-1.54203498	5.07576736
H	0.38068081	-0.05572620	5.81198558
H	-4.29540108	0.79046962	1.77000504
H	-4.21959531	0.73902156	3.53908435
H	-5.52751217	-0.10743207	2.69005433
H	-4.79514121	-2.36387443	3.91278069
H	-3.55858799	-1.40352071	4.75274375
H	-3.09242987	-2.85691693	3.84301583
H	-3.92751275	5.15843908	1.07372812
H	-6.02676259	4.10007923	0.29179008
H	-5.93796554	2.07060850	-1.13426534
H	-0.48680027	3.81660238	0.50944272
H	1.01956775	-0.02993111	-3.74044334
H	-2.22377348	5.53407217	2.36353493
H	-0.47856313	5.25091015	2.46516024
H	-1.60188836	3.90581266	2.73830410
H	-1.04176043	5.55619929	-1.26782932
H	-0.22705769	6.26983450	0.14200767
H	-1.98048181	6.45413445	-0.06687958
H	3.09548241	-1.74660597	-5.21160357
H	1.33243860	-1.92865683	-5.24050751
H	2.23134745	-2.24224261	-3.74103670
H	1.78676343	1.84227772	-5.23586124
H	1.16053734	0.46221429	-6.16521854
H	2.91018004	0.73450945	-6.03968145
H	4.65636610	-0.25577468	-4.60223286
H	6.51601220	0.55670756	-3.17567582
H	6.02145479	1.69806653	-1.02790127
H	-2.88942517	0.11852124	-1.87081969
H	2.67869644	1.95918283	0.54552714
H	-5.88039942	0.40258899	-2.50965652
H	-5.24165217	-0.47884711	-1.09877364
H	-4.83965522	-1.00905508	-2.73692297
H	-3.43542881	0.46352893	-4.26888124

H	-2.56908070	1.87417112	-3.63586852
H	-4.32763112	1.95156239	-3.87097759
H	4.98200577	1.20338349	1.37292473
H	4.38206281	2.71803127	2.06237629
H	5.63143216	2.76405724	0.81160209
H	2.51635425	3.92991147	-0.99674677
H	4.25578140	4.22770320	-0.79863763
H	3.15254586	4.39757087	0.58809249
O	-0.45341490	1.82088227	2.01001656
Hf	-0.05121515	-0.07469994	0.16166806
H	-1.18127523	-3.61574184	1.98148950
H	1.12695063	-3.06661552	2.69458780
H	-0.89357400	3.48442719	-2.26770636
H	1.31835139	2.73962642	-2.89516878
O	0.03825797	-1.59054822	-2.28449179

6. Singlet Ground States for NCCNO Complex

6.1 Two Oxygen Atoms

Bare Complex

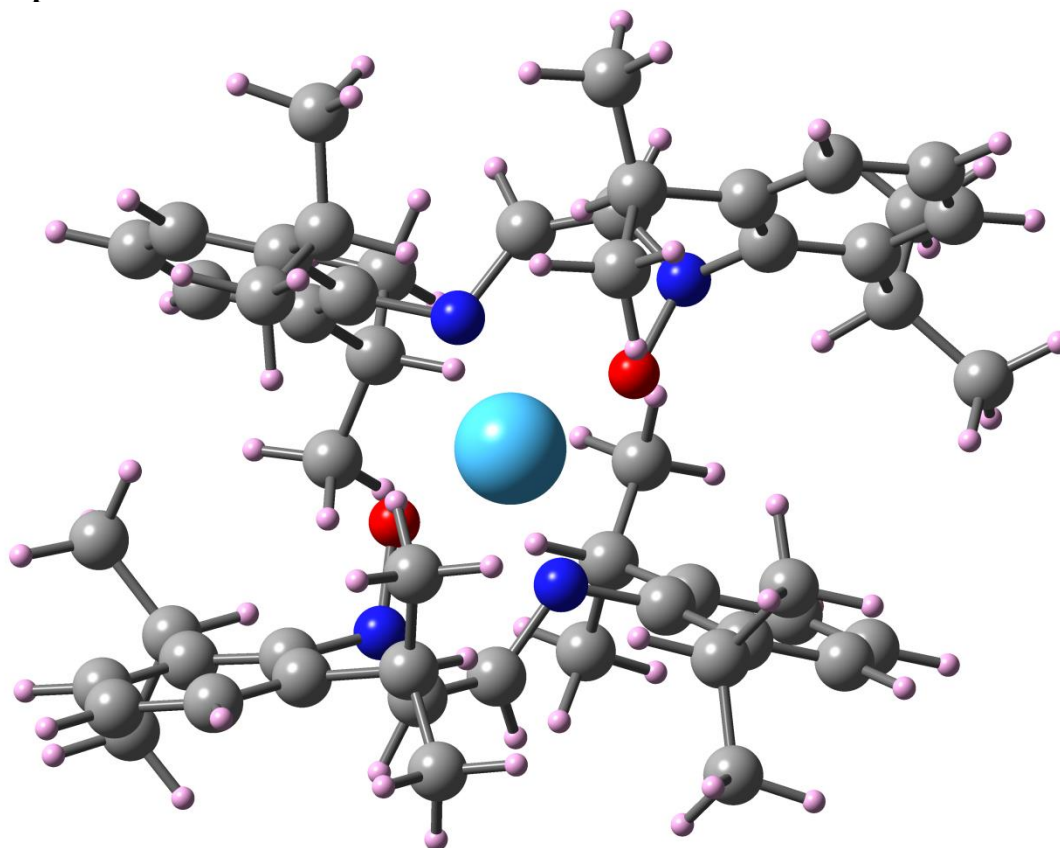


Fig. S37: NCCNO Bare Complex

E	E _{zp}	H	G
-2443.0036	-2441.8644	-2441.7972	-2441.9731
O	-1.87168508	-0.64669660	-0.12756398
O	1.70346835	-0.63984487	0.49883985
N	0.06130842	1.49868054	1.50921250
N	2.79467565	-0.06187107	1.25084209
N	-0.01459819	0.47923489	-2.01983005
N	-2.58737931	-1.09407810	-1.30013763
C	1.30800515	1.73274701	2.18009253
C	2.46379412	1.00414546	2.10337141
C	-1.22355931	0.36240477	-2.79066347
C	-2.34858535	-0.33847622	-2.46800477
C	-1.09075786	2.10558783	2.16870057
C	-1.51494948	3.41840817	1.81561878
C	-2.62431942	3.97726288	2.48634806
C	-3.30140032	3.26777260	3.48805129
C	-2.87128148	1.97855468	3.83557144

C	-1.76785359	1.37829396	3.19425156
C	-1.74951047	4.62615960	-0.41386896
C	-0.79672204	4.24939218	0.75051300
C	-0.15663747	5.52173901	1.36710841
C	5.96583498	-0.06190773	-1.47714909
C	5.28354083	0.38442735	-0.16073762
C	6.07370263	1.54991430	0.49488495
C	3.87892018	-0.97874922	1.51794945
C	5.10424756	-0.77027501	0.82748968
C	6.17757499	-1.64434814	1.10266808
C	6.02956094	-2.70764986	2.00632046
C	4.80459608	-2.91129397	2.66172757
C	3.71097352	-2.04978832	2.43866869
C	-2.45148868	-1.07428018	3.40906798
C	-1.33270219	-0.02349832	3.63525043
C	-0.86233684	-0.02541900	5.11349002
C	1.69126305	-3.57339062	2.60540333
C	2.38570088	-2.30171887	3.16237303
C	2.57059097	-2.40012632	4.69810555
C	1.17987427	0.64552636	-2.84159171
C	1.82775421	-0.51640910	-3.36114041
C	2.97658700	-0.35152778	-4.16196643
C	3.47927378	0.92412844	-4.45917390
C	2.82681268	2.05917141	-3.95841115
C	1.67312368	1.94520388	-3.15177892
C	2.36430401	-2.79816913	-2.35069581
C	1.31246445	-1.93565362	-3.09612772
C	0.86291970	-2.62291719	-4.41258990
C	-5.31261604	1.26983967	0.63519840
C	-4.92276865	0.68553155	-0.74704083
C	-5.79774378	1.29967872	-1.87144163
C	-3.87466010	-1.67208689	-0.99214960
C	-5.00527257	-0.84407377	-0.74543329
C	-6.24071642	-1.47120447	-0.47949935
C	-6.34831588	-2.87006245	-0.43613684
C	-5.21715339	-3.67092692	-0.65728525
C	-3.96296380	-3.09018160	-0.93913008
C	1.92768728	4.12407210	-1.84890167
C	0.97555228	3.22156932	-2.67495575
C	0.37732078	4.00972222	-3.87147025
C	-2.32062026	-4.66244611	0.18078771
C	-2.73787319	-3.98194224	-1.15056473
C	-2.96562312	-5.03565862	-2.26357614
H	1.31501976	2.57162267	2.87285452
H	3.29400156	1.29651141	2.73747393
H	-1.21281222	0.85372512	-3.76182901
H	-3.15863756	-0.38903763	-3.18848275
H	-2.95603984	4.97960505	2.22478423
H	-4.15396931	3.71433094	3.99456753
H	-3.39738816	1.43275828	4.61559200
H	0.01257129	3.63753258	0.34063449
H	4.28554282	0.75849161	-0.41219506

H	-2.58346210	5.24774486	-0.06253988
H	-2.17441145	3.73077513	-0.88577665
H	-1.21101789	5.19496411	-1.18342650
H	-0.91964492	6.18890203	1.78963751
H	0.39464499	6.08399549	0.60148352
H	0.54491518	5.26339846	2.17047618
H	7.00857663	-0.36709239	-1.31637768
H	5.96803202	0.76847264	-2.19461176
H	5.42835563	-0.90019235	-1.93604238
H	5.56291751	1.92438290	1.39107740
H	6.17792176	2.38492826	-0.21076348
H	7.08121891	1.22636009	0.79035146
H	7.12900176	-1.50061564	0.59764293
H	6.86488326	-3.37764392	2.19772544
H	4.70160765	-3.74145717	3.35632964
H	-0.46848319	-0.31838220	3.02732274
H	1.72188758	-1.45360480	2.96702396
H	-3.33795597	-0.84954504	4.01659522
H	-2.09738855	-2.07418701	3.69653227
H	-2.75737070	-1.10544267	2.35707892
H	-1.68081134	0.24930673	5.79180779
H	-0.04125323	0.68547716	5.26797193
H	-0.50968466	-1.02508608	5.40131943
H	1.52258077	-3.48177420	1.52607230
H	0.72085194	-3.72848887	3.09687381
H	2.30448307	-4.46758113	2.78001590
H	3.18943838	-3.26218392	4.97871246
H	1.59562062	-2.51824399	5.18930025
H	3.04763590	-1.49716652	5.09964116
H	3.47986023	-1.23021448	-4.55942852
H	4.36586005	1.03147073	-5.08007276
H	3.21179797	3.04684440	-4.20232498
H	0.42565987	-1.86271394	-2.45653603
H	-3.88565958	0.97785038	-0.93801806
H	3.27276850	-2.92864343	-2.95367020
H	1.95866555	-3.79793147	-2.14171482
H	2.64806071	-2.33450872	-1.39898184
H	0.08727939	-2.03469016	-4.91830409
H	0.45448972	-3.62093142	-4.20250511
H	1.70482337	-2.74348474	-5.10725017
H	-6.35440443	1.03568939	0.89243708
H	-5.20370936	2.36218080	0.62923792
H	-4.66641549	0.87393355	1.42658707
H	-5.50377106	0.92315465	-2.85966106
H	-5.69465931	2.39294148	-1.87856457
H	-6.86018845	1.06395018	-1.72566612
H	-7.12223279	-0.86132166	-0.29653138
H	-7.30941506	-3.33389229	-0.22524494
H	-5.31016632	-4.75331955	-0.61318416
H	0.14267681	2.92627031	-2.02880402
H	-1.91373989	-3.33296539	-1.46550708
H	2.77709489	4.46957176	-2.45266464

H	2.33021496	3.58855990	-0.97958570
H	1.39567684	5.01356000	-1.48654586
H	-0.15789388	4.90067908	-3.51604105
H	-0.32961740	3.39168650	-4.43954619
H	1.16274435	4.34176233	-4.56324737
H	-2.12133259	-3.91329377	0.95718621
H	-1.41063041	-5.26082968	0.03711184
H	-3.10979528	-5.33107517	0.55065469
H	-3.23701377	-4.55707841	-3.21309321
H	-3.76634444	-5.73890440	-1.99934344
H	-2.05020725	-5.62061943	-2.42487030
Hf	-0.05077022	0.09967903	0.00378973

6.2 Three Oxygen Atoms

Oxo Complex

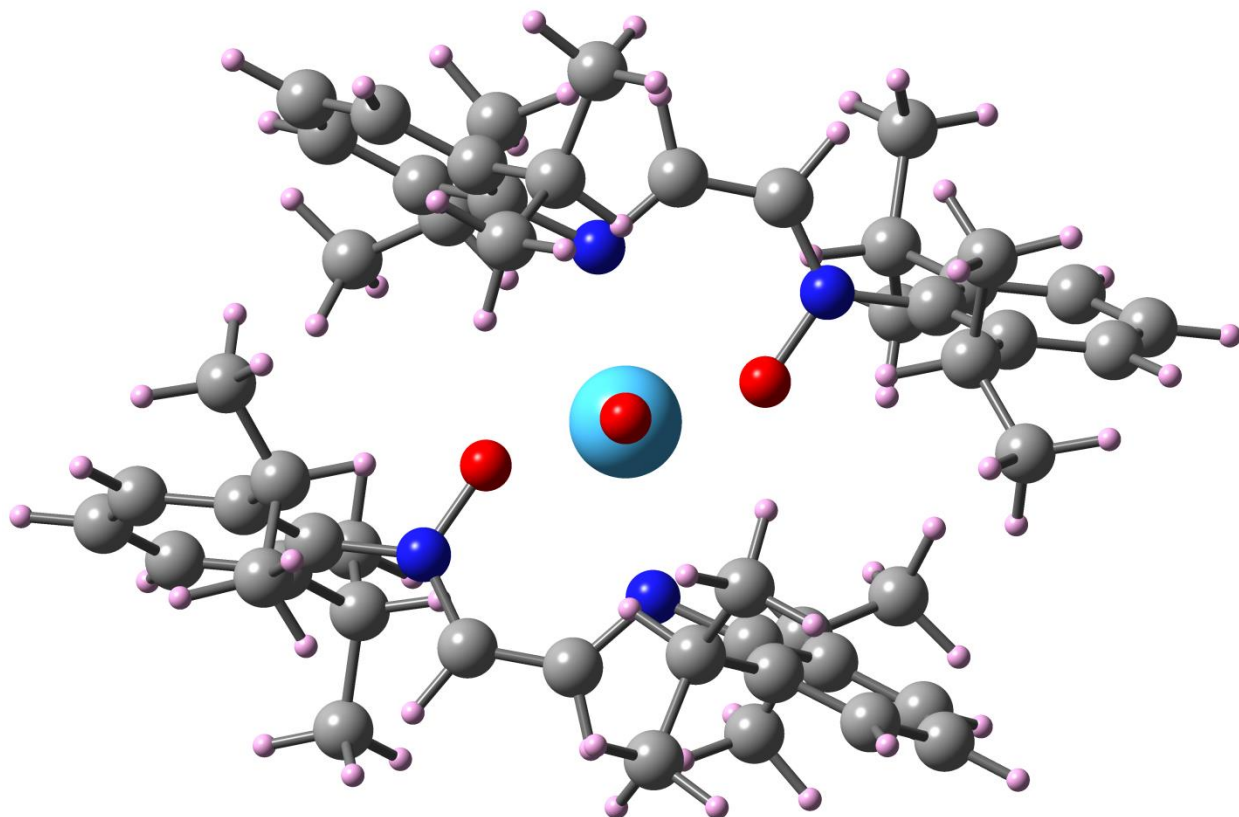


Fig. S38: NCCNO Oxo Complex

E	E_{zp}	H	G
-2518.2484	-2517.1045	-2517.0363	-2517.2102

N	-0.27906476	-2.24532913	-0.25150911
N	0.27885964	2.24652758	-0.24584268
C	0.77187971	-3.10556867	-0.15714075
C	2.10907286	-2.80929252	0.14145446
C	-0.77236658	3.10618024	-0.14965869
C	-2.10947430	2.80882782	0.14836345
C	-1.54119241	-2.88577860	-0.60631132
C	-2.48741094	-3.12960521	0.43149419
C	-3.68234484	-3.80216941	0.10538317
C	-3.93861178	-4.22774567	-1.20835197
C	-3.00042879	-3.97399288	-2.21814506
C	-1.78817893	-3.30141075	-1.94651110
C	-3.41469878	-2.26767857	2.67038822
C	-2.17746995	-2.75914237	1.88531573
C	-1.51706511	-3.96060946	2.61767855
C	3.53613652	-1.40335195	4.50926387
C	3.46664437	-2.22148494	3.19509169

C	3.72645428	-3.72631056	3.47778336
C	4.01866507	-1.38462296	0.81148401
C	4.43547641	-1.69250741	2.13234200
C	5.80155349	-1.51834947	2.44086683
C	6.70235456	-1.03955828	1.47720650
C	6.25881020	-0.72977390	0.18022515
C	4.90696146	-0.89675268	-0.18317219
C	-1.44677235	-2.25598487	-4.24764708
C	-0.79856486	-3.06245544	-3.09375285
C	-0.21728356	-4.40358119	-3.61699980
C	5.08719224	0.61734393	-2.25026185
C	4.43281268	-0.63163716	-1.61578675
C	4.68393929	-1.88437802	-2.50185110
C	1.54061721	2.88840261	-0.59942416
C	1.78685658	3.30802617	-1.93852884
C	2.99859881	3.98212156	-2.20866077
C	3.93705962	4.23342795	-1.19851517
C	3.68167363	3.80367973	0.11402648
C	2.48726613	3.12948834	0.43863963
C	1.44500333	2.26711961	-4.24157954
C	0.79706253	3.07156594	-3.08613253
C	0.21600860	4.41380945	-3.60672846
C	-3.53466742	1.38847424	4.51394366
C	-3.46529640	2.21002667	3.20194776
C	-3.72448677	3.71421342	3.48884519
C	-4.01843177	1.38193929	0.81565918
C	-4.43464490	1.68460453	2.13792308
C	-5.80054334	1.50914562	2.44636902
C	-6.70178861	1.03426469	1.48115613
C	-6.25882888	0.72960086	0.18278546
C	-4.90706913	0.89783095	-0.18047815
C	3.41606482	2.25933535	2.67362939
C	2.17836326	2.75407570	1.89137747
C	1.51893853	3.95309923	2.62857048
C	-5.08625758	-0.61055067	-2.25174608
C	-4.43345308	0.63771889	-1.61418941
C	-4.68712356	1.89259607	-2.49646667
H	0.57756130	-4.15897409	-0.36075664
H	2.83350383	-3.61400371	0.12112770
H	-0.57842988	4.16007039	-0.35113217
H	-2.83417538	3.61333499	0.12980335
H	-4.41427846	-4.00263456	0.88290543
H	-4.86231317	-4.75317078	-1.44072580
H	-3.20684404	-4.30237110	-3.23397209
H	-1.45021900	-1.93892936	1.87159362
H	2.44585764	-2.12587401	2.80844628
H	-4.15891995	-3.06347823	2.80749355
H	-3.89840675	-1.42686056	2.16110105
H	-3.11015404	-1.93553846	3.67216939
H	-2.20026660	-4.82041372	2.64601063
H	-1.26647282	-3.68944611	3.65264102
H	-0.59487895	-4.27750852	2.11560131

H	4.51397584	-1.50059425	4.99881480
H	2.77582726	-1.76292674	5.21519587
H	3.35493553	-0.33921389	4.32175837
H	3.62454374	-4.32952362	2.56688854
H	3.00982261	-4.10551358	4.21817803
H	4.73848107	-3.88403289	3.87355663
H	6.15928350	-1.74973866	3.44089025
H	7.75048345	-0.90678380	1.73562637
H	6.96887474	-0.35816246	-0.55262750
H	0.02438482	-2.44547407	-2.72497196
H	3.35218324	-0.45335302	-1.59290725
H	-2.31453760	-2.77468587	-4.67864216
H	-0.71333129	-2.09871952	-5.04970944
H	-1.75514220	-1.26953202	-3.88685269
H	-1.00347295	-5.04433766	-4.03942259
H	0.27912915	-4.96946935	-2.81701856
H	0.52095548	-4.21284024	-4.40755609
H	4.94421006	1.50482632	-1.62463980
H	4.62671644	0.81769315	-3.22577859
H	6.16372589	0.47616398	-2.41718490
H	5.75696697	-2.11201317	-2.56232252
H	4.31297822	-1.70632253	-3.51929709
H	4.16943779	-2.76848713	-2.10555537
H	3.20444065	4.31354533	-3.22361562
H	4.86036472	4.76006541	-1.42971731
H	4.41388571	4.00213746	0.89180777
H	-0.02597102	2.45407162	-2.71841192
H	-2.44466723	2.11506686	2.81470376
H	2.31270594	2.78656901	-4.67182871
H	0.71140260	2.11125486	-5.04376506
H	1.75342466	1.28004320	-3.88254774
H	-0.28019880	4.97827443	-2.80560314
H	-0.52235719	4.22476160	-4.39756947
H	1.00229012	5.05520776	-4.02800314
H	-4.51214153	1.48508392	5.00435778
H	-2.77373908	1.74570510	5.22039428
H	-3.35424679	0.32469928	4.32358472
H	-3.62243115	4.31991780	2.57963663
H	-3.00763204	4.09109116	4.23021123
H	-4.73643534	3.87111967	3.88515153
H	-6.15786287	1.73651315	3.44745627
H	-7.74981007	0.90051492	1.73951086
H	-6.96923167	0.36093761	-0.55123422
H	1.45084635	1.93413368	1.87529221
H	-3.35252714	0.46102819	-1.59250681
H	4.16068026	3.05435848	2.81311478
H	3.89907937	1.42025975	2.16080157
H	3.11219217	1.92355971	3.67440998
H	1.26876896	3.67816312	3.66263929
H	0.59664436	4.27234873	2.12817581
H	2.20258188	4.81245165	2.65978830
H	-4.94124497	-1.49957855	-1.62878188

H	-4.62632764	-0.80729420	-3.22826367
H	-6.16317898	-0.47076168	-2.41729641
H	-4.17389879	2.77641033	-2.09784514
H	-5.76055252	2.11865007	-2.55571564
H	-4.31643080	1.71814448	-3.51463334
O	0.00027015	0.00318749	-2.22110629
O	-1.79941611	0.47457610	0.52103587
O	1.79970794	-0.47583758	0.51980364
N	-2.63018491	1.58917430	0.46174013
N	2.63028527	-1.59045392	0.45731690
Hf	0.00019098	0.00069158	-0.41123989

6.3 Four Oxygen Atoms

Dioxo Complex (lower energy conformation)

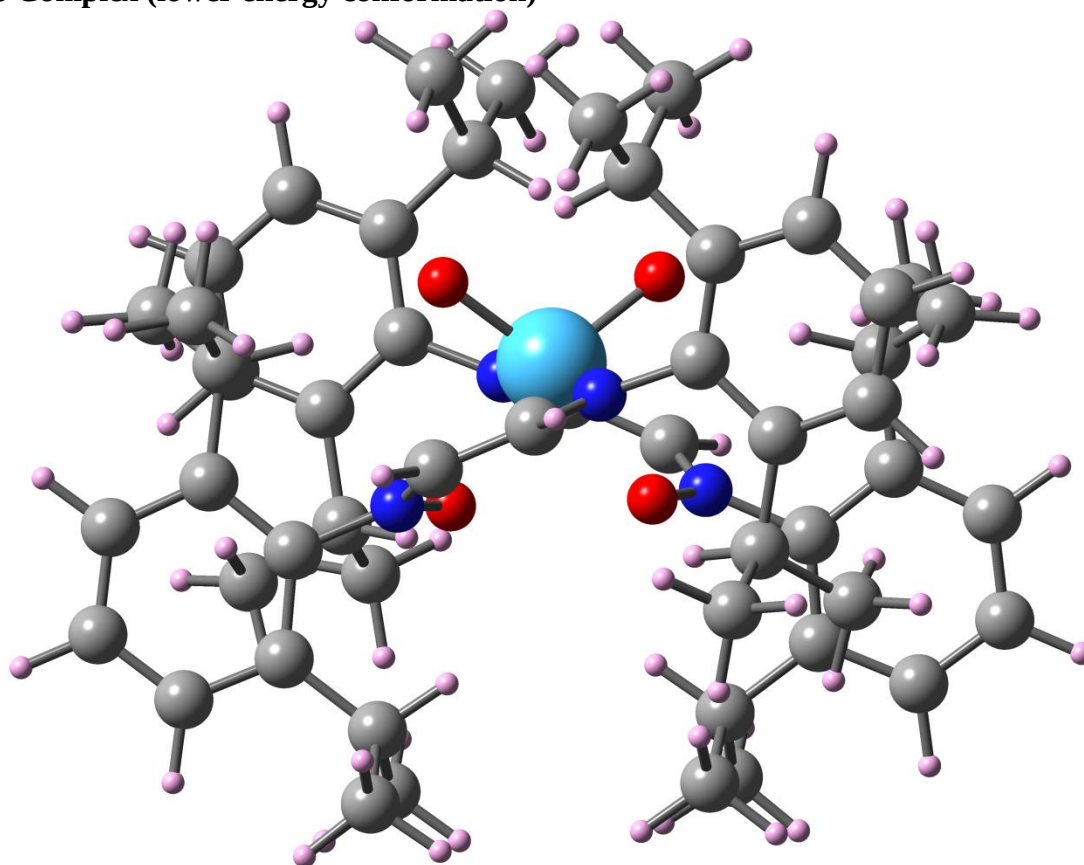


Fig. S39: NCCNO Dioxo Complex (lower energy conformation)

E	E_{zp}	H	G
-2593.4320	-2592.2839	-2592.2144	-2592.3910

N	0.62733351	0.47270140	2.28085802
N	-0.62566221	0.72254659	-2.22108741
C	-0.22238447	0.06703334	3.19210522
C	-1.53533371	-0.48921524	2.96794972
C	0.22167627	0.41391702	-3.17174228
C	1.53279886	-0.16768566	-3.00981381
C	1.92990985	0.92190435	2.78639791
C	2.93842462	-0.05590372	3.00414585
C	4.16942495	0.37969846	3.53634966
C	4.39191059	1.73463718	3.82938607
C	3.38448900	2.67848027	3.58334045
C	2.13150644	2.30065648	3.05309916
C	3.91851155	-2.20702010	2.00170356
C	2.70894669	-1.54371285	2.70450162
C	2.35505099	-2.32310746	4.00143524
C	-2.08723303	-4.68429029	0.56989573
C	-2.26250311	-3.88942857	1.89122001

C	-2.35389113	-4.84481302	3.10854105
C	-3.35873353	-1.54813263	1.76220557
C	-3.47539909	-2.95740873	1.80520460
C	-4.78014291	-3.48914703	1.74730236
C	-5.89809516	-2.64406999	1.65065931
C	-5.73624095	-1.25042556	1.59949000
C	-4.45445232	-0.65811857	1.64365743
C	1.56871560	4.43632177	1.80114501
C	1.06193790	3.37019166	2.80692356
C	0.60519411	4.01737231	4.14167474
C	-5.14614270	1.50686018	0.47080388
C	-4.28486958	0.86497326	1.58597916
C	-4.63289436	1.50102408	2.95985257
C	-1.92719070	1.22972120	-2.67115971
C	-2.11700086	2.62921676	-2.80183896
C	-3.37181734	3.06870883	-3.27737056
C	-4.39216304	2.16257310	-3.59926601
C	-4.18014912	0.78340909	-3.44245014
C	-2.94726283	0.28647280	-2.97214171
C	-1.51717323	4.61393890	-1.33879315
C	-1.03435150	3.65924206	-2.46157937
C	-0.59410070	4.44448755	-3.72543013
C	2.05899352	-4.57269804	-1.08168570
C	2.25698901	-3.65913250	-2.32069831
C	2.36362420	-4.49720505	-3.62006607
C	3.35589070	-1.34999289	-1.92202136
C	3.47116931	-2.74516177	-2.12694132
C	4.77507253	-3.28185705	-2.12315651
C	5.89330171	-2.45520681	-1.92400649
C	5.73252105	-1.07655807	-1.71302365
C	4.45138565	-0.48126670	-1.69589820
C	-3.94084750	-1.96154185	-2.22144328
C	-2.72327124	-1.22541886	-2.83048602
C	-2.35176026	-1.86066976	-4.19938460
C	5.12758405	1.53397101	-0.27341229
C	4.28249881	1.02538000	-1.46666069
C	4.65153256	1.81044889	-2.75522030
H	0.04670150	0.15585607	4.24778768
H	-2.19804595	-0.58671508	3.81823253
H	-0.04763889	0.61674168	-4.21155234
H	2.19269268	-0.17853864	-3.86784020
H	4.95925818	-0.34410136	3.71918190
H	5.34752920	2.05208786	4.24049341
H	3.56801550	3.72743143	3.80102143
H	1.85974954	-1.62562698	2.01555544
H	-1.35761345	-3.28360552	2.01637107
H	4.79918213	-2.25078927	2.65562586
H	4.19438751	-1.66487547	1.09100413
H	3.66788286	-3.23867837	1.72042809
H	3.17723508	-2.26153347	4.72684940
H	2.17717861	-3.38416482	3.77821637
H	1.45584089	-1.92163986	4.48671460

H	-2.95451993	-5.32891867	0.37499973
H	-1.19591104	-5.32315334	0.62763459
H	-1.96746352	-4.00079436	-0.27848743
H	-2.45722197	-4.28735901	4.04842366
H	-1.44729902	-5.46049356	3.17407267
H	-3.21162594	-5.52451512	3.02658087
H	-4.92121427	-4.56625205	1.77798697
H	-6.89660029	-3.07308200	1.61007466
H	-6.60994847	-0.61154232	1.51158711
H	0.18499744	2.90927193	2.34030547
H	-3.24241545	1.12783287	1.34725851
H	2.46139112	4.95976806	2.17325188
H	0.78284119	5.18486352	1.63077216
H	1.79416951	3.94871496	0.84554748
H	1.42965292	4.54734119	4.63878789
H	0.21750017	3.26734574	4.84611235
H	-0.19376650	4.74462660	3.94737530
H	-4.93176323	1.05964765	-0.50635748
H	-4.89951027	2.57288448	0.40263754
H	-6.22459043	1.42019544	0.66758566
H	-5.68061299	1.31525044	3.23696726
H	-4.47571096	2.58532957	2.90979970
H	-3.99804670	1.11110204	3.76737103
H	-3.54659367	4.13557892	-3.38965054
H	-5.34976794	2.52709526	-3.96411153
H	-4.98004403	0.08880567	-3.68442971
H	-0.15419223	3.14525834	-2.06076602
H	1.35622705	-3.03956299	-2.40239558
H	-2.40680091	5.18563383	-1.64130178
H	-0.71969784	5.32945462	-1.09664042
H	-1.74141843	4.02819321	-0.43989116
H	-0.21758780	3.77390918	-4.51131217
H	0.20869521	5.14652737	-3.46497065
H	-1.42407016	5.02526423	-4.15138597
H	2.92310793	-5.23381555	-0.93365143
H	1.16817559	-5.20140670	-1.21244406
H	1.92602237	-3.96979271	-0.17620911
H	2.49306538	-3.85599221	-4.50146672
H	1.45190226	-5.09231027	-3.76109528
H	3.21130996	-5.19330898	-3.58459752
H	4.91581711	-4.34842226	-2.27694053
H	6.89107092	-2.88782663	-1.92790997
H	6.60633297	-0.45338427	-1.54737537
H	-1.88299150	-1.38239703	-2.14350058
H	3.23723549	1.26241408	-1.21431544
H	-4.81121190	-1.93737096	-2.89010483
H	-4.23226504	-1.52089088	-1.26220699
H	-3.69088570	-3.01684788	-2.04822299
H	-2.18065952	-2.94055770	-4.09019094
H	-1.44395052	-1.41375689	-4.62502783
H	-3.16277912	-1.71651755	-4.92561703
H	4.89271851	0.98400051	0.64483741

H	4.88641888	2.58802853	-0.09270307
H	6.20873929	1.46048265	-0.46005353
H	4.03373402	1.50780562	-3.61179478
H	5.70507373	1.65937171	-3.03132151
H	4.48774083	2.88219693	-2.58964212
O	-1.41068473	1.93541561	0.68010722
O	1.40417215	2.00822185	-0.46162856
O	1.31148499	-0.88386644	-0.78669865
O	-1.31035858	-0.97109290	0.68386219
N	2.00495947	-0.76480270	-1.92132720
N	-2.00670467	-0.96867093	1.82286514
Hf	-0.00140956	0.88907878	0.04583420

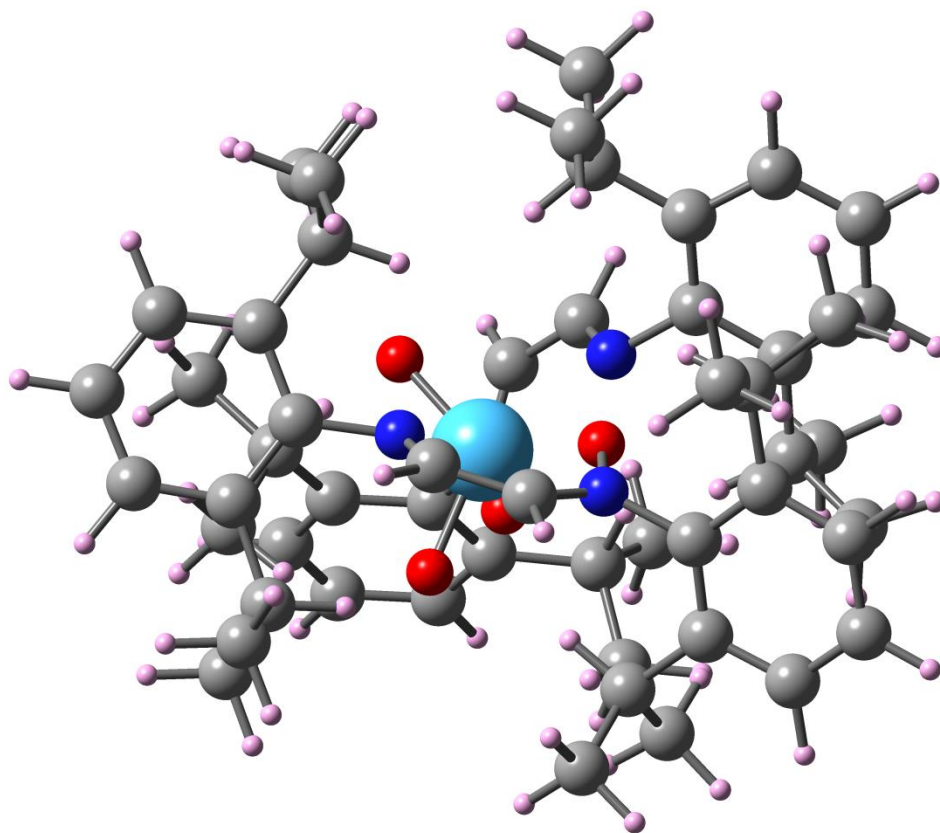
Dioxo Complex (higher energy conformation)

Fig. S40: NCCNO Dioxo Complex (higher energy conformation)

E	E_{zp}	H	G
-2593.4179	-2592.2697	-2592.2004	-2592.3766
O	-1.83155545	0.10926691	-0.15352208
O	1.80487450	-1.31716113	-0.57513576
O	0.75599728	1.00259596	-1.77249441
N	-0.06483304	-1.63664579	1.46344101
N	2.69691502	-1.75656779	0.33180902
N	-0.42136514	2.61940863	-0.11707690
N	-2.66643643	0.80526224	-0.97289983
C	1.01188091	-2.03808760	2.08860227
C	2.37256678	-1.93309994	1.60473778
C	-1.54488085	2.99282173	-0.70293563
C	-2.58270486	2.11478189	-1.16125238
C	-1.33247079	-2.08523697	2.02675784
C	-1.84023346	-1.49813909	3.21500517
C	-3.02577596	-2.03954504	3.75924688
C	-3.68883218	-3.11014515	3.14339660
C	-3.18572518	-3.64908688	1.94738602
C	-2.00686930	-3.14628295	1.36276365
C	-2.15738807	0.86640807	4.09221196

C	-1.16337316	-0.30914437	3.90831632
C	-0.55620880	-0.71913436	5.27661694
C	4.51181839	1.42768963	-0.79679429
C	4.63140261	0.45188592	0.40571939
C	5.64626346	0.97499348	1.45149097
C	4.05531989	-2.00435022	-0.16722159
C	4.99225179	-0.94602420	-0.10246638
C	6.28829607	-1.22372038	-0.59138040
C	6.61117002	-2.47990206	-1.12625274
C	5.64148462	-3.49427544	-1.19878465
C	4.33271579	-3.27738251	-0.72252444
C	-2.51860561	-4.11497287	-0.95960580
C	-1.43396700	-3.77758718	0.09022563
C	-0.60586571	-5.04558717	0.43856724
C	2.78598293	-4.42584748	-2.35623355
C	3.25900624	-4.35840644	-0.87784604
C	3.73207062	-5.74564432	-0.37807965
C	0.55631611	3.69041762	0.07948265
C	1.13513852	4.33552954	-1.05564380
C	2.07211958	5.36300033	-0.81241479
C	2.42033726	5.74860481	0.48927261
C	1.82883904	5.10498414	1.58603979
C	0.89387388	4.06670559	1.40780215
C	2.10496291	3.60259221	-3.29869386
C	0.82092141	3.96487971	-2.51191892
C	0.04657212	5.10723878	-3.22395922
C	-5.98574231	-0.57332724	1.23859521
C	-5.29059337	0.43684533	0.29373314
C	-6.17304444	1.70193117	0.10629786
C	-3.67676751	0.00721396	-1.67581805
C	-4.93914433	-0.18015526	-1.06395937
C	-5.89087533	-0.93007953	-1.78567089
C	-5.57935593	-1.47060441	-3.04463868
C	-4.31004883	-1.27376420	-3.61118864
C	-3.31838855	-0.52869746	-2.93702255
C	1.22946012	2.95376171	3.67630850
C	0.20588817	3.46606373	2.63451391
C	-0.77958158	4.49685783	3.25196342
C	-1.27225278	-1.63090426	-3.99764074
C	-1.94442167	-0.29950743	-3.57730154
C	-2.06386529	0.65774558	-4.79355418
H	0.92235690	-2.57986389	3.03631478
H	3.18239456	-2.19888300	2.27266575
H	-1.69710177	4.04132079	-0.95801760
H	-3.36076485	2.53733602	-1.78610875
H	-3.43161804	-1.61694207	4.67506611
H	-4.59365786	-3.51881944	3.58730828
H	-3.71250479	-4.47039605	1.46909100
H	-0.34380562	0.05678376	3.27875906
H	3.64071377	0.44719875	0.87931281
H	-2.98783405	0.59687846	4.75791465
H	-2.58077184	1.17684985	3.12862821

H	-1.64319860	1.72858756	4.53277865
H	-1.33341069	-1.07454910	5.96677628
H	-0.05369385	0.13854038	5.74211270
H	0.18327549	-1.52345150	5.16701052
H	5.45792764	1.50604758	-1.35256265
H	4.23713165	2.42451157	-0.43077947
H	3.72014159	1.10052195	-1.48012782
H	5.74690006	0.28444978	2.30035981
H	5.29629092	1.93904016	1.84066309
H	6.64589325	1.13203148	1.02234381
H	7.04295257	-0.44322401	-0.55763908
H	7.61589918	-2.66700122	-1.49833221
H	5.90213130	-4.45581468	-1.63239390
H	-0.75036744	-3.05124486	-0.36482012
H	2.38491508	-4.07632390	-0.27894012
H	-3.19118514	-4.91153357	-0.61496464
H	-2.04570850	-4.46732067	-1.88589822
H	-3.12537460	-3.23464935	-1.20057287
H	-1.24356226	-5.81291598	0.89774965
H	0.20283661	-4.81789117	1.14557073
H	-0.15681143	-5.47212366	-0.46862273
H	2.39960595	-3.45391991	-2.68341140
H	1.98888290	-5.17343104	-2.46837555
H	3.61322966	-4.70902976	-3.02033466
H	4.55293710	-6.13943205	-0.99061387
H	2.90616276	-6.46697848	-0.43274493
H	4.07999837	-5.70146601	0.66213938
H	2.53819407	5.86079530	-1.65886679
H	3.14297951	6.54606211	0.64760913
H	2.09156012	5.41414960	2.59419640
H	0.22640239	3.04608524	-2.52032900
H	-4.35932553	0.74332327	0.78512625
H	2.82092224	4.43488479	-3.34017691
H	1.84295612	3.33171640	-4.33081846
H	2.57955516	2.73352183	-2.83558388
H	-0.88720930	5.36316353	-2.70272282
H	-0.20682383	4.80997090	-4.25090634
H	0.64941973	6.02413528	-3.28071104
H	-6.97000813	-0.87645388	0.85814487
H	-6.14069483	-0.11463858	2.22384573
H	-5.37414189	-1.47113263	1.37556847
H	-5.67655801	2.45638942	-0.51755612
H	-6.39509763	2.15955791	1.07910174
H	-7.12633846	1.44539696	-0.37425029
H	-6.87619463	-1.09693808	-1.35988291
H	-6.32758023	-2.04718475	-3.58349990
H	-4.08307288	-1.70159461	-4.58372782
H	-0.37138012	2.59639578	2.30590076
H	-1.26173946	0.17379517	-2.86180861
H	1.87162815	3.76088739	4.05452424
H	1.84062719	2.17846546	3.20181339
H	0.70661107	2.51950776	4.54122891

H	-1.31509941	4.05657630	4.10401696
H	-1.52426876	4.83272062	2.51685393
H	-0.24458333	5.38511449	3.61390956
H	-1.19155470	-2.31803663	-3.14694084
H	-0.25807111	-1.42358279	-4.35871517
H	-1.82475844	-2.13957748	-4.79988835
H	-2.49612202	1.62522602	-4.50453635
H	-2.69581794	0.22903531	-5.58362877
H	-1.06791740	0.84666340	-5.21207317
O	1.57335068	0.85168331	1.32720042
Hf	0.38531859	0.37229949	-0.03004620

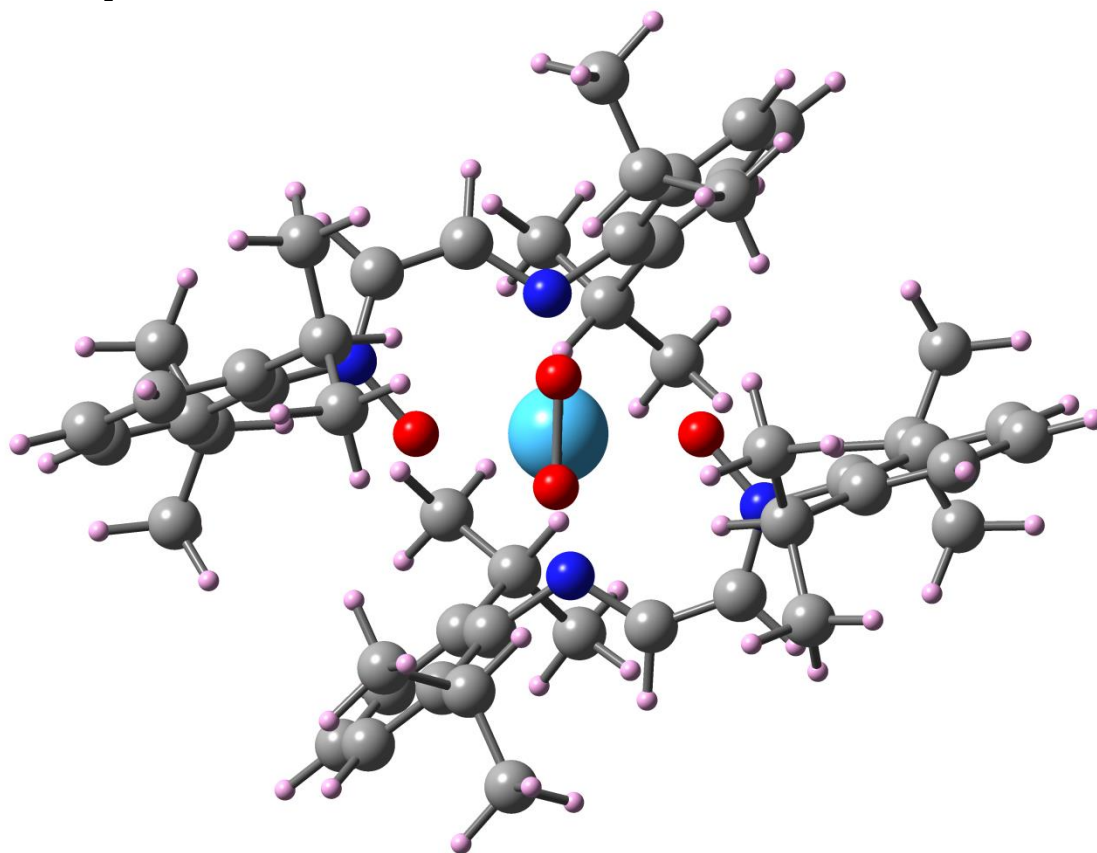
Peroxo Complex

Fig. S41: NCCNO Peroxo Complex

E	E_{zp}	H	G
-2593.4069	-2592.2606	-2592.1909	-2592.3706

O	2.02570130	0.27611105	0.04260586
O	-2.02759399	-0.27697561	0.05119438
O	-0.13067862	0.77810147	-2.22097038
O	0.11737233	-0.77770980	-2.22148323
N	0.10762640	-2.03060041	0.58884286
N	-2.78607314	-1.42781306	-0.15044406
N	-0.10666593	2.02899543	0.59298850
N	2.78734826	1.42677249	-0.14697037
C	-0.94332847	-2.90359177	0.55762647
C	-2.26907275	-2.63688105	0.18323539
C	0.94606251	2.90059345	0.56891684
C	2.27177653	2.63436955	0.19509893
C	1.36379534	-2.66002161	1.00577730
C	2.14073157	-3.38651765	0.06075756
C	3.30468051	-4.04198636	0.51735407
C	3.69424086	-3.98500102	1.86287614
C	2.92242464	-3.25372383	2.77828082
C	1.75385686	-2.57741774	2.37128569

C	2.90785701	-3.01961583	-2.34116853
C	1.75827471	-3.49857199	-1.41944182
C	1.33333043	-4.94715530	-1.78027076
C	-3.00405203	-0.71368760	-4.23369888
C	-3.10824817	-1.72523466	-3.06481726
C	-3.23343971	-3.17617100	-3.60294657
C	-4.10624216	-1.24486028	-0.72213573
C	-4.27155603	-1.39744371	-2.12348966
C	-5.57826821	-1.25274844	-2.63815963
C	-6.66099640	-0.95873611	-1.79554725
C	-6.46263108	-0.79696718	-0.41425786
C	-5.17875250	-0.92908844	0.15217201
C	1.78026893	-0.87843326	4.28338678
C	0.91838270	-1.82466251	3.41082035
C	0.12175315	-2.81758564	4.29984253
C	-5.64428804	0.49309464	2.22477743
C	-4.97557717	-0.78537246	1.66304774
C	-5.49207756	-2.04862926	2.40513962
C	-1.36284220	2.65860065	1.00963332
C	-1.75526464	2.57284171	2.37430752
C	-2.92422034	3.24861981	2.78100969
C	-3.69420052	3.98247636	1.86611737
C	-3.30211377	4.04299800	0.52149457
C	-2.13756736	3.38832772	0.06525811
C	-1.78522623	0.87094767	4.28404034
C	-0.92168212	1.81741667	3.41343234
C	-0.12453483	2.80814391	4.30450975
C	2.99853718	0.71842727	-4.23059950
C	3.10490344	1.72812009	-3.06034992
C	3.22865512	3.17995540	-3.59639965
C	4.10697237	1.24557318	-0.72019578
C	4.27008043	1.39935871	-2.12168632
C	5.57597978	1.25581714	-2.63857311
C	6.66026740	0.96219157	-1.79773644
C	6.46418897	0.79944107	-0.41627044
C	5.18097482	0.92993442	0.15220897
C	-2.89925400	3.03011646	-2.33987143
C	-1.75174164	3.50531437	-1.41368685
C	-1.32538247	4.95506609	-1.76820271
C	5.64690101	-0.49804003	2.22052816
C	4.98015212	0.78337501	1.66311583
C	5.50066362	2.04365226	2.40739798
H	-0.74151852	-3.94266187	0.81659514
H	-2.96587513	-3.46356611	0.11487313
H	0.74522988	3.93833512	0.83386695
H	2.97015861	3.46028187	0.13387370
H	3.90803388	-4.60405052	-0.19129666
H	4.58976131	-4.50486025	2.19562826
H	3.22840236	-3.21132859	3.82079791
H	0.90651805	-2.84243860	-1.61797766
H	-2.16399766	-1.65084506	-2.51783567
H	3.79103809	-3.66846487	-2.26401434

H	3.20832798	-1.99802012	-2.08422579
H	2.57423260	-3.02458098	-3.38672925
H	2.15648419	-5.65636545	-1.61838938
H	1.04039809	-5.00400121	-2.83706938
H	0.48112160	-5.27996687	-1.17288279
H	-3.88631282	-0.74520221	-4.88806252
H	-2.11999663	-0.94746623	-4.83892653
H	-2.88163475	0.30671219	-3.85639795
H	-3.25602862	-3.90935024	-2.78549749
H	-2.37627827	-3.41122345	-4.24682068
H	-4.14942678	-3.30517053	-4.19576992
H	-5.74454914	-1.36543911	-3.70607144
H	-7.65912984	-0.85197969	-2.21435417
H	-7.30957450	-0.56441006	0.22554549
H	0.18737627	-1.20930213	2.87409994
H	-3.90049905	-0.69760128	1.85535263
H	2.48836922	-1.43597571	4.91030286
H	1.14112260	-0.29117497	4.95520136
H	2.35483170	-0.18200432	3.66009360
H	0.80108844	-3.47668876	4.85679063
H	-0.53732268	-3.45080892	3.69247723
H	-0.49990963	-2.27626999	5.02591292
H	-5.27067452	1.38804250	1.71550342
H	-5.41918641	0.59348032	3.29480439
H	-6.73675468	0.46269323	2.11844026
H	-6.57077130	-2.18323152	2.24919245
H	-5.31404842	-1.95751966	3.48496153
H	-4.98578387	-2.95662979	2.05276006
H	-3.23203143	3.20365787	3.82287663
H	-4.59016869	4.50172989	2.19861755
H	-3.90386575	4.60736930	-0.18668249
H	-0.19098413	1.20194876	2.87641217
H	2.16188068	1.65295388	-2.51136068
H	-2.49241494	1.42841998	4.91205631
H	-1.14711077	0.28128752	4.95475586
H	-2.36084863	0.17674891	3.65927882
H	0.53607590	3.44121594	3.69865648
H	0.49566196	2.26513331	5.03056973
H	-0.80358671	3.46747876	4.86152608
H	3.87934542	0.75156491	-4.88683335
H	2.11303573	0.95268391	-4.83352234
H	2.87765557	-0.30269385	-3.85479388
H	3.25297790	3.91170278	-2.77773669
H	2.37002292	3.41592816	-4.23796973
H	4.14330540	3.30997293	-4.19105894
H	5.74059751	1.36943261	-3.70664874
H	7.65784314	0.85653337	-2.21814826
H	7.31231024	0.56708228	0.22206823
H	-0.89970102	2.84963262	-1.61246937
H	3.90517636	0.69767923	1.85716272
H	-3.78246339	3.67889337	-2.26236970
H	-3.20040536	2.00760137	-2.08748256

H	-2.56318038	3.03873046	-3.38461433
H	-1.02967084	5.01565556	-2.82402837
H	-0.47468735	5.28541898	-1.15735900
H	-2.14877700	5.66391438	-1.60595242
H	5.26983813	-1.39092868	1.71018799
H	5.42407590	-0.60021414	3.29086815
H	6.73917022	-0.47017765	2.11157637
H	4.99557896	2.95355543	2.05819445
H	6.57932964	2.17652139	2.24981881
H	5.32446485	1.95020588	3.48731231
Hf	-0.00103665	0.00062425	-0.37101407

6.4 Five Oxygen Atoms

Oxo Peroxo Complex (planar conformation, lower energy)

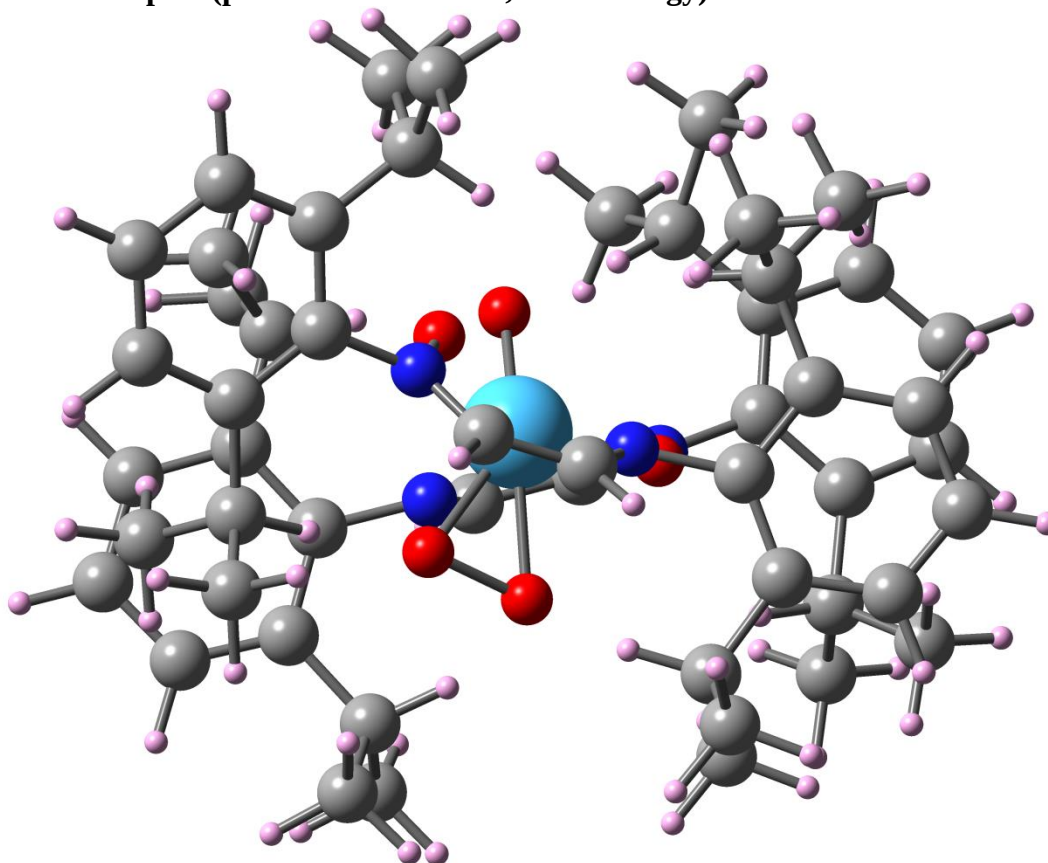


Fig. S42: NCCNO Oxo Peroxo Complex (planar conformation, lower energy)

E	E_{zp}	H	G
-2668.5875	-2667.4358	-2667.3655	-2667.5439

O	-2.07926151	0.24362653	-0.02909286
O	1.91865557	-1.07296686	-0.68754399
O	-0.13386814	0.36051768	-1.91937686
N	-0.14797757	-1.97468983	1.03869532
N	2.76104301	-1.71374928	0.17038061
N	-0.01708586	2.42490972	-0.21348510
N	-2.79339853	1.18738571	-0.65930309
C	0.92335871	-2.47786812	1.63141641
C	2.30252451	-2.28617276	1.27598264
C	-1.11386884	3.04072005	-0.57340027
C	-2.39469456	2.43711854	-0.85703409
C	-1.42741322	-2.52752851	1.46798004
C	-1.87828278	-2.38844059	2.81176021
C	-3.10236818	-3.00461613	3.15616411
C	-3.85204157	-3.72506698	2.21794628
C	-3.39079843	-3.83999730	0.89610155
C	-2.17678158	-3.25094315	0.49464728

C	-2.01161364	-0.41497114	4.40620158
C	-1.13636458	-1.58514540	3.88802217
C	-0.68120131	-2.49060201	5.06273652
C	5.11118842	1.46593627	1.38989420
C	4.67590151	0.00265513	1.65919065
C	5.25991817	-0.50215856	3.00599701
C	4.17001831	-1.72884690	-0.21206124
C	5.08580879	-0.91950985	0.50479544
C	6.43755596	-0.97862725	0.09917913
C	6.83870444	-1.77902359	-0.98014231
C	5.89569650	-2.54529231	-1.68560498
C	4.53586550	-2.54094478	-1.31688807
C	-2.74208395	-3.68304169	-1.97911427
C	-1.63542273	-3.46437037	-0.92356544
C	-0.64404904	-4.66238735	-0.94986531
C	3.14857618	-2.61713800	-3.43088520
C	3.51094780	-3.35519545	-2.11268401
C	3.99036336	-4.80102950	-2.39369774
C	1.17145725	3.27449994	-0.05721982
C	2.00674274	3.49186786	-1.18791619
C	3.12261174	4.34082075	-1.01594288
C	3.39660858	4.94966404	0.21655291
C	2.55345873	4.71421872	1.31325157
C	1.42797319	3.87154207	1.20693694
C	2.94158182	2.04301496	-3.06460074
C	1.73586527	2.88200148	-2.56942771
C	1.37533516	3.98680262	-3.59818163
C	-5.58122223	-0.00232046	2.18510571
C	-5.03520498	1.09374182	1.23669332
C	-5.72543811	2.45764436	1.51171365
C	-4.11181076	0.75681459	-1.15445760
C	-5.18538828	0.70146058	-0.23638361
C	-6.43767661	0.30264632	-0.74906372
C	-6.58847726	-0.03038589	-2.10478881
C	-5.49184695	0.02679273	-2.98079953
C	-4.21405767	0.42064262	-2.52806032
C	1.31710495	3.23628039	3.67704330
C	0.51783885	3.66436942	2.42204198
C	-0.32041554	4.94097693	2.70262208
C	-2.96457119	-0.67522622	-4.48276205
C	-3.02268959	0.51303079	-3.49228747
C	-3.07581974	1.84567634	-4.29139020
H	0.78397646	-3.16912737	2.46474050
H	3.04925219	-2.75502300	1.90583830
H	-1.09190080	4.11998510	-0.73858809
H	-3.14420349	3.07643245	-1.30696514
H	-3.46999608	-2.91066071	4.17505569
H	-4.78873376	-4.19389807	2.51080932
H	-3.97875571	-4.39790353	0.17449163
H	-0.26031502	-1.10645194	3.44188621
H	3.58518421	0.02143082	1.75248767
H	-2.93573833	-0.76921910	4.88373515

H	-2.27296548	0.25340415	3.57857107
H	-1.44915966	0.17183352	5.14410163
H	-1.53773006	-2.94012124	5.58354500
H	-0.11615321	-1.89982382	5.79583927
H	-0.03729432	-3.31294678	4.72045125
H	6.20417694	1.56924675	1.34604293
H	4.74100008	2.11394681	2.19363573
H	4.69060625	1.83693112	0.44836692
H	4.93291318	-1.52609059	3.23386896
H	4.92752842	0.14806466	3.82506832
H	6.35840311	-0.49870752	2.99388641
H	7.17487333	-0.37828287	0.62483381
H	7.88441123	-1.80115327	-1.27802908
H	6.21963108	-3.15347470	-2.52524824
H	-1.07679735	-2.56748615	-1.21857257
H	2.58671137	-3.42377021	-1.52717271
H	-3.25597482	-4.64392652	-1.84106776
H	-2.29547992	-3.69458645	-2.98130125
H	-3.49169195	-2.88346122	-1.94504468
H	-1.15881959	-5.59478277	-0.68053950
H	0.18538106	-4.51936209	-0.24734271
H	-0.21977201	-4.78258058	-1.95568543
H	2.71037069	-1.63807540	-3.21277316
H	2.41463764	-3.20156759	-4.00187696
H	4.03829243	-2.47858077	-4.06035276
H	4.85492806	-4.82228134	-3.06953014
H	3.18570049	-5.37101562	-2.87614882
H	4.27095085	-5.32163571	-1.46868693
H	3.77586370	4.52798760	-1.86442672
H	4.25939081	5.60356727	0.32221078
H	2.76917233	5.18920340	2.26680874
H	0.89549931	2.18207096	-2.50313557
H	-3.96914144	1.20502689	1.46347763
H	3.84880874	2.65091975	-3.18872990
H	2.70162704	1.58858044	-4.03476361
H	3.15970053	1.22982301	-2.36264857
H	0.50037426	4.56823778	-3.27520575
H	1.14013238	3.53223014	-4.56996119
H	2.20560227	4.69135720	-3.74731243
H	-6.66255535	-0.14632635	2.05936135
H	-5.40328771	0.28642540	3.22908328
H	-5.08101445	-0.96045947	2.00787906
H	-5.31429512	3.25358642	0.87677497
H	-5.58164907	2.75089225	2.55967204
H	-6.80515322	2.40037194	1.32063643
H	-7.29507552	0.24995421	-0.08399840
H	-7.56221240	-0.33728801	-2.47950877
H	-5.62483686	-0.24375363	-4.02402652
H	-0.15940612	2.83220239	2.21009527
H	-2.07972205	0.49331037	-2.92525667
H	2.03715746	4.00311995	3.99536430
H	1.84904863	2.30229997	3.46986405

H	0.62733848	3.05770432	4.51300391
H	-0.99066757	4.77608077	3.55716175
H	-0.93579498	5.22134165	1.83601896
H	0.32571565	5.79740140	2.94022010
H	-2.98634733	-1.63458932	-3.95658206
H	-2.02574333	-0.62361083	-5.04747147
H	-3.79139133	-0.65753529	-5.20676580
H	-3.05309583	2.72498670	-3.63481793
H	-3.98762238	1.90632784	-4.90219271
H	-2.20796357	1.90926968	-4.95959137
O	1.43746069	0.53500254	1.54120949
O	0.00791149	0.57172072	2.01206612
Hf	0.14320036	0.08943432	-0.09008591

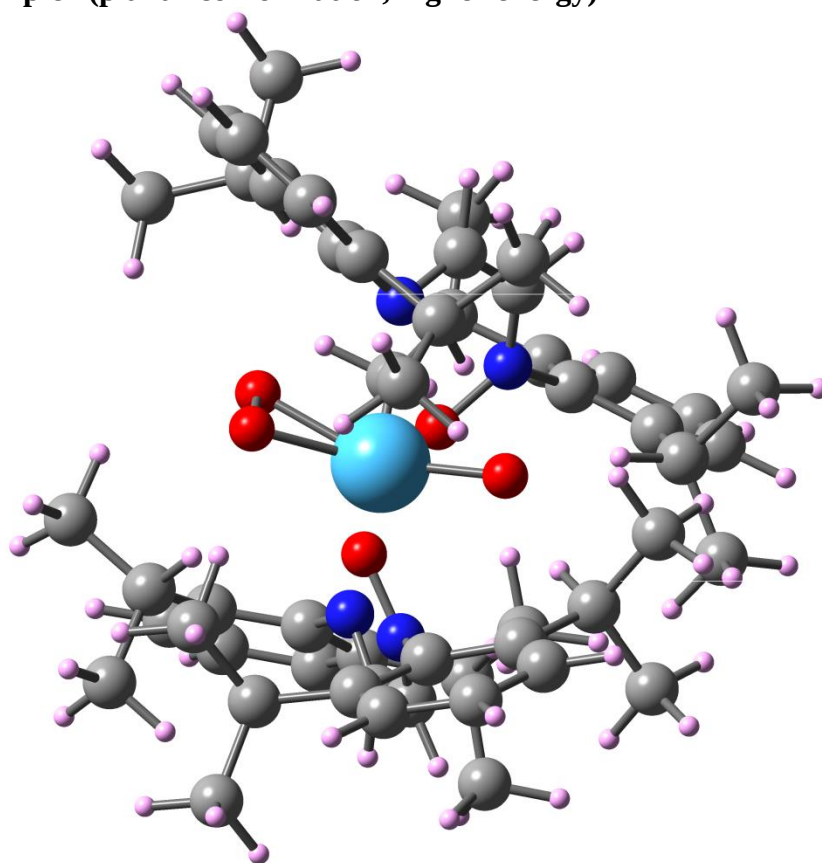
Oxo Peroxo Complex (planar conformation, higher energy)

Fig. S43: NCCNO Oxo Peroxo Complex (planar conformation, higher energy)

E	E_{zp}	H	G
-2668.5796	-2667.4283	-2667.3579	-2667.5355
O	-2.02249242	-0.00323589	-0.13033458
O	2.34787872	-0.28494163	0.30094402
O	0.39716084	-0.27277935	-1.52692391
N	0.15224900	-1.72886339	1.42933573
N	2.84568979	-1.48611670	0.05817589
N	-0.43212311	2.42181131	-0.68928163
N	-2.67022612	0.42325309	-1.24052745
C	1.02809456	-2.68382227	1.20814270
C	2.23272281	-2.61194872	0.42370119
C	-1.47160249	2.58453568	-1.48077145
C	-2.43385593	1.58098152	-1.84396779
C	-0.91187015	-2.04360855	2.39141046
C	-0.85684890	-1.40523996	3.66323782
C	-1.87830565	-1.70257335	4.58761216
C	-2.90733172	-2.60339563	4.27440988
C	-2.92475007	-3.23664832	3.02405764
C	-1.93237634	-2.97637015	2.05389092
C	-0.07654525	0.67454592	4.96293481

C	0.32778654	-0.52894659	4.08300455
C	1.39031683	-1.40820657	4.80256876
C	5.64633331	0.29717661	2.11592462
C	5.20960736	-1.15015049	1.76182399
C	6.03185338	-2.19390939	2.55999503
C	4.17112113	-1.52095152	-0.58209312
C	5.30582574	-1.38128927	0.25040329
C	6.56483547	-1.42006373	-0.38530782
C	6.66514239	-1.58063591	-1.77633891
C	5.50981479	-1.69048664	-2.56769932
C	4.22234258	-1.65206631	-1.99063960
C	-3.41567216	-3.70482022	0.09783908
C	-1.99452113	-3.72097384	0.71185102
C	-1.52129098	-5.19444163	0.86572291
C	3.05328145	-0.94980091	-4.15639402
C	2.95790279	-1.77243588	-2.84871958
C	2.67497340	-3.26403700	-3.17875943
C	0.31230078	3.64055521	-0.38310675
C	1.60199125	3.80670746	-0.95510390
C	2.28819019	5.01023322	-0.69696689
C	1.72650003	6.00984675	0.11067005
C	0.45776895	5.81691206	0.67488540
C	-0.28072775	4.63767301	0.44256724
C	3.67610620	2.42156148	-1.49248093
C	2.22404046	2.77269767	-1.89874660
C	2.16762056	3.27884011	-3.36642470
C	-5.72130640	-0.18445563	1.32351644
C	-5.29247344	0.60844770	0.06113033
C	-6.35233366	1.67951679	-0.30844162
C	-3.74744849	-0.44331560	-1.72813230
C	-5.01826877	-0.33254840	-1.11611224
C	-6.04926496	-1.14000463	-1.64109105
C	-5.80749916	-2.00712458	-2.71919549
C	-4.52584874	-2.10007007	-3.28633598
C	-3.45290671	-1.32498095	-2.79571277
C	-1.51215398	4.59739157	2.66517428
C	-1.64512480	4.47986791	1.12533499
C	-2.67632099	5.50154962	0.57552091
C	-1.60314692	-2.89863101	-3.58246287
C	-2.05290310	-1.42662338	-3.41171990
C	-2.00500459	-0.68935183	-4.77767050
H	0.87982274	-3.65244058	1.68971487
H	2.76556323	-3.52824802	0.20731090
H	-1.66381770	3.56491497	-1.91988703
H	-3.10689770	1.80793686	-2.66249649
H	-1.86158659	-1.22730411	5.56336234
H	-3.68574411	-2.81686726	5.00335792
H	-3.72076148	-3.93940445	2.79392424
H	0.79307429	-0.09764310	3.19277516
H	4.16311156	-1.24615467	2.07435054
H	-0.49504310	0.37067925	5.93312886
H	-0.79916155	1.29927088	4.42860371

H	0.80939074	1.29103697	5.16051125
H	0.98610042	-1.83851830	5.72947452
H	2.26709846	-0.80014764	5.06199643
H	1.72941049	-2.24079899	4.16916306
H	6.69242296	0.47613586	1.83428847
H	5.54982810	0.46732609	3.19585522
H	5.01819023	1.03144538	1.59972680
H	5.72035574	-3.21973147	2.32291091
H	5.89515865	-2.03510013	3.63734614
H	7.10523276	-2.11167800	2.34645756
H	7.46735002	-1.31648254	0.21081154
H	7.64535186	-1.60894015	-2.24645448
H	5.60640371	-1.79236323	-3.64443400
H	-1.33112748	-3.21764055	-0.00154760
H	2.09491133	-1.36394600	-2.30019580
H	-4.12166191	-4.29765764	0.69361521
H	-3.39530242	-4.13722898	-0.91036786
H	-3.80049858	-2.68467710	0.02225325
H	-2.16886628	-5.73594075	1.56775770
H	-0.49413282	-5.26905939	1.24527778
H	-1.56403188	-5.71192451	-0.10211342
H	3.29220659	0.09906583	-3.94587122
H	2.08191301	-0.97246040	-4.66535798
H	3.80638622	-1.34631245	-4.85181718
H	3.50175833	-3.71058407	-3.74901539
H	1.76103277	-3.34633178	-3.78054304
H	2.52982187	-3.86417033	-2.27070805
H	3.27151542	5.16569689	-1.13325074
H	2.27429299	6.93002275	0.30147657
H	0.03538634	6.58771207	1.31466449
H	1.64025867	1.84655211	-1.85675085
H	-4.36530460	1.13090886	0.32054041
H	4.35121949	3.28235912	-1.59219238
H	4.06338590	1.61975013	-2.13485849
H	3.70996993	2.06990504	-0.45574207
H	1.13468680	3.48435398	-3.67804934
H	2.58041170	2.52200153	-4.04701509
H	2.74739535	4.20389147	-3.49091396
H	-6.65604891	-0.73571617	1.15442399
H	-5.88307832	0.50514793	2.16192418
H	-4.94579320	-0.89971923	1.61990372
H	-6.04341797	2.26695496	-1.18306704
H	-6.49873525	2.37079361	0.53147837
H	-7.32320431	1.22129609	-0.53842278
H	-7.04361568	-1.08702097	-1.20560211
H	-6.61796344	-2.61517255	-3.11446232
H	-4.35373006	-2.78492282	-4.11178846
H	-2.01458270	3.46810788	0.93660010
H	-1.31382794	-0.95257051	-2.74868029
H	-1.14886727	5.58768798	2.97153051
H	-0.82220527	3.82941465	3.02623077
H	-2.49041947	4.43712552	3.14043840

H	-3.65083533	5.35883549	1.06262365
H	-2.81759616	5.39603443	-0.50952573
H	-2.35550705	6.53440265	0.76690339
H	-1.63963609	-3.43587158	-2.62672567
H	-0.56632629	-2.91934589	-3.93916501
H	-2.21911100	-3.44563765	-4.30968865
H	-2.27135946	0.37067051	-4.67462696
H	-2.69521030	-1.14149215	-5.50403729
H	-0.98949620	-0.73692097	-5.19091714
O	1.00909304	1.58728742	1.63519635
O	-0.51107991	1.63793975	1.80557623
Hf	0.13413694	0.33099012	0.24225537

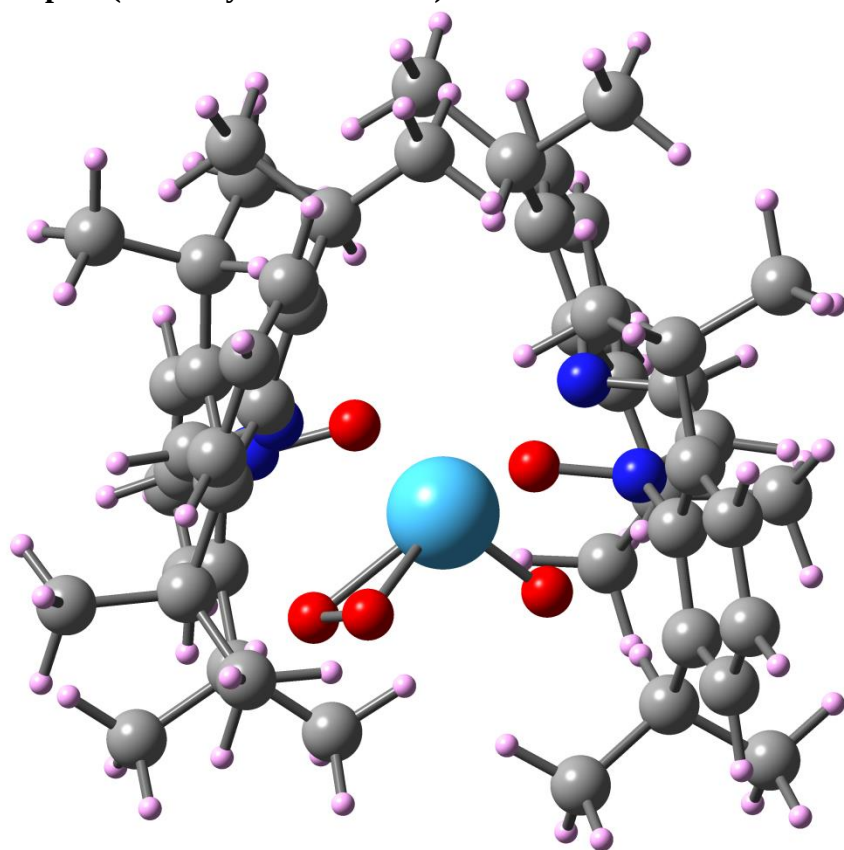
Oxo Peroxo Complex (butterfly conformation)

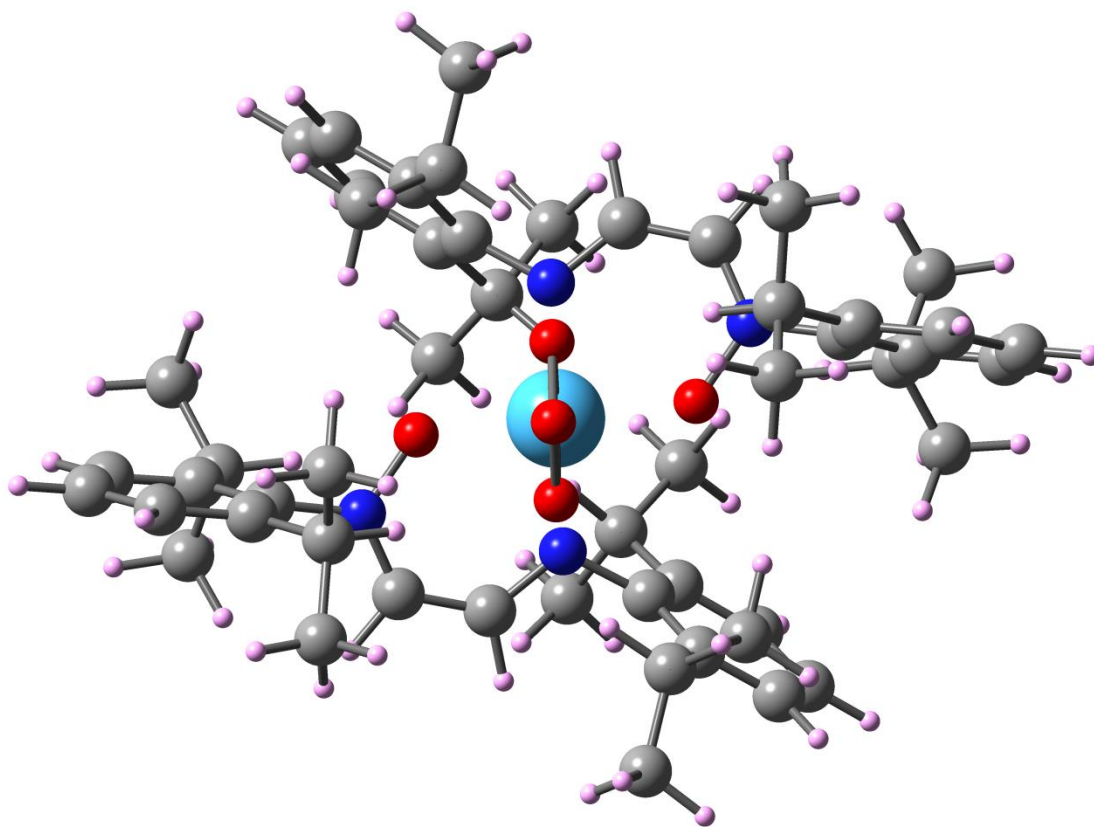
Fig. S44: NCCNO Oxo Peroxo Complex (butterfly conformation)

E	E_{zp}	H	G
-2668.5918	-2667.4397	-2667.3697	-2667.5462
O	-2.03614177	0.46536915	-0.00428011
O	-0.94416007	-1.37365069	1.92429774
N	0.17231170	2.14827633	-0.74922559
N	-2.68866534	1.64234559	0.10142793
N	2.66444629	-1.38599616	0.28645245
N	-0.20623184	-2.31747031	-0.50268406
C	-0.80200382	3.02141093	-0.71864385
C	-2.14789837	2.79815659	-0.22719717
C	2.10134247	-2.58113196	0.37608342
C	0.79307264	-3.03907860	-0.05191304
C	1.45087617	2.67925846	-1.23629923
C	2.22745979	3.53397233	-0.40343198
C	3.43634765	4.03370465	-0.93785607
C	3.85716115	3.71414993	-2.23481068
C	3.06420024	2.88005816	-3.03850592
C	1.85245674	2.34688235	-2.55810814
C	2.96984571	3.69951445	2.03096248
C	1.82128997	3.94005177	1.01871434

C	1.37607879	5.42732410	1.06428601
C	-3.04829310	0.64580909	3.97907527
C	-3.12884316	1.84845643	3.00166214
C	-3.28102295	3.18458325	3.77521368
C	-4.07189750	1.55657124	0.60101072
C	-4.27124008	1.66289251	1.99823323
C	-5.60788917	1.58563646	2.44759729
C	-6.66870693	1.40232805	1.54801863
C	-6.42185897	1.28012192	0.17050684
C	-5.10880781	1.34342493	-0.33805129
C	1.71101299	0.57986064	-4.41789196
C	0.93943853	1.54088648	-3.48556922
C	0.05458078	2.50716077	-4.32358768
C	-5.45786853	-0.12416268	-2.38974717
C	-4.85481172	1.19423009	-1.84120822
C	-5.39759307	2.42096023	-2.62250428
C	4.06773908	-1.14901703	0.63785795
C	4.44371029	-1.06693406	2.00246635
C	5.80999873	-0.82230071	2.27326228
C	6.74339459	-0.66645121	1.24109717
C	6.33610739	-0.75842167	-0.10099295
C	4.98962465	-1.00002406	-0.43274170
C	3.38953899	0.04345253	4.03839080
C	3.47465852	-1.24223298	3.17615065
C	3.87417782	-2.46449540	4.04512234
C	-1.91100465	-0.99336908	-4.10788568
C	-1.04575654	-1.91685988	-3.21925167
C	-0.16525673	-2.85363970	-4.09406655
C	-1.40745301	-3.01069422	-0.91823413
C	-1.87073926	-2.75795990	-2.24377452
C	-3.04309201	-3.39542221	-2.69132503
C	-3.75633993	-4.26718643	-1.85489611
C	-3.28929535	-4.51196664	-0.55733046
C	-2.11703795	-3.90510058	-0.05460776
C	5.32734373	-0.24553974	-2.86534746
C	4.55712221	-1.16943970	-1.89315698
C	4.71284888	-2.65427350	-2.32889884
C	-2.84804798	-3.91886073	2.38848383
C	-1.70885979	-4.23837571	1.38762484
C	-1.27336200	-5.72369204	1.51463725
H	-0.62187753	4.04910551	-1.04325962
H	-2.79387093	3.66104790	-0.11671795
H	2.76512345	-3.35518245	0.74852531
H	0.69672535	-4.12581301	0.02350222
H	4.05355091	4.68151932	-0.32123561
H	4.79044192	4.11736149	-2.62111454
H	3.38817393	2.65193310	-4.04989780
H	0.99471111	3.30407956	1.35667012
H	-2.16238764	1.87966309	2.48551616
H	3.82281501	4.37257988	1.86444409
H	3.32967509	2.66667569	1.97100476
H	2.60082663	3.86915008	3.05044174

H	2.19285765	6.10136478	0.76937200
H	1.06823179	5.69491226	2.08383329
H	0.52787868	5.62414846	0.39345952
H	-3.97623547	0.52324172	4.55564475
H	-2.22252659	0.80734064	4.68252413
H	-2.83392840	-0.28329439	3.44000416
H	-3.32331535	4.04617906	3.09422358
H	-2.41857720	3.32109202	4.43877514
H	-4.18992116	3.19850798	4.39243957
H	-5.81122896	1.66436357	3.51168006
H	-7.68901644	1.34612194	1.91982227
H	-7.25258666	1.12479834	-0.51233987
H	0.27145171	0.93465764	-2.86078777
H	-3.77276098	1.14093309	-2.01193310
H	2.35075103	1.12213537	-5.12569708
H	1.00777837	-0.01652943	-5.01114458
H	2.34169396	-0.10682496	-3.84219320
H	0.67977136	3.14977672	-4.95754920
H	-0.54888342	3.16043960	-3.68019630
H	-0.62872519	1.94516323	-4.97388413
H	-5.04231978	-0.99368494	-1.86848291
H	-5.22969443	-0.22576116	-3.45874745
H	-6.54957056	-0.14484145	-2.27912382
H	-6.48556186	2.51151559	-2.50923458
H	-5.17731498	2.31955608	-3.69325380
H	-4.94677102	3.35765880	-2.26836217
H	6.13660958	-0.75175598	3.30708772
H	7.78748686	-0.47524258	1.47797585
H	7.07049550	-0.63887978	-0.89128706
H	2.46339098	-1.42711495	2.80729892
H	-0.36997429	-1.28728996	-2.62904496
H	4.36520962	0.32157712	4.46095493
H	2.68980024	-0.11826491	4.86772368
H	3.00881715	0.88430766	3.44918517
H	3.92366660	-3.38639010	3.44953315
H	3.12789288	-2.61284619	4.83544296
H	4.85209687	-2.32263581	4.52499526
H	-2.56136976	-1.56461889	-4.78314392
H	-1.27192362	-0.35973936	-4.73514874
H	-2.54606836	-0.34199728	-3.49513432
H	0.48626124	-3.47811593	-3.46941580
H	0.47007834	-2.27310833	-4.77560366
H	-0.79281674	-3.52313320	-4.69755798
H	-3.39516494	-3.21986870	-3.70411242
H	-4.66065336	-4.75432132	-2.21238809
H	-3.84620032	-5.18647299	0.08803132
H	3.49638477	-0.90274051	-1.96189527
H	-0.87811402	-3.59761950	1.68576274
H	6.38888954	-0.51742534	-2.93403289
H	5.25502413	0.80289658	-2.55543254
H	4.90458075	-0.33338981	-3.87462277
H	4.36821805	-2.78842353	-3.36295143

H	4.13059413	-3.32857603	-1.68847468
H	5.76480504	-2.96526501	-2.27673402
H	-3.12252208	-2.86194046	2.31739992
H	-2.50250645	-4.10565770	3.41388667
H	-3.74169745	-4.53434036	2.21536195
H	-0.44177313	-5.96827565	0.83834114
H	-2.10023755	-6.40632895	1.27546649
H	-0.94971252	-5.93465702	2.54268271
O	0.02707225	1.55335295	1.91523753
O	0.54625592	-1.46915651	2.14081226
O	1.93888273	-0.27031725	-0.09293121
Hf	-0.00863803	0.09225455	0.81561816

η^2 -ozone ComplexFig. S45: NCCNO η^2 -ozone Complex

E	E_{zp}	H	G
-2668.5571	-2667.4065	-2667.3362	-2667.5148
O	-2.04328018	0.20679204	-0.13234806
O	2.04606913	-0.20266206	-0.13137006
O	0.01235699	1.18630507	-2.16545722
N	-0.04854107	-1.96562716	0.59720599
N	2.85535316	-1.32880916	-0.17780507
N	0.04704001	1.95059413	0.65461400
N	-2.85656122	1.33072014	-0.13706406
C	1.03155200	-2.81161425	0.57739099
C	2.35372911	-2.52660225	0.20640396
C	-1.03566206	2.79355022	0.66382300
C	-2.35816917	2.51659222	0.28741297
C	-1.28049417	-2.65123720	1.02650502
C	-1.67881520	-2.56034218	2.38964513
C	-2.82540030	-3.26772521	2.80708816
C	-3.56746737	-4.04641226	1.90799809
C	-3.15587234	-4.13516628	0.57225499
C	-2.00957324	-3.45570624	0.10450695
C	-1.74994418	-0.87750305	4.31556328

C	-0.86416313	-1.79086514	3.43248321
C	-0.04684608	-2.77685822	4.31218927
C	5.62129243	0.55071893	2.34516513
C	4.96836934	-0.71998616	1.74722308
C	5.44164136	-1.98840426	2.50849614
C	4.20504427	-1.14622117	-0.68253111
C	5.23798036	-0.85688117	0.24621497
C	6.54884246	-0.73220118	-0.25727607
C	6.81019946	-0.87197520	-1.63006718
C	5.76502237	-1.13983020	-2.52734524
C	4.43488329	-1.27987319	-2.07638521
C	-2.72731629	-3.16589321	-2.31888323
C	-1.60589521	-3.64261826	-1.36157816
C	-1.22091821	-5.11736138	-1.65377018
C	3.28062121	-0.57517111	-4.24066038
C	3.31376119	-1.59158419	-3.07148629
C	3.44841618	-3.04200530	-3.61018133
C	1.27819212	2.62701116	1.10057303
C	2.00130319	3.46237322	0.20132796
C	3.14841628	4.12917625	0.68517500
C	3.56683531	3.99842923	2.01544110
C	2.83018224	3.19039018	2.89284017
C	1.68294914	2.49431615	2.45851213
C	2.70873524	3.24706619	-2.23291422
C	1.59165815	3.69546024	-1.25630715
C	1.20702515	5.17886636	-1.50153017
C	-5.61785347	-0.63530096	2.32419813
C	-4.96842739	0.65688612	1.77036508
C	-5.44793344	1.89766922	2.57261614
C	-4.20634933	1.15986515	-0.64568910
C	-5.23854941	0.84227214	0.27452197
C	-6.54984250	0.73300215	-0.23160407
C	-6.81233352	0.91426117	-1.59924418
C	-5.76745844	1.20646218	-2.48915824
C	-4.43689334	1.33189917	-2.03512321
C	1.77201112	0.75016401	4.32701428
C	0.87670507	1.68965610	3.48098221
C	0.06497202	2.64517519	4.39857628
C	-3.28465527	0.69134310	-4.22132538
C	-3.31542325	1.67105217	-3.02070028
C	-3.44706123	3.13757229	-3.51336632
H	0.85421397	-3.85052532	0.85180301
H	3.06922415	-3.33985232	0.19324596
H	-0.86069403	3.82377229	0.97050702
H	-3.07733021	3.32654130	0.30633297
H	-3.13541732	-3.21470420	3.84758824
H	-4.44964245	-4.58418629	2.24760912
H	-3.72536839	-4.74600631	-0.12364406
H	-0.14838006	-1.15362810	2.90286517
H	3.88606526	-0.62448313	1.89111609
H	-2.44884524	-1.46092508	4.92847032
H	-2.33700321	-0.18246999	3.70184823

H	-1.12918612	-0.28852802	5.00178233
H	-0.71345615	-3.45568326	4.86059132
H	0.56342598	-2.23237319	5.04502733
H	0.62547596	-3.39024128	3.69892623
H	6.71734552	0.50692491	2.29653012
H	5.34121939	0.65239394	3.40190521
H	5.28645140	1.45079001	1.81834109
H	4.94312430	-2.89232532	2.13527411
H	5.22095334	-1.89619725	3.58031722
H	6.52444041	-2.13254529	2.39638813
H	7.36679253	-0.51835718	0.42531298
H	7.82797955	-0.76963221	-1.99966421
H	5.97917638	-1.23800521	-3.58804233
H	-0.73485114	-3.02314723	-1.58211517
H	2.34627412	-1.51842017	-2.56687925
H	-3.63708437	-3.77435924	-2.21985723
H	-2.38342327	-3.23299222	-3.35894331
H	-2.98648829	-2.12145412	-2.11391121
H	-2.06948729	-5.79693642	-1.49669517
H	-0.39943215	-5.45507844	-1.00729713
H	-0.89589419	-5.22035339	-2.69755926
H	3.18460822	0.45058997	-3.86784735
H	2.41044514	-0.77675512	-4.87582542
H	4.18388628	-0.63773014	-4.86355242
H	4.38847325	-3.17882533	-4.16222837
H	2.61740912	-3.26495131	-4.29111638
H	3.42576417	-3.77810836	-2.79544827
H	3.71275534	4.76375029	0.00647695
H	4.44971639	4.52684226	2.36770213
H	3.14475626	3.10461417	3.92989925
H	0.72022408	3.08306921	-1.49303217
H	-3.88597531	0.56098510	1.91355109
H	3.62023231	3.84987922	-2.11656621
H	2.36160121	3.34853320	-3.26907230
H	2.96640824	2.19593610	-2.06359221
H	0.38896910	5.49715639	-0.84098812
H	0.87717513	5.31393136	-2.54015725
H	2.05698723	5.85263338	-1.32796116
H	-6.71406658	-0.59050194	2.27910512
H	-5.33519445	-0.77463698	3.37586320
H	-5.28315346	-1.51538604	1.76458508
H	-4.95460536	2.81587829	2.22858612
H	-5.22562040	1.77242821	3.64079523
H	-6.53163251	2.03881026	2.46629513
H	-7.36707157	0.49797915	0.44478798
H	-7.83052262	0.82396019	-1.97090520
H	-5.98282247	1.33791419	-3.54590932
H	0.15779700	1.06964307	2.93534017
H	-2.34888818	1.57844015	-2.51721825
H	2.47708518	1.31502504	4.94996133
H	2.35338615	0.07554295	3.68624223
H	1.15869306	0.13968998	5.00114433

H	-0.53934904	2.07627215	5.11748734
H	-0.61201002	3.27801825	3.81078424
H	0.73577909	3.30576423	4.96367232
H	-3.18858428	-0.34546898	-3.88082235
H	-2.41546320	0.91249710	-4.85138543
H	-4.18818633	0.77322912	-4.84127043
H	-3.41306322	3.84797134	-2.67651726
H	-4.39131231	3.29541231	-4.05247836
H	-2.62093717	3.37665529	-4.19482438
O	0.00100197	0.04809099	-3.15957830
O	-0.00599405	-1.11832810	-2.19907122
Hf	0.00177397	0.00876699	-0.45137609

6.5 Six Oxygen Atoms

Bisperoxo Complex (spiro conformation)

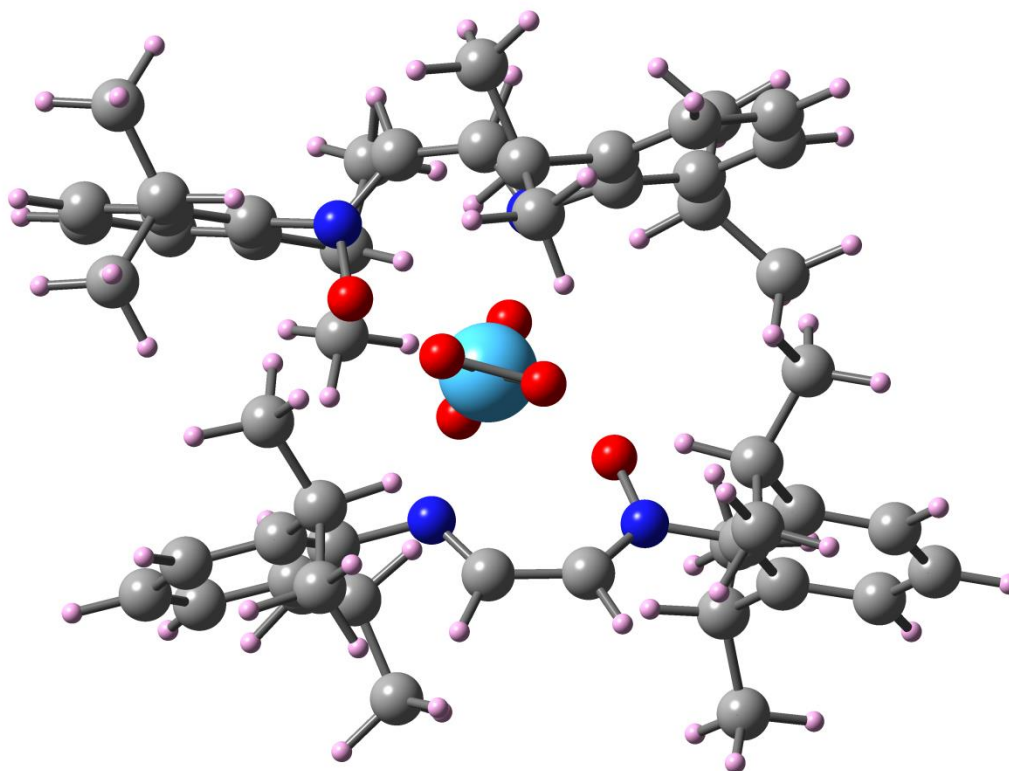


Fig. S46: NCCNO Bisperoxo Complex (spiro conformation)

E	E_{zp}	H	G
-2743.7624	-2742.6075	-2742.5361	-2742.7164
O	-2.19355503	0.55487654	0.12932926
O	1.94986692	-0.80273551	-0.73226315
O	-0.32774911	0.54345548	-2.00231952
O	-0.67695752	-0.93984897	-1.77246515
N	-0.08727763	-2.15654415	0.90570048
N	2.79689722	-1.52245416	0.03937946
N	0.05233494	2.40925105	-0.15416803
N	-2.80898604	1.45390670	-0.64496196
C	1.02947197	-2.64810115	1.39146217
C	2.38438360	-2.30125832	1.02911705
C	-0.94963549	3.09988049	-0.62443844
C	-2.26682052	2.60936805	-0.98814816
C	-1.32277482	-2.82870360	1.30597485
C	-1.78978253	-2.75043181	2.64923910
C	-3.00094557	-3.41107243	2.95609057
C	-3.71125475	-4.13174784	1.98763748
C	-3.20794242	-4.22591112	0.68021888

C	-2.00662542	-3.58829802	0.31295094
C	-1.95027937	-0.92947694	4.42774896
C	-1.05504968	-2.01239848	3.77621243
C	-0.53781765	-3.01287507	4.84542216
C	5.07103022	1.46677838	1.85423112
C	4.62878844	-0.01716236	1.81530425
C	5.16164998	-0.77401937	3.06253146
C	4.21186665	-1.42715863	-0.32555787
C	5.08699253	-0.70737820	0.52450062
C	6.44237475	-0.64886204	0.13251932
C	6.88226657	-1.25541006	-1.05359949
C	5.97807580	-1.94409353	-1.87923336
C	4.61593211	-2.05216904	-1.53264080
C	-2.46154399	-3.97977383	-2.18833745
C	-1.40208917	-3.80879380	-1.07724875
C	-0.45547722	-5.04274923	-1.05070259
C	3.29599944	-1.93822924	-3.69363015
C	3.63715920	-2.79788252	-2.44636732
C	4.17002976	-4.19340239	-2.85782466
C	1.26233722	3.18662845	0.14777239
C	2.18780505	3.43943625	-0.89933241
C	3.29890362	4.25764700	-0.59949096
C	3.48252845	4.79563424	0.68255373
C	2.56099461	4.50774384	1.70136581
C	1.43501632	3.69282810	1.46261438
C	3.27123375	2.13150709	-2.80434188
C	2.00985875	2.89049899	-2.32088417
C	1.64440675	4.02896111	-3.31116068
C	-5.16779758	0.18345158	2.28727013
C	-4.92657631	1.42923797	1.39532859
C	-5.78765242	2.63031321	1.86669092
C	-4.17672305	1.11084581	-1.06871927
C	-5.18770517	1.09683126	-0.07712576
C	-6.48857754	0.75995015	-0.50322343
C	-6.75257856	0.45411557	-1.84796866
C	-5.71947026	0.47190735	-2.79706231
C	-4.39333756	0.79279599	-2.43324178
C	1.12789184	2.91707921	3.87550749
C	0.43195972	3.41656009	2.58644850
C	-0.43461653	4.67354938	2.86912635
C	-3.24032483	-0.54622129	-4.27492827
C	-3.28433055	0.79044450	-3.49422630
C	-3.46478831	1.98576474	-4.46965712
H	0.97752886	-3.46400018	2.11643371
H	3.17502962	-2.81836439	1.55968731
H	-0.82772118	4.17430819	-0.78560177
H	-2.90473936	3.27029062	-1.56107171
H	-3.38708690	-3.35586820	3.97098479
H	-4.64295807	-4.62763654	2.25069912
H	-3.75016597	-4.80581845	-0.06031705
H	-0.20623422	-1.46875071	3.35554232
H	3.53428368	-0.01698819	1.86385078

H	-2.85124921	-1.35802302	4.88881910
H	-2.24875678	-0.19225698	3.67603972
H	-1.38753658	-0.40196521	5.20947458
H	-1.36552892	-3.53827988	5.34106773
H	0.03174875	-2.47871749	5.61775843
H	0.11892368	-3.77710090	4.40611039
H	6.16393354	1.56968552	1.89739852
H	4.65216490	1.95267818	2.74401315
H	4.70626961	2.01203836	0.97728778
H	4.82545644	-1.81957155	3.08292295
H	4.80240794	-0.28755101	3.97816440
H	6.25977341	-0.77788970	3.08682216
H	7.15248030	-0.11169102	0.75484008
H	7.92995370	-1.18923725	-1.33762712
H	6.33390347	-2.40583135	-2.79580173
H	-0.80554688	-2.93005951	-1.34228129
H	2.69487066	-2.94984305	-1.90832220
H	-3.00293717	-4.93277434	-2.10526062
H	-1.96999279	-3.96241643	-3.16918821
H	-3.19099683	-3.16252207	-2.16161169
H	-1.00927318	-5.95719891	-0.79621147
H	0.34940552	-4.92276305	-0.31351991
H	0.00766763	-5.18597221	-2.03646027
H	2.81652340	-1.00221870	-3.39222992
H	2.59813835	-2.48110189	-4.34406885
H	4.19947754	-1.70717555	-4.27478305
H	5.06314018	-4.11918172	-3.49154904
H	3.40317030	-4.72719162	-3.43374577
H	4.42636194	-4.80350381	-1.98173215
H	4.02147574	4.47685628	-1.38150244
H	4.34128573	5.43061262	0.88828687
H	2.71558289	4.91950875	2.69521444
H	1.19219405	2.16275057	-2.33049364
H	-3.87429269	1.70506355	1.52068970
H	4.14697643	2.79039370	-2.87839208
H	3.08782606	1.70437904	-3.79890129
H	3.51260849	1.30798667	-2.12316008
H	0.72076111	4.54413692	-3.01303820
H	1.49335101	3.61985200	-4.31871168
H	2.44217023	4.78234486	-3.36495559
H	-6.21132290	-0.15352338	2.22685163
H	-4.94925437	0.42301254	3.33583065
H	-4.51895437	-0.64516079	1.98421321
H	-5.60509405	3.52260403	1.25329872
H	-5.54738886	2.87742654	2.90886596
H	-6.86038927	2.40316851	1.81708950
H	-7.29761356	0.73786949	0.22180515
H	-7.76354603	0.19689187	-2.15504306
H	-5.93735206	0.22093995	-3.83118416
H	-0.22265806	2.59736186	2.27405360
H	-2.30553804	0.87839356	-3.01115204
H	1.81085281	3.66541154	4.30149691

H	1.68285071	1.99854539	3.65928543
H	0.37132138	2.68356649	4.63640079
H	-1.17368242	4.45682074	3.65207380
H	-0.97681863	5.00388650	1.97153180
H	0.18317572	5.51566733	3.21070870
H	-3.04534325	-1.37827241	-3.59283553
H	-2.41545084	-0.51567538	-4.99759290
H	-4.16977961	-0.74115539	-4.82771545
H	-3.46413943	2.95182647	-3.94502153
H	-4.41055877	1.91177171	-5.02383305
H	-2.64439772	1.99787818	-5.19821568
O	1.24496848	0.27083874	1.64054315
O	-0.22762488	0.32558794	2.00381410
Hf	0.00247560	0.01005198	-0.04788509

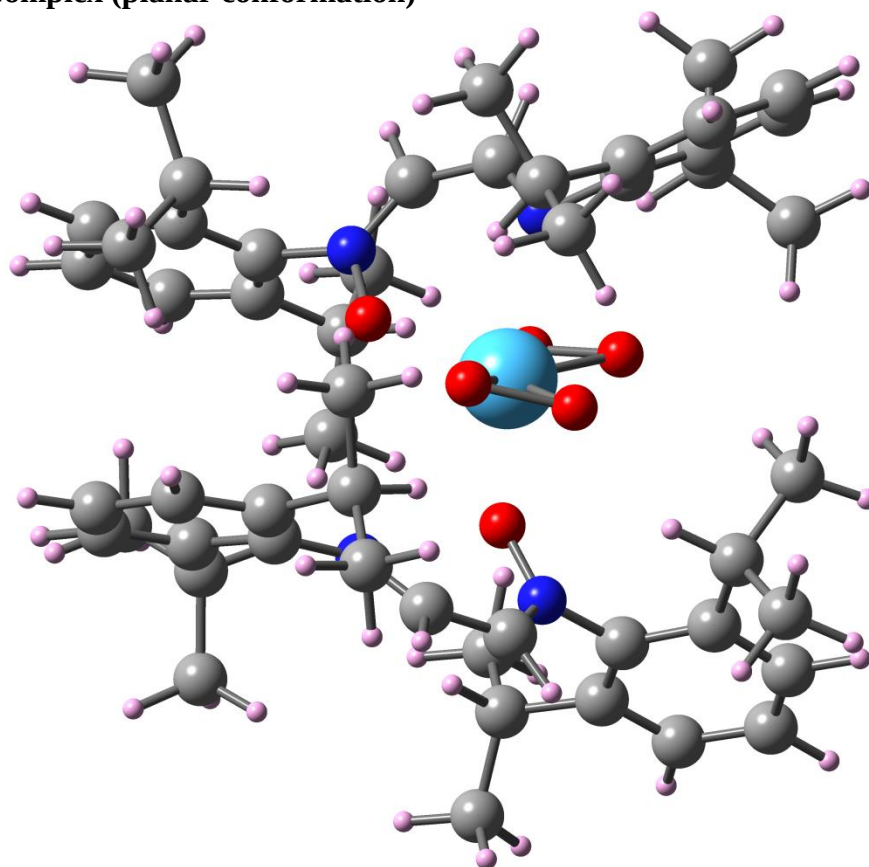
Bisperoxo Complex (planar conformation)

Fig. S47: NCCNO Bisperoxo Complex (planar conformation)

E	E_{zp}	H	G
-2743.7561	-2742.6021	-2742.5312	-2742.7114
O	-1.29956511	1.09075507	-0.41561245
O	0.61130209	-1.85266095	-0.52788839
O	2.29222051	0.58298925	-1.26167382
N	-1.41983525	-2.30522110	1.46651765
N	1.17684976	-2.91697226	0.10542981
N	1.16961578	2.58800643	0.01886301
N	-1.53970097	2.06721275	-1.33431535
C	-0.47042141	-3.03770965	1.97403654
C	0.72131883	-3.41383830	1.23934813
C	0.56372831	3.32663662	-0.88345918
C	-0.67866710	3.04268135	-1.56871592
C	-2.63442104	-2.02390815	2.13487569
C	-2.72471532	-1.63929404	3.51245423
C	-4.01326823	-1.44423417	4.05181526
C	-5.17118301	-1.60352470	3.27581015
C	-5.06313846	-1.91898536	1.91006484
C	-3.80652645	-2.11215871	1.31134111
C	-1.58581152	0.06581094	5.02161507

C	-1.50261264	-1.34891865	4.39404594
C	-1.33211677	-2.42287922	5.50185263
C	4.81526444	-1.14674189	0.56770466
C	3.94791938	-2.34090077	1.04805421
C	4.63864406	-3.10048046	2.21022093
C	2.31915466	-3.52808237	-0.59278817
C	3.63003768	-3.27586092	-0.12286401
C	4.68346831	-3.91273425	-0.81573407
C	4.43443369	-4.73083497	-1.92666250
C	3.12036851	-4.92955027	-2.38184717
C	2.02792123	-4.32943306	-1.72522396
C	-4.76218446	-1.85268041	-1.06388706
C	-3.68084586	-2.49445391	-0.16539923
C	-3.69135257	-4.04061592	-0.32735316
C	0.42616066	-3.64059790	-3.54557197
C	0.60673635	-4.50456220	-2.26786786
C	0.25210345	-5.98814557	-2.53643964
C	2.38096124	3.14672845	0.60915946
C	3.48718555	3.51570264	-0.21810614
C	4.61816863	4.06935978	0.41917279
C	4.66361374	4.25845663	1.80708422
C	3.56432098	3.88946282	2.59574951
C	2.40706768	3.32735895	2.02094984
C	4.76032325	2.46100153	-2.16207109
C	3.54278757	3.32307978	-1.74186938
C	3.56927764	4.69000139	-2.47905823
C	-4.70894618	2.13637594	1.09991278
C	-3.89325047	3.01226173	0.11389098
C	-4.35750827	4.49169193	0.16645261
C	-2.83298385	1.99322283	-2.01684858
C	-3.97090961	2.45583713	-1.31098927
C	-5.20868411	2.38848361	-1.98235645
C	-5.29422025	1.88235723	-3.28994088
C	-4.14529453	1.42110260	-3.95051952
C	-2.87962446	1.45447542	-3.32533865
C	1.55607338	2.36228073	4.23551417
C	1.18601211	3.03753819	2.89568247
C	0.38460755	4.34813508	3.13268555
C	-1.83231495	-0.56975813	-4.44758562
C	-1.64526168	0.91932196	-4.05899383
C	-1.32279344	1.77765101	-5.31074297
H	-0.53888147	-3.50236244	2.96304684
H	1.31022521	-4.23544261	1.63451616
H	0.98709536	4.29467214	-1.15486692
H	-0.99366389	3.75720265	-2.32060769
H	-4.11031900	-1.15241674	5.09430650
H	-6.15100320	-1.46233644	3.72651095
H	-5.96346389	-2.00689948	1.30925005
H	-0.60799260	-1.32944750	3.76488186
H	3.02316074	-1.90455046	1.43833456
H	-2.45037429	0.17720520	5.68941226
H	-1.64468539	0.82379840	4.23320310

H	-0.67956981	0.26055950	5.60913808
H	-2.19172972	-2.42439787	6.18578179
H	-0.43039825	-2.21742327	6.09377109
H	-1.24471620	-3.43666901	5.08684975
H	5.80306450	-1.47673448	0.21680205
H	4.96268139	-0.44260874	1.39577249
H	4.31610648	-0.61027796	-0.24698172
H	4.01911485	-3.92893307	2.58156775
H	4.82051383	-2.41291816	3.04577420
H	5.60601038	-3.51966031	1.90217977
H	5.70621834	-3.74877891	-0.48820858
H	5.26390100	-5.20445068	-2.44651788
H	2.94301458	-5.55287638	-3.25378707
H	-2.69998314	-2.13882621	-0.50097174
H	-0.10615760	-4.12478117	-1.52686733
H	-5.76593451	-2.24476874	-0.84967489
H	-4.54566429	-2.07289810	-2.11772549
H	-4.78623401	-0.76239918	-0.94696678
H	-4.64691685	-4.46331073	0.01250360
H	-2.88787197	-4.50722061	0.25599382
H	-3.55273761	-4.31701124	-1.38168800
H	0.62975919	-2.58668760	-3.32792258
H	-0.60251613	-3.72763402	-3.92058565
H	1.10792283	-3.97007349	-4.34127194
H	0.87323551	-6.41881705	-3.33218330
H	-0.79476743	-6.06956441	-2.85678946
H	0.38274797	-6.60336365	-1.63657314
H	5.47840357	4.34736644	-0.18415060
H	5.54823517	4.69006669	2.26993089
H	3.60143672	4.04404498	3.66995705
H	2.66497083	2.75994988	-2.06843810
H	-2.85232680	2.97716002	0.45299354
H	5.71597754	2.93385946	-1.89801793
H	4.74847203	2.30854349	-3.24972613
H	4.70159569	1.47802492	-1.68613932
H	2.70332991	5.31743034	-2.22306700
H	3.56634086	4.53315670	-3.56614040
H	4.47115863	5.26305972	-2.22521514
H	-5.77608487	2.12647123	0.84030395
H	-4.61456072	2.53164998	2.11947396
H	-4.34488070	1.10333334	1.10294760
H	-3.76849689	5.12348891	-0.51144358
H	-4.24412155	4.88556823	1.18462062
H	-5.41391480	4.59229838	-0.11509796
H	-6.10780360	2.73506704	-1.47995802
H	-6.25817535	1.84306870	-3.79167155
H	-4.22889561	1.02248470	-4.95775868
H	0.53896228	2.32853486	2.37188181
H	-0.77100851	0.96175339	-3.40148701
H	2.17748292	3.00392569	4.87552952
H	2.08476302	1.42197467	4.04564332
H	0.64040446	2.12833315	4.79167603

H	-0.51861305	4.13983374	3.72238964
H	0.07377038	4.80713586	2.18360976
H	0.98620378	5.08719560	3.68020991
H	-2.02669573	-1.18414161	-3.56019038
H	-0.91741572	-0.94401111	-4.92224806
H	-2.66349764	-0.70731955	-5.15249123
H	-1.15812325	2.83096127	-5.04697896
H	-2.13639623	1.73975920	-6.04766234
H	-0.41002424	1.40448424	-5.79112028
O	1.63936941	-0.17343682	1.69303158
O	0.12758986	0.16768058	1.93255248
O	1.00491682	0.65644914	-2.09197327
Hf	0.67838263	0.23814452	-0.05044558

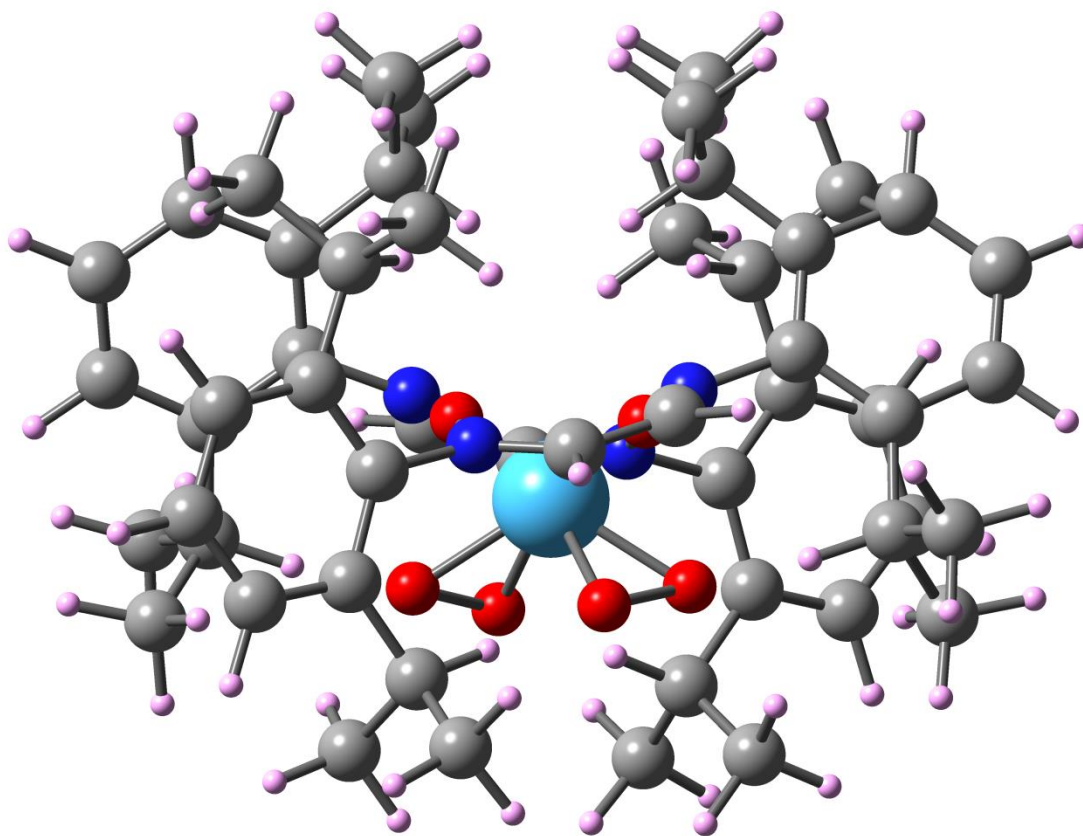
Bisperoxo Complex (butterfly conformation)

Fig. S48: NCCNO Bisperoxo Complex (butterfly conformation)

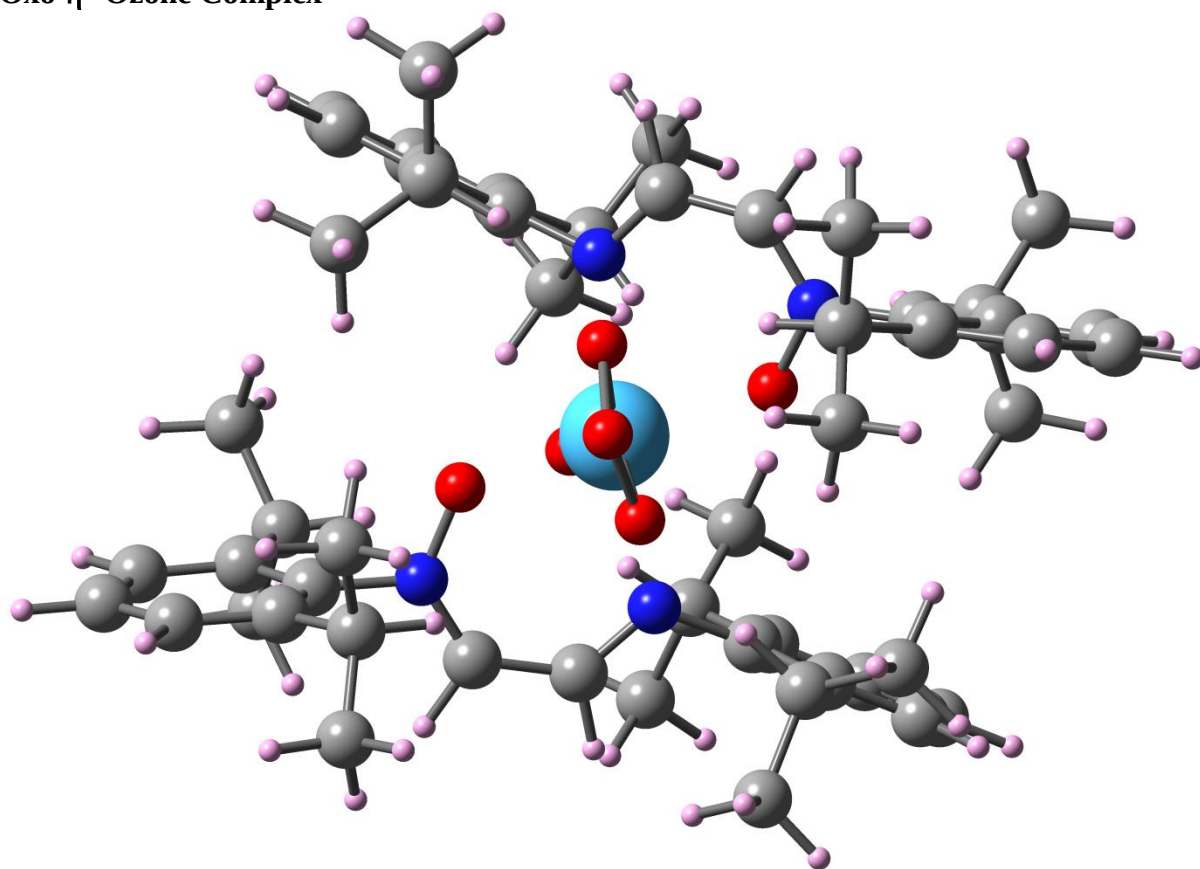
E	E_{zp}	H	G
-2743.7533	-2742.5985	-2742.5274	-2742.7052

O	1.90729392	0.46104634	0.17124284
O	1.03608842	-1.40161150	-1.88054160
N	-0.32450813	2.23980992	0.50106481
N	2.59337475	1.60117246	-0.17333990
N	-2.59340886	-1.60173692	-0.17106272
N	0.32436810	-2.23901356	0.50419522
C	0.62753471	3.08555950	0.17821280
C	1.97751301	2.76848305	-0.24092361
C	-1.97757997	-2.76916569	-0.23681230
C	-0.62757792	-3.08545087	0.18281469
C	-1.57226294	2.81691421	0.98237222
C	-2.35013035	3.70214112	0.17614844
C	-3.56086767	4.18773217	0.71976765
C	-3.98818953	3.83823788	2.00569242
C	-3.18960108	2.99710992	2.79637415
C	-1.97530731	2.48032766	2.30761649
C	-3.08315895	3.85932347	-2.26269623
C	-1.96588049	4.16820418	-1.23516027

C	-1.62559155	5.68384468	-1.24404127
C	3.44000722	0.20662318	-3.90268034
C	3.45222205	1.49838015	-3.04470365
C	3.80808421	2.73703986	-3.90975441
C	4.01456634	1.43146406	-0.49767015
C	4.41153595	1.37063221	-1.85705384
C	5.79171772	1.19308051	-2.10713499
C	6.71595579	1.08289481	-1.06087486
C	6.28507798	1.15065510	0.27495284
C	4.92309734	1.32145553	0.58774577
C	-1.78002770	0.86131246	4.29918862
C	-1.04076418	1.69470489	3.22986574
C	-0.04096400	2.67230185	3.91277016
C	5.22424106	0.50885289	3.00306571
C	4.46555698	1.45676912	2.04398491
C	4.61008039	2.93145289	2.51575137
C	-4.01471155	-1.43255108	-0.49524890
C	-4.41223758	-1.37409319	-1.85458972
C	-5.79255520	-1.19726863	-2.10441601
C	-6.71639094	-1.08531714	-1.05798411
C	-6.28495246	-1.15050752	0.27777841
C	-4.92282159	-1.32063771	0.59031273
C	-3.44221024	-0.21420007	-3.90333461
C	-3.45345362	-1.50400882	-3.04242404
C	-3.80917854	-2.74479166	-3.90449170
C	1.78090187	-0.85339037	4.29956287
C	1.04138958	-1.68857298	3.23180944
C	0.04146037	-2.66473537	3.91658537
C	1.57230516	-2.81509185	0.98629922
C	1.97567812	-2.47600621	2.31078749
C	3.19020427	-2.99172318	2.80012004
C	3.98865967	-3.83421675	2.01075541
C	3.56097927	-4.18615638	0.72561229
C	2.35000346	-3.70173449	0.18149328
C	-5.22245025	-0.50279693	3.00403356
C	-4.46466077	-1.45309749	2.04661264
C	-4.60958622	-2.92671735	2.52156338
C	3.08270055	-3.86412707	-2.25709544
C	1.96536745	-4.17039990	-1.22884691
C	1.62437769	-5.68589820	-1.23466830
H	0.44128693	4.16060778	0.23121216
H	2.59720291	3.59790410	-0.56307216
H	-2.59727881	-3.59913241	-0.55753287
H	-0.44117417	-4.16038133	0.23753958
H	-4.17745368	4.84907593	0.11677621
H	-4.92654641	4.22661497	2.39491065
H	-3.51103838	2.75455649	3.80478825
H	-1.09399942	3.60725911	-1.57570305
H	2.42802814	1.63744161	-2.69147244
H	-4.00545401	4.41935008	-2.05557452
H	-3.31072774	2.78929657	-2.26071570
H	-2.74448770	4.12900579	-3.27170064

H	-2.49329440	6.29190437	-0.95448674
H	-1.31818157	5.99477367	-2.25148187
H	-0.80970275	5.92784042	-0.54868044
H	4.43902223	-0.03869699	-4.28918738
H	2.76573262	0.34353324	-4.75737277
H	3.05964178	-0.64059948	-3.32273901
H	3.80890913	3.66147991	-3.31566211
H	3.06670865	2.85030178	-4.71034662
H	4.79727251	2.63783014	-4.37681770
H	6.13650792	1.13808523	-3.13582462
H	7.77164985	0.94472787	-1.28225990
H	7.01311078	1.06592186	1.07566461
H	-0.45576551	1.00727381	2.60697576
H	3.40446396	1.18643091	2.09396614
H	-2.30330900	1.49807279	5.02428737
H	-1.06446861	0.25395016	4.86555008
H	-2.51327773	0.18917823	3.84094884
H	-0.57879417	3.39377151	4.54233596
H	0.53642257	3.23821704	3.17135835
H	0.66694905	2.12381526	4.54774593
H	5.14097456	-0.53379300	2.67561967
H	4.80374845	0.58610928	4.01414080
H	6.28864135	0.76647794	3.07577929
H	5.66190938	3.24579061	2.49111020
H	4.24446468	3.04243124	3.54519234
H	4.03986826	3.61884664	1.87765901
H	-6.13778837	-1.14423929	-3.13305901
H	-7.77219242	-0.94769109	-1.27919162
H	-7.01266542	-1.06435382	1.07863079
H	-2.42904257	-1.64179003	-2.68937643
H	0.45641955	-1.00212286	2.60780369
H	-4.44146865	0.02973206	-4.29007862
H	-2.76814665	-0.35268452	-4.75794166
H	-3.06211223	0.63453509	-3.32543099
H	-3.80929739	-3.66787229	-3.30828980
H	-3.06812221	-2.85955875	-4.70516697
H	-4.79864342	-2.64709476	-4.37129956
H	2.30418013	-1.48892107	5.02573231
H	1.06553152	-0.24488621	4.86494980
H	2.51419470	-0.18220935	3.84000745
H	-0.53602963	-3.23195499	3.17625051
H	-0.66636304	-2.11492523	4.55052565
H	0.57917742	-3.38510294	4.54750805
H	3.51194832	-2.74721333	3.80795626
H	4.92720637	-4.22172000	2.40038429
H	4.17746702	-4.84851163	0.12363135
H	-3.40343015	-1.18309923	2.09551708
H	1.09370241	-3.60972527	-1.57040613
H	-6.28688200	-0.75992938	3.07798485
H	-5.13907618	0.53907408	2.67416077
H	-4.80135201	-0.57789699	4.01501884
H	-4.24361207	-3.03564843	3.55109375

H	-4.03989466	-3.61568830	1.88470673
H	-5.66154838	-3.24069300	2.49799986
H	3.31081760	-2.79422301	-2.25726065
H	2.74380155	-4.13562988	-3.26553278
H	4.00472762	-4.42421938	-2.04894014
H	0.80847344	-5.92812655	-0.53870900
H	2.49182868	-6.29380750	-0.94404453
H	1.31666905	-5.99867312	-2.24144555
O	0.46004092	1.53711154	-2.12397998
O	-1.03549876	1.39902464	-1.88213817
O	-0.46000082	-1.54017789	-2.12210966
O	-1.90724914	-0.46111261	0.17173415
Hf	0.00015486	-0.00071267	-0.79622984

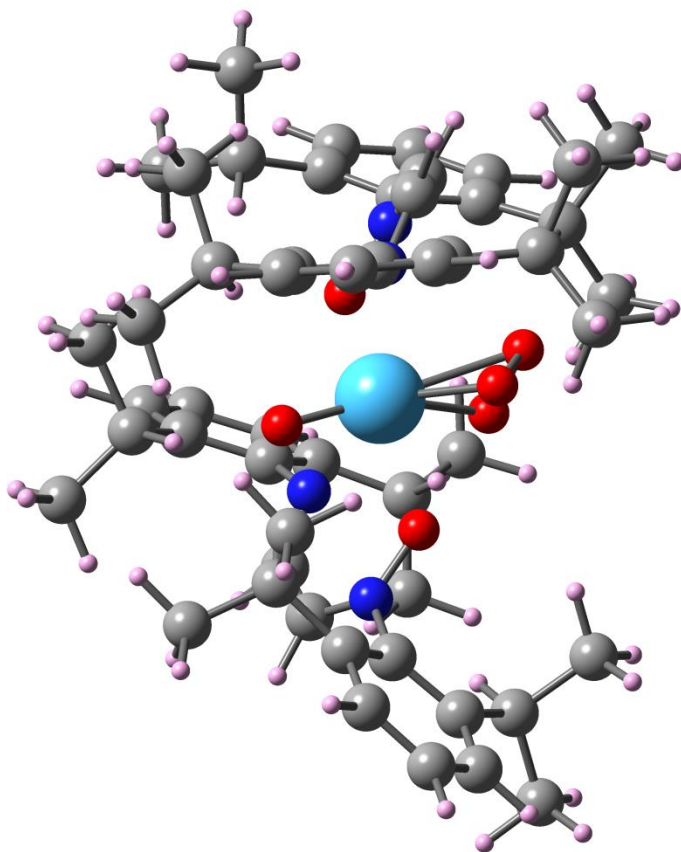
Oxo η^2 -Ozone ComplexFig. S49: NCCNO Oxo η^2 -Ozone Complex

E	E_{zp}	H	G
-2743.7441	-2742.5896	-2742.5178	-2742.7012
O	-2.05373302	0.49325983	0.04417604
O	2.11270342	-0.49535975	-0.53570924
O	0.02459470	0.95993893	-2.07098651
N	-0.20761761	-2.11929255	0.86437823
N	2.74938119	-1.58916055	-0.11629916
N	0.04552648	2.45676173	-0.04280077
N	-2.72524829	1.40242026	-0.70592278
C	0.86583931	-2.86030166	1.00461678
C	2.21242557	-2.61813720	0.53633955
C	-0.90748162	3.09869479	-0.67590981
C	-2.18453806	2.55669436	-1.07735806
C	-1.41746654	-2.62901857	1.52356204
C	-1.57733043	-2.44185317	2.92614882
C	-2.74101461	-2.97339829	3.52584700
C	-3.70494257	-3.65975690	2.77608736
C	-3.51554962	-3.84032025	1.39745822
C	-2.37289408	-3.33807539	0.74101009
C	-1.20456356	-0.60847387	4.65941064

C	-0.54834712	-1.72523230	3.80908070
C	0.18918556	-2.73838651	4.72576746
C	5.09366311	1.01203919	1.97580888
C	4.60426224	-0.45179113	1.83056641
C	5.06675292	-1.31195758	3.03642481
C	4.18179171	-1.59954301	-0.44687053
C	5.07695988	-1.06252662	0.50621190
C	6.44748798	-1.10217908	0.17314353
C	6.87637815	-1.62691277	-1.05743013
C	5.94637639	-2.11075493	-1.99244821
C	4.56357740	-2.10237093	-1.71170073
C	-3.43540736	-3.60180280	-1.58274494
C	-2.13933645	-3.65001760	-0.74015447
C	-1.46234474	-5.04200558	-0.88971793
C	3.56054422	-1.64233691	-3.99258340
C	3.54842760	-2.57944206	-2.75548264
C	3.80185055	-4.05211985	-3.16854068
C	1.20789028	3.23904001	0.37728760
C	2.15773394	3.68524353	-0.58438675
C	3.25149479	4.44777646	-0.11575541
C	3.39674285	4.76454009	1.24053732
C	2.44184893	4.31555701	2.16735079
C	1.33584043	3.54332338	1.76256793
C	3.30548006	2.55877982	-2.55570234
C	2.07224949	3.37280196	-2.08411863
C	1.91596357	4.67080709	-2.92018615
C	-5.06421133	0.17557142	2.28277167
C	-4.82149297	1.38333481	1.34109440
C	-5.67800738	2.60488359	1.76681415
C	-4.07737599	1.01653539	-1.11345586
C	-5.08585311	1.00061928	-0.11819158
C	-6.38095040	0.62358661	-0.52701305
C	-6.64583806	0.28335396	-1.86362276
C	-5.61967262	0.30827324	-2.82005137
C	-4.29971622	0.66821667	-2.47043093
C	0.84575832	2.71079426	4.13854009
C	0.26097672	3.13358316	2.77280945
C	-0.77514915	4.27872533	2.94564825
C	-3.07229589	-0.70246412	-4.23875074
C	-3.20211420	0.67529564	-3.54248541
C	-3.46352594	1.79532233	-4.58575388
H	0.78676667	-3.79335038	1.56671801
H	2.93054212	-3.39806047	0.76239272
H	-0.78010071	4.15699992	-0.91711199
H	-2.82917777	3.19026250	-1.67442748
H	-2.88699352	-2.84525814	4.59521620
H	-4.59255244	-4.05891366	3.26185067
H	-4.25843085	-4.38655906	0.82393612
H	0.18245890	-1.21741863	3.16899996
H	3.50870073	-0.41386678	1.84427259
H	-1.93621724	-1.00245295	5.37872303
H	-1.70961785	0.11852372	4.01225931

H	-0.43111049	-0.07413938	5.22545341
H	-0.50603820	-3.24047382	5.41321978
H	0.94615922	-2.21964441	5.32944017
H	0.69773218	-3.51793527	4.14198722
H	6.18974405	1.07429232	2.01322754
H	4.69785625	1.44411879	2.90325014
H	4.73937623	1.63039104	1.14338547
H	4.68918584	-2.34101058	2.96758544
H	4.69431079	-0.87703135	3.97259338
H	6.16240702	-1.36010536	3.09718074
H	7.17887688	-0.70959881	0.87433188
H	7.93766286	-1.64627851	-1.29406463
H	6.29405023	-2.49019240	-2.94936475
H	-1.45766016	-2.90136513	-1.15717001
H	2.53877714	-2.51852190	-2.33498221
H	-4.13519902	-4.40661305	-1.31857664
H	-3.18631608	-3.72305468	-2.64480678
H	-3.95331363	-2.64249584	-1.46188017
H	-2.10661420	-5.83946930	-0.49333929
H	-0.50485813	-5.08597493	-0.35455635
H	-1.26443046	-5.25336320	-1.94892087
H	3.31899441	-0.61422950	-3.70248830
H	2.80400408	-1.97139529	-4.71561458
H	4.53942249	-1.64726985	-4.49123506
H	4.77645676	-4.17210514	-3.66005740
H	3.02882991	-4.37973818	-3.87513129
H	3.77760051	-4.72516929	-2.30112108
H	3.99351038	4.79521781	-0.83024652
H	4.24463406	5.35815233	1.57500180
H	2.55652548	4.57027342	3.21688457
H	1.20624045	2.73508410	-2.27763043
H	-3.76789555	1.66153512	1.44971979
H	4.24218482	3.11761908	-2.42314135
H	3.20476331	2.31485901	-3.62177334
H	3.37937363	1.61768731	-1.99896033
H	1.02349331	5.23926497	-2.62264079
H	1.82081570	4.42272927	-3.98575793
H	2.78320585	5.33541787	-2.80628892
H	-6.11210931	-0.15183031	2.25052605
H	-4.82976527	0.45249529	3.31894899
H	-4.43075338	-0.67337817	2.00547356
H	-5.49114706	3.47303323	1.12105360
H	-5.43898293	2.89018590	2.79954162
H	-6.75135161	2.37905015	1.72286598
H	-7.18535998	0.59967594	0.20323022
H	-7.65228831	-0.00360065	-2.15901177
H	-5.83910110	0.03525663	-3.84845984
H	-0.24138330	2.24846084	2.37347381
H	-2.23055082	0.86815559	-3.07937811
H	1.35604477	3.53556432	4.65474919
H	1.54742891	1.88109045	4.00068752
H	0.03680438	2.36468110	4.79497181

H	-1.57765900	3.96877411	3.62899137
H	-1.23412779	4.55870062	1.98726567
H	-0.30216303	5.17855254	3.36306181
H	-2.79946838	-1.47426577	-3.51339928
H	-2.27143559	-0.65772650	-4.98628617
H	-4.00062979	-0.99982127	-4.74551922
H	-3.53049589	2.78658224	-4.11603845
H	-4.40005953	1.62351565	-5.13318026
H	-2.64429326	1.82141033	-5.31489886
O	0.73077981	0.17883431	1.69876159
O	0.02692077	-0.33308709	-2.80231571
O	-0.24097094	-1.33824098	-1.72520953
Hf	0.06441069	0.05687381	-0.04086929

Oxo η^3 -Ozone ComplexFig. S50: NCCNO Oxo η^3 -Ozone Complex

E	E_{zp}	H	G
-2743.7387	-2742.5838	-2742.5123	-2742.6920
O	-1.91422602	0.40885626	0.23111748
O	2.17305224	-0.99022403	-0.71531049
O	1.01342759	1.01687028	-1.94181729
N	-0.05752686	-2.10388444	0.80307343
N	2.88660808	-1.80903217	0.05294035
N	-0.17073950	2.56087206	-0.15970261
N	-2.77843618	1.14221831	-0.51295092
C	0.95662309	-2.82135154	1.22101445
C	2.35924552	-2.63259846	0.94492265
C	-1.25425732	3.07378711	-0.68458120
C	-2.48107859	2.35496079	-0.94200101
C	-1.35129722	-2.57193203	1.31263442
C	-1.69057645	-2.29302830	2.66460067
C	-2.90224422	-2.82902342	3.15344596
C	-3.74270241	-3.59695268	2.33552700
C	-3.38698699	-3.84327049	0.99932544
C	-2.18522353	-3.34250688	0.45872527
C	-1.58665375	-0.28181416	4.23262531

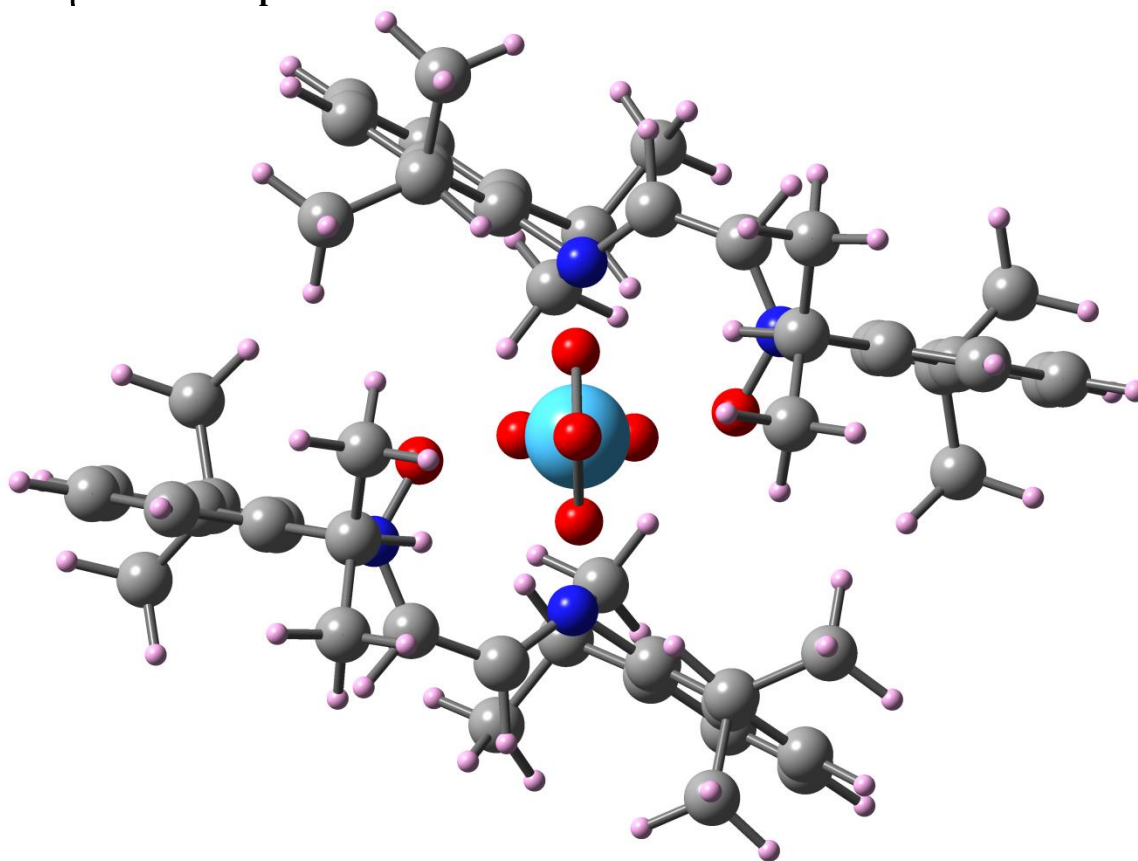
C	-0.80160341	-1.45797096	3.59812869
C	-0.17627526	-2.34265404	4.71062495
C	4.94009543	1.39241753	1.67272086
C	4.47893379	-0.08290167	1.78283093
C	4.80885400	-0.65824565	3.18611800
C	4.33972086	-1.76845400	-0.17141971
C	5.10744418	-0.94257301	0.67981452
C	6.50204774	-0.93644651	0.45780127
C	7.07200011	-1.69096515	-0.57939084
C	6.26311496	-2.46244372	-1.43161607
C	4.86589298	-2.51775962	-1.25114482
C	-2.94872929	-3.86892748	-1.93763915
C	-1.75614316	-3.69143802	-0.97024831
C	-0.88757698	-4.98143449	-0.97995621
C	3.65287063	-2.39084463	-3.46208065
C	3.96721152	-3.28312990	-2.22726191
C	4.56372016	-4.64375085	-2.65965846
C	0.92572442	3.48379767	0.11295197
C	1.58993218	4.16730572	-0.94838130
C	2.65185934	5.03126087	-0.59880966
C	3.02759108	5.23391664	0.73490666
C	2.33497808	4.57414769	1.76233561
C	1.27718646	3.68959521	1.47961629
C	2.44854285	3.54738664	-3.27000859
C	1.23467611	4.02818105	-2.43568677
C	0.67224329	5.36242723	-2.99759341
C	-5.34796355	0.08813995	2.82571358
C	-4.66536796	0.88621381	1.69233707
C	-5.06862355	2.38677824	1.78795105
C	-4.08697345	0.53452501	-0.80022805
C	-4.97976261	0.35018020	0.29019756
C	-6.21663573	-0.25797660	0.00616050
C	-6.54816977	-0.64907296	-1.30277210
C	-5.65519158	-0.42065895	-2.35697804
C	-4.39489375	0.18223856	-2.13916420
C	1.29684100	2.66731890	3.83704122
C	0.44879866	3.08486834	2.61647068
C	-0.67442756	4.07538117	3.03362200
C	-3.18897713	-0.81339160	-4.17311328
C	-3.48657867	0.46066814	-3.34496536
C	-4.11810896	1.56433753	-4.23941254
H	0.76266976	-3.67299254	1.87773772
H	3.06664240	-3.25774076	1.47526879
H	-1.29467212	4.13471332	-0.94016060
H	-3.26660585	2.86619112	-1.48438286
H	-3.18579901	-2.64181131	4.18637557
H	-4.66842284	-4.00504491	2.73551399
H	-4.04669599	-4.43640804	0.37348817
H	0.00907936	-1.00325747	3.01683847
H	3.38639358	-0.07300886	1.67244449
H	-2.41561238	-0.62958266	4.86432875
H	-1.99445600	0.37429619	3.45498737

H	-0.91362067	0.31630493	4.86055305
H	-0.95003475	-2.79515060	5.34612100
H	0.47824370	-1.73779614	5.35209658
H	0.42519218	-3.16038129	4.29076004
H	6.01878170	1.50411811	1.85008465
H	4.41073431	1.99914687	2.41698885
H	4.70653497	1.80388076	0.68391705
H	4.43809083	-1.68615228	3.29985275
H	4.33507466	-0.04401099	3.96241362
H	5.89176487	-0.66928283	3.37241802
H	7.13886017	-0.32510641	1.09089175
H	8.14816947	-1.66802155	-0.73477134
H	6.72024530	-3.02087018	-2.24288196
H	-1.14467963	-2.86594576	-1.35523553
H	3.00752757	-3.48896556	-1.73551793
H	-3.52707282	-4.77639936	-1.71421327
H	-2.57665482	-3.96301431	-2.96546809
H	-3.62718597	-3.00929632	-1.89992688
H	-1.45936038	-5.83920080	-0.59935542
H	0.01215552	-4.87541417	-0.36161649
H	-0.56556090	-5.21079675	-2.00427362
H	3.14135305	-1.47172547	-3.15854101
H	2.99818962	-2.93034931	-4.15889237
H	4.57662309	-2.12449393	-3.99368083
H	5.46674691	-4.51660924	-3.27044262
H	3.83356193	-5.18936474	-3.27085250
H	4.82283167	-5.26902778	-1.79509208
H	3.18887863	5.54925072	-1.38915249
H	3.84765565	5.90726993	0.97392863
H	2.61578469	4.75269116	2.79588743
H	0.47673468	3.25061641	-2.55272979
H	-3.58447809	0.81261151	1.84798701
H	3.29226263	4.24851459	-3.21507690
H	2.15999158	3.44871685	-4.32525843
H	2.77227461	2.56313766	-2.91873843
H	-0.20672669	5.70763400	-2.43426108
H	0.37671866	5.23498666	-4.04768314
H	1.42247861	6.16317999	-2.95571657
H	-6.43759575	0.22608178	2.82592508
H	-4.97581640	0.44000537	3.79629094
H	-5.12824800	-0.98156067	2.74548963
H	-4.56219472	2.99896317	1.03123575
H	-4.80331408	2.78677838	2.77510408
H	-6.15160678	2.50615339	1.65030820
H	-6.92708370	-0.42434477	0.80897249
H	-7.50777011	-1.12157775	-1.49881845
H	-5.93058648	-0.71407088	-3.36589213
H	-0.00409831	2.16457552	2.24016838
H	-2.51275922	0.81738459	-3.00310972
H	1.79219538	3.51870267	4.32428772
H	2.04757665	1.93306367	3.52784411
H	0.65166308	2.19178474	4.58802256

H	-1.30910034	3.62627583	3.80996341
H	-1.31678924	4.34202908	2.18264444
H	-0.25162087	5.00639257	3.43624753
H	-2.59115181	-1.51055737	-3.58128591
H	-2.59638491	-0.54202567	-5.05588503
H	-4.10406222	-1.31274620	-4.51929100
H	-4.32523210	2.48628950	-3.67715264
H	-5.06618343	1.22806232	-4.67966944
H	-3.43416376	1.81372842	-5.06032801
O	1.10249475	0.29007613	1.45239702
O	-0.35155713	0.57203531	-2.47742354
O	-0.51130130	-0.88264783	-2.02135272
Hf	0.25625703	0.10432960	-0.18331606

6.6 Seven Oxygen Atoms

Peroxo η^2 -Ozone Complex



Fis.S51: NCCNO Peroxo η^2 -Ozone Complex

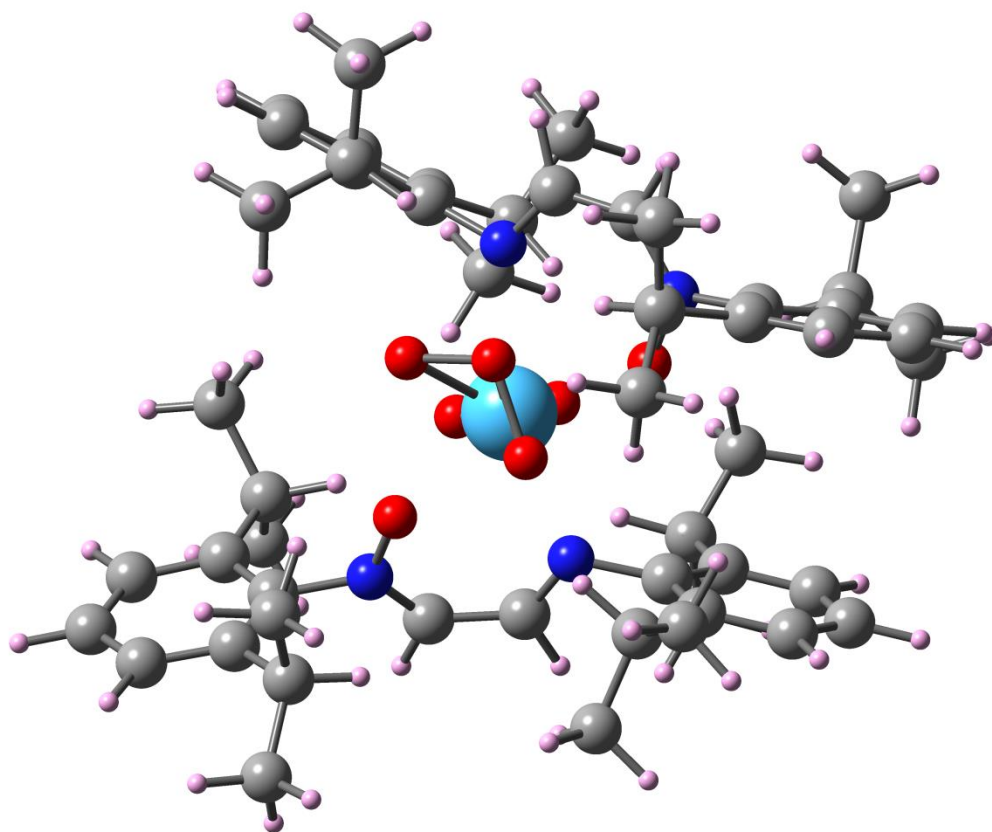
E	E_{zp}	H	G
-2818.9159	-2817.7574	-2817.6848	-2817.8682

O	-2.16427125	-0.32990278	0.18409654
O	2.16405029	0.32924349	0.18492606
O	0.02206484	-1.15999218	1.65453587
N	0.06338883	2.38195159	-0.54937314
N	2.78000634	1.43323259	0.61342289
N	-0.06333476	-2.38111693	-0.55218803
N	-2.78005534	-1.43435025	0.61166483
C	1.03807352	3.10627122	-0.06995466
C	2.27568099	2.65751231	0.54069672
C	-1.03770369	-3.10622383	-0.07324337
C	-2.27543526	-2.65844580	0.53782230
C	-1.03565365	3.11379294	-1.19532489
C	-1.00492638	3.27369391	-2.60781480
C	-2.06462858	3.98400189	-3.20791862
C	-3.11594279	4.51348054	-2.44394481
C	-3.11420711	4.35118861	-1.05219656

C	-2.07750178	3.65425392	-0.39262895
C	-0.31864903	2.03984044	-4.74254527
C	0.15920417	2.77193046	-3.46660769
C	1.10718719	3.94995956	-3.82494010
C	5.20907891	-0.48722340	-1.77989744
C	4.99368868	0.95145751	-1.23870839
C	5.92216627	1.96357614	-1.95774220
C	4.11678435	1.20972387	1.18484159
C	5.18383578	0.98801809	0.28127979
C	6.45772730	0.77584103	0.84767336
C	6.63968622	0.78314492	2.24044999
C	5.55009973	0.98988082	3.10074167
C	4.24921165	1.19854098	2.59368291
C	-3.44384528	2.96215067	1.65137243
C	-2.10692307	3.55256916	1.13763103
C	-1.84027539	4.94007011	1.78232869
C	2.91857407	0.17259199	4.50306941
C	3.06691829	1.38698385	3.55100288
C	3.21010500	2.70575416	4.35650247
C	1.03577607	-3.11210474	-1.19901786
C	2.07780279	-3.65336968	-0.39708985
C	3.11441496	-4.34955674	-1.05758951
C	3.11590811	-4.51035689	-2.44951073
C	2.06447013	-3.98004250	-3.21273699
C	1.00485731	-3.27041105	-2.61167660
C	3.44473889	-2.96350698	1.64724970
C	2.10758171	-3.55315677	1.13325102
C	1.84080971	-4.94120227	1.77672817
C	-5.20827780	0.48944253	-1.77902309
C	-4.99362869	-0.95013516	-1.23992782
C	-5.92255024	-1.96073804	-1.96050050
C	-4.11683831	-1.21162149	1.18333072
C	-5.18386299	-0.98873378	0.28000375
C	-6.45777397	-0.77731790	0.84661786
C	-6.63981761	-0.78653187	2.23938004
C	-5.55029336	-0.99447325	3.09944659
C	-4.24936472	-1.20241295	2.59217406
C	0.31817959	-2.03352944	-4.74452764
C	-0.15943863	-2.76766593	-3.46967592
C	-1.10712019	-3.94540936	-3.82975572
C	-2.91863467	-0.17834683	4.50240758
C	-3.06715669	-1.39198866	3.54938590
C	-3.21067240	-2.71135484	4.35383376
H	0.97023814	4.19556922	-0.13422787
H	2.92462966	3.42942604	0.93693376
H	-0.96943910	-4.19543476	-0.13844236
H	-2.92420083	-3.43089265	0.93331152
H	-2.06425526	4.12222005	-4.28559527
H	-3.92506384	5.05455451	-2.92946986
H	-3.92391009	4.77383650	-0.46257796
H	0.71985176	2.02862892	-2.89359822
H	3.95974422	1.22255214	-1.47852529

H	-0.85909947	2.70315159	-5.43246929
H	-0.96409140	1.20128670	-4.46358179
H	0.54838234	1.63570076	-5.28204727
H	0.58843584	4.71088364	-4.42477629
H	1.96300305	3.58389999	-4.40821785
H	1.49706284	4.44747140	-2.92513997
H	6.23063046	-0.83817491	-1.58012367
H	5.04577369	-0.50867486	-2.86468615
H	4.50392588	-1.18819763	-1.32075246
H	5.76788300	2.98612453	-1.58876943
H	5.71819738	1.95561637	-3.03600966
H	6.98148905	1.71173140	-1.81835486
H	7.30922096	0.60394185	0.19497997
H	7.63134110	0.61980912	2.65572928
H	5.70508712	0.97702219	4.17606577
H	-1.32226629	2.86712403	1.46971048
H	2.13550275	1.44042486	2.97909336
H	-4.30337084	3.59626022	1.39509824
H	-3.41400343	2.86918729	2.74536786
H	-3.61139389	1.96483868	1.23008643
H	-2.61949230	5.66516678	1.51014857
H	-0.87497351	5.35582945	1.46177578
H	-1.82497001	4.85299442	2.87708711
H	2.76624094	-0.74942128	3.93222504
H	2.04008488	0.31410950	5.14408838
H	3.79843554	0.04724588	5.14893148
H	4.10677608	2.69397714	4.99058583
H	2.33734387	2.84284873	5.00726722
H	3.27988156	3.58072813	3.69588967
H	3.92421432	-4.77282009	-0.46855125
H	3.92494391	-5.05091222	-2.93575550
H	2.06392368	-4.11707965	-4.29056385
H	1.32313150	-2.86787740	1.46616507
H	-3.95980292	-1.22141828	-1.48006558
H	4.30406670	-3.59764847	1.39039039
H	3.41508409	-2.87137956	2.74131935
H	3.61247699	-1.96591902	1.22669685
H	0.87535866	-5.35650785	1.45602866
H	1.82575091	-4.85513316	2.87157043
H	2.61983585	-5.66620302	1.50372558
H	-6.22961804	0.84063393	-1.57858816
H	-5.04510592	0.51239350	-2.86380316
H	-4.50268491	1.18936553	-1.31896377
H	-5.76892400	-2.98388700	-1.59291848
H	-5.71836402	-1.95140260	-3.03871643
H	-6.98176496	-1.70849700	-1.82100449
H	-7.30924498	-0.60454053	0.19412933
H	-7.63150102	-0.62376322	2.65481466
H	-5.70534282	-0.98311801	4.17477983
H	-0.72024542	-2.02538968	-2.89549311
H	-2.13571487	-1.44520103	2.97749272
H	0.85865960	-2.69571970	-5.43550523

H	0.96353927	-1.19531738	-4.46435187
H	-0.54896228	-1.62870329	-5.28333281
H	-1.96308817	-3.57871466	-4.41241404
H	-1.49678366	-4.44442745	-2.93069889
H	-0.58816320	-4.70524004	-4.43079767
H	-2.76599438	0.74405643	3.93228509
H	-2.04027065	-0.32057195	5.14343871
H	-3.79857962	-0.05331493	5.14821322
H	-3.28052096	-3.58580431	3.69253120
H	-4.10740365	-2.69994529	4.98783403
H	-2.33801139	-2.84909709	5.00459839
O	0.77899942	-0.01354819	-2.08892450
O	-0.77867778	0.01669329	-2.08913019
O	-0.00018702	-0.00162262	2.59516981
O	-0.02251654	1.15785635	1.65585138
Hf	-0.00010960	0.00012544	-0.20873350

Peroxo η^3 -Ozone ComplexFig. S52: NCCNO Peroxo η^3 -Ozone Complex

E	E_{zp}	H	G
-2818.9018	-2817.7439	-2817.6716	-2817.8540
O	-2.02951515	0.32068502	0.11874201
O	2.09894616	-1.06611408	-0.73797405
O	1.04054908	1.07200908	-1.82829114
N	0.06197800	-2.13507416	0.87994307
N	2.93575522	-1.74590813	0.05803300
N	-0.24156902	2.58980420	-0.02338800
N	-2.86824522	1.15199809	-0.51772204
C	1.12399009	-2.70441421	1.40678911
C	2.50650019	-2.45288119	1.09155508
C	-1.34955410	3.11384524	-0.47478604
C	-2.57909220	2.41335418	-0.78458206
C	-1.21418109	-2.73946321	1.27327710
C	-1.67978113	-2.64570520	2.61581920
C	-2.90651322	-3.27510125	2.92602122
C	-3.63624128	-3.97895231	1.96010615
C	-3.14068424	-4.08100931	0.65036705
C	-1.92350814	-3.47619526	0.28033402
C	-1.78633814	-0.78124106	4.34936733

C	-0.92985907	-1.91994915	3.74120329
C	-0.47732504	-2.91509522	4.84339537
C	5.08163039	1.48842411	1.37655911
C	4.75272836	-0.00669400	1.62555912
C	5.37171641	-0.49278404	2.96271023
C	4.35444933	-1.68700413	-0.31248102
C	5.22310440	-0.87204806	0.45127603
C	6.58138052	-0.85915607	0.06364100
C	7.02761653	-1.59769312	-1.04194108
C	6.12441448	-2.36484118	-1.79715414
C	4.75959236	-2.42763418	-1.45168711
C	-2.40369819	-3.90909630	-2.21147217
C	-1.33397610	-3.71093529	-1.11458908
C	-0.37530803	-4.93573938	-1.08944508
C	3.36852226	-2.37292818	-3.55888327
C	3.76848229	-3.21486424	-2.31465418
C	4.30771033	-4.60569235	-2.72888021
C	0.85253507	3.53560027	0.22401002
C	1.48444811	4.20580432	-0.86586507
C	2.55219620	5.07913839	-0.56028905
C	2.96269023	5.30817339	0.75883206
C	2.28951818	4.67581036	1.81452214
C	1.22560309	3.78407429	1.57599512
C	2.25550117	3.63544728	-3.23695325
C	1.07077908	4.07089531	-2.33894818
C	0.45118303	5.39904439	-2.85596222
C	-5.39600840	-0.27039202	2.65238520
C	-4.79927237	0.72070405	1.62652913
C	-5.31199241	2.16226117	1.90820615
C	-4.18226432	0.59101104	-0.87989307
C	-5.09896439	0.33566103	0.17280301
C	-6.34462651	-0.21176202	-0.18982201
C	-6.65092250	-0.48863704	-1.53327212
C	-5.72079543	-0.21322902	-2.54441920
C	-4.45330634	0.33638503	-2.24711317
C	1.32330310	2.70244321	3.90116630
C	0.42664203	3.22666825	2.75629921
C	-0.56200605	4.30782633	3.27616225
C	-3.18975424	-0.59446904	-4.26763233
C	-3.48210827	0.64961705	-3.39279026
C	-4.02932931	1.81740014	-4.25955233
H	0.98474007	-3.50168627	2.14054217
H	3.26606725	-2.96426922	1.66952213
H	-1.40908411	4.19078232	-0.64830205
H	-3.37262826	2.97977723	-1.25582009
H	-3.28700225	-3.21240525	3.94278430
H	-4.57646835	-4.45687734	2.22626117
H	-3.70065728	-4.64514036	-0.08873001
H	-0.04980000	-1.42491411	3.32452125
H	3.66350328	-0.06673801	1.71694513
H	-2.71600321	-1.15752509	4.79824637
H	-2.03478716	-0.04721200	3.57555427

H	-1.21723209	-0.26259502	5.13233039
H	-1.33510110	-3.38963126	5.33898743
H	0.10428901	-2.38829218	5.61168342
H	0.15031301	-3.71929329	4.43432034
H	6.16451950	1.66782513	1.32906110
H	4.66986136	2.09799116	2.19014917
H	4.63065935	1.83836714	0.44097803
H	5.11006739	-1.53867612	3.17471824
H	5.00130538	0.12264301	3.79240929
H	6.46766847	-0.41948703	2.94986123
H	7.28679257	-0.25189202	0.62413405
H	8.07739661	-1.56740412	-1.32435810
H	6.48254248	-2.91729322	-2.66083620
H	-0.74638106	-2.83146821	-1.39628210
H	2.84978122	-3.37798226	-1.73820513
H	-2.92732722	-4.86990837	-2.10957716
H	-1.92272815	-3.89918230	-3.19761224
H	-3.14852724	-3.10568623	-2.18865717
H	-0.91883407	-5.85111046	-0.81734706
H	0.43997503	-4.80143936	-0.36753903
H	0.07305301	-5.08493839	-2.08086316
H	2.90014222	-1.43259211	-3.25186725
H	2.64830220	-2.92838322	-4.17402932
H	4.24815932	-2.14914616	-4.17811732
H	5.16462339	-4.52525434	-3.40998726
H	3.52390827	-5.16333639	-3.25755525
H	4.62044735	-5.19660040	-1.85786714
H	3.06276823	5.58773545	-1.37375510
H	3.78807329	5.98625445	0.96360807
H	2.58575520	4.88194137	2.83911922
H	0.32537202	3.27850425	-2.43309419
H	-3.71373928	0.71126506	1.76866513
H	3.07777824	4.36321733	-3.21920824
H	1.91773015	3.53615227	-4.27754433
H	2.62885020	2.66030520	-2.91121122
H	-0.41168803	5.71415145	-2.25162417
H	0.11573801	5.28119540	-3.89528730
H	1.18346309	6.21684550	-2.83050122
H	-6.49366547	-0.24042702	2.66284021
H	-5.05233839	-0.00593300	3.66026528
H	-5.07444139	-1.29635210	2.44304319
H	-4.86404237	2.89566422	1.22507109
H	-5.06001139	2.46039919	2.93407322
H	-6.40287850	2.21737417	1.79401614
H	-7.07892154	-0.42471603	0.58046404
H	-7.61770658	-0.91535307	-1.78947614
H	-5.97258146	-0.43029103	-3.57848327
H	-0.14703401	2.36351618	2.40968419
H	-2.51604719	0.95620808	-2.98451623
H	1.92641315	3.49646527	4.36416833
H	1.98443215	1.91781815	3.52000027
H	0.69541605	2.26269517	4.68777236

H	-1.17397509	3.90077630	4.09264731
H	-1.23984610	4.65338535	2.48248719
H	-0.02417200	5.18621740	3.65957328
H	-2.69710521	-1.36880911	-3.67389228
H	-2.50536519	-0.31721802	-5.07915639
H	-4.10088131	-1.00912407	-4.71952736
H	-4.21469232	2.72174321	-3.66295428
H	-4.97420738	1.54434212	-4.74778836
H	-3.30491125	2.07099616	-5.04364638
O	1.51914812	0.42662403	1.43568911
O	0.07107601	0.30444202	1.93219815
O	-0.39395703	0.67182605	-2.19890517
O	-0.47833404	-0.83825106	-1.94265215
Hf	0.20293302	0.09325901	-0.11701001

Ligand Cyclization

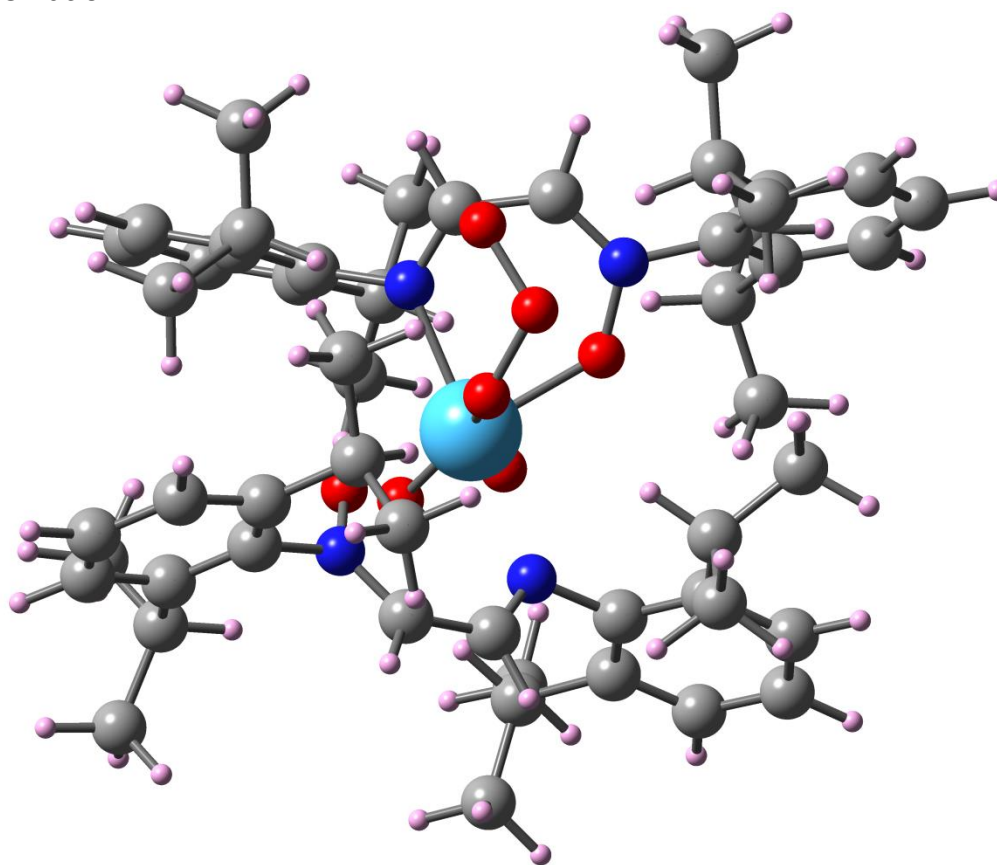


Fig. S53: NCCNO Ligand Cyclization

E	E_{zp}	H	G
-2818.8993	-2817.7410	-2817.6683	-2817.8510
O	2.18212414	0.48550902	0.04232395
O	-2.01062917	-0.32086413	-0.19158507
O	0.21143800	-0.22161207	1.53847007
N	0.16787503	-2.01843521	-0.99076513
N	-2.56592619	-1.48290523	0.31550297
N	-0.01882607	2.41924512	0.23029697
N	2.72658716	1.29018209	0.94803602
C	-0.61790201	-2.87310929	-0.34867008
C	-1.89483311	-2.63273530	0.27244997
C	0.92223699	2.99644319	0.92970402
C	2.18363909	2.43011617	1.35137905
C	1.24022512	-2.60071724	-1.81001719
C	1.08259211	-2.54513923	-3.22471130
C	2.09243220	-3.11403025	-4.02718336
C	3.21740530	-3.72737728	-3.45701132
C	3.34501431	-3.78401128	-2.06290421
C	2.36875323	-3.22506126	-1.20795614
C	0.15766801	-1.00073313	-5.05022344

C	-0.17196199	-1.97511721	-3.89448035
C	-1.08543204	-3.13477733	-4.38034539
C	-4.54406739	0.93066791	-2.08387221
C	-4.43011835	-0.58656520	-1.78626419
C	-5.24401439	-1.41754128	-2.81359527
C	-3.98488330	-1.38809425	0.66125100
C	-4.86529137	-0.90402823	-0.34898908
C	-6.22421350	-0.75250825	-0.00532805
C	-6.69946451	-1.10305028	1.26712605
C	-5.81824744	-1.62964431	2.22061412
C	-4.44072532	-1.78143529	1.95013810
C	3.97819834	-2.90015320	0.74664801
C	2.56211124	-3.34904626	0.30910197
C	2.30656926	-4.80648838	0.78443401
C	-3.68730927	-1.69513927	4.40156629
C	-3.54747524	-2.40309932	3.03117118
C	-3.85913824	-3.91839144	3.18190019
C	-1.18063818	3.27343216	-0.07883606
C	-2.24355927	3.34144615	0.85976001
C	-3.32374436	4.19689919	0.55564999
C	-3.34494938	4.94866125	-0.62831310
C	-2.27825930	4.85900126	-1.53467817
C	-1.17140119	4.02033722	-1.28610615
C	-3.60391134	1.98005701	2.55116614
C	-2.22130324	2.56745909	2.18386111
C	-1.71460923	3.47517117	3.34007720
C	5.35749239	0.46808909	-1.83327619
C	5.06882033	1.58282417	-0.79224111
C	6.01179540	2.79639828	-0.99672313
C	4.03574227	0.86979209	1.47613306
C	5.16127135	1.02704912	0.63290800
C	6.40491848	0.62719212	1.16462704
C	6.50064648	0.10351108	2.46416114
C	5.35390139	-0.04736995	3.26016920
C	4.07873029	0.32193505	2.78197216
C	-0.46801114	3.82113422	-3.73855834
C	0.00026989	3.98759224	-2.27322123
C	0.87596893	5.26101036	-2.11052621
C	2.74861721	-1.29034010	4.26218027
C	2.82951219	0.13203601	3.65327323
C	2.78049017	1.20116309	4.77906531
H	-0.35708397	-3.93117737	-0.37415608
H	-2.43056913	-3.50292938	0.62465900
H	0.78011095	4.02893126	1.25550604
H	2.78321313	3.00317422	2.04627510
H	1.99047220	-3.08174926	-5.10841744
H	3.98420537	-4.16325930	-4.09357436
H	4.21545439	-4.26806530	-1.62814918
H	-0.72932505	-1.38912018	-3.16076529
H	-3.37727526	-0.84734820	-1.90955720
H	0.69724506	-1.49203316	-5.87189951
H	0.75542204	-0.16594706	-4.67099441

H	-0.77349907	-0.58911712	-5.46153345
H	-0.58418799	-3.74022436	-5.14799544
H	-2.01033212	-2.73241531	-4.81550642
H	-1.36078205	-3.80578538	-3.55436033
H	-5.58165849	1.28056392	-1.98907421
H	-4.20369837	1.13864494	-3.10601929
H	-3.91516835	1.50725097	-1.39856416
H	-5.16825637	-2.49422136	-2.61121725
H	-4.85822337	-1.23251126	-3.82468834
H	-6.30836548	-1.14823728	-2.81055827
H	-6.91842954	-0.37338124	-0.75018111
H	-7.75271859	-0.98026530	1.50821806
H	-6.19826148	-1.91964534	3.19619219
H	1.83625917	-2.70973923	0.82053501
H	-2.50266816	-2.30677529	2.73926916
H	4.75977941	-3.55151723	0.33425697
H	4.06452735	-2.93928320	1.83976509
H	4.18407634	-1.87414211	0.42462398
H	3.01879332	-5.50379143	0.32219897
H	1.29492119	-5.14899042	0.53256199
H	2.41684627	-4.87367538	1.87452609
H	-3.44864127	-0.62934418	4.31936228
H	-2.98700620	-2.14280229	5.11844234
H	-4.69853635	-1.79000830	4.81923131
H	-4.88802131	-4.08088448	3.53015922
H	-3.17491917	-4.37205846	3.91010224
H	-3.74613421	-4.45823948	2.23176212
H	-4.15580743	4.27100218	1.24959504
H	-4.18878646	5.60011730	-0.84332512
H	-2.30300831	5.44287630	-2.45037624
H	-1.52845018	1.72378404	2.08701311
H	4.04531224	1.92585017	-0.98042713
H	-4.33773541	2.76459106	2.77821516
H	-3.51091232	1.35336697	3.44600921
H	-3.99987836	1.35891496	1.74158308
H	-0.70092216	3.85406222	3.15432819
H	-1.69635421	2.91393213	4.28356827
H	-2.37478930	4.34331022	3.47003421
H	6.37359849	0.06771908	-1.71703018
H	5.26344636	0.87136811	-2.84928427
H	4.64507334	-0.35755899	-1.73186319
H	5.80350134	3.59668734	-0.27440807
H	5.87896535	3.20456130	-2.00662321
H	7.06670649	2.51304728	-0.88987712
H	7.30052954	0.72725415	0.55792099
H	7.47046354	-0.19545092	2.85447816
H	5.44449040	-0.47116298	4.25599428
H	0.61695796	3.10944419	-2.06223321
H	1.93494912	0.23799100	3.02968118
H	-1.06974820	4.67198527	-4.08729136
H	-1.04852216	2.89871514	-3.83543835
H	0.40692893	3.73925323	-4.39671839

H	1.73070000	5.22294237	-2.79899127
H	1.26781796	5.36086240	-1.08768414
H	0.30058387	6.16995240	-2.33376723
H	2.74991423	-2.05389716	3.47787622
H	1.80766614	-1.39375713	4.81542432
H	3.57490028	-1.49497810	4.95646533
H	2.78479115	2.22447817	4.37897329
H	3.64077123	1.10659910	5.45555634
H	1.86616010	1.07620806	5.37258436
O	-0.73862410	0.82803398	-2.28929523
O	0.82871002	0.84377902	-2.27050822
O	-0.59486804	-1.18886216	2.34624813
O	-0.31505499	-2.53983226	1.96958010
Hf	0.02031998	0.17427695	-0.53686809

6.7 Eight Oxygen Atoms

Bis- η^2 -ozone Complex

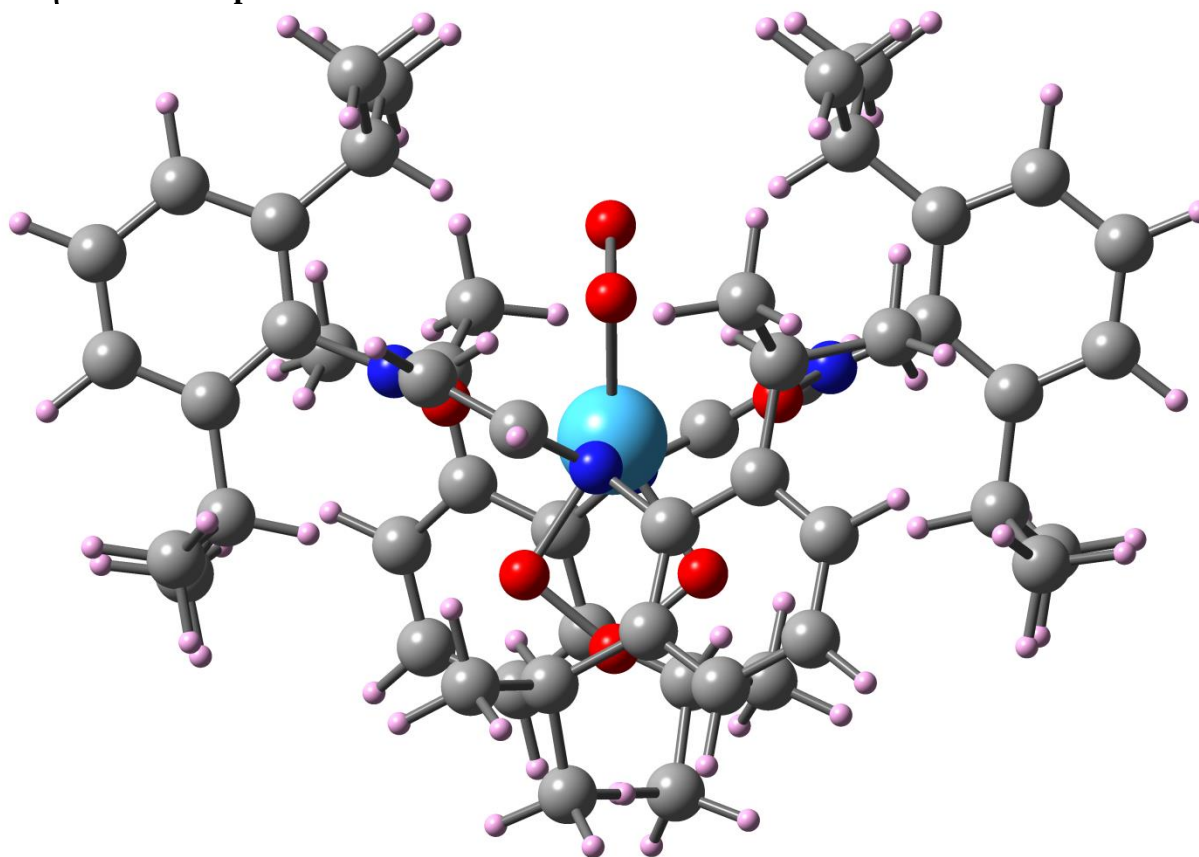


Fig. S54: NCCNO Bis- η^2 -ozone Complex

E	E_{zp}	H	G
-2894.0587	-2892.8971	-2892.8234	-2893.0118

O	2.15626185	0.01132815	0.40819271
O	-2.18734382	-0.12635392	0.36668245
O	0.03800444	0.92889177	1.85208011
N	-0.33628293	-2.24899158	-0.79611945
N	-2.91057062	-1.21749663	0.62118026
N	0.34393357	2.39942797	-0.18694644
N	2.89171271	0.99229921	0.93260136
C	-1.37056722	-2.92883287	-0.37640707
C	-2.52847443	-2.46020691	0.35922460
C	1.39118886	2.92943748	0.38816192
C	2.53355816	2.26801070	0.98717081
C	0.59212600	-2.97793317	-1.67401334
C	0.28795540	-3.07033148	-3.06024089
C	1.19247653	-3.77932605	-3.87850910
C	2.34469118	-4.37678524	-3.34800398
C	2.60761098	-4.28635813	-1.97356510

C	1.74243002	-3.58855243	-1.10467095
C	-0.73481822	-1.78895021	-5.03499988
C	-0.98979351	-2.48287339	-3.67493520
C	-2.06937803	-3.58990956	-3.84197373
C	-5.58726073	0.80234584	-1.76244541
C	-5.09757516	-0.55579546	-1.19830488
C	-5.81206808	-1.73761546	-1.90766936
C	-4.23402377	-0.95814458	1.21030052
C	-5.28846602	-0.64097298	0.32043432
C	-6.55582147	-0.41962208	0.89791906
C	-6.74036695	-0.49785536	2.28842453
C	-5.66015166	-0.78976354	3.13576072
C	-4.36802550	-1.02150873	2.61609113
C	3.49880967	-3.35541451	0.75476061
C	2.01171457	-3.59535635	0.40462722
C	1.52198176	-4.93328665	1.02721852
C	-2.95631139	-0.12723042	4.52816270
C	-3.19431406	-1.31195579	3.55677955
C	-3.41729305	-2.63380395	4.33779202
C	-0.55059868	3.34316743	-0.87274120
C	-1.73444164	3.77159889	-0.21265350
C	-2.56487645	4.68836196	-0.89006998
C	-2.23744653	5.16229080	-2.16889268
C	-1.05630558	4.73345453	-2.79030063
C	-0.18430936	3.81834387	-2.16294581
C	-3.57113104	3.06690717	1.43916737
C	-2.06783837	3.35738635	1.22442382
C	-1.58335315	4.45079749	2.21797000
C	5.55380339	-0.44570166	-1.86206880
C	5.07468839	0.74010631	-0.98649616
C	5.80401152	2.05151981	-1.38557219
C	4.20434677	0.56951296	1.44611823
C	5.25824806	0.45219925	0.50820787
C	6.51601612	0.06944321	1.01785872
C	6.69152416	-0.19301321	2.38694917
C	5.61119102	-0.09029173	3.27719762
C	4.32802053	0.28813580	2.82588329
C	0.89932895	3.08345983	-4.36847753
C	1.11548462	3.41020000	-2.87034897
C	2.19167391	4.52281781	-2.72255650
C	2.89072347	-1.00967393	4.46910842
C	3.15157032	0.36632567	3.80404786
C	3.38635787	1.46427919	4.87464698
H	-1.43564170	-3.99057755	-0.62531608
H	-3.24171174	-3.21676783	0.66383496
H	1.48319907	4.01784682	0.40744649
H	3.25886108	2.91042562	1.47232479
H	0.99168793	-3.85875266	-4.94298999
H	3.02864987	-4.91570737	-3.99983716
H	3.49268427	-4.76719889	-1.56628858
H	-1.37716116	-1.71053415	-3.00402016
H	-4.02919972	-0.61610766	-1.43183940

H	-0.44170489	-2.50229533	-5.81787670
H	0.04298161	-1.02683912	-4.93246091
H	-1.65364512	-1.28979576	-5.37056608
H	-1.71678025	-4.38214524	-4.51641516
H	-2.98693980	-3.16324942	-4.26979178
H	-2.32961641	-4.06293355	-2.88509839
H	-6.66628235	0.94228367	-1.61374856
H	-5.38630657	0.84956807	-2.83990187
H	-5.06060558	1.63778584	-1.28788151
H	-5.44299637	-2.70728509	-1.54783471
H	-5.63845471	-1.68836108	-2.99022258
H	-6.89631967	-1.70704672	-1.73634701
H	-7.39947378	-0.18063494	0.25632879
H	-7.72669508	-0.32372531	2.71194112
H	-5.81588472	-0.83195407	4.21031893
H	1.43794555	-2.79122970	0.87386246
H	-2.27411372	-1.41802004	2.97470558
H	4.14797224	-4.16968826	0.40513843
H	3.61558620	-3.28869767	1.84463741
H	3.85425866	-2.41475511	0.32102892
H	2.06558945	-5.79005177	0.60522295
H	0.45070228	-5.09392278	0.84655071
H	1.68061804	-4.92639443	2.11373280
H	-2.73865048	0.79151610	3.97243209
H	-2.08934616	-0.34223811	5.16430702
H	-3.82486048	0.05045593	5.17713452
H	-4.30400153	-2.57737226	4.98344358
H	-2.54841326	-2.84136635	4.97487483
H	-3.55054521	-3.48720164	3.65924490
H	-3.47319841	5.03709433	-0.40703556
H	-2.89470687	5.86606961	-2.67467256
H	-0.80764795	5.10725509	-3.77946826
H	-1.52269480	2.44102930	1.46683111
H	4.00800914	0.86670114	-1.20047978
H	-4.19100972	3.96730214	1.32929200
H	-3.73215249	2.68035401	2.45422235
H	-3.92707316	2.31028368	0.73179786
H	-0.50364891	4.62813591	2.12608141
H	-1.78419566	4.13962412	3.25162265
H	-2.09823228	5.40486915	2.03804426
H	6.63038037	-0.63036586	-1.74834268
H	5.35900287	-0.22699115	-2.91928358
H	5.01539904	-1.36529649	-1.60682177
H	5.44258801	2.90878427	-0.80198568
H	5.63477000	2.26836862	-2.44804294
H	6.88718654	1.96925996	-1.22465381
H	7.35875846	-0.02929117	0.33938272
H	7.67052434	-0.48661345	2.75828512
H	5.75956645	-0.31351517	4.33016667
H	1.49018916	2.49143722	-2.40951825
H	2.23745717	0.61846682	3.25811518
H	0.62027400	3.97135429	-4.95242470

H	0.12394628	2.32043559	-4.48075761
H	1.82979402	2.68646518	-4.79612586
H	3.12404619	4.21728774	-3.21678456
H	2.42149734	4.74077649	-1.67051545
H	1.85369164	5.45956772	-3.18638028
H	2.66066000	-1.76773291	3.71237244
H	2.02498566	-0.93656478	5.13840232
H	3.75329054	-1.34988884	5.05842854
H	3.54193667	2.45012533	4.41611291
H	4.26398703	1.24118787	5.49606645
H	2.51314948	1.53280671	5.53540966
O	-1.16580116	0.34911096	-1.86175510
O	1.15770807	0.18762551	-1.87642192
O	-0.01841097	-0.33635195	2.64329857
O	-0.07528490	-1.35759474	1.55609908
Hf	-0.01259709	0.02787138	-0.12923154
O	-0.00008433	0.41866346	-2.82830376

7. Triplet Ground States for NCCNO Complex

7.1 Two Oxygen Atoms

Bare Complex

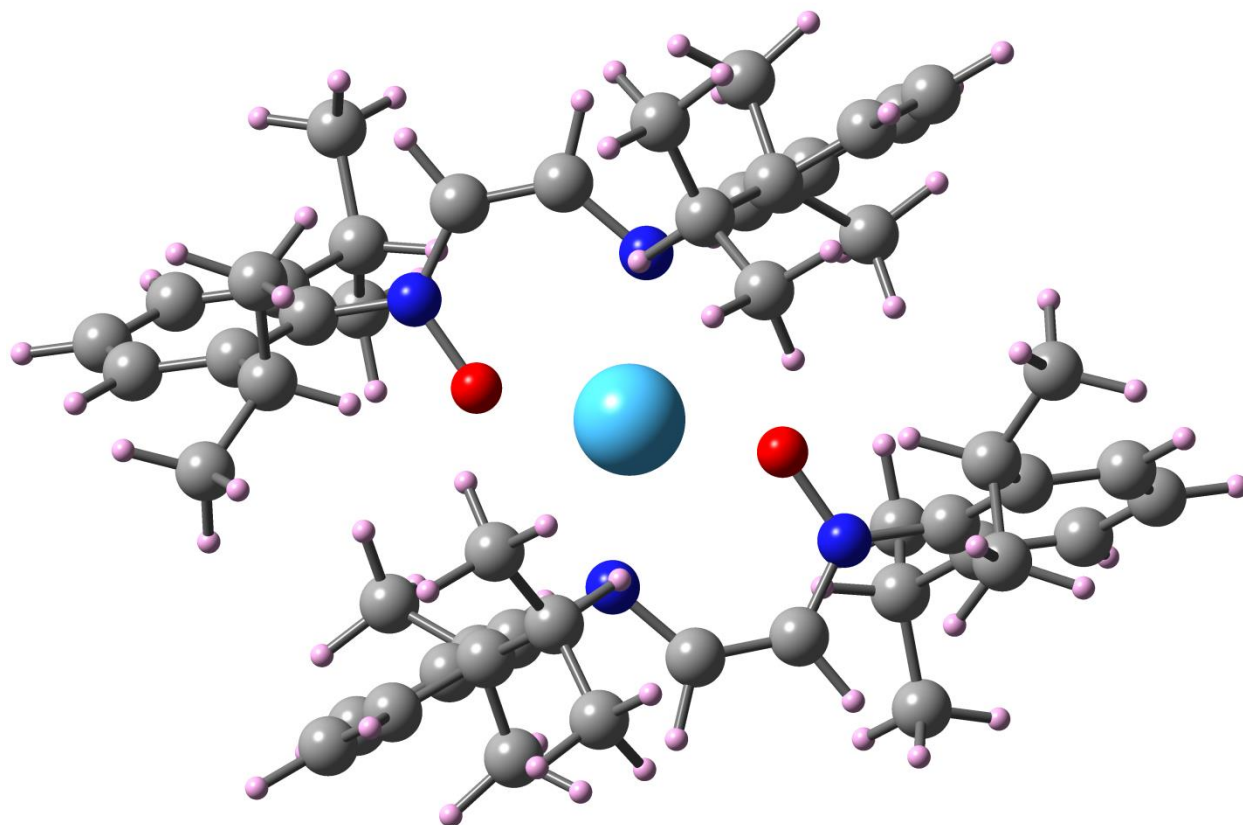


Fig. S55: NCCNO Bare Complex

E	E_{zp}	H	G
-2442.9596	-2441.8198	-2441.7526	-2441.9274
O	-1.96877028	0.40961052	-0.02028662
O	1.97003213	-0.41294313	-0.02781330
N	-0.21540391	-2.14973494	0.28062015
N	2.76653782	-1.54872165	-0.20731398
N	0.21670760	2.14567222	0.29427358
N	-2.76811590	1.54659410	-0.19289567
C	0.84773249	-3.05125758	0.20972962
C	2.18383540	-2.78373558	-0.02737280
C	-0.85019429	3.04916505	0.23232763
C	-2.18452635	2.78194039	-0.00427478
C	-1.48594520	-2.81158278	0.57302952
C	-1.84898692	-3.06231394	1.92762573
C	-3.05043117	-3.75556321	2.18613157
C	-3.87707779	-4.19113523	1.13986936
C	-3.51011370	-3.93139184	-0.18916849

C	-2.31781337	-3.24299033	-0.49822758
C	-1.73531992	-1.69368452	4.08005470
C	-0.97076905	-2.62681105	3.10648598
C	-0.38963678	-3.85223870	3.85997632
C	5.45240075	0.63055145	2.39314934
C	4.65867007	-0.52842091	1.74826083
C	4.79620710	-1.81928210	2.60484186
C	4.12873528	-1.34002653	-0.63320070
C	5.06678321	-0.81676224	0.30013068
C	6.39529613	-0.64179670	-0.13320927
C	6.78285666	-0.98830295	-1.43957265
C	5.84193135	-1.50373708	-2.34189380
C	4.49175180	-1.67590369	-1.96547716
C	-3.08868524	-2.36051459	-2.76907464
C	-1.93933486	-3.01591745	-1.96471770
C	-1.48781510	-4.34257651	-2.63320306
C	3.47680851	-1.38292912	-4.29281633
C	3.48461635	-2.21779477	-2.98654931
C	3.76088646	-3.71278009	-3.30266538
C	1.48618868	2.80721259	0.59068474
C	2.31666595	3.24913038	-0.47761458
C	3.50936463	3.93498109	-0.16417701
C	3.87819468	4.18309499	1.16655249
C	3.05234986	3.73919909	2.20996359
C	1.85055524	3.04823742	1.94693431
C	3.08170665	2.38377223	-2.75703804
C	1.93583825	3.03665899	-1.94563598
C	1.48897911	4.37092280	-2.60187802
C	-5.46053378	-0.65910056	2.38667167
C	-4.65801387	0.49719800	1.74812102
C	-4.78233506	1.78251354	2.61511113
C	-4.12828765	1.33874294	-0.62240626
C	-5.06628203	0.80064514	0.30309878
C	-6.39341617	0.62529990	-0.13399825
C	-6.78124129	0.98711931	-1.43624264
C	-5.84150812	1.51828559	-2.33056384
C	-4.49223358	1.69028016	-1.95059406
C	1.73569992	1.66493495	4.09048425
C	0.97245552	2.60551363	3.12317882
C	0.39325558	3.82673225	3.88509401
C	-3.47251660	1.42751178	-4.27932246
C	-3.48619185	2.24815719	-2.96406186
C	-3.76865098	3.74520502	-3.26423945
H	0.60519878	-4.10297567	0.35692533
H	2.88012683	-3.61237979	-0.07979887
H	-0.60697917	4.09921496	0.38867033
H	-2.88250792	3.60978621	-0.04771933
H	-3.33913559	-3.95824628	3.21523038
H	-4.79678950	-4.72957233	1.35764413
H	-4.15525862	-4.27046695	-0.99639450
H	-0.12563321	-2.05479375	2.70767808
H	3.60236427	-0.23947348	1.74403536

H	-2.59470811	-2.20145755	4.53790659
H	-2.10669064	-0.80383844	3.55604545
H	-1.07183399	-1.36192285	4.89042877
H	-1.18788395	-4.46705878	4.29688771
H	0.26952348	-3.52498838	4.67553727
H	0.19426318	-4.49080007	3.18504942
H	6.50992592	0.37294000	2.54149004
H	5.03131593	0.85961196	3.38045065
H	5.39478192	1.54025575	1.78456258
H	4.18312470	-2.63477472	2.20309941
H	4.47078330	-1.62778189	3.63623673
H	5.84091777	-2.15805270	2.63445949
H	7.13512836	-0.24014128	0.55221771
H	7.81613154	-0.85340773	-1.75137720
H	6.15308038	-1.76045625	-3.35142321
H	-1.08633577	-2.32823736	-1.98899955
H	2.48123871	-2.14979778	-2.55217583
H	-3.95719375	-3.02684327	-2.85527374
H	-2.75096714	-2.12732660	-3.78850066
H	-3.42029131	-1.43216471	-2.28995293
H	-2.29912022	-5.08322197	-2.62787946
H	-0.62932016	-4.77959333	-2.10771222
H	-1.19638683	-4.16689294	-3.67797573
H	3.27680566	-0.32571095	-4.08580563
H	2.69636672	-1.75407304	-4.97052756
H	4.43552604	-1.44949233	-4.82342681
H	4.75167710	-3.84280781	-3.75792340
H	3.01190379	-4.09954085	-4.00632270
H	3.72547260	-4.32939055	-2.39579624
H	4.15303946	4.28185659	-0.96930812
H	4.79823500	4.71956641	1.38786250
H	3.34190318	3.93380538	3.24041176
H	1.07998449	2.35282293	-1.97473888
H	-3.60413576	0.19952001	1.73905529
H	3.95465805	3.04538991	-2.83424970
H	2.74340283	2.16508300	-3.77951988
H	3.40699273	1.44757191	-2.28889791
H	0.63379885	4.80713760	-2.07044505
H	1.19398271	4.20519416	-3.64728849
H	2.30348580	5.10803833	-2.59277609
H	-6.51512758	-0.39259094	2.54042616
H	-5.03854182	-0.89940459	3.37092564
H	-5.41367948	-1.56485800	1.77124067
H	-4.16203661	2.59514508	2.21906460
H	-4.45733937	1.57971287	3.64453354
H	-5.82390138	2.13051812	2.64889708
H	-7.13233748	0.21191360	0.54538766
H	-7.81368986	0.85205797	-1.75078087
H	-6.15264926	1.78714018	-3.33695933
H	0.12634943	2.03784083	2.72034347
H	-2.48334469	2.18009313	-2.52860775
H	2.59539493	2.16862109	4.55236049

H	2.10655611	0.77828847	3.56063754
H	1.07154442	1.32823861	4.89830580
H	-0.26629023	3.49489407	4.69850905
H	-0.18991791	4.47036577	3.21445341
H	1.19245139	4.43748775	4.32599162
H	-3.26656463	0.36924097	-4.08348418
H	-2.69376085	1.81044658	-4.95244005
H	-4.43127706	1.49404408	-4.80990194
H	-3.73776325	4.35150572	-2.35030862
H	-4.75907532	3.87607541	-3.72009081
H	-3.01991532	4.14324711	-3.96187988
Hf	-0.00025911	0.00393224	0.14355335

7.2 Three Oxygen Atoms

Oxo Complex

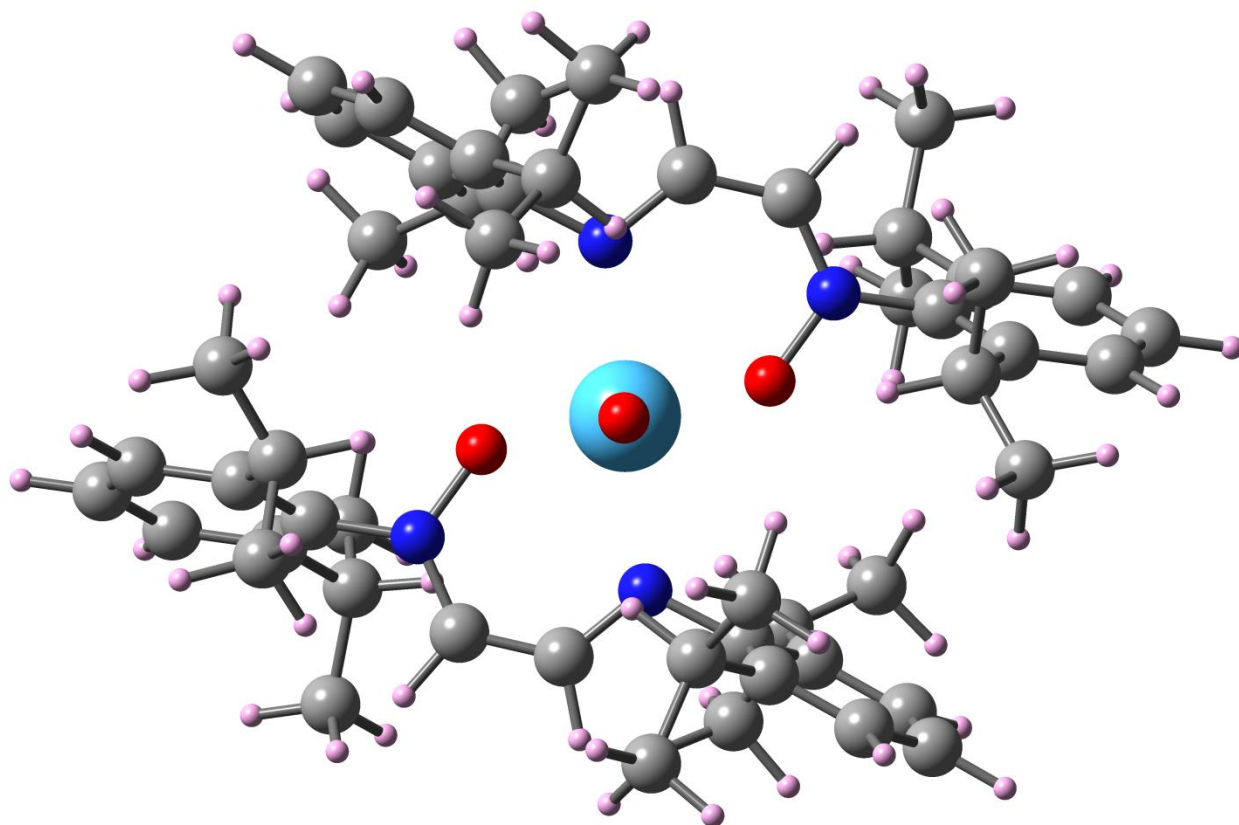


Fig. S56: NCCNO Oxo Complex

E	E_{zp}	H	G
-2518.2761	-2517.1314	-2517.0633	-2517.2380

N	-0.27337853	-2.24663115	-0.23674367
N	0.27309601	2.24668598	-0.23839426
C	0.76988737	-3.10956625	-0.11452649
C	2.11700966	-2.81505110	0.13348732
C	-0.77063318	3.10958397	-0.11974613
C	-2.11794266	2.81518007	0.12744628
C	-1.55825624	-2.89385668	-0.49613757
C	-2.43568321	-3.13569171	0.59845710
C	-3.65101226	-3.80455089	0.34738993
C	-3.99117121	-4.22693214	-0.94798357
C	-3.11643391	-3.97633251	-2.01437586
C	-1.88830608	-3.30689685	-1.81772117
C	-3.23089070	-2.19622528	2.85355020
C	-2.04675893	-2.75200800	2.02960075
C	-1.40218428	-3.96219586	2.76095845
C	3.59999658	-1.48945060	4.41907146
C	3.52382192	-2.28206175	3.08947941

C	3.79970577	-3.78911177	3.34423053
C	4.05566303	-1.38772626	0.71499462
C	4.47859875	-1.72465023	2.02719990
C	5.84550605	-1.55056333	2.33449436
C	6.74029091	-1.04304767	1.38101289
C	6.29016290	-0.70447753	0.09343413
C	4.93899581	-0.87159940	-0.27038405
C	-1.66530803	-2.30941122	-4.15781325
C	-0.95833092	-3.08362744	-3.01708347
C	-0.39029722	-4.43272821	-3.53453337
C	5.16599531	0.63203864	-2.34283965
C	4.45919592	-0.58131770	-1.69629176
C	4.63433163	-1.84631633	-2.58367771
C	1.55831375	2.89345601	-0.49728034
C	1.88931554	3.30609739	-1.81878211
C	3.11747584	3.97577856	-2.01460015
C	3.99153285	4.22645220	-0.94769371
C	3.65053506	3.80425484	0.34752315
C	2.43494840	3.13566653	0.59790502
C	1.66928895	2.30835283	-4.15892299
C	0.96056417	3.08221781	-3.01900445
C	0.39220182	4.43088264	-3.53717833
C	-3.58986873	1.49069954	4.41567486
C	-3.51915399	2.28516257	3.08685750
C	-3.79711428	3.79142774	3.34380666
C	-4.05581052	1.38885030	0.71422424
C	-4.47598465	1.72680568	2.02695452
C	-5.84221721	1.55249809	2.33728712
C	-6.73881101	1.04375465	1.38620251
C	-6.29127687	0.70392039	0.09800415
C	-4.94097318	0.87124846	-0.26875886
C	3.22867740	2.19843706	2.85435065
C	2.04487151	2.75235460	2.02878268
C	1.39817866	3.96228619	2.75874327
C	-5.17197615	-0.63478244	-2.33908288
C	-4.46321102	0.57865101	-1.69487061
C	-4.63822123	1.84248040	-2.58402900
H	0.55628682	-4.17221688	-0.23427854
H	2.82471706	-3.63408569	0.16870951
H	-0.55719997	4.17199004	-0.24184474
H	-2.82597315	3.63409276	0.15969548
H	-4.33393359	-4.00188497	1.16916585
H	-4.92942382	-4.74895867	-1.12245721
H	-3.38534089	-4.30521196	-3.01530935
H	-1.29089942	-1.96012202	1.96839037
H	2.49758225	-2.18881216	2.71700897
H	-3.99659264	-2.96066028	3.04093553
H	-3.70589056	-1.35268247	2.34057550
H	-2.87241835	-1.85140804	3.83313126
H	-2.11581391	-4.79376901	2.83796414
H	-1.09702431	-3.67954959	3.77805928
H	-0.51589953	-4.32671057	2.22736131

H	4.58261766	-1.59047368	4.89801610
H	2.84857300	-1.86853659	5.12440599
H	3.41097749	-0.42316827	4.25538028
H	3.69703936	-4.37942304	2.42511306
H	3.09346933	-4.18733798	4.08461931
H	4.81655302	-3.94320550	3.72857459
H	6.20754843	-1.80382656	3.32754834
H	7.78839736	-0.91016389	1.63941030
H	6.99539805	-0.31067629	-0.63196836
H	-0.12306262	-2.45362490	-2.70234226
H	3.38991690	-0.34933654	-1.65672053
H	-2.54409205	-2.84692329	-4.54053998
H	-0.96850223	-2.15985655	-4.99293875
H	-1.97127358	-1.31894268	-3.80536990
H	-1.19057415	-5.09287799	-3.89655986
H	0.15421872	-4.97037602	-2.74644050
H	0.30341626	-4.25634569	-4.36759779
H	5.08533177	1.52404510	-1.71183203
H	4.69353471	0.85978138	-3.30638898
H	6.22890783	0.43358330	-2.53696005
H	5.69386962	-2.12641173	-2.66101230
H	4.25538111	-1.65173433	-3.59511260
H	4.08278988	-2.70295533	-2.17735678
H	3.38711575	4.30446491	-3.01539881
H	4.92994932	4.74836245	-1.12163323
H	4.33300300	4.00155497	1.16968276
H	0.12538663	2.45167042	-2.70513763
H	-2.49381176	2.19442360	2.71138761
H	2.54852122	2.84613528	-4.54021713
H	0.97368526	2.15886779	-4.99507077
H	1.97482082	1.31785668	-3.80622109
H	-0.15317353	4.96845802	-2.74962305
H	-0.30080243	4.25390785	-4.37070143
H	1.19236132	5.09137831	-3.89883361
H	-4.57164593	1.58835130	4.89702944
H	-2.83776173	1.87089710	5.11968958
H	-3.39832070	0.42516837	4.25001506
H	-3.69854036	4.38258972	2.42475478
H	-3.08919841	4.19036010	4.08219998
H	-4.81293739	3.94342330	3.73165253
H	-6.20233302	1.80680125	3.33079590
H	-7.78630367	0.91064769	1.64696584
H	-6.99786428	0.30880456	-0.62535347
H	1.28995281	1.95960514	1.96716249
H	-3.39401612	0.34585814	-1.65612172
H	3.99354655	2.96370925	3.04171892
H	3.70487108	1.35480020	2.34262915
H	2.86946450	1.85429426	3.83389828
H	1.09202672	3.67978906	3.77558359
H	0.51219539	4.32571226	2.22391746
H	2.11090100	4.79458343	2.83631300
H	-5.09200270	-1.52603259	-1.70688789

H	-4.70066577	-0.86453336	-3.30272990
H	-6.23480043	-0.43517991	-2.53251802
H	-4.08570420	2.69938889	-2.17964603
H	-5.69767060	2.12306925	-2.66078333
H	-4.26039728	1.64602768	-3.59552854
O	-0.00121126	0.00000371	-2.28138653
O	-1.85434876	0.45490698	0.35629002
O	1.85398463	-0.45429054	0.35441462
N	-2.66739999	1.58825959	0.34930001
N	2.66637879	-1.58773854	0.35351111
Hf	-0.00047446	0.00020020	-0.47609889

7.3 Four Oxygen Atoms

Dioxo Complex (lower energy conformation)

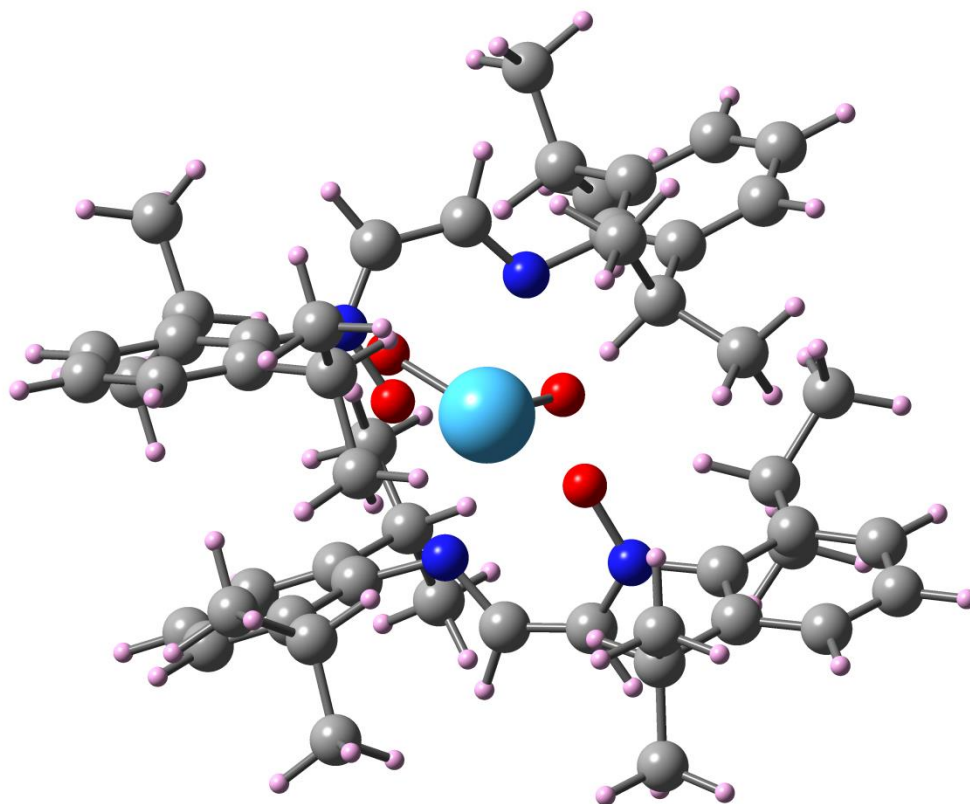


Fig. S57: NCCNO Dioxo Complex (lower energy conformation)

E	E_{zp}	H	G
-2593.4324	-2592.2867	-2592.2167	-2592.3966

N	-0.61445405	-1.89270314	-1.24435109
N	0.59089304	2.31337418	0.23849102
C	0.27200202	-2.92353822	-1.21963409
C	1.56446312	-2.94128222	-0.67536905
C	-0.30725002	3.10640624	0.77214506
C	-1.64576813	2.75501421	1.18251009
C	-1.92903815	-2.24557517	-1.77917713
C	-2.89502922	-2.83080422	-0.91012107
C	-4.14237432	-3.20748924	-1.45198511
C	-4.43444834	-3.00761923	-2.81000021
C	-3.47191327	-2.42833619	-3.64950428
C	-2.20597917	-2.04120916	-3.15926724
C	-3.76623529	-2.69510521	1.50256412
C	-2.59977320	-3.10651824	0.57011005
C	-2.24428017	-4.60262035	0.79120306
C	2.56938820	-2.98833223	4.04931131
C	2.57493520	-3.44328226	2.56813920

C	2.62125220	-4.99208338	2.47401019
C	3.51006527	-2.09531816	0.57422104
C	3.72520028	-2.81172021	1.77746914
C	5.05754439	-2.95175022	2.22140817
C	6.12013946	-2.38973118	1.49606212
C	5.87323245	-1.67388313	0.31227802
C	4.56054535	-1.50500212	-0.17598201
C	-1.71904313	-0.19690801	-4.84903337
C	-1.17501709	-1.45603411	-4.12943531
C	-0.70849006	-2.52771819	-5.15117139
C	5.08977039	0.55479404	-1.61505212
C	4.28268733	-0.75644806	-1.48335811
C	4.55348135	-1.68213213	-2.70199821
C	1.90963214	2.93253323	0.04114600
C	2.14581316	3.72226628	-1.11259109
C	3.40329826	4.35736833	-1.21513609
C	4.37837834	4.21313132	-0.21869202
C	4.11916432	3.41325526	0.90636007
C	2.88364022	2.75257721	1.06041908
C	1.66098813	3.48304427	-3.59870427
C	1.10588908	3.92328530	-2.22084417
C	0.61216705	5.39507641	-2.25731017
C	-1.90484415	-0.63760005	4.33726133
C	-2.30465017	0.85263206	4.15887432
C	-2.49698119	1.54404612	5.53119440
C	-3.45452326	1.28322610	1.88261914
C	-3.54188727	0.96990907	3.26159625
C	-4.83145437	0.72294406	3.77337529
C	-5.96199744	0.79010806	2.94154323
C	-5.82859445	1.09922508	1.57950912
C	-4.56248335	1.34885710	1.00469008
C	3.81068129	1.15976109	2.85741322
C	2.58201120	1.92824615	2.31890818
C	1.99903115	2.83552922	3.43920126
C	-5.23381740	0.71771505	-1.38382611
C	-4.43781134	1.69596713	-0.48378304
C	-4.90502438	3.15686924	-0.73288306
H	-0.03179800	-3.85768830	-1.69405313
H	2.17823917	-3.81979529	-0.83256106
H	-0.05105500	4.15284732	0.95636307
H	-2.31812918	3.55048727	1.47720511
H	-4.88971337	-3.66223028	-0.80643606
H	-5.40169642	-3.30419725	-3.20992325
H	-3.70057229	-2.27746918	-4.70195836
H	-1.72761313	-2.50846919	0.85664806
H	1.63016512	-3.10997924	2.12494616
H	-4.66043036	-3.31004425	1.33558910
H	-4.04226531	-1.64522413	1.35397810
H	-3.47266226	-2.82491522	2.55313119
H	-3.08337224	-5.24966240	0.50133504
H	-2.01781616	-4.79284737	1.84965014
H	-1.37103811	-4.89901537	0.19763602

H	3.46686827	-3.32876925	4.58232135
H	1.69548313	-3.40640926	4.56704235
H	2.52344419	-1.89556915	4.12369332
H	2.57795119	-5.33101739	1.43129311
H	1.77095713	-5.43329941	3.01083823
H	3.54398927	-5.38868141	2.91788122
H	5.26360240	-3.49955827	3.13758924
H	7.14081353	-2.50760019	1.85324814
H	6.70537352	-1.23968909	-0.23483202
H	-0.29637102	-1.13507309	-3.56333327
H	3.21952625	-0.49117604	-1.50477211
H	-2.59944820	-0.42475303	-5.46632642
H	-0.94443807	0.21877802	-5.50733141
H	-1.98681215	0.56602005	-4.10993631
H	-1.54147712	-2.87726822	-5.77697442
H	-0.27829802	-3.40324926	-4.64607535
H	0.05911000	-2.10629816	-5.81395243
H	4.92496737	1.21503709	-0.75715606
H	4.76499436	1.09148208	-2.51462819
H	6.16885547	0.36738103	-1.70829913
H	5.61269844	-1.97127715	-2.75352721
H	4.29093633	-1.15903809	-3.62988028
H	3.95143230	-2.59819120	-2.65196720
H	3.61506127	4.97003038	-2.08761116
H	5.33772439	4.71545136	-0.31859502
H	4.88397137	3.30091125	1.66906113
H	0.24235802	3.28069225	-2.02383916
H	-1.46036111	1.34781610	3.66268628
H	2.55219120	4.05778131	-3.88690629
H	0.89692407	3.63685828	-4.37262933
H	1.90639114	2.41652518	-3.56688827
H	0.17846001	5.70508241	-1.29570610
H	-0.15750701	5.51401344	-3.03106223
H	1.43297311	6.08724147	-2.48880719
H	-2.71525621	-1.20713109	4.81141237
H	-1.01396908	-0.71407806	4.97496838
H	-1.67778013	-1.09334008	3.36774026
H	-2.80007921	2.59280420	5.41759142
H	-1.55563412	1.51872312	6.09491644
H	-3.25565625	1.03679208	6.14046347
H	-4.95267338	0.47671904	4.82414137
H	-6.94820153	0.59581105	3.35623126
H	-6.71206549	1.13702109	0.94935307
H	1.82872314	1.17613809	2.05634916
H	-3.39149326	1.61787112	-0.81140506
H	4.58682435	1.83667214	3.23869325
H	4.25472532	0.52274604	2.08511616
H	3.50394927	0.51475904	3.69114828
H	1.75921413	2.23828417	4.32951533
H	1.08328009	3.34942625	3.11886724
H	2.72592821	3.60521628	3.73152929
H	-4.92488838	-0.31993502	-1.21878410

H	-5.03571838	0.95560907	-2.43568319
H	-6.31818548	0.79052306	-1.22124909
H	-4.32476933	3.87988430	-0.14350401
H	-5.96465147	3.28568325	-0.47256604
H	-4.77907837	3.41054226	-1.79262314
O	1.13639409	0.52963504	-2.27211817
O	-1.46892511	1.14489009	-1.69555413
O	-1.39282211	0.43299903	1.03705608
O	1.46305411	-0.82142806	0.43933503
N	-2.11417316	1.52300412	1.32760910
N	2.15422917	-1.96607515	0.07090801
Hf	0.00621800	0.22876202	-0.81279006

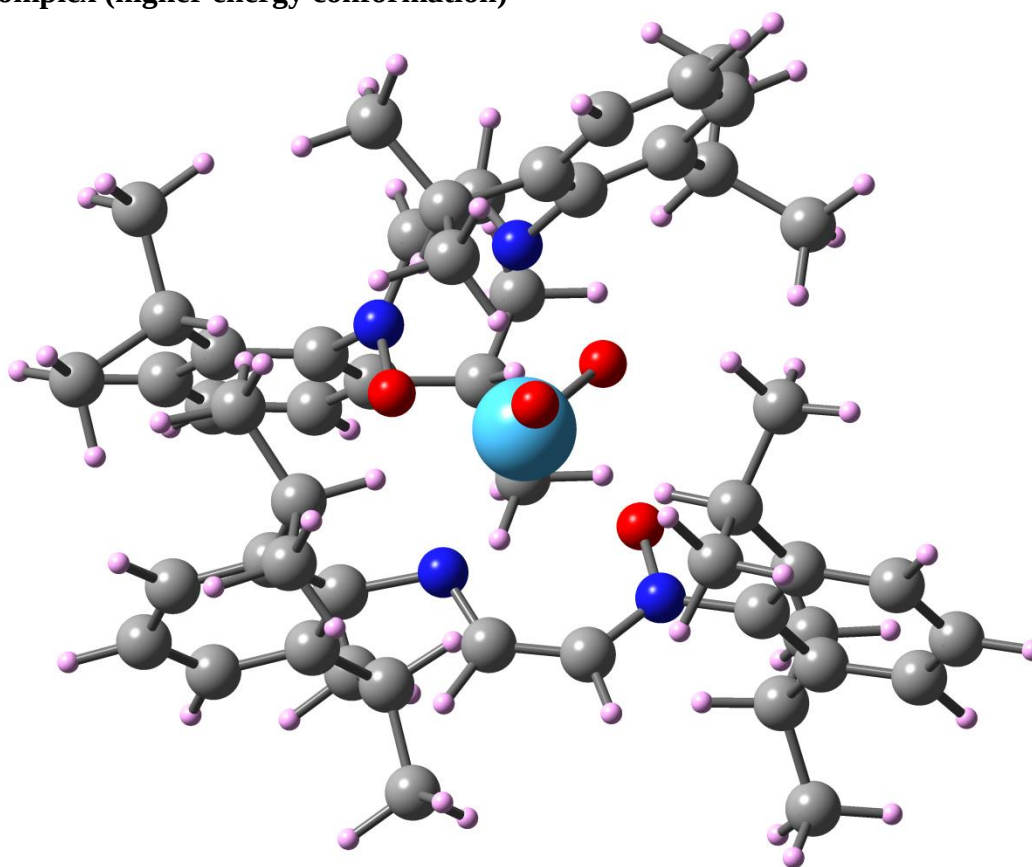
Dioxo Complex (higher energy conformation)

Fig. S58: NCCNO Dioxo Complex (higher energy conformation)

E	E_{zp}	H	G
-2593.4112	-2592.2644	-2592.1947	-2592.3738
O	-1.88336422	0.31719301	-0.10766565
O	1.80634114	-1.23627757	-0.52937704
O	0.41532419	0.57277951	-1.95830871
N	-0.25148690	-1.69405965	1.36366657
N	2.62251536	-1.94901322	0.34971888
N	-0.07805920	2.55343156	-0.50391325
N	-2.60845199	0.98719134	-1.02321225
C	0.74251770	-2.49416225	1.84749319
C	2.07843105	-2.56726808	1.43099740
C	-1.10827108	2.95912684	-1.19671491
C	-2.28272764	2.17210288	-1.50753358
C	-1.55711362	-1.99295841	1.94442602
C	-1.98077319	-1.30710645	3.11617519
C	-3.20348447	-1.68811399	3.71115667
C	-3.99250026	-2.71058133	3.16497557
C	-3.56930419	-3.36551530	1.99768171
C	-2.35382121	-3.02396226	1.36874105
C	-1.96075264	1.08612055	3.99174243

C	-1.13775882	-0.20860514	3.77248958
C	-0.53050972	-0.70061709	5.11349156
C	5.06685352	1.27304986	1.17927133
C	4.55306266	-0.12830700	1.59693004
C	5.05725952	-0.49597837	3.01778086
C	4.01457941	-2.06250428	-0.03354633
C	4.95754913	-1.19884420	0.57887768
C	6.31128813	-1.35570697	0.20804442
C	6.69450125	-2.30493251	-0.75157679
C	5.73055081	-3.12014265	-1.36900785
C	4.36816340	-3.01711815	-1.02272736
C	-3.04298314	-4.00496937	-0.89814315
C	-1.89886204	-3.79322366	0.12357610
C	-1.27854383	-5.16387695	0.51340151
C	2.98833261	-3.24937362	-3.12502442
C	3.31174937	-3.86511345	-1.73558330
C	3.72137898	-5.35228137	-1.86608697
C	1.01630254	3.51067951	-0.35056920
C	1.80934684	3.86887639	-1.48022278
C	2.84465835	4.80763005	-1.27696981
C	3.07900672	5.38155746	-0.02137096
C	2.27711019	5.01676578	1.07073938
C	1.24144096	4.07214285	0.93698888
C	2.91287027	2.53242771	-3.34295446
C	1.63313220	3.27924126	-2.88660541
C	1.23452640	4.37497075	-3.91058797
C	-5.85555555	0.45736674	1.70044851
C	-5.03962696	1.17007240	0.59632309
C	-5.60483846	2.59564182	0.33806340
C	-3.82131048	0.30449291	-1.50793618
C	-4.99033959	0.37514965	-0.71281245
C	-6.13781901	-0.26833110	-1.21879713
C	-6.10309202	-0.94667261	-2.44892724
C	-4.92091722	-0.99702370	-3.20303475
C	-3.73858794	-0.37301493	-2.74879728
C	1.14990056	3.46617915	3.41351405
C	0.33730399	3.76744195	2.13297049
C	-0.67060762	4.92836672	2.35851584
C	-2.09843873	-1.85048483	-4.04674695
C	-2.46085175	-0.41306297	-3.59723110
C	-2.60298282	0.51669993	-4.83369766
H	0.48964268	-3.16303294	2.67115395
H	2.76536103	-3.18899504	1.99267781
H	-1.12821339	3.97065129	-1.61045401
H	-2.99263873	2.58926251	-2.21096959
H	-3.53280203	-1.18476241	4.61721868
H	-4.92485556	-2.99887521	3.64576926
H	-4.18590561	-4.15532510	1.57626762
H	-0.30020948	0.04288430	3.11309074
H	3.46108762	-0.05222956	1.63321622
H	-2.79077646	0.93166416	4.69444781
H	-2.38191904	1.44820308	3.04433394

H	-1.31832240	1.87423966	4.40293917
H	-1.31424541	-0.96457519	5.83738900
H	0.09522108	0.08473062	5.55775888
H	0.09884825	-1.58647528	4.96029060
H	6.16450891	1.33071233	1.18322631
H	4.68254959	2.02697824	1.87711068
H	4.70918694	1.53747414	0.17713656
H	4.66110508	-1.46625713	3.34595028
H	4.72977419	0.26380418	3.73919255
H	6.15447921	-0.55029872	3.05426579
H	7.06498396	-0.71885340	0.66365047
H	7.74228131	-2.40393987	-1.02697184
H	6.04074367	-3.83965177	-2.12190824
H	-1.11466944	-3.20333114	-0.36569836
H	2.38707970	-3.82586290	-1.14804950
H	-3.82045643	-4.67309329	-0.50478054
H	-2.64926923	-4.46941955	-1.81247681
H	-3.51907863	-3.05549889	-1.16945963
H	-2.01853523	-5.79445950	1.02508200
H	-0.41976468	-5.03879240	1.18308608
H	-0.93582593	-5.69930840	-0.38266953
H	2.62579745	-2.22227496	-3.01021462
H	2.21118164	-3.83864938	-3.63122118
H	3.87974435	-3.23750864	-3.76729806
H	4.59370997	-5.47990776	-2.52031738
H	2.89685164	-5.93032634	-2.30417827
H	3.96461344	-5.78973505	-0.88906747
H	3.47307463	5.08799920	-2.11856563
H	3.87851453	6.10765459	0.10633890
H	2.45748876	5.47157358	2.04051890
H	0.85137489	2.51598747	-2.86856552
H	-4.01647668	1.27367277	0.97590062
H	3.78458744	3.19861976	-3.39399547
H	2.75748354	2.09944275	-4.34020687
H	3.13747295	1.71180136	-2.65338363
H	0.30664855	4.88772273	-3.61893684
H	1.08029877	3.92819606	-4.90206581
H	2.01533146	5.14114747	-4.00718279
H	-6.92125349	0.39181643	1.44441847
H	-5.77839368	1.02237223	2.63815916
H	-5.47530121	-0.55299320	1.88297219
H	-5.00936462	3.14391121	-0.40371253
H	-5.60446550	3.17759027	1.26858440
H	-6.63760904	2.54493931	-0.03135459
H	-7.06054173	-0.24311230	-0.64745397
H	-6.99996639	-1.43792568	-2.81845628
H	-4.90989277	-1.53071984	-4.14893821
H	-0.22255976	2.85642641	1.90496098
H	-1.61012624	-0.05179008	-3.00790586
H	1.77904507	4.31279741	3.71927327
H	1.77433766	2.58594696	3.23307479
H	0.47026366	3.24838119	4.24863377

H	-1.35248393	4.68527438	3.18472882
H	-1.27621128	5.12085349	1.46125177
H	-0.14937287	5.86133718	2.61296107
H	-1.98740301	-2.51774115	-3.18562372
H	-1.14300826	-1.83282938	-4.58531475
H	-2.85444601	-2.27886437	-4.71849890
H	-2.81698853	1.55416233	-4.54320681
H	-3.41415380	0.18171793	-5.49422406
H	-1.66953893	0.51571030	-5.41002371
O	1.30464511	0.91000999	1.44755434
Hf	0.34722952	0.12610786	0.10757245

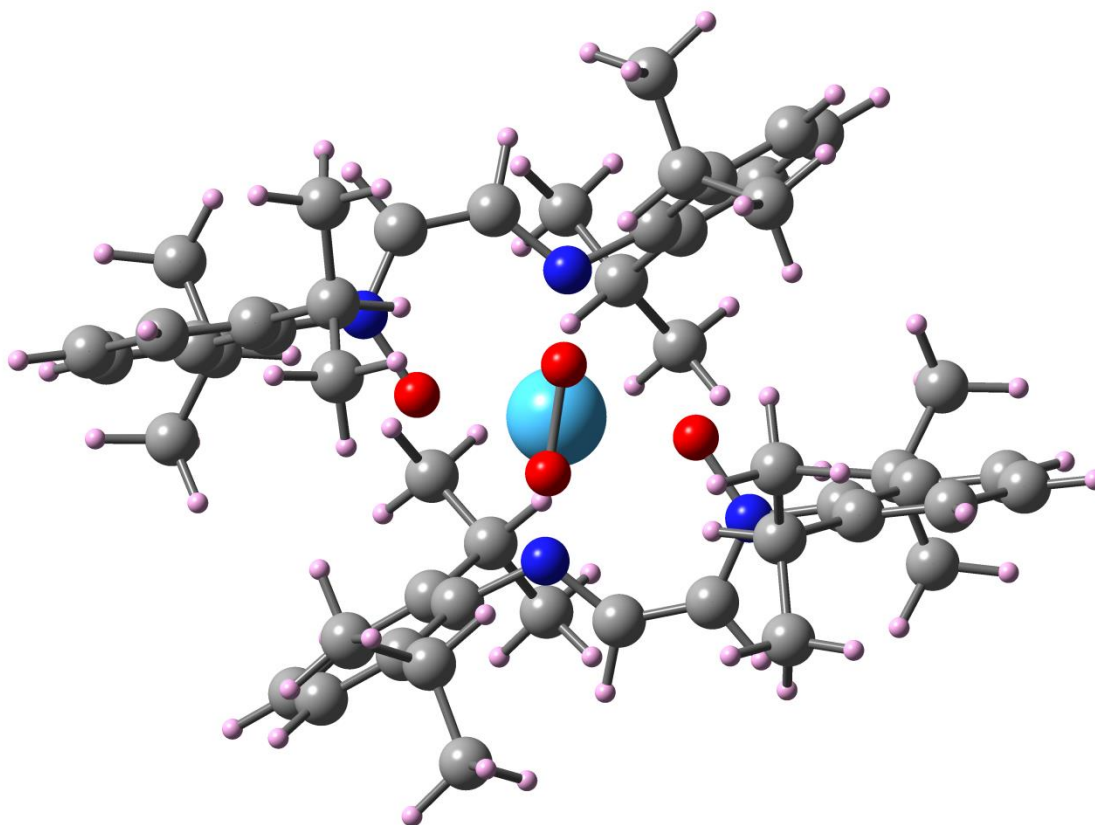
Peroxo Complex

Fig. S59: NCCNO Peroxo Complex

E	E_{zp}	H	G
-2593.4351	-2592.2885	-2592.2189	-2592.3989
O	2.00048906	-0.30359042	-0.05246628
O	-2.00077637	0.30962415	-0.05243948
O	-0.12090165	-0.81701441	2.23040111
O	0.10656800	0.74127572	2.25973858
N	0.15951819	2.10042826	-0.43209618
N	-2.76948127	1.45884843	0.14718078
N	-0.16156388	-2.07528756	-0.51127871
N	2.77037436	-1.45986409	0.08878274
C	-0.90053826	2.95873232	-0.43809960
C	-2.23596369	2.68145640	-0.11873843
C	0.89909010	-2.93161046	-0.55807741
C	2.23541044	-2.66896952	-0.23042568
C	1.41561784	2.72551831	-0.85183318
C	2.21212843	3.41725363	0.10146420
C	3.37418071	4.07648754	-0.35471208
C	3.74262578	4.05309808	-1.70758788
C	2.95222814	3.35240588	-2.63139369
C	1.78412005	2.67525538	-2.22456318

C	3.01739288	3.05953042	2.49573526
C	1.84088825	3.49291219	1.58622502
C	1.35320494	4.91703221	1.96642835
C	-3.14970882	0.57330895	4.18228840
C	-3.20603847	1.62322727	3.04458747
C	-3.34649444	3.05599717	3.62669637
C	-4.11615201	1.25657709	0.64713484
C	-4.33347828	1.33701627	2.04754511
C	-5.65876421	1.17175767	2.50443939
C	-6.70975542	0.92798349	1.60686746
C	-6.46019707	0.84130020	0.22732468
C	-5.15514605	0.99730105	-0.28230169
C	1.77069137	1.01137813	-4.16871356
C	0.92906363	1.94983626	-3.26867938
C	0.12965758	2.96344911	-4.13128294
C	-5.52190522	-0.32738515	-2.43616426
C	-4.89568158	0.93252774	-1.78955170
C	-5.40624200	2.22208998	-2.48882278
C	-1.41973794	-2.68457746	-0.94828101
C	-1.79547480	-2.58217888	-2.31601477
C	-2.96665876	-3.24223511	-2.74180890
C	-3.75257499	-3.97666279	-1.84074822
C	-3.37621117	-4.05253615	-0.49188681
C	-2.21095765	-3.41232520	-0.01733191
C	-1.78748295	-0.85486605	-4.20524253
C	-0.94366730	-1.82040242	-3.33669326
C	-0.14325457	-2.80411543	-4.23261487
C	3.16535441	-0.75081560	4.16617565
C	3.20516991	-1.74282211	2.97690106
C	3.32897431	-3.20405898	3.48786241
C	4.11765609	-1.28274468	0.59647123
C	4.33467948	-1.42225762	1.99234540
C	5.66111228	-1.28468276	2.45500432
C	6.71339749	-1.01035780	1.56773213
C	6.46385787	-0.86367347	0.19328529
C	5.15765075	-0.98987923	-0.32167761
C	-3.00277990	-3.19141240	2.40090162
C	-1.82614237	-3.54959392	1.45960557
C	-1.30127906	-4.97862774	1.76564197
C	5.53154185	0.42729350	-2.41376826
C	4.89783801	-0.85671421	-1.82431661
C	5.39993203	-2.11693944	-2.58072596
H	-0.70059275	3.99834557	-0.69821904
H	-2.93988849	3.50291195	-0.06285035
H	0.69892045	-3.95889127	-0.86315378
H	2.93902967	-3.49231581	-0.21255324
H	3.99326771	4.61440895	0.35894105
H	4.63729750	4.57504667	-2.03946719
H	3.24461977	3.33366086	-3.67855778
H	1.02072774	2.79607680	1.78011531
H	-2.24196019	1.56539562	2.53112349
H	3.86123581	3.76059887	2.43745301

H	3.37980963	2.06440788	2.21427825
H	2.68498397	3.02000858	3.54099756
H	2.14154032	5.66423538	1.80144100
H	1.06984773	4.95072489	3.02686900
H	0.47939705	5.21516376	1.37218053
H	-4.05624988	0.58645452	4.80320655
H	-2.28942559	0.78401258	4.82881883
H	-3.01604088	-0.43486130	3.77704266
H	-3.33683551	3.81610290	2.83416566
H	-2.51255792	3.26576842	4.30863103
H	-4.28333136	3.16835564	4.18949933
H	-5.86511143	1.22996219	3.56966897
H	-7.72322124	0.80361343	1.98168277
H	-7.28321470	0.64854720	-0.45554938
H	0.19865639	1.32909489	-2.73628849
H	-3.81272280	0.87182415	-1.94502869
H	2.47667303	1.57327875	-4.79407752
H	1.11673461	0.44287479	-4.84275916
H	2.34570388	0.29919555	-3.56463996
H	0.80798280	3.62722638	-4.68377991
H	-0.51856199	3.59066691	-3.50658498
H	-0.50278053	2.43857624	-4.86023898
H	-5.14737898	-1.24051061	-1.96100324
H	-5.26418944	-0.36829931	-3.50285898
H	-6.61729048	-0.32109501	-2.36117778
H	-6.49239830	2.33111243	-2.36914872
H	-5.18555504	2.18699046	-3.56403778
H	-4.93073149	3.11985492	-2.07313496
H	-3.26513114	-3.18307095	-3.78572029
H	-4.65003401	-4.48434911	-2.18692312
H	-3.99198812	-4.61723896	0.20362270
H	-0.21369515	-1.21625484	-2.78492295
H	2.24098437	-1.64762093	2.46906887
H	-2.49029598	-1.39793739	-4.85042360
H	-1.13474977	-0.26155751	-4.85881434
H	-2.36587480	-0.16558818	-3.57831298
H	0.50826432	-3.44902431	-3.62968954
H	0.48625059	-2.25512552	-4.94620507
H	-0.82128633	-3.45203938	-4.80392443
H	4.07027201	-0.81256984	4.78636412
H	2.30038150	-0.97861832	4.80055760
H	3.05162686	0.27918310	3.81308310
H	3.30827071	-3.92462186	2.65946332
H	2.49405245	-3.43649746	4.16118460
H	4.26572158	-3.35431335	4.04197474
H	5.86740743	-1.38889734	3.51668108
H	7.72779164	-0.90844873	1.94677986
H	7.28761486	-0.64686539	-0.48143133
H	-1.02069977	-2.84337434	1.67965130
H	3.81522123	-0.78249762	-1.97623412
H	-3.82490616	-3.91608895	2.32461008
H	-3.40008426	-2.19724245	2.16712329

H	-2.65715065	-3.18533870	3.44263121
H	-1.01030814	-5.05813899	2.82158029
H	-0.42451725	-5.22534431	1.15266675
H	-2.07285635	-5.73528880	1.56747733
H	5.16790430	1.31976759	-1.89295888
H	5.26774447	0.52193654	-3.47551007
H	6.62727876	0.40809261	-2.34600668
H	4.91709936	-3.02890604	-2.20640141
H	6.48503750	-2.23942584	-2.46478988
H	5.18100645	-2.03190533	-3.65351388
Hf	-0.00062183	-0.00366999	0.39967549

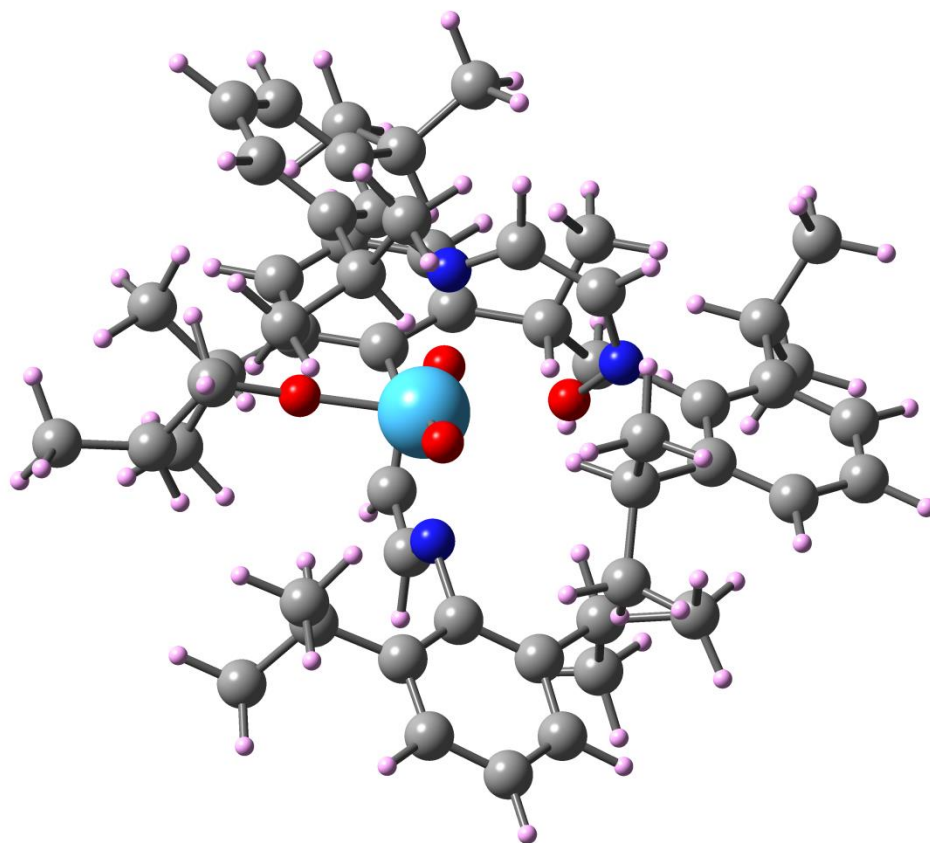
Propene Chemisorbed on Dioxo Complex forming Octahedral Complex

Fig. S60: NCCNO Propene Chemisorbed on Dioxo Complex forming Octahedral Complex

E	E_{zp}	H	G
-2711.3502	-2710.1212	-2710.0466	-2710.2356
N	0.39088226	-0.67005564	-2.28476366
N	-0.45795481	-0.30835942	2.21283504
C	-0.56545213	-0.38407872	-3.13889686
C	-1.86487390	0.15694808	-2.84231263
C	0.34822475	0.44268510	3.01107479
C	1.42539711	1.26651144	2.65598913
C	1.56378459	-1.33348950	-2.85915773
C	2.74160411	-0.56695737	-3.07272005
C	3.86221231	-1.22416981	-3.61861243
C	3.81343954	-2.58921357	-3.94753696
C	2.63403102	-3.31805798	-3.74026939
C	1.47990545	-2.71457114	-3.19223895
C	4.14696299	1.48477390	-2.40144263
C	2.75831496	0.94223454	-2.80669910
C	2.24374646	1.70994925	-4.05795343
C	-2.88178131	4.62069593	-0.90840510
C	-2.87417848	3.50577156	-1.98613530
C	-3.02743241	4.10803120	-3.40804029

C	-3.68183241	1.08809819	-1.53624158
C	-3.96158428	2.46383373	-1.70768011
C	-5.31406996	2.85340646	-1.61741820
C	-6.32021360	1.90933352	-1.35556026
C	-5.99608296	0.55658329	-1.16635921
C	-4.66015070	0.10637418	-1.24390155
C	0.46583134	-4.89516918	-2.29444761
C	0.20145925	-3.54769856	-3.01112099
C	-0.47636696	-3.80811299	-4.38556474
C	-4.98021858	-1.95115499	0.23564903
C	-4.31745168	-1.37415548	-1.03991807
C	-4.73445159	-2.20114727	-2.28656984
C	-1.62587226	-0.86273053	2.89191906
C	-1.66334884	-2.24559812	3.22617413
C	-2.79845724	-2.74409235	3.89950377
C	-3.86673611	-1.90641480	4.25003106
C	-3.81305274	-0.54348902	3.92255426
C	-2.70648801	0.00352388	3.23863056
C	-0.94346579	-4.39714009	2.05929706
C	-0.50065199	-3.19841245	2.93547354
C	0.16216951	-3.67743243	4.25507957
C	1.21302866	4.64364603	-1.11724894
C	1.35721419	4.32376005	0.39328413
C	1.02426056	5.56618333	1.25977692
C	2.98662802	2.47488597	1.19011411
C	2.75917928	3.78795598	0.69975689
C	3.88082612	4.62112933	0.51045060
C	5.17636300	4.17169344	0.81186671
C	5.37288711	2.87028985	1.29714983
C	4.28839811	1.98670586	1.48566177
C	-4.02474235	1.97494594	2.26318224
C	-2.69988667	1.50407673	2.91369270
C	-2.41371021	2.35137215	4.18431925
C	5.64809981	-0.16441828	1.18657085
C	4.55166358	0.56639697	2.00186282
C	4.94218897	0.58904959	3.50515899
H	-0.41717650	-0.61224675	-4.19621010
H	-2.59212725	0.18682837	-3.64365092
H	0.14527788	0.42035376	4.08292452
H	1.99447644	1.72497219	3.45530337
H	4.77674804	-0.66525146	-3.79245520
H	4.68874026	-3.07868275	-4.36857785
H	2.60452454	-4.37207775	-4.00356843
H	2.07596396	1.14629903	-1.97260805
H	-1.89395653	3.01857537	-1.93132663
H	4.86373875	1.44745282	-3.23321733
H	4.56367681	0.92088122	-1.56063653
H	4.06078366	2.53212957	-2.08710148
H	2.89506651	1.52150266	-4.92229020
H	2.23638456	2.79154488	-3.86701107
H	1.22514525	1.40962618	-4.33415867
H	-3.83080869	5.17207204	-0.90351272

H	-2.07865229	5.34238755	-1.10466467
H	-2.72744078	4.19737428	0.09084263
H	-2.99278205	3.32838587	-4.18017846
H	-2.21833178	4.82232133	-3.60882733
H	-3.98150954	4.64064001	-3.51347207
H	-5.57982864	3.89900961	-1.74870112
H	-7.35725591	2.23022020	-1.29111335
H	-6.78341753	-0.15835007	-0.94641797
H	-0.49681448	-3.00175383	-2.36630552
H	-3.23505590	-1.49957057	-0.90074963
H	1.13342475	-5.55186972	-2.86893047
H	-0.48410618	-5.42590368	-2.15061190
H	0.90443916	-4.73064453	-1.30468156
H	0.17739586	-4.39517776	-5.04537696
H	-0.71849791	-2.87328083	-4.90915792
H	-1.40967452	-4.36953680	-4.24585333
H	-4.70160136	-1.37516185	1.12492194
H	-4.62959125	-2.97884874	0.38789732
H	-6.07695056	-1.97493030	0.16356086
H	-5.81930940	-2.15295566	-2.45673184
H	-4.45603965	-3.25221051	-2.14099748
H	-4.23529194	-1.84554188	-3.19846791
H	-2.83827006	-3.79916386	4.15997839
H	-4.72986634	-2.30930510	4.77537196
H	-4.64264952	0.10324360	4.19761141
H	0.25969431	-2.65250959	2.37009494
H	0.62760247	3.54288682	0.62427229
H	-1.71412156	-5.00147375	2.55790900
H	-0.08426682	-5.05293089	1.85771747
H	-1.33226536	-4.02812955	1.10405496
H	0.50672317	-2.82868893	4.86178482
H	1.02933549	-4.31464819	4.03384800
H	-0.53882512	-4.26216087	4.86618162
H	1.92589296	5.41626514	-1.43590181
H	0.20134221	5.01030016	-1.33488356
H	1.38795768	3.74343536	-1.71715684
H	1.11139185	5.33854070	2.32985725
H	-0.00465626	5.89778591	1.06527110
H	1.69421859	6.40772153	1.03909009
H	3.73735156	5.63232991	0.13758426
H	6.02840124	4.83210213	0.66796177
H	6.38058431	2.53009005	1.51992233
H	-1.89998218	1.69162064	2.19001602
H	3.63528887	-0.02222863	1.89684205
H	-4.87233764	1.89372676	2.95651343
H	-4.25962343	1.38929086	1.36881744
H	-3.94398149	3.03039175	1.96863350
H	-2.39552381	3.42183165	3.93638430
H	-1.44925361	2.09121593	4.63656082
H	-3.19252105	2.19248121	4.94249359
H	5.39680454	-0.20205882	0.12038314
H	5.74038404	-1.19705345	1.54562197

H	6.62961523	0.31727495	1.28972188
H	4.16769847	1.06362041	4.12064949
H	5.87785079	1.14315245	3.66027804
H	5.08793605	-0.43470550	3.87384626
O	-1.17391698	-2.06096160	-0.34878175
O	1.74789136	-1.70041286	0.40304174
O	1.12077474	1.24493749	0.28157587
O	-1.51210227	0.73554704	-0.59197395
N	1.84014900	1.60799975	1.40145707
N	-2.28943183	0.63354300	-1.67683146
C	3.28623847	-3.00937163	1.77898494
H	2.79542117	-2.54920224	2.63462102
C	2.71922762	-2.74114667	0.40945235
H	3.53666459	-2.47921575	-0.29023871
H	2.27072615	-3.67279680	0.00607401
C	4.31268659	-4.09392899	1.97205288
H	5.07013622	-4.07881738	1.17239930
H	4.83173498	-3.99612040	2.93383621
H	3.86098956	-5.10361553	1.95128522
Hf	0.06541144	-0.75958333	0.07171472

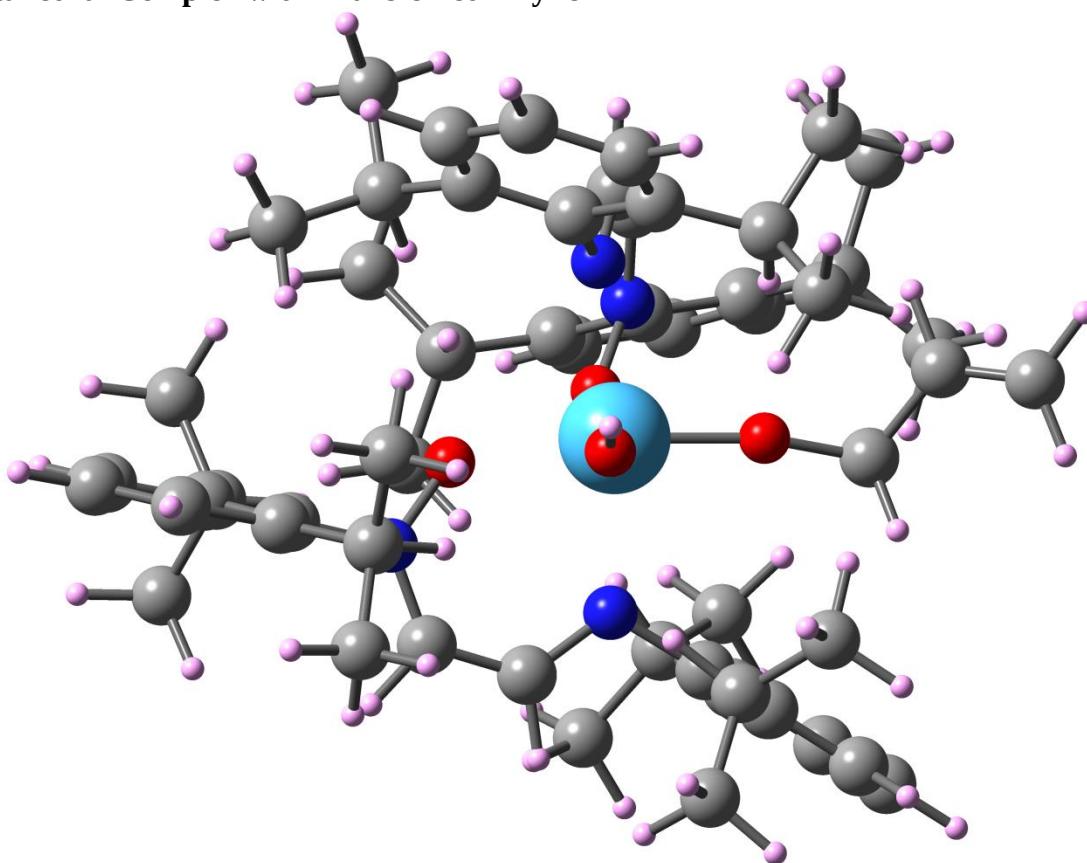
Octahedral Complex with Transferred Allylic H

Fig. S61: NCCNO Octahedral Complex with Transferred Allylic H

E	E_{zp}	H	G
-2711.4446	-2710.2140	-2710.1398	-2710.3266
N	-0.24415000	0.67812400	-2.26831700
N	0.30651300	0.36012700	2.24447100
C	0.72658900	0.28552900	-3.13799200
C	1.95033700	-0.32345600	-2.84387700
C	-0.51975000	-0.35676000	3.05314400
C	-1.57841500	-1.19524500	2.68895900
C	-1.36955700	1.35149400	-2.91073500
C	-2.52795900	0.60155400	-3.25993900
C	-3.59373600	1.27292300	-3.89572300
C	-3.52001000	2.64483500	-4.18622600
C	-2.36815700	3.36700800	-3.84141600
C	-1.27650700	2.74185000	-3.19974400
C	-4.01504000	-1.39570900	-2.61110500
C	-2.60260400	-0.90925600	-3.01306700
C	-2.11354100	-1.68762900	-4.26678000
C	2.85918500	-4.63113100	-0.29979800
C	2.86312000	-3.62094900	-1.47480300
C	2.97515500	-4.35953800	-2.83587300

C	3.73086700	-1.19343200	-1.38311200
C	3.98213300	-2.58754200	-1.32464900
C	5.31845200	-3.00541000	-1.15742900
C	6.35980500	-2.06984800	-1.04902700
C	6.08145300	-0.69521900	-1.09450800
C	4.76061000	-0.22445300	-1.25407600
C	-0.37442400	4.79485700	-1.97182800
C	-0.03177800	3.57039900	-2.85845000
C	0.70668200	4.01687800	-4.14867600
C	5.00211900	1.98659800	-0.00672700
C	4.48578400	1.28252600	-1.28818200
C	5.10137100	1.93053400	-2.55687700
C	1.39681100	1.02763000	2.95080200
C	1.25607300	2.39232000	3.33326000
C	2.31997300	3.01033900	4.02487900
C	3.49102500	2.30426900	4.33897900
C	3.60993500	0.95710500	3.96578700
C	2.57662600	0.29379200	3.26869500
C	0.20430300	4.59492100	2.52218300
C	-0.03875400	3.17297000	3.08343700
C	-0.88053000	3.24587800	4.38727800
C	-1.12036200	-4.48201800	-1.14662600
C	-1.32652700	-4.20086500	0.36440000
C	-0.98035500	-5.44857100	1.21884100
C	-3.05485500	-2.43398000	1.14255700
C	-2.75701900	-3.72612200	0.63419900
C	-3.83599300	-4.60111900	0.39191900
C	-5.15813400	-4.21601400	0.66227300
C	-5.42596100	-2.93559300	1.16808000
C	-4.38670700	-2.01100900	1.40548300
C	4.15083300	-1.55162100	2.41881100
C	2.73017100	-1.19191800	2.91641700
C	2.36769900	-2.08653000	4.13531300
C	-5.83202700	0.07280900	1.08133800
C	-4.73309300	-0.61349900	1.93277800
C	-5.17541000	-0.67092800	3.42053600
H	0.56662500	0.49506800	-4.19635200
H	2.65817100	-0.48632500	-3.64755400
H	-0.35279200	-0.28843100	4.12877600
H	-2.15784600	-1.66742000	3.47227300
H	-4.48677500	0.71789600	-4.16995300
H	-4.35072600	3.14353900	-4.68071600
H	-2.31220200	4.42813500	-4.07385700
H	-1.92595800	-1.14721600	-2.18526700
H	1.90431900	-3.09306600	-1.45420300
H	-4.72410800	-1.33634400	-3.44821600
H	-4.41991500	-0.80558300	-1.78056400
H	-3.97347900	-2.44371800	-2.28839500
H	-2.74315800	-1.45740000	-5.13736800
H	-2.16083500	-2.77100600	-4.08921800
H	-1.07794100	-1.43124800	-4.51953100
H	3.79259600	-5.20729500	-0.25429500

H	2.03618200	-5.34768500	-0.41842500
H	2.72841600	-4.11555400	0.65923400
H	2.94157200	-3.65339400	-3.67523300
H	2.14514900	-5.06861200	-2.95614600
H	3.91491500	-4.92349200	-2.90687500
H	5.54693600	-4.06727400	-1.11657100
H	7.38495800	-2.41160600	-0.92584700
H	6.89479400	0.01948200	-0.99796700
H	0.65135700	2.94590600	-2.27652000
H	3.40393000	1.43933300	-1.31976700
H	-1.06664600	5.48484700	-2.47334600
H	0.54022300	5.35535400	-1.73450900
H	-0.82713700	4.47398300	-1.02692200
H	0.07353600	4.66659000	-4.76820300
H	0.99847900	3.15329900	-4.76070200
H	1.61709100	4.57704700	-3.89443000
H	4.53649100	1.56721800	0.89278800
H	4.76333600	3.05836900	-0.04703500
H	6.09132000	1.89623300	0.09941800
H	6.19408800	1.82031200	-2.57324600
H	4.87034700	3.00362400	-2.58535300
H	4.70360900	1.47381800	-3.47225300
H	2.22594600	4.05045500	4.32682200
H	4.29954900	2.79632900	4.87505200
H	4.51684500	0.41399700	4.21761600
H	-0.62826500	2.63191900	2.33873700
H	-0.63351500	-3.40032000	0.63659000
H	0.73292400	5.23918800	3.23760200
H	-0.75774500	5.07009100	2.29150200
H	0.78874800	4.55993700	1.59421300
H	-1.11786700	2.24284600	4.76514100
H	-1.82492800	3.77532500	4.20239300
H	-0.33829300	3.78209700	5.17806900
H	-1.79261700	-5.27316300	-1.50554900
H	-0.08934600	-4.80548300	-1.33639600
H	-1.30629000	-3.57628800	-1.73439200
H	-1.11862700	-5.24793600	2.28907900
H	0.06703300	-5.73617100	1.06016600
H	-1.60782000	-6.30992700	0.95398700
H	-3.63735800	-5.59660700	0.00315200
H	-5.97544300	-4.90938100	0.47832100
H	-6.45397500	-2.64393100	1.36605700
H	2.03250000	-1.41910100	2.10295900
H	-3.83492100	0.00965200	1.87311400
H	4.90038000	-1.46083700	3.21638800
H	4.45775800	-0.91404400	1.58358500
H	4.17172900	-2.59216100	2.07029600
H	2.47369400	-3.14878000	3.87495300
H	1.33679300	-1.92158700	4.46895300
H	3.03499300	-1.87621300	4.98256500
H	-5.57018400	0.07555500	0.01671800
H	-5.96048300	1.11393900	1.40351100

H	-6.80143600	-0.43091200	1.18802800
H	-4.39590600	-1.10263900	4.06058200
H	-6.07934900	-1.28340500	3.53616500
H	-5.40013800	0.33764200	3.79192600
O	1.29404700	2.07300600	0.04831700
O	-1.64402400	1.71754800	0.16332700
O	-1.20220500	-1.10596000	0.33673800
O	1.50194600	-0.75194300	-0.53670900
N	-1.95834700	-1.52566400	1.42009500
N	2.37446500	-0.73488400	-1.61578500
C	-3.36319400	3.03372300	1.27819200
H	-3.25008600	2.44973200	2.19400400
C	-2.92179300	2.33688200	0.00800800
H	-3.65937200	1.56153800	-0.25716400
H	-2.89233900	3.05214300	-0.82542400
C	-3.88441800	4.27610900	1.32891900
H	-3.99450800	4.88587500	0.43293200
H	-4.21886400	4.72045200	2.26395300
H	1.89692500	2.70430700	0.45936700
Hf	-0.03285500	0.64487700	-0.00387800

7.4 Five Oxygen Atoms

Oxo Complex with Adsorbed Oxygen Molecule (planar conformation)

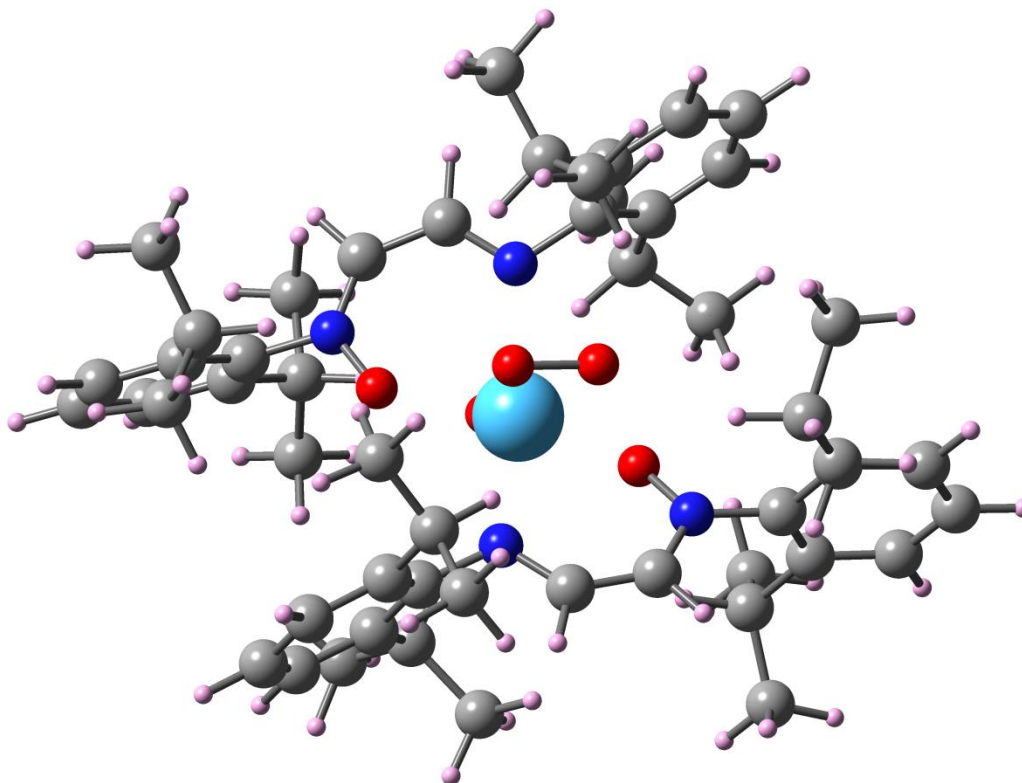


Fig. S62: NCCNO Oxo Complex with Adsorbed Oxygen Molecule (planar conformation)

E	E_{zp}	H	G
-2668.5989	-2667.4476	-2667.3770	-2667.5560
O	-2.12496678	0.42756750	0.20670625
O	1.97827068	-0.79098754	-0.55309524
O	-0.41343542	0.02228417	-1.84501671
N	-0.17937231	-2.03616977	0.85957891
N	2.80720818	-1.54323712	0.27525408
N	0.04540812	2.37471613	-0.35957435
N	-2.81988743	1.29885686	-0.52813533
C	0.90548379	-2.70781423	1.34724589
C	2.26509210	-2.47039090	1.11700893
C	-1.02992355	3.02483083	-0.71542202
C	-2.35708087	2.48231007	-0.90456240
C	-1.46024134	-2.64539938	1.20776078
C	-1.95876519	-2.54677777	2.53770827
C	-3.18524918	-3.17889681	2.84144082
C	-3.89978110	-3.88693518	1.86680599
C	-3.38975390	-3.98058264	0.56137929
C	-2.16730556	-3.37460253	0.20616959

C	-2.08717211	-0.65957104	4.25186793
C	-1.22171411	-1.79772903	3.65534027
C	-0.75451950	-2.76954063	4.77214611
C	5.06455125	1.46066509	2.01709897
C	4.61367268	-0.02144706	2.03005385
C	5.09187408	-0.73022776	3.32602488
C	4.22088053	-1.50458115	-0.05127727
C	5.09915013	-0.77483384	0.78885721
C	6.47051534	-0.77804705	0.45345302
C	6.93760867	-1.46341699	-0.67839352
C	6.04150579	-2.16739594	-1.49945747
C	4.66335103	-2.20567913	-1.20390746
C	-2.66341724	-3.86088442	-2.27286156
C	-1.59004968	-3.55158981	-1.20407350
C	-0.51720582	-4.67754421	-1.22348321
C	3.73004283	-2.49149171	-3.55781446
C	3.70921045	-3.00652693	-2.09588218
C	4.03812359	-4.52208757	-2.03845680
C	1.27430795	3.17313181	-0.26310749
C	2.17716138	3.15201488	-1.36121881
C	3.34344110	3.93910018	-1.25737489
C	3.60292303	4.71400981	-0.11721752
C	2.68905478	4.72120951	0.94638327
C	1.50556968	3.95450015	0.90215144
C	3.09754474	1.55980291	-3.14343831
C	1.88525511	2.39139035	-2.66070336
C	1.42583411	3.38369768	-3.76492102
C	-5.41626572	0.18750019	2.52242262
C	-4.92699498	1.27459854	1.53297263
C	-5.58825156	2.64539050	1.84325751
C	-4.18295694	0.89532559	-0.92170408
C	-5.18491734	0.87130775	0.07765799
C	-6.48301948	0.50522980	-0.33410198
C	-6.75053874	0.17474195	-1.67154632
C	-5.72591046	0.20331421	-2.63036726
C	-4.40500980	0.56180541	-2.28453883
C	1.22980704	3.72963159	3.43307834
C	0.52741772	4.01619809	2.08233037
C	-0.20486522	5.38538797	2.12153709
C	-3.35503562	-0.63322006	-4.29560943
C	-3.30543111	0.59753849	-3.35748648
C	-3.41548406	1.89234535	-4.21156841
H	0.70673622	-3.56232727	1.99462248
H	2.98939283	-3.09670128	1.62352800
H	-0.95761801	4.09101659	-0.94305417
H	-3.07788339	3.11336967	-1.40736916
H	-3.57924247	-3.11438348	3.85344080
H	-4.84229780	-4.36766283	2.11991102
H	-3.94710594	-4.53770600	-0.18493769
H	-0.33412963	-1.32035170	3.23432331
H	3.51996575	-0.01995406	2.03537812
H	-2.99634571	-1.04746170	4.73139913

H	-2.38053001	0.04881928	3.46939560
H	-1.51291932	-0.10768968	5.00747298
H	-1.60769015	-3.25643554	5.26360287
H	-0.19042032	-2.22303520	5.53989079
H	-0.10683055	-3.56105941	4.37254031
H	6.15760474	1.55699622	2.07305049
H	4.63651155	1.98599719	2.88058479
H	4.71990914	1.97059424	1.11025580
H	4.73053886	-1.76597696	3.37351860
H	4.71386199	-0.19861617	4.20907295
H	6.18849535	-0.75400893	3.38683202
H	7.17348975	-0.23352968	1.07850709
H	7.99783820	-1.44937861	-0.92115834
H	6.41556817	-2.69507412	-2.37326929
H	-1.09638112	-2.61487206	-1.49110232
H	2.68804818	-2.86808513	-1.72887198
H	-3.07093974	-4.87513565	-2.15993187
H	-2.21524320	-3.79805822	-3.27264406
H	-3.49840578	-3.15158802	-2.22459200
H	-0.96280173	-5.64027561	-0.93591898
H	0.30905462	-4.46363114	-0.53788640
H	-0.09852755	-4.78276519	-2.23388740
H	3.44499805	-1.43504480	-3.59971810
H	3.01569095	-3.06096852	-4.16695349
H	4.72347391	-2.60135052	-4.01372127
H	5.04184521	-4.72954721	-2.43312142
H	3.31577905	-5.08899786	-2.64057402
H	3.99590943	-4.90162065	-1.00933599
H	4.05016153	3.94813304	-2.08257719
H	4.50912367	5.31249507	-0.06025484
H	2.89587016	5.32645202	1.82502917
H	1.06758416	1.68224204	-2.49357737
H	-3.84794790	1.37885824	1.68669788
H	3.95916516	2.18917506	-3.40473347
H	2.81653456	0.99182788	-4.03996117
H	3.40533905	0.84487683	-2.37300735
H	0.53287661	3.94615261	-3.45803177
H	1.18082915	2.83601914	-4.68434316
H	2.21435550	4.11199519	-4.00004587
H	-6.50340683	0.04598849	2.46309542
H	-5.17456549	0.48334094	3.55114580
H	-4.93045011	-0.77321819	2.32083206
H	-5.22174001	3.43248061	1.17070380
H	-5.36520695	2.94787448	2.87460943
H	-6.67951363	2.59302623	1.73468679
H	-7.28616539	0.47872884	0.39678432
H	-7.75821674	-0.10746016	-1.96714195
H	-5.94834874	-0.06639568	-3.65830480
H	-0.22460654	3.23079816	1.96012514
H	-2.31896394	0.56817847	-2.87542471
H	1.97723899	4.49616869	3.67760145
H	1.72084509	2.75202170	3.40115069

H	0.48880059	3.71579154	4.24323217
H	-0.91986926	5.41124738	2.95474238
H	-0.75719357	5.58010212	1.19155214
H	0.50621786	6.21033603	2.26117446
H	-3.32269949	-1.56631811	-3.72737831
H	-2.47921014	-0.61473561	-4.95579172
H	-4.25164821	-0.64095473	-4.93087330
H	-3.33651639	2.80579277	-3.60779894
H	-4.37423820	1.93204580	-4.74685129
H	-2.60862929	1.91439682	-4.95497664
O	1.34033650	0.80078411	1.71064391
O	0.00855983	0.77953996	2.12985490
Hf	0.08883429	-0.00489197	-0.08366553

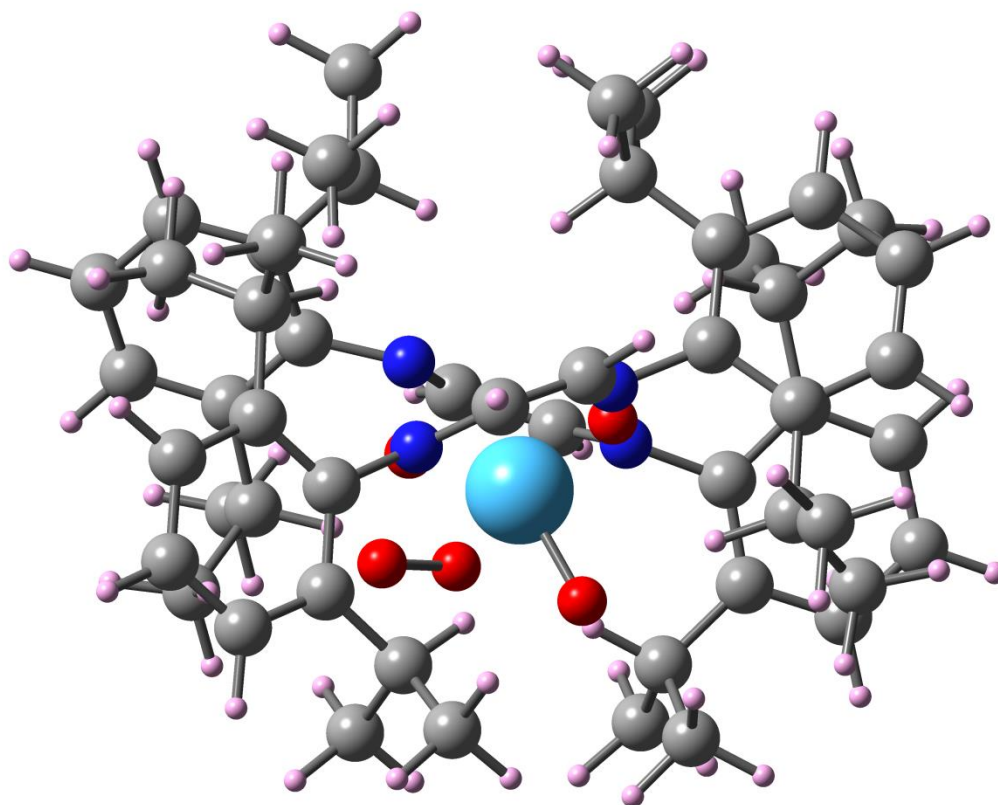
Oxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

Fig. S63: NCCNO Oxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

E	E_{zp}	H	G
-2668.5932	-2667.4430	-2667.3737	-2667.5494
O	-2.16094299	-0.53195319	-0.20656142
O	-1.06621964	1.17286005	-2.02839380
N	0.00012426	-1.93468018	0.98198845
N	-2.92629821	-1.65020349	0.10724911
N	2.75586261	1.14356248	-0.39710841
N	0.31394074	2.86951355	0.36059620
C	-1.05758350	-2.74301431	1.28193153
C	-2.38640441	-2.65278538	0.84938238
C	2.59904245	2.45260760	-0.45922361
C	1.44821264	3.27906636	-0.13279342
C	1.23526488	-2.39532220	1.62336109
C	2.02010141	-3.40835352	1.00148535
C	3.14333352	-3.90503006	1.69905241
C	3.48157703	-3.43211609	2.97459414
C	2.69697174	-2.43468968	3.57315585
C	1.57138454	-1.89844560	2.91378068
C	2.86604961	-4.03631473	-1.32691436
C	1.65836405	-4.02062077	-0.35669473

C	1.09262367	-5.45603387	-0.17838357
C	-3.15923386	-1.34803049	-3.81608441
C	-3.31424951	-2.40745535	-2.69317326
C	-3.47855776	-3.82874585	-3.28971399
C	-4.27906656	-1.65882102	-0.41244097
C	-4.47545222	-2.04446445	-1.76434752
C	-5.80120756	-2.06465160	-2.24645200
C	-6.87976113	-1.71686252	-1.41779477
C	-6.65361591	-1.32360007	-0.08944560
C	-5.34616419	-1.27338985	0.43826225
C	1.53784599	0.29077799	4.24352650
C	0.70340123	-0.86010569	3.63119018
C	-0.16604001	-1.53920383	4.72476643
C	-5.65728829	0.64031628	2.08220190
C	-5.12146835	-0.80038857	1.87725705
C	-5.75708683	-1.77737375	2.90126031
C	4.04789012	0.53261008	-0.78544410
C	4.23892946	0.14069158	-2.13245674
C	5.47615176	-0.46707522	-2.44318135
C	6.45954978	-0.66023515	-1.46432940
C	6.23876687	-0.23811330	-0.14278969
C	5.02381337	0.36789997	0.23190238
C	2.82193950	-0.90526785	-3.99271825
C	3.22647909	0.39594163	-3.25367663
C	3.79072107	1.44911551	-4.24748424
C	-2.18327607	1.82802897	3.25964508
C	-1.04795136	2.81683081	2.89281610
C	-0.59133422	3.63332174	4.13177494
C	-0.77320863	3.78554640	0.51133282
C	-1.47611754	3.74511901	1.75468904
C	-2.55923205	4.62029166	1.94803979
C	-2.96516188	5.50396521	0.93621260
C	-2.29721089	5.50291284	-0.29639637
C	-1.19901015	4.65532753	-0.55001265
C	5.42848982	-0.04910211	2.73374362
C	4.81609197	0.88209033	1.66132484
C	5.40178659	2.31536617	1.81362976
C	-1.68957228	4.38767648	-3.04046310
C	-0.60321522	4.66562261	-1.96751100
C	0.12803016	6.00331269	-2.26266974
H	-0.85639351	-3.60592488	1.91786363
H	-3.07266833	-3.45041681	1.10746586
H	3.46611168	2.97901029	-0.84296006
H	1.62635673	4.33863847	-0.34685165
H	3.74794051	-4.68293237	1.23951950
H	4.34050500	-3.84249384	3.50137211
H	2.95525912	-2.07784890	4.56735631
H	0.88856740	-3.40641360	-0.83040187
H	-2.37797031	-2.39849325	-2.12817116
H	3.66516554	-4.70917389	-0.98489865
H	3.28935516	-3.03147505	-1.44060221
H	2.53956630	-4.37872292	-2.31743639

H	1.83385803	-6.12564497	0.28052793
H	0.81390698	-5.87522703	-1.15456741
H	0.19768196	-5.45876855	0.45745446
H	-4.04561875	-1.31688017	-4.46559557
H	-2.28410702	-1.59031138	-4.43119440
H	-3.00198585	-0.35010563	-3.39160562
H	-3.56844471	-4.58653410	-2.50005953
H	-2.60007570	-4.07541017	-3.89929141
H	-4.36616069	-3.90333088	-3.93281609
H	-5.98852885	-2.35571216	-3.27675303
H	-7.89446305	-1.74478911	-1.80874646
H	-7.49623373	-1.04359716	0.53803770
H	0.02318072	-0.42190979	2.89249595
H	-4.04293558	-0.77487192	2.06759851
H	2.23255544	-0.07104934	5.01274496
H	0.87840240	1.02683417	4.72003472
H	2.12267872	0.80548021	3.47124670
H	0.46571935	-2.00884839	5.49080780
H	-0.80656178	-2.31776896	4.29300403
H	-0.81213470	-0.80263275	5.22228035
H	-5.18680370	1.33708048	1.37824715
H	-5.44073282	0.98329958	3.10271749
H	-6.74409188	0.68999084	1.93530210
H	-6.84529936	-1.84011817	2.76911740
H	-5.56134035	-1.43748551	3.92703322
H	-5.34841774	-2.79051121	2.79382788
H	5.66337441	-0.78909033	-3.46337763
H	7.40097579	-1.13537964	-1.72925198
H	7.01267632	-0.38964309	0.60296625
H	2.30691130	0.80882371	-2.83254948
H	-0.19298589	2.22768550	2.54561381
H	3.69389692	-1.43223208	-4.40371402
H	2.15389686	-0.65654016	-4.82736329
H	2.26786420	-1.57497090	-3.32777902
H	4.05896947	2.38679217	-3.74087605
H	3.03680035	1.67792974	-5.01084226
H	4.68813282	1.07673679	-4.75897879
H	-3.07405143	2.35674436	3.62376681
H	-1.85256550	1.14399618	4.05227436
H	-2.47469616	1.23047809	2.38778070
H	0.23893450	4.30638656	3.88069421
H	-0.25691432	2.96289578	4.93370809
H	-1.41040176	4.24654490	4.52990168
H	-3.08814471	4.61251256	2.89750594
H	-3.80299962	6.17711169	1.10071750
H	-2.64308744	6.16415278	-1.08616443
H	3.73844589	0.93021229	1.85700649
H	0.11939981	3.85114343	-2.06758636
H	6.52571255	-0.04877164	2.69448073
H	5.07260387	-1.07678627	2.61634784
H	5.13798011	0.29911992	3.73322911
H	5.23067592	2.68830316	2.83183754

H	4.94568900	3.02635878	1.11338548
H	6.48415372	2.31194922	1.62965464
H	-2.16590563	3.41909297	-2.85792405
H	-1.22609656	4.35381116	-4.03552306
H	-2.46221320	5.16699167	-3.05753589
H	0.93130234	6.20271355	-1.53935578
H	-0.56730444	6.85180866	-2.21934077
H	0.56887673	5.98173443	-3.26807782
O	0.15033196	-1.64680253	-1.98681086
O	0.31447794	1.34701199	-2.10640552
O	1.82154293	0.28707355	0.07900010
Hf	-0.13459344	-0.39388017	-0.73167752

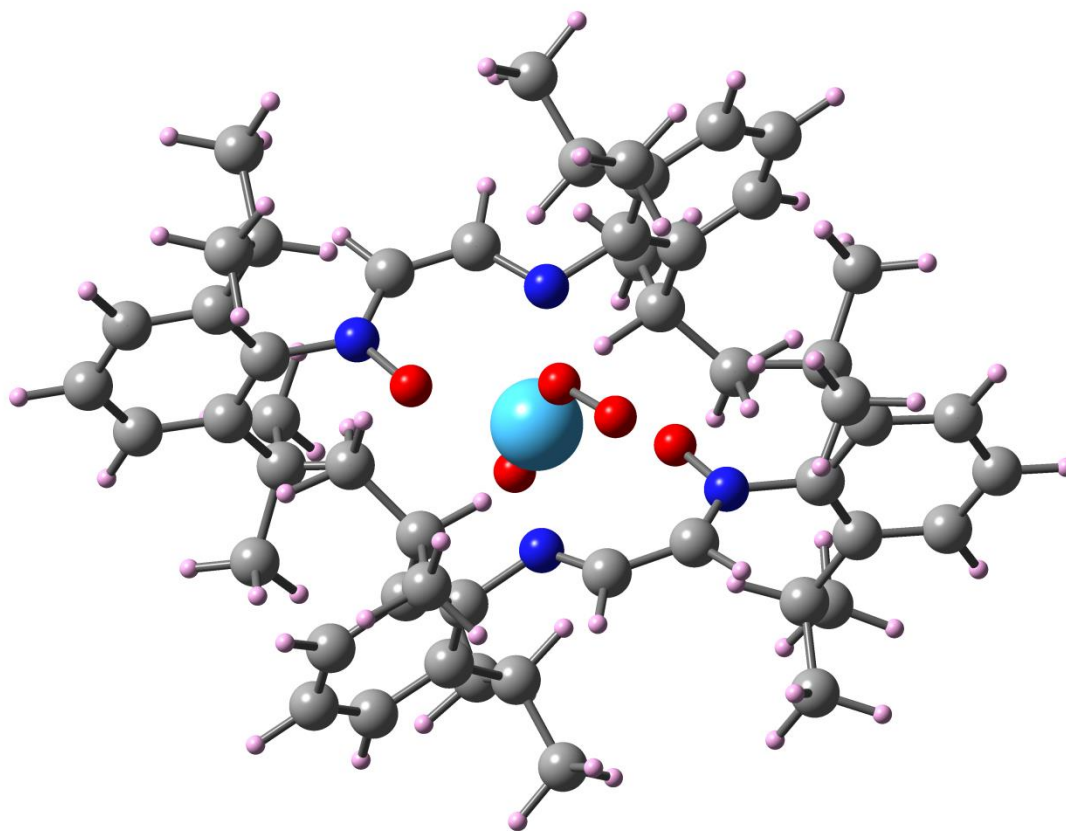
Oxo Complex with Weakly Adsorbed Oxygen Molecule

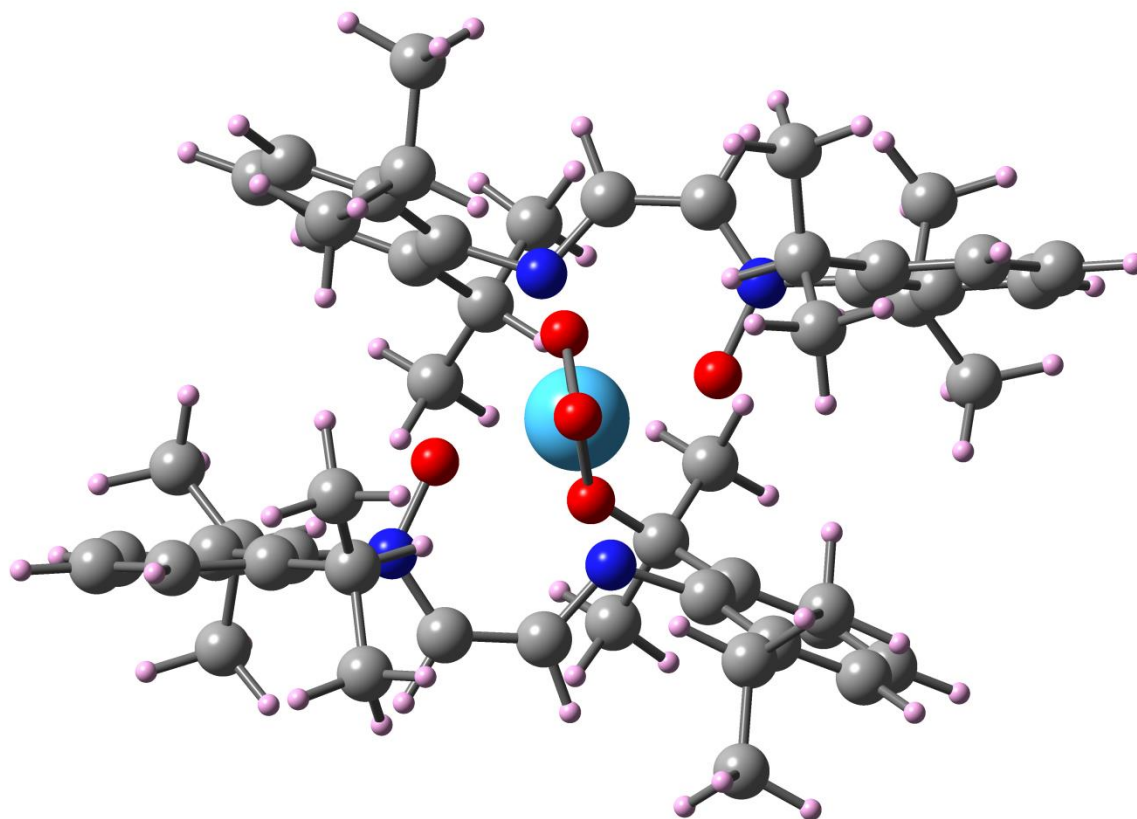
Fig. S64: NCCNO Oxo Complex with Weakly Adsorbed Oxygen Molecule

E	E_{zp}	H	G
-2668.6028	-2667.4525	-2667.3814	-2667.5623
O	-2.05201700	0.53465200	0.19356500
O	2.04046200	-0.38170800	-0.14017900
O	-0.44411400	-0.79132900	-1.90462000
N	-0.02869300	-2.01341400	0.96926100
N	2.83529400	-1.06438900	0.73156800
N	0.04785600	2.07550800	-0.95222700
N	-2.88863400	1.24947900	-0.67034500
C	0.98217700	-2.36257200	1.74495700
C	2.33638400	-1.89102200	1.64737800
C	-1.04643400	2.69283500	-1.47893900
C	-2.38276900	2.28290800	-1.40214700
C	-1.23892500	-2.84031500	1.04712100
C	-2.13414700	-2.72511100	2.14531500
C	-3.29662600	-3.52616900	2.13057300
C	-3.55481100	-4.41981700	1.08267600
C	-2.63599300	-4.54287900	0.02894000
C	-1.46174500	-3.76479300	-0.01329900
C	-2.99799700	-0.69148000	3.40209300

C	-1.90106500	-1.78361300	3.33173100
C	-1.80946300	-2.56772000	4.66763200
C	4.86920600	2.34100300	2.26574100
C	4.39361900	0.87123900	2.36731900
C	4.68795600	0.30059000	3.78222700
C	4.28280000	-0.93833600	0.51719000
C	5.02479800	-0.01403800	1.29012800
C	6.41746900	0.03511100	1.06125500
C	7.02526300	-0.78437400	0.09968900
C	6.25483100	-1.68130400	-0.65803500
C	4.86190800	-1.77990700	-0.46887100
C	-1.03472200	-3.98256200	-2.53893000
C	-0.42730900	-4.01829100	-1.11712600
C	0.30085500	-5.36505200	-0.84893200
C	4.41608300	-2.84571300	-2.76132100
C	4.04189100	-2.80661100	-1.25923200
C	4.20272200	-4.21822200	-0.62822900
C	1.27897800	2.85211400	-1.02405400
C	2.13899600	2.70046300	-2.14584500
C	3.30773700	3.49023300	-2.19946000
C	3.61296400	4.40720100	-1.18213100
C	2.74615000	4.54938500	-0.08656700
C	1.56883600	3.77953100	0.01686300
C	2.95980300	0.74857500	-3.56925100
C	1.80896500	1.74897700	-3.30118400
C	1.45802800	2.54298200	-4.58792900
C	-4.87571500	2.61934600	2.79506600
C	-4.42003100	2.75852100	1.32119800
C	-4.71697800	4.19267200	0.80134900
C	-4.31190300	0.98793800	-0.55763600
C	-5.06305200	1.71163200	0.40495700
C	-6.45081400	1.46703800	0.46414900
C	-7.05457300	0.53434100	-0.39411000
C	-6.28333500	-0.17484400	-1.32885300
C	-4.89078400	0.03082100	-1.42964400
C	1.32893700	3.95834600	2.56830200
C	0.61293800	3.99627800	1.19646700
C	-0.16573600	5.32957600	1.02605500
C	-4.47300500	-2.18995100	-2.63772900
C	-4.05753500	-0.70771200	-2.48202600
C	-4.15322600	0.02274300	-3.85093500
H	0.84005900	-3.15473300	2.48231400
H	3.06756100	-2.33066300	2.31443500
H	-0.88397300	3.62103900	-2.02786100
H	-3.12738900	2.84856900	-1.94877700
H	-4.00491700	-3.44506000	2.95128800
H	-4.45889000	-5.02417300	1.09155700
H	-2.82758200	-5.25702300	-0.76752200
H	-0.95129200	-1.26408400	3.19509900
H	3.30722300	0.86871600	2.23596900
H	-3.99213500	-1.13095300	3.56258100
H	-3.01725200	-0.11607000	2.47111300

H	-2.79151300	-0.00418000	4.23372400
H	-2.75229300	-3.07863100	4.90281500
H	-1.58724500	-1.87825600	5.49276100
H	-1.01785300	-3.32895000	4.63649600
H	5.94332000	2.43869700	2.47148600
H	4.33634400	2.95301600	3.00362000
H	4.66565400	2.75521500	1.27222500
H	4.30440000	-0.72157100	3.89626000
H	4.20700400	0.92377800	4.54623800
H	5.76752400	0.28074100	3.98342300
H	7.02607300	0.72646500	1.63629200
H	8.09906500	-0.72492500	-0.06097200
H	6.73867100	-2.30742300	-1.40174300
H	0.31411200	-3.21526900	-1.08982100
H	2.98392300	-2.52747800	-1.20560800
H	-1.85374200	-4.70392100	-2.66320100
H	-0.26052700	-4.22681500	-3.27927600
H	-1.39343300	-2.97173600	-2.75287900
H	-0.39956100	-6.20962700	-0.89538600
H	0.77419700	-5.38001100	0.14287500
H	1.08075200	-5.53233900	-1.60433000
H	4.34062200	-1.85272200	-3.21667900
H	3.73041500	-3.51613500	-3.29478000
H	5.43487700	-3.22239800	-2.92065200
H	5.24843000	-4.54958700	-0.67554800
H	3.58753700	-4.94850900	-1.16868100
H	3.89402600	-4.22969700	0.42520200
H	3.97870100	3.39057600	-3.04950800
H	4.51497200	5.01207900	-1.24556100
H	2.98370600	5.26897100	0.69348100
H	0.93001400	1.15538100	-3.03038100
H	-3.33454100	2.61085400	1.30152400
H	3.87459900	1.25530400	-3.90660600
H	2.65985400	0.03601100	-4.34911000
H	3.19108600	0.18569300	-2.65849000
H	0.60810300	3.21786900	-4.42148900
H	1.18902900	1.85159700	-5.39764700
H	2.30807000	3.15086100	-4.92756700
H	-5.94173700	2.85272200	2.91625600
H	-4.31246000	3.31884300	3.42674100
H	-4.70260900	1.60516400	3.17013000
H	-4.34890700	4.33400000	-0.22221600
H	-4.23067700	4.93989800	1.44253600
H	-5.79673600	4.39334300	0.80223100
H	-7.06052300	2.00483500	1.18510500
H	-8.12651700	0.35918000	-0.33378800
H	-6.76602100	-0.89650100	-1.98111100
H	-0.11542400	3.17978400	1.19704800
H	-3.00464400	-0.69213700	-2.17709400
H	2.07199200	4.76119900	2.66790300
H	1.83106100	2.99654300	2.71853600
H	0.59521200	4.08194800	3.37597600

H	-0.87402400	5.46888000	1.85436200
H	-0.73230600	5.34318900	0.08634300
H	0.51972400	6.18797700	1.01748800
H	-4.42835500	-2.71791800	-1.67787900
H	-3.78683900	-2.69088700	-3.33101100
H	-5.48758400	-2.29420800	-3.04592500
H	-3.80331700	1.05975900	-3.77777800
H	-5.18821100	0.03528400	-4.22086400
H	-3.52677400	-0.48911200	-4.59239600
O	0.24705300	0.56611500	2.04853000
O	1.11471100	0.05694100	2.93417100
Hf	-0.10499000	-0.06149800	-0.28620200

η^2 -ozone ComplexFig. S65: NCCNO η^2 -ozone Complex

E	E_{zp}	H	G
-2668.5820	-2667.4316	-2667.3612	-2667.5416
O	-2.00713899	0.26685904	0.00160372
O	2.00578713	-0.25020854	-0.06121866
O	-0.01217269	1.41037432	-2.02590109
N	-0.13228640	-2.09020708	0.23590712
N	2.80008962	-1.36639052	-0.31896118
N	0.13175848	1.96382424	0.75546876
N	-2.80444071	1.40830023	0.05371301
C	0.94096257	-2.93049960	0.12241947
C	2.27060571	-2.61065975	-0.17571602
C	-0.94082271	2.80367684	0.87542631
C	-2.27400724	2.57175250	0.51650318
C	-1.36947609	-2.79027119	0.60563621
C	-1.73855997	-2.84989479	1.97888452
C	-2.88927485	-3.58249275	2.33600575
C	-3.66335421	-4.23757176	1.36685951
C	-3.28509533	-4.17046406	0.01958085
C	-2.13665865	-3.45780510	-0.39016358
C	-1.73643786	-1.38951713	4.08366449

C	-0.88842876	-2.21099409	3.08157446
C	-0.06129948	-3.29444057	3.82681335
C	5.47007797	-0.04289727	2.63349355
C	4.83632620	-1.16668578	1.77741814
C	5.27144237	-2.56377731	2.29892043
C	4.17447965	-1.11637998	-0.71676096
C	5.16820012	-1.01946806	0.29023176
C	6.50043391	-0.82386803	-0.12834177
C	6.81896279	-0.71752336	-1.49180888
C	5.81156187	-0.80420046	-2.46523065
C	4.46235972	-1.00194942	-2.10185362
C	-2.90710237	-2.86344653	-2.74084096
C	-1.76705161	-3.46016947	-1.87707966
C	-1.40042501	-4.88855590	-2.36078520
C	3.46037152	-0.00005277	-4.23365762
C	3.38076095	-1.13065623	-3.17830125
C	3.46446998	-2.52127826	-3.86600324
C	1.37794663	2.54641202	1.27005694
C	2.12971589	3.44667578	0.46414500
C	3.29449712	4.02237888	1.01793458
C	3.70419953	3.73154400	2.32569624
C	2.94382474	2.85130747	3.11003016
C	1.77611623	2.24524950	2.60276384
C	2.84691988	3.50742378	-1.97774404
C	1.72513375	3.83673657	-0.96088009
C	1.33401080	5.33656872	-1.04095387
C	-5.46591324	-0.70464077	2.51685311
C	-4.83809952	0.61550188	2.00636186
C	-5.27984370	1.81173582	2.89374524
C	-4.17654988	1.26942500	-0.40096320
C	-5.16897291	0.88522766	0.53644866
C	-6.49897640	0.80016563	0.07667388
C	-6.81717687	1.07455819	-1.26331935
C	-5.81139497	1.44019152	-2.17114971
C	-4.46395211	1.54231407	-1.76383461
C	1.78626769	0.33067515	4.31067656
C	0.93425856	1.35227110	3.51931251
C	0.08736078	2.22199073	4.48967264
C	-3.43105046	1.14394542	-4.06949858
C	-3.38587827	1.97378697	-2.76247414
C	-3.51247696	3.49018935	-3.07387232
H	0.75308125	-3.99517912	0.25992617
H	2.97911134	-3.41840926	-0.31208932
H	-0.74976096	3.79605387	1.28329953
H	-2.98329094	3.38565579	0.60290805
H	-3.17840248	-3.64868150	3.38183232
H	-4.54679826	-4.79972737	1.66088910
H	-3.88270460	-4.68281038	-0.73029915
H	-0.17545107	-1.52616707	2.60848926
H	3.74915077	-1.08892205	1.89186865
H	-2.44813467	-2.02258334	4.62826163
H	-2.30565937	-0.60639253	3.56873718

H	-1.08855105	-0.91088365	4.82887295
H	-0.72212625	-4.01678109	4.32443257
H	0.57990057	-2.83582448	4.59151756
H	0.58035168	-3.85056159	3.13196128
H	6.56677025	-0.08976087	2.61778277
H	5.15114665	-0.14420011	3.67927166
H	5.16024717	0.94564361	2.27773183
H	4.78787100	-3.37215249	1.73566713
H	5.00244524	-2.67823682	3.35744111
H	6.35795574	-2.69504143	2.20898407
H	7.29082189	-0.75020945	0.61366019
H	7.85230969	-0.56516429	-1.79509827
H	6.07186141	-0.71344739	-3.51598442
H	-0.89728109	-2.81964054	-2.03503437
H	2.39480912	-1.05795779	-2.71055125
H	-3.81651406	-3.47896639	-2.70161536
H	-2.58632096	-2.79601485	-3.78843257
H	-3.16138405	-1.85440648	-2.39746844
H	-2.24710044	-5.58091213	-2.25727426
H	-0.55918082	-5.30276414	-1.78859737
H	-1.11137436	-4.86467547	-3.41987482
H	3.42691152	0.98745572	-3.76024185
H	2.60045104	-0.07209975	-4.90991366
H	4.37534767	-0.06423030	-4.83873898
H	4.42731125	-2.65475926	-4.37835188
H	2.66346846	-2.61758575	-4.60962579
H	3.35093674	-3.33719337	-3.14020513
H	3.88254488	4.70930619	0.41418895
H	4.60185321	4.19087352	2.73338599
H	3.25850646	2.63947110	4.12861834
H	0.85781036	3.24667233	-1.26340220
H	-3.75078050	0.51309978	2.09680998
H	3.74868273	4.11150501	-1.80590213
H	2.49507175	3.70486064	-2.99856737
H	3.12529277	2.44954765	-1.91325493
H	0.50523208	5.57328045	-0.36004486
H	1.01713615	5.58905384	-2.06162162
H	2.17820082	5.98882995	-0.77860760
H	-6.56290043	-0.66000522	2.51755685
H	-5.14323285	-0.89705493	3.54856142
H	-5.15374440	-1.55395708	1.89950307
H	-4.79769988	2.74617826	2.57905659
H	-5.01399221	1.62834231	3.94328742
H	-6.36657969	1.95966217	2.83962677
H	-7.28783167	0.51457118	0.76703694
H	-7.84896180	1.00172713	-1.59963519
H	-6.07121883	1.64468259	-3.20605038
H	0.23281243	0.78824225	2.89353429
H	-2.39789305	1.81300200	-2.32153561
H	2.46603220	0.82707551	5.01464665
H	2.38928912	-0.28836623	3.63577513
H	1.13775772	-0.33170026	4.89791915

H	-0.54217667	1.58977129	5.13004532
H	-0.56837081	2.90745639	3.93830303
H	0.73603508	2.82644526	5.13759493
H	-3.36055571	0.07108285	-3.85906024
H	-2.57720154	1.41314848	-4.70223999
H	-4.35098843	1.32672914	-4.64200520
H	-3.42088393	4.09625852	-2.16284979
H	-4.48020477	3.72259802	-3.53925035
H	-2.71721817	3.79668311	-3.76494604
O	0.00293579	0.39150120	-3.14445964
O	0.00966615	-0.86804577	-2.30717080
Hf	-0.00303387	0.05717590	-0.45196885

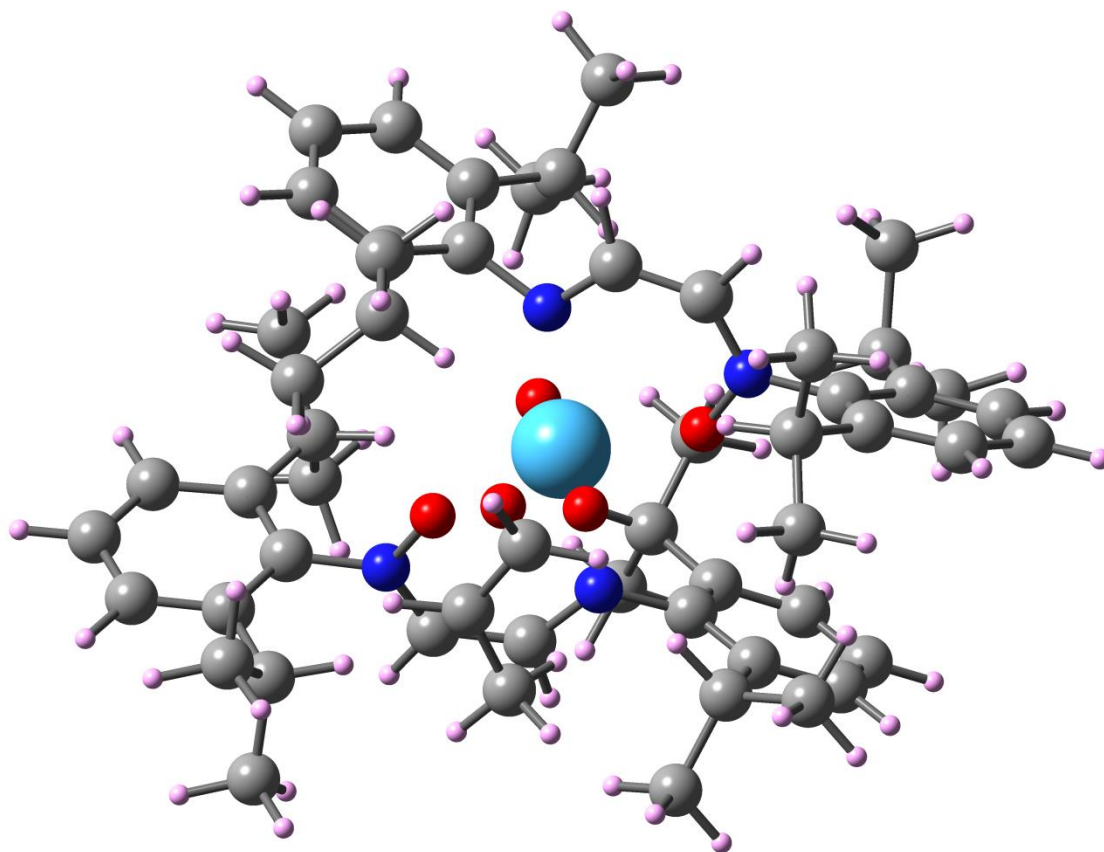
Propene Chemisorbed on Oxo Peroxo Complex forming Octahedral Complex

Fig. S66: NCCNO Propene Chemisorbed on Oxo Peroxo Complex forming Octahedral Complex

E	E_{zp}	H	G
-2786.4487	-2785.2152	-2785.1400	-2785.3294
O	1.98788543	0.38259335	-0.08140411
O	-1.91664570	-0.68873424	0.50948948
O	-0.52469340	-0.05553746	3.12589373
O	0.52932848	-0.32284308	2.10273494
N	0.25629718	-2.08907296	-0.87372101
N	-2.73164431	-1.57493090	-0.21266368
N	-0.12986821	2.30482970	0.36103311
N	2.77598815	1.31172473	0.57769960
C	-0.81888166	-2.88293321	-1.12353931
C	-2.17618996	-2.63942562	-0.85967503
C	0.95779819	2.98669029	0.80405955
C	2.27385366	2.52807086	0.94137941
C	1.49715635	-2.57125192	-1.47669657
C	1.67961934	-2.46078125	-2.88624513
C	2.86381840	-2.98775879	-3.44862220
C	3.84663820	-3.59188494	-2.65413339
C	3.65968969	-3.67578342	-1.26499840
C	2.49201706	-3.17466604	-0.65589565

C	1.28586142	-0.61503989	-4.59619189
C	0.65551722	-1.79702243	-3.81625567
C	0.03212577	-2.82776884	-4.79399402
C	-4.39228472	1.42866963	-2.66860761
C	-3.99208573	-0.03438500	-2.35916763
C	-4.17084934	-0.92465476	-3.61966033
C	-4.16336840	-1.35513117	-0.14491192
C	-4.78413788	-0.61461139	-1.18455524
C	-6.18657153	-0.46037124	-1.12094597
C	-6.93195314	-1.00618120	-0.06482228
C	-6.28965240	-1.72088440	0.95951762
C	-4.89219661	-1.90457743	0.94168131
C	3.57416393	-3.29786243	1.67594356
C	2.26945406	-3.34587915	0.84825639
C	1.51022265	-4.67307031	1.12972559
C	-4.59838660	-2.20747140	3.46018677
C	-4.20482048	-2.70959813	2.04757245
C	-4.51167105	-4.22494146	1.90442424
C	-1.28649629	3.14670229	0.05795803
C	-2.32355070	3.30043259	1.01873774
C	-3.42505991	4.12365989	0.70061937
C	-3.49781861	4.79274756	-0.52927419
C	-2.45720151	4.64756348	-1.45922338
C	-1.33893242	3.83009958	-1.19268571
C	-3.48778048	1.77109569	2.70121511
C	-2.25020883	2.65304956	2.40357114
C	-2.05952179	3.73142211	3.50462654
C	5.12231735	0.25036267	-2.91071824
C	4.44570784	1.09483267	-1.80719533
C	4.58342542	2.61104885	-2.12679001
C	4.17157064	0.96020943	0.75471308
C	4.98850102	0.81157934	-0.40165996
C	6.34315862	0.47959227	-0.20267517
C	6.87273297	0.32340422	1.08962330
C	6.04974963	0.48916428	2.21189704
C	4.67851883	0.79682576	2.07129352
C	-0.73725776	3.27928337	-3.61572016
C	-0.21642090	3.74484192	-2.23347124
C	0.53373452	5.10054376	-2.34032859
C	3.91732050	-0.26800025	4.26663825
C	3.81263428	0.96065098	3.32757991
C	4.19219939	2.25502169	4.09743552
H	-0.63498743	-3.82205537	-1.64818916
H	-2.89890423	-3.35432317	-1.23648426
H	0.82375962	4.04124771	1.05198704
H	3.01404584	3.21295530	1.33674282
H	3.01419144	-2.91747646	-4.52340672
H	4.74972930	-3.99282926	-3.10937499
H	4.42861892	-4.13880385	-0.65317845
H	-0.14178592	-1.35518173	-3.21379705
H	-2.92508934	-0.02230847	-2.11088137
H	2.11267076	-0.93776492	-5.24528581

H	1.65592450	0.14265335	-3.89667819
H	0.52370195	-0.13761626	-5.22593339
H	0.79050690	-3.26648975	-5.45763050
H	-0.72432333	-2.34016138	-5.42383042
H	-0.45455053	-3.65139080	-4.25435659
H	-5.42324637	1.50812999	-3.04203394
H	-3.72479209	1.83143157	-3.43965538
H	-4.29344795	2.06452519	-1.78157231
H	-3.83437773	-1.95315590	-3.43567642
H	-3.57550520	-0.51943057	-4.44767867
H	-5.22258949	-0.96167482	-3.93781474
H	-6.69539249	0.09621092	-1.90277543
H	-8.01138651	-0.87419053	-0.03833108
H	-6.87849311	-2.13700449	1.77329038
H	1.63975185	-2.51121369	1.17685160
H	-3.12446332	-2.57270293	1.93163203
H	4.21495563	-4.16833445	1.48231446
H	3.33697866	-3.30835736	2.74925626
H	4.15126060	-2.39136392	1.45879519
H	2.09188619	-5.53198155	0.76868879
H	0.53578789	-4.68904566	0.62781858
H	1.34462382	-4.80895427	2.20840618
H	-4.40359206	-1.13267517	3.56553551
H	-4.03471572	-2.75252693	4.23188621
H	-5.66341494	-2.37289517	3.66544599
H	-5.58878211	-4.41813180	1.99242444
H	-4.00004212	-4.80145023	2.68798186
H	-4.18025407	-4.60626187	0.93086766
H	-4.22553039	4.24920488	1.42658286
H	-4.35217210	5.42573149	-0.75886675
H	-2.51323667	5.17500443	-2.40848181
H	-1.37396594	2.00089731	2.42363037
H	3.38127383	0.84387001	-1.81185364
H	-4.41687224	2.35630284	2.69392783
H	-3.39642266	1.31201826	3.69804498
H	-3.57539652	0.97224209	1.95746703
H	-1.15492235	4.32672173	3.32424203
H	-1.97021619	3.26314679	4.49606369
H	-2.91252229	4.42219106	3.53674826
H	6.17383333	0.53119410	-3.06231287
H	4.60152836	0.41084477	-3.86319910
H	5.07306789	-0.81969659	-2.67936607
H	4.04824246	3.22763648	-1.39438167
H	4.16394519	2.82622264	-3.11834459
H	5.63903061	2.91644980	-2.12780457
H	6.99290272	0.35131241	-1.06268907
H	7.92382456	0.07526373	1.21851008
H	6.47194968	0.36601990	3.20616660
H	0.49604815	2.98377891	-1.90751920
H	2.76622522	1.04024563	3.01598065
H	-1.51490935	3.94666116	-4.01265230
H	-1.12927151	2.26172979	-3.52199250

H	0.08986937	3.26281707	-4.33977092
H	1.36476962	5.01862771	-3.05423853
H	0.94571888	5.41020728	-1.37016108
H	-0.13335055	5.90007211	-2.69070237
H	3.60649240	-1.18302449	3.75076665
H	3.27730593	-0.12302883	5.15001281
H	4.94009294	-0.41793055	4.63463447
H	4.09036356	3.14594018	3.46559003
H	5.23145118	2.21441320	4.44949814
H	3.54347946	2.38646520	4.97443563
O	-0.63634335	0.48393992	-1.93808681
C	-0.98462510	-1.38844168	4.03861849
H	-2.04145526	-1.23032047	4.22902180
C	-0.04130895	-0.36112012	4.54993028
H	-0.37787559	0.40560697	5.24253071
H	1.02105557	-0.58464331	4.55083635
C	-0.51368601	-2.68862882	3.47797572
H	0.07069151	-2.46461609	2.57187716
H	0.14897149	-3.21098653	4.17931931
H	-1.34679825	-3.33966339	3.20658533
Hf	-0.10823145	0.10705332	-0.23761206

7.5 Six Oxygen Atoms

Peroxo Complex with Adsorbed Oxygen Molecule (spiro conformation)

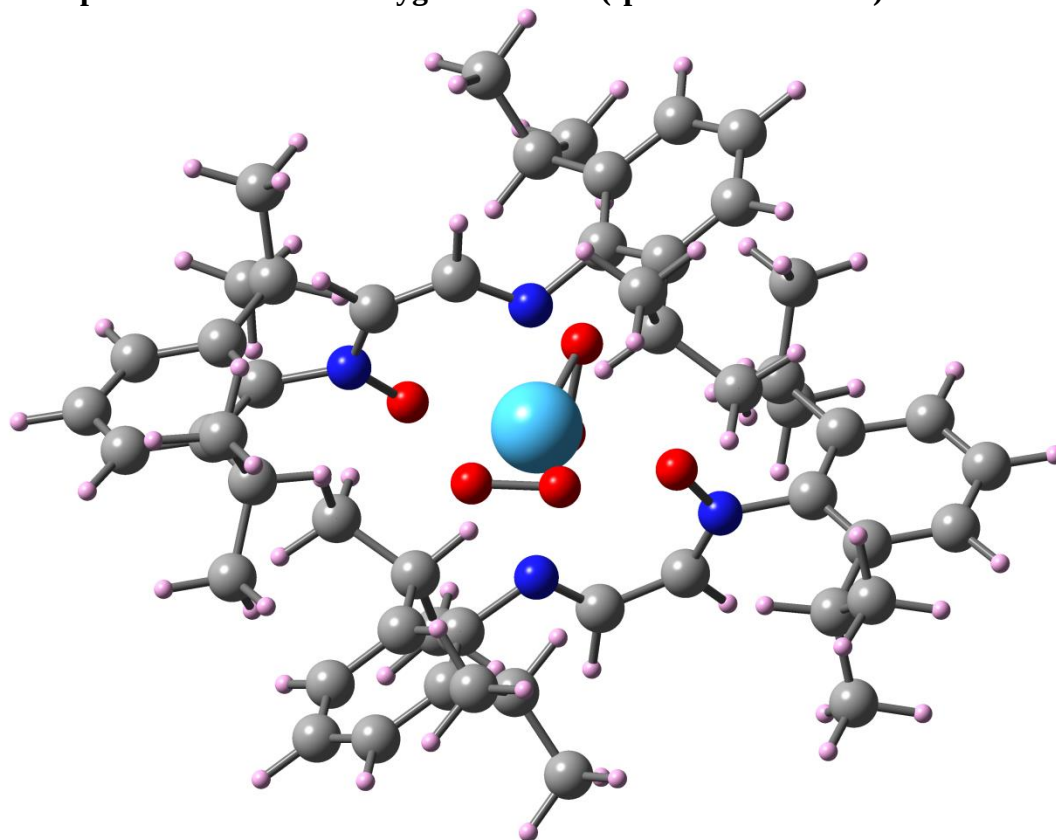


Fig. S67: NCCNO Peroxo Complex with Adsorbed Oxygen Molecule (spiro conformation)

E	E _{zp}	H	G
-2743.7619	-2742.6076	-2742.5360	-2742.7168
O	-1.98536315	0.53648304	-0.37738703
O	2.22853517	-0.51826604	0.13179501
O	0.74420306	1.45209811	-1.41552211
O	0.47189604	0.04786500	-1.99697715
N	0.03056300	-2.20658517	-0.70993205
N	2.91148022	-1.20226509	-0.79153606
N	-0.05989600	2.05349715	1.17290009
N	-2.90451922	1.07675208	0.52926404
C	1.02729208	-2.69197921	-1.40027611
C	2.36437918	-2.14359216	-1.54004812
C	-1.22904410	2.48314419	1.71449513
C	-2.51843719	1.99943615	1.46161311
C	-1.16717609	-3.05623523	-0.66138805
C	-1.34602910	-3.90639930	0.46292004
C	-2.48544519	-4.73668136	0.47726504
C	-3.40921426	-4.72282136	-0.57917604
C	-3.20027424	-3.88040829	-1.68027413

C	-2.07522716	-3.03089923	-1.75362913
C	-0.94817607	-3.94519930	2.99721223
C	-0.31003502	-4.00895631	1.58863912
C	0.53553704	-5.30269439	1.42521511
C	5.28127540	-2.56467420	2.36284018
C	4.69854836	-2.74957921	0.93904407
C	5.00107638	-4.17587632	0.40334903
C	4.35834133	-0.92681407	-0.87283007
C	5.21447040	-1.68411213	-0.03540600
C	6.59647752	-1.43255011	-0.15146701
C	7.08138856	-0.46627204	-1.04873508
C	6.19538545	0.27635502	-1.84313314
C	4.79987737	0.07122601	-1.77070713
C	-3.09988323	-1.28409010	-3.30547025
C	-1.86475414	-2.16625117	-3.00335123
C	-1.51083611	-3.05345223	-4.22823932
C	4.05775231	2.41026719	-2.42292118
C	3.84785629	0.89123807	-2.64484520
C	4.02009031	0.51932604	-4.14177631
C	1.06497208	2.97782623	1.29023110
C	1.14252209	4.08510631	0.39268603
C	2.25121917	4.95057238	0.49726504
C	3.25372625	4.74366136	1.45681811
C	3.14497224	3.66959328	2.35074418
C	2.05354516	2.77619521	2.29325617
C	0.60915705	4.59959135	-2.06443416
C	0.04807700	4.40516234	-0.63453005
C	-0.75894806	5.65391743	-0.18388401
C	-4.73720136	-2.20789917	2.39890518
C	-4.41627334	-0.69426405	2.33221718
C	-4.87962537	0.01188300	3.63620828
C	-4.30544333	0.82313606	0.23745302
C	-5.04089438	-0.02520500	1.10348608
C	-6.41120351	-0.21651502	0.81854406
C	-7.01251752	0.39591803	-0.28989002
C	-6.25762548	1.22672709	-1.13535008
C	-4.89091637	1.46475811	-0.88944507
C	3.19104024	0.75098806	3.35573226
C	1.94576015	1.67176413	3.34868426
C	1.69864413	2.27761718	4.75661136
C	-4.47433034	2.37833818	-3.25901925
C	-4.09854431	2.44791619	-1.75945513
C	-4.29401733	3.89694330	-1.22960209
H	0.89776007	-3.64384628	-1.92260215
H	3.02895723	-2.61832720	-2.25092817
H	-1.18842709	3.33382525	2.39595418
H	-3.34202926	2.42814218	2.01956616
H	-2.64744520	-5.40188740	1.32107610
H	-4.28257232	-5.36987143	-0.54674904
H	-3.91620730	-3.88071830	-2.49787319
H	0.36883503	-3.15357424	1.51901812
H	3.61089427	-2.64814820	1.03213708

H	-1.62335113	-4.79107536	3.18392424
H	-1.50704111	-3.01188923	3.11977324
H	-0.16203801	-3.97210130	3.76314829
H	-0.09565601	-6.19823248	1.49987511
H	1.29970110	-5.35999741	2.21208717
H	1.04366908	-5.33632440	0.45121603
H	6.36752348	-2.71999521	2.38143218
H	4.83056037	-3.29391125	3.04824323
H	5.07088039	-1.56062612	2.74684021
H	4.55347635	-4.34102033	-0.58572304
H	4.60090435	-4.93405637	1.08894708
H	6.08254047	-4.33935633	0.31026802
H	7.29528455	-1.98962615	0.46617804
H	8.15162865	-0.28889602	-1.12280909
H	6.58471550	1.02850908	-2.52307319
H	-1.02998408	-1.47848811	-2.83789022
H	2.81108322	0.68171005	-2.36624818
H	-3.98745231	-1.88472215	-3.54675127
H	-2.88734022	-0.63619205	-4.16594032
H	-3.32955725	-0.64837705	-2.44540318
H	-2.32602918	-3.75015029	-4.46573734
H	-0.60565205	-3.65123228	-4.05114131
H	-1.33405310	-2.42424319	-5.11024839
H	3.88483630	2.68157121	-1.37565610
H	3.33805426	2.96982823	-3.03139823
H	5.06903739	2.73363121	-2.70696321
H	5.03065438	0.75450006	-4.50348634
H	3.30074725	1.08428908	-4.74688237
H	3.83909329	-0.55003804	-4.31672333
H	2.32899218	5.79779442	-0.17980901
H	4.10263631	5.42140742	1.51542412
H	3.90993330	3.52595127	3.11039623
H	-0.63499005	3.55390127	-0.68774705
H	-3.32829025	-0.59845004	2.26800817
H	1.32470110	5.43132240	-2.12069116
H	-0.21249502	4.82094337	-2.76007421
H	1.09604708	3.67745428	-2.39418818
H	-1.20365009	5.50874543	0.80955106
H	-1.57035012	5.86119647	-0.89465507
H	-0.11675701	6.54386449	-0.13512801
H	-5.80960847	-2.39340419	2.54713319
H	-4.20304432	-2.66274420	3.24347825
H	-4.42137034	-2.71983221	1.48358012
H	-4.61715435	1.07744608	3.63544328
H	-4.40164533	-0.45236703	4.50872234
H	-5.96815944	-0.06547200	3.76225529
H	-7.00574453	-0.85687907	1.46448511
H	-8.06778760	0.23016002	-0.49525704
H	-6.73773853	1.69856513	-1.98755715
H	1.08467708	1.04332608	3.10954224
H	-3.03676423	2.19518917	-1.67831113
H	4.09996132	1.30006810	3.63866728

H	3.34485525	0.31194402	2.36384818
H	3.05053723	-0.06508500	4.07754231
H	1.57690712	1.47715911	5.49899042
H	0.79164706	2.89630222	4.77006637
H	2.53936819	2.90963622	5.07371339
H	-4.40513634	1.35425310	-3.64226528
H	-3.78583629	3.00568423	-3.83959529
H	-5.49133142	2.74879821	-3.44631726
H	-3.97151430	3.99107631	-0.18579301
H	-5.34950642	4.19570832	-1.28985310
H	-3.70401628	4.60224635	-1.82964214
O	0.39749503	-0.79112306	2.01414115
O	-0.98454208	-0.73621406	1.85199514
Hf	0.03788300	0.14065701	-0.01743900

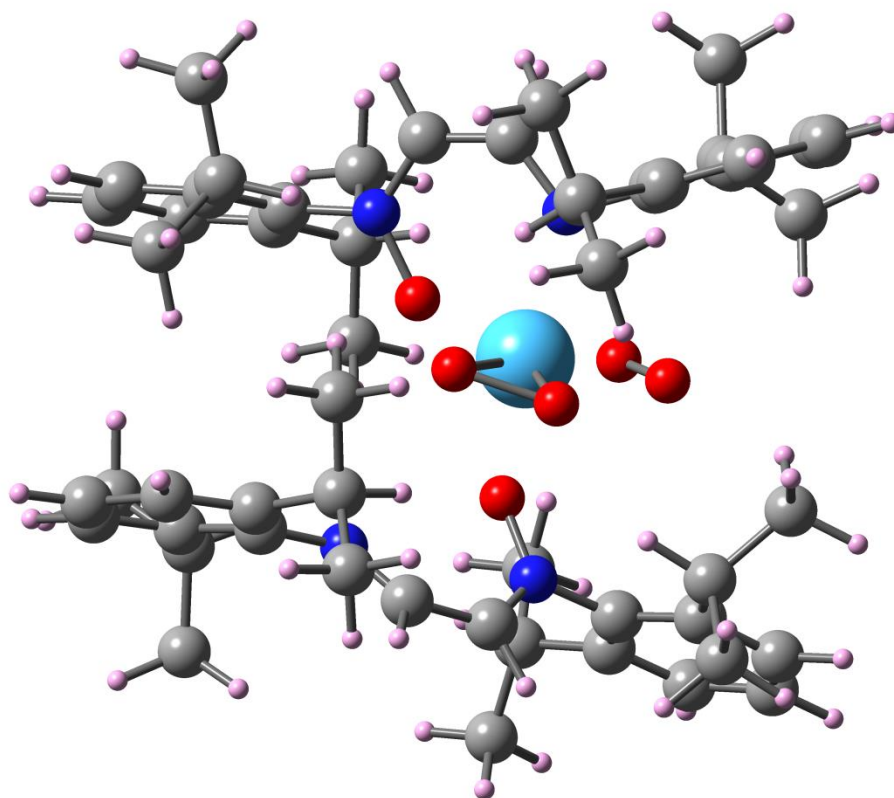
Peroxo Complex with Adsorbed Oxygen Molecule (planar conformation)

Fig. S68: NCCNO Peroxo Complex with Adsorbed Oxygen Molecule (planar conformation)

E	E_{zp}	H	G
-2743.7612	-2742.6084	-2742.5362	-2742.7214
O	-0.76823400	1.16000000	-1.07585800
O	0.46110200	-1.73551100	-0.72841800
O	2.86405800	-0.03365200	-0.73865200
N	-1.83687900	-2.43929300	0.97116800
N	0.91367700	-2.91593800	-0.22607300
N	1.39016200	2.42583600	0.23973000
N	-1.36716700	2.40857600	-1.09320700
C	-0.91949300	-3.22813200	1.44706600
C	0.30495800	-3.56772800	0.74349200
C	0.60194100	3.49155700	-0.06856200
C	-0.66706900	3.49556700	-0.66230800
C	-3.04865500	-2.17683900	1.65257200
C	-3.12841400	-1.88596800	3.05453100
C	-4.41279600	-1.70711800	3.60839300
C	-5.57399100	-1.79573200	2.82552200
C	-5.47334700	-2.01162100	1.43992900
C	-4.22054700	-2.18009800	0.82537200
C	-1.93783700	-0.26335100	4.61316000

C	-1.90172200	-1.66521100	3.95159200
C	-1.77496900	-2.77597900	5.02814000
C	4.65369600	-1.91567500	1.41321900
C	3.47757500	-2.92090500	1.30742400
C	3.65285100	-4.07115400	2.33613000
C	2.13000200	-3.45561600	-0.85776500
C	3.33815000	-3.47526700	-0.11640100
C	4.46247300	-4.03640100	-0.75976100
C	4.38436100	-4.52041700	-2.07367600
C	3.17529500	-4.45370700	-2.78433000
C	2.01415300	-3.91822500	-2.19235300
C	-5.15517500	-1.68836300	-1.51874000
C	-4.09850600	-2.44045700	-0.67762200
C	-4.15711500	-3.96565800	-0.97301000
C	0.84298600	-2.76772400	-4.11406700
C	0.71182700	-3.83569600	-2.99468900
C	0.30097300	-5.21162000	-3.57841600
C	2.67991200	2.77665100	0.84262700
C	3.78228600	3.09653700	-0.00067500
C	5.01166000	3.42762300	0.60848000
C	5.14902900	3.45240500	2.00369100
C	4.04458700	3.15886100	2.81741900
C	2.79262200	2.82071500	2.26136300
C	4.80246900	2.37494400	-2.24085100
C	3.66716500	3.15140900	-1.52881500
C	3.62633900	4.62585000	-2.01808100
C	-4.53853400	1.91203800	1.52491300
C	-3.63448300	2.88420800	0.72657700
C	-3.91099800	4.35425500	1.14267000
C	-2.69974600	2.46889400	-1.65513600
C	-3.79762900	2.70362300	-0.78653900
C	-5.08109300	2.77451200	-1.36943100
C	-5.26104500	2.59248300	-2.74930800
C	-4.15726100	2.34041900	-3.58047400
C	-2.85131600	2.27809900	-3.05335600
C	1.90772900	1.64697100	4.36536800
C	1.59087700	2.59862800	3.18692300
C	1.06534300	3.96439700	3.71085300
C	-1.70032200	0.54855800	-4.50573500
C	-1.65954400	2.00627200	-3.97529800
C	-1.58853100	3.02310600	-5.14312300
H	-1.04122900	-3.77959900	2.38632300
H	0.80697100	-4.48096700	1.04615700
H	0.98951700	4.48089900	0.17406600
H	-1.17013500	4.44356400	-0.80694000
H	-4.50388500	-1.48494000	4.66860500
H	-6.55079600	-1.67213900	3.28761400
H	-6.37560800	-2.03879700	0.83632300
H	-0.99947600	-1.66385600	3.33443900
H	2.57372600	-2.36162600	1.57233300
H	-2.81143800	-0.13200800	5.26545500
H	-1.94325200	0.51329600	3.84149200

H	-1.03536700	-0.12092100	5.22180700
H	-2.63725300	-2.76988800	5.70840500
H	-0.87039300	-2.61785400	5.62990300
H	-1.71825700	-3.77915300	4.58249000
H	5.62607600	-2.40763500	1.27595100
H	4.65075900	-1.45102100	2.40706500
H	4.55612600	-1.12176600	0.66614000
H	2.81068000	-4.77720300	2.31834900
H	3.72649000	-3.65935600	3.35065100
H	4.56779000	-4.64442100	2.13559600
H	5.41052900	-4.07365000	-0.23112400
H	5.26835800	-4.93943600	-2.54829700
H	3.13180300	-4.82051200	-3.80600500
H	-3.10499400	-2.08717600	-0.97833800
H	-0.09484800	-3.50246900	-2.33343500
H	-6.17119600	-2.06759800	-1.34228800
H	-4.93949100	-1.82117700	-2.58711300
H	-5.14682500	-0.61235500	-1.30577200
H	-5.12698400	-4.38533100	-0.67228200
H	-3.37091500	-4.50719400	-0.43230700
H	-4.02319100	-4.15325700	-2.04707700
H	1.10110900	-1.79152400	-3.68952700
H	-0.10612700	-2.67109300	-4.65777400
H	1.62221300	-3.04638400	-4.83628200
H	1.03262100	-5.57920000	-4.30930800
H	-0.66490400	-5.12546900	-4.09301900
H	0.20183300	-5.96981200	-2.79057600
H	5.86669800	3.67058600	-0.01718000
H	6.10596400	3.70820700	2.45343500
H	4.15213600	3.19769000	3.89828100
H	2.72524700	2.67829600	-1.82273700
H	-2.59949500	2.64965400	0.99703700
H	5.78635300	2.82691800	-2.05564500
H	4.63438700	2.37924600	-3.32612500
H	4.82735800	1.33344700	-1.90450300
H	2.78823300	5.17586900	-1.57031300
H	3.51471800	4.66337200	-3.11035700
H	4.55216600	5.15411100	-1.75310300
H	-5.60451000	2.10804000	1.34800500
H	-4.35285000	2.02830500	2.60048500
H	-4.33435600	0.86916300	1.25944700
H	-3.25056300	5.05536700	0.61613100
H	-3.74956800	4.48017800	2.22117100
H	-4.94761500	4.64070600	0.92018900
H	-5.94493600	2.95956400	-0.73642100
H	-6.26007100	2.64405200	-3.17611200
H	-4.31054400	2.20006200	-4.64726800
H	0.78950700	2.12423400	2.61489600
H	-0.73859500	2.10627200	-3.39238500
H	2.68701400	2.04683200	5.02902000
H	2.22334000	0.67121400	3.98270000
H	1.00293200	1.49617000	4.96954400

H	0.17888000	3.81397900	4.34222500
H	0.78570000	4.63190200	2.88468000
H	1.82835300	4.47762500	4.31234600
H	-1.69266900	-0.16349300	-3.67286900
H	-0.82273300	0.35044600	-5.13508100
H	-2.60030400	0.36975400	-5.11016700
H	-1.54233200	4.05516100	-4.77216800
H	-2.45831600	2.94276900	-5.80835300
H	-0.69056300	2.83700000	-5.74662000
O	1.24868100	-0.36826700	1.80482900
O	-0.23960000	0.13369300	1.68028300
O	2.15481000	0.26854800	-1.90862400
Hf	0.79707200	0.28527800	-0.04440400

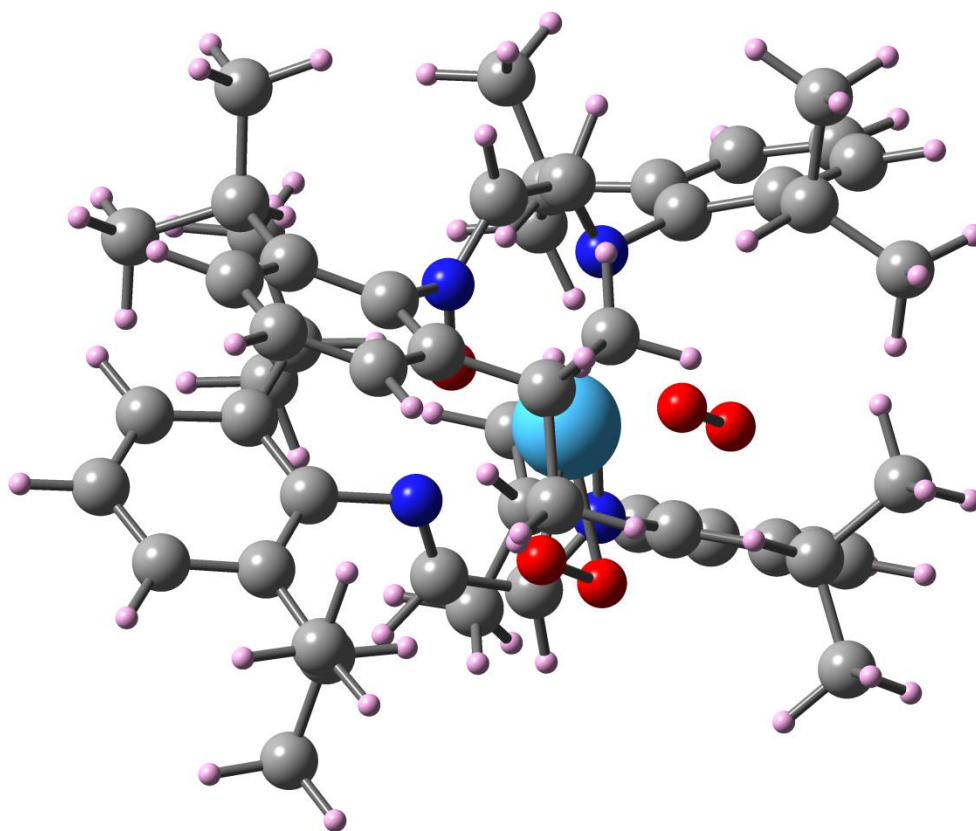
Peroxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

Fig. S69: NCCNO Peroxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

E	E_{zp}	H	G
-2743.7500	-2742.5959	-2742.5247	-2742.7036
O	1.94610429	0.20031438	-0.00015879
O	0.69781944	-0.26118689	-2.50534021
N	-0.08179525	1.77408378	1.19567078
N	2.83550863	1.09390767	0.59198721
N	-2.70775965	-1.18797814	-0.76732023
N	0.18763342	-2.04006186	-0.51392481
C	1.03765882	2.28330430	1.78290648
C	2.37723596	2.01298585	1.48282982
C	-2.08986940	-2.14727179	-1.44222198
C	-0.76573556	-2.66160724	-1.16709832
C	-1.31899169	2.42072421	1.64397684
C	-1.64353413	3.74381158	1.21367578
C	-2.88221322	4.28938593	1.61911352
C	-3.76399604	3.57990101	2.44463430
C	-3.39351629	2.31422236	2.92321897
C	-2.17104677	1.72449630	2.54704409
C	-1.35142564	5.28699987	-0.82619417
C	-0.68726944	4.64439378	0.41683081

C	-0.10482846	5.75271016	1.33964573
C	3.46514768	1.82399229	-3.29220940
C	3.66527570	2.44290765	-1.88471247
C	4.15253919	3.91255902	-1.99149683
C	4.22508769	0.98381817	0.18321786
C	4.62268645	1.61226162	-1.02637819
C	5.97263115	1.48060785	-1.41580124
C	6.88889737	0.77175092	-0.62505022
C	6.47385572	0.17939409	0.57816215
C	5.13239509	0.26397220	1.00507856
C	-2.85436828	-0.59914252	3.39989719
C	-1.71698899	0.42726036	3.21741040
C	-1.05424190	0.75826817	4.58493275
C	5.27218607	-1.79167991	2.52694115
C	4.70947501	-0.36251777	2.33728867
C	5.13889358	0.54004279	3.52780749
C	-4.16286912	-1.02706732	-0.79820243
C	-4.72775687	0.02155725	-1.56782139
C	-6.13621767	0.11891960	-1.58419960
C	-6.93851933	-0.78220903	-0.87190743
C	-6.34907969	-1.81234289	-0.12234382
C	-4.94872689	-1.95907521	-0.06157222
C	-4.21071748	2.46646093	-2.05197271
C	-3.90200985	0.99202976	-2.41206477
C	-4.13377325	0.73019534	-3.92498324
C	1.11998216	-2.38407368	3.59915287
C	0.46706045	-2.80805893	2.26291580
C	-0.56208331	-3.94838774	2.50183182
C	1.34261140	-2.87170556	-0.16308670
C	1.48605228	-3.23869696	1.20380136
C	2.53360235	-4.11120015	1.55627408
C	3.42167832	-4.60508471	0.58863809
C	3.26443976	-4.22889379	-0.75072086
C	2.22508708	-3.36545335	-1.16438373
C	-5.02857082	-3.30279335	2.12718743
C	-4.34657727	-3.11666359	0.74792950
C	-4.42542083	-4.44877657	-0.05046336
C	3.41255757	-2.30676790	-3.14086329
C	2.12302283	-3.01671974	-2.65361730
C	1.83358390	-4.27457672	-3.51452978
H	0.89759336	3.03914769	2.55548135
H	3.14655292	2.59752801	1.97199522
H	-2.70983754	-2.70934155	-2.12986268
H	-0.60176179	-3.68205840	-1.52260856
H	-3.15148385	5.28870742	1.28706181
H	-4.71606483	4.01882463	2.73432527
H	-4.05539290	1.78693720	3.60460851
H	0.14806233	4.04210577	0.05229135
H	2.68460782	2.46375890	-1.40427585
H	-2.16901736	5.96660504	-0.54956250
H	-1.74546679	4.51509121	-1.49314037
H	-0.60839258	5.87368172	-1.38292582

H	-0.89901119	6.41345908	1.71198008
H	0.61540890	6.36905111	0.78450396
H	0.40984195	5.32936746	2.21231449
H	4.41723685	1.74261215	-3.83515128
H	2.78752494	2.45501858	-3.88063567
H	3.00954978	0.83111263	-3.22580320
H	4.28601262	4.36516582	-0.99993134
H	3.41437264	4.50832238	-2.54318039
H	5.10912847	3.98313925	-2.52620178
H	6.30690702	1.94515977	-2.33975507
H	7.92577130	0.68486878	-0.94183847
H	7.19579150	-0.36059164	1.18415206
H	-0.95327745	-0.02899103	2.57953594
H	3.61586092	-0.43628749	2.34525809
H	-3.60021971	-0.25995348	4.13105502
H	-2.45147051	-1.55291980	3.76717545
H	-3.35876671	-0.77622239	2.44560130
H	-1.76765923	1.26581623	5.24797814
H	-0.18586813	1.41657254	4.45725414
H	-0.71555735	-0.15793127	5.08685823
H	5.01043647	-2.43505353	1.68105870
H	4.85381122	-2.23925048	3.43830079
H	6.36462978	-1.78675471	2.63625277
H	6.23170199	0.64289101	3.56254584
H	4.80859475	0.10136121	4.47892892
H	4.71031967	1.54688615	3.45189338
H	-6.60278722	0.90697311	-2.16807031
H	-8.02126191	-0.68606945	-0.90137108
H	-6.98300626	-2.50263068	0.42608483
H	-2.84036107	0.82759322	-2.22581583
H	-0.08531238	-1.94478208	1.87663442
H	-5.25197186	2.73397983	-2.27956706
H	-3.55621648	3.12639087	-2.63278685
H	-4.02614365	2.66223929	-0.98968229
H	-3.87269859	-0.30054197	-4.19653839
H	-3.49673268	1.40043138	-4.51455241
H	-5.17955676	0.90784973	-4.21199595
H	1.63738216	-3.22022707	4.08647485
H	0.35216307	-2.02663142	4.29631761
H	1.84491163	-1.57572210	3.44659930
H	-1.07166362	-4.22909736	1.57031126
H	-1.32347513	-3.63614334	3.22879589
H	-0.06398890	-4.84604117	2.89146114
H	2.65147471	-4.41482327	2.59276458
H	4.22460348	-5.27936693	0.87705325
H	3.95572474	-4.61128383	-1.49708467
H	-3.28957991	-2.89718379	0.94003842
H	1.31412177	-2.29852043	-2.80465215
H	-6.05939531	-3.66475108	2.02505255
H	-5.05055852	-2.36761760	2.69594926
H	-4.47764815	-4.04870901	2.71477613
H	-3.97894284	-5.26820291	0.52816726

H	-3.90166090	-4.38798624	-1.01248464
H	-5.47024974	-4.71157863	-0.26033782
H	3.61456192	-1.41798993	-2.53376070
H	3.29186446	-1.98687327	-4.18394669
H	4.28920168	-2.96713730	-3.08717642
H	0.90521963	-4.77636623	-3.20691397
H	2.64546994	-5.01107442	-3.44415826
H	1.72993665	-3.98980334	-4.56973952
O	0.35779695	2.35577675	-1.58387414
O	-1.03116476	2.14598079	-1.52428429
O	-0.79335741	-0.38285873	-2.54082047
O	-1.97790583	-0.32799982	0.03386000
Hf	-0.02087663	0.38840261	-0.69222249

Oxo Complex with Adsorbed Ozone Group

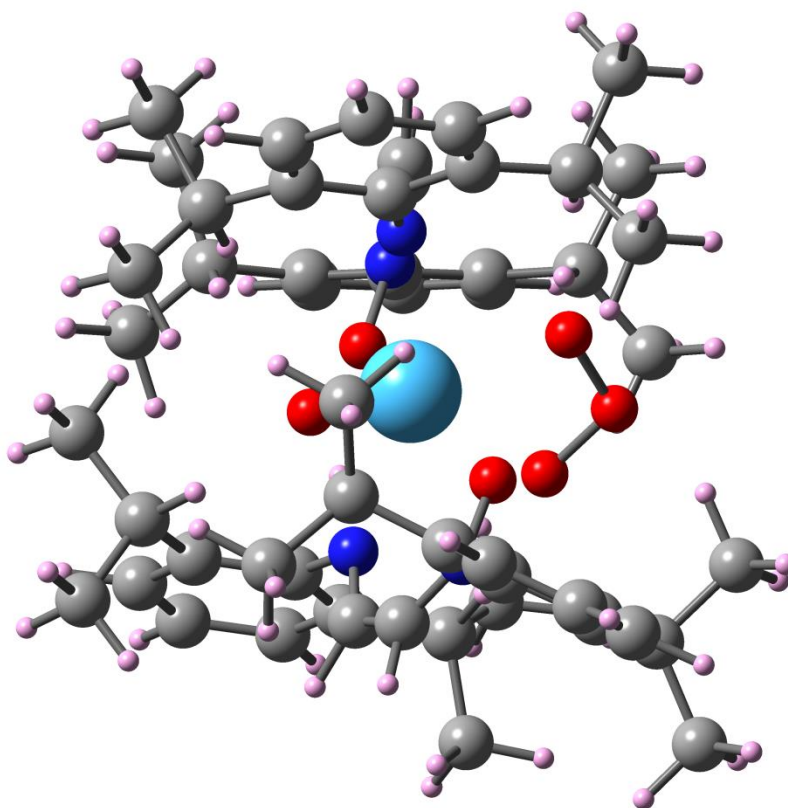


Fig. S70: NCCNO Oxo Complex with Adsorbed Ozone Group

E	E_{zp}	H	G
-2743.7456	-2742.5920	-2742.5198	-2742.7041
O	-1.92342373	0.41628064	-0.00151620
O	2.03689117	-0.89739996	-0.59937272
O	0.48748232	0.49349313	-2.38149431
N	-0.25260240	-2.00694061	1.02982227
N	2.71833074	-1.74274596	0.17966424
N	0.09232203	2.39176388	-0.38671982
N	-2.71373268	1.27919657	-0.77101753
C	0.77191057	-2.72347217	1.41374106
C	2.17013852	-2.55475909	1.06845116
C	-0.99589247	3.05667798	-0.84955297
C	-2.27508176	2.53348653	-1.07792968
C	-1.53811957	-2.42997204	1.61478024
C	-1.87824462	-1.97563228	2.91888370
C	-3.08633968	-2.44773781	3.47690169
C	-3.92380845	-3.32718639	2.77718612
C	-3.55998364	-3.76076995	1.49400024
C	-2.36310884	-3.32815711	0.88678663
C	-1.78001310	0.18614185	4.26948276

C	-0.98894349	-1.03954419	3.74689294
C	-0.33794004	-1.80567325	4.93075968
C	4.85853837	1.38216784	1.88352409
C	4.34068496	-0.07660624	1.94423702
C	4.62041588	-0.69773797	3.33950727
C	4.17548273	-1.73824637	-0.03127719
C	4.95578903	-0.93762671	0.83473331
C	6.35152661	-0.96790940	0.62581500
C	6.91223663	-1.73291853	-0.40940086
C	6.09278582	-2.48012232	-1.27201016
C	4.69247467	-2.49859162	-1.10644798
C	-3.12660251	-3.91499065	-1.48723718
C	-1.95587484	-3.89617280	-0.47544927
C	-1.35925284	-5.32179811	-0.31165174
C	3.70105192	-2.47460392	-3.42983361
C	3.79625151	-3.25643721	-2.09044066
C	4.27158666	-4.71157086	-2.32553579
C	1.24290651	3.24193026	-0.07006318
C	2.17370978	3.59538514	-1.08827243
C	3.26234348	4.42707722	-0.74200159
C	3.42192399	4.91465476	0.56147851
C	2.48184884	4.57603677	1.54663276
C	1.38379442	3.73965684	1.25806353
C	3.25147652	2.31231030	-3.01042107
C	2.03071976	3.14649657	-2.54606950
C	1.80402306	4.36071276	-3.48587371
C	-5.43257211	0.49275665	2.42510525
C	-4.74920954	1.32463318	1.31437305
C	-5.17056673	2.81750257	1.42026911
C	-4.04203394	0.80532066	-1.10682220
C	-5.03773628	0.79580913	-0.09398096
C	-6.32699512	0.35410759	-0.45156496
C	-6.61181694	-0.05662405	-1.76496184
C	-5.61059035	-0.03263809	-2.74682484
C	-4.29933000	0.39241502	-2.43988456
C	1.01906918	2.95314312	3.66217872
C	0.35571787	3.45303957	2.35671768
C	-0.52251987	4.70727232	2.61761040
C	-3.10652787	-0.92723910	-4.27887600
C	-3.23125995	0.42739123	-3.53817089
C	-3.51947421	1.57371000	-4.54572919
H	0.60779484	-3.55269191	2.10623693
H	2.87671855	-3.19485106	1.58327861
H	-0.88894538	4.12059929	-1.06371732
H	-3.02355456	3.16981579	-1.53459787
H	-3.36892369	-2.12016078	4.47391278
H	-4.84862727	-3.67694173	3.23004362
H	-4.20724667	-4.44852492	0.95726327
H	-0.18837993	-0.64070129	3.11481589
H	3.25239392	-0.02196040	1.81261485
H	-2.57903891	-0.10148451	4.96660926
H	-2.23120305	0.73991485	3.43771491

H	-1.10095304	0.86533558	4.79938241
H	-1.09655476	-2.19885031	5.62150802
H	0.32188804	-1.13493096	5.49681920
H	0.26401304	-2.65589575	4.58100797
H	5.93583380	1.44778928	2.08959226
H	4.33417579	1.98744665	2.63215078
H	4.66378410	1.83291792	0.90383935
H	4.21039858	-1.71368164	3.42369238
H	4.15564440	-0.08311042	4.12046909
H	5.69835636	-0.75330204	3.54447257
H	6.99779898	-0.37660039	1.26790777
H	7.99003030	-1.73686329	-0.55360363
H	6.54265416	-3.04845369	-2.08100339
H	-1.18085889	-3.25789962	-0.90538466
H	2.77909580	-3.30545204	-1.68345810
H	-3.90498440	-4.63656276	-1.20485283
H	-2.75495720	-4.20155938	-2.47957221
H	-3.59069224	-2.92545128	-1.56780391
H	-2.09848511	-6.01105709	0.11859479
H	-0.48134819	-5.32130021	0.34898605
H	-1.04913724	-5.71924616	-1.28733430
H	3.29588288	-1.47020755	-3.26618816
H	3.03653707	-3.00047427	-4.12718032
H	4.68846778	-2.38051361	-3.90122820
H	5.25188099	-4.74431028	-2.81783372
H	3.55990481	-5.23468977	-2.97686327
H	4.34814528	-5.27027102	-1.38353966
H	3.98346991	4.70198827	-1.50850387
H	4.26352721	5.55907484	0.80632432
H	2.59931214	4.97023493	2.55302771
H	1.15841153	2.49689985	-2.63271185
H	-3.66863003	1.26562968	1.48054202
H	4.18125878	2.89692806	-2.97592374
H	3.10289262	1.97076688	-4.04339582
H	3.37662421	1.42593557	-2.37759637
H	0.91691592	4.93607528	-3.18863756
H	1.65669939	4.01709511	-4.51882324
H	2.66280274	5.04554781	-3.47825358
H	-6.52669031	0.58244578	2.39048636
H	-5.10679262	0.85252012	3.40988547
H	-5.16701166	-0.56721795	2.34611060
H	-4.64769900	3.43606193	0.68056034
H	-4.93263403	3.20972873	2.41796212
H	-6.25089943	2.93146254	1.25712719
H	-7.11362662	0.33409673	0.29704574
H	-7.61412437	-0.39237042	-2.02154488
H	-5.84477139	-0.35282340	-3.75864069
H	-0.29231046	2.64427622	2.01128289
H	-2.26028742	0.63041384	-3.07688481
H	1.71637645	3.68886792	4.08550911
H	1.55146168	2.01805666	3.45972011
H	0.24984296	2.75562904	4.42141984

H	-1.28731286	4.48770718	3.37542087
H	-1.03346348	5.03437128	1.70226258
H	0.08314750	5.54854813	2.98193477
H	-2.87055446	-1.73602370	-3.57986081
H	-2.29444658	-0.87292403	-5.01490392
H	-4.02917168	-1.18724604	-4.81485666
H	-3.56539814	2.54886553	-4.04407014
H	-4.47567964	1.41616887	-5.06268349
H	-2.72635801	1.61900788	-5.30317092
O	0.94748493	0.38225023	1.54437620
O	0.12521546	-0.78002026	-2.91525485
O	-0.35849847	-1.57961129	-1.87914556
Hf	0.14867725	0.14442971	-0.08676198

7.6 Seven Oxygen Atoms

Ozone Complex with Adsorbed Oxygen Molecule

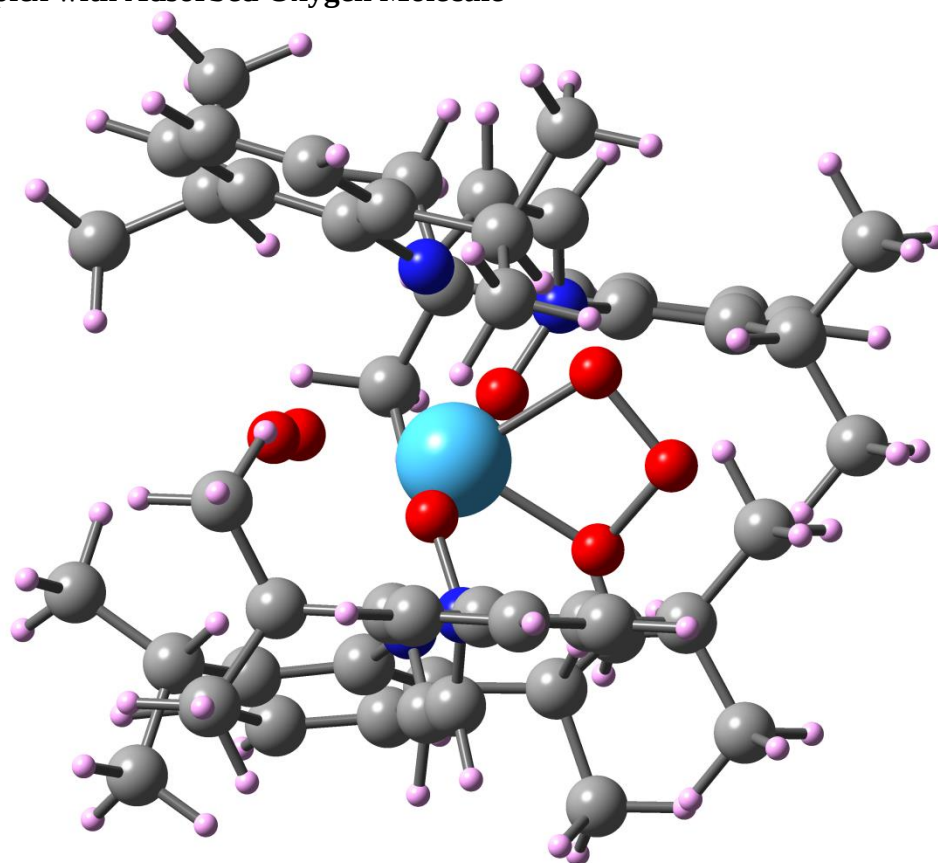


Fig. S71: NCCNO Ozone Complex with Adsorbed Oxygen Molecule

E	E _{zp}	H	G
-2818.9118	-2817.7547	-2817.6820	-2817.8660
O	-2.09909079	-0.31825652	0.06853161
O	2.13053906	0.27295517	0.18073982
O	0.11115481	-1.38738419	1.59744408
N	0.14761896	2.38251019	-0.10307566
N	2.78295604	1.19218444	0.90649184
N	-0.12605241	-2.15876124	-0.87878458
N	-2.80098460	-1.45661713	0.45224740
C	1.09099580	2.98522184	0.57574367
C	2.28584613	2.39804967	1.14602792
C	-1.14235331	-3.00018054	-0.54726707
C	-2.34691728	-2.69067154	0.09774634
C	-0.86126625	3.25284744	-0.72411129
C	-0.62079935	3.72653735	-2.04396856
C	-1.60416087	4.54573531	-2.63575659
C	-2.77593812	4.89041802	-1.94666189
C	-2.97438727	4.43283054	-0.63636443
C	-2.02685438	3.60922993	0.00874677

C	0.43219306	3.00410077	-4.26805771
C	0.68043362	3.44192957	-2.80440921
C	1.61591024	4.68190840	-2.75452892
C	5.13672313	-0.13441500	-1.93710553
C	4.96372859	1.12097066	-1.04158622
C	5.91490516	2.26143179	-1.48851172
C	4.11343026	0.79898988	1.38753088
C	5.16335227	0.76786040	0.43617564
C	6.43437714	0.38173529	0.90765497
C	6.63437624	0.04992686	2.25775469
C	5.56574687	0.08810789	3.16591260
C	4.26670941	0.45552025	2.75235353
C	-3.67554020	2.68353313	1.74313490
C	-2.24639997	3.21194476	1.47354412
C	-1.93342496	4.41737708	2.40418082
C	2.92243485	-0.93846828	4.40321649
C	3.11325944	0.45971680	3.76194094
C	3.33570609	1.54254610	4.85134214
C	0.90076521	-2.74319610	-1.74317239
C	2.05388239	-3.34977945	-1.16600294
C	3.03330241	-3.88052378	-2.03326691
C	2.87893927	-3.83263158	-3.42631923
C	1.71767633	-3.27126081	-3.97642842
C	0.70750044	-2.72606600	-3.15615550
C	3.63265707	-3.18741495	0.85459684
C	2.21294604	-3.53609186	0.34728498
C	1.84746317	-4.99452372	0.74219101
C	-5.18574022	0.74911507	-1.84742926
C	-4.95337734	-0.71475704	-1.39031267
C	-5.85261306	-1.69412980	-2.18937060
C	-4.12029367	-1.22313757	1.00569251
C	-5.16920872	-0.86530546	0.11889380
C	-6.44594617	-0.65092149	0.67744487
C	-6.66348834	-0.79412511	2.05793494
C	-5.60514205	-1.14654923	2.90964567
C	-4.30407398	-1.35899435	2.40461087
C	-0.31349302	-1.25836744	-4.99774557
C	-0.58136275	-2.21005185	-3.80641937
C	-1.47330103	-3.40151829	-4.25406710
C	-2.98247049	-0.66690865	4.46853927
C	-3.15893912	-1.72729813	3.35262054
C	-3.37654163	-3.13853887	3.96065707
H	1.03303731	4.06717292	0.71946022
H	2.91425133	3.04024924	1.75093416
H	-1.03626598	-4.04812021	-0.82817009
H	-3.02864418	-3.49907989	0.33277501
H	-1.44852420	4.91664936	-3.64501728
H	-3.52357215	5.51997901	-2.42342188
H	-3.87465834	4.72120390	-0.10076676
H	1.19628635	2.60943280	-2.31687292
H	3.93624110	1.47111698	-1.19045598
H	-0.01152785	3.80888058	-4.86915773

H	-0.23359390	2.13571119	-4.29930962
H	1.38319355	2.72495678	-4.74061609
H	1.14730633	5.54727186	-3.24177274
H	2.55992893	4.46972509	-3.27441993
H	1.85244491	4.97242899	-1.72148129
H	6.14662907	-0.55523173	-1.84157299
H	4.97693988	0.13020629	-2.99011909
H	4.41142286	-0.91060057	-1.67173173
H	5.78902670	3.15890948	-0.86860991
H	5.70735618	2.53401823	-2.53126720
H	6.96777431	1.95725503	-1.42932352
H	7.27067458	0.34119606	0.21527749
H	7.62355251	-0.24415659	2.60030202
H	5.73460923	-0.18233715	4.20443641
H	-1.55475283	2.40631397	1.73450336
H	2.17423900	0.68619165	3.24907990
H	-4.44220950	3.45335821	1.58200255
H	-3.75693474	2.35311493	2.78687267
H	-3.90300169	1.82601367	1.10211850
H	-2.61120915	5.25900411	2.20576233
H	-0.90487270	4.77929251	2.26915133
H	-2.05190571	4.12357375	3.45539855
H	2.69356559	-1.68701156	3.63744002
H	2.07597671	-0.90941185	5.09973452
H	3.81335021	-1.26117481	4.95886356
H	4.23742113	1.33816866	5.44381279
H	2.47893822	1.56278112	5.53628482
H	3.44407666	2.54482544	4.41427294
H	3.91989040	-4.34663955	-1.61102130
H	3.64742708	-4.24565865	-4.07621253
H	1.58998771	-3.26010695	-5.05584598
H	1.51204391	-2.87388137	0.86195917
H	-3.91064084	-0.95636218	-1.61913361
H	4.39621437	-3.86895066	0.45529999
H	3.66593531	-3.26533013	1.94949475
H	3.90879864	-2.16329197	0.58002250
H	0.82022703	-5.24344242	0.44666508
H	1.92638452	-5.12433229	1.82997189
H	2.52108796	-5.71676172	0.26014996
H	-6.21478954	1.07496541	-1.64318578
H	-5.01014162	0.83918887	-2.92750425
H	-4.49874003	1.43279992	-1.33672271
H	-5.67278688	-2.73548547	-1.89234182
H	-5.64521839	-1.60496352	-3.26392163
H	-6.91861480	-1.47997820	-2.03595973
H	-7.27437580	-0.37607430	0.02933553
H	-7.65710679	-0.62928845	2.46878984
H	-5.78625026	-1.24922560	3.97647983
H	-1.13919646	-1.63837888	-3.06001216
H	-2.22293404	-1.74670948	2.78735511
H	0.16803898	-1.77739289	-5.83753257
H	0.32713080	-0.42614092	-4.68832755

H	-1.26202344	-0.84463143	-5.36567532
H	-2.41025027	-3.03282895	-4.69371042
H	-1.72711830	-4.05344628	-3.40827244
H	-0.96201420	-4.01442591	-5.00869729
H	-2.78585141	0.32068444	4.03620893
H	-2.12282441	-0.93122103	5.09667638
H	-3.86909868	-0.59762733	5.11382998
H	-3.45294695	-3.90482383	3.17793639
H	-4.29459288	-3.18017540	4.56269484
H	-2.53212038	-3.40218287	4.61052902
O	0.70495759	0.27835119	-2.12791798
O	-0.66423225	0.55673934	-2.13522965
O	-0.01321606	-0.37778373	2.70007458
O	-0.00222337	0.88155589	1.89762303
Hf	-0.04382417	-0.05604078	-0.03986936

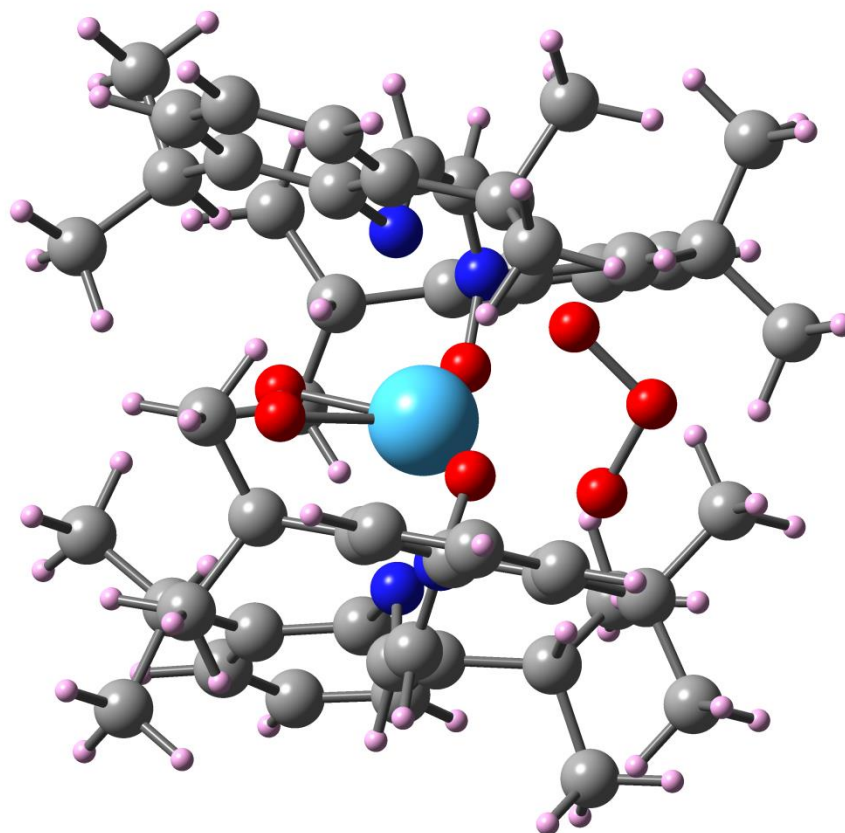
Peroxo Complex with Adsorbed Ozone Group

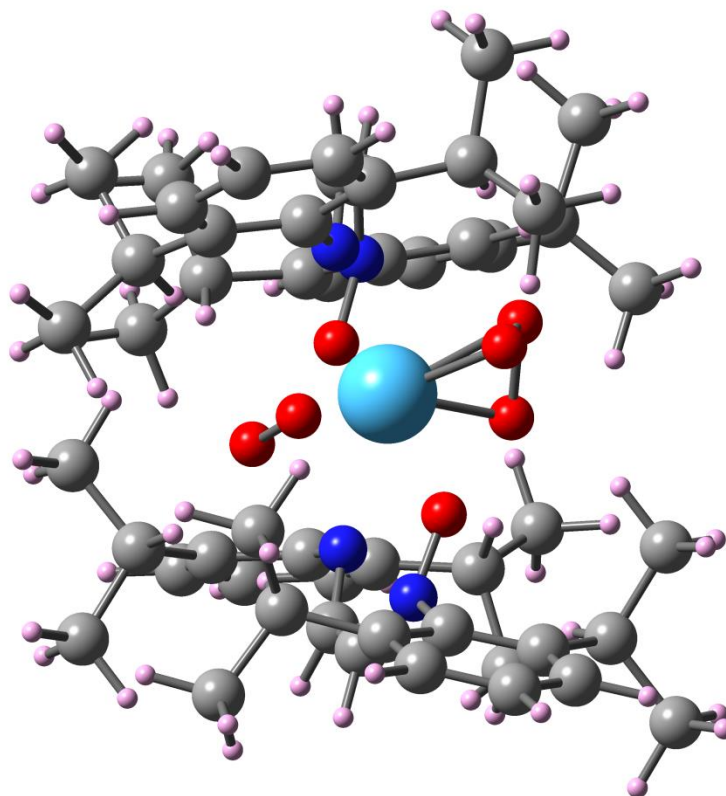
Fig. S72: NCCNO Peroxo Complex with Adsorbed Ozone Group

E	E_{zp}	H	G
-2818.9057	-2817.7488	-2817.6758	-2817.8617
O	-2.08895479	0.18802481	-0.41032998
O	1.94877616	-0.68036364	-0.68075844
O	-0.03434188	0.67164617	-2.18870327
N	-0.01636226	-2.17239033	0.84972327
N	2.84304446	-1.60579436	-0.15910689
N	0.02702486	2.40299068	-0.21592005
N	-2.80419195	1.24702542	-0.80105996
C	1.08658120	-2.96318461	0.94149004
C	2.39533272	-2.70151782	0.51215905
C	-1.07085843	3.04380001	-0.51356043
C	-2.36521053	2.49431582	-0.87068147
C	-1.18794113	-2.70248129	1.55783116
C	-1.30172159	-2.49469433	2.96569216
C	-2.43471965	-3.01579310	3.62640162
C	-3.42383049	-3.73066033	2.93490308
C	-3.27615827	-3.95937503	1.56033492
C	-2.15871092	-3.46668431	0.85093810
C	-0.78778367	-0.71895880	4.74137087

C	-0.21427665	-1.80434487	3.79824519
C	0.58591322	-2.85937207	4.61311035
C	4.92759789	1.19653722	2.09863634
C	4.55199690	-0.27599949	1.80015336
C	5.07088041	-1.21172373	2.92573576
C	4.23162580	-1.38939244	-0.50781439
C	5.06929492	-0.74022791	0.43478863
C	6.42165889	-0.55491643	0.07670209
C	6.90348653	-0.98036672	-1.17203697
C	6.04311147	-1.60083222	-2.09267793
C	4.68462348	-1.81741602	-1.78116462
C	-3.21155753	-3.34514193	-1.47187739
C	-2.00945889	-3.83494008	-0.62732381
C	-1.80555250	-5.36489161	-0.79662385
C	3.61032807	-1.62992967	-4.07718255
C	3.75398135	-2.48954050	-2.79443036
C	4.23367005	-3.92402359	-3.13751465
C	1.13780754	3.23613889	0.24618299
C	2.27371295	3.39549521	-0.59857271
C	3.31141242	4.23712834	-0.15227128
C	3.23920358	4.89230378	1.08671275
C	2.11722992	4.71014898	1.90477813
C	1.04158561	3.88444182	1.51210675
C	3.75050201	2.31839203	-2.40774193
C	2.33399458	2.78369240	-2.00003889
C	1.77458886	3.79125943	-3.04369365
C	-5.11160295	-0.21390297	2.23847668
C	-4.73401954	1.02869379	1.39248389
C	-5.37230903	2.31655187	1.97883308
C	-4.20692592	0.94595096	-1.14348210
C	-5.12988078	0.84411428	-0.07597149
C	-6.46986361	0.57690939	-0.42542856
C	-6.84873970	0.41161400	-1.76750956
C	-5.89533036	0.50149119	-2.79386667
C	-4.53888454	0.76477178	-2.50673048
C	0.36215704	3.14117612	3.84478413
C	-0.12971619	3.70488592	2.48639745
C	-0.90977531	5.03171800	2.68378926
C	-3.49702746	-0.45618022	-4.48438784
C	-3.51005084	0.84419581	-3.64019352
C	-3.77078287	2.08208418	-4.53985138
H	0.96662863	-3.92153858	1.44674637
H	3.16471129	-3.42874687	0.74280674
H	-1.07450965	4.13615873	-0.48628837
H	-3.11601911	3.20685736	-1.19153048
H	-2.53636964	-2.86520824	4.69812516
H	-4.28955504	-4.12077817	3.46588611
H	-4.02478645	-4.54268037	1.02932646
H	0.47660691	-1.29495994	3.12348041
H	3.45814473	-0.32752916	1.79927963
H	-1.46948292	-1.13875440	5.49470043
H	-1.31484361	0.04042058	4.15603044

H	0.03325207	-0.22292879	5.27671916
H	-0.06218837	-3.38393431	5.32877135
H	1.39014268	-2.36972959	5.17912837
H	1.04261918	-3.61487518	3.96014540
H	6.01451960	1.33546042	2.17949023
H	4.47802723	1.50561833	3.05065291
H	4.54891102	1.86745081	1.31960055
H	4.76640879	-2.25245485	2.75535832
H	4.66697416	-0.89509339	3.89607794
H	6.16752903	-1.18656650	2.98801214
H	7.09794932	-0.06837871	0.77450320
H	7.94890640	-0.82474654	-1.42928431
H	6.42878030	-1.91848247	-3.05830590
H	-1.11887175	-3.34374877	-1.02131878
H	2.75566194	-2.56779018	-2.35210853
H	-4.14861095	-3.83016040	-1.16513254
H	-3.04449229	-3.57651786	-2.53254660
H	-3.33649189	-2.26118496	-1.37082229
H	-2.67665482	-5.92954665	-0.43761411
H	-0.92752768	-5.71371880	-0.23706424
H	-1.65506614	-5.61217307	-1.85630648
H	3.21353379	-0.63790261	-3.83445135
H	2.91637698	-2.11201621	-4.77809594
H	4.57477652	-1.50296903	-4.58766272
H	5.21943081	-3.91486136	-3.62151552
H	3.52624131	-4.40407922	-3.82641991
H	4.30769177	-4.54675494	-2.23645979
H	4.18099304	4.38576554	-0.78505120
H	4.05237579	5.53769571	1.41065784
H	2.07272022	5.20749605	2.87012785
H	1.68563380	1.90427427	-2.02869479
H	-3.64577134	1.13278229	1.46302842
H	4.44766234	3.15889805	-2.52783083
H	3.70066485	1.79722591	-3.37249935
H	4.16829215	1.62213777	-1.67176170
H	0.74434980	4.08747009	-2.80594392
H	1.76972252	3.33632101	-4.04268413
H	2.38910361	4.70163338	-3.08106322
H	-6.19785152	-0.37527930	2.25808899
H	-4.77282249	-0.07672194	3.27284532
H	-4.63338910	-1.11848851	1.84855400
H	-5.08315726	3.20881203	1.40738383
H	-5.04689371	2.45748953	3.01729060
H	-6.46854643	2.25619207	1.97432455
H	-7.21764302	0.49493691	0.35828306
H	-7.88770625	0.20591913	-2.01323877
H	-6.20220808	0.35727791	-3.82593501
H	-0.81097551	2.94703093	2.09062450
H	-2.50761823	0.95094805	-3.21304645
H	1.04408638	3.83570300	4.35441752
H	0.87319042	2.18741315	3.68363210
H	-0.49533113	2.96403486	4.50775118

H	-1.76018899	4.87434237	3.36100788
H	-1.29786915	5.42508060	1.73336079
H	-0.27236469	5.80972351	3.12473541
H	-3.29810326	-1.33110561	-3.85641971
H	-2.70582271	-0.39783004	-5.24191837
H	-4.45169581	-0.61251699	-5.00378874
H	-3.73613578	3.01716428	-3.96469666
H	-4.75475153	2.02364957	-5.02336969
H	-3.00961056	2.14125685	-5.32795139
O	1.03676618	0.49056102	1.68292609
O	-0.50808067	0.62964964	1.80523986
O	-0.23866112	-0.55403521	-2.91459009
O	-0.41196991	-1.57201584	-1.99174651
Hf	0.07704030	-0.08272721	-0.00092146

η^3 -ozone Complex with Adsorbed Oxygen MoleculeFig. S73: NCCNO η^3 -ozone Complex with Adsorbed Oxygen Molecule

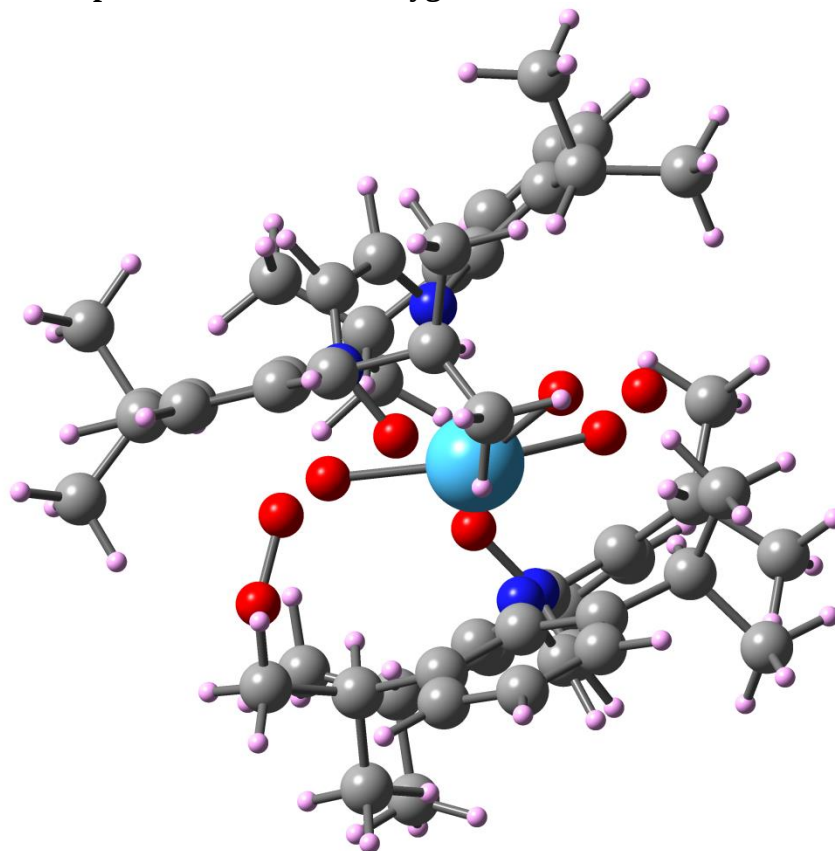
E	E_{zp}	H	G
-2818.8918	-2817.7345	-2817.6622	-2817.8438
O	-1.82749712	0.34099067	0.14756179
O	2.12137420	-1.01526843	-0.63764532
O	1.12054284	0.85334497	-2.12786835
N	-0.07340430	-2.06219730	0.85751797
N	2.85627102	-1.83112904	0.11230992
N	-0.16020999	2.51314114	-0.16258116
N	-2.79910566	1.10990625	-0.51282751
C	0.92748866	-2.77565119	1.31188575
C	2.33720795	-2.63158347	1.02809199
C	-1.33300186	3.07873853	-0.54273879
C	-2.54571076	2.42101085	-0.77198629
C	-1.37722618	-2.55511091	1.33290667
C	-1.74532904	-2.35080288	2.69095152
C	-2.95254792	-2.93151550	3.13504658
C	-3.76156101	-3.68215624	2.27210986
C	-3.37556589	-3.86424358	0.93517531
C	-2.17768899	-3.31415773	0.43634968
C	-1.69961393	-0.36062059	4.29052841

C	-0.90182348	-1.54732951	3.69197800
C	-0.35695469	-2.45789006	4.82575885
C	5.25569307	0.84683599	2.08673217
C	4.79856576	-0.63397949	2.03579954
C	5.34876409	-1.43046682	3.24871126
C	4.29202699	-1.85050717	-0.21181840
C	5.20775258	-1.29112445	0.71186422
C	6.57126582	-1.33194458	0.34766278
C	6.97929323	-1.87790517	-0.87790200
C	6.03333413	-2.39692955	-1.77704024
C	4.65809370	-2.39692728	-1.46855403
C	-2.88481808	-3.76040902	-1.99360251
C	-1.71612239	-3.62237347	-0.99120785
C	-0.85149191	-4.91466530	-1.01419794
C	3.38717798	-1.89103581	-3.59880136
C	3.63668808	-2.93622323	-2.47577379
C	4.06049540	-4.30412866	-3.06734875
C	0.88817585	3.47867027	0.17483263
C	1.65224997	4.11532079	-0.84459999
C	2.65934142	5.02469163	-0.45124430
C	2.89600780	5.32012766	0.89811348
C	2.09925422	4.72441996	1.88731706
C	1.08249172	3.80833188	1.55064906
C	2.67013389	3.45498369	-3.09365216
C	1.39636186	3.91561329	-2.34317462
C	0.82576420	5.21313684	-2.97812771
C	-5.39676443	-0.16700217	2.75939585
C	-4.66517633	0.65214112	1.67266986
C	-5.03200356	2.15663276	1.83082050
C	-4.06254269	0.46858965	-0.82398975
C	-4.96195464	0.18491887	0.24302127
C	-6.17254103	-0.45851902	-0.07636887
C	-6.49126978	-0.78283325	-1.40687946
C	-5.60927831	-0.45106097	-2.44302347
C	-4.37357053	0.18314181	-2.18002273
C	0.90580632	2.88070762	3.94356575
C	0.15708428	3.26950363	2.64674426
C	-0.96117566	4.30420949	2.95561607
C	-3.10587180	-0.62713103	-4.25589399
C	-3.47535059	0.57920248	-3.35776143
C	-4.15252135	1.70044322	-4.19360017
H	0.71677979	-3.61702811	1.97727700
H	3.03368339	-3.28132149	1.54216480
H	-1.35584042	4.15882496	-0.68658197
H	-3.38244770	2.97804888	-1.17460268
H	-3.25817481	-2.79155561	4.16888826
H	-4.68539457	-4.12482826	2.63722648
H	-4.00805415	-4.44672809	0.27277433
H	-0.04375582	-1.10931886	3.17661634
H	3.70723818	-0.61591859	2.11244387
H	-2.57883804	-0.70315931	4.85171480
H	-2.03796728	0.31733326	3.49917152

H	-1.06178478	0.20976623	4.97831149
H	-1.17398753	-2.90458385	5.40717827
H	0.26700540	-1.87417938	5.51538496
H	0.25249741	-3.28184604	4.42953667
H	6.34822936	0.93826227	2.02999541
H	4.92549060	1.30529652	3.02733717
H	4.81247579	1.41861140	1.26473379
H	4.99923066	-2.47223958	3.24575434
H	5.02048344	-0.96398245	4.18622067
H	6.44621028	-1.44983846	3.24950113
H	7.31359381	-0.91621267	1.02315373
H	8.03482986	-1.89065989	-1.13831806
H	6.36498073	-2.80603919	-2.72644057
H	-1.09548563	-2.78998586	-1.34018454
H	2.67577817	-3.08381475	-1.96905822
H	-3.47591845	-4.66922623	-1.81394271
H	-2.48626367	-3.82562866	-3.01372420
H	-3.55542637	-2.89549112	-1.94656778
H	-1.43650775	-5.78162885	-0.67741498
H	0.03015413	-4.83260334	-0.36529779
H	-0.49997965	-5.11446330	-2.03494859
H	2.96608415	-0.96885603	-3.18646806
H	2.66936956	-2.29088727	-4.32658946
H	4.32040182	-1.65704908	-4.12962401
H	4.95540226	-4.21787529	-3.69687413
H	3.25415236	-4.69520151	-3.70054323
H	4.26807122	-5.04257380	-2.28145480
H	3.25863444	5.51131072	-1.21705018
H	3.67959120	6.02190268	1.17545399
H	2.26339355	4.98053619	2.93052896
H	0.66134813	3.11923994	-2.46859535
H	-3.58711541	0.54679700	1.83690279
H	3.47411730	4.20206653	-3.03715969
H	2.43984144	3.28606533	-4.15408024
H	3.03506239	2.50994368	-2.67871369
H	-0.09980203	5.53291544	-2.48031985
H	0.60123691	5.04677247	-4.04047240
H	1.54269635	6.04285096	-2.91109336
H	-6.48020897	0.01450137	2.74435053
H	-5.03224993	0.13047097	3.75118827
H	-5.22022674	-1.24064754	2.63980992
H	-4.47301428	2.78836135	1.13265903
H	-4.80204194	2.49679136	2.84954805
H	-6.10495192	2.31199250	1.65361634
H	-6.87659220	-0.70128387	0.71293944
H	-7.43221588	-1.27984039	-1.63256743
H	-5.87592221	-0.68667047	-3.46994776
H	-0.32786709	2.36491345	2.26796254
H	-2.53358369	0.97531641	-2.97315434
H	1.33352418	3.75582908	4.45087779
H	1.71355123	2.17245821	3.72865171
H	0.20950398	2.40403426	4.64659697

H	-1.64852883	3.91175406	3.71808500
H	-1.54661809	4.53728090	2.05747257
H	-0.53262029	5.24275117	3.33278697
H	-2.51662563	-1.35480183	-3.69114058
H	-2.49037953	-0.28335269	-5.09714825
H	-3.99466008	-1.12440162	-4.66825689
H	-4.39447269	2.57680615	-3.57711067
H	-5.08574522	1.34853517	-4.65361307
H	-3.48094294	2.02628279	-4.99855005
O	1.92756354	0.99965827	1.02325576
O	0.93506538	0.34129858	1.75515305
O	-0.33653750	0.52646060	-2.46200057
O	-0.45857434	-0.93007560	-1.99189073
Hf	0.20743003	0.22848495	-0.33625823

7.7 Eight Oxygen Atoms

Oxo η^2 -ozone Complex with Adsorbed Oxygen MoleculeFig. S74: NCCNO Oxo η^2 -ozone Complex with Adsorbed Oxygen Molecule

E	E_{zp}	H	G
-2894.0562	-2892.8957	-2892.8217	-2893.0096
O	-2.10331316	0.16311301	-0.21452202
O	1.93008915	-0.70224405	-0.40372503
O	-0.36003503	-0.33571703	-1.86256614
N	-0.07464201	-1.92063715	1.19040609
N	2.83704322	-1.48698911	0.30313702
N	-0.00317300	2.30991518	-0.62311505
N	-2.81963222	1.04514208	-0.90874707
C	1.03137708	-2.64875120	1.52369512
C	2.36543918	-2.43138418	1.16144209
C	-1.09387908	2.84457521	-1.11169408
C	-2.38878318	2.23354817	-1.30644410
C	-1.32628810	-2.47393819	1.71637313
C	-1.67461613	-2.26463617	3.08039523
C	-2.86508822	-2.85524622	3.55918327
C	-3.68621728	-3.62362728	2.72293921
C	-3.32110325	-3.82518329	1.38244610

C	-2.13845116	-3.26596325	0.85539407
C	-1.59572512	-0.34314103	4.76460736
C	-0.80017406	-1.46806011	4.05611031
C	-0.14398301	-2.41067119	5.10198839
C	5.05746639	1.67522913	1.90576514
C	4.61566835	0.19086101	1.93138215
C	5.10726439	-0.50432304	3.23016925
C	4.23308432	-1.38399011	-0.08420401
C	5.09902939	-0.57743604	0.69887705
C	6.45888948	-0.53388504	0.32127602
C	6.92625051	-1.25230410	-0.78982806
C	6.04217647	-2.03354816	-1.55162012
C	4.67420336	-2.11482216	-1.21897809
C	-2.89819122	-3.69711628	-1.56286612
C	-1.71048813	-3.58082527	-0.58108004
C	-0.86586007	-4.88477237	-0.62100905
C	3.85287429	-2.73312521	-3.56042127
C	3.73237628	-3.00068323	-2.03981816
C	3.98728630	-4.50091935	-1.72814413
C	1.11845908	3.24008825	-0.43942803
C	2.24299617	3.11705324	-1.30167110
C	3.30563225	4.02447531	-1.12881209
C	3.25760925	5.01916539	-0.13951301
C	2.13617316	5.12204639	0.69375505
C	1.03922508	4.24146632	0.57063204
C	3.66303828	1.55806812	-2.77839421
C	2.25781317	2.11256916	-2.45695019
C	1.62821812	2.75070421	-3.72729629
C	-5.17977240	0.18408201	2.35613418
C	-4.77613736	1.20683809	1.26452610
C	-5.42631041	2.59133020	1.53372011
C	-4.20602332	0.63571305	-1.19881209
C	-5.13973139	0.70766505	-0.13839601
C	-6.46556452	0.33297803	-0.44220803
C	-6.81907154	-0.09427201	-1.73173113
C	-5.85565144	-0.16165901	-2.75151421
C	-4.51258734	0.19707702	-2.51127019
C	0.28495102	4.51866335	3.00225723
C	-0.15635701	4.41257434	1.52006711
C	-0.99948907	5.65950744	1.13121709
C	-3.57429027	-1.17713309	-4.46244134
C	-3.46930126	0.12832001	-3.63527828
C	-3.59913128	1.35492410	-4.58193735
H	0.87386507	-3.51216727	2.16897617
H	3.12594224	-3.07947023	1.57928012
H	-1.07349908	3.89318830	-1.41282211
H	-3.13575224	2.83164422	-1.81194114
H	-3.14731024	-2.71071221	4.59909335
H	-4.59873835	-4.06961231	3.11283024
H	-3.95689430	-4.43084034	0.74304705
H	-0.00121000	-0.97666007	3.49659727
H	3.52215027	0.19304501	1.94445015

H	-2.41086018	-0.74341606	5.38344742
H	-2.01207415	0.34661403	4.02358031
H	-0.92570307	0.22926802	5.41936041
H	-0.90322307	-2.91212122	5.71771144
H	0.50967504	-1.83603414	5.77176144
H	0.46306804	-3.18990224	4.62203035
H	6.14959146	1.78541914	1.95860415
H	4.62542635	2.20076217	2.76677721
H	4.70149136	2.17671717	0.99837508
H	4.75238336	-1.54170612	3.28883725
H	4.72795536	0.03204300	4.10963532
H	6.20467246	-0.51961804	3.28603625
H	7.15267853	0.06902701	0.90082507
H	7.97829960	-1.20471009	-1.06234808
H	6.41664452	-2.58389120	-2.41052219
H	-1.07318908	-2.76880021	-0.94247607
H	2.70020721	-2.77058921	-1.76018613
H	-3.51044727	-4.58798235	-1.36693810
H	-2.51393619	-3.78200429	-2.58729519
H	-3.54811827	-2.81525321	-1.50641311
H	-1.45593911	-5.74360741	-0.27155702
H	0.02567100	-4.80478037	0.01207100
H	-0.53353104	-5.08751539	-1.64762513
H	3.68164028	-1.67445013	-3.78665829
H	3.09648623	-3.31568225	-4.09949531
H	4.84055737	-3.01544823	-3.94926730
H	5.00938638	-4.79518037	-2.00290215
H	3.28757625	-5.12864639	-2.29515017
H	3.84981929	-4.71797936	-0.66096405
H	4.17386632	3.95429830	-1.77645714
H	4.08937731	5.70949644	-0.02078000
H	2.11077516	5.89060645	1.46108811
H	1.63544113	1.25764910	-2.18077217
H	-3.69029228	1.32544910	1.33876310
H	4.32768133	2.32899618	-3.19161724
H	3.57766228	0.76294406	-3.52916927
H	4.13593031	1.12963309	-1.88828014
H	0.60304605	3.09798024	-3.54344627
H	1.59317212	2.01503215	-4.54073034
H	2.22086417	3.61210227	-4.06442031
H	-6.26771747	0.03890900	2.39599719
H	-4.85358337	0.54590404	3.33920525
H	-4.70562836	-0.78747306	2.18253716
H	-5.11625939	3.33681426	0.78890806
H	-5.12952439	2.95790323	2.52451519
H	-6.52233751	2.52881119	1.51002411
H	-7.22137457	0.37401403	0.33689203
H	-7.84672058	-0.38020703	-1.94249915
H	-6.14505345	-0.50859804	-3.73889329
H	-0.79028106	3.52239627	1.45788611
H	-2.46781419	0.13595501	-3.18897025
H	0.87300407	5.42605042	3.19428324

H	0.87242007	3.64205328	3.28830525
H	-0.60248805	4.55641935	3.64814328
H	-1.86313914	5.75658342	1.80256114
H	-1.37491011	5.60655744	0.09984201
H	-0.40288303	6.57772152	1.21544409
H	-3.52484827	-2.06053716	-3.81953929
H	-2.73861221	-1.22824709	-5.17134840
H	-4.50458734	-1.22177310	-5.04403738
H	-3.47576026	2.30798718	-4.05134231
H	-4.58354835	1.37086211	-5.06842339
H	-2.83271722	1.30606010	-5.36576941
O	1.41393111	0.74805006	1.67058413
O	-0.86231207	1.05365508	1.80933414
O	0.59560904	-0.81104906	-2.90297322
O	0.51630504	-2.13820016	-3.09722224
Hf	0.10130001	0.06334200	0.21482802
O	0.38296703	1.29382410	2.62588920

8. Singlet Ground States for ONCCNO Complex

8.1 Four Oxygen Atoms

Bare Complex (lower energy conformation)

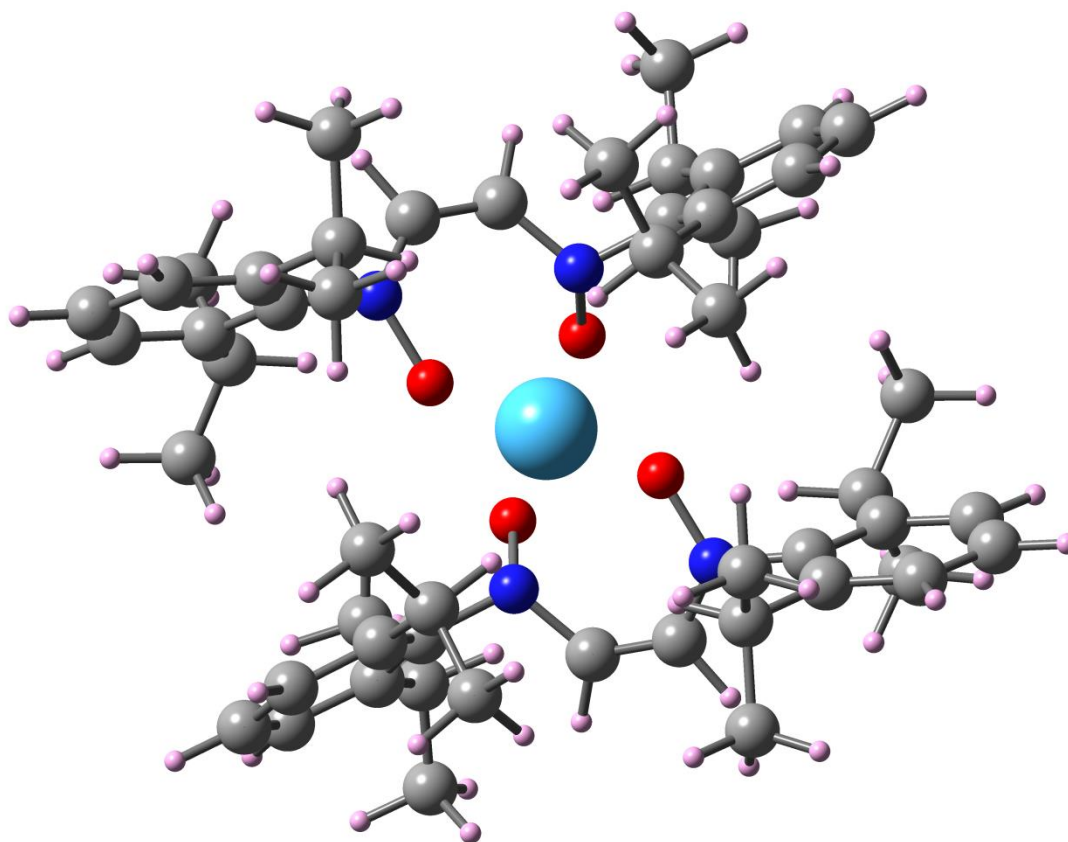


Fig. S75: ONCCNO Bare Complex (lower energy conformation)

E	E_{zp}	H	G
-2593.4106	-2592.2615	-2592.1932	-2592.3669
O	-0.48764500	-1.28737500	-2.08981100
O	-1.61793800	0.64792300	0.37457700
N	0.45628800	2.25324000	-0.82720100
N	-2.35711000	1.86785600	0.40595500
N	2.36335500	-1.87148800	0.36777900
N	-0.45577800	-2.24355500	-0.85618600
C	-0.64921000	3.17448500	-0.84395000
C	-1.86943200	2.95995900	-0.25972000
C	1.87241800	-2.95631000	-0.30655000
C	0.64945400	-3.16471600	-0.88746400
C	1.75742400	2.92561200	-0.67284400
C	2.31883200	2.98937900	0.63246100
C	3.56694200	3.62849800	0.78769500
C	4.23328400	4.19617300	-0.30742100
C	3.63732200	4.16415400	-1.57604200

C	2.38334900	3.55203400	-1.78815200
C	2.47410500	1.66290500	2.82838300
C	1.57980400	2.49494000	1.88086900
C	0.95841600	3.70406600	2.63437800
C	-2.89487600	1.90355400	4.56847900
C	-2.86004000	2.59683200	3.18417500
C	-2.92961300	4.14002100	3.34836400
C	-3.71032900	1.75985300	0.89844100
C	-3.97066100	2.10793400	2.25138400
C	-5.30428300	2.04016800	2.70597900
C	-6.33722700	1.62693000	1.84951500
C	-6.05635100	1.27597800	0.51975900
C	-4.73936200	1.33169000	0.01746400
C	2.58770900	2.75346300	-4.19497900
C	1.77381600	3.61671400	-3.19724200
C	1.65723300	5.08081100	-3.69745200
C	-5.04101400	-0.40335200	-1.83206800
C	-4.46113500	0.97996200	-1.44605900
C	-5.00913900	2.08583900	-2.38886100
C	3.71212000	-1.77316400	0.87288000
C	3.96515500	-2.16101900	2.21625800
C	5.29525800	-2.09923200	2.68227800
C	6.33137700	-1.65313500	1.84663400
C	6.05771900	-1.26401900	0.52588000
C	4.74498000	-1.31351500	0.01225000
C	2.85720700	-2.00524200	4.52041500
C	2.85209700	-2.68292600	3.12792800
C	2.94668000	-4.22647500	3.27385000
C	-2.59057900	-2.69804500	-4.22677800
C	-1.77947800	-3.57614300	-3.23999400
C	-1.66909000	-5.03485200	-3.75720500
C	-1.75741200	-2.91630500	-0.70743600
C	-2.38734500	-3.52622500	-1.82958700
C	-3.64340500	-4.13607400	-1.62341800
C	-4.23753200	-4.18211100	-0.35431700
C	-3.56691800	-3.63181500	0.74703300
C	-2.31657400	-2.99561700	0.59793600
C	5.05976400	0.46470800	-1.79472100
C	4.47454200	-0.92530600	-1.44353700
C	5.02411700	-2.01064900	-2.40926100
C	-2.46404000	-1.68938000	2.80573200
C	-1.57454000	-2.51884500	1.85134300
C	-0.96235600	-3.73938300	2.59395100
H	-0.48479900	4.12294700	-1.34496200
H	-2.58811300	3.77342400	-0.31011500
H	2.59140200	-3.76857900	-0.37038900
H	0.48374100	-4.10666700	-1.40017300
H	4.01801100	3.68337400	1.77445300
H	5.20070700	4.67366300	-0.17040200
H	4.14723400	4.62986900	-2.41555500
H	0.75022900	1.85307100	1.56697300
H	-1.90080900	2.35386100	2.71438600

H	3.28743700	2.26347300	3.25603900
H	2.90996300	0.80921500	2.30106400
H	1.87223600	1.28286700	3.66531700
H	1.74171400	4.39217700	2.97889100
H	0.39897800	3.35844100	3.51423800
H	0.27300300	4.26452600	1.98732400
H	-3.79735500	2.16731700	5.13553400
H	-2.02923900	2.21744800	5.16715100
H	-2.86455800	0.81264800	4.46723000
H	-2.84464900	4.64961500	2.38033500
H	-2.11376500	4.49542100	3.99144700
H	-3.88106100	4.44254500	3.80617300
H	-5.53614900	2.30836000	3.73329000
H	-7.35968500	1.57966100	2.21774700
H	-6.86540600	0.95797800	-0.13255500
H	0.77149000	3.18824200	-3.17054800
H	-3.37685000	0.92843000	-1.58956800
H	3.63129200	3.09088500	-4.26268700
H	2.14577100	2.81425600	-5.19870800
H	2.57591200	1.70479500	-3.87932700
H	2.64027800	5.55142200	-3.82803900
H	1.08106300	5.70148300	-2.99789500
H	1.14828800	5.10190800	-4.67053900
H	-4.65908100	-1.19267800	-1.17546800
H	-4.75712700	-0.65352900	-2.86191500
H	-6.13799400	-0.41210400	-1.77789100
H	-6.09966500	2.17837600	-2.29659300
H	-4.77567100	1.84328600	-3.43377800
H	-4.56751300	3.06439400	-2.16093300
H	5.52147300	-2.39759600	3.70259500
H	7.35085800	-1.61052400	2.22358500
H	6.86950000	-0.92152700	-0.11038800
H	1.89431000	-2.45087200	2.65006800
H	-0.77539500	-3.15201100	-3.20911800
H	3.76326000	-2.24887600	5.09067000
H	1.99667200	-2.35031400	5.10918900
H	2.79613800	-0.91458900	4.43009400
H	2.88420900	-4.72523600	2.29840700
H	2.12810800	-4.60395000	3.90074400
H	3.89649200	-4.51913900	3.74129900
H	-3.63571800	-3.02999000	-4.29746500
H	-2.14984000	-2.74893000	-5.23159300
H	-2.57390800	-1.65329300	-3.89870800
H	-1.09461800	-5.66572100	-3.06542400
H	-1.16132700	-5.04679700	-4.73106100
H	-2.65415000	-5.50006300	-3.89195100
H	-4.15647300	-4.58882200	-2.46809400
H	-5.20681800	-4.65714400	-0.22198400
H	-4.01659700	-3.69745300	1.73379700
H	3.39101700	-0.86823700	-1.59058600
H	-0.74004100	-1.88017800	1.54396800
H	6.15665200	0.46861500	-1.73796500

H	4.67875300	1.23945500	-1.12050100
H	4.77929700	0.74052900	-2.81895900
H	4.79651300	-1.74315800	-3.44937300
H	4.57830200	-2.99275800	-2.20623000
H	6.11392200	-2.10853400	-2.31372000
H	-2.89436700	-0.82907200	2.28487000
H	-1.86035000	-1.31944400	3.64580300
H	-3.28115400	-2.28884000	3.22777900
H	-0.28055800	-4.29893000	1.94219700
H	-1.75057600	-4.42519200	2.93177200
H	-0.40121600	-3.40596300	3.47745200
Hf	0.00020800	0.00374500	-0.62472600
O	0.48646800	1.31298200	-2.07369500
O	1.62049600	-0.65354300	0.36233100

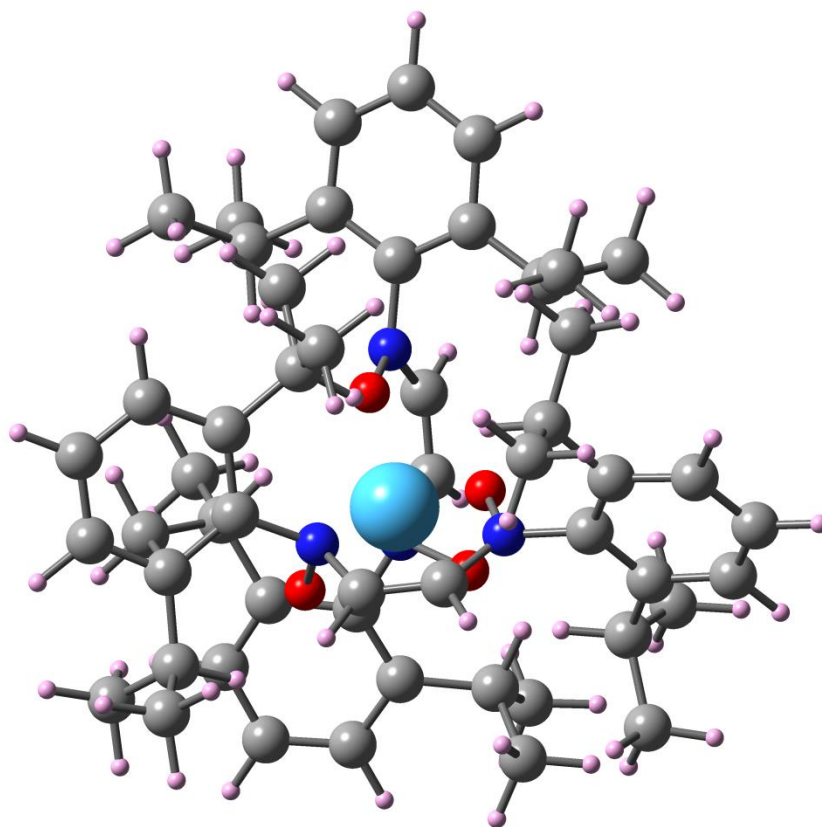
Bare Complex (higher energy conformation)

Fig. S76: ONCCNO Bare Complex (higher energy conformation)

E	E_{zp}	H	G
-2593.4064	-2592.2575	-2592.1892	-2592.3628
O	-0.99882799	1.33880353	-0.38969783
O	1.88698757	-0.02312914	-0.29648029
O	-0.15793897	-1.60405216	-1.69039481
O	-0.58444137	-1.65555877	1.44019688
N	0.52402557	-0.76448104	2.12259682
N	3.03388597	-0.59206570	0.32270278
N	-1.65148575	-1.19251900	-1.54819546
N	-1.73654357	1.88235184	-1.48919578
C	1.78319572	-1.43657553	2.29987475
C	2.88170006	-1.28815025	1.48639209
C	-2.07880802	-0.31665217	-2.60490044
C	-2.10534351	1.05055085	-2.51786757
C	-0.04481760	-0.21436387	3.36526366
C	0.01958936	1.19019691	3.57280263
C	-0.54943622	1.71443572	4.75419223
C	-1.14839911	0.87984837	5.70580733
C	-1.15778901	-0.50836343	5.50346858
C	-0.60202132	-1.08957869	4.34552228

C	-0.11078043	3.35641333	2.20373786
C	0.75906990	2.15089054	2.63436578
C	2.07274008	2.63425474	3.30898827
C	5.20859271	2.89152139	0.65365251
C	5.02159603	1.41712609	1.09421376
C	5.95571780	1.07796797	2.28634524
C	4.25514515	-0.51409423	-0.44202122
C	5.23458722	0.44609174	-0.06919228
C	6.44010945	0.48049202	-0.80140916
C	6.65077253	-0.38614765	-1.88491918
C	5.65773359	-1.30680693	-2.25512619
C	4.44326508	-1.39260549	-1.54290443
C	-1.98282128	-3.25444501	4.40766661
C	-0.57629861	-2.62405415	4.24753448
C	0.39232257	-3.21401868	5.31082250
C	2.86528328	-2.10094744	-3.39904604
C	3.38410282	-2.41056347	-1.97051144
C	3.92088179	-3.86284898	-1.87690894
C	-2.52286176	-2.36177037	-1.33727566
C	-3.58168205	-2.21611778	-0.39697396
C	-4.39897840	-3.33552711	-0.13924140
C	-4.18857735	-4.55600441	-0.79626907
C	-3.18088751	-4.65589060	-1.76515187
C	-2.34353222	-3.56275701	-2.07782900
C	-4.04072617	-0.97716415	1.80554915
C	-3.93711771	-0.87883230	0.26507594
C	-5.25627147	-0.32742278	-0.34335185
C	1.97506168	3.36616575	-1.92489209
C	0.68035185	3.05633603	-2.72055146
C	0.90653519	3.25236614	-4.24234445
C	-1.64304944	3.31974984	-1.61035417
C	-0.49255957	3.89900536	-2.21175273
C	-0.44512555	5.30395606	-2.32704017
C	-1.49941599	6.10342545	-1.85759693
C	-2.62044455	5.51172861	-1.25511424
C	-2.71068818	4.11134694	-1.10984286
C	-0.22602855	-4.76039239	-2.81406773
C	-1.32152610	-3.73748645	-3.21045461
C	-2.01510379	-4.15304102	-4.53500823
C	-4.21006808	4.07517345	0.95657175
C	-3.94296036	3.48714192	-0.45248401
C	-5.19309949	3.64347228	-1.35921526
H	1.88557612	-2.08420958	3.16221318
H	3.78783792	-1.80491188	1.79124469
H	-2.41714258	-0.78451243	-3.52439592
H	-2.48980233	1.59468405	-3.37635313
H	-0.51612956	2.78639015	4.92937678
H	-1.58878770	1.30391949	6.60519222
H	-1.59745385	-1.15292213	6.26018352
H	1.05064208	1.61224890	1.72731941
H	3.98863160	1.30835525	1.43845121
H	-0.40937925	3.96967094	3.06413255

H	-1.01086140	3.01928708	1.68029828
H	0.45241953	4.00061469	1.51585300
H	1.85925976	3.21155455	4.21823353
H	2.63680449	3.27999460	2.62299397
H	2.70923926	1.78573765	3.59029131
H	6.23856907	3.09201889	0.33076679
H	4.98732196	3.56643244	1.49130159
H	4.53771410	3.14270310	-0.17656391
H	5.79812754	0.05016960	2.63791089
H	5.76640220	1.75835881	3.12722286
H	7.01216932	1.17649981	2.00312326
H	7.21265881	1.19526925	-0.52903538
H	7.58413753	-0.34156425	-2.44169285
H	5.82936022	-1.96900117	-3.09995296
H	-0.22410643	-2.90935873	3.25532725
H	2.52653343	-2.33034340	-1.29604135
H	-2.42453627	-3.03271165	5.38829622
H	-1.91402503	-4.34649877	4.31336351
H	-2.66490317	-2.89152029	3.63294758
H	0.03551265	-3.01127081	6.32936355
H	1.40179001	-2.79014293	5.22711682
H	0.46742257	-4.30319879	5.19106668
H	2.44294418	-1.09112652	-3.44650600
H	2.07340250	-2.80812489	-3.67207477
H	3.66967692	-2.17867685	-4.14334045
H	4.76269995	-4.02717222	-2.56273435
H	3.12788870	-4.57408820	-2.14168139
H	4.26404306	-4.09771250	-0.86081530
H	-5.20793864	-3.24825233	0.58153913
H	-4.81758323	-5.41407038	-0.57096996
H	-3.04721222	-5.59289355	-2.29984319
H	-3.15151673	-0.15192993	0.04101964
H	0.45034077	1.99882561	-2.55775677
H	-4.82668249	-1.67706052	2.11862791
H	-4.28461861	0.00622311	2.23006518
H	-3.08856820	-1.30692786	2.23092567
H	-5.17201203	-0.20692151	-1.43064832
H	-5.49784882	0.65022747	0.09481885
H	-6.09677544	-1.00436498	-0.14119389
H	2.29009624	4.40917531	-2.06488849
H	2.78944066	2.71257197	-2.26158120
H	1.82373020	3.18990399	-0.85391655
H	0.00416089	3.00609912	-4.81687230
H	1.72002732	2.60205592	-4.58930931
H	1.18243483	4.28874425	-4.47772597
H	0.42060198	5.77479458	-2.78602562
H	-1.44582006	7.18513641	-1.95847063
H	-3.42769893	6.14195898	-0.89064078
H	-0.81520409	-2.78618822	-3.37909082
H	-3.74838859	2.41656242	-0.33298732
H	-0.65558345	-5.74936359	-2.60388754
H	0.30397617	-4.41703478	-1.91873868

H	0.50272654	-4.87670126	-3.62832901
H	-1.27535209	-4.20151713	-5.34572867
H	-2.79124104	-3.43179910	-4.82435385
H	-2.48947569	-5.14005292	-4.45922995
H	-3.33452879	3.95911184	1.60666930
H	-5.05635292	3.55740614	1.42747973
H	-4.45975673	5.14352028	0.91101874
H	-5.03194974	3.18367036	-2.34268369
H	-5.43726364	4.70219183	-1.51914597
H	-6.06474620	3.16141338	-0.89708516
Hf	-0.07996238	-0.41462608	-0.07021092

8.2 Five Oxygen Atoms

Oxo Complex

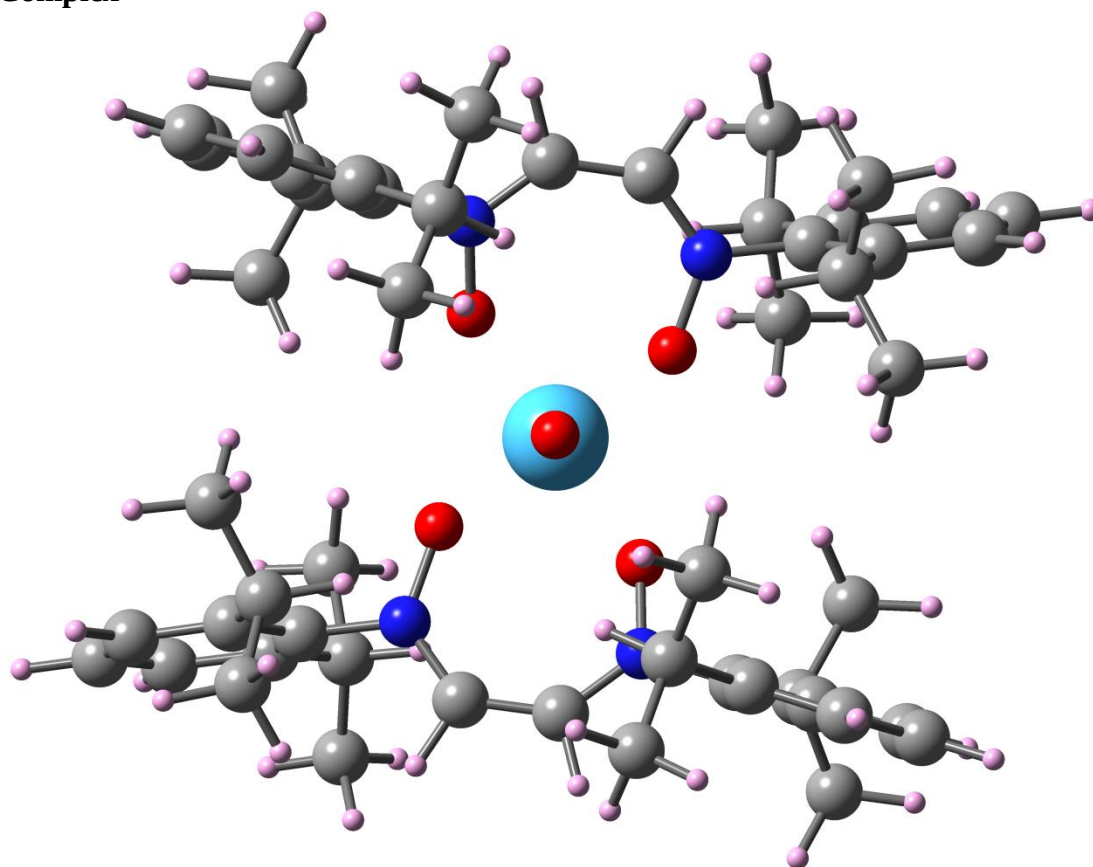


Fig. S77: ONCCNO Oxo Complex

E	E_{zp}	H	G
-2668.6093	-2667.4575	-2667.3865	-2667.5730

N	-1.00596897	-2.98334034	-0.13915479
N	1.00675655	2.98298583	-0.14092547
C	0.13199754	-3.73016256	-0.21666003
C	1.47364338	-3.47090641	0.08887258
C	-0.13181237	3.72886122	-0.21811383
C	-1.47332534	3.46892119	0.08759114
C	-2.27348650	-3.45542850	-0.65917243
C	-3.29573103	-3.78556130	0.27150008
C	-4.52883848	-4.23019888	-0.24481763
C	-4.73115989	-4.35104156	-1.62994411
C	-3.70699859	-4.01005774	-2.52572081
C	-2.45843255	-3.53770285	-2.06527475
C	-3.86472310	-2.41785211	2.32248019
C	-3.09359188	-3.65253398	1.78337793
C	-3.49788389	-4.93988187	2.54510496
C	3.13767653	-1.52522486	4.19868325
C	3.00200113	-2.75519904	3.26144420

C	3.14704808	-4.07900252	4.05421694
C	3.59415476	-2.44639861	0.76962161
C	4.00485673	-2.66351227	2.10890761
C	5.38987243	-2.75742731	2.35876393
C	6.32062705	-2.63049843	1.31476788
C	5.88497008	-2.38833851	0.00218795
C	4.51067360	-2.27804855	-0.29822228
C	-1.90018515	-2.02060098	-4.03801642
C	-1.38540184	-3.12601102	-3.08114222
C	-0.87524276	-4.35668451	-3.87728952
C	4.66409815	-0.65177858	-2.24826912
C	4.05454257	-1.97960196	-1.72916778
C	4.39659322	-3.15350088	-2.68453175
C	2.27377193	3.45681316	-0.66073874
C	2.45902071	3.53833603	-2.06681248
C	3.70662963	4.01329679	-2.52717753
C	4.72966482	4.35724164	-1.63122380
C	4.52725358	4.23662764	-0.24608781
C	3.29497596	3.78949010	0.27009267
C	1.90521524	2.02009803	-4.03999064
C	1.38701215	3.12326875	-3.08236491
C	0.87230084	4.35238286	-3.87797594
C	-3.14350122	1.53242719	4.19898849
C	-3.00701354	2.76046784	3.25932513
C	-3.15480085	4.08589815	4.04885283
C	-3.59398247	2.44439877	0.76718943
C	-4.00748161	2.66522495	2.10497837
C	-5.39306347	2.75919474	2.35172317
C	-6.32159026	2.62881090	1.30617038
C	-5.88314092	2.38288119	-0.00479533
C	-4.50819000	2.27218100	-0.30203000
C	3.86600661	2.42228228	2.32067566
C	3.09271358	3.65575833	1.78189127
C	3.49432851	4.94353667	2.54429074
C	-4.66061328	0.64393294	-2.25090380
C	-4.04867095	1.97040153	-1.73121339
C	-4.38434789	3.14425323	-2.68892935
H	-0.05537393	-4.72892430	-0.59575100
H	2.12600159	-4.32999848	-0.02763753
H	0.05471777	4.72755945	-0.59774849
H	-2.12624518	4.32732890	-0.03078540
H	-5.33223476	-4.49072693	0.43915070
H	-5.68792654	-4.70295638	-2.00924723
H	-3.88204770	-4.09176677	-3.59526074
H	-2.03072739	-3.47113975	1.97389854
H	1.99071052	-2.72674556	2.84178673
H	-4.94610332	-2.52349411	2.15897244
H	-3.52283166	-1.50677133	1.82014505
H	-3.69415673	-2.30465425	3.40193358
H	-4.57285300	-5.14578967	2.45913059
H	-3.26864438	-4.82979692	3.61345120
H	-2.95534691	-5.81665070	2.16793512

H	4.12840637	-1.49057798	4.67173031
H	2.38316823	-1.57060833	4.99537036
H	2.99191930	-0.59402452	3.63909633
H	3.02412658	-4.95171890	3.39989769
H	2.38493224	-4.13357697	4.84281363
H	4.13050261	-4.15605628	4.53634416
H	5.74097492	-2.92671411	3.37364300
H	7.38470645	-2.70986402	1.52565355
H	6.61687910	-2.27489172	-0.79346566
H	-0.53782289	-2.68434704	-2.54921964
H	2.96678380	-1.85249760	-1.73089618
H	-2.78938254	-2.34037766	-4.59865162
H	-1.11406141	-1.76372243	-4.75926444
H	-2.13289875	-1.11154681	-3.47478960
H	-1.68046897	-4.81080333	-4.47056188
H	-0.47344717	-5.13285013	-3.21185373
H	-0.07769422	-4.05437839	-4.56853558
H	4.40387232	0.18527313	-1.59016598
H	4.27614794	-0.42864953	-3.25029746
H	5.75894911	-0.70792660	-2.31582873
H	5.48124398	-3.31501842	-2.74554383
H	4.03013383	-2.93704126	-3.69640115
H	3.93577243	-4.09184727	-2.34908969
H	3.88186865	4.09475161	-3.59670235
H	5.68572341	4.71119759	-2.01041816
H	5.32995538	4.49910528	0.43793666
H	0.54126322	2.67835521	-2.55021390
H	-1.99485283	2.73193699	2.84176466
H	2.79122146	2.34427495	-4.60312816
H	1.11857170	1.75865012	-4.75897083
H	2.14467834	1.11257435	-3.47708673
H	0.46789564	5.12686615	-3.21218011
H	0.07560570	4.04754683	-4.56909888
H	1.67579586	4.80957881	-4.47126138
H	-4.13526104	1.49778861	4.66986864
H	-2.39083665	1.58037654	4.99726928
H	-2.99551399	0.60014511	3.64178035
H	-3.03106745	4.95725198	3.39287455
H	-2.39450844	4.14278000	4.83905099
H	-4.13938217	4.16330120	4.52860641
H	-5.74633569	2.93120728	3.36539324
H	-7.38613475	2.70841483	1.51461318
H	-6.61338426	2.26675254	-0.80158092
H	2.03011616	3.47228530	1.97203067
H	-2.96130514	1.83993163	-1.72955999
H	4.94726324	2.53022085	2.15783260
H	3.52627584	1.51083474	1.81751975
H	3.69505027	2.30801841	3.39995153
H	3.26483292	4.83264480	3.61249636
H	2.95037243	5.81946519	2.16722183
H	4.56895800	5.15140403	2.45887518
H	-4.40543813	-0.19325947	-1.59099530

H	-4.26962630	0.41846237	-3.25119358
H	-5.75502235	0.70340010	-2.32268075
H	-3.92160072	4.08157477	-2.35329488
H	-5.46834687	3.30894608	-2.75315647
H	-4.01560264	2.92547916	-3.69947105
O	-0.00384419	0.00127672	-1.86332563
O	-1.63942964	1.10353370	0.63576196
O	1.64124083	-1.10419835	0.62993580
N	-2.16914431	2.36423969	0.48775030
N	2.16990583	-2.36585615	0.48738073
Hf	-0.00002922	-0.00015177	-0.05238971
O	-1.04888668	-1.75059278	0.48614507
O	1.05088418	1.74970136	0.48298060

8.3 Six Oxygen Atoms

Dioxo Complex

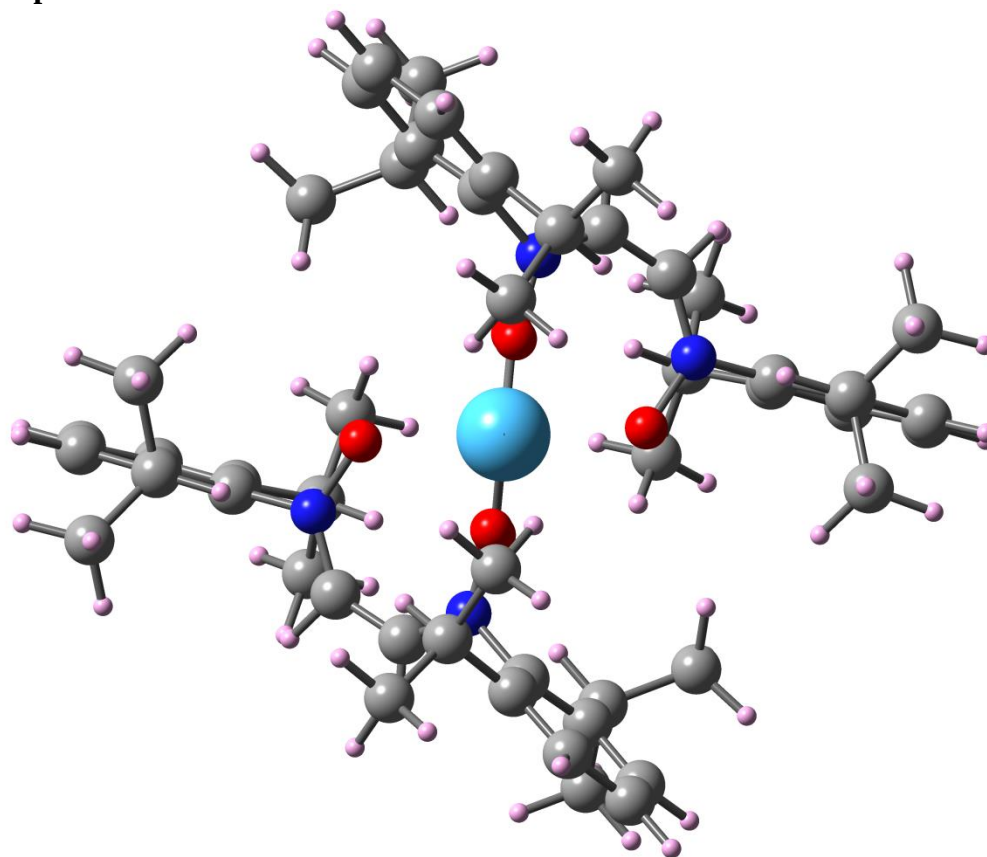


Fig. S78: ONCCNO Dioxo Complex

E	E_{zp}	H	G
-2743.7754	-2742.6189	-2742.5472	-2742.7328
O	-0.18177296	-1.46177643	1.23397242
O	2.18802032	0.10061715	-0.26425836
O	-0.13988100	-1.53739022	-1.67773539
N	0.53392236	2.74093176	1.02206899
N	2.91074299	1.17621265	-0.64706717
N	-2.91105011	-1.17722336	-0.64479348
N	-0.53347204	-2.73961315	1.02563553
C	1.53269049	3.13787303	0.24015630
C	2.57200925	2.44806506	-0.47492152
C	-2.57220001	-2.44879411	-0.47114436
C	-1.53298376	-3.13754071	0.24508181
C	-0.32030550	3.74288070	1.67694636
C	-1.29087908	4.41626745	0.89620958
C	-2.09125447	5.36668446	1.56932762
C	-1.93971421	5.60501526	2.94341808
C	-0.98386274	4.89262285	3.68769160
C	-0.14971538	3.93973350	3.06941401

C	-2.94854933	3.59352662	-0.83728562
C	-1.51606487	4.13721764	-0.59469818
C	-1.25492812	5.40578029	-1.44758991
C	2.34035883	-0.32119767	-4.26203234
C	2.80772205	0.99880634	-3.59090627
C	3.00398874	2.11963323	-4.64460593
C	4.14646024	0.84227847	-1.37085077
C	4.08944353	0.76403439	-2.78370253
C	5.29332107	0.42757536	-3.44214029
C	6.47143140	0.17214755	-2.72390859
C	6.47760240	0.23674771	-1.32071170
C	5.30693384	0.56803952	-0.60821586
C	0.11491144	2.06830922	4.74708390
C	0.85692544	3.13411396	3.89620956
C	1.74928787	4.03682106	4.78433586
C	5.59009421	-0.82283928	1.49562015
C	5.31636934	0.59298762	0.92340407
C	6.33735688	1.62250175	1.47331010
C	-4.14632503	-0.84392729	-1.36957472
C	-4.08924110	-0.76921375	-2.78262533
C	-5.29270051	-0.43281739	-3.44187392
C	-6.47048703	-0.17415582	-2.72429053
C	-6.47677905	-0.23553102	-1.32094635
C	-5.30655781	-0.56660872	-0.60764724
C	-2.33978352	0.30901821	-4.26589618
C	-2.80800247	-1.00791996	-3.58942540
C	-3.00569813	-2.13279788	-4.63856777
C	-0.11496592	-2.06307529	4.74909182
C	-0.85714927	-3.13030223	3.90009741
C	-1.74916138	-4.03162081	4.78993103
C	0.32049896	-3.74107834	1.68170191
C	0.14939449	-3.93697531	3.07422618
C	0.98321115	-4.88960546	3.69336573
C	1.93926729	-5.60251230	2.94983752
C	2.09138678	-5.36499221	1.57566632
C	1.29129907	-4.41493751	0.90169989
C	-5.58896579	0.82858713	1.49349850
C	-5.31623112	-0.58852106	0.92401760
C	-6.33813186	-1.61617715	1.47572632
C	2.94932987	-3.59275602	-0.83167418
C	1.51689166	-4.13667450	-0.58929455
C	1.25638331	-5.40576177	-1.44158669
H	1.60796376	4.21679048	0.16246172
H	3.27240841	3.12708562	-0.95052099
H	-3.27236262	-3.12849931	-0.94611377
H	-1.60869218	-4.21658118	0.16953540
H	-2.84577571	5.91243327	1.00930918
H	-2.57144194	6.33940083	3.43792061
H	-0.88570304	5.07904031	4.75374065
H	-0.83697834	3.34927974	-0.94710952
H	1.98705341	1.30770591	-2.93100721
H	-3.72290713	4.30805648	-0.52352512

H	-3.09860881	2.64970447	-0.30050300
H	-3.08436255	3.38803937	-1.90638228
H	-1.95602090	6.21661329	-1.20454012
H	-1.37214520	5.16393413	-2.51122128
H	-0.23564057	5.78991069	-1.30127557
H	3.11485310	-0.74312104	-4.91905263
H	1.44503160	-0.12444572	-4.86521853
H	2.06052767	-1.06452349	-3.50726578
H	3.33595309	3.05867061	-4.18027239
H	2.05022473	2.31357819	-5.15065060
H	3.74185113	1.84322435	-5.41074752
H	5.30003094	0.36044108	-4.52652676
H	7.38399259	-0.08575749	-3.25650291
H	7.39376226	0.02202414	-0.77661016
H	1.51705976	2.58820216	3.21251034
H	4.32220889	0.88828657	1.27783038
H	-0.57170026	2.54431793	5.46012695
H	0.83518801	1.46585787	5.31657513
H	-0.46089455	1.39714708	4.10081837
H	1.16438719	4.55912897	5.55227163
H	2.27418602	4.79450905	4.18809453
H	2.50110791	3.42685717	5.30229724
H	4.84236695	-1.53882055	1.13632524
H	5.54766356	-0.80336412	2.59266100
H	6.58317866	-1.18746196	1.20180775
H	7.36370409	1.36477095	1.18149899
H	6.29854411	1.64685993	2.57039490
H	6.12815295	2.63379014	1.10049608
H	-5.29928114	-0.36824153	-4.52641898
H	-7.38269748	0.08368560	-3.25751615
H	-7.39270200	-0.01845742	-0.77737927
H	-1.98721509	-1.31472243	-2.92869466
H	-1.51757091	-2.58551763	3.21574355
H	-3.11394737	0.72901790	-4.92453171
H	-1.44467382	0.10915551	-4.86838400
H	-2.05940734	1.05511992	-3.51406624
H	-3.33791092	-3.06980083	-4.17029033
H	-2.05244586	-2.32936295	-5.14457646
H	-3.74401799	-1.85898889	-5.40521142
H	0.57203762	-2.53791732	5.46253762
H	-0.83513327	-1.45993950	5.31799121
H	0.46044039	-1.39275114	4.10160541
H	-2.27399167	-4.79050610	4.19515434
H	-2.50103485	-3.42089371	5.30690389
H	-1.16402756	-4.55237230	5.55874336
H	0.88469021	-5.07539852	4.75948649
H	2.57073179	-6.33667710	3.44500528
H	2.84607569	-5.91114790	1.01626641
H	-4.32236631	-0.88392174	1.27917184
H	0.83764583	-3.34919554	-0.94242132
H	-6.58176285	1.19338196	1.19891284
H	-4.84067227	1.54331285	1.13291186

H	-5.54665426	0.81117913	2.59057934
H	-6.29945472	-1.63850025	2.57285960
H	-6.12971265	-2.62833839	1.10484673
H	-7.36423539	-1.35814093	1.18332577
H	3.09892899	-2.64847223	-0.29557912
H	3.08557123	-3.38806384	-1.90087484
H	3.72370979	-4.30687763	-0.51703670
H	0.23716074	-5.79008341	-1.29535413
H	1.95765628	-6.21625398	-1.19793056
H	1.37382685	-5.16442037	-2.50530607
O	0.13932782	1.53667377	-1.67922578
Hf	-0.00048023	0.00017519	-0.59623090
O	-2.18866643	-0.10128648	-0.26199684
O	0.18350408	1.46299309	1.23298131

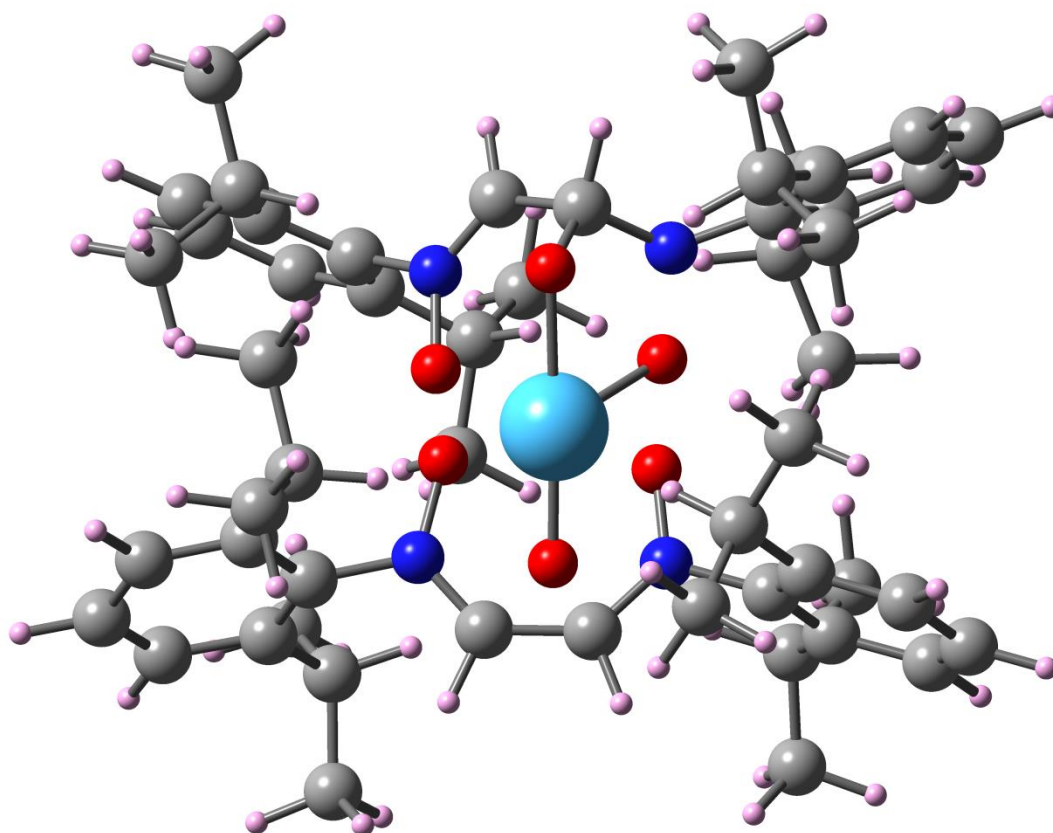
Dioxo Complex (octahedral conformation)

Fig. S79: ONCCNO Dioxo Complex (octahedral conformation)

E	E_{zp}	H	G
-2743.8166	-2742.6592	-2742.5885	-2742.7701

O	0.31737855	2.00257713	-0.39873567
O	-0.22146893	0.69060658	1.85761946
N	-2.72859416	1.33990215	0.54775266
N	0.08094321	2.83858766	0.78600646
C	-2.11650892	2.12219660	1.40251659
C	-0.63996426	2.03223674	1.80375319
C	-4.15527763	1.47434036	0.24510681
C	-5.08066292	0.81750762	1.08987428
C	-6.44808918	0.96240862	0.77279713
C	-6.85467172	1.70842301	-0.34472895
C	-5.90289310	2.31776924	-1.17893139
C	-4.52301648	2.21003990	-0.90674514
C	-5.05450461	-1.53123977	2.04605378
C	-4.65193102	-0.05042501	2.27737861
C	-5.23254641	0.48099857	3.61345027
C	0.70137640	4.86055891	-2.28930533
C	0.05119649	5.14243522	-0.90845083
C	-0.63575807	6.53116027	-0.89094457

C	1.10396209	3.81844664	1.04406412
C	1.07959235	4.98252587	0.21288700
C	2.04062692	5.98949836	0.42276452
C	2.99231474	5.87896175	1.44913277
C	3.00756975	4.73530373	2.25789146
C	2.09476876	3.67421845	2.06278064
C	-3.39198427	1.96922120	-3.15315450
C	-3.48823787	2.81938942	-1.85668146
C	-3.79245970	4.30198111	-2.18485666
C	3.66237665	1.81965628	2.83143497
C	2.24208681	2.43041619	2.94892869
C	1.91196121	2.74984820	4.43242809
H	-2.73808910	2.89568058	1.84590027
H	-0.54629389	2.55901983	2.76603374
H	-7.19538832	0.48106554	1.39813658
H	-7.91359038	1.80639594	-0.57235772
H	-6.23276542	2.87747949	-2.04969919
H	-3.55992226	-0.03026783	2.35899176
H	-0.71620282	4.37821466	-0.75137508
H	-6.14460211	-1.64556806	1.97827484
H	-4.70029974	-2.15184309	2.87963543
H	-4.61053659	-1.91727503	1.12112629
H	-4.92593732	1.51841869	3.80061569
H	-4.87874537	-0.13437651	4.45070311
H	-6.33003603	0.45065339	3.61511790
H	1.51495891	5.57009289	-2.49682683
H	-0.04416877	4.95534734	-3.09201426
H	1.10432818	3.84323289	-2.31082630
H	-1.08792505	6.74149082	0.08750967
H	-1.42881019	6.56843552	-1.65026650
H	0.07018093	7.34196475	-1.11546561
H	2.03600702	6.87450428	-0.20877501
H	3.71763325	6.67337068	1.61171635
H	3.75687044	4.65050794	3.04151580
H	-2.50095342	2.78091737	-1.38354578
H	1.55122856	1.65525972	2.61147435
H	-4.35147959	1.95254415	-3.68844771
H	-3.10123406	0.94001680	-2.91836285
H	-2.63129960	2.39125969	-3.82220351
H	-2.98919931	4.71465540	-2.80815067
H	-3.86397549	4.91116769	-1.27451654
H	-4.73225078	4.41196790	-2.74183461
H	3.88179877	1.55033377	1.79130019
H	3.72106165	0.90736984	3.44125557
H	4.44197097	2.50945346	3.18180459
H	0.90019194	3.16346275	4.54141069
H	2.61555613	3.48266882	4.85120975
H	1.97083213	1.83681064	5.04002800
O	0.20974757	-0.75586107	-1.89070678
Hf	0.00514917	-0.03116799	-0.19432705
O	-2.13455364	0.31607324	-0.16505225
O	2.11575864	-0.61595958	0.18047629

N	-0.04260312	-3.16253277	-0.19189891
N	2.79421742	-1.54051478	-0.51568388
C	1.06704317	-3.38783470	-0.88092256
C	2.31381457	-2.68449534	-0.99862607
C	-1.15785596	-4.11767033	-0.24324748
C	-1.96110671	-4.16258381	-1.40924921
C	-3.01749708	-5.10117775	-1.40767009
C	-3.26415564	-5.92027239	-0.29655110
C	-2.46224030	-5.82029748	0.85307422
C	-1.38679560	-4.91178242	0.90934594
C	-3.02719534	-2.38275164	-2.86771658
C	-1.75951481	-3.24205145	-2.61875150
C	-1.38794791	-4.05771350	-3.88467724
C	5.54264108	-1.82510505	2.64734347
C	4.86171346	-2.40599339	1.38305288
C	5.24796037	-3.89867745	1.19301454
C	4.19690712	-1.18422243	-0.79675628
C	5.18990646	-1.59582635	0.12409892
C	6.52126296	-1.24583729	-0.18026142
C	6.82672889	-0.50711086	-1.33584985
C	5.80846714	-0.10129765	-2.21179760
C	4.45721002	-0.42811844	-1.96332684
C	-1.33744081	-3.98815974	3.26188691
C	-0.54735082	-4.77980625	2.18418618
C	-0.07858421	-6.15203404	2.72902853
C	3.25827433	1.57975420	-2.94174350
C	3.35580327	0.03161656	-2.92409775
C	3.58948025	-0.52565077	-4.35243991
H	1.03706660	-4.31039358	-1.44973141
H	3.04427088	-3.21512837	-1.59937539
H	-3.65830990	-5.17469139	-2.28184655
H	-4.08730449	-6.63056987	-0.32044195
H	-2.67299525	-6.45287511	1.71066227
H	-0.95303319	-2.52343617	-2.42473230
H	3.78019967	-2.35693463	1.55756181
H	-3.90800086	-2.99824806	-3.09865428
H	-2.84804532	-1.71046933	-3.71595318
H	-3.25196572	-1.76191638	-1.99259419
H	-0.47593737	-4.65239131	-3.73298202
H	-1.20741391	-3.37437228	-4.72382935
H	-2.19119126	-4.74854894	-4.17647493
H	6.63565722	-1.91185469	2.59837346
H	5.20771439	-2.37357772	3.53741103
H	5.28896632	-0.76790784	2.78080121
H	4.73111414	-4.34512403	0.33323669
H	4.98454471	-4.47824351	2.08753293
H	6.32772819	-4.00558708	1.02563824
H	7.32039676	-1.54216892	0.49330682
H	7.85984904	-0.24296684	-1.54894220
H	6.05889905	0.47781715	-3.09618581
H	0.34944083	-4.19123373	1.95853711
H	2.37874613	-0.33685576	-2.58835257

H	-2.26336456	-4.51266664	3.53484346
H	-1.59201089	-2.98990621	2.89078875
H	-0.72977718	-3.87264031	4.16898339
H	0.58016052	-6.00350975	3.59452954
H	0.47528159	-6.72006581	1.97009475
H	-0.92257506	-6.76920394	3.06247597
H	3.01542702	1.96864270	-1.94679937
H	2.45493209	1.88750204	-3.62232288
H	4.19455783	2.04425797	-3.28195534
H	3.64487353	-1.62292261	-4.35467352
H	4.51710630	-0.13999705	-4.79742594
H	2.75529859	-0.22994476	-5.00038255
O	-0.24321556	-2.08830718	0.60431831

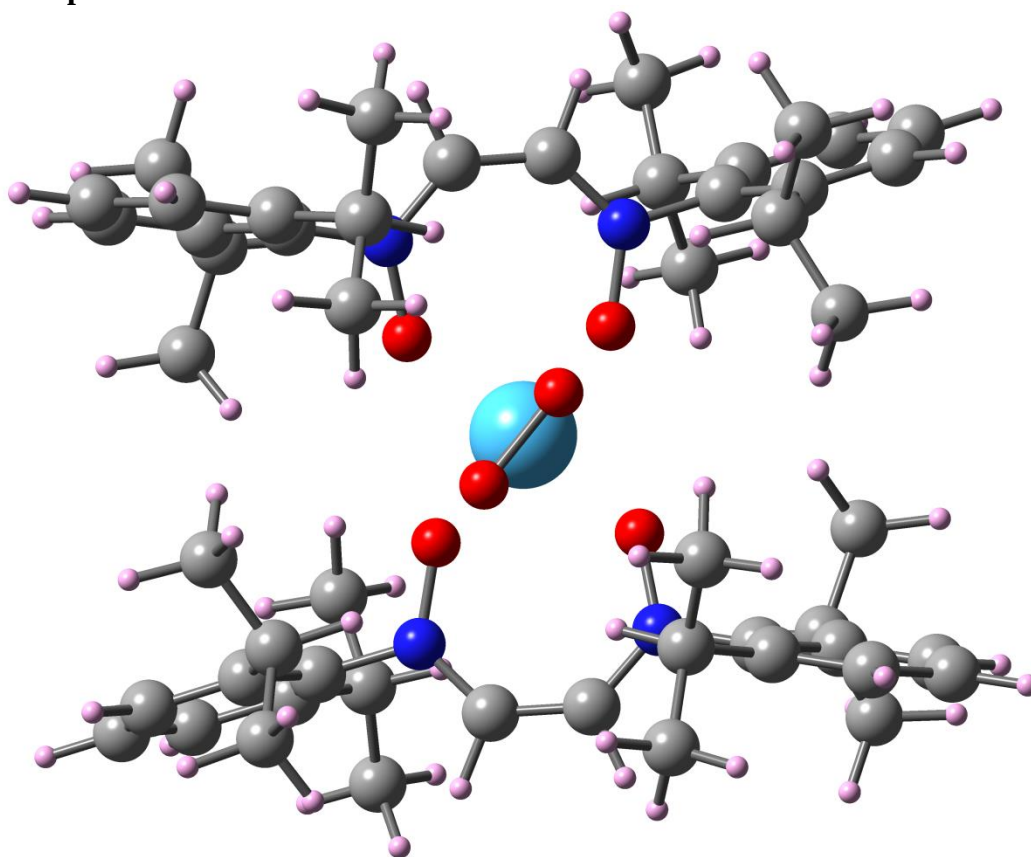
Peroxo Complex

Fig. S80: ONCCNO Peroxo Complex

E	E_{zp}	H	G
-2743.7721	-2742.6175	-2742.5455	-2742.7329
O	-1.46987700	-1.41339100	0.25478100
O	1.43063400	1.42587900	0.22265600
O	0.58456700	-0.68841600	-2.08555100
O	-0.50107800	0.46360700	-2.17903700
N	-1.57709200	2.72505200	0.57441600
N	1.60660600	2.71528300	-0.24513400
N	1.56352000	-2.65394000	0.70723700
N	-1.61958000	-2.73076100	-0.13143200
C	-0.68329700	3.70085300	0.23833900
C	0.66184300	3.69265600	-0.14676100
C	0.68956500	-3.65333800	0.39772400
C	-0.65666100	-3.68318200	0.01345300
C	-2.94625800	3.05162400	0.93792400
C	-3.94150300	3.00409800	-0.07093800
C	-5.26129800	3.33172900	0.30496900
C	-5.57060700	3.68018900	1.62962700
C	-4.56748400	3.69487100	2.61201600
C	-3.23264200	3.37217200	2.28868100

C	-4.32760600	1.25324500	-1.86265200
C	-3.62802500	2.59271100	-1.51178400
C	-4.01280100	3.70331100	-2.52282100
C	2.18049500	1.75874000	-4.14402300
C	1.93630200	2.94985800	-3.18054400
C	1.69512800	4.26559600	-3.96700200
C	2.92891900	2.98086200	-0.78122400
C	3.09129500	3.10613400	-2.18536000
C	4.39508400	3.36397900	-2.66310500
C	5.48376800	3.46448500	-1.78436700
C	5.29520200	3.30797300	-0.40064000
C	4.01374700	3.06451400	0.13223400
C	-2.46266500	2.21308400	4.40821100
C	-2.16168900	3.33824300	3.38256900
C	-2.01376700	4.71019300	4.08884400
C	4.35774300	1.48283900	2.07904100
C	3.82263500	2.87217400	1.63924900
C	4.47729000	4.00809200	2.46521900
C	2.94983400	-2.94487500	1.03742200
C	3.28869300	-3.17812800	2.39399400
C	4.63722100	-3.47094900	2.68608500
C	5.60183100	-3.51653000	1.66636900
C	5.24034000	-3.25355100	0.33546900
C	3.90575100	-2.95107600	-0.00949000
C	2.53874700	-1.82041700	4.39409200
C	2.25786900	-3.07343500	3.52127200
C	2.20633300	-4.35650400	4.38846400
C	-2.21775300	-1.96420300	-4.09405600
C	-1.92832500	-3.07789600	-3.05431700
C	-1.61710300	-4.42650100	-3.75648200
C	-2.93291300	-3.05338800	-0.66111900
C	-3.08501100	-3.23152800	-2.06060600
C	-4.37766200	-3.54982300	-2.53193400
C	-5.46526000	-3.65762600	-1.65236000
C	-5.28716000	-3.44788600	-0.27438400
C	-4.01644200	-3.14197800	0.25231600
C	4.32432700	-1.40433200	-1.98164300
C	3.53674600	-2.63454700	-1.46154500
C	3.75952600	-3.86423500	-2.38049700
C	-4.42772500	-1.50970100	2.14317300
C	-3.83621300	-2.89061000	1.75182200
C	-4.44627400	-4.02303400	2.61578500
H	-1.13863700	4.68512500	0.25287300
H	1.04866900	4.66273800	-0.43991200
H	1.16404000	-4.62789300	0.43413100
H	-1.02457200	-4.67140600	-0.24037900
H	-6.05015700	3.31066900	-0.44263100
H	-6.59424400	3.93147500	1.89807200
H	-4.82435900	3.94941400	3.63734600
H	-2.55092100	2.42066400	-1.60485300
H	1.01861100	2.71044100	-2.63514600
H	-5.42116600	1.34690900	-1.81192400

H	-4.01593100	0.45858300	-1.17571100
H	-4.05688800	0.94447100	-2.87999100
H	-5.09399400	3.89566500	-2.52145200
H	-3.72846000	3.39882100	-3.53822900
H	-3.50241100	4.64833400	-2.29462700
H	3.11019300	1.88155900	-4.71686100
H	1.34681100	1.68243800	-4.85331500
H	2.21809300	0.81624700	-3.58785900
H	1.49663500	5.11008100	-3.29286400
H	0.83091800	4.15104300	-4.63395100
H	2.56345400	4.52915500	-4.58577800
H	4.55783000	3.46986400	-3.73255900
H	6.48000500	3.65651600	-2.17652100
H	6.14877900	3.38043800	0.26814200
H	-1.19915000	3.09804600	2.91801000
H	2.74851800	2.88132700	1.85394200
H	-3.40853900	2.39474500	4.93574100
H	-1.66231000	2.15931400	5.15818800
H	-2.53159500	1.23974700	3.90812800
H	-2.93852700	4.99890900	4.60528000
H	-1.76813000	5.50427700	3.37191000
H	-1.21243400	4.66710100	4.83822900
H	3.82800000	0.68301800	1.55108200
H	4.20720000	1.34250200	3.15834700
H	5.43253100	1.38905300	1.87150700
H	5.57067700	4.00655900	2.36659200
H	4.24375400	3.87829000	3.53034300
H	4.11169900	4.99499700	2.15275300
H	4.93460500	-3.65781000	3.71484400
H	6.63635900	-3.74716600	1.91060500
H	6.00020300	-3.27479700	-0.44153700
H	1.26779100	-2.93470900	3.07320900
H	-1.02893200	-2.76004200	-2.51835600
H	3.51725700	-1.89123000	4.88792200
H	1.77180900	-1.72009400	5.17383100
H	2.52841000	-0.91165200	3.78124100
H	1.99033000	-5.24335900	3.77871400
H	1.42125200	-4.26655200	5.15077800
H	3.15660500	-4.53065400	4.90986500
H	-3.12264000	-2.17578500	-4.68054800
H	-1.37095800	-1.88062700	-4.78659100
H	-2.32482700	-0.99408800	-3.59796500
H	-1.37977400	-5.21619200	-3.03055700
H	-0.75591100	-4.31021100	-4.42694500
H	-2.46852200	-4.77138300	-4.35883500
H	-4.53314900	-3.69907500	-3.59721700
H	-6.45285300	-3.89773700	-2.03986300
H	-6.13999400	-3.52707000	0.39459100
H	2.47597400	-2.36998100	-1.51245400
H	-2.76288200	-2.84911300	1.96715100
H	5.40615900	-1.59467500	-2.00297900
H	4.14038900	-0.52680900	-1.35139000

H	4.00009000	-1.16003600	-3.00059500
H	3.44842700	-3.62649500	-3.40575500
H	3.17710300	-4.73063900	-2.04012600
H	4.81724500	-4.15924300	-2.40788900
H	-3.93080600	-0.70782100	1.58695200
H	-4.28396500	-1.32569800	3.21668900
H	-5.50511700	-1.46603600	1.93278400
H	-4.03801000	-5.00397800	2.33965200
H	-5.53822400	-4.07114300	2.51320700
H	-4.22347500	-3.84593100	3.67637800
Hf	-0.01368000	-0.00596000	-0.28800400
O	-1.29800400	1.38389800	0.56569900
O	1.24179000	-1.32176100	0.72864500

8.4 Seven Oxygen Atoms

Oxo Peroxo Complex (lower energy conformation)

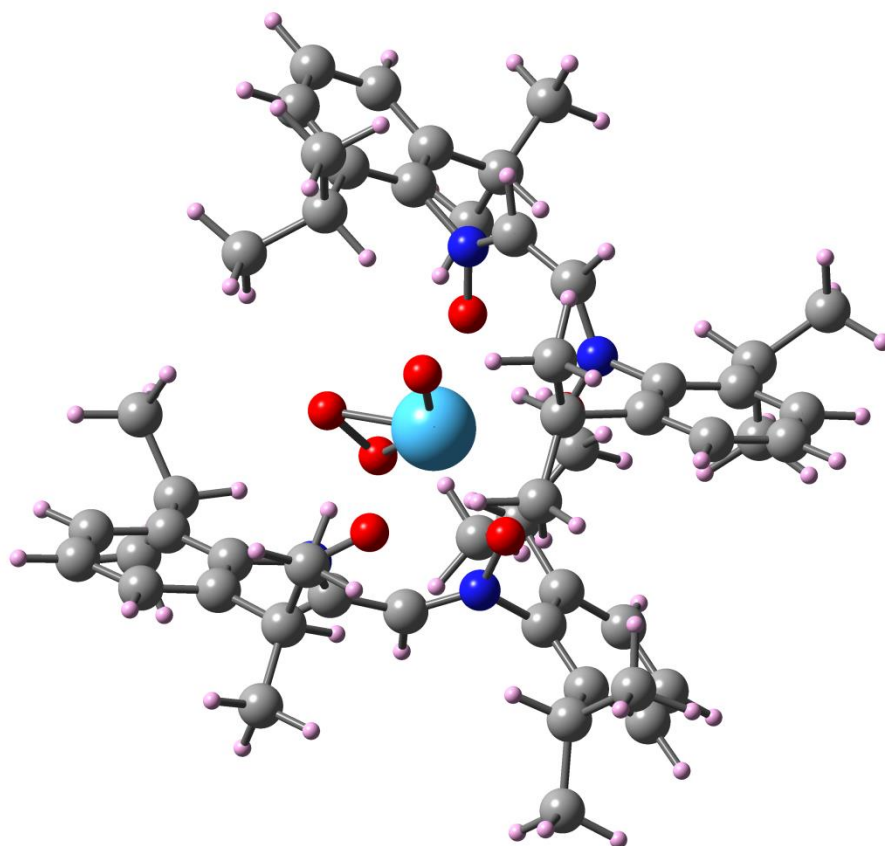


Fig. S81: ONCCNO Oxo Peroxo Complex (lower energy conformation)

E	E_{zp}	H	G
-2818.9306	-2817.7705	-2817.6981	-2817.8836
O	1.88177314	0.43086203	0.56816304
O	-1.43812711	-1.63156913	0.89014107
O	-0.53913004	1.02696408	1.74231513
N	0.43121903	-2.54842819	-1.45131611
N	-2.42873419	-2.10197916	0.05366800
N	0.23332902	3.23881925	-0.07826501
N	2.42020119	1.33603710	1.38858711
C	-0.82626806	-2.90332622	-1.71361813
C	-2.10417716	-2.64320720	-1.11486409
C	1.01492008	3.41842026	0.97628508
C	2.01170315	2.58858020	1.58578812
C	1.51593412	-3.11734624	-2.26061317
C	1.81705414	-2.51770619	-3.50680627
C	2.86573722	-3.09630523	-4.25486632
C	3.58318127	-4.19902632	-3.76639829
C	3.27594525	-4.74622736	-2.50939119
C	2.23331217	-4.21394032	-1.72323413

C	2.06623316	-0.07810201	-4.13594031
C	1.08820108	-1.27858510	-4.03558831
C	0.40680303	-1.55300112	-5.40067542
C	-5.33036142	0.43239403	-1.72842913
C	-4.71281236	-0.98504408	-1.63049112
C	-5.35108141	-1.92746815	-2.68837920
C	-3.79715129	-2.09493916	0.56974305
C	-4.86339937	-1.57327412	-0.21966102
C	-6.15582548	-1.60449112	0.34756003
C	-6.38424749	-2.10306216	1.63633512
C	-5.31430840	-2.61025220	2.38699718
C	-4.00254131	-2.63555120	1.87283814
C	3.03398523	-4.28234433	0.67112405
C	1.94685015	-4.76999636	-0.32537902
C	1.82683714	-6.31385951	-0.31185102
C	-2.49581919	-2.26348117	3.87142829
C	-2.89054022	-3.24609225	2.73656921
C	-3.28710525	-4.63170335	3.30805525
C	-0.68983205	4.29665633	-0.50945304
C	-1.82502814	4.58048235	0.29025702
C	-2.66883021	5.61948741	-0.16307801
C	-2.40396318	6.30931250	-1.35419310
C	-1.28673610	5.97176843	-2.13625816
C	-0.40194903	4.95261238	-1.73345913
C	-3.56129827	3.08784924	1.36707210
C	-2.19679917	3.80129929	1.55711912
C	-2.21835517	4.72435136	2.80266121
C	5.16022739	0.00962800	-0.75916406
C	5.07443539	1.25982909	0.15947801
C	6.32597148	2.15686217	0.00097900
C	3.54506027	0.82583406	2.19227217
C	4.83388837	0.82269306	1.60745612
C	5.88952645	0.32869102	2.40094218
C	5.65401342	-0.13908201	3.70512128
C	4.35522633	-0.14322701	4.23677633
C	3.25730425	0.32943703	3.48432327
C	0.28238702	3.72963729	-3.83179029
C	0.78384806	4.56481835	-2.62216320
C	1.60394112	5.79307046	-3.08979724
C	1.43945011	-1.19323309	4.38127633
C	1.83575414	0.27021702	4.05428031
C	1.69433213	1.17194109	5.30807141
H	-0.89249907	-3.55295827	-2.58115520
H	-2.93643623	-3.04302823	-1.67957013
H	0.90528207	4.39155134	1.44119511
H	2.57282720	3.08987324	2.36680018
H	3.12471624	-2.67257420	-5.22157140
H	4.38754833	-4.62705435	-4.36022633
H	3.84946029	-5.59032842	-2.13663717
H	0.30254602	-0.98319508	-3.33326626
H	-3.65561728	-0.84923806	-1.86050014
H	2.86942922	-0.26863402	-4.86126237

H	2.52379520	0.13220501	-3.16166724
H	1.52091011	0.81829706	-4.45546034
H	1.14009609	-1.80007214	-6.18045149
H	-0.14576501	-0.66263205	-5.72569344
H	-0.30620802	-2.38533818	-5.33320940
H	-6.41658747	0.43157403	-1.56373312
H	-5.14070139	0.84459806	-2.72801821
H	-4.85765637	1.09819308	-1.00041808
H	-4.91749938	-2.93828622	-2.66527820
H	-5.19908640	-1.51778212	-3.69558828
H	-6.43213650	-2.03597915	-2.52646619
H	-6.98975655	-1.21122909	-0.22652202
H	-7.38895956	-2.09832916	2.05252016
H	-5.49958643	-3.00496223	3.38180126
H	0.99247707	-4.36121533	0.02591000
H	-1.99818915	-3.38380626	2.12187116
H	4.02796331	-4.64918535	0.38107903
H	2.81563221	-4.65218236	1.68175113
H	3.06097723	-3.18773424	0.70328405
H	2.77708821	-6.79930851	-0.56924504
H	1.06568408	-6.66487849	-1.02078908
H	1.54400912	-6.65829251	0.69139505
H	-2.13033816	-1.32335610	3.44556426
H	-1.69935113	-2.70147221	4.48892734
H	-3.35309726	-2.04924816	4.52517434
H	-4.11030131	-4.56446135	4.03108531
H	-2.42821018	-5.07163339	3.83268529
H	-3.59263727	-5.32426741	2.51237019
H	-3.55107527	5.87306243	0.41809303
H	-3.07379224	7.10108655	-1.68159113
H	-1.10222209	6.50400649	-3.06510724
H	-1.47606212	2.99475623	1.73763813
H	4.20918532	1.84328614	-0.17930601
H	-4.38270733	3.79961229	1.20221709
H	-3.79116829	2.49673319	2.26219617
H	-3.51396727	2.39881418	0.51652104
H	-1.24817710	5.21607340	2.96416923
H	-2.44824519	4.13088832	3.69660828
H	-2.97965923	5.51206543	2.71628821
H	6.00744143	-0.62804805	-0.47273204
H	5.30179643	0.31475102	-1.80454214
H	4.24084232	-0.58210504	-0.69298705
H	6.28135347	3.03348023	0.66028105
H	6.40188650	2.51120619	-1.03519008
H	7.25054753	1.61063812	0.22714402
H	6.89795551	0.30734702	1.99773115
H	6.48349849	-0.51057104	4.30235733
H	4.18608032	-0.52543504	5.23977940
H	1.45824611	3.91724430	-2.05035316
H	1.11250308	0.62338305	3.30834525
H	-0.40766103	4.31560333	-4.45395834
H	-0.23777002	2.83063221	-3.48476727

H	1.13115808	3.42503826	-4.45942834
H	2.48519919	5.45987739	-3.65359928
H	1.94930115	6.39576048	-2.23940517
H	1.02074908	6.44641349	-3.75104929
H	1.51091111	-1.82549214	3.48791127
H	0.39999203	-1.22090409	4.72855136
H	2.07596616	-1.62687512	5.16533639
H	1.93997215	2.21873417	5.08258339
H	2.35098118	0.84157806	6.12488645
H	0.65930105	1.14101108	5.67038542
O	-2.15477817	0.47781004	-0.86548807
O	-1.29541310	-0.25932702	-1.87345814
Hf	-0.35299503	0.15165301	0.11771501
O	0.22405202	2.11413716	-0.82314806
O	0.86782407	-1.65880413	-0.52070704

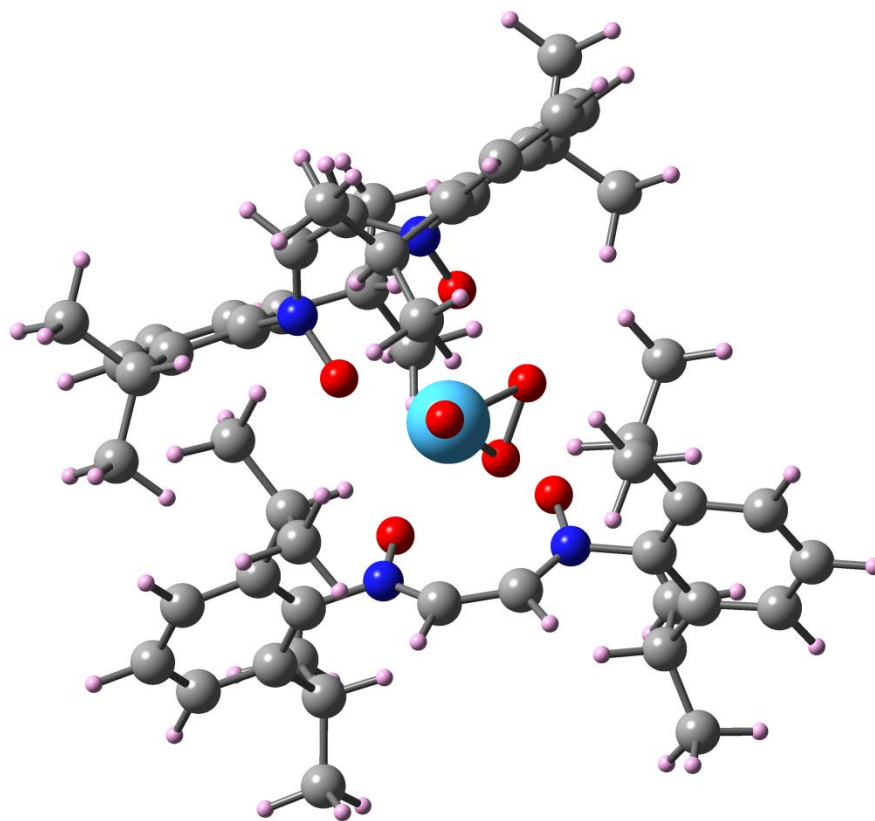
Oxo Peroxo Complex (higher energy conformation 1)

Fig. S82: Oxo Peroxo Complex (higher energy conformation 1)

E	E_{zp}	H	G
-2818.9197	-2817.7611	-2817.6890	-2817.8731
O	-0.35991600	-2.06773100	-0.25054400
O	-0.01345200	2.27110100	-0.49515500
O	0.84689900	0.12963900	1.18639800
N	-2.88608300	1.36524800	-0.47337200
N	-0.44377400	3.12428400	0.44291600
N	2.91311100	-1.72490600	-0.26054100
N	0.01061700	-2.81219900	0.83389800
C	-2.83763900	2.55021200	0.15981600
C	-1.74904400	3.26829000	0.72063700
C	2.53066300	-2.56939600	0.72139500
C	1.27820900	-3.00688000	1.21589100
C	-4.08832300	0.98682100	-1.22560200
C	-4.09975400	1.25887300	-2.61547100
C	-5.26906800	0.90625900	-3.32221800
C	-6.35591100	0.30292500	-2.66971100
C	-6.29277400	0.01893600	-1.29599100
C	-5.14686000	0.34500900	-0.54056200
C	-2.36155300	0.93352500	-4.44390500

C	-2.91054600	1.88625400	-3.34996100
C	-3.29002200	3.26660400	-3.94874200
C	1.98070700	4.31197200	-2.21471000
C	0.87911100	5.00282000	-1.36518700
C	0.65630500	6.46653300	-1.82460000
C	0.56900600	4.00990600	1.01592100
C	1.21500000	4.91255400	0.12803600
C	2.21299200	5.74267900	0.67614400
C	2.54291900	5.67809700	2.03974700
C	1.88672000	4.77110100	2.88383700
C	0.88706400	3.90296900	2.39270700
C	-5.13904500	-1.55670400	1.13624800
C	-5.07251200	-0.01919600	0.94460600
C	-6.17764000	0.69362000	1.76678600
C	1.30184700	1.89955700	3.89547700
C	0.24224000	2.89130000	3.34699800
C	-0.51885000	3.61209700	4.49128600
C	4.34215500	-1.60121100	-0.57402800
C	5.08800300	-0.64336200	0.15010100
C	6.46100900	-0.53817600	-0.16194500
C	7.03536600	-1.33444800	-1.16490400
C	6.24963900	-2.24659400	-1.89058200
C	4.87496900	-2.39955400	-1.61509800
C	4.55982100	1.75757300	0.75845700
C	4.45110100	0.27405400	1.19936400
C	5.08712000	0.06401000	2.59768600
C	-2.40491200	-4.53809300	-1.54447400
C	-1.34515600	-5.01738100	-0.51532100
C	-1.14035200	-6.55077300	-0.59820400
C	-1.08652400	-3.46865000	1.53945900
C	-1.73029700	-4.55527600	0.89314700
C	-2.77674700	-5.19069600	1.59205800
C	-3.15260400	-4.76362500	2.87653100
C	-2.50481900	-3.67477500	3.47873500
C	-1.46386700	-2.98586300	2.81754100
C	3.50800700	-2.55937700	-3.73326300
C	3.98993600	-3.31782400	-2.46306100
C	4.68175300	-4.65011900	-2.83716700
C	-1.87115400	-0.70387000	3.85604900
C	-0.80822200	-1.76749800	3.47851500
C	0.01125400	-2.18552900	4.72811300
H	-3.80363700	3.04104100	0.22135300
H	-1.99336900	4.10874200	1.35895900
H	3.38014000	-3.02266900	1.21963200
H	1.35855800	-3.67284700	2.06848000
H	-5.32319000	1.09869800	-4.39015500
H	-7.24753200	0.04134400	-3.23468200
H	-7.13338800	-0.46889100	-0.80964100
H	-2.09063500	2.04490400	-2.64173500
H	-0.04939800	4.45348100	-1.55505500
H	-3.12491300	0.70487500	-5.20041000
H	-1.99762200	-0.00159100	-4.00554000

H	-1.50681200	1.40265300	-4.94569800
H	-4.07527100	3.17267500	-4.71075800
H	-2.41187100	3.71806200	-4.42756600
H	-3.65278100	3.95806800	-3.17594600
H	2.96251600	4.77238300	-2.03709700
H	1.74654300	4.40701000	-3.28302900
H	2.03727100	3.24473000	-1.98041800
H	-0.10577200	6.97177000	-1.21632900
H	0.32300600	6.47761200	-2.87044800
H	1.57914100	7.05801600	-1.77031600
H	2.73203800	6.44697200	0.03259000
H	3.31550200	6.32964300	2.44121500
H	2.16188700	4.72120000	3.93389000
H	-4.10258200	0.30694900	1.33803100
H	-0.47464500	2.27802100	2.79242900
H	-6.10098200	-1.96115900	0.79450500
H	-5.02173100	-1.81381200	2.19656200
H	-4.33936000	-2.05595800	0.57748100
H	-7.17932900	0.37765200	1.44783700
H	-6.12186300	1.78505300	1.65835100
H	-6.07400800	0.45091700	2.83238600
H	1.64292300	1.25520200	3.07687300
H	0.84770700	1.25854700	4.66416900
H	2.15189900	2.42162200	4.35493800
H	0.16440900	4.19071700	5.12675800
H	-1.02399200	2.87613700	5.13072500
H	-1.27901300	4.30530200	4.10426500
H	7.07640200	0.17950500	0.37430100
H	8.09436300	-1.23593200	-1.39286600
H	6.70659500	-2.83753800	-2.67879300
H	3.38026300	0.05378400	1.28020400
H	-0.40038800	-4.53921600	-0.79475700
H	5.60649800	2.08522800	0.68832200
H	4.04718100	2.40110700	1.48444200
H	4.08505400	1.90771300	-0.21804500
H	4.99257000	-0.97856900	2.93021300
H	4.58393700	0.70144000	3.33608900
H	6.15505600	0.32224900	2.60010700
H	-3.39422100	-4.96055700	-1.32032000
H	-2.11939300	-4.85425000	-2.55626200
H	-2.47660100	-3.44552100	-1.53753500
H	-0.39820000	-6.89873800	0.13227400
H	-0.78731400	-6.82469700	-1.60088400
H	-2.07417000	-7.09925100	-0.41829100
H	-3.29458300	-6.02854000	1.13322900
H	-3.95437400	-5.27594100	3.40360800
H	-2.81601300	-3.34659200	4.46708900
H	3.09120200	-3.56628000	-1.88421600
H	-0.12916400	-1.27887900	2.76848300
H	4.36524100	-2.23851900	-4.34135900
H	2.91266600	-1.68076400	-3.46456800
H	2.87891600	-3.21742400	-4.34750700

H	3.96681500	-5.30663100	-3.34960600
H	5.05759000	-5.17766500	-1.95034700
H	5.52519200	-4.49288000	-3.52213900
H	-2.44318300	-0.39980900	2.97096500
H	-1.37310600	0.18694800	4.25817700
H	-2.57548300	-1.06995800	4.61588900
H	0.79542800	-2.91083400	4.47275500
H	-0.62751300	-2.64235400	5.49683200
H	0.49962200	-1.30684200	5.16870400
O	0.70819600	0.78824100	-2.44379300
O	0.30820700	-0.58178100	-2.73227200
Hf	0.17490000	0.00142400	-0.54303300
O	2.13216000	-0.94678900	-1.00742800
O	-1.92821700	0.42051200	-0.44998400

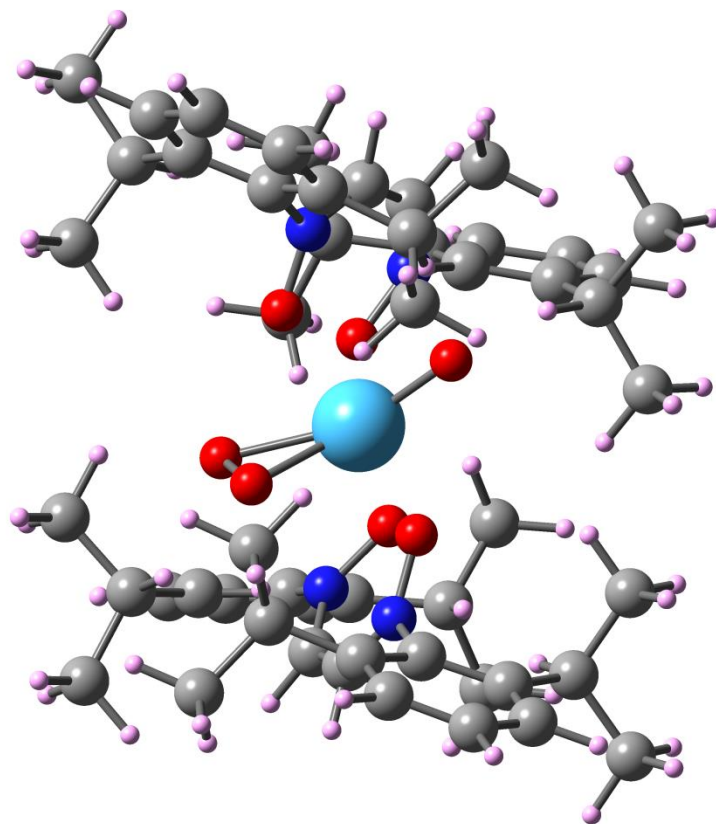
Oxo Peroxo Complex (higher energy conformation 2)

Fig. S83: ONCCNO Oxo Peroxo Complex (higher energy conformation 2)

E	E_{zp}	H	G
-2818.9259	-2817.7668	-2817.6940	-2817.8807
O	-1.96760622	0.51583470	-0.09061804
O	2.05096637	-0.98429067	-0.66522809
O	0.33351187	0.98687116	-1.66796917
N	-0.14851549	-2.67893521	1.13758905
N	2.76676660	-1.95817962	-0.08583004
N	-0.32052262	3.36678123	0.05099797
N	-2.54293039	1.24352465	-1.08141812
C	1.08343168	-3.09408801	1.44461607
C	2.34747573	-2.82002776	0.85444703
C	-1.29795671	3.44008505	-0.85808210
C	-2.23719860	2.50023681	-1.38027114
C	-1.32479848	-3.21310446	1.82772210
C	-1.49951753	-2.99430048	3.22301021
C	-2.66515552	-3.53065073	3.81330325
C	-3.61075046	-4.24136396	3.06266720
C	-3.39462040	-4.46257094	1.69431109
C	-2.24355141	-3.97185569	1.04659104
C	-1.19221486	-1.10197628	4.90632934

C	-0.50570459	-2.24553924	4.11919628
C	0.20422364	-3.23061618	5.08720735
C	5.18116826	0.91251605	1.49556108
C	4.74927650	-0.57397514	1.58847508
C	5.35950564	-1.24494808	2.84711618
C	4.17443272	-1.98752536	-0.50391408
C	5.12779767	-1.33516013	0.31324599
C	6.47321377	-1.39106689	-0.11207705
C	6.82916395	-2.03946387	-1.30462214
C	5.84643296	-2.64029710	-2.10959820
C	4.48915086	-2.62566635	-1.72835017
C	-3.07176754	-3.61976782	-1.32916014
C	-2.02392533	-4.32509868	-0.43069407
C	-2.04224205	-5.86073582	-0.65227108
C	3.05890667	-2.19432658	-3.76313532
C	3.40747288	-3.21140159	-2.64019424
C	3.79859417	-4.58673662	-3.23291828
C	0.45842722	4.57869746	0.35445999
C	1.51989324	4.90533868	-0.52049808
C	2.25518608	6.07052492	-0.20997305
C	1.95346192	6.83397592	0.92836503
C	0.91505591	6.44827667	1.79387510
C	0.13978506	5.30068844	1.52911908
C	3.36835562	3.59590092	-1.67157716
C	1.88615943	4.04544868	-1.73659917
C	1.60193926	4.80392369	-3.05995227
C	-5.15987428	-0.43721596	1.23338206
C	-5.08213650	0.79573715	0.29428399
C	-6.34832974	1.68000098	0.42647200
C	-3.60867335	0.55735440	-1.82074218
C	-4.84135141	0.35145416	-1.15190812
C	-5.85828235	-0.30684508	-1.87236718
C	-5.64646624	-0.73327607	-3.19395528
C	-4.40748321	-0.52298783	-3.81730333
C	-3.34528125	0.11949642	-3.14306428
C	-0.29689972	3.95766527	3.62624924
C	-0.93988993	4.82461122	2.50603115
C	-1.76870621	5.98558715	3.10526220
C	-1.42378088	-1.05914532	-4.32158937
C	-1.99179518	0.30143968	-3.84097633
C	-2.11093037	1.29269174	-5.02895542
H	1.12071281	-3.79155006	2.27297214
H	3.15132990	-3.44014966	1.23566206
H	-1.39330189	4.43206511	-1.28457514
H	-2.85308272	2.90562472	-2.17584020
H	-2.83330557	-3.37635476	4.87531833
H	-4.50508046	-4.63140316	3.54299823
H	-4.11775736	-5.03914812	1.12400405
H	0.23699037	-1.74571207	3.49355623
H	3.66076341	-0.56776134	1.70624610
H	-1.97341085	-1.46787645	5.58739339
H	-1.62846102	-0.37905330	4.21006128

H	-0.44242890	-0.56944110	5.50517438
H	-0.50970933	-3.69729635	5.77971043
H	0.95215760	-2.69345400	5.68493341
H	0.71789183	-4.04244415	4.55191731
H	6.27319234	1.02067226	1.44026507
H	4.82753513	1.45486803	2.38101515
H	4.74242314	1.39020901	0.61175901
H	5.03284883	-2.28888822	2.94831919
H	5.04448854	-0.70365610	3.74822425
H	6.45759876	-1.23965988	2.81472818
H	7.24123576	-0.91089571	0.48843500
H	7.87131499	-2.06701068	-1.61460916
H	6.13613110	-3.12084608	-3.03969627
H	-1.04516732	-3.95446147	-0.74364509
H	2.49409384	-3.35565577	-2.05044619
H	-4.09349056	-3.93693703	-1.07916612
H	-2.89265948	-3.86332180	-2.38496422
H	-3.00857273	-2.53325373	-1.21166413
H	-3.02517104	-6.29627400	-0.43126007
H	-1.30089489	-6.36666171	-0.01961404
H	-1.80796299	-6.08806878	-1.70092617
H	2.70053147	-1.25292457	-3.33328529
H	2.26936168	-2.60121975	-4.40932037
H	3.93846169	-1.98617140	-4.38785237
H	4.64798922	-4.50738746	-3.92369334
H	2.95484518	-4.99989281	-3.80078533
H	4.06689132	-5.30492964	-2.44703823
H	3.07663709	6.36928109	-0.85566310
H	2.53585580	7.72532906	1.15038705
H	0.71020479	7.04132667	2.68025717
H	1.28906755	3.12420650	-1.74195817
H	-4.22525955	1.39010835	0.62903501
H	4.06230552	4.44451612	-1.74937917
H	3.57776777	2.90573991	-2.49806823
H	3.57367873	3.06746292	-0.73318909
H	0.54556713	5.09473552	-3.14110228
H	1.84008640	4.16011468	-3.91600933
H	2.20795815	5.71705187	-3.14023127
H	-6.00128922	-1.08965716	0.96294904
H	-5.30145035	-0.11312896	2.27277114
H	-4.23546510	-1.02175683	1.18085705
H	-6.29630395	2.55885206	-0.22970805
H	-6.45266185	2.03151699	1.46129808
H	-7.26071371	1.12486977	0.17294598
H	-6.82018540	-0.48341827	-1.39860815
H	-6.44566322	-1.23498826	-3.73477132
H	-4.25328414	-0.87131082	-4.83493441
H	-1.63715087	4.17248804	1.96375111
H	-1.25176119	0.70018785	-3.13451928
H	0.44329423	4.54075545	4.19136628
H	0.19419748	3.07504429	3.20389421
H	-1.07036272	3.61566111	4.32681729

H	-2.59362620	5.57951198	3.70478825
H	-2.19580436	6.62726611	2.32336014
H	-1.16515928	6.61604432	3.77080125
H	-1.32736575	-1.75848235	-3.48267730
H	-0.42342984	-0.90507012	-4.74473040
H	-2.05383384	-1.52510947	-5.09241043
H	-2.47622358	2.27665574	-4.70311640
H	-2.79919736	0.92103558	-5.80105648
H	-1.12643032	1.43730993	-5.49174148
O	1.45384312	0.14442230	1.68740309
O	0.05715604	-0.00684196	2.19481913
Hf	0.21179202	0.14459008	-0.01421604
O	-0.38977264	-1.95999920	-0.01693304
O	0.08436361	2.28898422	0.71092202

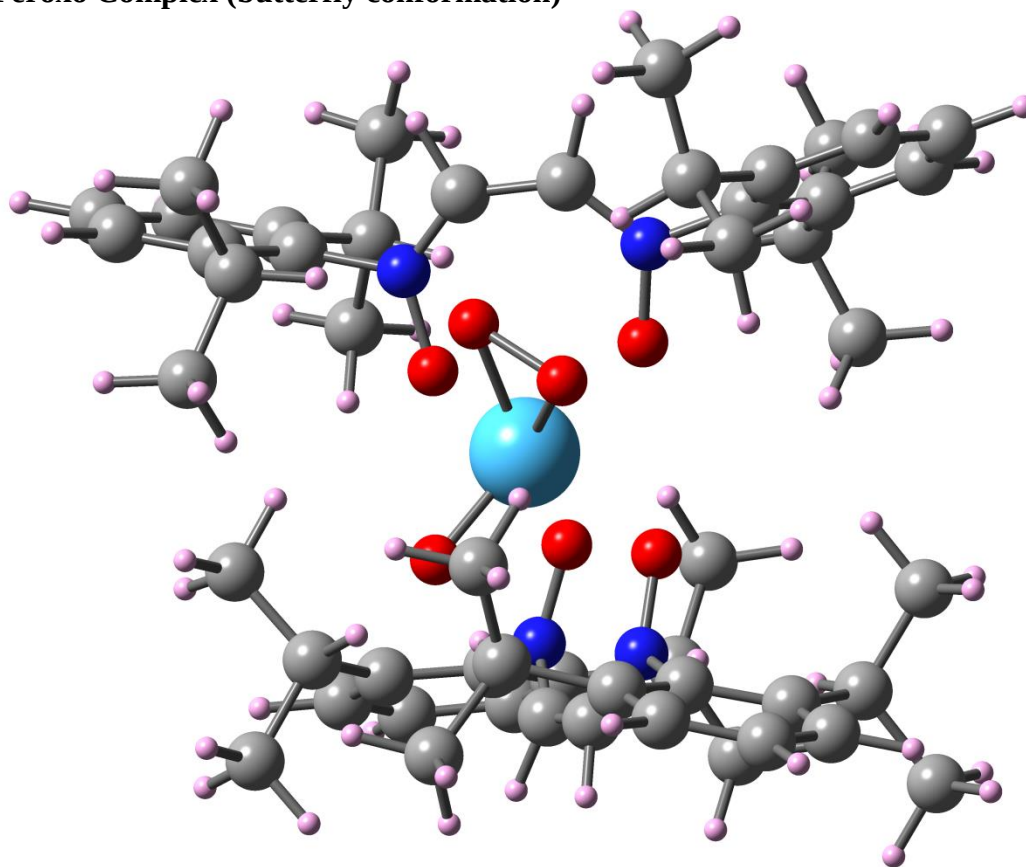
Oxo Peroxo Complex (butterfly conformation)

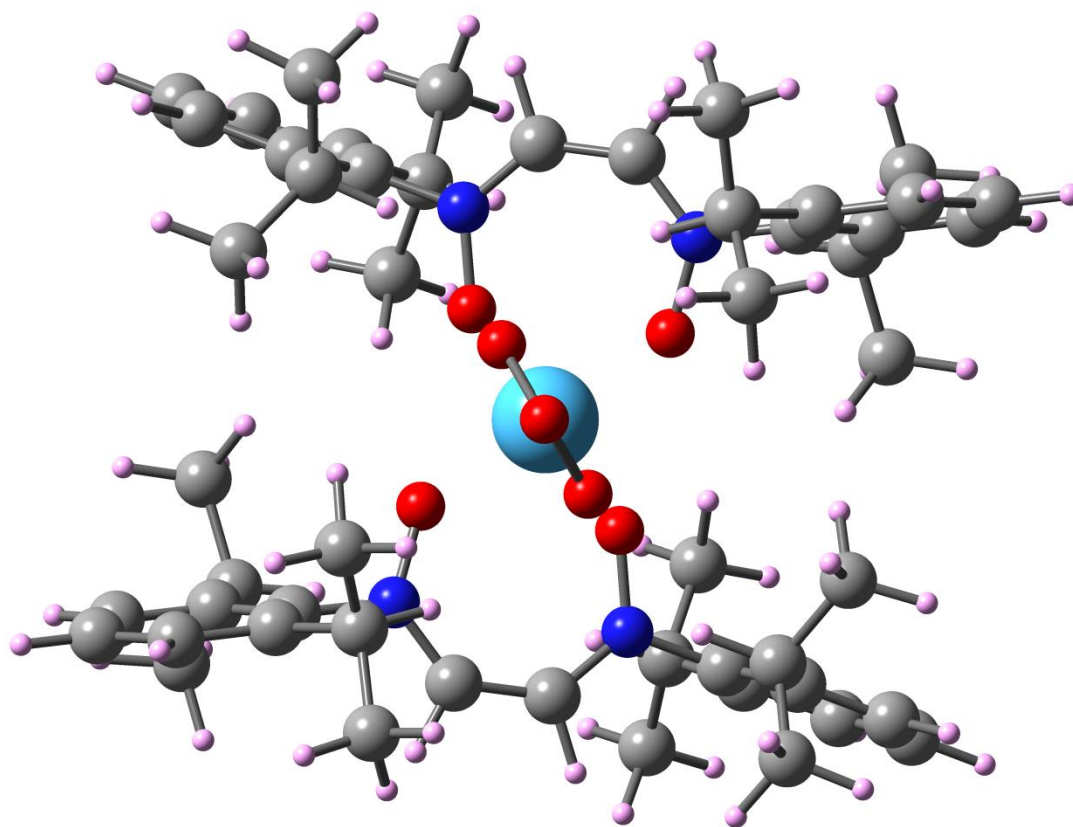
Fig. S84: ONCCNO Oxo Peroxo Complex (butterfly conformation)

E	E_{zp}	H	G
-2818.9493	-2817.7891	-2817.7166	-2817.9019
O	-0.03383300	1.52869500	1.13838900
O	-2.26525500	-0.51858400	-0.05687600
O	-1.22734800	1.48421000	-1.71873000
N	-0.02972400	-2.71554100	0.97370900
N	-2.81150500	-1.69386600	-0.41108400
N	2.71435600	1.37704600	-0.61208700
N	0.14080900	2.83715500	0.82921300
C	-1.02783100	-3.33247300	0.35093100
C	-2.24570400	-2.88452300	-0.26568000
C	2.30050400	2.63628400	-0.48874800
C	1.16106300	3.28335800	0.10031800
C	1.05165500	-3.52129300	1.56715400
C	2.04238100	-4.05138800	0.70637000
C	3.05998300	-4.81837400	1.31671900
C	3.08825700	-5.01914800	2.70485300
C	2.09865700	-4.45279700	3.52567800
C	1.05300900	-3.68545500	2.97360400
C	3.37270300	-3.13341100	-1.25064100

C	2.05520400	-3.82099500	-0.80922600
C	1.84616800	-5.15544600	-1.57281000
C	-2.82492400	-0.45953900	-4.21406500
C	-3.00242800	-1.74532600	-3.36210600
C	-3.10648100	-3.00443500	-4.26128900
C	-4.14156300	-1.58434900	-1.03281900
C	-4.22373100	-1.61724300	-2.44527000
C	-5.51735000	-1.49291000	-3.00014700
C	-6.64693200	-1.32494500	-2.18591800
C	-6.51530200	-1.26709300	-0.78800300
C	-5.25218700	-1.39079200	-0.17565100
C	0.62915200	-1.83385200	4.64075300
C	0.00503800	-3.03509300	3.88128700
C	-0.63399200	-4.04790400	4.86395100
C	-5.23109600	0.23547500	1.75780700
C	-5.10504000	-1.25611300	1.34302500
C	-6.11291200	-2.13958400	2.11922200
C	4.04688800	1.10217900	-1.16846300
C	4.19855300	1.03031100	-2.57519400
C	5.49563000	0.74415300	-3.05602800
C	6.56967200	0.53241700	-2.17841100
C	6.37345900	0.59236600	-0.78907700
C	5.10074500	0.87147400	-0.25061800
C	2.69566300	-0.13642200	-4.24857100
C	3.03979500	1.21233500	-3.56011800
C	3.34735800	2.31026000	-4.61032600
C	-0.76693500	1.90047000	4.45526300
C	0.05398500	3.00955000	3.74593800
C	0.81521900	3.88471900	4.77463000
C	-0.81941000	3.77915700	1.42104700
C	-0.85599400	3.84706800	2.84038000
C	-1.78032000	4.73724800	3.42108000
C	-2.61934800	5.53338200	2.62510800
C	-2.55078000	5.44774700	1.22828400
C	-1.65614800	4.56361100	0.58405800
C	5.22958900	-0.46558600	1.90825000
C	4.89707200	0.90712400	1.26767200
C	5.72727000	2.04282000	1.92140500
C	-3.05916200	4.17789700	-1.50373800
C	-1.64963700	4.50299600	-0.94800900
C	-1.11432100	5.82992200	-1.55007000
H	-0.91271700	-4.41060600	0.33704100
H	-2.85039300	-3.69232600	-0.66289800
H	3.00853300	3.34185100	-0.91220500
H	1.16227400	4.35840800	-0.03539900
H	3.84007700	-5.25050000	0.69595300
H	3.88504100	-5.61103800	3.14938700
H	2.13892400	-4.60809900	4.60031500
H	1.24761200	-3.13624900	-1.09823100
H	-2.08535700	-1.83363600	-2.76760600
H	4.25810000	-3.74228200	-1.01987900
H	3.47770300	-2.15681000	-0.76549800

H	3.35127100	-2.96426200	-2.33438100
H	2.65966500	-5.86863700	-1.37907700
H	1.81401500	-4.96162400	-2.65211900
H	0.90168100	-5.64173100	-1.29081800
H	-3.70532900	-0.25694700	-4.84093000
H	-1.95459600	-0.57853300	-4.87205500
H	-2.63025000	0.40604200	-3.57076900
H	-3.21843500	-3.92212200	-3.66640000
H	-2.19341200	-3.10137000	-4.86174200
H	-3.95929300	-2.94708800	-4.95199800
H	-5.63198000	-1.51510700	-4.08028900
H	-7.63046800	-1.22699200	-2.63965800
H	-7.39767100	-1.12031200	-0.17133200
H	-0.79953100	-2.62841700	3.25780100
H	-4.09686300	-1.57906400	1.62979700
H	1.45070900	-2.16276300	5.29149100
H	-0.12899700	-1.34698500	5.26808000
H	1.01725500	-1.09406400	3.93218200
H	0.10184100	-4.44524100	5.57467100
H	-1.08040900	-4.89804600	4.33188300
H	-1.42300300	-3.55617400	5.44787500
H	-4.46774600	0.83974600	1.25618400
H	-5.09876000	0.34150500	2.84284400
H	-6.21993800	0.63376200	1.49388100
H	-7.14874500	-1.81898600	1.95037000
H	-5.91979000	-2.06848400	3.19771000
H	-6.03491600	-3.19452300	1.82542100
H	5.65939700	0.68194800	-4.12839000
H	7.55796900	0.31381500	-2.57632300
H	7.21100500	0.41614700	-0.11896000
H	2.13554900	1.51720000	-3.02448700
H	0.79882700	2.49951800	3.12788900
H	3.55770200	-0.54296100	-4.79679400
H	1.87378200	0.01384200	-4.95966400
H	2.35876300	-0.87449900	-3.51260900
H	3.59554000	3.26853400	-4.13384900
H	2.46578100	2.46668200	-5.24431200
H	4.18503400	2.03243500	-5.26466700
H	-1.55853100	2.33290100	5.08243700
H	-0.11291300	1.29732000	5.09873000
H	-1.22712800	1.23972000	3.71299700
H	1.38740300	4.68063700	4.28012000
H	1.51803700	3.26281500	5.34491000
H	0.13512600	4.35729900	5.49520200
H	-1.83676500	4.81438800	4.50333900
H	-3.32363800	6.21702400	3.09345400
H	-3.20839400	6.06319400	0.62095600
H	3.83981800	1.10142700	1.47702000
H	-1.01471300	3.68098200	-1.28384900
H	6.28354700	-0.73526100	1.75949100
H	4.60765700	-1.25765000	1.47628600
H	5.03948500	-0.43368100	2.98919800

H	5.53792700	2.07813500	3.00243800
H	5.47034500	3.02232600	1.49701600
H	6.80400300	1.88680100	1.77466200
H	-3.40894700	3.21681400	-1.11294700
H	-3.00657100	4.08563400	-2.59531900
H	-3.79604100	4.95578800	-1.25895700
H	-0.09879400	6.06249200	-1.19835500
H	-1.75715800	6.68108000	-1.28664500
H	-1.08259600	5.75467100	-2.64436000
O	-0.11500700	-1.50169400	-1.71452200
O	0.27622800	1.65327900	-1.94510300
O	2.02533100	0.26023100	-0.26745100
O	0.12300400	-1.38994300	1.09761600
Hf	-0.16736100	0.03152900	-0.67990000

η^2 -ozone ComplexFig. S85: ONCCNO η^2 -ozone Complex

E	E_{zp}	H	G
-2818.9278	-2817.7697	-2817.6966	-2817.8871
O	1.67704926	1.15767684	-0.08812254
O	-1.67727600	-1.16528587	-0.09895440
O	-0.59018639	1.00582179	2.09690418
N	1.10173950	-2.85255567	-0.70034568
N	-2.03528744	-2.45768689	0.22281742
N	-1.10336574	2.84717658	-0.69260250
N	2.03313216	2.45057008	0.23275011
C	0.08974848	-3.71290831	-0.39060892
C	-1.23310824	-3.54137042	0.03467973
C	-0.09367121	3.70672922	-0.37491708
C	1.22927087	3.53389915	0.05011460
C	2.41271880	-3.33881567	-1.10079775
C	2.66418538	-3.54140532	-2.48147749
C	3.94080170	-4.01691342	-2.84629261
C	4.92104711	-4.26799560	-1.87227810
C	4.64939930	-4.03471805	-0.51486597
C	3.38925836	-3.55589237	-0.09648895
C	2.05233910	-1.95087026	-4.35273926

C	1.62426731	-3.21323018	-3.55646019
C	1.36299222	-4.40909522	-4.50631076
C	-4.60196522	-0.80026667	-2.09145561
C	-4.18738098	-2.25332865	-1.73512285
C	-4.89150015	-3.27830710	-2.65938429
C	-3.40105731	-2.60516905	0.69912010
C	-4.45146661	-2.52857225	-0.25267562
C	-5.77005299	-2.68221992	0.22091186
C	-6.02547151	-2.90430296	1.58444680
C	-4.96718652	-2.95693120	2.50399688
C	-3.62826243	-2.79345653	2.08610876
C	4.07023935	-2.16014323	1.91034963
C	3.12393105	-3.27060900	1.38430127
C	3.24709646	-4.55756881	2.24077877
C	-2.72425819	-1.73255765	4.21515264
C	-2.49767282	-2.80694266	3.12047597
C	-2.33811373	-4.21444706	3.75470294
C	-2.41433223	3.33403565	-1.09263493
C	-3.38848848	3.55865297	-0.08766706
C	-4.64650577	4.04324874	-0.50571955
C	-4.91962518	4.27147911	-1.86374620
C	-3.94244633	4.01110625	-2.83840491
C	-2.66705934	3.53217250	-2.47363292
C	-4.12592554	2.26265720	1.97220818
C	-3.11732094	3.28879087	1.39507687
C	-3.13686904	4.60567991	2.21537535
C	4.58673914	0.83911288	-2.11763236
C	4.17424664	2.28747555	-1.73997704
C	4.87305768	3.32426244	-2.65494174
C	3.40086435	2.59971596	0.70347698
C	4.44603718	2.54330837	-0.25538341
C	5.76645136	2.69671502	0.21315588
C	6.02830795	2.89875729	1.57863498
C	4.97497967	2.93200524	2.50478489
C	3.63454796	2.76868845	2.09165609
C	-2.06337005	1.94489669	-4.35157609
C	-1.62830948	3.20040258	-3.54861975
C	-1.35772549	4.39933745	-4.49220983
C	2.73965423	1.65908186	4.19833689
C	2.50931328	2.76074793	3.13174710
C	2.35604843	4.15266384	3.80051556
H	0.40285543	-4.74787757	-0.47321999
H	-1.74693190	-4.46806859	0.26631410
H	-0.40811739	4.74182603	-0.45015626
H	1.74205528	4.45984789	0.28705433
H	4.17100379	-4.18548022	-3.89523121
H	5.89961231	-4.63590440	-2.17253930
H	5.42309042	-4.21809066	0.22613107
H	0.67757248	-2.97236112	-3.06022955
H	-3.10949436	-2.32894737	-1.91452954
H	2.99897084	-2.11912652	-4.88361120
H	2.18257397	-1.09487752	-3.68056585

H	1.28656866	-1.69310293	-5.09657807
H	2.26026052	-4.67566587	-5.07996171
H	0.57379357	-4.15385879	-5.22575377
H	1.04298170	-5.29964861	-3.95008189
H	-5.67525639	-0.64139668	-1.91952274
H	-4.39357062	-0.59357547	-3.14997372
H	-4.04156091	-0.08166178	-1.48380094
H	-4.60046079	-4.30771192	-2.41258518
H	-4.61996823	-3.08754057	-3.70619976
H	-5.98466739	-3.21044540	-2.58567536
H	-6.60016557	-2.62978525	-0.47862883
H	-7.04949473	-3.02613149	1.93032358
H	-5.18075704	-3.10943450	3.55855555
H	2.10553197	-2.88857095	1.50351294
H	-1.55463380	-2.55274612	2.62629267
H	5.12424647	-2.46665295	1.85953885
H	3.82846861	-1.93317456	2.95598117
H	3.94778741	-1.23849366	1.33030498
H	4.26503820	-4.96917818	2.20998062
H	2.55795457	-5.33870956	1.89308732
H	3.00633249	-4.33301588	3.28769204
H	-2.79680421	-0.73395468	3.77120122
H	-1.87150390	-1.72253177	4.90426434
H	-3.63511328	-1.92980799	4.79723243
H	-3.24589766	-4.51470013	4.29551423
H	-1.50456292	-4.21157920	4.46872158
H	-2.13203833	-4.98021101	2.99468276
H	-5.41764444	4.23389973	0.23611720
H	-5.89684582	4.64309222	-2.16382754
H	-4.17367034	4.17618286	-3.88769852
H	-2.12538097	2.84074709	1.50669332
H	3.09532207	2.36573628	-1.91252701
H	-5.15508615	2.64726834	1.95593140
H	-3.86348010	2.03301981	3.01228431
H	-4.09730233	1.32560519	1.40442225
H	-2.39485657	5.32329960	1.84054071
H	-2.90411990	4.39506853	3.26701271
H	-4.12247441	5.08930612	2.17635719
H	5.66102412	0.67830336	-1.95391989
H	4.37222540	0.64634684	-3.17759083
H	4.03006558	0.11238943	-1.51626074
H	4.58384607	4.35043011	-2.39301616
H	4.59517349	3.14720332	-3.70247551
H	5.96663102	3.25521223	-2.58888185
H	6.59295383	2.65925015	-0.49159255
H	7.05365840	3.02025017	1.92068057
H	5.19355614	3.06968726	3.56037862
H	-0.68405753	2.95067164	-3.05213714
H	1.56284179	2.52124001	2.63680368
H	-3.00823320	2.12121748	-4.88296282
H	-2.19947157	1.08650011	-3.68371102
H	-1.29826442	1.68609914	-5.09574233

H	-0.57051990	4.14200686	-5.21309625
H	-1.03087365	5.28433645	-3.93110853
H	-2.25314558	4.67589841	-5.06400610
H	2.80661344	0.67180195	3.72888555
H	1.89115206	1.63416059	4.89212664
H	3.65510791	1.83957259	4.77867234
H	2.14743147	4.93672549	3.06010241
H	3.26683281	4.43844363	4.34406874
H	1.52603963	4.13387522	4.51838778
O	-0.01447413	0.00214376	3.07950229
O	0.57141053	-1.00448413	2.10566461
Hf	-0.00246265	-0.00334866	0.38576045
O	-0.99219707	1.48577630	-0.64064693
O	0.99600481	-1.49157872	-0.63260524

8.5 Eight Oxygen Atoms

Bisperoxo Complex (spiro conformation)

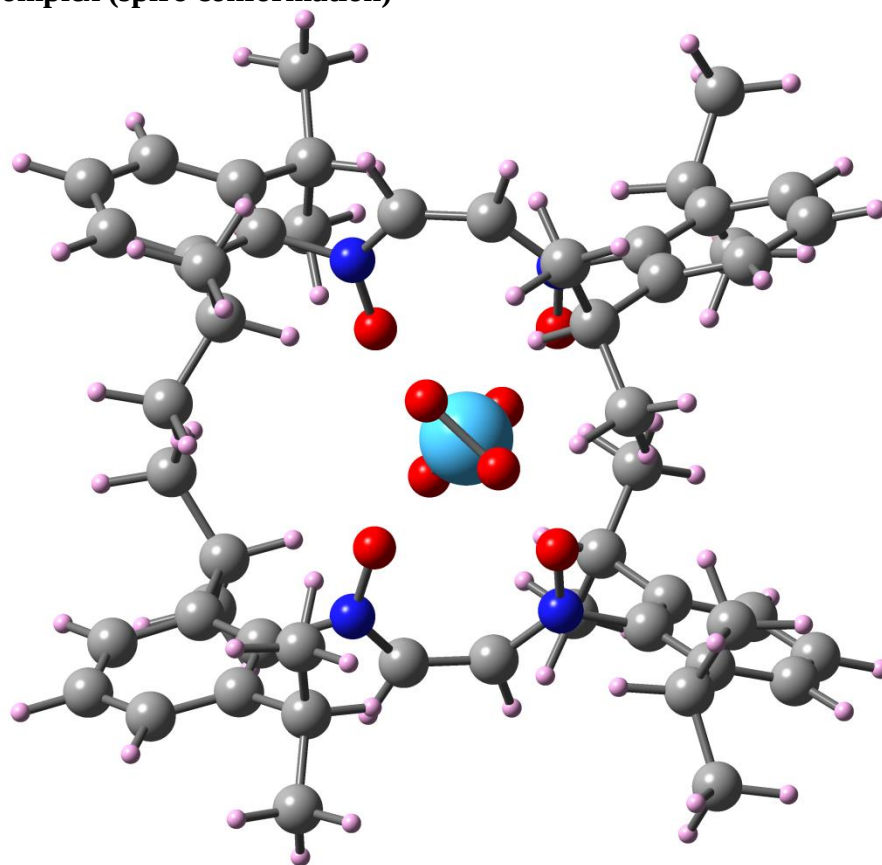


Fig. S86: ONCCNO Bisperoxo Complex (spiro conformation)

E	E_{zp}	H	G
-2894.0979	-2892.9351	-2892.8614	-2893.0493

O	1.54372105	-1.70007273	0.20636817
O	-1.24750061	1.52518858	-0.80099503
O	-0.43635287	-1.02920819	-1.71811317
O	0.67204706	-0.03769592	-2.02925887
N	1.58551147	2.84253011	0.49987034
N	-1.59232623	2.72964674	-0.32949355
N	-1.59181226	-2.73004467	0.32978673
N	1.58606995	-2.84231440	-0.49945046
C	0.55196494	3.66432982	0.69143710
C	-0.81831582	3.62082862	0.30531234
C	-0.81754259	-3.62141171	-0.30442316
C	0.55279114	-3.66470127	-0.69033666
C	2.92113096	3.21739315	0.98253135
C	3.19174379	3.14328923	2.37125748
C	4.49094226	3.51684191	2.78145268
C	5.46333064	3.91227723	1.85134255
C	5.16266176	3.94506000	0.47950960

C	3.88009495	3.59858140	0.00928166
C	2.71437953	1.50988976	4.26604478
C	2.16502300	2.68054126	3.41233806
C	1.72944286	3.86421726	4.31771618
C	-4.39177531	1.07532784	2.11813228
C	-3.58257398	2.36077759	1.80707996
C	-3.80120899	3.42929708	2.91061315
C	-2.99184389	3.08516354	-0.61097906
C	-3.94202480	2.91469181	0.42307984
C	-5.27628174	3.26402869	0.11895060
C	-5.63037592	3.72810583	-1.15711957
C	-4.66076091	3.84673433	-2.16763324
C	-3.31089512	3.52360673	-1.91950382
C	4.23604400	2.38937436	-2.18434505
C	3.57679266	3.61325490	-1.49262169
C	4.01135363	4.93826970	-2.16815130
C	-2.34520139	2.30649034	-3.91545815
C	-2.26472925	3.58642609	-3.03666324
C	-2.38606587	4.86597230	-3.89961544
C	-2.99138272	-3.08540824	0.61104404
C	-3.94127005	-2.91536151	-0.42330392
C	-5.27559552	-3.26479868	-0.11947358
C	-5.62998830	-3.72856666	1.15659662
C	-4.66063259	-3.84675565	2.16744456
C	-3.31076803	-3.52350183	1.91966152
C	-4.39213969	-1.07774643	-2.12018770
C	-3.58143111	-2.36185053	-1.80735500
C	-3.79773211	-3.43131314	-2.91042499
C	4.23878347	-2.38844970	2.18377062
C	3.57846879	-3.61198585	1.49254194
C	4.01248037	-4.93731613	2.16775744
C	2.92161938	-3.21700417	-0.98251913
C	3.88104572	-3.59753145	-0.00954225
C	5.16360741	-3.94374707	-0.48006913
C	5.46376356	-3.91138939	-1.85199533
C	4.49085664	-3.51659326	-2.78188183
C	3.19169839	-3.14333390	-2.37137411
C	-2.34498344	-2.30541168	3.91496050
C	-2.26482138	-3.58601797	3.03703185
C	-2.38683155	-4.86482119	3.90093388
C	2.71323764	-1.50972578	-4.26561132
C	2.16460754	-2.68110353	-3.41232378
C	1.72989264	-3.86481111	-4.31800915
H	0.82333293	4.56332137	1.23290299
H	-1.36865087	4.51471704	0.57674833
H	-1.36760186	-4.51559069	-0.57546244
H	0.82452867	-4.56395476	-1.23117533
H	4.74277247	3.48019709	3.83759027
H	6.45839374	4.18776879	2.19311433
H	5.92880850	4.24386254	-0.23044524
H	1.28007058	2.28563144	2.90574263
H	-2.52730886	2.06844601	1.82823960

H	3.59571142	1.80083054	4.85505633
H	2.97329859	0.66058789	3.62566048
H	1.93571466	1.16916499	4.95936945
H	2.57705863	4.26450858	4.89068119
H	0.96638083	3.52771207	5.03110622
H	1.30333317	4.69209893	3.73341016
H	-5.47166566	1.27131990	2.16547712
H	-4.07626450	0.66749076	3.08638034
H	-4.21160526	0.30607908	1.35848324
H	-3.20494705	4.33259580	2.72311316
H	-3.50336801	3.02489934	3.88621043
H	-4.85527409	3.73186447	2.97592377
H	-6.04064244	3.15888796	0.88418837
H	-6.66483150	3.98832068	-1.36938658
H	-4.95507245	4.19191712	-3.15447588
H	2.49632279	3.50720689	-1.63798914
H	-1.26617797	3.59051796	-2.58289423
H	5.32782449	2.40756272	-2.06274418
H	4.00994688	2.39570413	-3.25867332
H	3.84862880	1.45786262	-1.75947137
H	5.10092400	5.06972692	-2.14871103
H	3.55755265	5.80975648	-1.67802403
H	3.70022885	4.93670760	-3.22093000
H	-2.14174024	1.41379128	-3.31583346
H	-1.59462157	2.35330942	-4.71513634
H	-3.33735604	2.21317039	-4.37900498
H	-3.31757453	4.88072210	-4.48012455
H	-1.55589691	4.90796985	-4.61630931
H	-2.35474676	5.77543721	-3.28510262
H	-6.03971008	-3.15987537	-0.88498294
H	-6.66444187	-3.98894143	1.36867237
H	-4.95518077	-4.19181767	3.15426352
H	-2.52655574	-2.06807404	-1.82773618
H	2.49812820	-3.50535286	1.63846340
H	-5.47163661	-1.27557073	-2.16931150
H	-4.07561872	-0.66988103	-3.08809347
H	-4.21462555	-0.30786493	-1.36056231
H	-3.20030963	-4.33368520	-2.72212899
H	-3.49986270	-3.02706707	-3.88608122
H	-4.85132502	-3.73542464	-2.97621919
H	5.33049556	-2.40725480	2.06166145
H	4.01326055	-2.39442474	3.25822444
H	3.85173066	-1.45675647	1.75894411
H	3.55740593	-5.80836866	1.67803284
H	3.70223409	-4.93541254	3.22080547
H	5.10189669	-5.06989678	2.14739204
H	5.93003661	-4.24199681	0.22982108
H	6.45877401	-4.18662529	-2.19411844
H	4.74231506	-3.48028104	-3.83812576
H	-1.26618831	-3.59082121	2.58343068
H	1.27938973	-2.28691657	-2.90560424
H	-3.33723042	-2.21151551	4.37818990

H	-2.14097717	-1.41320148	3.31482242
H	-1.59461711	-2.35201821	4.71485616
H	-1.55678620	-4.90658020	4.61778724
H	-2.35582492	-5.77482109	3.28720411
H	-3.31842523	-4.87866720	4.48133863
H	2.97058313	-0.66019970	-3.62490439
H	1.93470331	-1.16988496	-4.95952385
H	3.59535477	-1.79964199	-4.85393635
H	1.30439376	-4.69315670	-3.73392095
H	2.57777325	-4.26438041	-4.89109062
H	0.96662980	-3.52864089	-5.03133720
O	-0.43699799	1.02900186	1.71856187
O	0.67170316	0.03768623	2.02966048
Hf	0.14999002	0.00006103	0.00020523
O	1.54330423	1.70051718	-0.20650877
O	-1.24694538	-1.52552958	0.80092152

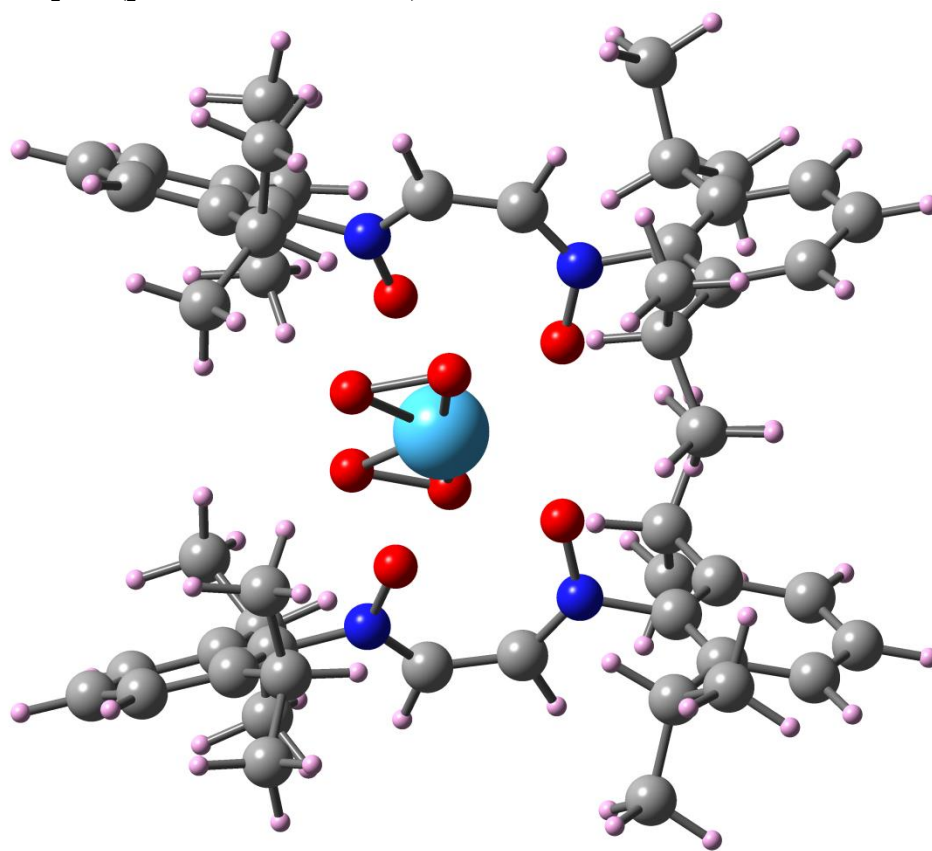
Bisperoxo Complex (planar conformation)

Fig. S87: ONCCNO Bisperoxo Complex (planar conformation)

E	E_{zp}	H	G
-2894.0935	-2892.9296	-2892.8568	-2893.0394
O	-1.68410615	0.58241954	1.50205441
O	-0.22707942	0.84367916	1.90628115
O	-0.22543983	-0.84315110	-1.90229751
O	-1.68227408	-0.58273812	-1.49943863
C	-2.86543973	3.27898698	0.13372186
C	-3.44154084	3.59948613	-1.13084927
C	-4.81329671	3.92205907	-1.14876903
C	-5.57274995	3.95500619	0.02930785
C	-4.96904404	3.66150764	1.25913512
C	-3.60660549	3.30615598	1.35068373
C	-2.98286934	2.37805033	-3.30694698
C	-2.66259940	3.63539178	-2.45392970
C	-2.93345034	4.93780652	-3.25086856
C	3.93628773	3.81187385	-2.97593553
C	3.12821645	4.00753977	-1.67024234
C	2.78860858	5.51084928	-1.46801639
C	3.16488121	2.73098778	0.57218774
C	3.84929606	3.45108861	-0.43723990

C	5.22589553	3.67910434	-0.23525520
C	5.87609504	3.19839596	0.91422619
C	5.16348004	2.48230042	1.88792700
C	3.78251380	2.22702578	1.74013271
C	-3.88061127	1.88633897	3.45263647
C	-3.03960318	2.97397762	2.73871721
C	-2.94585032	4.25416444	3.61394154
C	3.55402070	-0.00324365	2.92699167
C	3.02055567	1.44707685	2.81597924
C	3.08305938	2.17290691	4.18544300
C	3.16350770	-2.73188033	-0.57346547
C	3.85089902	-3.45103079	0.43479015
C	5.22718191	-3.67796671	0.22969101
C	5.87438193	-3.19732919	-0.92157830
C	5.15894245	-2.48258025	-1.89407368
C	3.77800105	-2.22873349	-1.74340368
C	3.94728511	-3.81577299	2.97278887
C	3.13288959	-4.00617628	1.67025880
C	2.78574071	-5.50761717	1.46752476
C	-3.88315057	-1.88476461	-3.45458884
C	-3.04110999	-2.97044874	-2.73902161
C	-2.94411531	-4.25099004	-3.61339234
C	-2.86767960	-3.27714191	-0.13422285
C	-3.60879647	-3.30289806	-1.35129141
C	-4.97164687	-3.65671151	-1.26015846
C	-5.57609001	-3.94950809	-0.03051437
C	-4.81676042	-3.91803078	1.14766387
C	-3.44441452	-3.59793293	1.13002112
C	3.54664895	0.00087484	-2.93085957
C	3.01337411	-1.44928510	-2.81773312
C	3.07261962	-2.17593809	-4.18695895
C	-2.98411041	-2.38057569	3.30831715
C	-2.66566073	-3.63690328	2.45318374
C	-2.93820422	-4.94043900	3.24774977
H	-5.28630258	4.16211599	-2.09622305
H	-6.62908420	4.21025264	-0.01087310
H	-5.56660196	3.68642835	2.16555670
H	-1.59170897	3.59845458	-2.23825176
H	2.18359384	3.46439520	-1.79205695
H	-4.05712140	2.31970951	-3.53392136
H	-2.67725079	1.46796995	-2.78066948
H	-2.43738511	2.42276413	-4.25990553
H	-3.96527066	4.99206313	-3.62131071
H	-2.27199464	4.97456677	-4.12676913
H	-2.74534646	5.83252216	-2.64205607
H	4.85485892	4.41321911	-2.98324507
H	3.33189462	4.12655823	-3.83653885
H	4.21208979	2.76190761	-3.11892992
H	2.16122920	5.66797365	-0.58142187
H	2.24561879	5.89892972	-2.33966703
H	3.70306544	6.10597762	-1.34307304
H	5.79295589	4.22967185	-0.98034984

H	6.93933299	3.38291516	1.04924943
H	5.68028268	2.11564824	2.77079481
H	-2.04642166	2.53581913	2.63011376
H	1.96489438	1.36812035	2.53795835
H	-4.91015708	2.21301699	3.65233961
H	-3.41393469	1.63678020	4.41475702
H	-3.89928025	0.97633988	2.84612652
H	-3.93915834	4.68468923	3.79917391
H	-2.33516696	5.03964661	3.14459902
H	-2.49672635	4.01183603	4.58605099
H	3.41973102	-0.53159385	1.97729833
H	2.99010828	-0.54392835	3.69800044
H	4.61830128	-0.02517697	3.20035743
H	4.11048790	2.22930176	4.56983518
H	2.47663235	1.62911974	4.92041874
H	2.69328550	3.19753683	4.11776745
H	5.79672596	-4.22716613	0.97388562
H	6.93755739	-3.38068912	-1.05866942
H	5.67338655	-2.11548714	-2.77813954
H	2.19213580	-3.45764021	1.79745038
H	-2.04877218	-2.53065131	-2.62922844
H	4.86445827	-4.41927759	2.97482193
H	3.34594265	-4.13124126	3.83524217
H	4.22591893	-2.76668318	3.11709266
H	2.15413072	-5.66107582	0.58333640
H	2.24472331	-5.89448760	2.34092331
H	3.69735913	-6.10612251	1.33826028
H	-4.91120861	-2.21426469	-3.65730122
H	-3.41469419	-1.63347195	-4.41538990
H	-3.90651381	-0.97508374	-2.84772914
H	-2.33161872	-5.03467706	-3.14344299
H	-2.49553392	-4.00825850	-4.58564971
H	-3.93637010	-4.68407218	-3.79833793
H	-5.56902486	-3.68069133	-2.16671819
H	-6.63286158	-4.20297284	0.00941331
H	-5.29029667	-4.15747035	2.09501340
H	1.95840858	-1.36996356	-2.53736059
H	-1.59474568	-3.60097249	2.23762784
H	4.60994970	0.02273688	-3.20801220
H	3.41578178	0.52928297	-1.98070671
H	2.98000440	0.54153070	-3.69986654
H	2.46595647	-1.63153056	-4.92129457
H	2.68113797	-3.19986701	-4.11822522
H	4.09934168	-2.23434960	-4.57290918
H	-2.67774595	-1.47007083	2.78318443
H	-2.43823670	-2.42735989	4.26095224
H	-4.05816948	-2.32116537	3.53593031
H	-2.75113941	-5.83421230	2.63722858
H	-3.97013206	-4.99419758	3.61794353
H	-2.27681095	-4.97967043	4.12359060
O	-1.02860240	-2.01860769	0.78954945
N	-1.45107601	-2.91465196	-0.14334774

O	1.46287109	-1.33298133	0.27640819
O	-1.02748585	2.01709309	-0.78741918
O	1.46320730	1.33012305	-0.27111744
N	1.72467887	-2.47993859	-0.38701553
N	1.72567621	2.47867781	0.38889294
N	-1.44902979	2.91520755	0.14331327
C	0.86779206	3.34720437	0.93356951
H	1.38042708	4.10785686	1.51384529
C	-0.55034803	3.52277897	0.90755032
H	-0.92781982	4.30426073	1.55336641
C	-0.55233495	-3.52112278	-0.90831624
H	-0.92988143	-4.30088527	-1.55614544
C	0.86589393	-3.34630877	-0.93372905
H	1.37787722	-4.10556710	-1.51642433
Hf	-0.34874281	-0.00107409	0.00313286

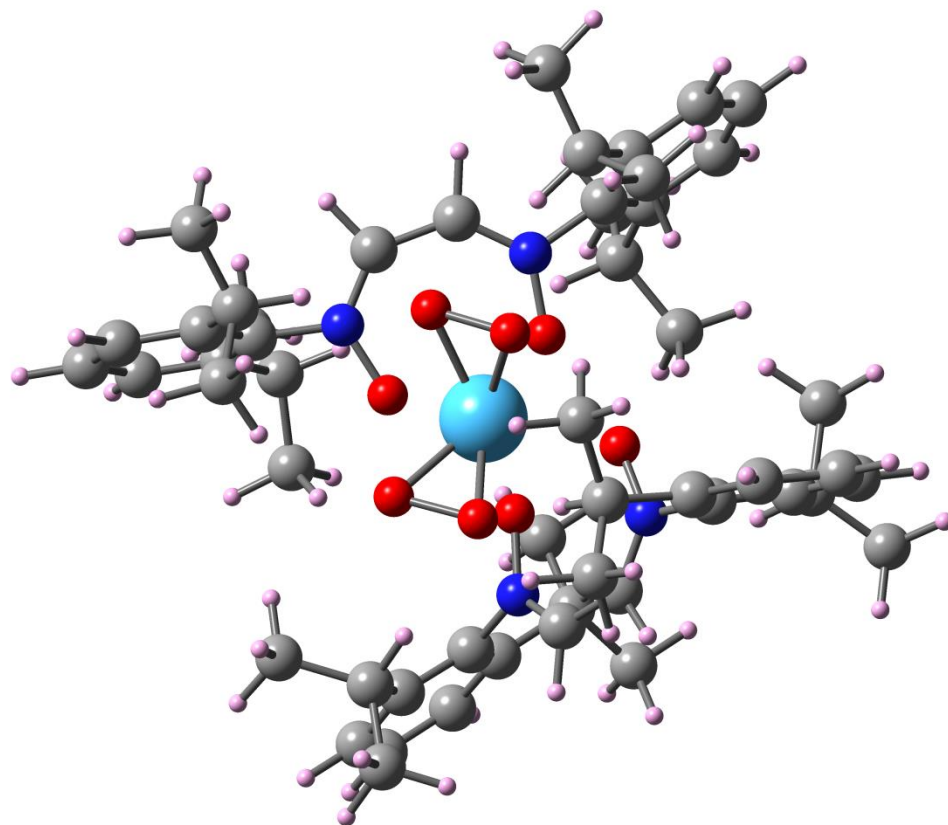
Bisperoxo Complex (butterfly conformation)

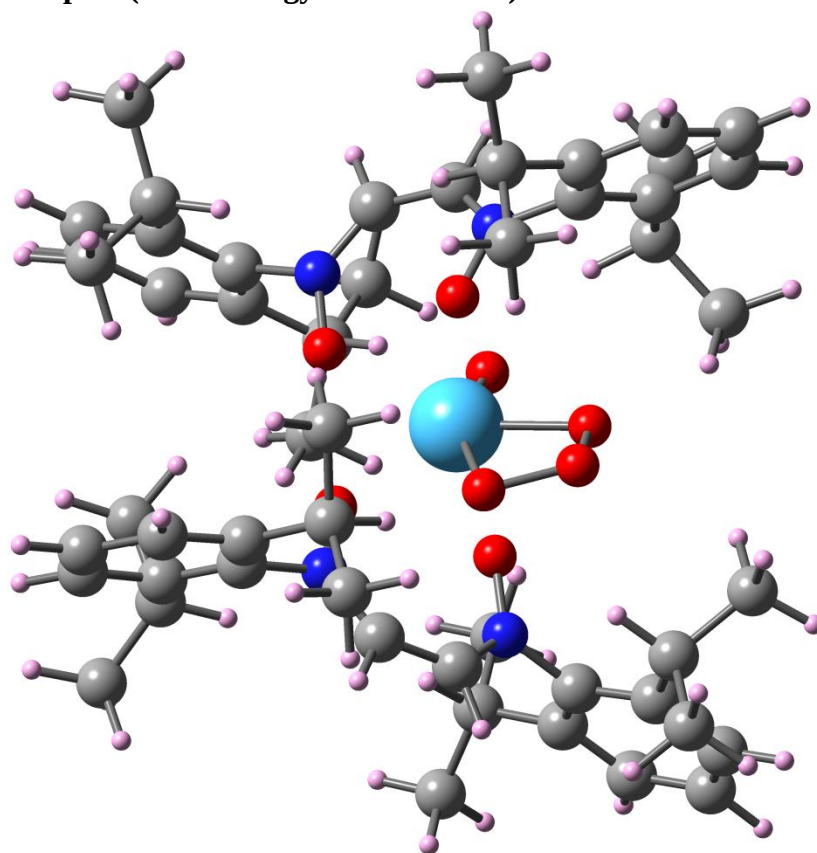
Fig. S88: ONCCNO Bisperoxo Complex (butterfly conformation)

E	E_{zp}	H	G
-2894.1072	-2892.9468	-2892.8739	-2893.0595
O	0.37064200	-1.40115700	0.96712600
O	2.02830400	0.67578000	0.00941900
O	1.19417800	-1.22651300	-1.93652800
N	-0.35834900	2.77903400	0.78589900
N	2.55367200	1.85916100	-0.38367300
N	-2.56768400	-1.85713300	-0.37795600
N	0.34969400	-2.74625900	0.80569300
C	0.65671600	3.43124200	0.22765800
C	1.93020000	3.02916300	-0.30535500
C	-1.93356900	-3.02137200	-0.27419100
C	-0.64714300	-3.41313200	0.23442200
C	-1.49039300	3.53837400	1.34120900
C	-2.40900700	4.15467900	0.45555700
C	-3.46642400	4.88180500	1.04675500
C	-3.60566500	4.96717300	2.43916700
C	-2.68804100	4.32079300	3.28349400
C	-1.60620300	3.58944600	2.75361300
C	-3.61409800	3.45826600	-1.67085100

C	-2.31764700	4.05948100	-1.07138200
C	-2.01169000	5.44688900	-1.69637300
C	3.05810000	0.72845600	-4.20850200
C	3.12838400	2.00487500	-3.32731600
C	3.36308700	3.27078600	-4.19263200
C	3.94314600	1.78509500	-0.86167900
C	4.20911000	1.85835400	-2.25154900
C	5.56440100	1.75437900	-2.63910200
C	6.58432000	1.57441200	-1.69477900
C	6.27653600	1.48680300	-0.32689300
C	4.94544900	1.58651800	0.12294800
C	-1.32758600	1.62107600	4.31059400
C	-0.63606100	2.86620300	3.69269100
C	-0.07636400	3.80099300	4.79389900
C	4.73892400	-0.05362000	2.03426800
C	4.62325900	1.43649600	1.61334700
C	5.51147600	2.34071900	2.50425900
C	-3.97022800	-1.82725700	-0.82729900
C	-4.24527700	-1.84709900	-2.21602200
C	-5.60772800	-1.81213000	-2.58864300
C	-6.62506800	-1.73665200	-1.62647900
C	-6.30776400	-1.68483600	-0.25868200
C	-4.96752800	-1.72542400	0.17506500
C	-3.24060700	-0.64174600	-4.21411800
C	-3.15698000	-1.88726300	-3.29276200
C	-3.23300200	-3.19895900	-4.11630100
C	1.37846800	-1.44912900	4.27403400
C	0.70296800	-2.72489200	3.70492100
C	0.18991700	-3.64398200	4.84237200
C	1.50631400	-3.47058300	1.35264600
C	1.66523800	-3.45635000	2.76309100
C	2.77456400	-4.14438100	3.29355800
C	3.67543300	-4.81974600	2.45454500
C	3.48776400	-4.81035900	1.06555300
C	2.40343300	-4.12676100	0.47115000
C	-4.75031000	-0.11047000	2.10486700
C	-4.62705500	-1.59474300	1.66317100
C	-5.49086300	-2.51746200	2.55785400
C	3.54702800	-3.57712200	-1.73410800
C	2.26595100	-4.12492800	-1.05578300
C	1.93146200	-5.54674800	-1.58199200
H	0.50244100	4.50427600	0.19820900
H	2.52067300	3.85566600	-0.68531300
H	-2.53119000	-3.85753800	-0.62062600
H	-0.47493900	-4.48231500	0.18477800
H	-4.19260600	5.37210600	0.40438500
H	-4.43171900	5.53028300	2.86724300
H	-2.81145500	4.38706500	4.36103800
H	-1.51938500	3.36920900	-1.35461400
H	2.14251100	2.09830200	-2.86231700
H	-4.49356400	4.08874000	-1.47841100
H	-3.79719800	2.45881700	-1.26174800

H	-3.49679800	3.35283500	-2.75598900
H	-2.81626300	6.16761800	-1.49514900
H	-1.90811200	5.34883200	-2.78427300
H	-1.07708900	5.87509900	-1.30682000
H	4.01931600	0.51737300	-4.69845400
H	2.29837500	0.86558800	-4.98882000
H	2.75844100	-0.13991200	-3.61104000
H	3.41276200	4.18104000	-3.57847300
H	2.53597600	3.38745900	-4.90410300
H	4.29509900	3.20602800	-4.77064000
H	5.81417400	1.80417800	-3.69528100
H	7.61799000	1.49385700	-2.02308100
H	7.07505700	1.33713900	0.39442400
H	0.21338100	2.49508700	3.10928000
H	3.58121700	1.73092500	1.78198800
H	-2.21068600	1.90977000	4.89639300
H	-0.63243300	1.09482400	4.97753100
H	-1.63942700	0.93032700	3.51988300
H	-0.86445500	4.14806600	5.47433700
H	0.40907000	4.68600100	4.36215100
H	0.66688500	3.26412000	5.39793500
H	4.04716500	-0.66980100	1.45075700
H	4.49178100	-0.16914800	3.09809900
H	5.75977900	-0.42760900	1.87853700
H	6.56797700	2.04710100	2.45855700
H	5.19399500	2.25944700	3.55223300
H	5.44189100	3.39497700	2.20576300
H	-5.86651300	-1.83261400	-3.64373700
H	-7.66578500	-1.70720900	-1.94094100
H	-7.10591800	-1.60885200	0.47426100
H	-2.17158600	-1.84358300	-2.82015800
H	-0.16681800	-2.38709900	3.13268800
H	-4.21066400	-0.57117900	-4.72598100
H	-2.45411300	-0.70060200	-4.97699300
H	-3.06716800	0.27492200	-3.63983300
H	-3.15096300	-4.08730000	-3.47470300
H	-2.40752900	-3.22838400	-4.83812300
H	-4.17623200	-3.27403000	-4.67514400
H	2.28369300	-1.69922400	4.84376800
H	0.68731800	-0.92371600	4.94593900
H	1.65113400	-0.77153200	3.45801200
H	-0.28424400	-4.55043400	4.44375000
H	-0.55233400	-3.10864800	5.44912100
H	1.00051200	-3.95597700	5.51329400
H	2.93055600	-4.15654100	4.36884200
H	4.52383200	-5.34814400	2.88312400
H	4.19857200	-5.32616100	0.42615000
H	-3.57928700	-1.88180200	1.81219000
H	1.46644500	-3.44421400	-1.35597400
H	-5.77743200	0.25404300	1.96946500
H	-4.07469500	0.52177000	1.51919300
H	-4.48806900	-0.00665600	3.16638900

H	-5.15258400	-2.44977900	3.60015200
H	-5.42151700	-3.56671000	2.24235100
H	-6.54957500	-2.22897500	2.53892800
H	3.75564600	-2.55887900	-1.38997100
H	3.39183200	-3.53064900	-2.81874800
H	4.42535700	-4.20840500	-1.53930300
H	1.00760600	-5.94463700	-1.13800200
H	2.73785000	-6.25925000	-1.35999000
H	1.79552800	-5.51701500	-2.67039000
O	0.28926900	1.73777500	-1.90416100
O	-1.14080700	1.17998700	-2.02996200
O	-0.25045400	-1.75817100	-1.89909800
O	-2.05785300	-0.64567200	-0.07103800
O	-0.45192800	1.43773000	0.91403900
Hf	0.00347600	-0.00252800	-0.79096600

Oxo η^2 -Ozone Complex (lower energy conformation)Fig. S89: ONCCNO Oxo η^2 -Ozone Complex (lower energy conformation)

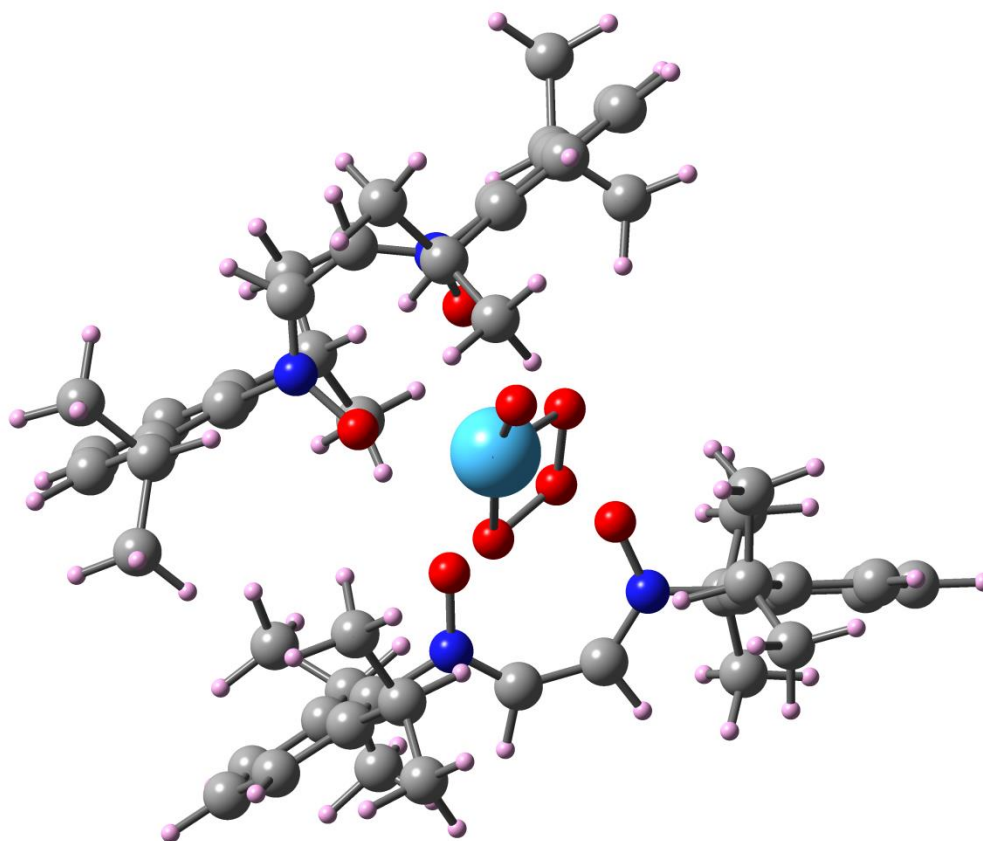
E	E_{zp}	H	G
-2894.0923	-2892.9290	-2892.8554	-2893.0431

O	2.32749652	-0.77774427	0.26600456
O	-1.77534726	0.64848992	-0.10901856
O	0.23479191	-1.27908346	-1.68440646
N	-0.48372303	3.48033731	0.20976156
N	-2.77354312	1.50572272	-0.32006677
N	-0.26165130	-2.79380017	0.67049686
N	2.79903749	-1.94321595	-0.18306424
C	-1.77110832	3.63941515	0.51795594
C	-2.81732191	2.79042523	0.04993369
C	0.75291811	-3.42267477	0.06891094
C	2.08583801	-3.07482769	-0.28258692
C	0.56601226	4.34080212	0.74261552
C	0.72786598	4.46527049	2.15125588
C	1.76729907	5.30870616	2.59505802
C	2.61116597	5.97068669	1.69244605
C	2.42711852	5.81677628	0.31039578
C	1.39762757	5.00471672	-0.20423493
C	0.76229011	2.92171036	4.17754353

C	-0.12209567	3.74002051	3.20289858
C	-1.02887271	4.74415272	3.96541524
C	-5.14393381	-1.08063616	1.83219709
C	-4.95611259	0.35923245	1.29056037
C	-6.01925103	1.31750333	1.89171597
C	-3.93648820	0.93082974	-1.01708981
C	-4.98831221	0.39151779	-0.24080613
C	-6.09952023	-0.11847701	-0.94469819
C	-6.13187836	-0.10396254	-2.34876788
C	-5.05083828	0.41104372	-3.08199957
C	-3.91636524	0.94277704	-2.43229645
C	2.34919344	4.06618605	-2.36393012
C	1.21639106	4.91485858	-1.72567140
C	1.13610632	6.32184051	-2.37437449
C	-2.04773276	0.32826815	-4.04054560
C	-2.73118585	1.47358532	-3.24614200
C	-3.16557676	2.62801195	-4.18637887
C	-1.47942018	-3.53487893	1.00355021
C	-2.32927712	-3.98048947	-0.04145675
C	-3.47080896	-4.72156630	0.33679707
C	-3.75881073	-4.97994555	1.68491690
C	-2.90666159	-4.50299521	2.69411439
C	-1.74257422	-3.77315986	2.37806657
C	-3.29581010	-3.05109814	-2.20697542
C	-2.06528702	-3.70112789	-1.52638451
C	-1.66620123	-5.00351418	-2.27288977
C	4.64821195	-0.02786554	2.47821770
C	4.57607274	-1.53122995	2.09502864
C	5.32419396	-2.40940743	3.12997262
C	4.24454558	-1.94954094	-0.44736839
C	5.09863294	-1.74475366	0.66957106
C	6.48529547	-1.72467023	0.41944584
C	6.99234211	-1.90786003	-0.87720448
C	6.11843329	-2.10551103	-1.95489550
C	4.71778287	-2.12142410	-1.77186923
C	-1.50369760	-2.09794395	4.26144437
C	-0.82733130	-3.26810616	3.49842900
C	-0.41468333	-4.40451785	4.46815762
C	4.01700530	-1.12464007	-3.99720474
C	3.80799536	-2.28832380	-2.99370765
C	4.03030816	-3.66307281	-3.67723078
H	-2.03859055	4.53143582	1.06925333
H	-3.80386932	3.23357124	-0.03315675
H	0.51812189	-4.45824095	-0.15207501
H	2.66162689	-3.90125116	-0.68287947
H	1.93168253	5.42531450	3.66205355
H	3.41389683	6.60250559	2.06542653
H	3.08432809	6.33902559	-0.37869223
H	-0.74968342	2.99775715	2.70321923
H	-3.96974857	0.69755453	1.62878736
H	1.47211781	3.55186178	4.73015304
H	1.29446130	2.16312622	3.59475335

H	0.12354508	2.41335625	4.91376038
H	-0.42824806	5.47392953	4.52427290
H	-1.66067391	4.20875542	4.68658825
H	-1.68660656	5.31125812	3.29013624
H	-6.13317067	-1.48186407	1.57604090
H	-5.05463935	-1.08390001	2.92622273
H	-4.38478503	-1.75859150	1.42740864
H	-5.87040643	2.35236988	1.55545599
H	-5.96543677	1.30546568	2.98797695
H	-7.03372705	1.01577134	1.60034453
H	-6.93698265	-0.53542669	-0.39171127
H	-6.99684763	-0.50419380	-2.87230653
H	-5.08323203	0.39725848	-4.16789025
H	0.27902207	4.39622073	-1.94756796
H	-1.97168418	1.87159883	-2.56476891
H	3.33748536	4.48451328	-2.12726718
H	2.23719183	4.05621420	-3.45680806
H	2.30452265	3.03000761	-2.01469805
H	2.08524779	6.86668145	-2.29281668
H	0.35236327	6.93794210	-1.91303565
H	0.90777454	6.22103182	-3.44358615
H	-1.64288953	-0.43249695	-3.36471744
H	-1.20504142	0.73068666	-4.61578867
H	-2.74874103	-0.14550406	-4.74223134
H	-3.88738066	2.28764710	-4.94051793
H	-2.29017447	3.02233528	-4.71742103
H	-3.62686644	3.45377944	-3.62764637
H	-4.14362747	-5.08849015	-0.43337063
H	-4.64659160	-5.54976201	1.94957429
H	-3.14118466	-4.70803593	3.73517323
H	-1.24190421	-2.98581766	-1.62733594
H	3.51765917	-1.81022280	2.13287294
H	-4.16257548	-3.72562383	-2.22437889
H	-3.04954751	-2.79485676	-3.24481153
H	-3.58748800	-2.12890286	-1.69303984
H	-0.77753858	-5.47565105	-1.83241046
H	-1.44038383	-4.77900043	-3.32314109
H	-2.47949806	-5.74168677	-2.24939055
H	5.68001777	0.34499878	2.41315238
H	4.29472951	0.11488780	3.50791663
H	4.00776553	0.56538772	1.81896809
H	5.29706696	-3.47233679	2.85502651
H	4.85373308	-2.29803770	4.11564227
H	6.37609805	-2.11386213	3.23559943
H	7.17228523	-1.56870151	1.24625119
H	8.06654335	-1.89048231	-1.04628724
H	6.52145738	-2.23197238	-2.95600934
H	0.08523117	-2.86043012	3.05327227
H	2.76347068	-2.22396483	-2.68100136
H	-2.44518816	-2.41942626	4.72859949
H	-1.71087148	-1.26902124	3.57638966
H	-0.83832056	-1.72744964	5.05207709

H	0.29811958	-4.02022964	5.20937774
H	0.06381412	-5.23533309	3.93311930
H	-1.27529685	-4.80849059	5.01698432
H	3.78794854	-0.16537976	-3.52122060
H	3.33575166	-1.24428630	-4.84916872
H	5.04559298	-1.09460440	-4.38220546
H	3.85845587	-4.49724663	-2.98235285
H	5.05293606	-3.76087445	-4.06534875
H	3.33875835	-3.77664072	-4.52212656
O	0.87357789	1.23074949	1.56133614
O	1.17555168	-0.51614167	-2.51864806
O	1.37769102	0.77671570	-1.81181134
Hf	0.41987073	0.30685680	0.05528650
O	-0.24800100	-1.49724838	1.08557402
O	-0.13374166	2.54755622	-0.68410756

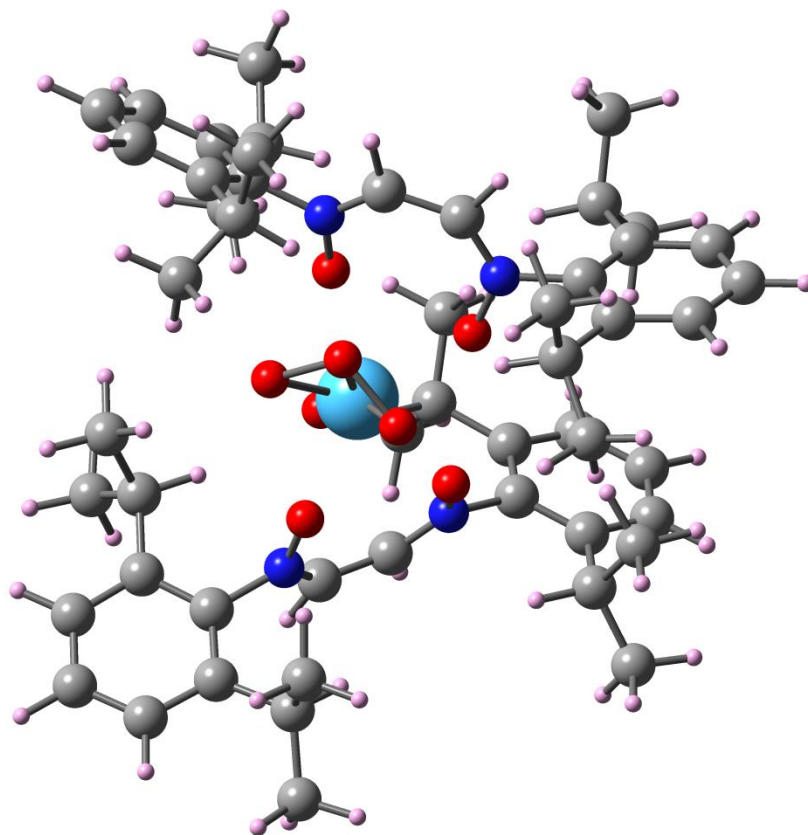
Oxo η^2 -Ozone Complex (higher energy conformation)Fig. S90: ONCCNO Oxo η^2 -Ozone Complex (higher energy conformation)

E	E_{zp}	H	G
-2894.0815	-2892.9184	-2892.8448	-2893.0312
O	2.32749652	-0.77774427	0.26600456
O	-1.77534726	0.64848992	-0.10901856
O	0.23479191	-1.27908346	-1.68440646
N	-0.48372303	3.48033731	0.20976156
N	-2.77354312	1.50572272	-0.32006677
N	-0.26165130	-2.79380017	0.67049686
N	2.79903749	-1.94321595	-0.18306424
C	-1.77110832	3.63941515	0.51795594
C	-2.81732191	2.79042523	0.04993369
C	0.75291811	-3.42267477	0.06891094
C	2.08583801	-3.07482769	-0.28258692
C	0.56601226	4.34080212	0.74261552
C	0.72786598	4.46527049	2.15125588
C	1.76729907	5.30870616	2.59505802
C	2.61116597	5.97068669	1.69244605
C	2.42711852	5.81677628	0.31039578
C	1.39762757	5.00471672	-0.20423493
C	0.76229011	2.92171036	4.17754353

C	-0.12209567	3.74002051	3.20289858
C	-1.02887271	4.74415272	3.96541524
C	-5.14393381	-1.08063616	1.83219709
C	-4.95611259	0.35923245	1.29056037
C	-6.01925103	1.31750333	1.89171597
C	-3.93648820	0.93082974	-1.01708981
C	-4.98831221	0.39151779	-0.24080613
C	-6.09952023	-0.11847701	-0.94469819
C	-6.13187836	-0.10396254	-2.34876788
C	-5.05083828	0.41104372	-3.08199957
C	-3.91636524	0.94277704	-2.43229645
C	2.34919344	4.06618605	-2.36393012
C	1.21639106	4.91485858	-1.72567140
C	1.13610632	6.32184051	-2.37437449
C	-2.04773276	0.32826815	-4.04054560
C	-2.73118585	1.47358532	-3.24614200
C	-3.16557676	2.62801195	-4.18637887
C	-1.47942018	-3.53487893	1.00355021
C	-2.32927712	-3.98048947	-0.04145675
C	-3.47080896	-4.72156630	0.33679707
C	-3.75881073	-4.97994555	1.68491690
C	-2.90666159	-4.50299521	2.69411439
C	-1.74257422	-3.77315986	2.37806657
C	-3.29581010	-3.05109814	-2.20697542
C	-2.06528702	-3.70112789	-1.52638451
C	-1.66620123	-5.00351418	-2.27288977
C	4.64821195	-0.02786554	2.47821770
C	4.57607274	-1.53122995	2.09502864
C	5.32419396	-2.40940743	3.12997262
C	4.24454558	-1.94954094	-0.44736839
C	5.09863294	-1.74475366	0.66957106
C	6.48529547	-1.72467023	0.41944584
C	6.99234211	-1.90786003	-0.87720448
C	6.11843329	-2.10551103	-1.95489550
C	4.71778287	-2.12142410	-1.77186923
C	-1.50369760	-2.09794395	4.26144437
C	-0.82733130	-3.26810616	3.49842900
C	-0.41468333	-4.40451785	4.46815762
C	4.01700530	-1.12464007	-3.99720474
C	3.80799536	-2.28832380	-2.99370765
C	4.03030816	-3.66307281	-3.67723078
H	-2.03859055	4.53143582	1.06925333
H	-3.80386932	3.23357124	-0.03315675
H	0.51812189	-4.45824095	-0.15207501
H	2.66162689	-3.90125116	-0.68287947
H	1.93168253	5.42531450	3.66205355
H	3.41389683	6.60250559	2.06542653
H	3.08432809	6.33902559	-0.37869223
H	-0.74968342	2.99775715	2.70321923
H	-3.96974857	0.69755453	1.62878736
H	1.47211781	3.55186178	4.73015304
H	1.29446130	2.16312622	3.59475335

H	0.12354508	2.41335625	4.91376038
H	-0.42824806	5.47392953	4.52427290
H	-1.66067391	4.20875542	4.68658825
H	-1.68660656	5.31125812	3.29013624
H	-6.13317067	-1.48186407	1.57604090
H	-5.05463935	-1.08390001	2.92622273
H	-4.38478503	-1.75859150	1.42740864
H	-5.87040643	2.35236988	1.55545599
H	-5.96543677	1.30546568	2.98797695
H	-7.03372705	1.01577134	1.60034453
H	-6.93698265	-0.53542669	-0.39171127
H	-6.99684763	-0.50419380	-2.87230653
H	-5.08323203	0.39725848	-4.16789025
H	0.27902207	4.39622073	-1.94756796
H	-1.97168418	1.87159883	-2.56476891
H	3.33748536	4.48451328	-2.12726718
H	2.23719183	4.05621420	-3.45680806
H	2.30452265	3.03000761	-2.01469805
H	2.08524779	6.86668145	-2.29281668
H	0.35236327	6.93794210	-1.91303565
H	0.90777454	6.22103182	-3.44358615
H	-1.64288953	-0.43249695	-3.36471744
H	-1.20504142	0.73068666	-4.61578867
H	-2.74874103	-0.14550406	-4.74223134
H	-3.88738066	2.28764710	-4.94051793
H	-2.29017447	3.02233528	-4.71742103
H	-3.62686644	3.45377944	-3.62764637
H	-4.14362747	-5.08849015	-0.43337063
H	-4.64659160	-5.54976201	1.94957429
H	-3.14118466	-4.70803593	3.73517323
H	-1.24190421	-2.98581766	-1.62733594
H	3.51765917	-1.81022280	2.13287294
H	-4.16257548	-3.72562383	-2.22437889
H	-3.04954751	-2.79485676	-3.24481153
H	-3.58748800	-2.12890286	-1.69303984
H	-0.77753858	-5.47565105	-1.83241046
H	-1.44038383	-4.77900043	-3.32314109
H	-2.47949806	-5.74168677	-2.24939055
H	5.68001777	0.34499878	2.41315238
H	4.29472951	0.11488780	3.50791663
H	4.00776553	0.56538772	1.81896809
H	5.29706696	-3.47233679	2.85502651
H	4.85373308	-2.29803770	4.11564227
H	6.37609805	-2.11386213	3.23559943
H	7.17228523	-1.56870151	1.24625119
H	8.06654335	-1.89048231	-1.04628724
H	6.52145738	-2.23197238	-2.95600934
H	0.08523117	-2.86043012	3.05327227
H	2.76347068	-2.22396483	-2.68100136
H	-2.44518816	-2.41942626	4.72859949
H	-1.71087148	-1.26902124	3.57638966
H	-0.83832056	-1.72744964	5.05207709

H	0.29811958	-4.02022964	5.20937774
H	0.06381412	-5.23533309	3.93311930
H	-1.27529685	-4.80849059	5.01698432
H	3.78794854	-0.16537976	-3.52122060
H	3.33575166	-1.24428630	-4.84916872
H	5.04559298	-1.09460440	-4.38220546
H	3.85845587	-4.49724663	-2.98235285
H	5.05293606	-3.76087445	-4.06534875
H	3.33875835	-3.77664072	-4.52212656
O	0.87357789	1.23074949	1.56133614
O	1.17555168	-0.51614167	-2.51864806
O	1.37769102	0.77671570	-1.81181134
Hf	0.41987073	0.30685680	0.05528650
O	-0.24800100	-1.49724838	1.08557402
O	-0.13374166	2.54755622	-0.68410756

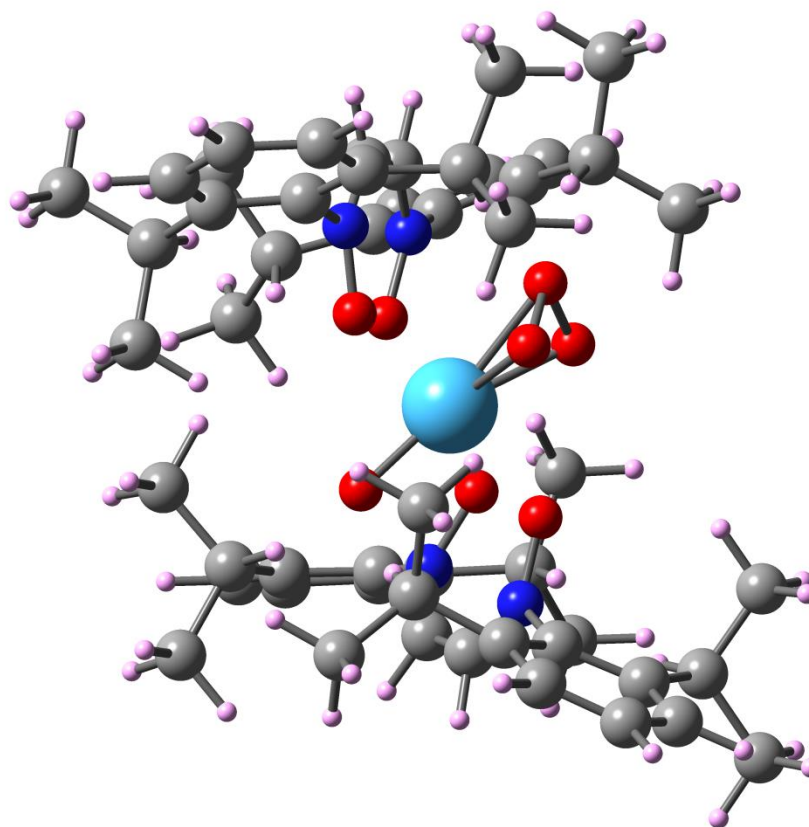
Oxo η^3 -Ozone Complex (lower energy conformation)Fig. S91: ONCCNO Oxo η^3 -Ozone Complex (lower energy conformation)

E	E_{zp}	H	G
-2894.0766	-2892.9140	-2892.8402	-2893.0289
O	-1.83890714	0.06418100	-0.27956602
O	2.34046818	-0.96860007	-0.75465806
O	1.54558212	1.63098513	-1.22071710
N	0.17445301	-2.79611822	0.97819407
N	3.09532323	-1.73303213	0.03119200
N	-0.79797106	3.19395424	0.06931201
N	-2.76919221	0.82409306	-0.86194807
C	1.39732211	-2.97668023	1.45404111
C	2.68736221	-2.55041919	0.99968008
C	-1.88491314	3.20769425	-0.69654805
C	-2.77120721	2.14872516	-1.05934408
C	-0.97256008	-3.41755526	1.65410113
C	-1.36422210	-2.93907722	2.93044723
C	-2.46359519	-3.58666427	3.53781127
C	-3.14161024	-4.63276135	2.89541822
C	-2.73614021	-5.06292839	1.62125312
C	-1.63794913	-4.46670534	0.96981807
C	-1.68481013	-0.65054605	3.99222730

C	-0.67349305	-1.77529114	3.65290028
C	0.04583500	-2.26733517	4.93656538
C	4.41176734	1.79081014	0.85556507
C	4.50073535	0.37397003	1.48776411
C	5.18614140	0.42427603	2.87568122
C	4.54190535	-1.57852012	-0.20660402
C	5.21931940	-0.57625704	0.52397204
C	6.60305048	-0.44232103	0.27491702
C	7.25089255	-1.25423810	-0.66858705
C	6.52911849	-2.21028017	-1.40396711
C	5.14625939	-2.39067118	-1.19595909
C	-2.23961717	-4.42707434	-1.48251411
C	-1.22344309	-4.93855838	-0.42705403
C	-1.06103308	-6.47749450	-0.50469004
C	3.88888530	-2.60904320	-3.37049426
C	4.32778133	-3.34454826	-2.07156816
C	5.06899839	-4.66176935	-2.39999618
C	-0.03750200	4.41954134	0.33823003
C	0.56717704	5.12475739	-0.73665006
C	1.29745210	6.28543047	-0.39937903
C	1.43428111	6.70466252	0.93020107
C	0.83238106	5.97390848	1.96683315
C	0.07752801	4.81491637	1.70111813
C	1.92278315	4.50934234	-2.80328621
C	0.50343604	4.70265836	-2.21053717
C	-0.31526502	5.72730246	-3.04223423
C	-5.18855340	-0.76211406	2.10270616
C	-4.91681838	0.37146003	1.08174709
C	-5.89055745	1.56011912	1.30564410
C	-3.96398830	0.07101801	-1.30736410
C	-4.99681738	-0.13501201	-0.36219003
C	-6.14277349	-0.82444406	-0.81065906
C	-6.23373445	-1.28964410	-2.13231316
C	-5.17623240	-1.08408309	-3.03209723
C	-4.00294531	-0.40288703	-2.64040720
C	0.48468904	3.19722924	3.61166227
C	-0.57270305	4.05613231	2.86559422
C	-1.31376410	5.00594838	3.84126429
C	-2.49356419	-1.46280011	-4.41093834
C	-2.86058322	-0.17487801	-3.63372128
C	-3.21592924	0.96829108	-4.62314635
H	1.43275911	-3.60945528	2.33391418
H	3.51181127	-2.99452223	1.54684212
H	-2.15811816	4.18321232	-1.07899608
H	-3.64714628	2.48041919	-1.60419812
H	-2.79505822	-3.25707525	4.51889134
H	-3.98769030	-5.11061339	3.38407026
H	-3.27316325	-5.87082443	1.13188009
H	0.07124001	-1.30993710	2.99422423
H	3.46614127	0.04372200	1.64062513
H	-2.45745719	-0.98109808	4.70087236
H	-2.17657217	-0.28897702	3.08156824

H	-1.14902209	0.19576901	4.44000834
H	-0.66055805	-2.69313121	5.66288042
H	0.56299005	-1.42738111	5.41779039
H	0.79618906	-3.03868023	4.71301136
H	5.41055744	2.20515417	0.65711005
H	3.88751230	2.46790519	1.54195312
H	3.84819230	1.76625013	-0.08436101
H	5.25917340	-0.57417004	3.32813325
H	4.59962435	1.05987108	3.55106727
H	6.19969147	0.84463906	2.81965522
H	7.16932057	0.31041902	0.81629706
H	8.31724064	-1.13238909	-0.84474006
H	7.04176155	-2.81188722	-2.14853617
H	-0.25747102	-4.48909834	-0.67981705
H	3.40906326	-3.61246627	-1.53354612
H	-3.24318625	-4.83274337	-1.29502210
H	-1.92867015	-4.73659036	-2.48916819
H	-2.29337317	-3.33400925	-1.45632311
H	-2.01489516	-6.99809252	-0.34963303
H	-0.34959403	-6.84670253	0.24567202
H	-0.68938405	-6.76254953	-1.49765511
H	3.29361525	-1.72067813	-3.13433524
H	3.27948025	-3.27555925	-3.99541331
H	4.76602236	-2.29859418	-3.95446830
H	5.93824844	-4.48889834	-3.04755023
H	4.39550534	-5.34173640	-2.93749923
H	5.41738943	-5.17079440	-1.49162511
H	1.78087514	6.85099352	-1.19051509
H	2.01308315	7.59596359	1.16061109
H	0.94461907	6.31088146	2.99294623
H	0.02180200	3.72635928	-2.29488518
H	-3.89937530	0.73069806	1.27359710
H	2.51598819	5.43316939	-2.77097521
H	1.84120614	4.19492932	-3.85180530
H	2.44438218	3.71655729	-2.25868117
H	-1.33512710	5.85948146	-2.65169420
H	-0.39120803	5.38760940	-4.08310531
H	0.16442001	6.71508852	-3.04539423
H	-6.21451246	-1.14368209	2.02056315
H	-5.05450339	-0.38485103	3.12476424
H	-4.49796834	-1.60012712	1.95589315
H	-5.67785444	2.39093418	0.62002904
H	-5.80307344	1.93563915	2.33356118
H	-6.93230451	1.25283710	1.14521409
H	-6.96327355	-1.00212708	-0.12076501
H	-7.12669857	-1.81745214	-2.45899619
H	-5.25372440	-1.46234511	-4.04727231
H	-1.31395810	3.35704126	2.46485419
H	-1.95188815	0.10775801	-3.09107424
H	1.30011110	3.82540329	3.99693630
H	0.89921207	2.43387218	2.94576922
H	0.01724800	2.68793820	4.46598734

H	-1.85564614	4.41271434	4.58952035
H	-2.03983716	5.64133645	3.31661225
H	-0.62233105	5.66143444	4.38581233
H	-2.26516518	-2.28386817	-3.72234028
H	-1.59573412	-1.27416610	-5.01109638
H	-3.29561125	-1.78700314	-5.08903539
H	-3.42817326	1.91120314	-4.10095931
H	-4.09741431	0.71405905	-5.22854640
H	-2.37229818	1.14577209	-5.30161540
O	1.06705408	-0.14909501	1.54521312
O	0.31164302	1.49299412	-2.15403716
O	0.14015101	0.00309300	-2.38886818
O	-0.38609403	2.10438316	0.73821206
O	-0.11294601	-2.06209016	-0.12028001
Hf	0.44591703	0.17311901	-0.17314701

Oxo η^3 -Ozone Complex (higher energy conformation)Fig. S92: ONCCNO Oxo η^3 -Ozone Complex (higher energy conformation)

E	E_{zp}	H	G
-2894.0758	-2892.9128	-2892.8401	-2893.0241
O	-1.82805300	0.21888900	0.00490200
O	2.37711300	-0.91506700	-0.76858700
O	1.35515900	1.40856800	-1.66739300
N	0.26419700	-2.82822100	0.97019800
N	3.15242200	-1.62400300	0.05149200
N	-0.77068400	3.23551800	0.05926300
N	-2.70177300	0.80365700	-0.84781700
C	1.49143000	-2.93911600	1.45836900
C	2.76408500	-2.44830500	1.02214600
C	-1.91442500	3.18668800	-0.63969100
C	-2.73248600	2.11173700	-1.09387900
C	-0.85240000	-3.49774900	1.64777100
C	-1.22995100	-3.06274100	2.94463400
C	-2.28301000	-3.76992400	3.56621300
C	-2.93689400	-4.82622500	2.91551300
C	-2.55627100	-5.20351800	1.61715400
C	-1.49967200	-4.55060700	0.95063700
C	-1.63030200	-0.82302700	4.08412400

C	-0.57419500	-1.88054700	3.67218400
C	0.22043500	-2.36346100	4.91451900
C	4.25325700	1.98952700	0.86440200
C	4.38401400	0.58414300	1.51365700
C	5.00689100	0.68008900	2.92832100
C	4.59347400	-1.38734400	-0.14496000
C	5.18843000	-0.33681900	0.59006700
C	6.56952300	-0.12633600	0.38329300
C	7.29348900	-0.91280400	-0.52615300
C	6.65221600	-1.91972200	-1.26785600
C	5.27604700	-2.17748500	-1.10030900
C	-2.14346400	-4.42681100	-1.49180900
C	-1.10817800	-4.97035300	-0.46993000
C	-0.94050300	-6.50465300	-0.60618200
C	4.13098000	-2.51520100	-3.32114200
C	4.54490700	-3.19319900	-1.98353100
C	5.36270000	-4.48095100	-2.23973900
C	-0.25812600	4.55913500	0.46832500
C	0.51184700	5.29684100	-0.45953700
C	0.96994200	6.56288200	-0.03214800
C	0.69445800	7.03538400	1.25966200
C	-0.03921300	6.24969100	2.16504900
C	-0.53420800	4.98354700	1.79144400
C	2.39100000	4.80581600	-2.10398100
C	0.86162200	4.77536700	-1.85731800
C	0.10890600	5.57344300	-2.95483700
C	-5.06341700	-1.47399900	1.93863800
C	-4.64594500	-0.29454200	1.03036100
C	-5.56051500	0.93648800	1.29338200
C	-3.75572800	-0.06848000	-1.39651500
C	-4.66474900	-0.64413200	-0.46376100
C	-5.67381700	-1.47747400	-0.98143200
C	-5.77854600	-1.72059300	-2.36122200
C	-4.87971100	-1.12129000	-3.25095300
C	-3.84020100	-0.27646800	-2.79741700
C	-0.24056900	3.32725200	3.67876500
C	-1.26907000	4.09452300	2.80018800
C	-2.27304000	4.88142300	3.67681900
C	-2.25375900	-0.70075400	-4.74967300
C	-2.91156800	0.36354800	-3.83693200
C	-3.68504800	1.41485900	-4.67998700
H	1.54987500	-3.56223300	2.34360400
H	3.59840700	-2.83892300	1.59471800
H	-2.28948800	4.17043700	-0.89485500
H	-3.56069500	2.41735500	-1.72208700
H	-2.60066800	-3.47727200	4.56331000
H	-3.74765800	-5.35119400	3.41556800
H	-3.07750800	-6.01752300	1.12128100
H	0.11461500	-1.35706400	2.99601000
H	3.36094700	0.20524600	1.62653600
H	-2.35646100	-1.21483300	4.81035900
H	-2.17455500	-0.46101800	3.20426700

H	-1.12324000	0.03703800	4.53952600
H	-0.43451800	-2.84573000	5.65364400
H	0.70886000	-1.50868100	5.39969100
H	1.00247300	-3.08714700	4.64503500
H	5.23649800	2.45988500	0.72161200
H	3.64825900	2.63914300	1.50929500
H	3.75349200	1.92246000	-0.10896800
H	5.10203100	-0.30938700	3.39581600
H	4.36594000	1.29725200	3.57048300
H	6.00372800	1.14169000	2.90926000
H	7.07392500	0.66561500	0.93007800
H	8.35621900	-0.73184100	-0.67037600
H	7.22245600	-2.50174300	-1.98571500
H	-0.14876700	-4.50750700	-0.72333600
H	3.61611700	-3.49116500	-1.48013200
H	-3.14649200	-4.82750500	-1.28993000
H	-1.85708400	-4.71942600	-2.51058000
H	-2.18530400	-3.33392000	-1.44914800
H	-1.89101200	-7.03564800	-0.46595000
H	-0.22184800	-6.89957400	0.12408400
H	-0.57499300	-6.74878500	-1.61210800
H	3.48528900	-1.65010000	-3.13648300
H	3.58082300	-3.22638700	-3.95153200
H	5.01746200	-2.17916500	-3.87603400
H	6.25290800	-4.28346500	-2.85067400
H	4.74840600	-5.20658600	-2.78835800
H	5.69073400	-4.94870200	-1.30207000
H	1.55875600	7.17084500	-0.71325200
H	1.06150100	8.01163900	1.56767800
H	-0.22633000	6.62272300	3.16756300
H	0.57442100	3.72278500	-1.93430900
H	-3.62330000	-0.02415200	1.30599900
H	2.79057200	5.82942400	-2.10634400
H	2.61232700	4.34903200	-3.07590200
H	2.91703700	4.22370200	-1.33951300
H	-0.98067100	5.52161400	-2.82226600
H	0.34751100	5.16311900	-3.94406600
H	0.39644600	6.63376700	-2.94770400
H	-6.12444200	-1.73128500	1.81952800
H	-4.91086700	-1.19997600	2.99034600
H	-4.46373200	-2.36788200	1.73383500
H	-5.25281700	1.80628000	0.69831200
H	-5.51880200	1.22067800	2.35328000
H	-6.60513600	0.70828100	1.04230000
H	-6.38692400	-1.93526600	-0.30331400
H	-6.56431900	-2.37073700	-2.73875500
H	-4.97300600	-1.31333800	-4.31577300
H	-1.84176300	3.33697000	2.25006000
H	-2.08345700	0.86273700	-3.33151200
H	0.40013900	4.02988100	4.22901500
H	0.38926000	2.67640200	3.06350700
H	-0.76731300	2.70002700	4.41064000

H	-2.84983900	4.18264200	4.29616700
H	-2.97789700	5.46207400	3.06741400
H	-1.76300700	5.57374200	4.35880200
H	-1.63146500	-1.36855500	-4.14743900
H	-1.59422200	-0.20320100	-5.47200500
H	-2.99453800	-1.28564000	-5.31227600
H	-4.13600000	2.19913200	-4.05448100
H	-4.49496400	0.94953700	-5.25747400
H	-3.00061800	1.89903800	-5.38808500
O	1.00939000	-0.12215900	1.48237500
O	-0.01586200	1.16203800	-2.32216400
O	-0.17806100	-0.35508500	-2.34820100
O	-0.02751400	2.22327800	0.48394100
O	-0.05247100	-2.12590200	-0.14049200
Hf	0.39788200	0.10192600	-0.26418400

Ligand Cyclization

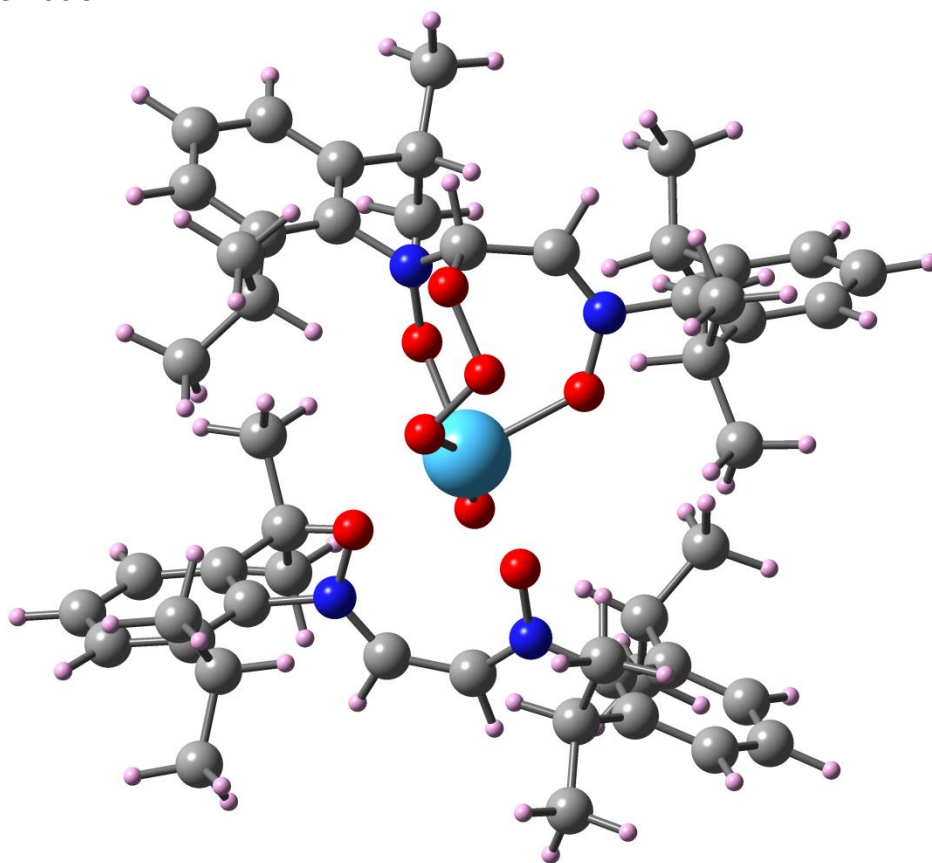


Fig. S93: ONCCNO Ligand Cyclization

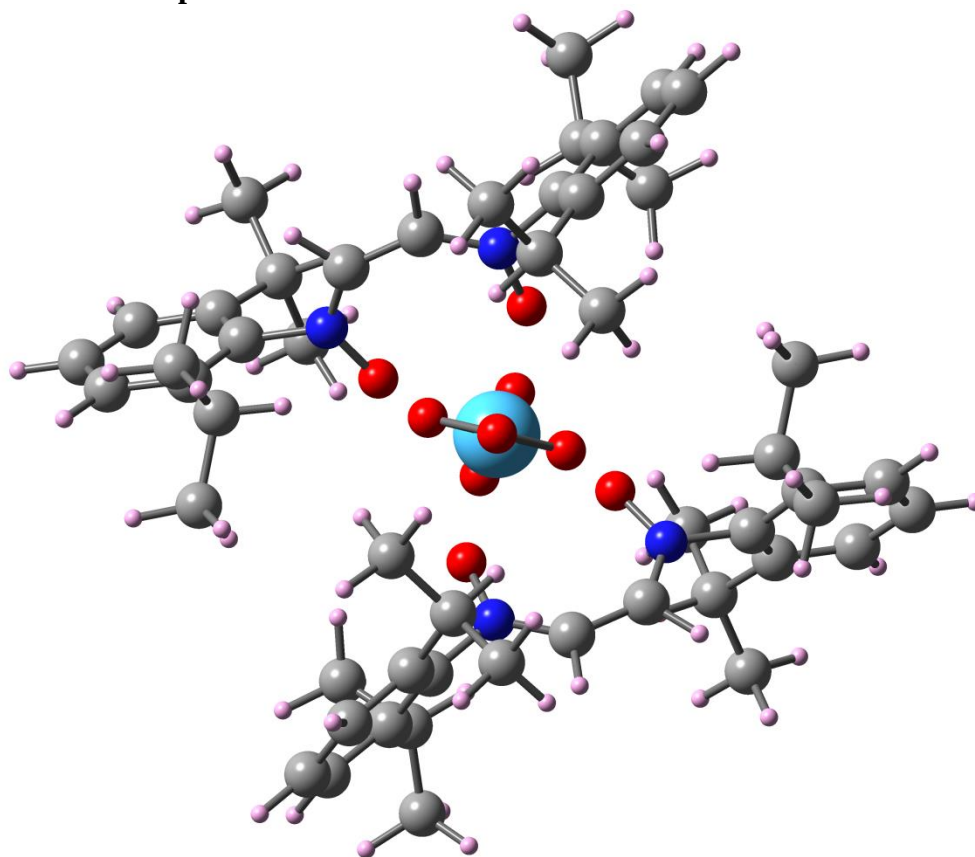
E	E_{zp}	H	G
-2894.0910	-2892.9276	-2892.8542	-2893.0426
O	-1.97121987	0.53404848	-0.12831714
O	2.08768450	-1.04833724	-0.32520494
O	-0.36126437	2.16677129	-2.94200427
N	-0.40195166	-3.19915409	0.39793497
N	2.64776246	-1.95033489	0.49071356
N	0.41655853	2.98865539	-0.67293253
N	-2.55828941	1.66867688	-0.59135598
C	0.69270646	-3.48281790	1.08777860
C	2.02843326	-2.94773865	1.11125687
C	-0.57820366	2.97345298	-1.67109797
C	-2.00464733	2.68568746	-1.21098993
C	-1.61531937	-4.00987241	0.57672716
C	-2.38517189	-3.82632750	1.75090134
C	-3.54451294	-4.62392716	1.87448906
C	-3.91565521	-5.52897011	0.86896661
C	-3.13595730	-5.66176507	-0.29247706
C	-1.96165127	-4.90259756	-0.46825274
C	-3.17976066	-1.80360908	3.06555089

C	-2.02576937	-2.81501866	2.84566310
C	-1.66770231	-3.53587339	4.17225360
C	3.59660241	1.23439117	2.69168814
C	3.49665503	-0.31178939	2.77321567
C	3.71470509	-0.80476766	4.22737254
C	4.09192564	-1.75439347	0.70556014
C	4.49285554	-0.96736449	1.81045838
C	5.88299725	-0.79009652	1.98306348
C	6.80401068	-1.35752160	1.08837644
C	6.35967462	-2.11120075	-0.01056404
C	4.98355080	-2.32351182	-0.23375481
C	-1.85237257	-4.31446804	-2.92699270
C	-1.13533344	-5.03208257	-1.75172345
C	-0.82255205	-6.50807671	-2.10330611
C	4.88150779	-2.37293619	-2.76933226
C	4.50930289	-3.11313038	-1.45774169
C	5.06784372	-4.55994732	-1.45490426
C	1.49459007	3.94603515	-0.60548677
C	2.64033876	3.81170328	-1.43659340
C	3.65234581	4.79312205	-1.33287464
C	3.54894187	5.85019546	-0.41874417
C	2.42711011	5.94752068	0.42189944
C	1.38444671	5.00280266	0.34705114
C	4.12813850	1.86717044	-2.12096073
C	2.82250045	2.64901750	-2.41519403
C	2.79643633	3.14267191	-3.88504190
C	-3.78499623	2.28159629	3.27834981
C	-3.58204025	2.91394891	1.87758452
C	-3.79852932	4.44972417	1.93073148
C	-4.01395962	1.66997909	-0.35248138
C	-4.49870289	2.26851524	0.83332580
C	-5.89685873	2.25667616	1.02335844
C	-6.74953156	1.65769420	0.08219030
C	-6.22355165	1.04975460	-1.06892790
C	-4.83402823	1.03494023	-1.31396839
C	0.52161772	4.29190419	2.61145381
C	0.19779894	5.08049386	1.31132369
C	-0.24141618	6.52792822	1.63569323
C	-4.58061944	-1.17831913	-2.52239271
C	-4.27359110	0.34190777	-2.55987720
C	-4.81776004	0.98763544	-3.86073078
H	0.56363748	-4.32882042	1.75417836
H	2.69434736	-3.50513034	1.76136972
H	-0.59046916	3.97637497	-2.11415271
H	-2.72755189	3.44906953	-1.48313544
H	-4.16454741	-4.52096534	2.76065948
H	-4.81638020	-6.12705364	0.98559831
H	-3.44017484	-6.36096777	-1.06615634
H	-1.15885583	-2.21693367	2.53831480
H	2.46921080	-0.56961728	2.48775979
H	-4.10092616	-2.29161385	3.41266703
H	-3.40063276	-1.26067964	2.13893272

H	-2.87714114	-1.07034565	3.82360545
H	-2.51924742	-4.10661032	4.56800083
H	-1.37408549	-2.79662706	4.92812487
H	-0.82962204	-4.23502297	4.04279908
H	4.59605044	1.59527162	2.97200688
H	2.86488458	1.68609004	3.37285193
H	3.36863571	1.59028205	1.68067321
H	3.63126386	-1.89782848	4.30131115
H	2.95413762	-0.36364008	4.88357391
H	4.70207963	-0.51604469	4.61321602
H	6.24187796	-0.19676446	2.81955417
H	7.86970666	-1.20430868	1.24142502
H	7.08445774	-2.53020167	-0.70347439
H	-0.17835728	-4.51708303	-1.60978231
H	3.41540979	-3.17803052	-1.43733084
H	-2.83234320	-4.76868939	-3.12790611
H	-1.24735051	-4.38695926	-3.83996749
H	-1.99454945	-3.25396365	-2.69646337
H	-1.73239826	-7.07144315	-2.34726841
H	-0.31916932	-7.02330411	-1.27458351
H	-0.16599983	-6.55006709	-2.98197810
H	4.43644346	-1.37244403	-2.78829688
H	4.50481197	-2.93001696	-3.63689357
H	5.96948074	-2.27114088	-2.87752618
H	6.16323100	-4.56689783	-1.52521031
H	4.67545527	-5.11825568	-2.31483337
H	4.78822778	-5.09911616	-0.53997776
H	4.53139943	4.71871382	-1.96828115
H	4.34157377	6.59282344	-0.35376188
H	2.36507042	6.76348713	1.13620266
H	1.99380952	1.94818331	-2.29730852
H	-2.53822719	2.73038699	1.59936377
H	5.02319204	2.48896364	-2.26171411
H	4.20242075	1.01003303	-2.80255857
H	4.13401600	1.48164140	-1.09425125
H	1.84157056	3.62829782	-4.11932109
H	2.90931221	2.28963546	-4.56643430
H	3.60820186	3.85565137	-4.08896284
H	-4.79858830	2.45962934	3.66082742
H	-3.07473523	2.71890389	3.99164212
H	-3.61304164	1.20048261	3.24726500
H	-3.61545936	4.91945174	0.95529524
H	-3.11490553	4.90342757	2.65939039
H	-4.82536956	4.69443531	2.23248783
H	-6.31778283	2.71139124	1.91597794
H	-7.82398458	1.65922332	0.24951207
H	-6.89435885	0.57941351	-1.78271690
H	-0.64765900	4.56811607	0.83454885
H	-3.18374366	0.44270425	-2.57438137
H	1.39185843	4.72801009	3.12158234
H	0.73719100	3.24517776	2.37442422
H	-0.33115500	4.32630265	3.30502522

H	-1.16958607	6.51564908	2.22253226
H	-0.42125355	7.11216085	0.72341252
H	0.51109576	7.05873417	2.23364769
H	-4.15290773	-1.64121752	-1.62551361
H	-4.14229655	-1.66814145	-3.40113276
H	-5.66175777	-1.37198793	-2.52961444
H	-4.58440157	2.05926799	-3.90545000
H	-5.90707492	0.87457291	-3.94444018
H	-4.36012869	0.50718775	-4.73438848
O	0.29259876	-0.72724409	1.72758877
O	-0.68670645	0.68341841	-2.71270502
O	0.48870579	-0.01647107	-2.17549896
Hf	0.09382963	-0.10161495	-0.00240049
O	0.53651580	1.86920317	0.21000371
O	-0.51146229	-2.20012807	-0.50180120

8.6 Nine Oxygen Atoms

Peroxo η^2 -Ozone ComplexFig. S94: ONCCNO Peroxo η^2 -Ozone Complex

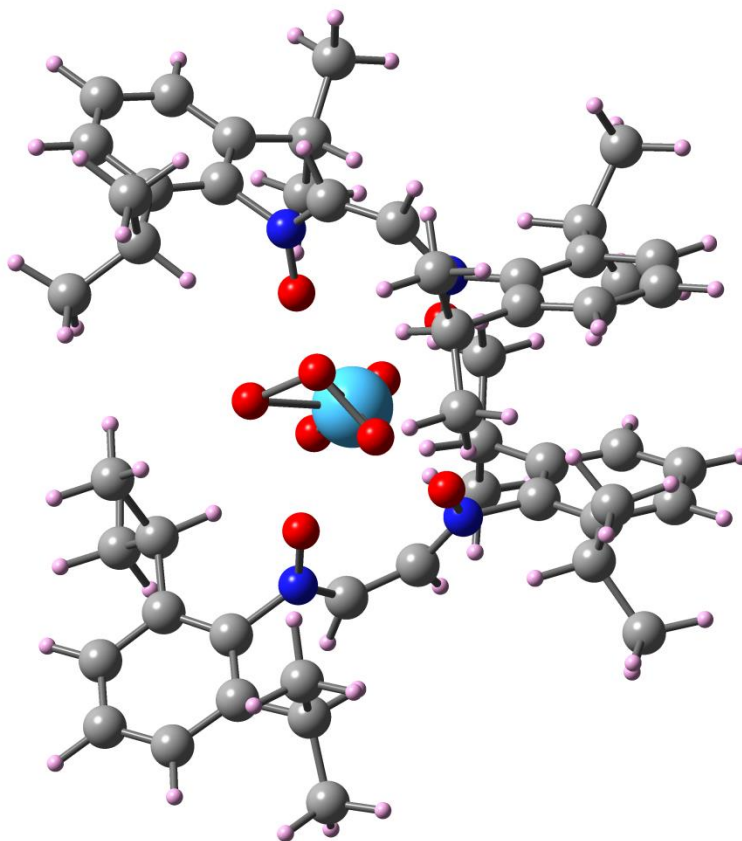
E	E_{zp}	H	G
-2969.2488	-2968.0828	-2968.0080	-2968.1973

O	0.49584779	2.10942055	-0.26470298
O	-0.49420341	-2.10220129	-0.26262682
O	-1.13058976	0.27522397	1.26551420
N	2.79378875	-1.76728191	-0.46916618
N	-0.04588922	-3.05127085	0.57301649
N	-2.79097904	1.75488005	-0.47682174
N	0.03982343	3.06115625	0.56232004
C	2.46998361	-2.75614801	0.37461872
C	1.24161350	-3.29845138	0.84381232
C	-2.47416708	2.74891909	0.36276723
C	-1.24959753	3.30134691	0.83083841
C	4.19914239	-1.58273024	-0.85845463
C	4.58283481	-2.03148324	-2.14709433
C	5.93326692	-1.84488389	-2.50706906
C	6.84154342	-1.23883865	-1.62281077
C	6.41445579	-0.78327596	-0.36643609

C	5.07082883	-0.92862792	0.04315298
C	3.13389405	-1.56363194	-4.16685530
C	3.58356846	-2.63803264	-3.13696172
C	4.13941374	-3.89661889	-3.84772279
C	-2.53592533	-4.05635247	-2.12164370
C	-1.43349478	-4.79407511	-1.31477472
C	-1.22265340	-6.23470459	-1.84592767
C	-1.09326812	-3.93091245	1.10809957
C	-1.76292463	-4.77308858	0.18194251
C	-2.78233600	-5.60152232	0.69305855
C	-3.10729786	-5.59253953	2.05939395
C	-2.42466787	-4.74471731	2.94313618
C	-1.40400353	-3.88016040	2.48948167
C	4.91426726	1.15299825	1.48941479
C	4.61116122	-0.36486587	1.39257592
C	5.26554044	-1.13150194	2.57251256
C	-1.73209145	-1.99531431	4.16458977
C	-0.71132005	-2.94478410	3.48691376
C	0.08532448	-3.75292711	4.54567879
C	-4.19406656	1.55848863	-0.86777225
C	-5.06365824	0.90372060	0.03539268
C	-6.40497864	0.74599435	-0.37715153
C	-6.83168680	1.19031040	-1.63767161
C	-5.92532217	1.79756449	-2.52302638
C	-4.57742907	1.99652507	-2.16024528
C	-4.89905614	-1.16687911	1.49655732
C	-4.60407397	0.35185560	1.38966328
C	-5.26541269	1.12323571	2.56267810
C	2.52026859	4.06256531	-2.13888946
C	1.41406746	4.80081049	-1.33771807
C	1.19537882	6.23607765	-1.88014471
C	1.08048703	3.95266572	1.09140930
C	1.74359207	4.79316761	0.15913060
C	2.75697560	5.63260931	0.66426512
C	3.08210915	5.63577078	2.03057915
C	2.40600478	4.78912307	2.92045510
C	1.39193212	3.91367078	2.47295340
C	-3.12083037	1.52941740	-4.17500151
C	-3.58026462	2.60518341	-3.15095017
C	-4.14384154	3.85642507	-3.86876155
C	1.73719820	2.04061514	4.15688954
C	0.70766345	2.97870516	3.47655675
C	-0.09311012	3.78631667	4.53252294
H	3.34309998	-3.27775180	0.75021411
H	1.36885840	-4.13272040	1.52442416
H	-3.35084867	3.26669220	0.73550245
H	-1.38283384	4.13853587	1.50669931
H	6.27539213	-2.17464335	-3.48371708
H	7.87990343	-1.11064873	-1.91979164
H	7.12328871	-0.29471942	0.29668199
H	2.68231718	-2.93959989	-2.59010029
H	-0.50367389	-4.24086754	-1.48300007

H	3.99599996	-1.17342455	-4.72587567
H	2.62337491	-0.73534990	-3.66622864
H	2.42902229	-2.00467586	-4.88339205
H	4.97817549	-3.65364566	-4.51292963
H	3.35324523	-4.34613721	-4.46783667
H	4.48394392	-4.65231816	-3.12913189
H	-3.51433281	-4.53819662	-1.98734971
H	-2.29071249	-4.06708812	-3.19125271
H	-2.60754553	-3.01130608	-1.80468912
H	-0.45192255	-6.76833810	-1.27412993
H	-0.90585190	-6.19804060	-2.89622588
H	-2.14597414	-6.82649748	-1.80263560
H	-3.32061614	-6.26160574	0.01891097
H	-3.89467075	-6.24317693	2.43272430
H	-2.69250208	-4.74066978	3.99626948
H	3.52395119	-0.46862683	1.47997118
H	-0.01350056	-2.29251335	2.95540652
H	5.99199295	1.35968961	1.44511557
H	4.53421689	1.54885789	2.43949363
H	4.42450763	1.70227875	0.67697363
H	6.35891043	-1.02666706	2.56133059
H	5.03341319	-2.20468810	2.53774380
H	4.89786576	-0.73722589	3.52871234
H	-2.21253631	-1.36037893	3.41305969
H	-1.20989179	-1.33706537	4.87040745
H	-2.50377946	-2.54715214	4.71854787
H	-0.57795135	-4.37940843	5.15696996
H	0.61597610	-3.06770369	5.21925212
H	0.82872416	-4.41436933	4.07935303
H	-7.11210561	0.25631422	0.28693916
H	-7.86814358	1.05234931	-1.93690409
H	-6.26694112	2.11877461	-3.50271568
H	-3.51764865	0.46233284	1.47873807
H	0.48711312	4.24146262	-1.50156736
H	-5.97551871	-1.37995539	1.45137745
H	-4.51902359	-1.55409680	2.45013837
H	-4.40450782	-1.71919350	0.68907969
H	-5.03862290	2.19731348	2.52120396
H	-4.89839122	0.73728624	3.52252505
H	-6.35819678	1.01279080	2.54917063
H	3.49637020	4.54985196	-2.00745886
H	2.27552370	4.06459990	-3.20864947
H	2.59642694	3.02008512	-1.81468638
H	0.42226293	6.77024906	-1.31206516
H	0.87803041	6.18933066	-2.92987711
H	2.11561714	6.83302102	-1.84239454
H	3.29057553	6.29163856	-0.01459112
H	3.86470532	6.29485390	2.39910494
H	2.67417612	4.79444840	3.97349331
H	-2.68231084	2.91572549	-2.60375138
H	0.01364563	2.31868801	2.94968453
H	-3.97896765	1.13006430	-4.73366496

H	-2.60493405	0.70732797	-3.66968184
H	-2.41814564	1.97243869	-4.89246792
H	-3.35962064	4.30891894	-4.48917796
H	-4.49568161	4.61282997	-3.15448207
H	-4.97922149	3.60403168	-4.53473251
H	2.22283053	1.40706783	3.40746100
H	1.22153069	1.38051716	4.86574273
H	2.50450276	2.60152251	4.70775870
H	-0.84327674	4.43842351	4.06389143
H	0.56606179	4.42220398	5.13849330
H	-0.61627077	3.10061755	5.21146813
O	-0.27599306	-0.68465676	-2.51658503
O	0.30536354	0.68825781	-2.51162924
O	0.00961087	0.01371387	2.20588783
O	1.14336342	-0.26255213	1.26192165
Hf	0.00482613	0.00147028	-0.56221820
O	-1.94513714	0.91959209	-1.09079087
O	1.95501348	-0.92842324	-1.08653315

Peroxo η^3 -Ozone ComplexFig. S95: ONCCNO Peroxo η^3 -Ozone Complex

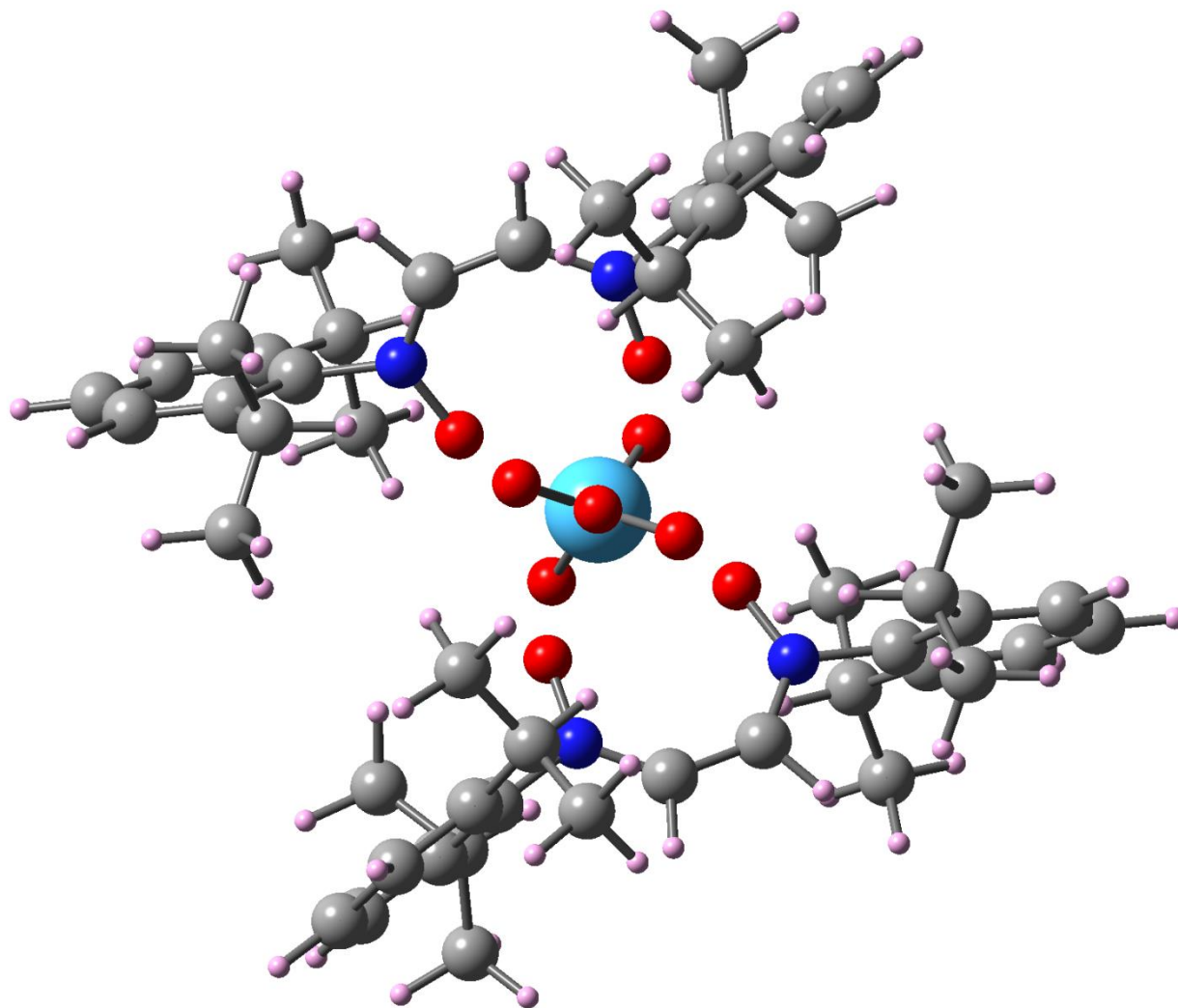
E	E_{zp}	H	G
-2969.2377	-2968.0719	-2967.9973	-2968.1864
O	-1.75892933	-0.81327487	-0.19259609
O	2.48799811	0.52541708	-0.71417474
O	0.38525178	2.00162722	-1.49502840
N	1.74122197	-2.08198056	1.19740422
N	3.56247155	0.33062413	0.04228029
N	-2.48666810	2.30443659	0.01160736
N	-2.72759031	-0.71940580	-1.13403848
C	2.87398654	-1.53859071	1.62106823
C	3.70424419	-0.51345202	1.06838669
C	-3.33636568	1.70771257	-0.84030890
C	-3.40742391	0.39515988	-1.39214926
C	1.16417871	-3.25019642	1.87153108
C	0.75888464	-3.16497855	3.23126443
C	0.23042800	-4.33889809	3.81236760
C	0.10014696	-5.52646202	3.08041148
C	0.51532524	-5.57537281	1.74099545
C	1.06879339	-4.44630033	1.10500672
C	-0.51302215	-1.51345072	4.69423616

C	0.86220434	-1.90145912	4.09560029
C	1.91892510	-2.08676261	5.21802267
C	2.77679307	4.01557245	0.49289937
C	3.68275777	2.99976947	1.24278873
C	4.27508918	3.62457478	2.52972550
C	4.69804072	1.20222449	-0.31332952
C	4.76453975	2.47830030	0.29238609
C	5.85422562	3.29613777	-0.07850047
C	6.80204431	2.85853182	-1.01636968
C	6.67604741	1.59757921	-1.62348632
C	5.60966461	0.73665577	-1.29110876
C	0.34050161	-4.64277278	-1.31539917
C	1.55032280	-4.56985497	-0.34667533
C	2.49512194	-5.78376064	-0.54171983
C	4.59875569	-0.33275908	-3.34013708
C	5.40055974	-0.58838443	-2.03155087
C	6.72121158	-1.33892757	-2.32415140
C	-2.84305403	3.64071336	0.53121735
C	-2.50546915	4.77307765	-0.24442042
C	-2.87599538	6.02993152	0.28242740
C	-3.51405627	6.13351929	1.52802511
C	-3.79091456	4.98310833	2.28579382
C	-3.45873791	3.69965150	1.80520694
C	-0.52193209	5.58787320	-1.61973159
C	-1.77286525	4.67474265	-1.58682965
C	-2.72781823	5.00706875	-2.76452313
C	-3.04287655	-3.61017716	1.46201393
C	-3.97025352	-2.71284170	0.60271571
C	-5.45972636	-2.92553451	0.97812139
C	-3.13652911	-1.98988280	-1.75187943
C	-3.72478218	-2.95494793	-0.89122655
C	-4.10951573	-4.18085730	-1.46923936
C	-3.92747531	-4.42420029	-2.83983435
C	-3.35760614	-3.44169868	-3.66103545
C	-2.93984393	-2.19627593	-3.14135248
C	-2.53262844	2.28674691	3.68710030
C	-3.69220321	2.45220886	2.66396706
C	-5.06744198	2.46337544	3.37497381
C	-1.10380001	-1.74062720	-4.84910024
C	-2.32525939	-1.16217945	-4.09213163
C	-3.39289899	-0.63071961	-5.08755582
H	3.27636718	-1.99403742	2.51849628
H	4.65798809	-0.40222893	1.57219500
H	-4.15373797	2.35586057	-1.13250978
H	-4.20746363	0.25902644	-2.11061912
H	-0.09232092	-4.31268693	4.84935493
H	-0.31910440	-6.41214423	3.55208090
H	0.42305855	-6.50399305	1.18499941
H	1.14553507	-1.05511280	3.46751486
H	3.03031607	2.17598170	1.55108888
H	-0.91992550	-2.29446633	5.35129816
H	-1.22419213	-1.30973078	3.88776084

H	-0.40840749	-0.59380994	5.28435550
H	1.63540059	-2.89244755	5.90859165
H	2.01231523	-1.16080382	5.80003422
H	2.91218276	-2.33510202	4.81659552
H	3.35068381	4.89574076	0.16949401
H	1.97099835	4.35051314	1.15833722
H	2.31748596	3.55375857	-0.38850915
H	4.92220061	2.91515764	3.06301049
H	3.45983655	3.91390631	3.20470327
H	4.86512404	4.52639781	2.31751360
H	5.95195455	4.28366049	0.36355422
H	7.63263255	3.50633348	-1.28725812
H	7.40518005	1.28586973	-2.36525085
H	2.10792154	-3.66898954	-0.61609812
H	4.78390220	-1.24676291	-1.40633803
H	-0.28848417	-5.51770874	-1.10023334
H	0.69139331	-4.72194886	-2.35284215
H	-0.27087499	-3.73933044	-1.23018566
H	1.97667769	-6.73975998	-0.39270584
H	3.34590626	-5.74978185	0.15181851
H	2.88972845	-5.78178067	-1.56639113
H	3.62460729	0.11705845	-3.12097654
H	4.42826132	-1.27967254	-3.86966987
H	5.15405015	0.33884603	-4.00900695
H	7.34368717	-0.80058761	-3.05031323
H	6.49953685	-2.32358858	-2.75536274
H	7.31482214	-1.48921183	-1.41277860
H	-2.64745466	6.93026067	-0.28095647
H	-3.78501525	7.11258086	1.91626649
H	-4.26531183	5.08309005	3.25748844
H	-1.39764565	3.65521573	-1.71998008
H	-3.71089390	-1.67765163	0.84454338
H	-0.78393818	6.65295253	-1.55740841
H	0.02355023	5.42599909	-2.55734055
H	0.15666841	5.34564051	-0.79448453
H	-3.59574731	4.33381457	-2.78807794
H	-2.19604882	4.90389264	-3.71881048
H	-3.10551471	6.03639399	-2.69416402
H	-3.22938026	-4.67577193	1.27117720
H	-3.21600058	-3.42136879	2.52954497
H	-1.99184089	-3.39725732	1.24432702
H	-6.12254373	-2.28781225	0.37826425
H	-5.61528728	-2.68023673	2.03694322
H	-5.77284335	-3.96713241	0.83113322
H	-4.56253299	-4.94515001	-0.84369156
H	-4.23231163	-5.37678831	-3.26675074
H	-3.22267171	-3.64210971	-4.72008021
H	-3.66764876	1.56708767	2.01596665
H	-1.94143326	-0.31810269	-3.51613385
H	-2.45894478	3.17094388	4.33520847
H	-1.57778193	2.13390552	3.17422503
H	-2.71672636	1.40957525	4.32149707

H	-5.22635945	1.50496271	3.88575614
H	-5.89220864	2.61545174	2.66619339
H	-5.12560648	3.25043815	4.13773390
H	-0.32727464	-2.03349382	-4.13648798
H	-0.67628725	-0.96701834	-5.49940984
H	-1.37317053	-2.60183640	-5.47614123
H	-4.25554895	-0.18727291	-4.56971656
H	-3.77335733	-1.43249555	-5.73446535
H	-2.95079187	0.14080638	-5.73064469
O	1.14421497	0.87053718	1.56591554
O	-0.06486200	-0.00055268	1.89230757
O	-0.56428145	0.99316288	-2.15891567
O	0.22622767	-0.32175376	-2.23729524
Hf	0.19156748	0.29141550	-0.17546980
O	-1.35863496	1.82851045	0.50580823
O	1.15526176	-1.70905311	0.02132125

8.7 Ten Oxygen Atoms

Bis- η^2 -ozone ComplexFig. S96: ONCCNO Bis- η^2 -ozone Complex

E	E_{ZP}	H	G
-3044.3955	-3043.2266	-3043.1512	-3043.3417
O	0.67305741	2.03428607	-0.01122002
O	-0.67032924	-2.01655769	-0.01219173
O	-1.09362282	0.36594322	1.39496432
N	2.65643894	-2.01714426	-0.42985018
N	-0.27509206	-3.15306658	0.53961059
N	-2.65351867	1.99819654	-0.43898175
N	0.26345877	3.16984253	0.53125892
C	2.24795828	-3.12026858	0.20232850
C	0.98280372	-3.60420874	0.63747544
C	-2.25943675	3.10581862	0.19413195

C	-1.00011232	3.60638098	0.62709600
C	4.08109785	-1.85715298	-0.75627749
C	4.47086353	-2.06869462	-2.10178729
C	5.84205973	-1.91617576	-2.39463199
C	6.76273575	-1.56760899	-1.39301542
C	6.33025945	-1.33866735	-0.07759977
C	4.96835480	-1.46151494	0.27313225
C	3.24176875	-1.15459746	-4.11239194
C	3.47167844	-2.40094056	-3.21400881
C	3.91561351	-3.62596715	-4.05250485
C	-2.95746479	-3.75323862	-2.14182372
C	-1.85589813	-4.59811630	-1.44631906
C	-1.71793136	-5.99307866	-2.10731698
C	-1.38132000	-3.99293351	1.02634915
C	-2.13379734	-4.70033222	0.05711146
C	-3.19796635	-5.49186340	0.53658051
C	-3.48597381	-5.56186816	1.90966354
C	-2.72868716	-4.82648864	2.83443260
C	-1.65880890	-4.00684137	2.41341426
C	4.95807902	0.26552699	2.14075237
C	4.50679891	-1.15110044	1.70194417
C	5.02326062	-2.22220036	2.69970838
C	-1.82266320	-2.16714472	4.15495116
C	-0.88322901	-3.16912739	3.43575181
C	-0.14133828	-4.07273680	4.45537899
C	-4.07519452	1.81754004	-0.76580870
C	-4.95945773	1.41808815	0.26481647
C	-6.31913657	1.27543919	-0.08744040
C	-6.75208754	1.48901002	-1.40518219
C	-5.83413313	1.84248881	-2.40760261
C	-4.46568770	2.01530945	-2.11349572
C	-4.93333082	-0.29469592	2.14525997
C	-4.49764360	1.12382153	1.69706697
C	-5.02947292	2.19590659	2.68569634
C	2.92510604	3.80418901	-2.16374785
C	1.81339044	4.63364538	-1.46574912
C	1.65057436	6.02457005	-2.12976468
C	1.35940889	4.02743000	1.01061568
C	2.09603371	4.74417180	0.03615411
C	3.15030405	5.55295210	0.50867422
C	3.44427069	5.63011022	1.88007683
C	2.70347568	4.88458968	2.81007433
C	1.64426289	4.04772389	2.39601608
C	-3.20794356	1.10175572	-4.10681272
C	-3.46925234	2.35461206	-3.22607531
C	-3.93530747	3.55827624	-4.08324119
C	1.85049826	2.20650812	4.12982362
C	0.88947098	3.19713701	3.42325107
C	0.14541304	4.08712440	4.45304012
H	3.06556825	-3.79833846	0.41953123
H	1.03209297	-4.57010359	1.12679830
H	-3.08562382	3.77305635	0.41251987

H	-1.06064080	4.57369182	1.11234645
H	6.18922377	-2.06870311	-3.41264308
H	7.81615699	-1.46108094	-1.64147468
H	7.05087837	-1.04423094	0.68047628
H	2.50099660	-2.64079665	-2.76622806
H	-0.91469325	-4.06047131	-1.60407932
H	4.18084486	-0.82969751	-4.58238967
H	2.82470815	-0.32764136	-3.52957615
H	2.52169559	-1.39333788	-4.90486161
H	4.84007388	-3.42647965	-4.60995331
H	3.13700203	-3.87154718	-4.78587501
H	4.08479952	-4.50993185	-3.42279588
H	-3.94989796	-4.20516382	-2.00582391
H	-2.75120460	-3.68371692	-3.21691926
H	-2.96947938	-2.73422956	-1.74294777
H	-0.94030939	-6.59702945	-1.62081817
H	-1.44921620	-5.87656283	-3.16494435
H	-2.65831532	-6.55783054	-2.06634836
H	-3.80396930	-6.05360638	-0.16875477
H	-4.30910233	-6.18174215	2.25747584
H	-2.97696005	-4.87518656	3.89119056
H	3.41187562	-1.14635616	1.73612763
H	-0.13870078	-2.55703486	2.91745279
H	6.05194439	0.35709946	2.17381849
H	4.57235058	0.48157866	3.14499736
H	4.56773814	1.02876812	1.45792791
H	6.12108817	-2.24350186	2.72889166
H	4.67821339	-3.22975644	2.43025329
H	4.66182880	-2.00059597	3.71223023
H	-2.25915868	-1.47213575	3.43072551
H	-1.24662567	-1.57480010	4.87686130
H	-2.63049106	-2.67894212	4.69615747
H	-0.84527467	-4.66934762	5.05076431
H	0.44417922	-3.45437951	5.14764879
H	0.54666436	-4.76886341	3.95617817
H	-7.03742721	0.97757618	0.67151325
H	-7.80356935	1.36701762	-1.65474884
H	-6.18144497	1.98364608	-3.42714152
H	-3.40281812	1.13234307	1.73385191
H	0.88011169	4.08084748	-1.61818714
H	-6.02608001	-0.39931530	2.17490317
H	-4.54906228	-0.49828371	3.15265453
H	-4.53104355	-1.05846868	1.47001789
H	-4.69587202	3.20562155	2.40995895
H	-4.66809511	1.98592076	3.70071367
H	-6.12755435	2.20429585	2.71193267
H	3.91132467	4.27022737	-2.03029737
H	2.71718326	3.73146365	-3.23832604
H	2.95212793	2.78542801	-1.76503855
H	0.86603113	6.61771086	-1.64104792
H	1.37853407	5.90107538	-3.18576087
H	2.58223024	6.60412445	-2.09501821

H	3.74425471	6.12214267	-0.20090353
H	4.25957783	6.26321486	2.22243727
H	2.95672135	4.93875771	3.86538194
H	-2.50626753	2.62201164	-2.77720511
H	0.14818434	2.57643363	2.91053963
H	-4.13807352	0.74981915	-4.57514876
H	-2.77393743	0.29231480	-3.51187887
H	-2.49097305	1.34627132	-4.90038030
H	-3.15711028	3.81197627	-4.81427639
H	-4.12913989	4.44620359	-3.46633906
H	-4.85066330	3.33065401	-4.64488900
H	2.29050213	1.52054406	3.39906671
H	1.29036265	1.60326997	4.85520734
H	2.65576390	2.72893377	4.66463467
H	-0.55675186	4.77529110	3.96270755
H	0.84672406	4.69125262	5.04394807
H	-0.42475608	3.45827627	5.14867434
O	-0.61738624	-0.96265531	-2.27334533
O	0.66497593	0.97230290	-2.26195223
O	0.00799125	0.01170522	2.34262299
O	1.10825402	-0.34922120	1.39531426
Hf	0.00949668	0.00560113	-0.45392923
O	-1.86754463	1.01991592	-0.89765129
O	1.88684050	-1.02530753	-0.88387656
O	0.03331114	0.00420049	-3.20839914

9. Triplet Ground States for ONCCNO Complex

9.1 Four Oxygen Atoms

Bare Complex

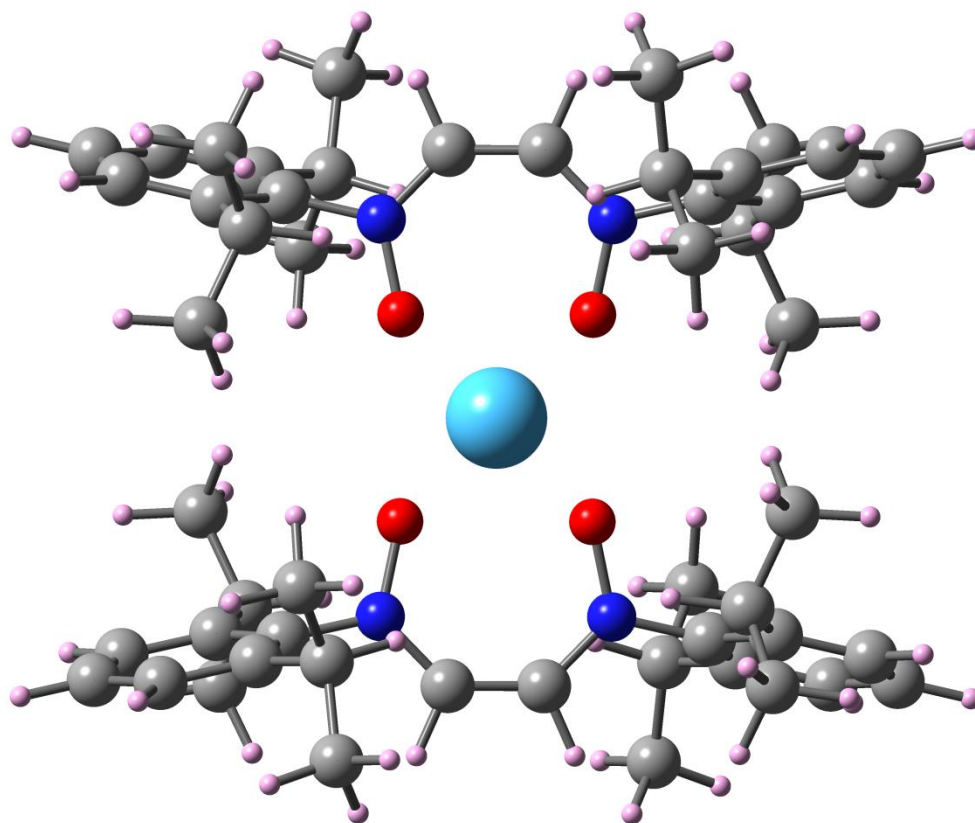


Fig. S97: ONCCNO Bare Complex

E	E_{zp}	H	G
-2593.3220	-2592.1744	-2592.1044	-2592.2900
O	1.36845909	1.46428969	0.10423040
O	-1.36834930	-1.46418700	0.10435667
N	1.63432811	-2.81946158	-0.26829688
N	-1.64921394	-2.81136532	0.27208658
N	-1.63436601	2.81945724	-0.26785899
N	1.64913762	2.81144642	0.27238809
C	0.67388400	-3.79973592	-0.10883029
C	-0.69366837	-3.79630286	0.11222527
C	-0.67393734	3.79976601	-0.10872947
C	0.69362638	3.79637479	0.11231111
C	3.01632507	-3.13090574	-0.55465303
C	3.38750629	-3.46036655	-1.88507559
C	4.74068424	-3.77512974	-2.13303539
C	5.69161173	-3.73735736	-1.10135715
C	5.30584543	-3.38409906	0.20213462

C	3.96279891	-3.07760507	0.50296941
C	2.76706397	-2.41372415	-4.11666632
C	2.38043699	-3.46031984	-3.03881431
C	2.23095694	-4.87071719	-3.66659907
C	-4.19898070	-1.32176197	-2.34329101
C	-3.56735569	-2.67776749	-1.93216487
C	-3.92786776	-3.79100739	-2.94955131
C	-3.03370681	-3.11629741	0.55356344
C	-3.97610593	-3.05855631	-0.50743375
C	-5.32160544	-3.35896351	-0.21142261
C	-5.71364498	-3.71023618	1.09073334
C	-4.76664327	-3.75209248	2.12586214
C	-3.41113066	-3.44375360	1.88267105
C	4.20091416	-1.34312445	2.33914465
C	3.56091947	-2.69555504	1.92932340
C	3.91925563	-3.81136079	2.94469596
C	-2.79228039	-2.39535155	4.11345008
C	-2.40823801	-3.44740274	3.03996565
C	-2.26985036	-4.85695946	3.67210852
C	-3.01635173	3.13074926	-0.55443190
C	-3.96291452	3.07751367	0.50311511
C	-5.30594867	3.38392081	0.20212899
C	-5.69161009	3.73703234	-1.10143136
C	-4.74059032	3.77474246	-2.13303013
C	-3.38742692	3.46004555	-1.88492599
C	-4.20118050	1.34314531	2.33935071
C	-3.56115346	2.69556461	1.92952830
C	-3.91958683	3.81140086	2.94482892
C	4.19864666	1.32294521	-2.34367704
C	3.56713814	2.67886699	-1.93209224
C	3.92770433	3.79241254	-2.94912709
C	3.03363878	3.11641906	0.55384189
C	3.97595676	3.05915300	-0.50724982
C	5.32146590	3.35948720	-0.21120714
C	5.71358396	3.71020552	1.09107565
C	4.76665534	3.75159558	2.12629109
C	3.41113254	3.44333760	1.88305673
C	-2.76678605	2.41389378	-4.11677205
C	-2.38020237	3.46008889	-3.03853253
C	-2.23042633	4.87065974	-3.66589677
C	2.79256115	2.39431790	4.11364411
C	2.40828110	3.44650700	3.04038662
C	2.26963424	4.85591472	3.67281398
H	1.11045866	-4.79027721	-0.18835685
H	-1.13524373	-4.78467497	0.19114897
H	-1.11052029	4.79029083	-0.18841738
H	1.13520878	4.78475320	0.19111186
H	5.05379845	-4.03753864	-3.14080101
H	6.73123759	-3.97714090	-1.31324408
H	6.05235450	-3.35246316	0.99205284
H	1.40278069	-3.16825705	-2.64138135
H	-2.48054815	-2.54659042	-1.95150326

H	3.73512135	-2.64938280	-4.57842152
H	2.83467625	-1.41039112	-3.67925172
H	2.01068324	-2.39188993	-4.91270164
H	3.17590800	-5.21498631	-4.10755907
H	1.47481190	-4.85564051	-4.46280811
H	1.92152008	-5.61037953	-2.91693010
H	-5.29623689	-1.37456633	-2.34131470
H	-3.87723373	-1.04495344	-3.35657599
H	-3.89236631	-0.52596583	-1.65528380
H	-3.46590967	-4.74791573	-2.67403444
H	-3.57272713	-3.51616481	-3.95182439
H	-5.01305536	-3.94653479	-3.01214963
H	-6.06513662	-3.32401926	-1.00399202
H	-6.75511787	-3.94518156	1.29894029
H	-5.08460043	-4.01271485	3.13256578
H	2.47488460	-2.55888154	1.95255751
H	-1.42730672	-3.16256569	2.64531757
H	5.29787285	-1.40151482	2.33308425
H	3.88432883	-1.06542929	3.35380846
H	3.89584304	-0.54525474	1.65284209
H	5.00385871	-3.97231719	3.00362118
H	3.45165962	-4.76575032	2.66995115
H	3.56873594	-3.53555626	3.94832797
H	-2.85236388	-1.39297362	3.67278203
H	-2.03858389	-2.37564428	4.91208457
H	-3.76339957	-2.62386606	4.57240274
H	-3.21825753	-5.19408186	4.11116560
H	-1.51611345	-4.84445579	4.47064066
H	-1.96284409	-5.60069003	2.92547222
H	-6.05252210	3.35233171	0.99198728
H	-6.73122346	3.97675791	-1.31344459
H	-5.05363414	4.03706142	-3.14084064
H	-2.47511601	2.55890725	1.95285711
H	2.48032346	2.54776523	-1.95146065
H	-5.29813770	1.40156311	2.33322510
H	-3.88465404	1.06547511	3.35404043
H	-3.89608677	0.54525810	1.65308290
H	-3.45201137	4.76579845	2.67007790
H	-3.56911475	3.53564171	3.94848988
H	-5.00419756	3.97232242	3.00370116
H	5.29590732	1.37565889	-2.34172568
H	3.87682711	1.04648300	-3.35703281
H	3.89199607	0.52696082	-1.65590162
H	3.46578814	4.74925477	-2.67331026
H	3.57255839	3.51790127	-3.95148797
H	5.01289882	3.94790992	-3.01166548
H	6.06494591	3.32489325	-1.00384067
H	6.75506845	3.94507565	1.29931089
H	5.08467988	4.01177229	3.13308809
H	-1.40265315	3.16776763	-2.64102855
H	1.42740389	3.16155670	2.64568131
H	-3.73472057	2.64981882	-4.57864337

H	-2.83459867	1.41042334	-3.67970494
H	-2.01026351	2.39222513	-4.91267515
H	-1.47420603	4.85569594	-4.46203695
H	-1.92095010	5.61005609	-2.91598516
H	-3.17529872	5.21517059	-4.10683730
H	2.85289036	1.39204676	3.67276684
H	2.03886485	2.37425210	4.91227050
H	3.76361922	2.62296653	4.57266106
H	1.96246310	5.59972730	2.92632901
H	3.21799361	5.19312906	4.11190377
H	1.51592373	4.84311356	4.47136553
Hf	0.00008289	-0.00000479	0.00501398
O	-1.36049568	1.47129678	-0.09654093
O	1.36059624	-1.47127534	-0.09693578

9.2 Five Oxygen Atoms

Oxo Complex

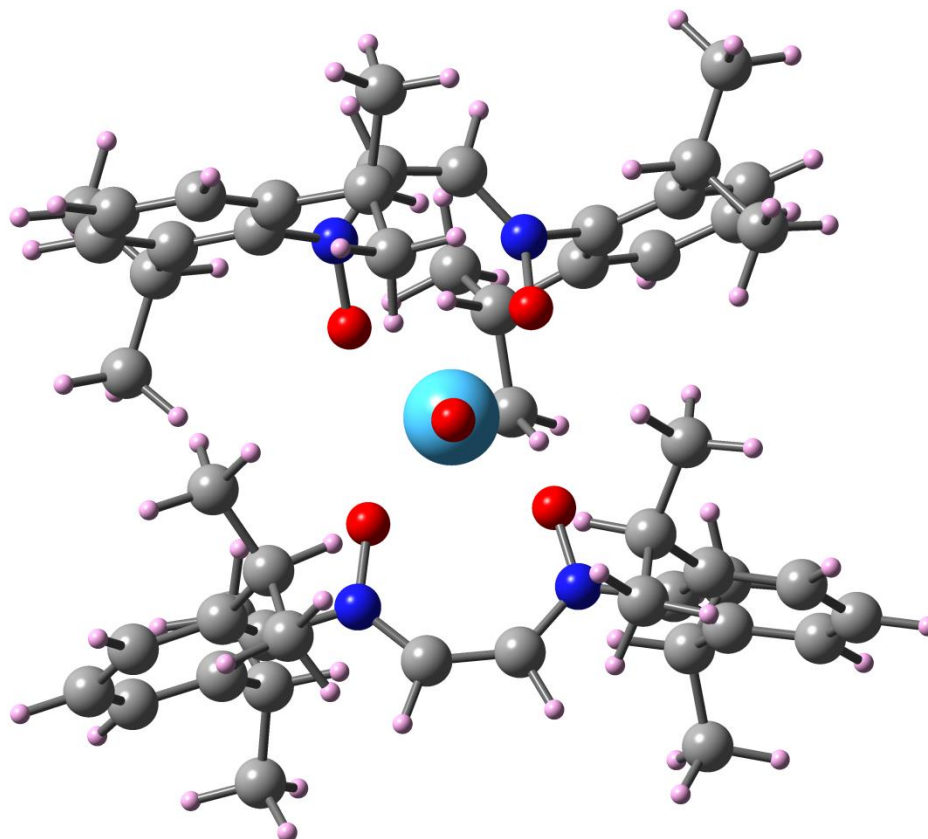


Fig. S98: ONCCNO Oxo Complex

E	E_{zp}	H	G
-2668.6327	-2667.4816	-2667.4106	-2667.5983
N	-1.63865096	-2.60524622	-0.53803814
N	1.51600990	2.84100936	0.08066505
C	-0.64915587	-3.53984017	-0.57242916
C	0.70008822	-3.55364471	-0.19532481
C	0.65339236	3.86799483	0.30856954
C	-0.68317519	3.82116865	0.71671793
C	-2.95489282	-2.88560698	-1.08984911
C	-3.97319311	-3.33077484	-0.21002802
C	-5.23585425	-3.61782496	-0.76840172
C	-5.46794179	-3.45736345	-2.14445947
C	-4.44659408	-2.98884954	-2.98589273
C	-3.16707401	-2.67831455	-2.47617218
C	-4.58697001	-2.43360799	2.07845982
C	-3.74180598	-3.47394781	1.29643807
C	-4.03145342	-4.91374050	1.79230214
C	2.57640756	-2.35787767	4.01687961
C	2.34266763	-3.52107673	3.01456649

C	2.39511995	-4.89292199	3.73173852
C	2.95229733	-2.96134825	0.57330351
C	3.33898091	-3.42405877	1.85658798
C	4.69800387	-3.74750855	2.04809111
C	5.62533265	-3.60962037	1.00174456
C	5.21604767	-3.12400578	-0.25008005
C	3.86997819	-2.77241240	-0.49024834
C	-2.55081931	-0.85677664	-4.14444243
C	-2.07713871	-2.13411931	-3.40501143
C	-1.61701556	-3.21608446	-4.41793979
C	4.30376239	-0.97646654	-2.24402088
C	3.44758248	-2.20678254	-1.85020709
C	3.51487058	-3.29793049	-2.95178212
C	2.81943228	3.01821543	-0.52673209
C	2.90113788	3.25032712	-1.92552843
C	4.19000358	3.40551033	-2.48106105
C	5.34081463	3.30830004	-1.68564234
C	5.22911106	3.06134711	-0.30707127
C	3.96801207	2.91737331	0.30443052
C	1.71905860	2.24998889	-3.95208553
C	1.67396038	3.33128774	-2.84060411
C	1.52912945	4.75504921	-3.44234285
C	-1.94394386	0.44160745	3.76437510
C	-1.76529042	1.96469591	3.51504480
C	-1.53217018	2.72114247	4.84637424
C	-2.86103447	2.87296673	1.36182510
C	-2.95970985	2.51528663	2.73032731
C	-4.22729102	2.62151383	3.34015358
C	-5.34572190	3.05205959	2.60836202
C	-5.22273856	3.37181538	1.24638047
C	-3.97727424	3.28262919	0.59023418
C	4.35789957	1.22518466	2.15125628
C	3.87138459	2.65871277	1.81089098
C	4.64893378	3.72125280	2.62952379
C	-4.61348485	2.50277648	-1.73132686
C	-3.86632254	3.58444345	-0.90611811
C	-4.38052640	5.00487994	-1.25309995
H	-0.99009341	-4.46858503	-1.01764263
H	1.20118901	-4.49460431	-0.39680065
H	1.08893032	4.85280357	0.17280687
H	-1.11456756	4.75081381	1.07444365
H	-6.04023211	-3.96618430	-0.12535254
H	-6.44705691	-3.68803371	-2.55842579
H	-4.64547137	-2.85096292	-4.04553943
H	-2.68982665	-3.25306299	1.50584262
H	1.33195097	-3.39500121	2.61074176
H	-5.66230653	-2.59719484	1.92608696
H	-4.34590893	-1.41518000	1.75292007
H	-4.38251572	-2.50949767	3.15500543
H	-5.08512270	-5.18649436	1.64802417
H	-3.80987612	-4.99749831	2.86465871
H	-3.41786997	-5.65103526	1.25849135

H	3.57753970	-2.41773676	4.46510309
H	1.83708482	-2.40044200	4.82818497
H	2.48064642	-1.39109253	3.51017829
H	2.22554270	-5.71942147	3.02953963
H	1.62096076	-4.94059086	4.50907632
H	3.36349822	-5.05994225	4.22122020
H	5.03288957	-4.10773896	3.01733801
H	6.66834714	-3.87126437	1.16581589
H	5.94806864	-3.00454254	-1.04439798
H	-1.20650329	-1.83584294	-2.81231200
H	2.41247391	-1.85492263	-1.79027252
H	-3.38856578	-1.06200303	-4.82528768
H	-1.72143349	-0.44625000	-4.73306593
H	-2.86460818	-0.08654213	-3.43004651
H	-2.44134727	-3.53025527	-5.07312634
H	-1.23544700	-4.10965258	-3.90599302
H	-0.81278183	-2.81886721	-5.05043030
H	4.26058125	-0.20157324	-1.46982747
H	3.91594192	-0.54104336	-3.17303236
H	5.35714636	-1.24344837	-2.40698375
H	4.53942880	-3.67288093	-3.08254069
H	3.17928209	-2.88321042	-3.91093160
H	2.87128067	-4.15412302	-2.70988052
H	4.28996967	3.58742625	-3.54790968
H	6.32346106	3.42015495	-2.13839890
H	6.12852708	2.98778213	0.29885864
H	0.77687009	3.12530429	-2.24860662
H	-0.86213331	2.08869387	2.90742644
H	2.63571922	2.32149005	-4.55347379
H	0.86228091	2.37888225	-4.62791125
H	1.64236305	1.25143749	-3.50780240
H	1.46812572	5.52257526	-2.65869462
H	0.61821769	4.81599855	-4.05215247
H	2.38185012	5.00377779	-4.08807166
H	-2.81894582	0.24638862	4.39902851
H	-1.05809930	0.03446060	4.26989952
H	-2.08180607	-0.10292932	2.82222789
H	-1.38938200	3.79598014	4.67578649
H	-0.63542824	2.33270775	5.34657906
H	-2.37604257	2.59878078	5.53806396
H	-4.34225496	2.35836799	4.38851785
H	-6.31483150	3.12746679	3.09634953
H	-6.10052387	3.68846453	0.68889249
H	2.81880620	2.71416886	2.10570781
H	-2.81104749	3.52918202	-1.19375936
H	5.40912993	1.08340778	1.86537593
H	3.75074725	0.47939268	1.62756683
H	4.27343968	1.04182052	3.23122490
H	4.50013478	3.54913267	3.70393901
H	4.30624750	4.73777724	2.39534492
H	5.72846469	3.67729184	2.43462878
H	-4.21418166	1.50621607	-1.51195151

H	-4.49155775	2.69417493	-2.80573387
H	-5.68884418	2.50122315	-1.50689787
H	-3.84193145	5.77649737	-0.68743485
H	-5.45076951	5.11322808	-1.03349482
H	-4.23960011	5.20554786	-2.32328404
O	0.44194182	-0.12457871	-1.94765336
O	-1.38188905	1.64710070	-0.06124307
O	1.17959776	-1.37041175	0.76922415
N	-1.56350943	2.77806486	0.71744320
N	1.55247956	-2.63977856	0.34643836
Hf	0.01672160	0.07088556	-0.20357728
O	-1.51512125	-1.35565022	0.05247797
O	1.26229750	1.57586281	0.61575951

9.3 Six Oxygen Atoms

Dioxo Complex (lower energy conformation)

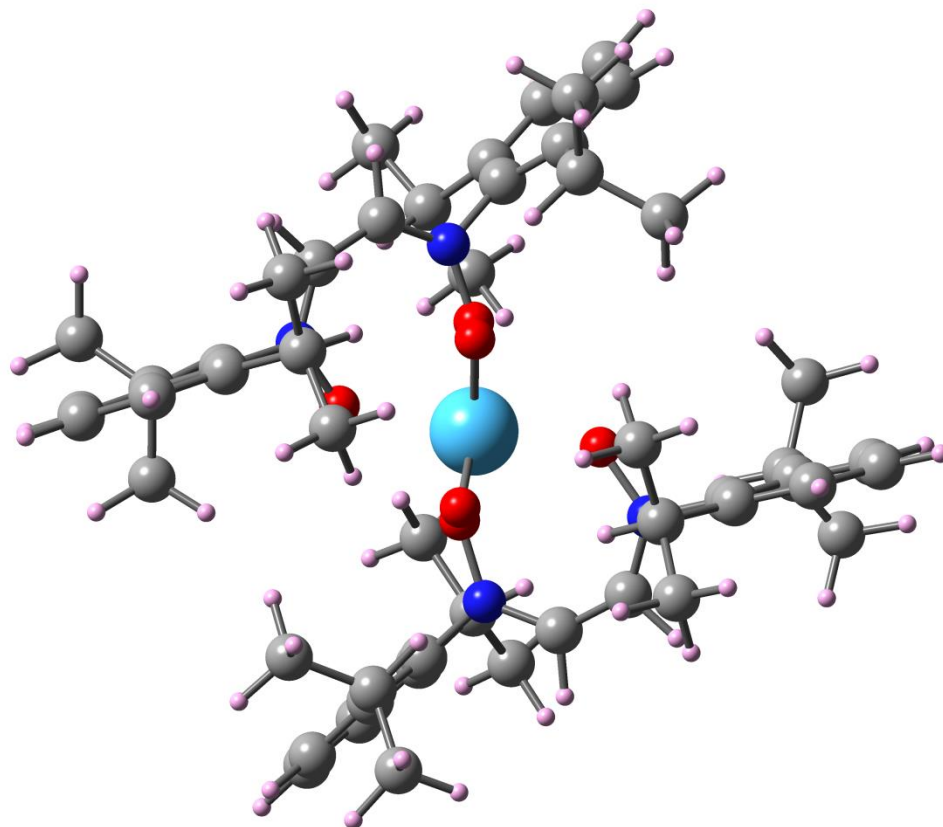


Fig. S99: ONCCNO Dioxo Complex (lower energy conformation)

E	E_{zp}	H	G
-2743.7767	-2742.6234	-2742.5506	-2742.7408

O	0.29759049	-1.48813179	1.04212412
O	2.06824254	0.56821263	-0.09942579
O	0.33786757	-1.24611024	-1.97606218
N	0.02469345	2.97382556	0.80069304
N	2.65602921	1.65983519	-0.62630461
N	-2.71769162	-1.72941391	-0.41824497
N	0.03514758	-2.83781815	1.06327178
C	1.07821659	3.48388863	0.15839583
C	2.21076722	2.90651045	-0.50323713
C	-2.26759468	-2.95084800	-0.02716886
C	-1.10825295	-3.42214661	0.60712766
C	-0.96497816	3.89433373	1.39019337
C	-2.00854392	4.36680978	0.56035970
C	-2.94591445	5.23529828	1.16232896
C	-2.84588796	5.58577416	2.51720170
C	-1.81092488	5.06707656	3.31342820
C	-0.84319993	4.19924353	2.76744570

C	-3.45851731	3.08448017	-1.07033427
C	-2.17633972	3.94355433	-0.90259161
C	-2.20015235	5.16822123	-1.85275145
C	2.31262343	0.27664131	-4.40826657
C	2.64964068	1.55934357	-3.60203581
C	2.80687405	2.78612931	-4.53878238
C	3.91790651	1.39538184	-1.33678017
C	3.90789516	1.35235313	-2.75175454
C	5.14353916	1.07880810	-3.38014146
C	6.30627068	0.84455781	-2.63209042
C	6.26654709	0.87281005	-1.22800647
C	5.06594127	1.14705955	-0.54335951
C	-0.37999759	2.42782373	4.50765331
C	0.23548575	3.57257003	3.65633786
C	0.95052022	4.61379439	4.55203901
C	5.17558258	-0.31204889	1.52348000
C	5.03122252	1.13798114	0.98846024
C	6.10842867	2.06926685	1.60070203
C	-4.01317874	-1.57645757	-1.06227218
C	-4.07873024	-1.61871913	-2.47743834
C	-5.35238646	-1.47280048	-3.06898607
C	-6.49981070	-1.28114616	-2.28328499
C	-6.39803584	-1.21749827	-0.88383951
C	-5.14908605	-1.35497020	-0.24339310
C	-2.57931481	-0.50433373	-4.19289437
C	-2.83544479	-1.78516095	-3.35502146
C	-2.94373873	-3.03414027	-4.26679183
C	0.83360130	-1.75352717	4.53364604
C	0.16773795	-3.03811376	3.96774024
C	-0.38293674	-3.92964989	5.10684977
C	1.09599725	-3.64928951	1.64386383
C	1.15148448	-3.77598677	3.05538311
C	2.18803474	-4.56404935	3.59627393
C	3.12612482	-5.19353961	2.76032523
C	3.05666629	-5.03120304	1.36814616
C	2.04529898	-4.24298664	0.77610362
C	-5.51099845	0.15340204	1.76780323
C	-5.04781399	-1.24445974	1.28056980
C	-5.84621435	-2.37088338	1.98728441
C	3.32351693	-3.37635060	-1.24182397
C	2.01533195	-4.04206855	-0.74223809
C	1.75797148	-5.38017372	-1.48295412
H	1.06514316	4.56756421	0.12961579
H	2.85276435	3.63640680	-0.98353907
H	-2.97154487	-3.73569120	-0.28477148
H	-1.09535846	-4.49714688	0.75252009
H	-3.76364263	5.62860148	0.56473354
H	-3.58180635	6.25428590	2.95775645
H	-1.75844091	5.33325628	4.36534767
H	-1.34267467	3.30183779	-1.21080255
H	1.78384066	1.74042071	-2.95588980
H	-4.36180620	3.64578200	-0.79320261

H	-3.40479282	2.17749442	-0.45761547
H	-3.55611858	2.76995425	-2.11653367
H	-3.06297407	5.81925336	-1.65784579
H	-2.26668342	4.82565365	-2.89274422
H	-1.29064261	5.77629337	-1.75338221
H	3.14469944	-0.02912314	-5.05807156
H	1.43538445	0.46468671	-5.04052907
H	2.05360636	-0.54563758	-3.73209991
H	3.03221225	3.70351872	-3.97652489
H	1.87316048	2.94887997	-5.09146133
H	3.61050675	2.63880832	-5.27330562
H	5.18522455	1.03789159	-4.46491609
H	7.24288827	0.63062876	-3.14158520
H	7.17282923	0.67751425	-0.66132577
H	0.99853769	3.11328543	3.01626613
H	4.05283575	1.50048778	1.32409086
H	-1.15947112	2.81309215	5.17855516
H	0.39598670	1.95261512	5.12227090
H	-0.82408128	1.66224624	3.86197685
H	0.26668216	5.05689714	5.28705279
H	1.38141553	5.42994083	3.95760022
H	1.76263405	4.13068486	5.11053377
H	4.36496235	-0.94502639	1.14741148
H	5.13382080	-0.31837133	2.62063901
H	6.13311045	-0.75327587	1.21639266
H	7.12351731	1.72349499	1.36739907
H	6.01015034	2.08843978	2.69400354
H	6.01084510	3.09806116	1.22968728
H	-5.44264098	-1.50381825	-4.15178521
H	-7.47115555	-1.17226688	-2.76085828
H	-7.29187183	-1.05318781	-0.28669548
H	-1.95373679	-1.91446091	-2.71983175
H	-0.68415969	-2.71125762	3.36054563
H	-3.41751579	-0.28895212	-4.87105637
H	-1.67065430	-0.63450888	-4.79366146
H	-2.41747506	0.36090475	-3.54032515
H	-3.10377801	-3.94808417	-3.67892419
H	-2.01458877	-3.15657788	-4.83780996
H	-3.77087139	-2.94660738	-4.98495486
H	1.71079124	-2.00262709	5.14683882
H	0.12181893	-1.20151623	5.16279749
H	1.15086541	-1.10007464	3.71371944
H	-0.84378691	-4.84510314	4.71371379
H	-1.14468617	-3.38109276	5.67660347
H	0.40463528	-4.22390529	5.81286455
H	2.26270325	-4.68769352	4.67332806
H	3.91488295	-5.80327628	3.19567604
H	3.79768829	-5.51101401	0.73369344
H	-3.99568679	-1.34867556	1.56592432
H	1.20543640	-3.35380644	-1.00440338
H	-6.57029753	0.32956158	1.53741244
H	-4.92075480	0.94541825	1.29226159

H	-5.38405714	0.23749145	2.85552515
H	-5.73108518	-2.29411481	3.07680358
H	-5.49580577	-3.36373415	1.67662144
H	-6.91813283	-2.30671834	1.75760585
H	3.48148926	-2.41177838	-0.74580508
H	3.25185655	-3.18694224	-2.31983582
H	4.20214538	-4.01126531	-1.06046607
H	0.81237887	-5.83902961	-1.16468198
H	2.56265617	-6.10546406	-1.29878526
H	1.70192915	-5.20322862	-2.56458856
O	-0.18459125	1.43645504	-1.82723193
Hf	-0.04545850	-0.05714054	-0.57052929
O	-2.05919159	-0.53101426	-0.18331473
O	-0.25828005	1.68051971	0.96786094

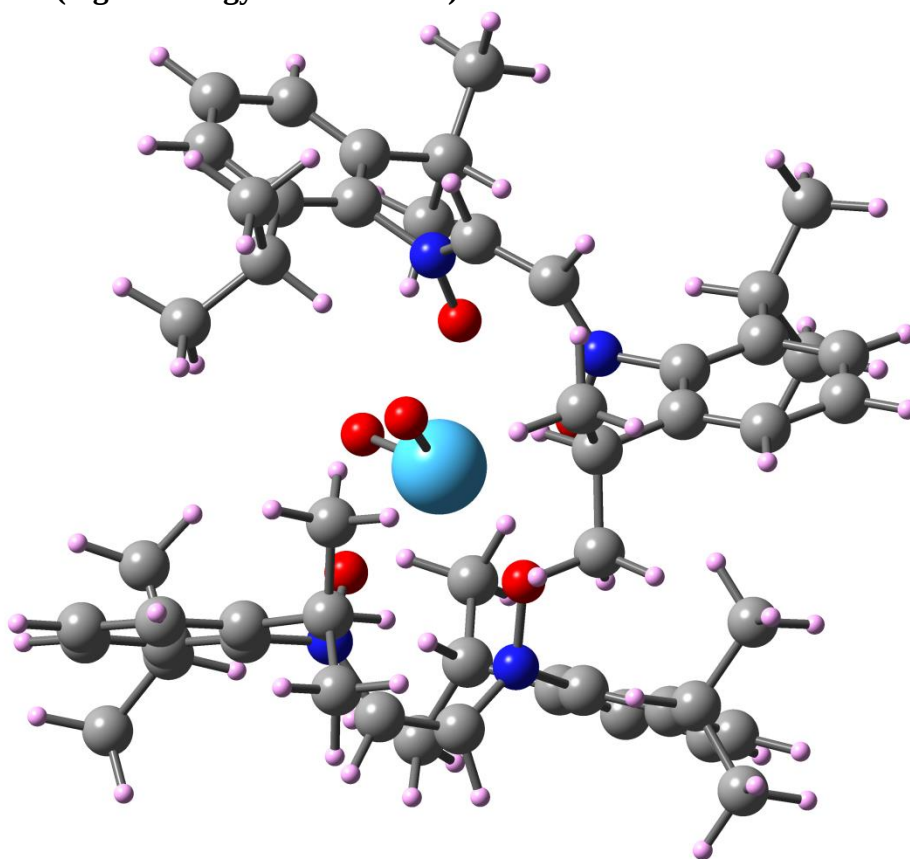
Dioxo Complex (higher energy conformation)

Fig. S100: ONCCNO Dioxo Complex (higher energy conformation)

E	E_{zp}	H	G
-2743.7604	-2742.6054	-2742.5345	-2742.7172
O	0.95209710	-1.65912404	-0.27637284
O	-0.01119988	2.27851762	-1.12250108
O	-1.47675734	0.56043605	-1.96553758
N	2.09707606	1.77929067	1.02708648
N	-0.41839230	3.26220347	-0.29335288
N	-1.97188409	-2.56624012	0.46683660
N	0.83654811	-2.94456783	-0.79929101
C	1.41088240	2.87954091	1.34640740
C	0.23167996	3.50940187	0.83294787
C	-1.22151630	-3.69794700	0.39679398
C	-0.01764876	-3.88093951	-0.28721185
C	3.38326549	1.54649562	1.71053443
C	3.35639873	0.86004003	2.94594797
C	4.59954462	0.65793482	3.58297245
C	5.79510832	1.10346229	2.99718471
C	5.77930608	1.75324051	1.75225483
C	4.56562242	1.98712590	1.07229056
C	2.09435272	-1.21920711	3.64577793

C	2.06363743	0.33089799	3.57628181
C	1.82887448	0.94892061	4.97872936
C	-4.15103690	2.23974389	1.13293298
C	-2.94472886	3.19613998	1.32822309
C	-3.12874846	4.06519116	2.59963945
C	-1.57121071	4.06345488	-0.71579220
C	-2.74570667	4.06607333	0.08091961
C	-3.80510638	4.89038500	-0.35877809
C	-3.70676690	5.64018284	-1.53831547
C	-2.54215843	5.57910822	-2.32105417
C	-1.44377485	4.78842950	-1.93206948
C	5.24789441	1.72575220	-1.35397547
C	4.56684717	2.64958588	-0.30889789
C	5.23722640	4.04688335	-0.27692771
C	-0.47981784	3.76971552	-4.02853076
C	-0.20179632	4.71477736	-2.82646864
C	0.27279006	6.10882015	-3.30675967
C	-3.24641512	-2.50377732	1.15862346
C	-4.43205774	-2.59433580	0.37903635
C	-5.66406445	-2.50973707	1.05771166
C	-5.71406213	-2.35168196	2.45281567
C	-4.52789059	-2.26254097	3.19520975
C	-3.26597636	-2.32481271	2.56413149
C	-4.77081198	-1.41939899	-1.84140639
C	-4.40386623	-2.75724973	-1.14388369
C	-5.32311788	-3.90919320	-1.62426010
C	4.41221566	-2.27031021	0.41033352
C	3.54633588	-3.53359398	0.15793215
C	4.26255916	-4.81336610	0.65631770
C	1.85222757	-3.29919468	-1.77302743
C	3.15941606	-3.61490317	-1.32037588
C	4.11788403	-3.96952782	-2.29179164
C	3.78551814	-4.00131702	-3.65650569
C	2.49082946	-3.66105720	-4.07801181
C	1.49676339	-3.29172834	-3.14626944
C	-1.94721121	-0.76380051	4.06430080
C	-1.99575707	-2.16767345	3.40503341
C	-1.87387086	-3.29855690	4.45999202
C	0.18582209	-1.64275321	-4.57295688
C	0.10537525	-2.87406064	-3.63253909
C	-0.62569032	-4.05225994	-4.32765225
H	1.87828915	3.42836946	2.15746579
H	-0.13658623	4.34988537	1.40834290
H	-1.65873304	-4.56247633	0.88512682
H	0.29699024	-4.90595159	-0.46023618
H	4.62979378	0.14213920	4.53902122
H	6.74121935	0.93550549	3.50626170
H	6.71467984	2.07542755	1.30236254
H	1.20660220	0.59664403	2.94635315
H	-2.08135246	2.53714770	1.47335408
H	2.92970221	-1.58164586	4.26058036
H	2.18643447	-1.64711333	2.64144001

H	1.16145727	-1.58953871	4.08796274
H	2.62063428	0.66625150	5.68549365
H	0.87263792	0.59857269	5.38624624
H	1.79378176	2.04583892	4.93512944
H	-5.10022057	2.78345235	1.02718527
H	-4.23308306	1.57238104	1.99970263
H	-4.00526195	1.61457533	0.24514831
H	-2.26666534	4.72499185	2.77622581
H	-3.24217680	3.41766341	3.47857394
H	-4.02218083	4.70123341	2.53258393
H	-4.72284450	4.92191276	0.22158964
H	-4.54098058	6.26063862	-1.85736332
H	-2.48611819	6.15157958	-3.24216108
H	3.53043121	2.78630869	-0.63833232
H	0.61951110	4.26529392	-2.25824608
H	6.29989537	1.54208609	-1.09866065
H	5.21656636	2.19137159	-2.34756700
H	4.73578433	0.75861768	-1.41255444
H	6.29706623	3.97838129	-0.00019503
H	4.74489321	4.71286111	0.44379229
H	5.18197610	4.51515775	-1.26817483
H	-0.77061774	2.77519695	-3.67522543
H	0.42189920	3.67246461	-4.64853065
H	-1.28609482	4.16691434	-4.66053244
H	-0.45876711	6.58653327	-3.97073941
H	1.20703300	6.00477322	-3.87413485
H	0.45741244	6.78727010	-2.46321031
H	-6.59009834	-2.57341921	0.49263417
H	-6.67587141	-2.29244749	2.95750069
H	-4.57835982	-2.12783809	4.27276066
H	-3.38019566	-2.99879358	-1.44833281
H	2.62992450	-3.41344412	0.74646410
H	-5.77315048	-1.07996475	-1.54425131
H	-4.76503903	-1.54800870	-2.93244967
H	-4.04110893	-0.64300394	-1.59026554
H	-5.07906413	-4.85590408	-1.12400468
H	-5.20406523	-4.05341419	-2.70632426
H	-6.38318887	-3.69268947	-1.43750660
H	5.34303590	-2.30627256	-0.17258092
H	4.68027651	-2.19500998	1.47275481
H	3.85640799	-1.36835091	0.13250480
H	3.65410212	-5.70978749	0.47855199
H	4.45480340	-4.73946557	1.73500317
H	5.23059687	-4.96020504	0.15932637
H	5.12819312	-4.22239769	-1.98058655
H	4.53788019	-4.28179346	-4.39039636
H	2.25175243	-3.67049868	-5.13840857
H	-1.12730805	-2.23266116	2.74108350
H	-0.49508481	-2.57606046	-2.76718843
H	-2.84259739	-0.57344785	4.67157366
H	-1.85252300	0.00684618	3.29003730
H	-1.07351319	-0.69135991	4.72751026

H	-0.92889922	-3.20294401	5.01171273
H	-1.89583424	-4.29162014	3.99122064
H	-2.69193026	-3.25560134	5.19123314
H	0.68578997	-0.80103174	-4.07991589
H	-0.82456237	-1.31094093	-4.84081613
H	0.73000022	-1.87588001	-5.49845494
H	-0.73253447	-4.91097197	-3.65198591
H	-0.08187587	-4.39067170	-5.21995746
H	-1.62929891	-3.73922461	-4.64368966
O	-0.81955441	0.80421008	1.29537687
O	1.76138163	0.78869911	0.19267367
O	-1.72360120	-1.52297956	-0.41462117
Hf	-0.32107551	0.07314459	-0.32106695

Octahedral Complex

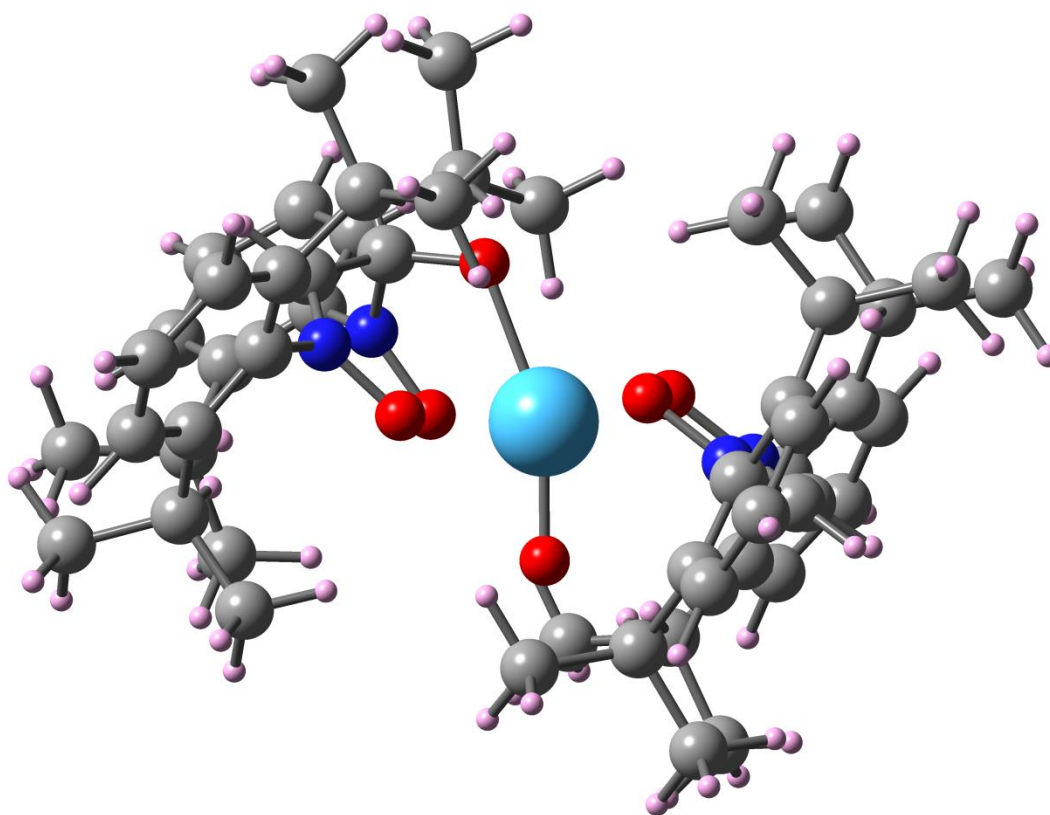


Fig. S101: ONCCNO Octahedral Complex

E	E_{zp}	H	G
-2743.8274	-2742.6722	-2742.6022	-2742.7866
O	-1.09202166	1.86887047	0.43895410
O	-0.00938228	0.92547903	-1.74602307
N	2.31393243	1.93870477	-0.51111597
N	-0.84316086	2.77893114	-0.51083598
C	1.55652857	2.67533798	-1.28981503
C	0.11480741	2.28717244	-1.62749706
C	3.76883110	2.12000333	-0.43028497
C	4.55057431	1.65004820	-1.51403905
C	5.94679798	1.83144661	-1.41553504
C	6.52117560	2.42291606	-0.28085496
C	5.71374949	2.83956312	0.79041612
C	4.31204274	2.69419170	0.74571912
C	4.54915953	-0.49499897	-2.87362116
C	3.96229000	0.93430771	-2.73583214
C	4.18973702	1.75363633	-4.03336724
C	-1.06157394	4.44920574	2.76301227
C	-0.37305902	4.91084745	1.44845818
C	0.43319487	6.21236850	1.67449819

C	-1.65141584	3.97974726	-0.58882898
C	-1.40820340	5.03665594	0.32864809
C	-2.19932629	6.19681809	0.20869008
C	-3.18930661	6.29870170	-0.78230399
C	-3.42461403	5.22972504	-1.65964506
C	-2.67085907	4.03987578	-1.57695706
C	3.44745346	1.96169453	3.00764430
C	3.44619870	3.09507762	1.94377221
C	3.87977745	4.44259677	2.57073326
C	-4.45436710	2.35373631	-2.21786811
C	-3.01315722	2.85951686	-2.49460713
C	-2.84122111	3.23056931	-3.99119524
H	2.04646162	3.49577823	-1.80424808
H	-0.17710402	2.86730477	-2.51642413
H	6.58614083	1.49214415	-2.22591011
H	7.59967132	2.54935869	-0.22478695
H	6.17648848	3.28023928	1.66798819
H	2.88192122	0.81316407	-2.60414514
H	0.33780496	4.12273212	1.16890916
H	5.63153455	-0.47394533	-3.05669917
H	4.07464576	-1.01234517	-3.71700922
H	4.36521295	-1.08370646	-1.96750608
H	3.74703955	2.75613032	-3.96175924
H	3.73277124	1.24020317	-4.88885131
H	5.25970480	1.87668794	-4.24662326
H	-1.81142579	5.18305497	3.08847630
H	-0.31807862	4.34104154	3.56383533
H	-1.55480563	3.48174846	2.62370227
H	0.89590204	6.57061567	0.74534612
H	1.22904537	6.03359644	2.40747825
H	-0.19765714	7.01857406	2.07061622
H	-2.04121729	7.02524354	0.89278013
H	-3.78479087	7.20525731	-0.86059900
H	-4.21071729	5.31178714	-2.40553712
H	2.40908235	3.20554210	1.60479119
H	-2.34233413	2.02187243	-2.27726811
H	4.46826304	1.75587401	3.35850832
H	3.01890766	1.04425742	2.59511226
H	2.83970069	2.25826907	3.87224136
H	3.17196770	4.72693707	3.35978132
H	3.90802348	5.24927991	1.82662320
H	4.87081769	4.37499418	3.03696030
H	-4.56866236	2.04531901	-1.17215502
H	-4.67558400	1.48587470	-2.85171916
H	-5.20208204	3.12909454	-2.43063012
H	-1.82122687	3.57360882	-4.21066826
H	-3.53302311	4.03014068	-4.28761326
H	-3.04608700	2.35631074	-4.62176529
O	-0.10059570	-0.54734031	1.94228721
Hf	-0.06811244	-0.24229120	0.15006208
O	1.83720186	0.92371453	0.25742408
O	-1.90176042	-1.12694674	-0.33916996

N	0.60970003	-3.28524878	0.14485508
N	-2.51210393	-2.16802730	0.34963109
C	-0.56634383	-3.79211768	0.60808211
C	-1.88342407	-3.32193586	0.70024012
C	1.83990999	-4.05343685	0.23526508
C	2.58755792	-3.99829201	1.43838218
C	3.76620690	-4.77392021	1.50066718
C	4.18696280	-5.54283725	0.40453609
C	3.43898277	-5.55263708	-0.78493900
C	2.24655686	-4.80826191	-0.89465600
C	3.29046750	-2.16168116	3.04994930
C	2.16254279	-3.13924499	2.63316126
C	1.73787592	-4.02719109	3.83275036
C	-4.41717412	-1.73883392	-2.84633415
C	-4.37339237	-2.86694689	-1.78093107
C	-5.17481141	-4.10756394	-2.24851811
C	-3.93128151	-1.97461375	0.59644511
C	-4.84674271	-2.33234200	-0.42661497
C	-6.21833031	-2.12921333	-0.17170395
C	-6.65132563	-1.59313635	1.05325114
C	-5.71994843	-1.23963005	2.04184222
C	-4.33359491	-1.41209368	1.83315420
C	2.17535460	-3.88266601	-3.24493118
C	1.45743475	-4.78600183	-2.20624210
C	1.21127919	-6.20503251	-2.77617915
C	-3.45862653	0.51126359	3.24930431
C	-3.33069985	-0.99706621	2.91341028
C	-3.49843075	-1.86335768	4.18951938
H	-0.43190239	-4.78735343	1.01935014
H	-2.56533342	-4.02141257	1.17273716
H	4.36273792	-4.76482575	2.40939425
H	5.10138830	-6.12822408	0.47312610
H	3.78257124	-6.14440229	-1.62941706
H	1.30379721	-2.51908803	2.35468124
H	-3.32416056	-3.16683036	-1.68314206
H	4.18020385	-2.69031804	3.42068133
H	2.92718586	-1.50245700	3.84798336
H	3.59040298	-1.53185838	2.20379623
H	0.91269550	-4.69951215	3.56260134
H	1.39896636	-3.39440987	4.66280242
H	2.57285149	-4.64504310	4.19205339
H	-5.44284011	-1.36963038	-2.98718617
H	-4.05196418	-2.11357205	-3.81225923
H	-3.78020611	-0.90290130	-2.53681613
H	-5.16461947	-4.90386398	-1.49277805
H	-4.73887340	-4.50904291	-3.17293818
H	-6.22223009	-3.85862247	-2.46209912
H	-6.95061775	-2.38947513	-0.93171601
H	-7.71412707	-1.44537693	1.23263816
H	-6.06739251	-0.81645386	2.98090829
H	0.48057656	-4.32954218	-2.01214509
H	-2.30969742	-1.14008973	2.54489326

H	3.17767162	-4.26821460	-3.47784320
H	2.27242913	-2.86402870	-2.85454415
H	1.59827846	-3.84222341	-4.17868226
H	0.57852900	-6.14543006	-3.67171822
H	0.70765472	-6.85007683	-2.04453909
H	2.14939445	-6.69492629	-3.06816517
H	-3.30997901	1.12230300	2.35118624
H	-2.68285115	0.79055551	3.97287637
H	-4.43941520	0.75568922	3.68211835
H	-3.37050014	-2.93145645	3.96761737
H	-4.49003215	-1.73047409	4.64469942
H	-2.74175738	-1.58028082	4.93240344
O	0.74744004	-2.05334535	-0.48915997

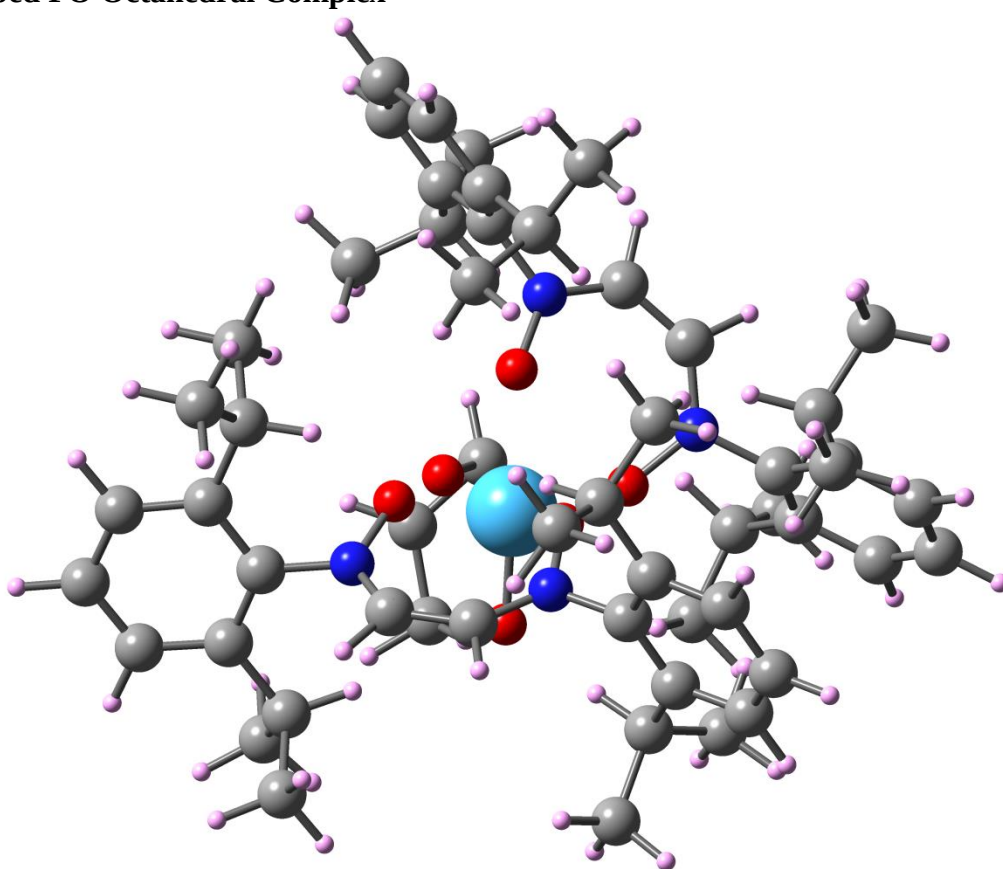
Adsorbed PO Octahedral Complex

Fig. S102: ONCCNO Adsorbed PO Octahedral Complex

E	E_{zp}	H	G
-2861.7111	-2860.4721	-2860.3956	-2860.5910

O	0.50763472	-1.22622931	0.84785419
O	1.65761784	0.93192011	-1.18289246
O	0.02813084	-1.36209069	-2.08607870
N	-0.09562958	3.00084742	0.74824997
N	2.60175805	1.77240901	-0.60768294
N	-2.65041782	-1.91170121	-0.09032496
N	0.39300960	-2.59499080	1.04295528
C	1.15310140	3.51710616	0.54282814
C	2.31537486	2.96326539	-0.00045580
C	-2.04211374	-3.02004793	0.41806831
C	-0.75480714	-3.30967497	0.88213271
C	-1.11730648	3.77235557	1.44389256
C	-1.85637397	4.75304377	0.73720935
C	-2.84692076	5.46545423	1.44709350
C	-3.09789378	5.19906386	2.80108125
C	-2.36086042	4.21060885	3.47359262
C	-1.35446317	3.47737514	2.81248963
C	-2.89354291	4.57672300	-1.56677598

C	-1.65011687	5.02847347	-0.75461528
C	-1.31331355	6.51644771	-1.02924226
C	3.13487241	0.54670770	-4.16484564
C	3.60136271	1.79814987	-3.37308091
C	4.31351638	2.81462839	-4.30099279
C	3.97974178	1.37886466	-0.84983248
C	4.47108256	1.38465365	-2.18407373
C	5.80526270	0.98456949	-2.39579114
C	6.63001672	0.61297238	-1.32171645
C	6.12540092	0.62242146	-0.01384037
C	4.78772103	0.98838123	0.25133994
C	-1.49199969	1.14585605	3.77922941
C	-0.58340616	2.38434042	3.55693339
C	0.01104418	2.89232081	4.89441716
C	4.52163939	-0.43188853	2.35319573
C	4.27164918	0.94751939	1.69407209
C	4.90789159	2.08077925	2.54405311
C	-4.03012538	-1.97220779	-0.54384678
C	-4.32012866	-2.61461808	-1.77642345
C	-5.67600571	-2.69569125	-2.16194013
C	-6.69033520	-2.13120230	-1.37308614
C	-6.36905926	-1.47235878	-0.17537558
C	-5.03362446	-1.38356051	0.26864782
C	-3.41680703	-2.78479130	-4.15637693
C	-3.22748548	-3.20452522	-2.67678218
C	-3.19101372	-4.75408113	-2.57491518
C	1.42561673	-1.66408377	4.88815062
C	0.76218985	-2.70008899	3.94535854
C	0.05256164	-3.81175940	4.76386134
C	1.59104670	-3.23676376	1.55946675
C	1.77407756	-3.29986720	2.96399654
C	2.92730850	-3.95601982	3.44239301
C	3.86039591	-4.51196376	2.55180588
C	3.66114746	-4.41667400	1.16506319
C	2.52300093	-3.77112401	0.63432445
C	-4.90426723	0.87115828	1.40884062
C	-4.70468512	-0.65868512	1.57611482
C	-5.53152540	-1.20289189	2.76870706
C	3.53281724	-3.07617334	-1.60269338
C	2.30803054	-3.69014647	-0.87976955
C	1.97673992	-5.09225584	-1.45808227
H	1.25555636	4.53357523	0.90814041
H	3.19570356	3.59133817	0.09925906
H	-2.71118993	-3.87336114	0.43139958
H	-0.62040668	-4.34678467	1.17200495
H	-3.43257656	6.22429097	0.93367448
H	-3.86886365	5.75528831	3.32939775
H	-2.56744932	4.00959469	4.52154208
H	-0.79999718	4.42913416	-1.09689394
H	2.70637257	2.28793356	-2.97473494
H	-3.79510271	5.11314804	-1.24415020
H	-3.06991597	3.50220628	-1.43902624

H	-2.75028866	4.78391148	-2.63732243
H	-2.14280886	7.17660115	-0.74505030
H	-1.11661548	6.67318605	-2.09849866
H	-0.42510148	6.83525129	-0.46860641
H	3.99707577	-0.01062085	-4.55618363
H	2.51367796	0.84416815	-5.02215217
H	2.54803251	-0.11930069	-3.52393780
H	4.66362076	3.69264470	-3.74253999
H	3.62124300	3.15864544	-5.08158243
H	5.17954539	2.37000655	-4.80789854
H	6.20586888	0.97410183	-3.40594972
H	7.65959742	0.31434732	-1.50506592
H	6.76901386	0.32518969	0.80968262
H	0.24719444	2.05288630	2.92575666
H	3.18831894	1.10431182	1.68063621
H	-2.36249708	1.39877759	4.40123501
H	-0.92845594	0.35196417	4.28678810
H	-1.84124448	0.75771468	2.81707455
H	-0.77187013	3.17300364	5.61135866
H	0.65639221	3.76717026	4.74065328
H	0.61365536	2.10054185	5.35911892
H	4.05425814	-1.23683715	1.77638516
H	4.09317632	-0.44734188	3.36347626
H	5.59321757	-0.65244303	2.44529305
H	5.99795879	1.96218982	2.60694809
H	4.50681231	2.06224460	3.56618608
H	4.70308378	3.07079277	2.11657578
H	-5.93703339	-3.18977304	-3.09400224
H	-7.72762061	-2.19979763	-1.69349529
H	-7.16169465	-1.03208211	0.42412096
H	-2.25457622	-2.81537174	-2.35462098
H	-0.00180212	-2.16805187	3.36889965
H	-4.29748946	-3.26012736	-4.60912810
H	-2.53748649	-3.08479500	-4.74030128
H	-3.53379263	-1.69835096	-4.24544798
H	-2.99660869	-5.09072070	-1.54920106
H	-2.39514980	-5.15547378	-3.21582370
H	-4.14514444	-5.19320980	-2.89803902
H	2.20978958	-2.12194886	5.50522407
H	0.67578867	-1.23475982	5.56633267
H	1.87560840	-0.84723769	4.31180590
H	-0.45165604	-4.53089830	4.10579711
H	-0.70220296	-3.37336797	5.43028437
H	0.76798661	-4.36863582	5.38362512
H	3.09774131	-4.03020593	4.51378820
H	4.74374811	-5.01557687	2.93847033
H	4.39541983	-4.84388343	0.48705262
H	-3.64577276	-0.81714081	1.80183418
H	1.45794253	-3.03433059	-1.09610120
H	-5.94887067	1.11224965	1.16723395
H	-4.26163339	1.25256541	0.60818222
H	-4.63913385	1.39494982	2.33659202

H	-5.22073351	-0.70510415	3.69696346
H	-5.38720119	-2.28377782	2.89597179
H	-6.60641277	-1.01936396	2.63904786
H	3.76601035	-2.08112725	-1.20593904
H	3.30716527	-2.96506924	-2.67059525
H	4.42894479	-3.70568660	-1.50789764
H	1.08040516	-5.51754490	-0.98728711
H	2.80607556	-5.79761048	-1.30617169
H	1.78618375	-5.01420925	-2.53612626
O	-1.14670773	1.35141649	-2.30531713
O	-2.08047957	-0.64700302	-0.10496672
O	-0.40757384	1.68687344	0.53662417
C	-0.45774756	2.29951124	-3.24504299
H	-0.75628207	3.33452225	-3.10798788
C	-1.41153182	1.31234356	-3.82884255
H	-2.42408167	1.67120478	-4.00449435
C	-0.94632833	0.10322954	-4.60553848
H	-0.40536253	-0.58388031	-3.93298465
H	-1.79636762	-0.43700505	-5.03206915
H	-0.28069491	0.41022602	-5.42357461
H	0.60726080	2.10932669	-3.33052124
Hf	-0.15793346	-0.08659056	-0.78906757

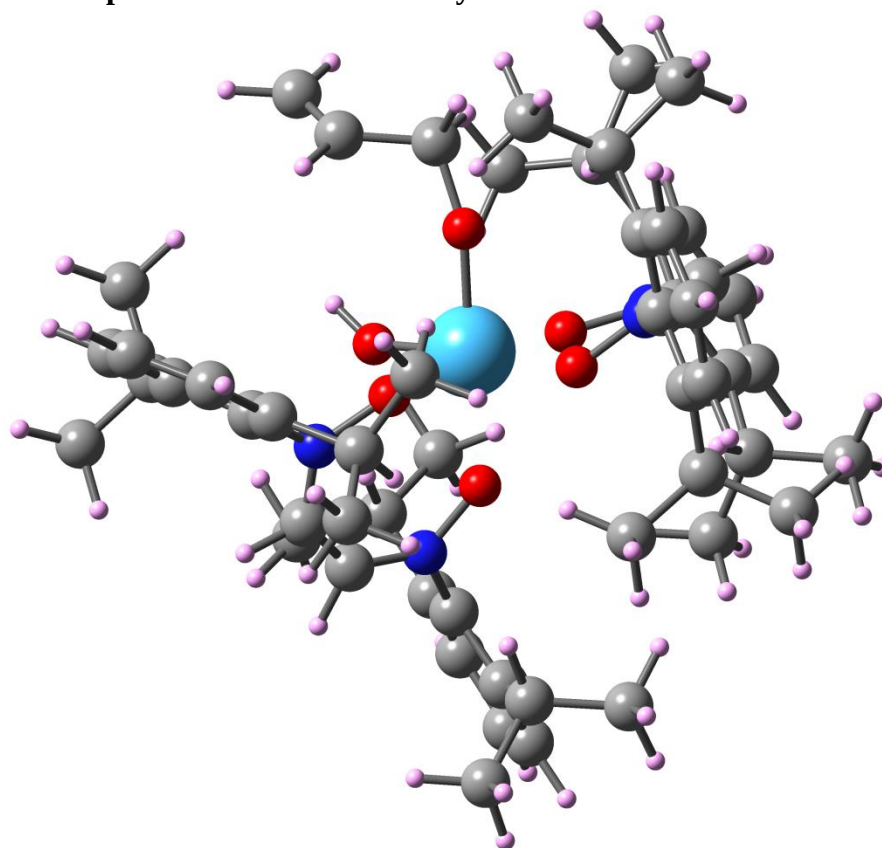
Octahedral Complex with Transferred Allylic H

Fig. S103: ONCCNO Octahedral Complex with Transferred Allylic H

E	E_{zp}	H	G
-2861.7892	-2860.5522	-2860.4748	-2860.6750
O	0.44951178	-1.38928353	0.77082785
O	1.87511329	0.59180541	-0.83439484
O	0.00436994	-1.37954645	-2.08097355
N	0.06470016	2.82801850	0.93289889
N	2.73724420	1.62591621	-0.55928036
N	-2.74832366	-1.78593038	-0.05024053
N	0.23249925	-2.72116610	1.02140272
C	1.27025274	3.36452669	0.60042507
C	2.41396987	2.83239523	-0.00325416
C	-2.23756437	-2.93829379	0.47079003
C	-0.97396654	-3.34414175	0.91117470
C	-0.94579181	3.61515193	1.62131466
C	-1.73135294	4.53508080	0.88165898
C	-2.67343723	5.30871241	1.59404518
C	-2.84794068	5.14619387	2.97623698
C	-2.07991858	4.20261687	3.67779479
C	-1.10909464	3.42141687	3.01857571
C	-2.96224112	4.53671673	-1.34569719

C	-1.59531923	4.70679596	-0.63467794
C	-0.96248149	6.07984087	-0.98674169
C	3.01251765	0.65052323	-4.25259566
C	3.38097408	1.89470189	-3.39986004
C	3.83353965	3.07281504	-4.29803934
C	4.10612222	1.36571379	-0.98142311
C	4.43270069	1.51884353	-2.35292763
C	5.76635780	1.26967219	-2.73660985
C	6.73011165	0.88260592	-1.79070691
C	6.37302735	0.71818151	-0.44364039
C	5.04831844	0.94350541	-0.01095694
C	-1.18989641	1.18072537	4.18200409
C	-0.29357007	2.38938850	3.80137873
C	0.38137836	3.00223454	5.05425734
C	4.95992428	-0.74924147	1.88560583
C	4.67138034	0.71206164	1.45550876
C	5.39574365	1.71789190	2.38853221
C	-4.13026188	-1.72227253	-0.49613040
C	-4.50086841	-2.38883258	-1.69383863
C	-5.85412688	-2.31436864	-2.08900636
C	-6.78831163	-1.58185727	-1.34090066
C	-6.38768047	-0.91140933	-0.17368282
C	-5.05365487	-0.97182303	0.27831146
C	-3.50736050	-2.69323146	-4.02627034
C	-3.50033573	-3.17232190	-2.55225500
C	-3.77872374	-4.69793352	-2.48074047
C	1.52648858	-1.84538414	4.79577102
C	0.72574547	-2.83704052	3.91316296
C	-0.02606515	-3.87355957	4.78934537
C	1.40070418	-3.45020255	1.49594102
C	1.63508812	-3.52605594	2.89177818
C	2.75483537	-4.26608191	3.32658421
C	3.61520802	-4.88205829	2.40360020
C	3.37696429	-4.76026904	1.02564868
C	2.26617661	-4.03773619	0.53944313
C	-4.63842370	1.29939585	1.31506119
C	-4.63914442	-0.23350164	1.55375674
C	-5.53417700	-0.61144926	2.76142745
C	3.19979054	-3.10788590	-1.62757836
C	2.03903345	-3.89794796	-0.96774480
C	1.85451902	-5.28317424	-1.64046748
H	1.35356046	4.40977522	0.87888152
H	3.25210467	3.52104500	-0.04160501
H	-2.98867013	-3.71969908	0.51947317
H	-0.92599237	-4.38138875	1.22587482
H	-3.28480085	6.03184582	1.06017181
H	-3.58466619	5.74740934	3.50428895
H	-2.22970066	4.07886645	4.74725229
H	-0.93700115	3.91780331	-1.01236472
H	2.47034388	2.20584543	-2.87640316
H	-3.68895897	5.29307099	-1.02188681
H	-3.38547934	3.54575724	-1.14387211

H	-2.83939205	4.64230195	-2.43183614
H	-1.59589947	6.90873665	-0.64307781
H	-0.83976601	6.17715598	-2.07373962
H	0.02516184	6.19910229	-0.52238517
H	3.88742210	0.27334379	-4.79947496
H	2.23784472	0.90837369	-4.98786443
H	2.62791656	-0.15041791	-3.61211101
H	4.09557952	3.95552164	-3.70034457
H	3.02392615	3.35370710	-4.98472963
H	4.70607948	2.80847456	-4.90978975
H	6.05373582	1.37891299	-3.77915419
H	7.75514905	0.70063499	-2.10575874
H	7.12414153	0.40106673	0.27558849
H	0.49481709	2.00204464	3.14919465
H	3.59350636	0.86973177	1.56465828
H	-2.02336656	1.49106635	4.82751270
H	-0.60089144	0.42912145	4.72344209
H	-1.59589372	0.71399689	3.27824735
H	-0.35707448	3.34372095	5.79148197
H	1.01497224	3.85896596	4.78982321
H	1.01305213	2.24960001	5.54478827
H	4.41682426	-1.46041716	1.25324178
H	4.63813310	-0.90730814	2.92338674
H	6.03096611	-0.98492948	1.82704486
H	6.48612660	1.59987396	2.33245526
H	5.09339492	1.55540418	3.43158525
H	5.15617742	2.75545720	2.12196227
H	-6.17485586	-2.82094137	-2.99587287
H	-7.82423626	-1.53004232	-1.66833010
H	-7.11878536	-0.34358369	0.39587530
H	-2.49285133	-2.99201116	-2.16356065
H	-0.02235652	-2.25067083	3.36933102
H	-4.47439976	-2.87758396	-4.51224968
H	-2.73984346	-3.23150781	-4.59873001
H	-3.29078659	-1.62128041	-4.09175380
H	-3.74123313	-5.06787199	-1.44807679
H	-3.03247027	-5.25071753	-3.06666883
H	-4.77140708	-4.93722800	-2.88508724
H	2.29571932	-2.35876974	5.38760226
H	0.85314994	-1.33468218	5.49677491
H	2.01930732	-1.08611191	4.17653272
H	-0.63260661	-4.55008394	4.17370591
H	-0.69505947	-3.36318709	5.49500867
H	0.67427170	-4.48696598	5.37169471
H	2.95804376	-4.35587111	4.39090861
H	4.47372068	-5.44848606	2.75767599
H	4.05774722	-5.22865340	0.31929007
H	-3.61013690	-0.51524382	1.79663989
H	1.13217696	-3.31123277	-1.14175025
H	-5.64302908	1.66346632	1.05774522
H	-3.95158347	1.55459814	0.50144781
H	-4.30507091	1.82728362	2.21802005

H	-5.16538068	-0.11502407	3.66885500
H	-5.53087155	-1.69488668	2.93947123
H	-6.57587871	-0.29723295	2.61324281
H	3.25951710	-2.09390492	-1.21667607
H	3.02392614	-3.02010279	-2.70800152
H	4.16799529	-3.60679205	-1.48120764
H	1.01666835	-5.83600610	-1.19496246
H	2.75555926	-5.90450021	-1.54572192
H	1.64747408	-5.15662496	-2.71153839
O	-0.72741463	1.39791430	-1.99443009
O	-2.07908728	-0.57651563	-0.11735024
O	-0.19280554	1.47569441	0.85184761
C	-0.94708318	1.92783963	-3.30084112
H	-1.49656493	2.87934749	-3.21014987
C	-1.75073129	0.97753632	-4.16575504
H	-2.68256082	0.63094452	-3.71495418
C	-1.39247517	0.56435991	-5.39886595
H	-0.05643954	-1.55601870	-3.03076853
H	-2.01940226	-0.10388314	-5.98568955
H	-0.46039670	0.88860846	-5.86097501
H	0.01689909	2.14842575	-3.78929673
Hf	-0.15265183	0.02787250	-0.70718049

Peroxo Complex

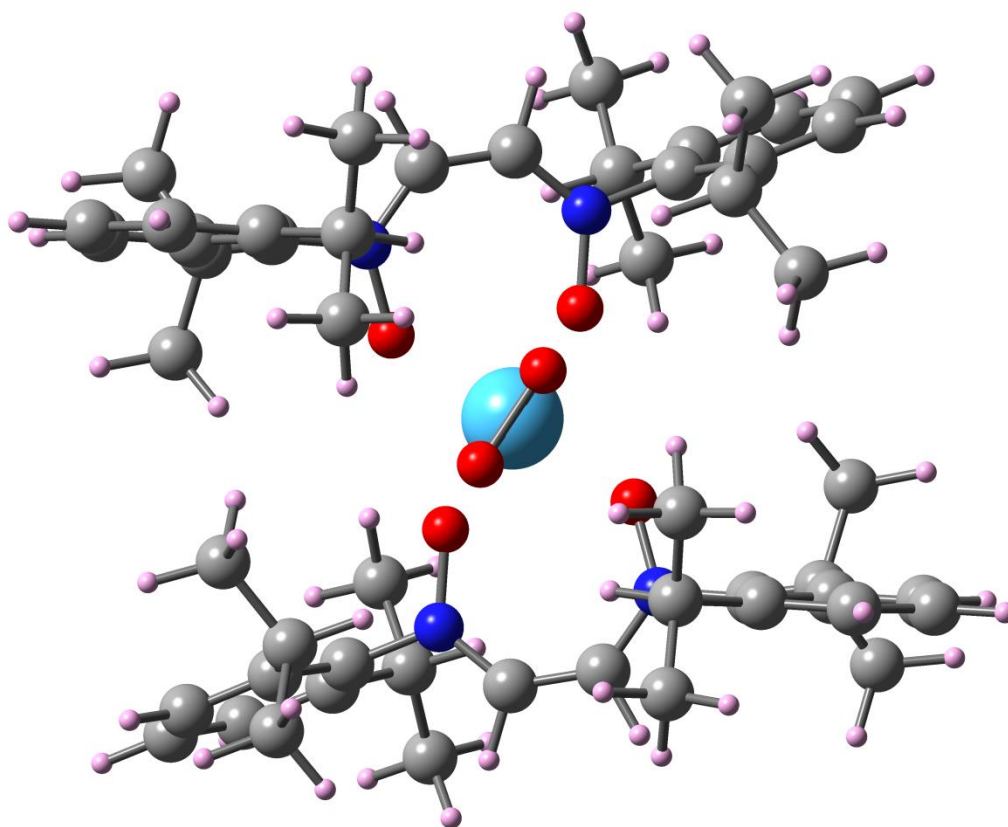


Fig. S104: ONCCNO Peroxo Complex

E	E_{zp}	H	G
-2743.7920	-2742.6377	-2742.5655	-2742.7560
O	-1.62813688	-1.27761902	0.11909224
O	1.62658403	1.27755972	0.12005560
O	0.48613986	-0.63418028	-2.08125517
O	-0.47994208	0.62454769	-2.08574371
N	-1.22246780	2.86021016	0.72120506
N	1.88744215	2.56578310	-0.32003817
N	1.22168837	-2.85743733	0.72921407
N	-1.88866913	-2.56828329	-0.31345353
C	-0.27134362	3.74690404	0.31728692
C	1.04574988	3.62037461	-0.14318054
C	0.27131810	-3.74582180	0.32736777
C	-1.04607318	-3.62156387	-0.13291172
C	-2.54535255	3.29854305	1.13525013
C	-3.56409497	3.38041712	0.15350190
C	-4.83825592	3.81284092	0.57886443
C	-5.08214107	4.12842776	1.92511209
C	-4.05932486	4.00694589	2.87998706
C	-2.76735114	3.58239822	2.50586283

C	-4.18905716	1.76401336	-1.69865891
C	-3.32724957	2.99372552	-1.30905994
C	-3.59213136	4.18531505	-2.26506081
C	2.27899986	1.50321226	-4.22100800
C	2.13129838	2.71398202	-3.26296203
C	1.93089882	4.03324757	-4.05507025
C	3.20873272	2.73998764	-0.90284049
C	3.32912138	2.82013869	-2.31312214
C	4.62892576	2.98995564	-2.83903548
C	5.75010285	3.05079036	-1.99810177
C	5.59927808	2.94047600	-0.60553781
C	4.32403210	2.78300001	-0.02636437
C	-2.00785264	2.15883880	4.45329911
C	-1.67798141	3.38772656	3.56336647
C	-1.45918277	4.65733785	4.42420890
C	4.68161025	1.23601024	1.94404472
C	4.17453459	2.63099817	1.48982169
C	4.89018404	3.76520675	2.26615417
C	2.54600277	-3.29337243	1.14114754
C	2.77174494	-3.57277334	2.51210860
C	4.06507546	-3.99480597	2.88423686
C	5.08556838	-4.11836189	1.92710137
C	4.83797174	-3.80721052	0.58052853
C	3.56229829	-3.37728113	0.15706181
C	2.01242088	-2.13558007	4.44889891
C	1.68506954	-3.37435835	3.57167238
C	1.47520934	-4.63665753	4.44523632
C	-2.28189469	-1.51321364	-4.21522722
C	-2.13278357	-2.72264793	-3.25568849
C	-1.93122951	-4.04260629	-4.04631064
C	-3.20989027	-2.74573321	-0.89549098
C	-3.33039252	-2.82877721	-2.30558143
C	-4.63004097	-3.00145183	-2.83093524
C	-5.75096028	-3.06224972	-1.98963548
C	-5.60006840	-2.94887588	-0.59731913
C	-4.32492763	-2.78840114	-0.01871888
C	4.18375939	-1.76908522	-1.70370553
C	3.32136213	-2.99579655	-1.30621811
C	3.58130056	-4.19177493	-2.25813309
C	-4.68213747	-1.23576953	1.94719930
C	-4.17518591	-2.63211534	1.49699842
C	-4.89058962	-3.76402917	2.27685864
H	-0.63682686	4.76804606	0.34482475
H	1.50124998	4.55715302	-0.44614324
H	0.63788468	-4.76652829	0.35657332
H	-1.50106427	-4.55966468	-0.43252589
H	-5.64419178	3.89487261	-0.14586585
H	-6.07188845	4.45881631	2.23220952
H	-4.26787742	4.23651521	3.92183021
H	-2.28124806	2.69526443	-1.43393934
H	1.22291519	2.52569897	-2.68292736
H	-5.26266952	1.98348114	-1.62011019

H	-3.96183234	0.90782717	-1.05359052
H	-3.97425021	1.46999422	-2.73350503
H	-4.64118985	4.50795984	-2.22724137
H	-3.36841229	3.89265519	-3.29890392
H	-2.96500764	5.05054796	-2.01224220
H	3.19488455	1.56776546	-4.82484709
H	1.41958350	1.46713908	-4.90215711
H	2.28112262	0.56656660	-3.65389811
H	1.79842666	4.89274513	-3.38361765
H	1.03911728	3.95641968	-4.69040114
H	2.78957412	4.24688570	-4.70604753
H	4.76140866	3.05989293	-3.91553077
H	6.74202015	3.17572037	-2.42670964
H	6.47743746	2.97815859	0.03379003
H	-0.73453790	3.16722505	3.05190130
H	3.10894311	2.67807095	1.73934825
H	-2.94331441	2.31060757	5.00851077
H	-1.20388472	1.98941224	5.18211678
H	-2.11407368	1.25573826	3.84093005
H	-2.35179571	4.90779227	5.01227763
H	-1.21315728	5.52640286	3.80036629
H	-0.63267200	4.49793513	5.12923146
H	4.11828676	0.44168965	1.44283228
H	4.55202496	1.11825794	3.02854302
H	5.74795011	1.10755771	1.71331597
H	5.97787688	3.73509623	2.12030675
H	4.69913963	3.66206946	3.34259003
H	4.53536145	4.75455347	1.94900536
H	4.27654338	-4.22084862	3.92624605
H	6.07640482	-4.44684443	2.23273521
H	5.64214456	-3.89065641	-0.14599506
H	0.73875934	-3.16304979	3.06158504
H	-1.22446598	-2.53289324	-2.67600624
H	2.95082813	-2.27804695	5.00163917
H	1.21051354	-1.96325899	5.17930925
H	2.11191201	-1.23784386	3.82763200
H	1.23221081	-5.51309807	3.83059156
H	0.64959837	-4.47460554	5.15071294
H	2.37039944	-4.87667151	5.03375346
H	-3.19779774	-1.57959765	-4.81883761
H	-1.42258116	-1.47702621	-4.89649172
H	-2.28497768	-0.57580786	-3.64937737
H	-1.79802014	-4.90122391	-3.37388972
H	-1.03950487	-3.96569655	-4.68170321
H	-2.78970095	-4.25771192	-4.69707603
H	-4.76263758	-3.07374961	-3.90726500
H	-6.74277534	-3.18948868	-2.41780193
H	-6.47808427	-2.98642751	0.04221062
H	2.27549028	-2.69607828	-1.42907157
H	-3.10951850	-2.67848474	1.74641376
H	5.25732796	-1.98954828	-1.62735736
H	3.95950655	-0.90971866	-1.06181907

H	3.96622639	-1.47933611	-2.73917198
H	3.35478888	-3.90300906	-3.29245846
H	2.95358463	-5.05493048	-1.99972911
H	4.62996030	-4.51595884	-2.22218554
H	-4.11874188	-0.44295950	1.44366978
H	-4.55254880	-1.11487822	3.03134924
H	-5.74846055	-1.10791708	1.71606761
H	-4.53614132	-4.75431304	1.96223754
H	-5.97835923	-3.73409138	2.13157972
H	-4.69891471	-3.65795888	3.35289234
Hf	-0.00045627	-0.00069159	-0.23741963
O	-1.04474392	1.49160159	0.75551159
O	1.04111792	-1.48912506	0.76449483

9.4 Seven Oxygen Atoms

Oxo Complex with Adsorbed Oxygen Molecule (planar conformation)

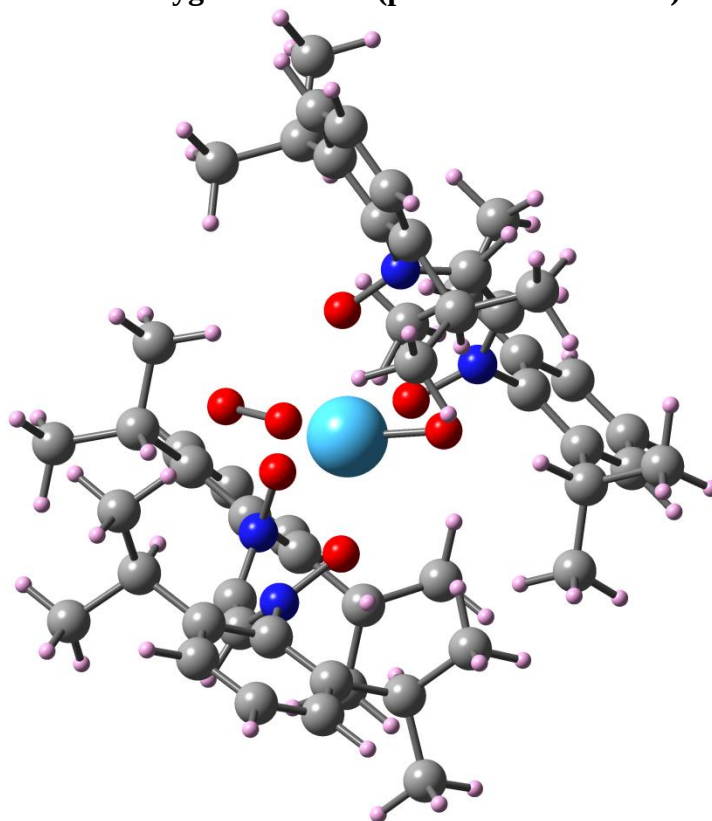


Fig. S105: ONCCNO Oxo Complex with Adsorbed Oxygen Molecule (planar conformation)

E	E_{zp}	H	G
-2818.9461	-2817.7881	-2817.7148	-2817.9045
O	1.69456426	0.20738904	0.38853694
O	-1.70148102	-1.31889062	0.69094892
O	-0.51572238	1.07952294	1.70133531
N	0.28685693	-2.59135033	-1.41949294
N	-2.53406227	-2.21070447	0.01141147
N	0.46571892	3.29300098	0.00611027
N	2.38528169	0.96688766	1.24360305
C	-0.76915316	-3.44654019	-1.27428086
C	-2.03530247	-3.24450838	-0.72135727
C	1.30893563	3.26939096	1.02438676
C	2.18313742	2.25112498	1.53243168
C	1.54606712	-3.05075643	-1.98131171
C	1.86507790	-2.67954864	-3.31497380
C	3.09028653	-3.13653778	-3.84254017
C	3.95358251	-3.94119705	-3.08104392
C	3.61173953	-4.29424591	-1.76681904
C	2.40738991	-3.84641101	-1.18212375

C	1.54495293	-0.40981263	-4.39697164
C	0.93456937	-1.81912168	-4.17520961
C	0.60370819	-2.50127200	-5.52731801
C	-5.12667170	-0.15590198	-2.52023297
C	-4.54380090	-1.51748307	-2.06216692
C	-5.01272694	-2.66093619	-3.00221657
C	-3.93462702	-2.14374660	0.38696523
C	-4.90171140	-1.82517551	-0.60372072
C	-6.25510512	-1.78635997	-0.20344463
C	-6.62631343	-2.02071865	1.12794899
C	-5.64662648	-2.31079063	2.09134453
C	-4.28316045	-2.38808753	1.74422106
C	3.22734085	-3.85406249	1.23424518
C	2.07791326	-4.22843163	0.26517665
C	1.73918492	-5.73918937	0.38031737
C	-3.01662911	-1.48983798	3.74347165
C	-3.24280802	-2.71706805	2.81962162
C	-3.62948418	-3.97371000	3.64056950
C	-0.28895690	4.51185790	-0.31559040
C	-1.33670918	4.91460336	0.55008340
C	-2.02110200	6.09927676	0.19753107
C	-1.69274619	6.81506519	-0.96211884
C	-0.67026432	6.36094221	-1.81183274
C	0.05763719	5.19334973	-1.51048549
C	-3.26393563	3.70686381	1.67348522
C	-1.77510965	4.12818793	1.79181803
C	-1.53076702	4.94705302	3.08649795
C	5.43425489	-0.44618739	-1.00869961
C	5.01536458	0.69120746	-0.04076202
C	6.09366404	1.80551743	0.00655952
C	3.45099740	0.25535798	1.97405646
C	4.71926958	0.14285495	1.35857346
C	5.72610064	-0.51475440	2.09608749
C	5.46148641	-1.03522041	3.37371199
C	4.18009958	-0.92421428	3.93659686
C	3.13195007	-0.28034594	3.24379753
C	0.47802310	4.02936695	-3.71226055
C	1.13934495	4.68807193	-2.47056069
C	2.12801917	5.80468463	-2.88965526
C	1.16323249	-1.59988294	4.15278030
C	1.72960119	-0.18743426	3.85552018
C	1.73833130	0.68128808	5.14060646
H	-0.58356629	-4.43246820	-1.68679539
H	-2.75369339	-4.04062771	-0.88954622
H	1.37785271	4.21238421	1.55495535
H	2.84140062	2.60701586	2.31737375
H	3.36420401	-2.87167765	-4.86056923
H	4.88963178	-4.29102902	-3.51067022
H	4.29095583	-4.91191306	-1.18480855
H	-0.00429010	-1.67143856	-3.63408039
H	-3.45625441	-1.43387741	-2.14825289
H	2.50213875	-0.46862987	-4.93411731

H	1.71167561	0.08777646	-3.43554304
H	0.85864525	0.21047607	-4.98833369
H	1.49606877	-2.61689979	-6.15684621
H	-0.11876578	-1.89150083	-6.08560763
H	0.16559942	-3.49667835	-5.37724319
H	-6.22516781	-0.15741380	-2.51226247
H	-4.79745889	0.06143794	-3.54449748
H	-4.76838170	0.65291661	-1.87540137
H	-4.56579196	-3.62451150	-2.72305955
H	-4.72699606	-2.44052846	-4.03932883
H	-6.10444650	-2.77732079	-2.96992990
H	-7.01985827	-1.54892673	-0.93797596
H	-7.67404618	-1.97246479	1.41626227
H	-5.94562221	-2.48832998	3.12104879
H	1.19361817	-3.66357087	0.57915417
H	-2.28656564	-2.91962703	2.32796161
H	4.13916072	-4.42923476	1.02575770
H	2.93052982	-4.06802047	2.26937998
H	3.47226015	-2.78840579	1.16425378
H	2.59492912	-6.35961238	0.08219491
H	0.88938837	-6.01118780	-0.25847093
H	1.48048123	-5.99466873	1.41643938
H	-2.61513782	-0.64878185	3.16872132
H	-2.29716487	-1.74096109	4.53560699
H	-3.95420235	-1.17898361	4.22545757
H	-4.53672185	-3.81259625	4.23755199
H	-2.81905940	-4.22587507	4.33776384
H	-3.80351774	-4.84138698	2.99030797
H	-2.83185507	6.44806934	0.83090769
H	-2.24121490	7.72004195	-1.21266391
H	-0.43831219	6.91760122	-2.71536131
H	-1.21134112	3.19102116	1.86780858
H	4.09820020	1.12997143	-0.44989070
H	-3.93825570	4.57374334	1.63365232
H	-3.54052771	3.09966910	2.54458293
H	-3.42203388	3.09642697	0.77738716
H	-0.47324664	5.22547631	3.20193652
H	-1.81919063	4.35070082	3.96128302
H	-2.12099899	5.87371522	3.09976830
H	6.36274215	-0.93108205	-0.67921074
H	5.60586872	-0.03999613	-2.01396613
H	4.65416019	-1.21214098	-1.08064846
H	5.79271697	2.63051180	0.66565150
H	6.26045637	2.21464851	-0.99836892
H	7.05264439	1.41724885	0.37332811
H	6.71886442	-0.62202346	1.66708240
H	6.25296364	-1.53521075	3.92699270
H	3.98613703	-1.34600282	4.91906634
H	1.72026577	3.90445967	-1.97093419
H	1.03675729	0.28120223	3.14509352
H	-0.12441123	4.75949026	-4.26945909
H	-0.17145803	3.20229766	-3.40750233

H	1.24920290	3.63618623	-4.38817571
H	2.92716882	5.37995109	-3.51132678
H	2.59068068	6.28401433	-2.01685233
H	1.63446613	6.58623064	-3.48130310
H	1.13394059	-2.20920541	3.24152704
H	0.13660871	-1.51035095	4.52708064
H	1.75858575	-2.13274043	4.90735520
H	2.10319035	1.69754769	4.93833643
H	2.37454995	0.24540547	5.92344222
H	0.71890188	0.76480552	5.53678611
O	-2.45354591	1.21936550	-0.67553188
O	-1.92653021	0.80093904	-1.90946565
Hf	-0.58362837	0.33298455	0.02067585
O	0.24466808	2.23732768	-0.80836215
O	0.15696088	-1.23111762	-1.28678573

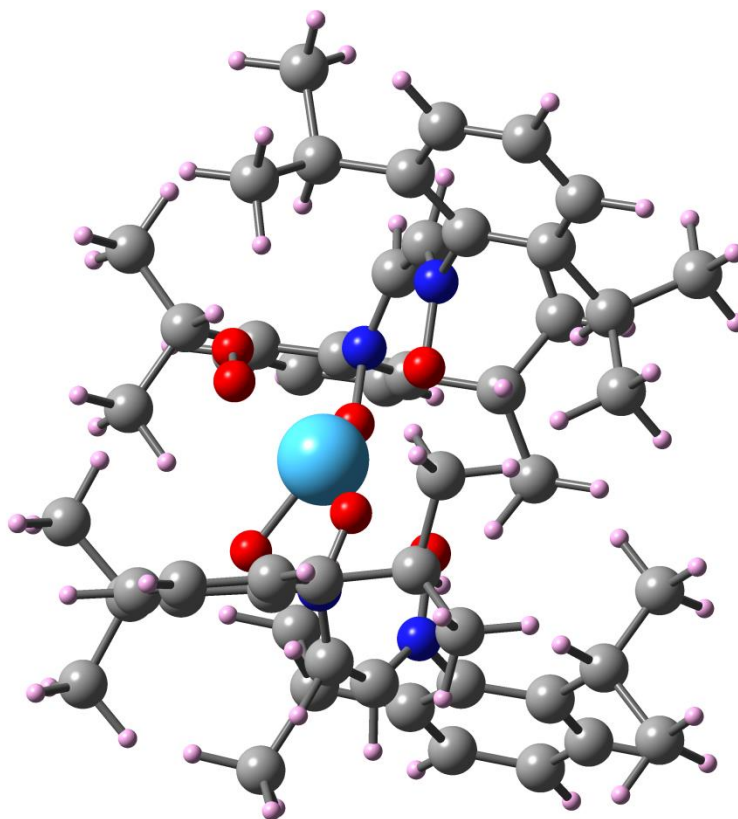
Oxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

Fig. S106: ONCCNO Oxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

E	E_{zp}	H	G
-2818.9562	-2817.7981	-2817.7247	-2817.9144
O	-0.39575876	1.55554198	0.81560488
O	-2.20059432	-0.63820943	-0.04999125
O	-1.41033151	1.26801692	-2.05298094
N	0.12322327	-2.73840195	0.87348874
N	-2.71823394	-1.81648482	-0.44061028
N	2.69972167	1.56627028	-0.45355324
N	-0.03782311	2.88184814	0.90787234
C	-0.87936976	-3.39398070	0.29995307
C	-2.12179743	-2.99146075	-0.30006818
C	2.34962738	2.79284133	0.03140007
C	1.20283339	3.35907790	0.59975372
C	1.24543183	-3.50352545	1.44662284
C	2.23905076	-3.98821881	0.56305304
C	3.29917367	-4.71468440	1.14932703
C	3.36234501	-4.91960650	2.53585619
C	2.36843621	-4.39543606	3.37912262
C	1.28223183	-3.66773855	2.85200731
C	3.47042904	-2.95356493	-1.40018667

C	2.21434303	-3.74386901	-0.95025933
C	2.09311072	-5.08174437	-1.72667834
C	-2.85703254	-0.95680419	-4.45255188
C	-2.94220332	-2.08095604	-3.38721475
C	-2.99311312	-3.47744805	-4.06191995
C	-4.05105209	-1.73698250	-1.06083660
C	-4.15067195	-1.87343509	-2.46681180
C	-5.45040348	-1.78892109	-3.01408181
C	-6.56985715	-1.55706345	-2.20168489
C	-6.42134715	-1.39734765	-0.81364224
C	-5.15240978	-1.48089792	-0.20673073
C	0.84093709	-1.84372677	4.54410327
C	0.23394156	-3.05391033	3.78428229
C	-0.35868747	-4.09292514	4.76901618
C	-5.13350493	0.25209148	1.63385279
C	-4.99581862	-1.25839969	1.30066870
C	-5.99094280	-2.10789907	2.13017414
C	4.05380421	1.32335848	-0.92900733
C	4.30717579	1.39829593	-2.32214045
C	5.62646239	1.15055579	-2.75667454
C	6.64485321	0.84252663	-1.84021936
C	6.36083145	0.75954783	-0.46769561
C	5.05484338	0.98514997	0.01638161
C	2.82508616	0.41974220	-4.12945300
C	3.20060822	1.70012284	-3.33520848
C	3.58431710	2.85492097	-4.29425852
C	-1.72086015	1.44943273	4.06378910
C	-0.72009125	2.58783590	3.72983991
C	-0.13802238	3.21768349	5.02049014
C	-1.06003482	3.76110068	1.45387681
C	-1.38855631	3.62934870	2.82873097
C	-2.38312683	4.48168734	3.34881106
C	-3.02125379	5.43097447	2.53326370
C	-2.68547407	5.53136522	1.17520260
C	-1.70722916	4.69084867	0.59959843
C	5.14486742	-0.53946871	2.05672936
C	4.75659686	0.85960560	1.51371072
C	5.46426914	1.98020737	2.32104536
C	-2.67518808	4.55142895	-1.75052656
C	-1.40402352	4.80255308	-0.89871433
C	-0.77168565	6.17752842	-1.24248750
H	-0.73651993	-4.46885812	0.31003300
H	-2.70633324	-3.81880041	-0.68599280
H	3.17122775	3.49580056	-0.06616428
H	1.30472639	4.41300982	0.83597517
H	4.08455923	-5.11065904	0.51158394
H	4.19142098	-5.47965513	2.96194378
H	2.43832801	-4.55033836	4.45228297
H	1.35499999	-3.11868699	-1.22083300
H	-2.01084429	-2.01741873	-2.81140166
H	4.40130383	-3.49390696	-1.17865422
H	3.50474883	-1.97285631	-0.91337678

H	3.42602862	-2.78332440	-2.48308680
H	2.96027551	-5.73396856	-1.55365592
H	2.03194665	-4.87897258	-2.80312401
H	1.19185321	-5.64055491	-1.43746349
H	-3.72601689	-0.95604451	-5.12540185
H	-1.95566662	-1.10150983	-5.06115659
H	-2.78089263	0.02664763	-3.97519248
H	-3.02193901	-4.28845122	-3.32023602
H	-2.09939571	-3.62102778	-4.68192290
H	-3.87557054	-3.58571534	-4.70761618
H	-5.57841452	-1.88927292	-4.08818305
H	-7.55834940	-1.48992753	-2.64993702
H	-7.29624976	-1.20477477	-0.19923301
H	-0.59310991	-2.66265173	3.18038330
H	-3.98323160	-1.55465073	1.59927765
H	1.68452194	-2.15566682	5.17422519
H	0.08331144	-1.38510736	5.19300063
H	1.19491292	-1.08533545	3.83700444
H	0.40233483	-4.47811370	5.45948331
H	-0.79393784	-4.94911066	4.23733510
H	-1.14768985	-3.62799290	5.37423974
H	-4.37984047	0.83506311	1.09440554
H	-4.99167155	0.41765038	2.70993219
H	-6.12853222	0.62722790	1.35924302
H	-7.03159245	-1.81230138	1.94610186
H	-5.79594035	-1.96964937	3.20166881
H	-5.89904810	-3.17749208	1.89988733
H	5.85734031	1.20085858	-3.81757608
H	7.65678886	0.66129387	-2.19588753
H	7.15584989	0.50930646	0.23056561
H	2.30322419	2.00995464	-2.79157239
H	0.10524256	2.12957996	3.17610460
H	3.68721848	0.03605287	-4.69336449
H	2.02062194	0.64445815	-4.84156024
H	2.46535448	-0.36581579	-3.45630311
H	3.85412821	3.76449290	-3.74141894
H	2.73440726	3.09212317	-4.94711137
H	4.43246903	2.58694329	-4.93872585
H	-2.59259817	1.83472354	4.61076123
H	-1.23477493	0.68839895	4.68931660
H	-2.06668204	0.97019663	3.14144918
H	0.57565253	4.01848216	4.78719764
H	0.38714725	2.45255568	5.60798680
H	-0.92408377	3.64262660	5.65873754
H	-2.65620381	4.40663744	4.39837981
H	-3.78210344	6.08454208	2.95411115
H	-3.19634480	6.25839178	0.54917279
H	3.67726218	0.97125471	1.65945758
H	-0.68451588	4.02701481	-1.17575649
H	6.22541161	-0.71932739	1.97861810
H	4.62564331	-1.33270570	1.50631311
H	4.86831282	-0.62240197	3.11642645

H	5.21796827	1.89708185	3.38806143
H	5.15536453	2.97567855	1.97707745
H	6.55594053	1.91417152	2.22032585
H	-3.08561022	3.55536192	-1.55127827
H	-2.42386765	4.59997521	-2.81780627
H	-3.45457021	5.29906588	-1.54997960
H	0.15139347	6.35022123	-0.67305912
H	-1.46127545	7.00284691	-1.01958240
H	-0.52570373	6.22321975	-2.31140563
O	-0.09905114	-1.48568989	-1.80869208
O	-0.08347958	1.66721845	-2.23701508
O	1.90594321	0.43315310	-0.48915443
O	0.25474088	-1.40829157	0.96726778
Hf	-0.14015530	0.01048192	-0.73476952

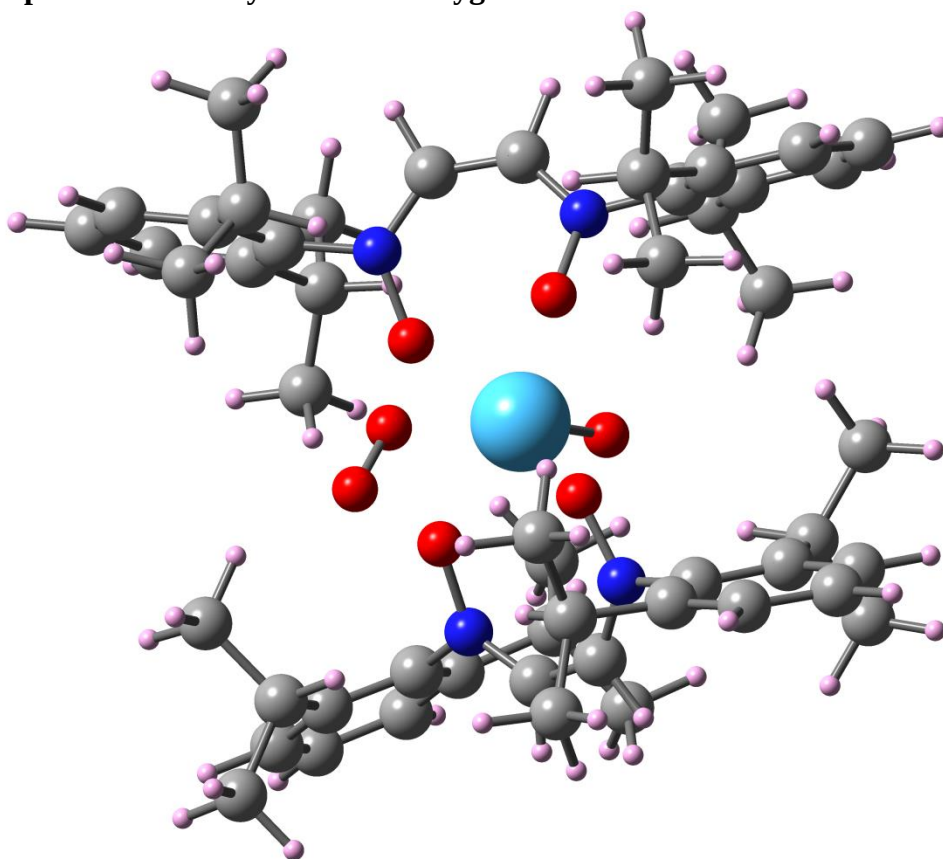
Oxo Complex with Weakly Adsorbed Oxygen Molecule

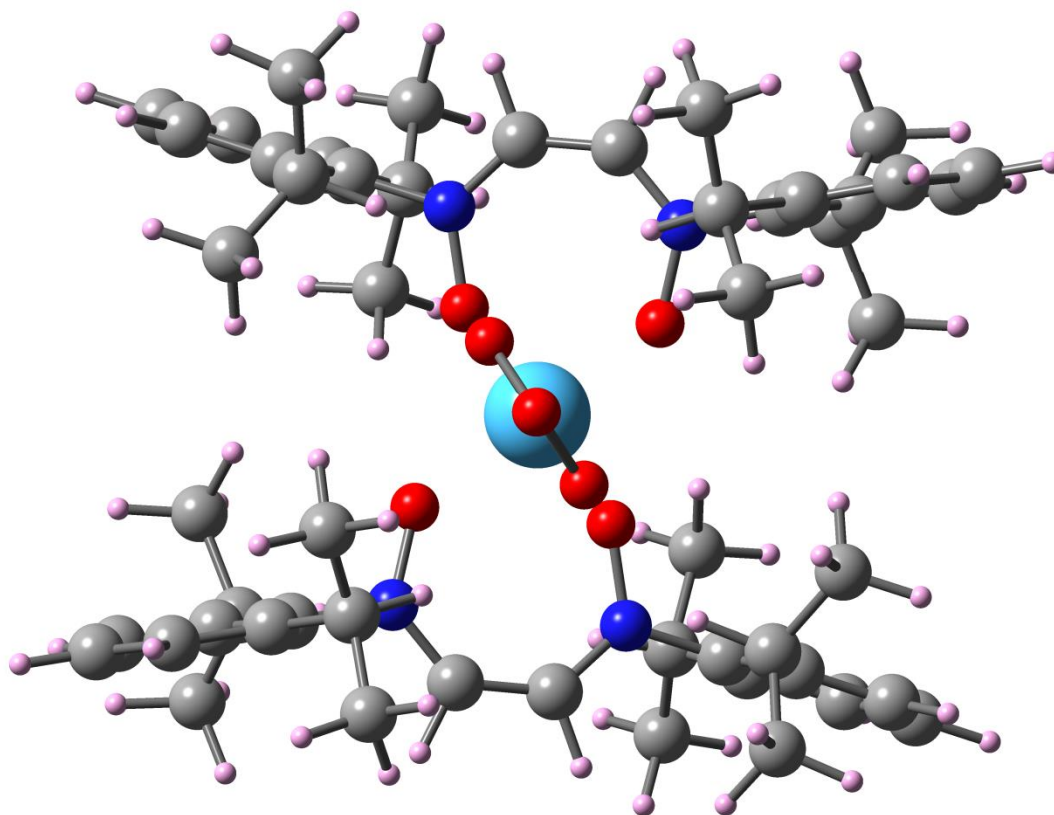
Fig. S107: ONCCNO Oxo Complex with Weakly Adsorbed Oxygen Molecule

E	E_{zp}	H	G
-2818.9530	-2817.7973	-2817.7224	-2817.9198
O	0.91640191	1.82024993	0.45846947
O	-1.11886333	-1.73199427	0.21857028
O	-0.36308872	-1.08242098	3.64889310
O	-0.36852990	-0.16598130	2.76823359
N	2.13329201	-2.30083711	0.43199749
N	-0.99793897	-2.97360221	-0.38030966
N	-2.17247649	2.47944080	0.37093572
N	0.94616599	3.01396015	-0.26378121
C	1.48024440	-3.40364645	-0.02862622
C	0.15669439	-3.68834939	-0.39625308
C	-1.46891533	3.61275964	0.06881753
C	-0.13544527	3.83745002	-0.28697900
C	3.56558816	-2.35027606	0.69457026
C	4.45226359	-2.04261113	-0.36738142
C	5.83489631	-2.13093170	-0.09967020
C	6.30352806	-2.48608900	1.17550848
C	5.39841573	-2.75022091	2.21614690
C	4.00599202	-2.68250045	1.99935758

C	4.55922591	-0.27647384	-2.19921939
C	3.95641745	-1.63438510	-1.75778942
C	4.26521985	-2.73877050	-2.80386595
C	-2.09496209	-1.79801303	-4.22858392
C	-1.42601369	-2.83060050	-3.28680407
C	-0.68810158	-3.92012042	-4.11067848
C	-2.23275978	-3.51692653	-0.92385398
C	-2.43841731	-3.46447191	-2.32617919
C	-3.63584266	-4.02530586	-2.82127023
C	-4.59113008	-4.57762913	-1.95380523
C	-4.37323205	-4.57929892	-0.56601470
C	-3.18683960	-4.04913370	-0.01921853
C	3.16999930	-1.81964463	4.22990194
C	3.03169322	-2.92958608	3.15415742
C	3.21939463	-4.33620716	3.77781743
C	-3.86851889	-2.92713393	2.14216732
C	-2.97353934	-4.01954507	1.49648999
C	-3.21745182	-5.40065912	2.15469739
C	-3.54111435	2.56707237	0.85607749
C	-3.75798483	2.83320365	2.23181018
C	-5.09480114	2.94504806	2.66978135
C	-6.16398450	2.77070334	1.77727740
C	-5.91804434	2.47670652	0.42631841
C	-4.60059409	2.36857147	-0.06543196
C	-2.76012596	2.02819480	4.43430411
C	-2.60685068	2.99214494	3.22991805
C	-2.48509309	4.46158528	3.71462047
C	1.55162710	2.03484212	-4.17541426
C	1.22484094	3.21440057	-3.22327409
C	0.87560033	4.50173761	-4.01770028
C	2.23050053	3.37948876	-0.82565801
C	2.36957869	3.47528146	-2.23650365
C	3.64277071	3.82458313	-2.73808400
C	4.72925765	4.04331184	-1.87936494
C	4.56467522	3.92802897	-0.48887851
C	3.31303253	3.60253743	0.06955753
C	-4.81028086	0.58427025	-1.84973239
C	-4.35295972	2.03389227	-1.53837615
C	-5.04089585	3.05091476	-2.48508996
C	3.84910009	2.21474186	2.12163095
C	3.15606452	3.49740248	1.58988137
C	3.68462878	4.76004464	2.31719692
H	2.15928990	-4.23985766	-0.15721740
H	0.01374583	-4.68720407	-0.79407548
H	-2.09035716	4.50167090	0.10570932
H	0.09236591	4.84011060	-0.63402843
H	6.54660928	-1.91135332	-0.89121075
H	7.37356716	-2.54723076	1.36087655
H	5.77479321	-3.00615321	3.20342411
H	2.87046163	-1.49911451	-1.72529231
H	-0.68185449	-2.27133661	-2.71066267
H	5.64952086	-0.33422200	-2.32140413

H	4.33623150	0.51116588	-1.47037171
H	4.12686115	0.02540405	-3.16097218
H	5.34685608	-2.90291528	-2.90338366
H	3.87420104	-2.44590112	-3.78676979
H	3.80361516	-3.69583289	-2.52692461
H	-2.80449003	-2.26902199	-4.92308256
H	-1.32254105	-1.29124053	-4.81966496
H	-2.62564968	-1.03275979	-3.65124048
H	-0.15537418	-4.62718582	-3.46092525
H	0.04810025	-3.45268349	-4.77720509
H	-1.39047365	-4.49620356	-4.72883873
H	-3.82703892	-4.01326082	-3.89093547
H	-5.50958523	-4.99789561	-2.35757875
H	-5.12814876	-4.99670135	0.09498358
H	2.00951242	-2.87145751	2.76539836
H	-1.93435340	-3.73479137	1.69415372
H	4.16921207	-1.82760094	4.68561709
H	2.43116225	-1.97032552	5.02783482
H	3.00223413	-0.82998056	3.78928173
H	4.21713412	-4.45043008	4.22152736
H	3.09347848	-5.12682038	3.02668819
H	2.47995040	-4.49942535	4.57281194
H	-3.64635725	-1.94552103	1.70976001
H	-3.68668806	-2.87805314	3.22423730
H	-4.93399410	-3.14429461	1.98571735
H	-4.26310594	-5.72044384	2.05627228
H	-2.98806425	-5.35016709	3.22727970
H	-2.58416598	-6.17689753	1.70569498
H	-5.29947096	3.15605163	3.71621420
H	-7.18742986	2.85607804	2.13536784
H	-6.75500489	2.33342110	-0.25221318
H	-1.67144544	2.72935974	2.72435084
H	0.33419530	2.91244167	-2.66486547
H	-3.64588919	2.26830829	5.03710641
H	-1.88189603	2.10155841	5.08911234
H	-2.84948193	0.98855856	4.09791625
H	-2.32248919	5.14741499	2.87340746
H	-1.63955665	4.56658561	4.40711506
H	-3.39470875	4.78260436	4.23965277
H	2.49014678	2.19811592	-4.72282401
H	0.74544023	1.92106836	-4.91315081
H	1.60700964	1.10254855	-3.60389611
H	0.61877670	5.33497653	-3.34912053
H	0.01797111	4.31598210	-4.67749265
H	1.71657427	4.82553897	-4.64518897
H	3.78469864	3.90904182	-3.81236139
H	5.70268852	4.30023279	-2.29103528
H	5.41309230	4.10289565	0.16751518
H	-3.27590251	2.07497341	-1.72940807
H	2.09125543	3.39923189	1.82185778
H	-5.88668662	0.45778852	-1.67057382
H	-4.26875604	-0.13501836	-1.22532693

H	-4.61199343	0.34243755	-2.90215854
H	-4.79320745	2.81839107	-3.52912535
H	-4.71287726	4.07784991	-2.27722156
H	-6.13419817	3.02081851	-2.38845715
H	3.41330264	1.32476402	1.65589240
H	3.71688426	2.13592313	3.20957520
H	4.92756149	2.22905377	1.91179455
H	3.20144195	5.67161751	1.94152555
H	4.76922821	4.87930519	2.19635045
H	3.48025851	4.68376708	3.39357966
O	0.30453625	-0.09405950	-1.92360817
O	1.55409344	-1.08043994	0.69701172
O	-1.74442276	1.19786168	0.11043215
Hf	-0.01548074	0.02960366	-0.14937699

η^2 -ozone ComplexFig. S108: ONCCNO η^2 -ozone Complex

E	E_{zp}	H	G
-2818.9460	-2817.7886	-2817.7152	-2817.9070
O	-1.79928700	1.01970500	-0.01350000
O	1.79919000	-1.01944000	-0.01142900
O	0.51153300	1.04323900	-2.04708100
N	-0.82190900	-2.95655900	0.69604100
N	2.26266800	-2.29231300	-0.26981100
N	0.82181400	2.95649100	0.69584000
N	-2.26291400	2.29279400	-0.27006500
C	0.24843700	-3.72178600	0.35272800
C	1.55604200	-3.43779200	-0.06226600
C	-0.24830500	3.72191200	0.35233700
C	-1.55601500	3.43811600	-0.06247600
C	-2.09693900	-3.54486900	1.07201300
C	-2.36584300	-3.74287300	2.45037700
C	-3.60727800	-4.31618400	2.79392100
C	-4.53662100	-4.67008300	1.80144100
C	-4.25001300	-4.44140000	0.44673800
C	-3.02600700	-3.86068700	0.04948700
C	-1.89108700	-2.01534700	4.23410300

C	-1.38148600	-3.30736600	3.53908800
C	-1.10797100	-4.42659100	4.57410500
C	4.69959700	-0.70080400	2.25423800
C	4.34498200	-2.13315800	1.77198200
C	5.05105600	-3.20591700	2.63882200
C	3.65141600	-2.33880100	-0.70631200
C	4.66616900	-2.28571400	0.28272700
C	6.00427400	-2.33497700	-0.15835500
C	6.30884200	-2.42907100	-1.52655700
C	5.28126200	-2.45916000	-2.48191600
C	3.92457500	-2.40159300	-2.09509400
C	-3.82716100	-2.65276600	-2.03929500
C	-2.74855200	-3.58545100	-1.43111800
C	-2.64398300	-4.90821600	-2.23568600
C	3.00097600	-1.23702400	-4.16110100
C	2.82019200	-2.40402400	-3.15678300
C	2.76459200	-3.76687500	-3.89731200
C	2.09702900	3.54444400	1.07172100
C	3.02597300	3.86068900	0.04920900
C	4.25004200	4.44120500	0.44656900
C	4.53685400	4.66931400	1.80131600
C	3.60763200	4.31502600	2.79377100
C	2.36613700	3.74190500	2.45014100
C	3.82747500	2.65378800	-2.03995100
C	2.74854300	3.58588200	-1.43146600
C	2.64351400	4.90889900	-2.23557900
C	-4.69732500	0.70277500	2.25456600
C	-4.34485500	2.13567800	1.77230000
C	-5.05232500	3.20739000	2.63925300
C	-3.65176300	2.33953700	-0.70623300
C	-4.66634100	2.28757000	0.28304200
C	-6.00451200	2.33684600	-0.15785900
C	-6.30928900	2.42981900	-1.52609300
C	-5.28187700	2.45877600	-2.48167400
C	-3.92514800	2.40121100	-2.09502000
C	1.89111400	2.01371600	4.23319100
C	1.38180400	3.30618900	3.53880000
C	1.10878200	4.42501000	4.57439500
C	-3.00179400	1.23390400	-4.15956100
C	-2.82090800	2.40226900	-3.15684900
C	-2.76539300	3.76412000	-3.89921600
H	0.01847600	-4.78081800	0.40240200
H	2.15065900	-4.31821900	-0.28116600
H	-0.01810200	4.78090700	0.40170700
H	-2.15058300	4.31864700	-0.28109200
H	-3.84967500	-4.48542200	3.83979500
H	-5.48758600	-5.11505600	2.08564900
H	-4.98502900	-4.70421700	-0.30961100
H	-0.42737500	-3.05692000	3.06160700
H	3.26484200	-2.25620100	1.90759600
H	-2.85106600	-2.19034800	4.73862700
H	-2.02737100	-1.21284100	3.50043900

H	-1.16696400	-1.67719400	4.98764500
H	-2.01060300	-4.68370800	5.14348600
H	-0.34763200	-4.09577000	5.29385900
H	-0.74422300	-5.34154200	4.08889000
H	5.77385800	-0.50013900	2.14369700
H	4.43939800	-0.58074300	3.31468600
H	4.14656200	0.04852500	1.67726900
H	4.79720700	-4.22094400	2.30644700
H	4.74482000	-3.10303200	3.68828500
H	6.14339600	-3.10350100	2.60264600
H	6.81076300	-2.29710300	0.56930100
H	7.34729100	-2.46943900	-1.84767700
H	5.53195600	-2.51548500	-3.53790200
H	-1.79563300	-3.05688300	-1.53039100
H	1.85231100	-2.24878300	-2.66986900
H	-4.82152900	-3.12013200	-2.03538900
H	-3.56536900	-2.41514200	-3.07773100
H	-3.88446100	-1.70965500	-1.48403200
H	-3.58782600	-5.46988400	-2.21018100
H	-1.85452300	-5.56000500	-1.83809700
H	-2.40787000	-4.69043700	-3.28513300
H	2.99709300	-0.27307900	-3.64113500
H	2.16559500	-1.22963700	-4.87102700
H	3.93694900	-1.32980900	-4.72940400
H	3.69973900	-3.96737300	-4.43778400
H	1.94551400	-3.76269600	-4.62778800
H	2.59433800	-4.59846700	-3.20030100
H	4.98498100	4.70426100	-0.30977400
H	5.48787500	5.11413900	2.08557100
H	3.85014000	4.48385900	3.83968200
H	1.79584000	3.05697000	-1.53091000
H	-3.26487200	2.26033200	1.90782700
H	4.82166600	3.12155200	-2.03605800
H	3.56563300	2.41630200	-3.07840500
H	3.88520000	1.71054900	-1.48495000
H	1.85370400	5.56018400	-1.83785500
H	2.40765800	4.69140400	-3.28514200
H	3.58710100	5.47097800	-2.20971300
H	-5.77128900	0.50054800	2.14400800
H	-4.43695000	0.58311300	3.31502100
H	-4.14318000	-0.04572200	1.67758500
H	-4.80027800	4.22278300	2.30663000
H	-4.74546300	3.10513700	3.68859500
H	-6.14450900	3.10319700	2.60362500
H	-6.81089600	2.29978700	0.56994600
H	-7.34778400	2.47018600	-1.84706500
H	-5.53274600	2.51426000	-3.53766500
H	0.42756400	3.05622700	3.06133200
H	-1.85297700	2.24771100	-2.66983100
H	2.85119400	2.18825000	4.73770000
H	2.02706100	1.21148700	3.49916900
H	1.16697600	1.67548400	4.98668500

H	0.34851400	4.09403600	5.29415800
H	0.74517800	5.34029300	4.08970200
H	2.01160700	4.68158500	5.14370800
H	-2.99773500	0.27063800	-3.63833400
H	-2.16656200	1.22563500	-4.86965100
H	-3.93791600	1.32586000	-4.72776100
H	-2.59514200	4.59663700	-3.20331400
H	-3.70055200	3.96386500	-4.43994500
H	-1.94633500	3.75896600	-4.62970400
O	0.00102100	0.00092300	-3.02404800
O	-0.50969600	-1.04217700	-2.04801400
Hf	-0.00002300	0.00009800	-0.32883700
O	0.79399000	1.57451500	0.73072900
O	-0.79513800	-1.57459900	0.72926700

9.5 Eight Oxygen Atoms

Bare Complex with Two Adsorbed Oxygen Molecules

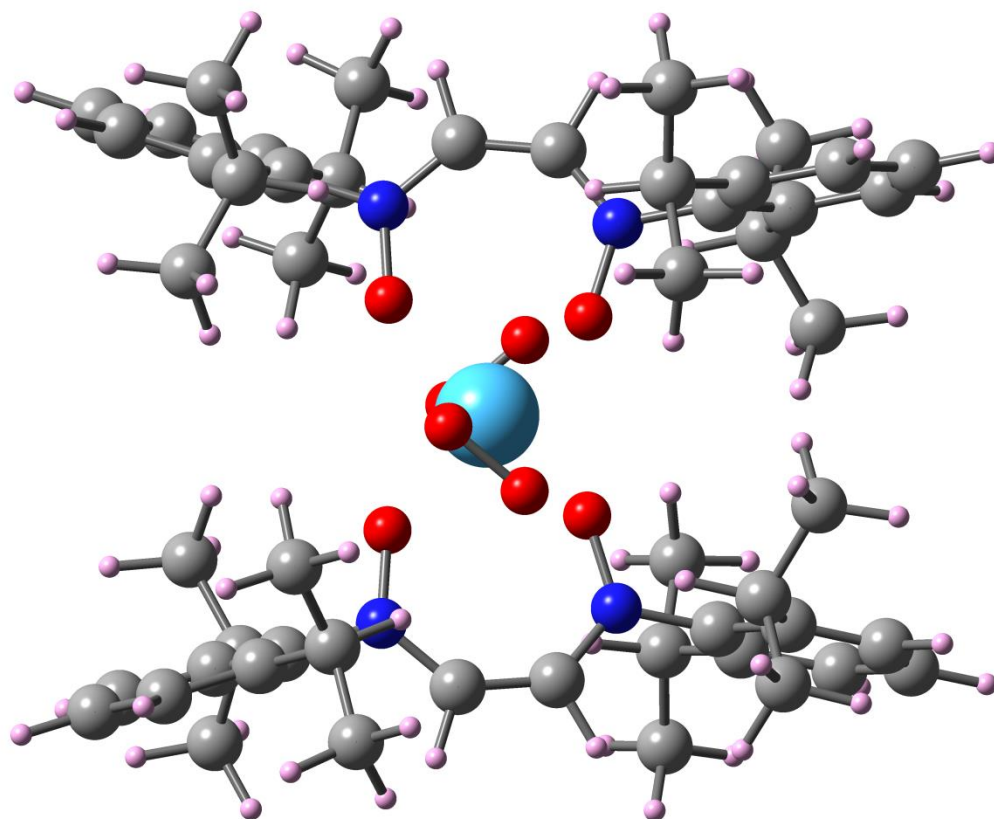


Fig. S109: ONCCNO Bare Complex with Two Adsorbed Oxygen Molecules

E	E_{zp}	H	G
-2894.1185	-2892.9588	-2892.8839	-2893.0768

O	-1.52284493	-1.57276383	-0.14401337
O	1.23253417	1.35616998	0.77458804
O	0.35868282	-1.03479414	1.89865456
O	-0.68643847	-0.15439850	2.17334595
N	-1.58020515	2.87239551	-0.35522370
N	1.63883161	2.63299305	0.42603381
N	1.61612483	-2.64316567	-0.41189849
N	-1.60641499	-2.85040390	0.37047373
C	-0.53335630	3.74390395	-0.33851085
C	0.82199869	3.63611925	-0.00575782
C	0.79693275	-3.62853788	0.05365891
C	-0.56030877	-3.72223532	0.38625785
C	-2.91815801	3.29856141	-0.73653025
C	-3.21932185	3.48216254	-2.11020033
C	-4.52632236	3.90609639	-2.43572795
C	-5.49138497	4.11160192	-1.43897518
C	-5.16915980	3.89976167	-0.08833139

C	-3.87508382	3.49304384	0.29465565
C	-2.71610257	2.13613008	-4.20806089
C	-2.20637772	3.22762065	-3.23157647
C	-1.87024843	4.53708712	-3.99371093
C	4.37983830	1.21645829	-2.20987654
C	3.63281766	2.48952983	-1.73493972
C	3.91148661	3.68165321	-2.68809575
C	3.03396906	2.89961960	0.74715574
C	3.99753801	2.83868776	-0.28933418
C	5.33951915	3.10748754	0.05730264
C	5.69933010	3.40054241	1.38173488
C	4.72366909	3.42861279	2.39212710
C	3.36765731	3.17873205	2.09753677
C	-4.26192497	1.97882904	2.28718939
C	-3.54893092	3.25771737	1.77235755
C	-3.90471610	4.48559635	2.64891102
C	2.50049184	1.94298497	4.13168037
C	2.31922507	3.18128589	3.21350922
C	2.34594011	4.49490422	4.03522297
C	3.00597110	-2.92850610	-0.74064921
C	3.97842318	-2.87001407	0.28762904
C	5.31403768	-3.15937971	-0.06723048
C	5.65942891	-3.46879853	-1.39168309
C	4.67545242	-3.49315019	-2.39410571
C	3.32507547	-3.22393645	-2.09109873
C	4.39831974	-1.23343887	2.18728989
C	3.63116882	-2.50215009	1.73309119
C	3.90462875	-3.68768330	2.69586779
C	-4.23969075	-1.97926273	-2.32133832
C	-3.54197676	-3.25648545	-1.78183587
C	-3.89113400	-4.49161393	-2.65075968
C	-2.95113037	-3.26931595	0.73704779
C	-3.89210610	-3.47367028	-0.30679520
C	-5.19337444	-3.87159002	0.06064902
C	-5.53767174	-4.06564205	1.40849564
C	-4.58769134	-3.85123895	2.41776496
C	-3.27431937	-3.43534275	2.10791904
C	2.45060650	-1.98793357	-4.12124859
C	2.26768646	-3.22281255	-3.19861603
C	2.27868386	-4.53865893	-4.01692403
C	-2.79997650	-2.07462497	4.20398472
C	-2.27766192	-3.17301659	3.24212907
C	-1.95400306	-4.47751176	4.01831865
H	-0.82765135	4.73302553	-0.67267057
H	1.37242205	4.56340378	-0.12677275
H	1.34393680	-4.55346603	0.20404677
H	-0.85818269	-4.70118318	0.74614889
H	-4.79119023	4.06105194	-3.47847368
H	-6.49439409	4.43057030	-1.71319830
H	-5.92755715	4.05664216	0.67410962
H	-1.27849673	2.84874952	-2.79433295
H	2.56258508	2.26710466	-1.78546757

H	-3.64381952	2.44170985	-4.71021580
H	-2.90000925	1.19563486	-3.67701018
H	-1.95947707	1.94237239	-4.97919270
H	-2.75843603	4.95287164	-4.48792424
H	-1.11608792	4.34070668	-4.76697341
H	-1.47286764	5.30674482	-3.31836961
H	5.46886769	1.35893821	-2.20124464
H	4.08025074	0.96823184	-3.23615337
H	4.14025759	0.35806917	-1.57161744
H	3.36619200	4.58198230	-2.37550882
H	3.59624048	3.43009338	-3.70904492
H	4.98086161	3.93041492	-2.71709208
H	6.10597789	3.07737620	-0.71296634
H	6.73959303	3.60068009	1.62849482
H	5.01749995	3.64621240	3.41570058
H	-2.47343393	3.07980789	1.86906757
H	1.32708571	3.09229535	2.75894429
H	-5.35424477	2.07956386	2.22463848
H	-3.99596102	1.79345580	3.33636638
H	-3.95799606	1.10729584	1.69763787
H	-4.98456698	4.68394401	2.65522669
H	-3.39746209	5.39234019	2.29405306
H	-3.59603938	4.30542536	3.68711673
H	2.39765281	1.01949400	3.55241340
H	1.73392583	1.93971320	4.91774943
H	3.48680227	1.94757154	4.61595009
H	3.29391737	4.61770275	4.57526749
H	1.53960092	4.48702771	4.78031532
H	2.20831423	5.37402981	3.39219824
H	6.08700911	-3.13206802	0.69661511
H	6.69502599	-3.68447372	-1.64485828
H	4.95835985	-3.72360130	-3.41792633
H	2.56415308	-2.26635116	1.79186866
H	-2.46412243	-3.08536903	-1.86379617
H	5.48534585	-1.38902236	2.16758938
H	4.11371662	-0.97164644	3.21446075
H	4.16164237	-0.37844374	1.54339998
H	3.34528442	-4.58447230	2.39818528
H	3.60272437	-3.42180520	3.71721214
H	4.97102510	-3.94954556	2.71692976
H	-5.33340784	-2.07399670	-2.27600158
H	-3.95518591	-1.80581392	-3.36764609
H	-3.94089664	-1.10340054	-1.73569400
H	-3.39498148	-5.39754661	-2.27855175
H	-3.56507766	-4.32421234	-3.68576994
H	-4.97190946	-4.68373579	-2.67232463
H	-5.94011749	-4.03532643	-0.71173106
H	-6.54596697	-4.37795062	1.67070222
H	-4.86950694	-3.99263096	3.45796939
H	1.27983477	-3.12539756	-2.73646806
H	-1.34306565	-2.79817595	2.81594501
H	3.43348223	-2.00056404	-4.61235367

H	2.35773354	-1.06242398	-3.54357899
H	1.67848429	-1.98160909	-4.90181714
H	1.46545674	-4.52752859	-4.75443646
H	2.14165576	-5.41532220	-3.37040547
H	3.22059199	-4.66872484	-4.56580430
H	-2.97831241	-1.13838190	3.66364982
H	-2.05271783	-1.87459019	4.98254989
H	-3.73337868	-2.37698069	4.69748408
H	-1.54661250	-5.25215030	3.35468348
H	-2.85013339	-4.88939922	4.50126695
H	-1.21185266	-4.27625453	4.80188292
O	0.36367920	1.03509407	-1.90110415
O	-0.67483039	0.14200061	-2.17173657
Hf	-0.15925993	0.00316263	-0.00311687
O	-1.50605343	1.58728773	0.14368292
O	1.21569459	-1.37212165	-0.78231394

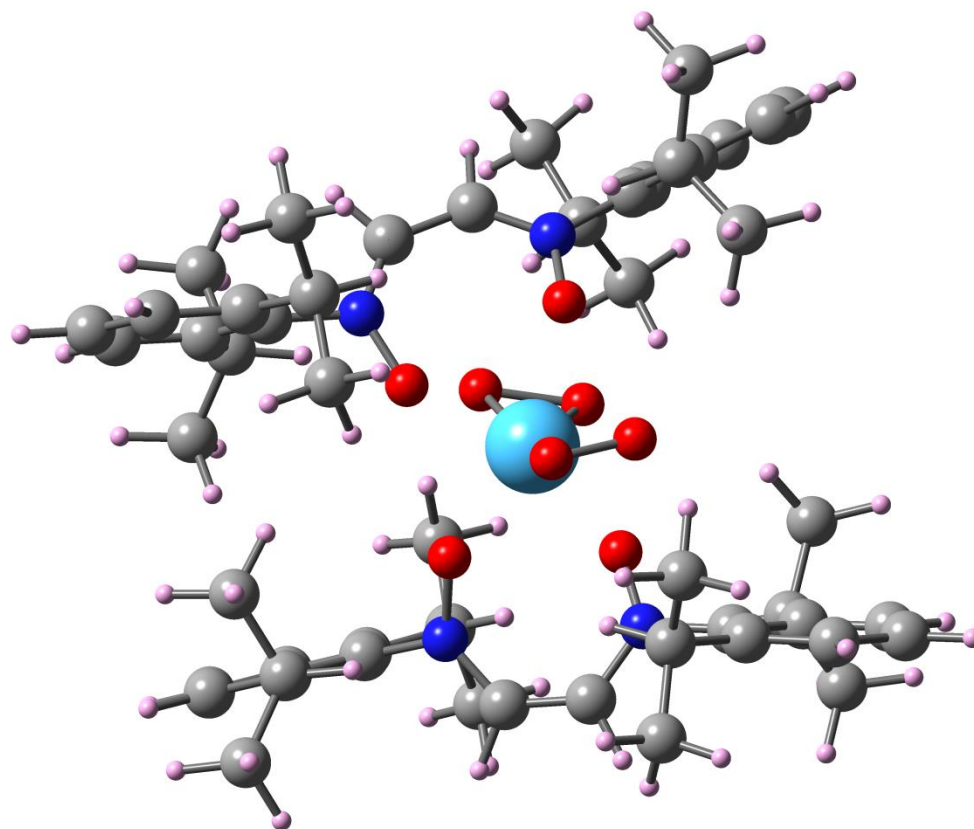
Peroxo Complex with Adsorbed Oxygen Molecule (planar conformation)

Fig. S110: ONCCNO Peroxo Complex with Adsorbed Oxygen Molecule (planar conformation)

E	E_{zp}	H	G
-2894.1053	-2892.9439	-2892.8708	-2893.0568
O	1.09453851	0.64168486	-1.72215960
O	-0.44920650	0.86269674	-1.55395465
O	0.72472463	-0.17828199	2.29700119
O	1.97755011	0.11807699	1.74553896
C	1.86961366	3.85281228	-0.76802091
C	2.81711362	4.35717451	0.16690749
C	3.97662940	4.95966565	-0.35978012
C	4.17524367	5.06993562	-1.74402779
C	3.21284711	4.57567438	-2.63515078
C	2.03589612	3.94504340	-2.17834069
C	3.61575584	3.28402194	2.32298558
C	2.63450267	4.30616161	1.68960125
C	2.79672312	5.70886105	2.33225041
C	-2.58549588	0.97809102	4.23428533
C	-2.83471683	2.29757766	3.45336296
C	-3.17432730	3.46201469	4.41681845
C	-3.62039813	1.93345710	1.01523131
C	-3.91772350	2.08532280	2.39120624

C	-5.27625808	1.99368488	2.75741857
C	-6.27198132	1.76367271	1.79379369
C	-5.93131537	1.60395257	0.44197041
C	-4.58719080	1.67148744	0.01594850
C	1.73107594	2.48278973	-4.24813266
C	1.03995505	3.40789735	-3.21545982
C	0.31662789	4.58175803	-3.93281269
C	-4.82844527	0.13755747	-2.00486832
C	-4.23469192	1.46105415	-1.46203362
C	-4.71066208	2.66255646	-2.32311129
C	-2.19810194	-3.16578687	-1.10254210
C	-2.19961130	-3.11383468	-2.51993212
C	-3.41640923	-3.39907346	-3.17709656
C	-4.57615745	-3.70847320	-2.45011637
C	-4.54848044	-3.73175339	-1.04524352
C	-3.35827875	-3.46059834	-0.33958706
C	-1.15957381	-1.42301367	-4.11221884
C	-0.95398639	-2.75006220	-3.33430784
C	-0.54991376	-3.90411124	-4.28878724
C	2.75805859	-1.95048308	4.36979192
C	2.55272643	-2.97428924	3.22512946
C	2.42726925	-4.41361541	3.79521389
C	3.42993485	-2.76580488	0.78767671
C	3.67277325	-2.89583405	2.18107375
C	5.01828141	-2.95772781	2.60289483
C	6.07309455	-2.86442591	1.68360003
C	5.80270064	-2.72386643	0.31298946
C	4.47906097	-2.68348924	-0.16924175
C	-4.09482764	-2.23263150	1.74923475
C	-3.34255643	-3.46985831	1.19135915
C	-3.92118296	-4.78438359	1.77338259
C	4.55675407	-1.13083840	-2.17287013
C	4.22316767	-2.56222391	-1.67554994
C	5.00414079	-3.63115297	-2.48250471
H	4.72513491	5.35269799	0.32184636
H	5.07867114	5.53849815	-2.12703416
H	3.38351594	4.65873135	-3.70430445
H	1.62571719	3.95251849	1.91998131
H	-1.89116224	2.54823231	2.95521042
H	4.65982073	3.55077430	2.10861324
H	3.42255977	2.27625287	1.94289228
H	3.48691630	3.26510205	3.41341561
H	3.81960040	6.09325409	2.22887997
H	2.57546229	5.64978011	3.40606043
H	2.11414857	6.44191294	1.88175805
H	-3.49505918	0.65239774	4.75756928
H	-1.79377875	1.12564868	4.97965923
H	-2.26484532	0.18331848	3.55344188
H	-3.36681544	4.39575400	3.87219598
H	-2.33395352	3.63284030	5.10174461
H	-4.05674651	3.24065013	5.03088660
H	-5.55595259	2.10401772	3.80127040

H	-7.31383284	1.70121468	2.09887004
H	-6.71188499	1.40988056	-0.28812251
H	0.29803671	2.77882480	-2.71806690
H	-3.14688682	1.38028594	-1.56702357
H	2.49613170	3.00674267	-4.83731132
H	0.97919094	2.09242651	-4.94676096
H	2.17992749	1.62956300	-3.73237151
H	1.02622078	5.20069608	-4.49824484
H	-0.20545383	5.24698531	-3.22906675
H	-0.42539804	4.18902950	-4.64018666
H	-4.50698244	-0.71830952	-1.40285658
H	-4.48469438	-0.02852798	-3.03315892
H	-5.92650372	0.15707323	-2.01765152
H	-5.80214966	2.77363944	-2.27778897
H	-4.42867554	2.50869148	-3.37235200
H	-4.26665143	3.61048657	-1.98981061
H	-3.45432145	-3.37318419	-4.26319783
H	-5.50323272	-3.92551318	-2.97626662
H	-5.45572991	-3.96742018	-0.49490860
H	-0.12003366	-2.58139803	-2.64574397
H	1.60540455	-2.71652100	2.74169913
H	-2.02018831	-1.48388311	-4.79343549
H	-0.26601088	-1.20404977	-4.71136204
H	-1.30008415	-0.58680294	-3.41819500
H	-0.37717578	-4.83902280	-3.73912188
H	0.37516111	-3.64448029	-4.81967334
H	-1.32521186	-4.09557130	-5.04305009
H	3.65820504	-2.17118591	4.95961433
H	1.89720912	-1.97819646	5.05066171
H	2.83801204	-0.93662169	3.96612236
H	2.22771725	-5.14890422	3.00434599
H	1.60521717	-4.46391155	4.52161694
H	3.35052487	-4.71680018	4.30720583
H	5.23925455	-3.05873906	3.66197806
H	7.10256676	-2.89954406	2.03313556
H	6.62774412	-2.65670187	-0.39113514
H	-2.30368576	-3.38287096	1.52654762
H	3.15622006	-2.71391725	-1.86183368
H	-5.14986969	-2.23519513	1.44223228
H	-3.62761134	-1.30849104	1.39308470
H	-4.06105045	-2.23226169	2.84711364
H	-3.83065919	-4.78194998	2.86766867
H	-3.38749277	-5.66346617	1.38890444
H	-4.98524979	-4.90440657	1.53020404
H	3.92048265	-0.39728368	-1.66814017
H	4.37337008	-1.05274756	-3.25303359
H	5.60988745	-0.87808213	-1.98540693
H	4.77511901	-4.64625563	-2.13153968
H	6.09046252	-3.48784138	-2.41230167
H	4.73193836	-3.56722625	-3.54453950
O	1.70428459	-1.59309526	-0.43850377
N	2.06031322	-2.71792070	0.30876477

O	-0.87223660	-1.67509299	0.23196645
O	0.87706512	2.19688861	0.65740984
O	-1.50124936	0.93249327	0.94133290
N	-0.95308717	-2.90948877	-0.40459684
N	-2.20218282	2.01914786	0.61132929
N	0.67848081	3.20219172	-0.21691114
C	-1.80089939	3.13395516	-0.00451376
H	-2.62445435	3.81826742	-0.17620240
C	-0.54546085	3.62413355	-0.48972117
H	-0.60649801	4.50911935	-1.11057537
C	1.27057050	-3.82425141	0.25849618
H	1.75817660	-4.74685981	0.55338042
C	-0.05011222	-3.90785216	-0.18382674
H	-0.43527798	-4.90080424	-0.39448527
Hf	0.38414662	0.00491529	0.08931041

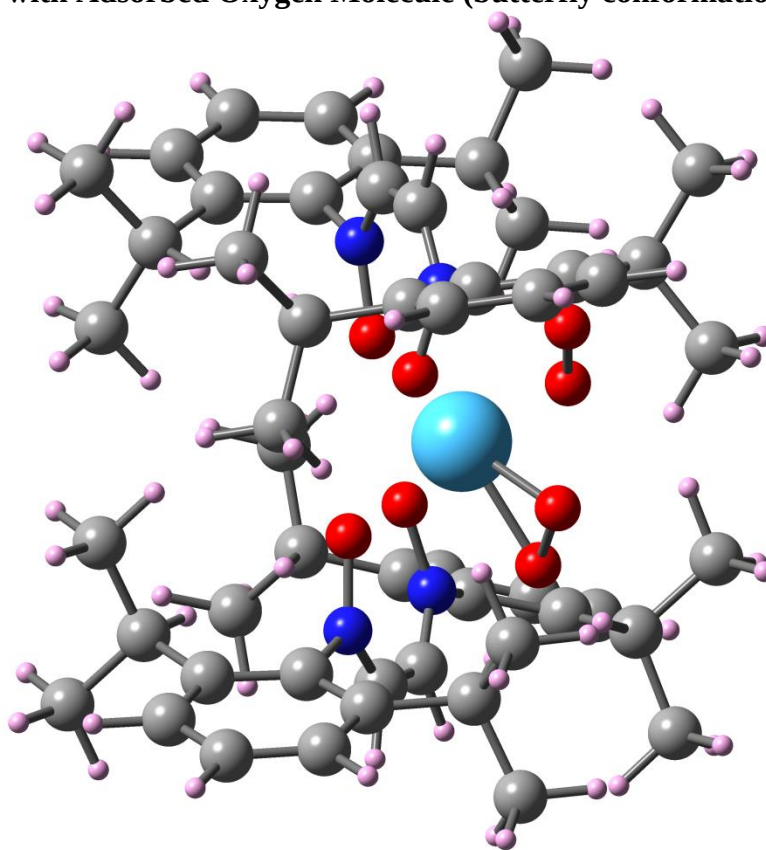
Peroxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

Fig. S111: ONCCNO Peroxo Complex with Adsorbed Oxygen Molecule (butterfly conformation)

E	E_{zp}	H	G
-2894.1152	-2892.9543	-2892.8800	-2893.0709

O	0.66227500	-1.40421900	0.85923600
O	1.83592900	0.89499200	-0.06286000
O	1.17911500	-0.97786000	-2.12322600
N	-0.61521500	2.83730200	0.75599700
N	2.35604900	2.12998100	-0.41385600
N	-2.35708500	-2.10234300	-0.33935000
N	0.60820200	-2.75096400	0.85201500
C	0.47770900	3.58610200	0.43233400
C	1.73958500	3.29858000	-0.10450700
C	-1.66703600	-3.22851000	-0.19549400
C	-0.37774900	-3.50388400	0.37123800
C	-1.77094100	3.47144500	1.37959700
C	-2.76470300	4.04811800	0.55000800
C	-3.86518000	4.66110500	1.18706900
C	-3.97238400	4.68311600	2.58634700
C	-2.98225900	4.08304800	3.38118500
C	-1.86163800	3.45970200	2.79374900

C	-3.86160300	3.18170400	-1.56749200
C	-2.68877600	4.00817000	-0.97847700
C	-2.65434500	5.43494200	-1.58537000
C	2.75572300	1.30761900	-4.29671600
C	2.86263100	2.50566000	-3.31546200
C	3.06459600	3.83914500	-4.08146600
C	3.72544300	2.09068400	-0.90703500
C	3.97501800	2.27263500	-2.29021000
C	5.31877800	2.20433200	-2.72007300
C	6.35891000	1.95083300	-1.81431000
C	6.07864000	1.75994700	-0.45075800
C	4.75684200	1.82584300	0.03294600
C	-1.42034800	1.57029500	4.42515200
C	-0.80854200	2.78149400	3.67354700
C	-0.15704300	3.78062300	4.66379500
C	4.61818700	0.07774300	1.85725400
C	4.46482500	1.58406900	1.51679900
C	5.34986600	2.45914100	2.43976700
C	-3.72835700	-2.12137700	-0.86982000
C	-3.94451800	-2.38025300	-2.24724700
C	-5.28707800	-2.36566200	-2.68774300
C	-6.34300600	-2.09149700	-1.80805800
C	-6.08558600	-1.82494000	-0.45317300
C	-4.77057800	-1.83386900	0.05138200
C	-2.84612900	-1.58968500	-4.39818500
C	-2.82665600	-2.64534200	-3.26136800
C	-2.92792100	-4.08304000	-3.83679000
C	1.36355400	-1.55761500	4.41438400
C	0.80993900	-2.85559900	3.76678800
C	0.30741800	-3.84986400	4.84312800
C	1.79080200	-3.40405400	1.43771100
C	1.86885600	-3.47415300	2.84988200
C	3.00520600	-4.10460000	3.39568900
C	4.00770200	-4.62991700	2.56348600
C	3.90341100	-4.51973900	1.16883600
C	2.79306300	-3.88991500	0.56417400
C	-4.67761600	-0.00554100	1.80045900
C	-4.51520000	-1.52559200	1.53084800
C	-5.42346900	-2.36123300	2.46820800
C	3.95400000	-2.97595900	-1.50344800
C	2.72440400	-3.74769200	-0.96016400
C	2.59649000	-5.13562900	-1.64225900
H	0.30942800	4.64003100	0.62759900
H	2.35365200	4.16818600	-0.31342600
H	-2.19442000	-4.11079500	-0.53936700
H	-0.15882500	-4.56394900	0.44093100
H	-4.64472700	5.11727400	0.58204100
H	-4.82884000	5.16119500	3.05655800
H	-3.08172900	4.09705900	4.46385400
H	-1.76594800	3.50137800	-1.27446100
H	1.90407900	2.56829800	-2.79424000
H	-4.83354200	3.63761000	-1.33297600

H	-3.85158100	2.15914000	-1.17403300
H	-3.76517300	3.11996700	-2.65857500
H	-3.57588400	5.99087100	-1.36596900
H	-2.55048400	5.37518600	-2.67641900
H	-1.80955500	6.01763100	-1.19472200
H	3.69311000	1.15904300	-4.85108100
H	1.95479800	1.49480100	-5.02401200
H	2.50825200	0.38330100	-3.76263600
H	3.12609900	4.69440400	-3.39470300
H	2.22112700	4.00883800	-4.76312500
H	3.98307800	3.82572500	-4.68350700
H	5.54572500	2.33909700	-3.77435900
H	7.38569900	1.89623600	-2.16924300
H	6.89269400	1.55948300	0.24108400
H	-0.01771500	2.38795300	3.02663500
H	3.41965700	1.84673500	1.71102500
H	-2.22096100	1.88448800	5.10851300
H	-0.64743300	1.06541800	5.01976500
H	-1.83567100	0.84707000	3.71368600
H	-0.89421800	4.19149200	5.36629700
H	0.30625200	4.62224000	4.13304000
H	0.62175400	3.27791900	5.25263100
H	3.92429500	-0.51850000	1.25593700
H	4.39365700	-0.09780600	2.91834700
H	5.64229800	-0.27016700	1.66444600
H	6.41320000	2.20098400	2.35067600
H	5.06148100	2.30812200	3.48870000
H	5.24205800	3.52634300	2.20560500
H	-5.49840000	-2.55650200	-3.73599100
H	-7.36585300	-2.07948100	-2.17703900
H	-6.91245100	-1.61116600	0.21804400
H	-1.84957700	-2.53825300	-2.78101100
H	-0.05485600	-2.56016700	3.16135900
H	-3.77985700	-1.62104400	-4.97663000
H	-2.01267700	-1.77938400	-5.08617400
H	-2.71647500	-0.58075800	-3.99121000
H	-2.89371400	-4.84438600	-3.04440800
H	-2.08949600	-4.26862000	-4.51993200
H	-3.86004300	-4.23115100	-4.39898300
H	2.24160200	-1.77123600	5.03852000
H	0.59713700	-1.09540500	5.05008100
H	1.65206800	-0.83773700	3.64047100
H	-0.08691600	-4.76868100	4.38982300
H	-0.49405500	-3.38837600	5.43454400
H	1.10726700	-4.13465800	5.53845200
H	3.10751300	-4.18220800	4.47465400
H	4.87550800	-5.11542600	3.00369400
H	4.69669500	-4.91227200	0.53876600
H	-3.47623800	-1.77663900	1.77168600
H	1.85180700	-3.15140100	-1.24071200
H	-5.69543700	0.33203900	1.56242500
H	-3.96579100	0.56810600	1.19869200

H	-4.48651500	0.21448000	2.85927700
H	-5.15232600	-2.17077900	3.51489300
H	-5.31999500	-3.43765000	2.27776600
H	-6.48272900	-2.09914600	2.35220300
H	4.01855500	-1.98109800	-1.04986800
H	3.84548500	-2.83527300	-2.58518300
H	4.89446000	-3.51293600	-1.31621000
H	1.70540600	-5.67863500	-1.29729700
H	3.47210700	-5.76771700	-1.44055500
H	2.51349500	-5.00740400	-2.72857400
O	-0.15332700	1.64553500	-2.22918600
O	-1.31437200	0.86297700	-2.24611400
O	-0.11656200	-1.76675700	-1.85443300
O	-1.91442400	-0.88938100	0.06308100
O	-0.76971400	1.48502700	0.55833200
Hf	0.02105500	-0.01746200	-0.73971100

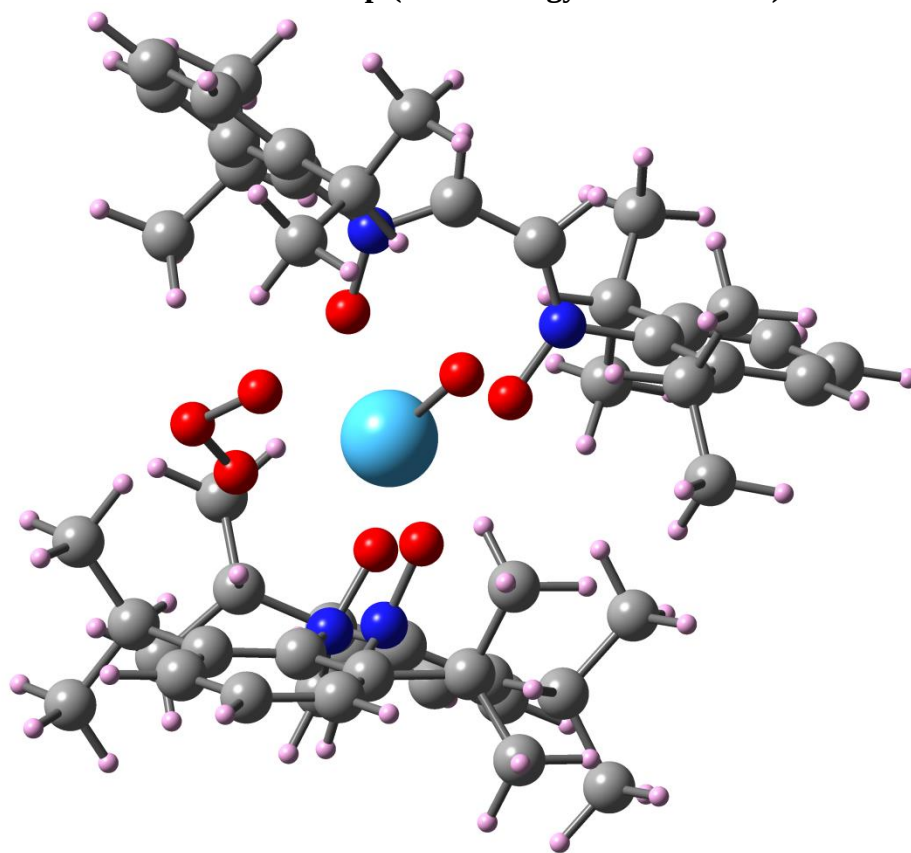
Oxo Complex with Adsorbed Ozone Group (lower energy conformation)

Fig. S112: ONCCNO Oxo Complex with Adsorbed Ozone Group (lower energy conformation)

E	E_{zp}	H	G
-2894.0939	-2892.9324	-2892.8580	-2893.0493
O	-0.10719300	-1.61059300	0.64513300
O	-0.90738200	1.90110700	0.82598100
O	1.80784000	2.00909500	0.35223200
N	-2.82682300	0.38088400	-1.20355200
N	-1.34773700	2.95611100	0.09394100
N	3.11440100	-1.38894600	-0.23224200
N	0.52968700	-2.54378800	1.43330300
C	-2.93643500	1.69750800	-1.39301400
C	-2.24901200	2.83745400	-0.86655300
C	2.95123800	-2.39857200	0.66511000
C	1.85019700	-2.88312000	1.37633500
C	-3.78518100	-0.49447900	-1.90935100
C	-3.44702500	-0.91039400	-3.21792300
C	-4.38735500	-1.72913900	-3.87988800
C	-5.58130400	-2.11696200	-3.25055700
C	-5.86248800	-1.70377400	-1.93793200
C	-4.96246600	-0.88067900	-1.22897500
C	-1.32027300	-1.75998600	-4.31506100

C	-2.13586400	-0.50814400	-3.90160400
C	-2.40461900	0.40190600	-5.12913900
C	1.96720700	4.39054100	-2.01572600
C	0.42653900	4.38958400	-1.83946400
C	-0.25419900	5.18452000	-2.98659100
C	-0.80395600	4.26983700	0.45844100
C	0.02328600	4.95286600	-0.47044300
C	0.50295800	6.21926000	-0.06957100
C	0.19673700	6.75257200	1.19044000
C	-0.60376300	6.03111800	2.09118200
C	-1.12686600	4.76941900	1.74677300
C	-5.32157500	-1.70128800	1.14690600
C	-5.26511000	-0.46328500	0.21351100
C	-6.57411300	0.36363900	0.30380200
C	-1.10613100	3.41783200	3.88701700
C	-1.99071300	3.99773400	2.75018400
C	-3.13882200	4.86623800	3.32407200
C	4.40604300	-1.12346700	-0.84663700
C	5.40195300	-0.44737800	-0.09769400
C	6.64654500	-0.22110500	-0.72518000
C	6.87309400	-0.62156500	-2.04987000
C	5.85688100	-1.26278100	-2.77743500
C	4.60374000	-1.53356800	-2.19169100
C	5.39361400	1.58666900	1.42851000
C	5.17418200	0.05456700	1.33172100
C	6.07828700	-0.69714000	2.34458300
C	-2.23077700	-4.14303100	-0.57023200
C	-1.00110200	-4.69574000	0.19922400
C	-0.81458400	-6.21188600	-0.05611800
C	-0.38298200	-3.30163600	2.27979700
C	-1.11963200	-4.36040500	1.68830000
C	-2.01003900	-5.07544400	2.51542800
C	-2.15477300	-4.74774300	3.87416800
C	-1.41917500	-3.68934100	4.42845800
C	-0.52203900	-2.93486700	3.64083700
C	2.85961700	-1.20002100	-3.99302600
C	3.50103800	-2.21426700	-3.00721400
C	4.00991800	-3.47361000	-3.75261900
C	-0.72327800	-0.68399400	4.80631400
C	0.24575600	-1.76520900	4.26208900
C	1.20945200	-2.25208200	5.37618400
H	-3.72381300	1.95139900	-2.09354300
H	-2.54324700	3.77981200	-1.31390100
H	3.88159600	-2.91682900	0.87182400
H	2.08013500	-3.70878400	2.04146100
H	-4.17749800	-2.06903900	-4.89041200
H	-6.29034600	-2.74869100	-3.78044700
H	-6.78335700	-2.02555300	-1.45874700
H	-1.50420900	0.05725000	-3.20488700
H	0.12394500	3.33913400	-1.91707800
H	-1.84753900	-2.36686900	-5.06425900
H	-1.10756900	-2.39276200	-3.44497600

H	-0.36157700	-1.44518700	-4.74421700
H	-2.98907600	-0.11739100	-5.90127100
H	-1.45137200	0.71249700	-5.57430200
H	-2.95374400	1.31013900	-4.84560700
H	2.38390800	5.40728500	-2.03238600
H	2.22322100	3.90493700	-2.96588600
H	2.44147400	3.82318800	-1.20869100
H	-1.35100600	5.17099200	-2.90762900
H	0.01851100	4.74577100	-3.95475900
H	0.06324200	6.23629900	-2.98917700
H	1.14052000	6.77946900	-0.74732200
H	0.58831100	7.72631800	1.47514000
H	-0.82733800	6.45267500	3.06697300
H	-4.44737800	0.16873100	0.57896300
H	-2.44708700	3.14187900	2.24143200
H	-6.13510100	-2.38103800	0.86110900
H	-5.49545600	-1.38477800	2.18352200
H	-4.37936500	-2.25927800	1.11408000
H	-7.44324400	-0.22589400	-0.01538100
H	-6.52838800	1.26052300	-0.32797900
H	-6.74966200	0.68343500	1.33917100
H	-0.34698100	2.74368000	3.47803700
H	-1.72553200	2.85241800	4.59622900
H	-0.60024100	4.22001100	4.44124600
H	-2.75792500	5.69757900	3.93076600
H	-3.77949400	4.25435100	3.97271100
H	-3.76339100	5.28960100	2.52634500
H	7.43505600	0.28797200	-0.17675500
H	7.83574600	-0.42814600	-2.51787800
H	6.04166700	-1.56013800	-3.80611400
H	4.13317000	-0.13533400	1.61051200
H	-0.11985400	-4.18210100	-0.20044200
H	6.43257100	1.86219900	1.20247600
H	5.16477200	1.93419100	2.44422900
H	4.73417200	2.11858900	0.73403900
H	5.90281200	-1.78082600	2.31508300
H	5.87608300	-0.34708900	3.36540800
H	7.14222800	-0.52524700	2.13358600
H	-3.16097200	-4.60230700	-0.20726100
H	-2.14045500	-4.36483500	-1.64249700
H	-2.29859000	-3.05713200	-0.44735800
H	0.04849800	-6.60941900	0.49364300
H	-0.65081900	-6.39305900	-1.12666400
H	-1.69981900	-6.78870200	0.24213500
H	-2.59055400	-5.89336300	2.09689300
H	-2.84307400	-5.31446900	4.49739100
H	-1.54575000	-3.43989900	5.47903200
H	2.70899600	-2.53168300	-2.32060500
H	0.84950300	-1.28331600	3.48821000
H	3.61190800	-0.79158400	-4.68226300
H	2.39387300	-0.37539700	-3.44368900
H	2.08431000	-1.69727900	-4.59213000

H	3.16895200	-3.97947200	-4.24544300
H	4.48237200	-4.18680100	-3.06430800
H	4.74111700	-3.22051700	-4.53143900
H	-1.38236300	-0.31661400	4.01086900
H	-0.15022500	0.16932600	5.19026600
H	-1.34784900	-1.07216100	5.62275500
H	1.92036900	-2.99677000	4.99451800
H	0.66118000	-2.70859600	6.21151200
H	1.78460700	-1.40540000	5.77287200
O	0.00812800	1.05054500	-1.82731400
O	2.03423300	1.74084300	1.73255000
O	1.33704500	0.57259300	2.07642500
O	2.07652800	-0.65090500	-0.76431300
O	-1.92513000	-0.27166800	-0.47965400
Hf	0.33621400	0.33787700	-0.17311800

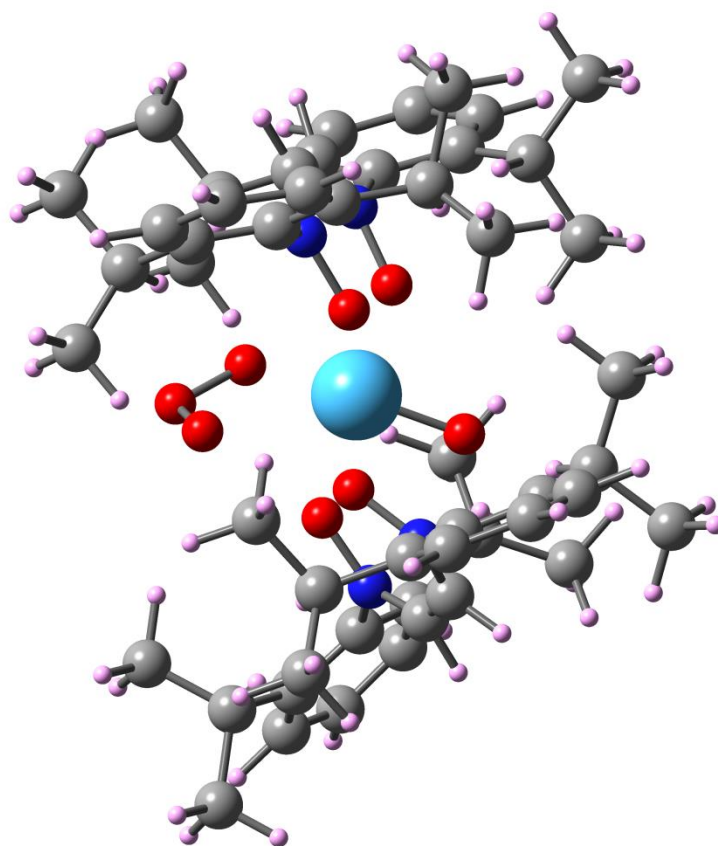
Oxo Complex with Adsorbed Ozone Group (higher energy conformation)

Fig. S113: ONCCNO Oxo Complex with Adsorbed Ozone Group (higher energy conformation)

E	E_{zp}	H	G
-2894.0918	-2892.9304	-2892.8558	-2893.0488
O	-1.62253751	0.91335544	-0.10141981
O	1.72037368	-1.62221973	-0.72509837
O	1.48707428	0.88015921	-1.79496128
N	-1.04615635	-2.77078577	0.79905256
N	2.11306491	-2.69453366	-0.03904765
N	0.83705617	3.18209456	0.09869939
N	-2.15022560	2.03312769	-0.72923629
C	0.01875964	-3.43522303	1.21799567
C	1.39346820	-3.43112304	0.80330863
C	-0.26778846	3.73635058	-0.47435579
C	-1.52918476	3.24448633	-0.82484318
C	-2.35582721	-2.99786691	1.42566582
C	-2.55249518	-2.58489242	2.76871771
C	-3.82696980	-2.83637803	3.32349687
C	-4.84530004	-3.43948631	2.57124725
C	-4.61735660	-3.80766143	1.23516050
C	-3.36405453	-3.59612080	0.62689810
C	-1.99569776	-0.51486923	4.14144134

C	-1.48272846	-1.87917794	3.61301415
C	-1.01987599	-2.78130367	4.78749195
C	4.62919048	-0.04400414	1.38119898
C	4.08393561	-1.45525954	1.73127408
C	4.57591074	-1.90823069	3.12895411
C	3.53393568	-3.03779756	-0.24058861
C	4.47635658	-2.45315202	0.63658713
C	5.82960914	-2.79389774	0.42243574
C	6.20386277	-3.64996275	-0.62522643
C	5.23656885	-4.17726305	-1.49728064
C	3.86885225	-3.87676246	-1.32925419
C	-3.87737878	-2.98046046	-1.76937233
C	-3.14580853	-3.98480684	-0.83884737
C	-3.58434795	-5.44211011	-1.13142017
C	2.90396389	-3.53140979	-3.63654046
C	2.82645086	-4.37564832	-2.33438739
C	2.96415976	-5.88799602	-2.63649198
C	1.99255382	3.99732388	0.44500773
C	2.90133507	4.38245535	-0.57195116
C	4.00864168	5.17060785	-0.18738483
C	4.21223022	5.52952130	1.15288075
C	3.30501670	5.11390843	2.14207407
C	2.17116163	4.34456310	1.81127030
C	3.97450090	3.21505637	-2.56385384
C	2.73037946	3.97608340	-2.03912097
C	2.42302925	5.21033017	-2.92798001
C	-4.96743245	1.20160389	2.20847633
C	-4.25541873	2.22155678	1.28525358
C	-4.63703242	3.67513787	1.67769193
C	-3.53077014	1.87939051	-1.16857037
C	-4.55851021	1.96477354	-0.19373266
C	-5.89178911	1.84896733	-0.63700602
C	-6.18637917	1.64886374	-1.99560956
C	-5.14976429	1.55398634	-2.93599289
C	-3.79728004	1.65819742	-2.54363330
C	1.77971855	2.67902420	3.68147838
C	1.19683563	3.88990319	2.90273781
C	0.80966099	5.04117098	3.86441258
C	-2.81656232	0.26856706	-4.44738581
C	-2.68814381	1.55534060	-3.59427513
C	-2.66845473	2.81449157	-4.50248725
H	-0.19582809	-4.14916354	2.00500829
H	1.98462543	-4.20820134	1.27589683
H	-0.12153275	4.78558283	-0.70708394
H	-2.17332077	3.98368011	-1.28955346
H	-4.02303546	-2.53937424	4.34987499
H	-5.81920991	-3.61541104	3.02196381
H	-5.41792115	-4.26457556	0.66050784
H	-0.61337319	-1.63603485	2.99049548
H	2.99275608	-1.35931885	1.77871604
H	-2.85639636	-0.62301394	4.81627500
H	-2.28332059	0.13601331	3.30859582

H	-1.19008875	-0.01411331	4.69276609
H	-1.84429096	-3.00107566	5.47993167
H	-0.22732090	-2.27657591	5.35455186
H	-0.62063134	-3.74306534	4.43469422
H	5.72765595	-0.03084041	1.35307338
H	4.29406147	0.68031553	2.13339023
H	4.25429020	0.28977466	0.40681782
H	4.18452236	-2.89988702	3.39376497
H	4.23270957	-1.19497353	3.88866375
H	5.67210747	-1.95334871	3.18288597
H	6.59203814	-2.37527251	1.07348316
H	7.25286760	-3.89589857	-0.77258098
H	5.54673522	-4.81838800	-2.31752213
H	-2.07899361	-3.90669793	-1.07380364
H	1.82538981	-4.21515883	-1.91577643
H	-4.96276785	-3.00404421	-1.60227397
H	-3.68820915	-3.23305440	-2.82103436
H	-3.51914584	-1.96184889	-1.58893205
H	-4.66524179	-5.57886205	-0.99893583
H	-3.07116898	-6.15802348	-0.47574766
H	-3.34641674	-5.69976587	-2.17170162
H	2.74056383	-2.46978380	-3.42218287
H	2.13365165	-3.85897371	-4.34673756
H	3.88438517	-3.64262716	-4.11880560
H	3.91265260	-6.11807065	-3.13816653
H	2.15447042	-6.21083420	-3.30346950
H	2.91347780	-6.48956673	-1.71941946
H	4.72234290	5.49039779	-0.94238290
H	5.07707988	6.12904494	1.42850754
H	3.47577766	5.39704146	3.17718374
H	1.89256359	3.27757364	-2.11375460
H	-3.17858392	2.10067843	1.43977965
H	4.87958185	3.83726761	-2.53801905
H	3.80832932	2.90140269	-3.60260938
H	4.15214296	2.31275026	-1.96859237
H	1.51796833	5.73468887	-2.59263397
H	2.26880723	4.89831375	-3.96938406
H	3.25158774	5.93123806	-2.91100736
H	-6.06024433	1.28991736	2.14629601
H	-4.68034834	1.37770589	3.25352930
H	-4.69138338	0.17331797	1.94736225
H	-4.10074783	4.40901525	1.06267939
H	-4.38461077	3.86420265	2.72961201
H	-5.71398275	3.85029622	1.55038621
H	-6.70358617	1.91912228	0.08229011
H	-7.22152634	1.56589392	-2.31941817
H	-5.38986332	1.39063289	-3.98321642
H	0.27828844	3.53796056	2.42081905
H	-1.72574384	1.49615231	-3.07770452
H	2.74695964	2.93345567	4.13770480
H	1.90688024	1.82448880	3.00952268
H	1.09183002	2.37978051	4.48447538

H	0.03280244	4.69780448	4.56038911
H	0.41920866	5.90965255	3.31763208
H	1.66295258	5.37729833	4.46805306
H	-2.80649170	-0.62287320	-3.81132062
H	-1.96632677	0.19382514	-5.13646703
H	-3.73864159	0.26444926	-5.04460998
H	-2.53211824	3.73286034	-3.91656263
H	-3.60682872	2.91146648	-5.06524407
H	-1.84470640	2.74738616	-5.22504288
O	0.69643038	-0.65134693	1.59831917
O	0.94881932	0.18748799	-2.93789062
O	-0.15273386	-0.55744906	-2.53395967
O	0.90177911	1.89637451	0.59282701
O	-1.02086332	-1.87061224	-0.20325946
Hf	0.26403545	-0.01571986	-0.06819568

9.6 Nine Oxygen Atoms

η^2 -ozone Complex with Adsorbed Oxygen Molecule

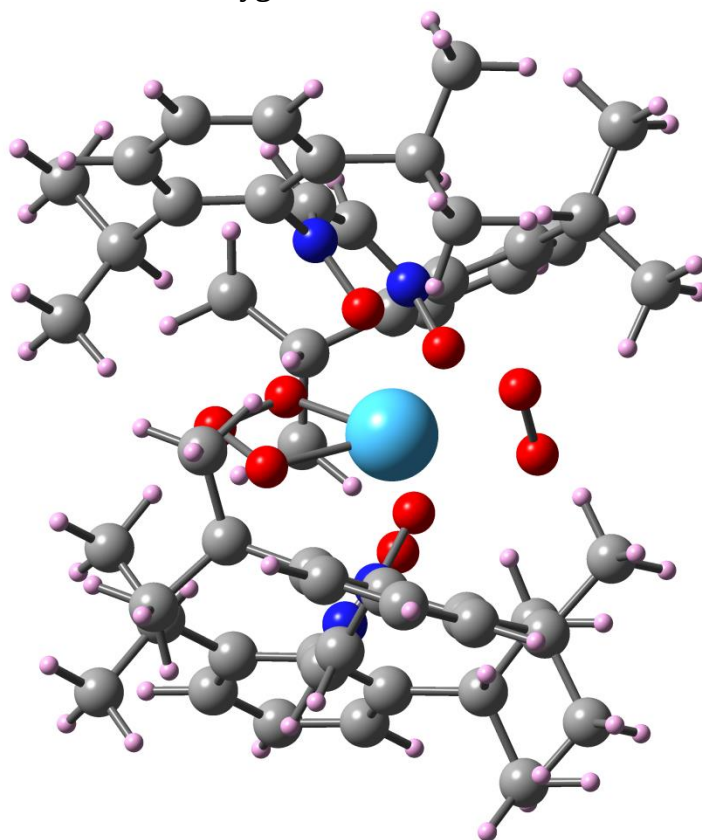


Fig. S114: ONCCNO η^2 -ozone Complex with Adsorbed Oxygen Molecule

E	E_{zp}	H	G
-2969.2636	-2968.0993	-2968.0239	-2968.2169
O	0.86506360	1.97515507	-0.26065150
O	-0.81932871	-1.94418769	-0.36148289
O	-1.00011598	0.51937331	1.29203018
N	2.47549820	-2.20181948	-0.48062472
N	-0.58346427	-3.00534332	0.48974354
N	-2.45309368	2.07437004	-0.50422087
N	0.54052134	3.04063260	0.47998235
C	1.93419697	-3.23318190	0.21942498
C	0.64338624	-3.56607588	0.65425187
C	-1.99832691	3.06419950	0.26681910
C	-0.70526925	3.48159954	0.69881661
C	3.89096824	-2.20057527	-0.82645420
C	4.25559307	-2.60380858	-2.13664794
C	5.62910383	-2.60173523	-2.45542674
C	6.59072192	-2.21499711	-1.50729259
C	6.19517442	-1.80205694	-0.22574392

C	4.83204002	-1.77055367	0.14090133
C	3.10415135	-1.88265556	-4.27234104
C	3.21654061	-2.99232162	-3.19226328
C	3.52229499	-4.36935932	-3.83400651
C	-3.44990999	-3.32070466	-2.06593095
C	-2.47949837	-4.28651667	-1.33510763
C	-2.61299297	-5.73040158	-1.88366644
C	-1.77674817	-3.60574979	1.06365497
C	-2.70048471	-4.22613567	0.17953724
C	-3.85878247	-4.79589159	0.74544695
C	-4.07779557	-4.76678339	2.13245276
C	-3.14529393	-4.15163656	2.98037176
C	-1.97930248	-3.54242426	2.46713157
C	4.91884987	0.18269957	1.76050511
C	4.41949890	-1.26653710	1.52729255
C	4.93250264	-2.21189776	2.64551238
C	-1.71136063	-1.76521336	4.27410989
C	-1.00301520	-2.85313600	3.42786497
C	-0.30125134	-3.89139571	4.34397677
C	-3.88156802	2.01429393	-0.84493028
C	-4.78988100	1.48899169	0.10498553
C	-6.15335015	1.47484860	-0.26236045
C	-6.57107198	1.93175749	-1.52121700
C	-5.63306837	2.40994682	-2.45094071
C	-4.26011126	2.46310575	-2.13556048
C	-4.83853945	-0.52971896	1.64499207
C	-4.35498092	0.93235401	1.46479148
C	-4.86867991	1.82641657	2.62490111
C	3.30053688	3.46430278	-2.16046487
C	2.25575549	4.38294392	-1.47152653
C	2.23747530	5.79146329	-2.11789646
C	1.68907932	3.79958153	0.99525347
C	2.51455459	4.44631421	0.03798729
C	3.62266019	5.16388135	0.53129621
C	3.88589789	5.23469636	1.90879017
C	3.04975847	4.57884253	2.82338119
C	1.93139527	3.83237388	2.39165974
C	-3.04462029	1.86828358	-4.27295866
C	-3.24536384	2.94871656	-3.17526426
C	-3.64705676	4.31032004	-3.79645795
C	1.91912092	2.08399810	4.23702459
C	1.07228705	3.10075410	3.42946490
C	0.36057703	4.10620517	4.37313770
H	2.69176543	-3.95172114	0.51409736
H	0.60043044	-4.47020396	1.25177570
H	-2.79521846	3.71044013	0.61847645
H	-0.72424093	4.37703819	1.30941366
H	5.94719259	-2.90478812	-3.44943516
H	7.64600391	-2.22667511	-1.77091841
H	6.94812951	-1.48765672	0.49255875
H	2.23599649	-3.06015193	-2.70968790
H	-1.46594335	-3.93858711	-1.55504883

H	4.05782766	-1.74445178	-4.80058420
H	2.81113513	-0.93097489	-3.81706824
H	2.33877916	-2.15237268	-5.01175286
H	4.46604571	-4.35738514	-4.39505765
H	2.72356890	-4.63857455	-4.53758766
H	3.59087119	-5.16044990	-3.07561485
H	-4.49822463	-3.59393905	-1.88091382
H	-3.27368668	-3.35483719	-3.14908451
H	-3.28896220	-2.29125145	-1.72936429
H	-1.92974321	-6.41966670	-1.37026114
H	-2.37170190	-5.74493941	-2.95470474
H	-3.63340711	-6.11966045	-1.77015257
H	-4.58772174	-5.27554873	0.09763810
H	-4.97366461	-5.22109886	2.54976317
H	-3.32871008	-4.13017082	4.05146918
H	3.32703703	-1.23153853	1.58467525
H	-0.23499216	-2.33504089	2.84756232
H	6.01543682	0.24611567	1.74363376
H	4.57565500	0.54403180	2.73859363
H	4.52259620	0.85853186	0.99359709
H	6.03016023	-2.25434478	2.66428754
H	4.56050187	-3.23605461	2.50880621
H	4.59170732	-1.85623819	3.62677665
H	-2.13476302	-0.99319379	3.62302352
H	-0.98282852	-1.27898551	4.93534598
H	-2.51104958	-2.18506701	4.89936214
H	-1.02532902	-4.41355261	4.98398898
H	0.42571675	-3.38928035	4.99562403
H	0.23465719	-4.65155563	3.75981734
H	-6.88793734	1.08724479	0.43811454
H	-7.62619670	1.90523626	-1.78315320
H	-5.96904518	2.74451916	-3.42828016
H	-3.26116320	0.90588761	1.51491063
H	1.27626081	3.92715434	-1.64854705
H	-5.93453033	-0.60117077	1.65779031
H	-4.46482222	-0.93191728	2.59438030
H	-4.46119981	-1.17109782	0.84030789
H	-4.50382594	2.85887220	2.53539473
H	-4.52240540	1.42847231	3.58742271
H	-5.96629504	1.86157122	2.64857711
H	4.31974412	3.85128906	-2.02458362
H	3.09693661	3.40377065	-3.23708823
H	3.25219389	2.45043647	-1.75028866
H	1.50253937	6.44864206	-1.63445028
H	1.97458161	5.70709662	-3.18023419
H	3.21768439	6.28171326	-2.06015269
H	4.28022504	5.67343587	-0.16734803
H	4.74518387	5.79633437	2.26737933
H	3.27243580	4.63159209	3.88550050
H	-2.27303798	3.08236898	-2.68810965
H	0.30780908	2.50830329	2.92009963
H	-3.98575696	1.66394575	-4.80148661

H	-2.67442655	0.93566793	-3.83530175
H	-2.30592279	2.21183243	-5.00860856
H	-2.85769687	4.65552957	-4.47657170
H	-3.79658364	5.07902875	-3.02661478
H	-4.57292688	4.23409438	-4.38101028
H	2.35298325	1.33413550	3.56744448
H	1.27738447	1.55808699	4.95491726
H	2.72770785	2.57320833	4.79674125
H	-0.26641862	4.81680508	3.81647827
H	1.08360745	4.69101984	4.95692229
H	-0.28355986	3.56682498	5.07940877
O	-0.35653086	-0.47894788	-2.68671040
O	0.51204090	0.60625063	-2.59496392
O	0.08130021	0.17155499	2.25953777
O	1.10545712	-0.39698117	1.33489903
Hf	0.06633132	-0.05445496	-0.49120842
O	-1.70438957	1.12812669	-1.10404894
O	1.77882512	-1.14894598	-1.02583816

Adsorbed Oxygen Molecule and Ozone Group

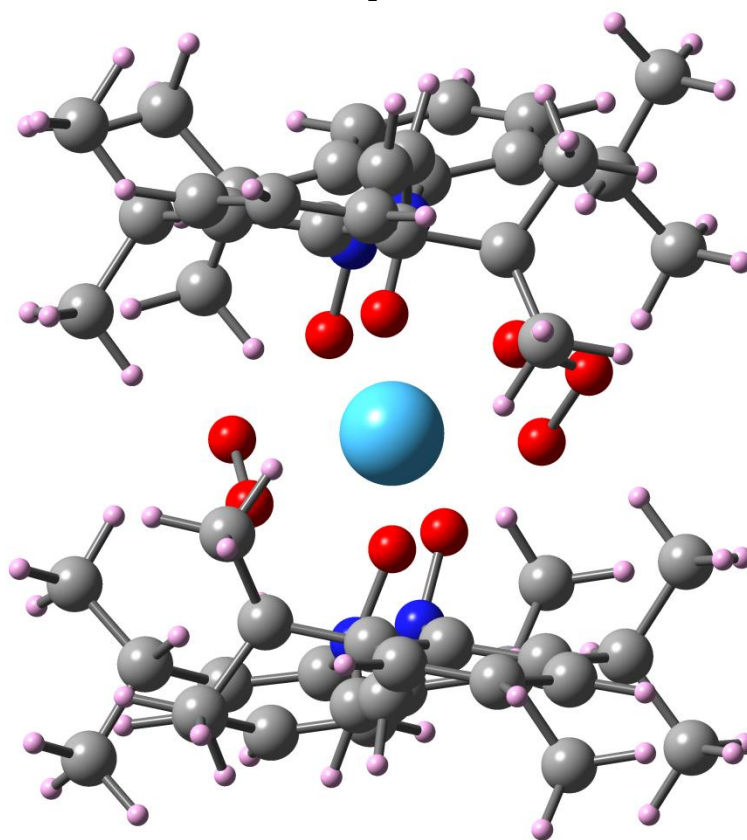


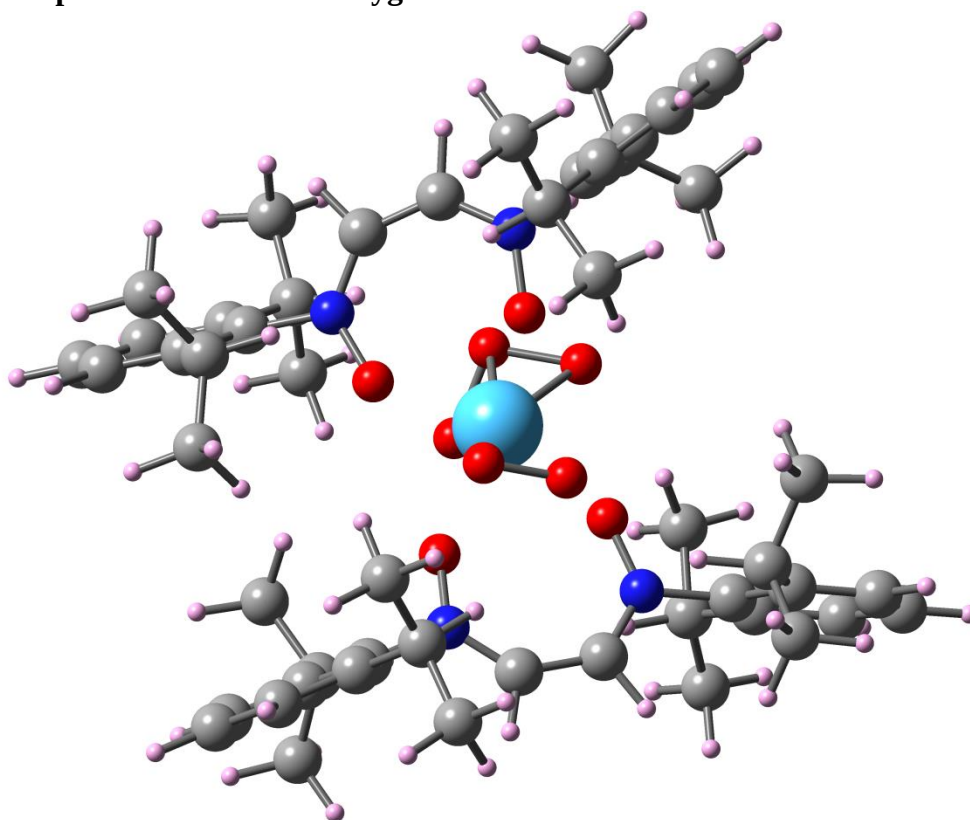
Fig. S115: ONCCNO Adsorbed Oxygen Molecule and Ozone Group

E	E_{zp}	H	G
-2969.2610	-2968.0979	-2968.0220	-2968.2176
O	-1.68427731	1.42279207	-0.03092742
O	1.36920657	-1.23511227	-0.78998194
O	0.51816251	1.26684920	-1.79924449
N	-1.24264141	-3.07171752	0.35936850
N	1.91830264	-2.45748318	-0.45243721
N	1.33683827	2.74392766	0.49339991
N	-1.86943829	2.73575619	-0.33049725
C	-0.09751592	-3.80893405	0.35320906
C	1.23105675	-3.54452263	0.00295185
C	0.47521245	3.67264532	0.02054311
C	-0.89128450	3.67569822	-0.31532136
C	-2.52286482	-3.65355970	0.73359087
C	-2.81870909	-3.84794142	2.10684137
C	-4.06726166	-4.42588721	2.42401063
C	-4.98379502	-4.76847634	1.41867583
C	-4.67098966	-4.54124001	0.06841496
C	-3.43264951	-3.98123853	-0.30611140
C	-2.50682055	-2.42253735	4.19165217

C	-1.85708627	-3.45352218	3.23287574
C	-1.36589711	-4.70127320	4.01382907
C	4.53133365	-0.89069130	2.27129276
C	3.88258992	-2.18864123	1.72537347
C	4.24032283	-3.40235262	2.62370725
C	3.33408912	-2.55842301	-0.77554548
C	4.28394235	-2.44059447	0.26886832
C	5.64719217	-2.55457938	-0.07983465
C	6.03813800	-2.74907535	-1.41352999
C	5.07280678	-2.83253797	-2.43085997
C	3.69734390	-2.74045733	-2.13496274
C	-3.99649737	-2.57333176	-2.33414095
C	-3.11821368	-3.72813919	-1.78343587
C	-3.28035515	-5.01084939	-2.63851053
C	2.67974328	-1.48469980	-4.08285685
C	2.65565924	-2.79821997	-3.25553090
C	2.84299551	-4.03719843	-4.16695920
C	2.69278923	3.11264496	0.88843860
C	3.70001973	3.20352913	-0.10350975
C	4.99415524	3.57022364	0.32684346
C	5.26740221	3.80900534	1.68204487
C	4.25025761	3.68654190	2.64310323
C	2.93718591	3.33677435	2.26820590
C	4.34349832	1.77019984	-2.10197410
C	3.43737028	2.91711903	-1.58476486
C	3.62247405	4.19651988	-2.44316519
C	-4.28806426	1.46337883	2.38813167
C	-3.70084694	2.82820859	1.93842819
C	-4.07427053	3.95334341	2.93671779
C	-3.25850111	3.10115597	-0.59706912
C	-4.14558626	3.15416370	0.50966404
C	-5.48735757	3.49688401	0.24738050
C	-5.91992425	3.77736970	-1.05893798
C	-5.01976490	3.70685533	-2.13206162
C	-3.66728575	3.35492895	-1.93007178
C	2.08449796	1.89780621	4.17068762
C	1.84581510	3.18174784	3.33125717
C	1.73612302	4.43214352	4.24033843
C	-3.21368618	2.13437052	-4.10919355
C	-2.72895448	3.24020504	-3.13533501
C	-2.57849253	4.59978614	-3.86721394
H	-0.26834293	-4.82085230	0.70431273
H	1.88978755	-4.39758574	0.12800699
H	0.95265860	4.63945414	-0.09957037
H	-1.26504840	4.64820112	-0.61661338
H	-4.32684219	-4.59560743	3.46579051
H	-5.94291880	-5.20601917	1.68641467
H	-5.39230881	-4.80450896	-0.70082721
H	-0.98121008	-2.96510473	2.79661787
H	2.79818354	-2.04636343	1.77276911
H	-3.39555812	-2.83286393	4.68969419
H	-2.79757885	-1.51751773	3.64686348

H	-1.78739373	-2.12996409	4.96731449
H	-2.19921666	-5.21853989	4.50789831
H	-0.64719294	-4.40372459	4.78860444
H	-0.87130491	-5.42364886	3.35061154
H	5.62684059	-0.96443550	2.29745437
H	4.18242261	-0.70009107	3.29430877
H	4.26058794	-0.02574280	1.65491035
H	3.75657412	-4.32204134	2.26912369
H	3.91047255	-3.22061347	3.65484252
H	5.32409919	-3.57976693	2.64191983
H	6.40484667	-2.47785144	0.69583299
H	7.09413956	-2.82813846	-1.66191599
H	5.39030842	-2.97222396	-3.46082593
H	-2.07892404	-3.39732759	-1.87031445
H	1.66098677	-2.86622032	-2.80266185
H	-5.06577647	-2.81745848	-2.26582513
H	-3.75299729	-2.38439385	-3.38754112
H	-3.80813648	-1.65117997	-1.77493614
H	-4.32086302	-5.36089262	-2.65707185
H	-2.65609445	-5.82983695	-2.25738919
H	-2.98157923	-4.80738863	-3.67523587
H	2.46883095	-0.62367314	-3.44044193
H	1.91338507	-1.51925418	-4.86820215
H	3.65701771	-1.33761768	-4.56357689
H	3.79461524	-4.00207554	-4.71355994
H	2.03687537	-4.07798388	-4.91111880
H	2.82078793	-4.96972892	-3.58785222
H	5.79333124	3.65775732	-0.40445198
H	6.27314652	4.08469078	1.99100547
H	4.47724319	3.86553246	3.69073089
H	2.40495009	2.57725059	-1.70734441
H	-2.61139099	2.72219573	1.95312816
H	5.40903552	2.02892756	-2.03636798
H	4.11180115	1.55911952	-3.15374003
H	4.17628371	0.85010470	-1.53023246
H	2.95981897	5.00621122	-2.10885593
H	3.38995505	3.98076827	-3.49400503
H	4.65497834	4.56821802	-2.39531630
H	-5.38628762	1.48862594	2.40111671
H	-3.93910603	1.21679112	3.39931918
H	-3.96612964	0.66472647	1.71144084
H	-3.65635333	4.92022421	2.62702351
H	-3.68043428	3.71358452	3.93310027
H	-5.16154512	4.07079787	3.03145419
H	-6.19646630	3.54576411	1.06931771
H	-6.95869823	4.04355603	-1.24015622
H	-5.37054031	3.91206205	-3.13996011
H	0.88183943	3.05149084	2.82816432
H	-1.73698333	2.93673847	-2.78922124
H	3.04893023	1.94105757	4.69555143
H	2.07134937	1.01183159	3.52769314
H	1.29159764	1.78459726	4.92170831

H	0.89885737	4.31345354	4.94056167
H	1.56392978	5.34335330	3.65249407
H	2.64532218	4.58329177	4.83677676
H	-3.25794479	1.16355752	-3.60327332
H	-2.51316759	2.04282630	-4.94906919
H	-4.20753432	2.36209590	-4.51748590
H	-2.21276628	5.38478365	-3.19146748
H	-3.53489848	4.93956401	-4.28604919
H	-1.86487304	4.50383728	-4.69559428
O	0.40546191	-0.96348949	1.86445025
O	-0.74877871	-0.20944283	2.07861199
O	-0.37625189	0.77950565	-2.81364555
O	-1.10114083	-0.27608850	-2.18625889
Hf	-0.19058384	-0.05570147	-0.10303065
O	1.00492972	1.44686859	0.79303000
O	-1.32091341	-1.79158676	-0.14272446

η^3 -ozone Complex with Adsorbed Oxygen MoleculeFig. S116: ONCCNO η^3 -ozone Complex with Adsorbed Oxygen Molecule

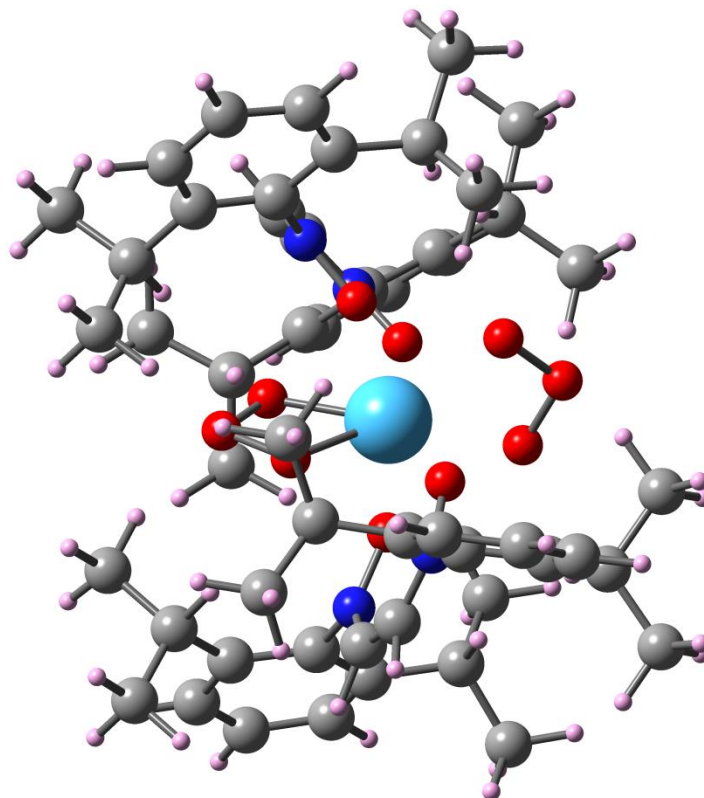
E	E_{zp}	H	G
-2969.2397	-2968.0762	-2968.0015	-2968.1919
O	-1.79324407	0.86654111	0.20868597
O	1.91103485	-1.29868743	-0.86299735
O	1.49419347	1.14394196	-1.59154920
N	-0.61516834	-3.02049504	0.44177979
N	2.45381758	-2.44426301	-0.47195396
N	0.42898315	3.27231295	0.54494967
N	-2.43710814	1.95428592	-0.35902219
C	0.51327323	-3.71988461	0.55690787
C	1.85175919	-3.48093477	0.12411060
C	-0.73177639	3.78988481	0.06105390
C	-1.95367511	3.22539100	-0.32919549
C	-1.87667879	-3.57025770	0.96251194
C	-2.05848713	-3.69228680	2.36402671
C	-3.29036593	-4.22749543	2.79929686
C	-4.28724556	-4.59803368	1.88589868
C	-4.07448021	-4.44901883	0.50634249
C	-2.86120059	-3.93514851	0.00624371
C	-1.60138142	-2.24544041	4.41133724
C	-1.01622805	-3.27333593	3.40943708

C	-0.45147610	-4.51140431	4.15659418
C	5.02226878	-0.66744449	2.11019749
C	4.43969895	-2.04374303	1.69247146
C	4.88382822	-3.15589231	2.67820129
C	3.89038126	-2.55349932	-0.79360880
C	4.83061264	-2.38345335	0.24960728
C	6.19301045	-2.49444381	-0.10371849
C	6.57952104	-2.73310352	-1.43103452
C	5.61329350	-2.85327346	-2.44388051
C	4.23706346	-2.76009655	-2.15186263
C	-3.50763574	-2.61052042	-2.05192449
C	-2.66167639	-3.79207325	-1.50650589
C	-2.98495024	-5.10787062	-2.25999071
C	3.10940619	-1.44574982	-3.99250702
C	3.19244764	-2.82062557	-3.27063630
C	3.46208002	-3.96685062	-4.27654663
C	1.54404246	4.13464567	0.91147778
C	2.33814224	4.71827131	-0.10867685
C	3.40708902	5.54635331	0.29932726
C	3.68534203	5.75888995	1.65739824
C	2.89231512	5.15029481	2.64403566
C	1.80086530	4.32993099	2.29472481
C	3.34522299	3.90845888	-2.30270695
C	2.08974481	4.48672765	-1.60301971
C	1.61947664	5.79306967	-2.29721592
C	-4.57008884	-0.17186400	2.17581517
C	-4.45345106	1.28174630	1.64897373
C	-5.36106433	2.24340043	2.45937273
C	-3.79018708	1.68217568	-0.82279520
C	-4.76706003	1.34164790	0.15092059
C	-6.07262490	1.06490017	-0.30188042
C	-6.39523459	1.13660828	-1.66671060
C	-5.41218910	1.48403212	-2.60447567
C	-4.08407543	1.75792821	-2.20952407
C	1.75251351	2.54996354	4.09614557
C	0.95235614	3.67651022	3.38987914
C	0.42626152	4.71499349	4.41356891
C	-2.90557298	1.00801394	-4.34152522
C	-3.04592749	2.12469975	-3.27618405
C	-3.39346563	3.48444850	-3.94032368
H	0.37681846	-4.67121707	1.05795043
H	2.52962890	-4.30364200	0.31852422
H	-0.68196060	4.86713341	-0.05300198
H	-2.67239463	3.94443371	-0.70707232
H	-3.47312644	-4.33672094	3.86458535
H	-5.23112624	-4.99832341	2.24801696
H	-4.85524165	-4.73798047	-0.19108281
H	-0.18530413	-2.76606525	2.91205903
H	3.35186220	-1.94605234	1.76380068
H	-2.42970047	-2.66757864	4.99533323
H	-1.95835991	-1.35547895	3.88366555
H	-0.81968489	-1.92767725	5.11263460

H	-1.24141991	-5.03931673	4.70644371
H	0.31192177	-4.19899519	4.88076713
H	0.00905992	-5.23320038	3.46747663
H	6.12035114	-0.67339357	2.10851546
H	4.68501804	-0.41290005	3.12286577
H	4.68105300	0.12361565	1.43277682
H	4.44844303	-4.12966330	2.41499841
H	4.56470944	-2.90461562	3.69785407
H	5.97551104	-3.27183769	2.68740950
H	6.95283310	-2.37475846	0.66377831
H	7.63509598	-2.81005021	-1.68051405
H	5.93005217	-3.01638322	-3.46965267
H	-1.61483493	-3.54422627	-1.70875470
H	2.20590673	-3.00044804	-2.82635857
H	-4.57956786	-2.77630986	-1.87738812
H	-3.34982039	-2.50380606	-3.13280933
H	-3.21382696	-1.67192619	-1.57261119
H	-4.04686010	-5.37469213	-2.18271736
H	-2.39604224	-5.95131721	-1.87540660
H	-2.75400331	-4.98783771	-3.32630206
H	2.80903551	-0.65538175	-3.29710637
H	2.36084122	-1.49054146	-4.79422232
H	4.07777272	-1.18219865	-4.44043610
H	4.38197721	-3.79818269	-4.85105567
H	2.63598537	-4.02535003	-4.99656103
H	3.54889811	-4.93956411	-3.77405521
H	4.03407468	6.01343484	-0.45557097
H	4.52014501	6.39318783	1.94722378
H	3.11881708	5.31867184	3.69363975
H	1.30672817	3.73371754	-1.71910282
H	-3.41531907	1.58934013	1.80188528
H	4.20375074	4.59118206	-2.24054659
H	3.12844666	3.72957114	-3.36368369
H	3.61875883	2.94739812	-1.85550542
H	0.70764828	6.19413220	-1.83360905
H	1.40500459	5.60050011	-3.35658734
H	2.39003902	6.57432256	-2.24559954
H	-5.59044336	-0.56117590	2.05531090
H	-4.31773970	-0.21001662	3.24424163
H	-3.88156632	-0.83046663	1.63550646
H	-5.27347236	3.27607153	2.09716094
H	-5.07316739	2.22823259	3.51915437
H	-6.41859263	1.95417899	2.39742932
H	-6.84291923	0.80228854	0.41904265
H	-7.40950454	0.92396334	-1.99731758
H	-5.67220399	1.53346321	-3.65860921
H	0.08551438	3.19884622	2.92331554
H	-2.06593052	2.22171424	-2.80313786
H	2.65131252	2.94855707	4.58726798
H	2.05376111	1.78717536	3.37078558
H	1.13045377	2.06682799	4.86149207
H	-0.22967339	4.22129511	5.14305045

H	-0.14931034	5.50876993	3.91939899
H	1.24343068	5.18987803	4.97247123
H	-2.56338064	0.08072292	-3.87181328
H	-2.15275663	1.29935774	-5.08549828
H	-3.85115812	0.82198371	-4.86918712
H	-3.46591135	4.29224797	-3.19908478
H	-4.35167648	3.43670517	-4.47516036
H	-2.61603559	3.75768395	-4.66567041
O	1.26289835	-0.65516251	1.60211422
O	-0.04602995	-0.42113363	2.03003985
O	0.04469087	1.39508614	-2.00663368
O	-0.51307192	-0.02907274	-2.17787682
Hf	0.17608307	0.17106761	-0.18866667
O	0.60157033	1.95031459	0.89024456
O	-0.73968923	-1.86639187	-0.23676304

9.7 Ten Oxygen Atoms

 η^2 -ozone Complex with Adsorbed Ozone GroupFig. S117: ONCCNO η^2 -ozone Complex with Adsorbed Ozone Group

E	E_{zp}	H	G
-3044.4060	-3043.2380	-3043.1616	-3043.3564

O	1.00893058	1.91580938	-0.08754646
O	-0.94086867	-1.85437514	-0.20276546
O	-0.94250944	0.61997131	1.37710213
N	2.33014828	-2.36544262	-0.46607195
N	-0.75683837	-2.98965407	0.55775564
N	-2.31235754	2.18992677	-0.49318206
N	0.70407448	3.04311396	0.54394878
C	1.73068882	-3.38624523	0.20359042
C	0.43077772	-3.64690397	0.65310054
C	-1.82667730	3.18038732	0.25252986
C	-0.52354496	3.55518991	0.69793489
C	3.74468615	-2.42838463	-0.80527252
C	4.09895396	-2.81504204	-2.12265832
C	5.47356694	-2.88772083	-2.42899983
C	6.44619658	-2.58481475	-1.46208925
C	6.06239263	-2.18231521	-0.17340194
C	4.69989412	-2.08008588	0.18167437
C	3.06072709	-2.00165361	-4.28197071

C	3.05048166	-3.11248591	-3.19781552
C	3.24775404	-4.51389880	-3.82971729
C	-3.65747173	-3.10805767	-1.97822290
C	-2.72317657	-4.13032576	-1.27779083
C	-2.91761805	-5.55371576	-1.86005321
C	-1.97625365	-3.53864186	1.12743707
C	-2.93273623	-4.09822695	0.23908766
C	-4.11326791	-4.62244447	0.80368730
C	-4.32233293	-4.60231970	2.19261019
C	-3.35918402	-4.04069861	3.04408737
C	-2.16859434	-3.48083348	2.53153567
C	4.90967699	-0.20258706	1.88164444
C	4.30125865	-1.59590836	1.57927572
C	4.71113398	-2.62398023	2.66691939
C	-1.80231868	-1.71606926	4.33119767
C	-1.15482566	-2.84437578	3.48874031
C	-0.50821559	-3.91572178	4.40696281
C	-3.73953627	2.17811370	-0.84765756
C	-4.67600394	1.71538992	0.10760946
C	-6.03595271	1.75105063	-0.27102254
C	-6.42469367	2.19674295	-1.54312558
C	-5.46013415	2.61026059	-2.47644166
C	-4.08827946	2.60922005	-2.15194727
C	-4.79432431	-0.28233270	1.66688715
C	-4.27755315	1.16815324	1.48237641
C	-4.79378178	2.08548108	2.62262646
C	3.54373212	3.35349634	-2.07623832
C	2.47528107	4.27580050	-1.43025197
C	2.44422248	5.66456500	-2.11805556
C	1.86834097	3.79181904	1.04724798
C	2.71401087	4.39148506	0.07930179
C	3.82783624	5.10640927	0.56504594
C	4.07695920	5.21177848	1.94293713
C	3.22394105	4.59114148	2.86733316
C	2.09796115	3.85187676	2.44379085
C	-2.95497618	1.94993384	-4.31493737
C	-3.04855829	3.02416788	-3.19754926
C	-3.34493423	4.42557284	-3.78955677
C	2.04311173	2.11939632	4.30009283
C	1.21921703	3.14922405	3.48489845
C	0.52780871	4.17577049	4.42029099
H	2.44272135	-4.16588559	0.45301328
H	0.33339469	-4.57579414	1.20463430
H	-2.59820349	3.87636766	0.56391914
H	-0.51276945	4.48337583	1.25768576
H	5.78333841	-3.18206276	-3.42834979
H	7.50170273	-2.65271552	-1.71622619
H	6.82519629	-1.93183702	0.55943490
H	2.05848608	-3.09093381	-2.73514365
H	-1.69805371	-3.81665227	-1.49687889
H	4.02911691	-1.95896245	-4.79969836
H	2.86106530	-1.02316466	-3.83252004

H	2.28149487	-2.19666397	-5.03023968
H	4.20351017	-4.58761447	-4.36541259
H	2.44615273	-4.71491814	-4.55254194
H	3.22688957	-5.30437940	-3.06790635
H	-4.71530525	-3.34270178	-1.79385588
H	-3.48598580	-3.12156609	-3.06222244
H	-3.45104757	-2.09453410	-1.61907586
H	-2.25716610	-6.28148963	-1.37044246
H	-2.68714446	-5.55116475	-2.93345719
H	-3.95149370	-5.90531980	-1.74490783
H	-4.86807922	-5.05738759	0.15390733
H	-5.23585877	-5.02095136	2.60911610
H	-3.53659327	-4.02369900	4.11631580
H	3.21440283	-1.47380045	1.61857222
H	-0.35961990	-2.37303536	2.90463520
H	6.00782773	-0.22752843	1.89526160
H	4.56886713	0.14775260	2.86471770
H	4.59045412	0.53142141	1.13249086
H	5.80041893	-2.76361665	2.69784342
H	4.25278082	-3.60529313	2.48534104
H	4.38624405	-2.27709614	3.65667868
H	-2.18403228	-0.92420772	3.67799079
H	-1.04855946	-1.26739212	4.99070603
H	-2.62370854	-2.09054385	4.95765500
H	-1.25677042	-4.39336597	5.05372407
H	0.24924068	-3.45207004	5.05228781
H	-0.01890455	-4.70672735	3.82301556
H	-6.79148203	1.41143402	0.43207535
H	-7.47811174	2.21025129	-1.81262150
H	-5.77353286	2.93429178	-3.46484045
H	-3.18595385	1.11810408	1.55505545
H	1.50809790	3.79546599	-1.60958234
H	-5.89122173	-0.33270852	1.64410213
H	-4.45921441	-0.67777575	2.63334659
H	-4.40242644	-0.94126521	0.88382011
H	-4.40893607	3.11013804	2.52684271
H	-4.47017324	1.69288079	3.59509230
H	-5.89075303	2.14073069	2.62917831
H	4.55599607	3.75686446	-1.93532521
H	3.35534182	3.25967135	-3.15272789
H	3.49889541	2.34953865	-1.64222941
H	1.68786198	6.32187887	-1.66871124
H	2.20482622	5.54467593	-3.18240268
H	3.41425975	6.17402961	-2.05371802
H	4.50204691	5.58373551	-0.14050400
H	4.94080673	5.77052719	2.29502315
H	3.43938728	4.66631634	3.92960850
H	-2.06172179	3.06698128	-2.72400919
H	0.44163543	2.57150167	2.97760842
H	-3.90911848	1.85045592	-4.85021002
H	-2.68538511	0.97546164	-3.89477493
H	-2.18245459	2.23033413	-5.04225842

H	-2.54964021	4.70920281	-4.49088620
H	-3.39941618	5.19259930	-3.00551159
H	-4.29312136	4.44201504	-4.34215852
H	2.46727807	1.35883329	3.63618422
H	1.38878025	1.60835045	5.01723970
H	2.85821046	2.59665307	4.86055879
H	-0.08401739	4.89412327	3.85698200
H	1.26177830	4.74993035	5.00103252
H	-0.12772064	3.65458894	5.12967762
O	-0.61989163	-0.81004597	-2.60875925
O	0.83789618	0.93335181	-2.39871703
O	0.11478697	0.19885544	2.34330421
O	1.08824091	-0.44936074	1.41572277
Hf	0.07519153	-0.06315218	-0.40060114
O	-1.59728944	1.19318881	-1.04863527
O	1.69433801	-1.24537806	-0.95612534
O	0.14914325	0.11146714	-3.33245070

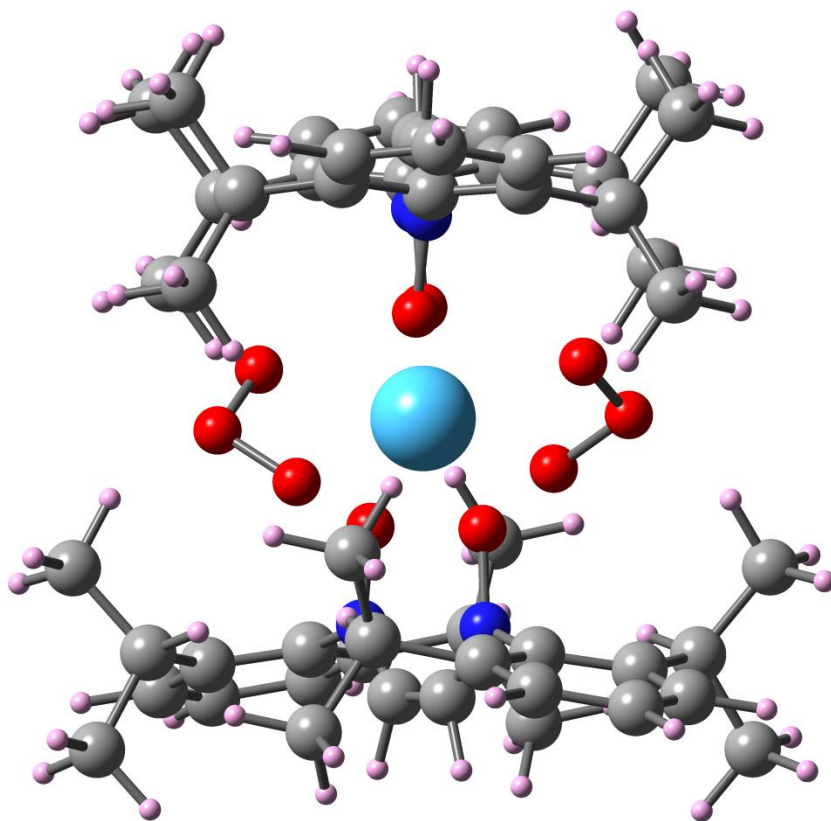
Bare Complex with Two Adsorbed Ozone Groups

Fig. S118: ONCCNO Bare Complex with Two Adsorbed Ozone Groups

E	E_{zp}	H	G
-3044.4054	-3043.2399	-3043.1622	-3043.3633
O	1.32294893	1.48429839	0.48628066
O	-1.36360758	-1.49949868	0.33324779
O	-0.91952730	0.66595611	2.05794869
N	1.63595535	-2.79313483	-0.41491181
N	-1.58047775	-2.84305267	0.39264996
N	-1.63236061	2.83269668	-0.39152009
N	1.58793342	2.82797631	0.42125942
C	0.72982910	-3.77106470	-0.14856327
C	-0.62917767	-3.79309237	0.19042673
C	-0.69898916	3.79862374	-0.15500553
C	0.65979387	3.79567546	0.16895695
C	3.01668835	-3.12575616	-0.74644622
C	3.35246317	-3.32848156	-2.10808757
C	4.69006530	-3.66964320	-2.39909311
C	5.64426502	-3.78686419	-1.37556979
C	5.28497126	-3.54930308	-0.03927955
C	3.96142710	-3.20270816	0.30644179
C	2.72738482	-1.96280970	-4.14892482

C	2.33616343	-3.15876714	-3.24076430
C	2.17722127	-4.45994519	-4.06887328
C	-4.32865908	-1.79293781	-2.31474739
C	-3.52349135	-3.01112168	-1.79149289
C	-3.72903047	-4.24897288	-2.70279994
C	-2.95179454	-3.21377546	0.72121753
C	-3.88891972	-3.31719667	-0.33652401
C	-5.20446933	-3.69770662	0.00271584
C	-5.56318798	-3.94677475	1.33730105
C	-4.61754119	-3.80433309	2.36522317
C	-3.28882169	-3.42380548	2.08117777
C	4.39852133	-1.69060699	2.29613395
C	3.59582680	-2.90608342	1.76322731
C	3.80524388	-4.14992934	2.66562664
C	-2.74048443	-2.07865859	4.16060019
C	-2.28475867	-3.22557117	3.22027033
C	-2.05610072	-4.53821794	4.01404481
C	-3.00686580	3.17765639	-0.72547960
C	-3.95614731	3.25608655	0.32361040
C	-5.27638325	3.61276595	-0.02420575
C	-5.62970921	3.85954862	-1.36045040
C	-4.67279354	3.74086665	-2.38127119
C	-3.33855513	3.38902721	-2.08730960
C	-4.41097747	1.74193590	2.30863971
C	-3.59651634	2.95138293	1.77996991
C	-3.79450805	4.19489530	2.68538608
C	4.38558467	1.79986744	-2.28107786
C	3.56312109	2.99877817	-1.74105513
C	3.76313589	4.25573384	-2.62715934
C	2.95924346	3.17698317	0.76538678
C	3.91207374	3.28267720	-0.27781444
C	5.22774209	3.64442051	0.08284820
C	5.57350513	3.86834986	1.42491152
C	4.61313389	3.72281901	2.43918312
C	3.28296962	3.36721895	2.13250568
C	-2.70454781	1.99623165	-4.10538986
C	-2.32143606	3.21054765	-3.21788646
C	-2.17190120	4.49807082	-4.06832324
C	2.63882065	1.93067634	4.11664079
C	2.26068501	3.16446799	3.25423793
C	2.10759726	4.43274842	4.13253736
H	1.17953247	-4.75572789	-0.21705132
H	-1.03217693	-4.79136228	0.32254154
H	-1.12670660	4.79095288	-0.25037283
H	1.09465063	4.78642826	0.24703429
H	4.98663560	-3.83678898	-3.43136578
H	6.67003305	-4.05279003	-1.62077718
H	6.03819478	-3.62429928	0.74074902
H	1.35987910	-2.91970408	-2.80610018
H	-2.46723369	-2.72955169	-1.84254669
H	3.69793180	-2.13126513	-4.63506860
H	2.78486500	-1.03647843	-3.56711070

H	1.97242579	-1.82262013	-4.93315512
H	3.11439578	-4.73640270	-4.56981002
H	1.41256141	-4.32170943	-4.84431462
H	1.87319794	-5.30438458	-3.43625672
H	-5.40891984	-1.99290659	-2.31623732
H	-4.02321527	-1.55705728	-3.34198891
H	-4.14062250	-0.90892982	-1.69512581
H	-3.13829149	-5.10632429	-2.35383704
H	-3.41744802	-4.01524696	-3.72911026
H	-4.78257589	-4.55735695	-2.73430882
H	-5.95181771	-3.79257820	-0.78075107
H	-6.58241977	-4.24091989	1.57744694
H	-4.91430591	-3.97966167	3.39608265
H	2.53943364	-2.62621908	1.81675711
H	-1.32276203	-2.92195228	2.79432761
H	5.47928729	-1.88753671	2.29761044
H	4.09207164	-1.46364288	3.32517507
H	4.20962273	-0.80174527	1.68358097
H	4.85962968	-4.45619198	2.69232467
H	3.21581951	-5.00627587	2.31194174
H	3.49496225	-3.92444444	3.69418042
H	-2.85261326	-1.14153318	3.60434130
H	-1.99118873	-1.91701558	4.94603955
H	-3.69771840	-2.31358417	4.64534465
H	-2.97965549	-4.88038964	4.49948356
H	-1.30477611	-4.37862512	4.79834627
H	-1.70120506	-5.34670035	3.36126388
H	-6.03164441	3.68911503	0.75380531
H	-6.65287342	4.13362986	-1.60774865
H	-4.96492336	3.91483590	-3.41373411
H	-2.54276860	2.66176732	1.83197673
H	2.51084628	2.70614101	-1.80503983
H	-5.48989656	1.94894649	2.30995894
H	-4.10707672	1.50870396	3.33705386
H	-4.22911802	0.85366384	1.69315964
H	-3.19492293	5.04535456	2.33477807
H	-3.48922407	3.96369810	3.71422732
H	-4.84562229	4.51244421	2.71010638
H	5.46400630	2.00925379	-2.26915546
H	4.09186601	1.58205604	-3.31582996
H	4.20019656	0.90150937	-1.68146305
H	3.15860898	5.09937393	-2.26852590
H	3.46495800	4.03826198	-3.66106304
H	4.81329512	4.57713962	-2.64101233
H	5.98579089	3.74184658	-0.69004550
H	6.59336733	4.14595169	1.68177007
H	4.89909977	3.88056883	3.47598142
H	-1.34333499	2.98663170	-2.77933982
H	1.28459750	2.95068812	2.80643779
H	-3.67850065	2.14857648	-4.59013248
H	-2.75113055	1.07882922	-3.50856249
H	-1.95111417	1.85052826	-4.89022306

H	-1.40481577	4.35231290	-4.84004182
H	-1.87570481	5.35589639	-3.45020596
H	-3.11001525	4.75833071	-4.57619289
H	2.68607044	1.02656797	3.50011297
H	1.88262353	1.76969084	4.89587182
H	3.61141536	2.07122712	4.60773447
H	1.81582727	5.30452952	3.53214881
H	3.04272008	4.68047804	4.65205285
H	1.33580266	4.27027026	4.89624342
O	-0.81518823	-0.70419639	-2.11367238
O	0.87971220	0.80037020	-2.02502996
O	-0.10228513	-0.13628484	2.88820702
O	0.79423977	-0.81821317	2.02547844
Hf	-0.01448544	0.01353555	-0.01319367
O	-1.37228897	1.48761574	-0.41474021
O	1.35946101	-1.45834899	-0.45644530
O	0.07371729	0.04757580	-2.91759301

10. Molecules and Bare Ligands

O₂ Triplet

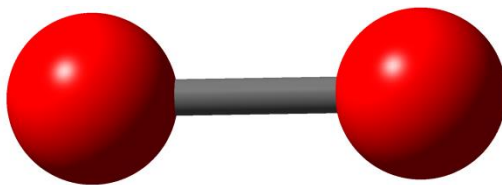


Fig. S119: O₂ Triplet

E	E_{ZP}	H	G
-150.3147	-150.3114	-150.3081	-150.3315

O	0.00000000	0.00000000	0.63422700
O	0.00000000	0.00000000	-0.63422700

O₂ Singlet



Fig. S120: O₂ Singlet

E	E_{ZP}	H	G
-150.2523	-150.2490	-150.2457	-150.2681

O	0.00000000	0.00000000	0.63532800
O	0.00000000	0.00000000	-0.63532800

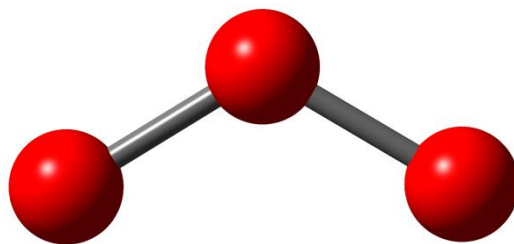
Ozone

Fig. S121: Ozone

E	E_{ZP}	H	G
-225.3955	-225.3891	-225.3851	-225.4124

O	0.00000000	0.00000000	0.45657800
O	0.00000000	1.13809000	-0.22828900
O	0.00000000	-1.13809000	-0.22828900

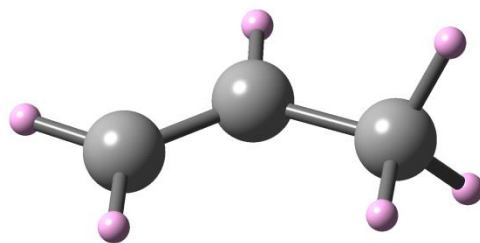
Propene

Fig. S122: Propene

E	E_{ZP}	H	G
-117.8913	-117.8111	-117.8061	-117.8362

C	-0.13128000	-0.45886400	-0.00008400
H	-0.16081500	-1.55115200	0.00012700
C	-1.29659400	0.22180900	-0.00003600
H	-2.25616100	-0.29082800	0.00028100
H	-1.32356100	1.31039200	0.00002500
C	1.24615100	0.16543900	0.00001300
H	1.19036600	1.26028600	-0.00080800
H	1.81989200	-0.14881100	0.88404800
H	1.82061800	-0.15018800	-0.88303300

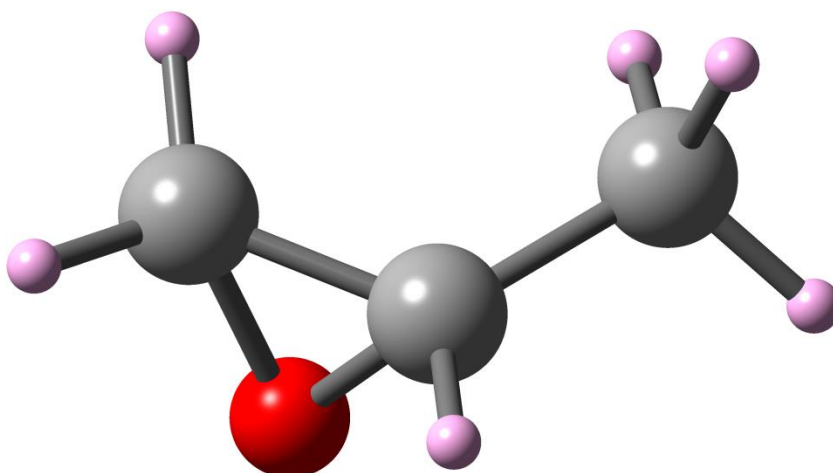
Propylene Oxide

Fig. S123: Propylene Oxide

E	E_{ZP}	H	G
-193.0741	-192.9886	-192.9832	-193.0151
C	0.16847400	-0.00532200	0.50100300
H	0.17015800	-0.18410900	1.57652400
C	-1.03954600	0.65225100	-0.08081900
H	-1.85786500	0.95938100	0.56752000
H	-0.94344800	1.20490300	-1.01412300
C	1.52675800	0.08205200	-0.15864600
H	1.42298000	0.23317600	-1.23919500
H	2.10446900	0.91909200	0.25726300
H	2.09638000	-0.84154500	0.00242700
O	-0.86584900	-0.83309800	-0.21495600

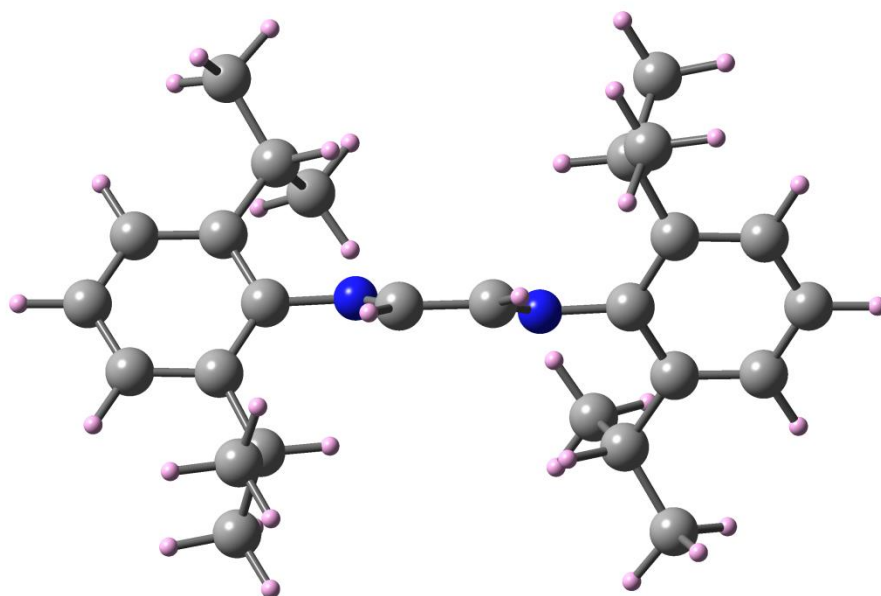
NCCN Ligand

Fig. S124: NCCN Ligand

E	Ezp	H	G
-1121.7494	-1121.1845	-1121.1531	-1121.2482
N	1.44881500	0.16072700	-0.05964200
N	-1.44881900	-0.16078900	-0.05970400
C	0.74080300	0.00836400	-1.13150800
C	-0.74077700	-0.00832000	-1.13153200
C	2.87547600	0.14308200	-0.06412700
C	3.63484200	-0.93754000	-0.60580000
C	5.04370100	-0.85956500	-0.52479200
C	5.68464700	0.23713500	0.06416300
C	4.91927700	1.27798100	0.62333100
C	3.51546000	1.24498600	0.58797200
C	3.45319500	-3.47175900	-0.40794100
C	3.00657000	-2.20956000	-1.19263100
C	3.32374000	-2.36313300	-2.70369600
C	-3.45314700	3.47172300	-0.40790900
C	-3.00655800	2.20954700	-1.19266000
C	-3.32377500	2.36317200	-2.70370700
C	-2.87546700	-0.14310900	-0.06417800
C	-3.63483000	0.93752300	-0.60583800
C	-5.04368800	0.85958700	-0.52477500
C	-5.68464400	-0.23709000	0.06420900
C	-4.91928100	-1.27795200	0.62335800
C	-3.51546600	-1.24499300	0.58795000
C	2.16184200	1.84809700	2.63365100
C	2.66696200	2.33920900	1.24762400
C	3.38981100	3.69852100	1.38180200

C	-2.16184800	-1.84811600	2.63361800
C	-2.66698100	-2.33922900	1.24759600
C	-3.38985100	-3.69852900	1.38177800
H	5.64312200	-1.67249800	-0.92810300
H	6.77067000	0.27937300	0.10018800
H	5.42503600	2.11793500	1.08908200
H	1.91787700	-2.15124100	-1.08951100
H	-1.91786200	2.15121500	-1.08958000
H	4.53459800	-3.63882400	-0.49047100
H	2.94633400	-4.36315800	-0.80181900
H	3.20712100	-3.37929800	0.65704000
H	2.97490900	-1.49474200	-3.27799300
H	2.83963000	-3.26174000	-3.10937900
H	4.40405800	-2.45820700	-2.87362400
H	-4.53455600	3.63877900	-0.49037700
H	-2.94631300	4.36313700	-0.80178800
H	-3.20701600	3.37922900	0.65705600
H	-2.97498100	1.49479200	-3.27804300
H	-2.83965800	3.26178200	-3.10937700
H	-4.40409500	2.45827700	-2.87360300
H	-5.64310000	1.67253900	-0.92806400
H	-6.77066700	-0.27929800	0.10027400
H	-5.42504500	-2.11788700	1.08914000
H	1.77777800	2.49711200	0.62433000
H	-1.77780100	-2.49714200	0.62430100
H	3.00783200	1.64834300	3.30530300
H	1.57348500	0.93163200	2.52324100
H	1.52625700	2.61231500	3.10160100
H	2.68559600	4.45585800	1.75022300
H	3.78946300	4.04430700	0.41931900
H	4.21949500	3.65181000	2.09998000
H	-1.57347100	-0.93166300	2.52319700
H	-1.52627800	-2.61234000	3.10157600
H	-3.00783300	-1.64833500	3.30527000
H	-3.78952100	-4.04430100	0.41929700
H	-4.21952600	-3.65180900	2.09996600
H	-2.68564500	-4.45588000	1.75018600
H	1.19642000	-0.07981000	-2.12956700
H	-1.19636100	0.07998300	-2.12959400

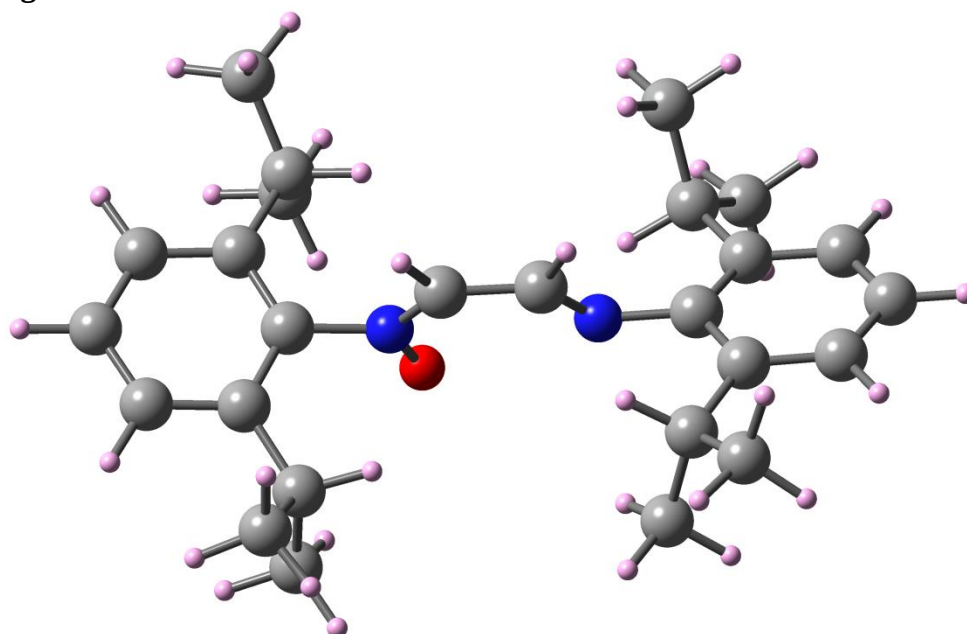
NCCNO Ligand

Fig. S125: NCCNO Ligand

E	E_{zp}	H	G
-1196.9200	-1196.3503	-1196.3179	-1196.4162

O	-1.03473700	-0.26839900	1.33093300
N	1.57518500	-0.05506400	0.04550200
N	-1.43895300	-0.03624500	0.09618600
C	0.80306600	0.13786600	-0.98371200
C	-0.64574400	0.14641200	-0.96483700
C	2.99784200	-0.01674200	-0.07209400
C	3.70212000	-1.21468700	0.24314000
C	5.10848200	-1.20566800	0.17143200
C	5.80661700	-0.03672700	-0.17178900
C	5.09977200	1.14955400	-0.43197300
C	3.69121300	1.19308300	-0.38929800
C	3.61608100	-3.34837500	1.67482200
C	2.92135300	-2.48199400	0.59904500
C	2.63372000	-3.32459200	-0.67510200
C	-2.90989000	2.71783100	2.04716600
C	-2.78311500	2.52737400	0.50961100
C	-3.23555500	3.79781200	-0.24939300
C	-2.90407000	0.02221800	-0.09291000
C	-3.54686700	1.26981000	0.08262700
C	-4.94934100	1.29207300	-0.07077400
C	-5.66171600	0.11979100	-0.37119600
C	-4.98981000	-1.10561300	-0.51015400
C	-3.58832700	-1.18497300	-0.36764700
C	2.50834400	3.03848700	0.86555100
C	2.93896500	2.52526500	-0.53792200

C	3.73022000	3.61683900	-1.29308000
C	-2.98164600	-3.24292600	0.95857300
C	-2.86612000	-2.53519000	-0.42079100
C	-3.37340400	-3.45021900	-1.56073000
H	5.66191100	-2.11401700	0.39330600
H	6.89291800	-0.04373800	-0.22297000
H	5.65490500	2.05210500	-0.66786200
H	1.95409800	-2.15372600	1.00196500
H	-1.71769100	2.38157000	0.29432100
H	4.54894200	-3.79578100	1.30558000
H	2.95558200	-4.17279000	1.97512400
H	3.85125500	-2.75826600	2.56938200
H	2.08916100	-2.73790700	-1.42619200
H	2.02802700	-4.20689900	-0.42639700
H	3.57049600	-3.67109500	-1.13268800
H	-3.95835900	2.86681100	2.33811700
H	-2.33762600	3.59771800	2.36954400
H	-2.52242400	1.84080400	2.57739100
H	-3.16561500	3.66531600	-1.33686700
H	-2.59921000	4.64635600	0.03329100
H	-4.27025700	4.07241700	-0.00747700
H	-5.48650000	2.22826800	0.05070100
H	-6.74240200	0.15897800	-0.48557400
H	-5.55806400	-2.00586200	-0.72502500
H	2.01919800	2.35226800	-1.11048900
H	-1.79875100	-2.35512600	-0.59803500
H	3.39134600	3.23256900	1.48876600
H	1.88378400	2.29974900	1.38132800
H	1.93876600	3.97401400	0.77680400
H	3.08731900	4.49119400	-1.45907500
H	4.08278900	3.26198500	-2.27035500
H	4.60109100	3.95939200	-0.71919200
H	-2.55989000	-2.61474300	1.75100600
H	-2.43576000	-4.19555300	0.94397300
H	-4.03141200	-3.45488600	1.20222200
H	-3.32129700	-2.94827300	-2.53551800
H	-4.41107500	-3.76876200	-1.39825100
H	-2.75846100	-4.35802600	-1.61055800
H	1.21892900	0.30157300	-1.99021900
H	-1.16458400	0.31846400	-1.90073600

ONCCNO Ligand

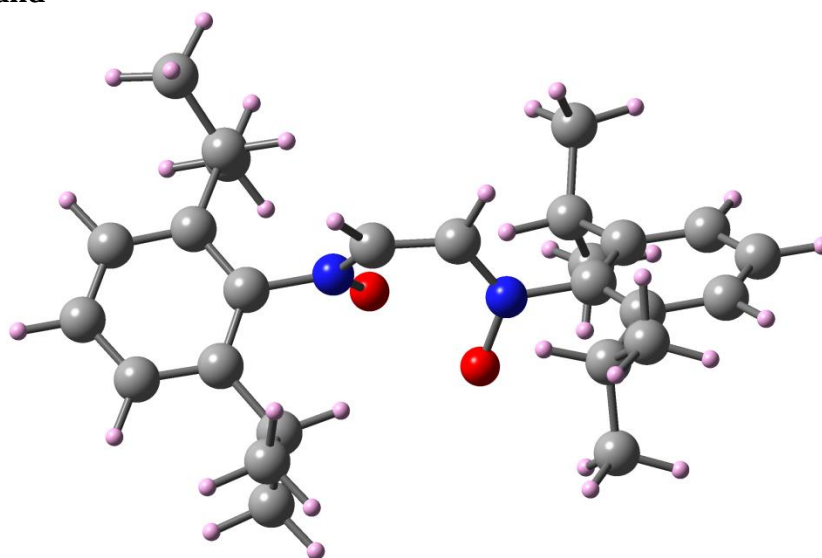


Fig. S126: ONCCNO Ligand

E	Ezp	H	G
-1272.0942	-1271.5198	-1271.4866	-1271.5853

O	1.01339000	0.78755600	0.95164600
N	-1.47638900	-0.18912800	-0.13860900
N	1.47648600	0.18916000	-0.13849500
C	-0.70881700	0.07596600	-1.21062000
C	0.70894400	-0.07554100	-1.21061300
C	-2.89282800	0.19984800	-0.12968000
C	-3.22266600	1.49592700	0.32900100
C	-4.59113500	1.84330900	0.33520800
C	-5.57063400	0.92870500	-0.08188900
C	-5.20676400	-0.36353300	-0.49800700
C	-3.85444900	-0.76217300	-0.52369400
C	-2.38872100	2.73982800	2.37004200
C	-2.16973500	2.47588800	0.85617700
C	-2.16857200	3.80172800	0.05329100
C	2.38835300	-2.73917700	2.37020500
C	2.16963800	-2.47577700	0.85622100
C	2.16858500	-3.80194800	0.05386700
C	2.89291000	-0.19987700	-0.12970000
C	3.22266700	-1.49599800	0.32891100
C	4.59111300	-1.84346800	0.33502700
C	5.57063500	-0.92892700	-0.08216300
C	5.20684900	0.36336000	-0.49821600
C	3.85457000	0.76212000	-0.52370800
C	-3.60368000	-3.10883600	0.36644000
C	-3.45939000	-2.19745400	-0.88471200
C	-4.25607900	-2.76748800	-2.08243500
C	3.60371000	3.10871100	0.36663600
C	3.45937900	2.19739700	-0.88458600

C	4.25602400	2.76760800	-2.08223500
H	-4.88943900	2.83120400	0.67642500
H	-6.61934400	1.21665100	-0.07103500
H	-5.97910300	-1.06541000	-0.79905700
H	-1.17743300	2.02308200	0.76049200
H	1.17734700	-2.02300800	0.76020900
H	-3.35960600	3.21608200	2.56317600
H	-1.60258500	3.40399700	2.75182700
H	-2.34500700	1.80209600	2.93599700
H	-1.98510600	3.62251000	-1.01434900
H	-1.37924800	4.46682200	0.42731100
H	-3.12519700	4.33333700	0.14586300
H	3.35925900	-3.21527300	2.56366900
H	1.60220700	-3.40330400	2.75205000
H	2.34443200	-1.80129700	2.93589400
H	1.98518600	-3.62317000	-1.01385800
H	1.37925700	-4.46690100	0.42811900
H	3.12521900	-4.33348900	0.14673400
H	4.88939100	-2.83138900	0.67618600
H	6.61932200	-1.21696600	-0.07144200
H	5.97923600	1.06516100	-0.79932100
H	-2.39831200	-2.20585400	-1.16368200
H	2.39829100	2.20572700	-1.16351800
H	-4.64702600	-3.14050600	0.70815800
H	-2.97992400	-2.73588900	1.18623600
H	-3.29081000	-4.13459800	0.12913500
H	-3.86297300	-3.75567300	-2.35462200
H	-4.18397600	-2.11591800	-2.96297300
H	-5.31930300	-2.89598300	-1.84210300
H	2.98043000	2.73538800	1.18662000
H	3.29027700	4.13434200	0.12952500
H	4.64717600	3.14085300	0.70794600
H	4.18377000	2.11626500	-2.96292900
H	5.31927700	2.89588000	-1.84191900
H	3.86302300	3.75590900	-2.35415800
O	-1.01326600	-0.78790800	0.95130100
H	-1.23121900	0.36183200	-2.11650400
H	1.23140700	-0.36110800	-2.11655700

11. Singlet Transition States for NCCN Complex

Bisperoxo Complex (spiro conformation) to Oxo Peroxo Complex

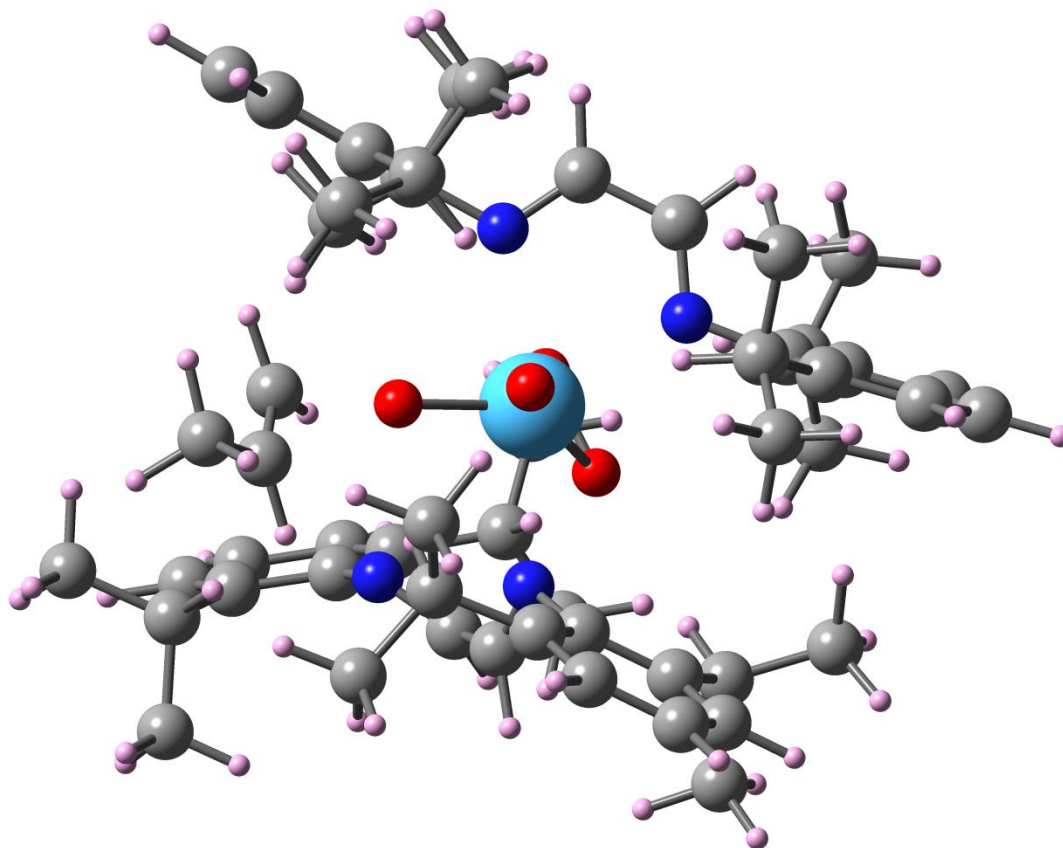


Fig. S127: NCCN Bisperoxo Complex (spiro conformation) to Oxo Peroxo Complex

E	E_{ZP}	H	G	<i>f</i>
-2711.2456	-2710.0186	-2709.9439	-2710.1297	-394

O	1.40433940	1.32475535	1.34235687
O	-0.61202207	1.25974212	1.61432017
O	-0.61898633	-0.04687615	-1.78583765
O	0.12388863	-1.29415912	-1.21347577
N	0.46573097	-1.64028823	1.45098678
N	-2.61015852	-1.91154013	0.54192725
N	0.01408312	2.56914865	-0.97430021
N	2.17584147	0.89876736	-1.45835437
C	-0.39322292	-2.61460087	1.38736255
C	-1.62436734	-2.74487610	0.57210994
C	0.90906542	2.90263116	-1.85037514
C	2.04038130	2.00909981	-2.11738936
C	1.67890660	-1.95118029	2.23009786
C	2.57878369	-2.93367448	1.71641674
C	3.71227747	-3.25367714	2.49516843
C	3.94932293	-2.63616204	3.73042888
C	3.04821904	-1.67544896	4.21129420

C	1.90054622	-1.31053811	3.47779335
C	3.66465879	-3.65740762	-0.48628192
C	2.38056190	-3.66886358	0.37944929
C	1.93051036	-5.13997149	0.60536234
C	-2.61734358	-1.95782526	-3.73310117
C	-2.54417396	-2.77029585	-2.41589247
C	-2.28321890	-4.26989344	-2.72848786
C	-3.81428902	-2.20393511	-0.19253309
C	-3.81221943	-2.60327380	-1.56621475
C	-5.06254865	-2.83960837	-2.17955127
C	-6.27041189	-2.69252639	-1.48477247
C	-6.25394929	-2.29197779	-0.13910988
C	-5.04030830	-2.03750719	0.52521082
C	1.58284060	0.95023703	4.62336743
C	0.89826030	-0.32940094	4.08680732
C	0.07098821	-1.03803458	5.19535669
C	-6.17131350	-0.73490312	2.43653857
C	-5.03413401	-1.69540316	2.01707719
C	-5.07653065	-2.99704144	2.86553255
C	-1.03872629	3.54077284	-0.68389119
C	-0.81569002	4.47624358	0.36272400
C	-1.83536676	5.41795502	0.61367712
C	-3.02074539	5.42953844	-0.14016182
C	-3.20944773	4.49080838	-1.16572900
C	-2.22585311	3.52148864	-1.46013820
C	0.28900472	4.82632612	2.65650306
C	0.49402531	4.49673468	1.15968454
C	1.49422803	5.50713112	0.53072280
C	1.76652370	-2.36694862	-4.03947346
C	2.11485919	-0.87243617	-3.82925291
C	2.30373448	-0.15666722	-5.19421889
C	3.36355068	0.10427258	-1.77648788
C	3.35687203	-0.70188858	-2.94490599
C	4.56387140	-1.34907808	-3.28732461
C	5.71672929	-1.20639412	-2.50074053
C	5.68145549	-0.42270598	-1.33579324
C	4.50522761	0.25005622	-0.94350939
C	-3.87202099	1.92928211	-2.61656744
C	-2.44069697	2.51976465	-2.60187655
C	-2.12408653	3.17951826	-3.97283910
C	5.25237086	0.55802079	1.49308832
C	4.49413274	1.16312759	0.28824605
C	5.07798329	2.55832913	-0.06907251
H	4.41565079	-3.99562998	2.12719153
H	4.82685230	-2.90369387	4.31441186
H	3.23237151	-1.20633159	5.17377333
H	1.60556336	-3.15760616	-0.20240319
H	-1.67859304	-2.37462719	-1.87943423
H	4.46251326	-4.26508713	-0.03935059
H	4.04576491	-2.64210832	-0.62155648
H	3.44871364	-4.07418332	-1.47825686
H	2.69138138	-5.69593310	1.16900097

H	1.78784815	-5.64505905	-0.35922077
H	0.99040141	-5.21192090	1.16725552
H	-3.43101272	-2.29362277	-4.39093523
H	-1.67177229	-2.06668712	-4.27937918
H	-2.74782777	-0.89343650	-3.51520576
H	-2.19388160	-4.87253030	-1.81361461
H	-1.35069009	-4.37717533	-3.29837624
H	-3.09796644	-4.70193708	-3.32598229
H	-5.08512263	-3.14040109	-3.22359972
H	-7.21574106	-2.88659145	-1.98631600
H	-7.19194724	-2.18071940	0.39742483
H	0.22119141	-0.00073012	3.29650994
H	-4.08314516	-1.19854602	2.22995358
H	2.30984244	0.73630060	5.41850568
H	0.82979771	1.63099031	5.04420208
H	2.07993580	1.46524486	3.79553170
H	0.71499102	-1.37320132	6.02004818
H	-0.45537327	-1.92086906	4.80564597
H	-0.67879009	-0.35161623	5.61214328
H	-6.16518758	0.17813382	1.82826965
H	-6.04690710	-0.44453414	3.48847864
H	-7.16130142	-1.20049797	2.34316147
H	-6.00979987	-3.54825561	2.68780679
H	-5.01730357	-2.76299031	3.93739927
H	-4.24081729	-3.66294164	2.61416937
H	-1.70029087	6.14678915	1.40752535
H	-3.79227790	6.16637770	0.07103157
H	-4.13042586	4.50627647	-1.74162388
H	0.93288880	3.49272701	1.12669672
H	1.25079320	-0.43444382	-3.32093226
H	-0.06370071	5.85461488	2.81914616
H	1.24383028	4.71701256	3.18648934
H	-0.42496220	4.13198418	3.11059064
H	1.71628650	5.26912372	-0.51824613
H	2.44203901	5.49512171	1.08511638
H	1.09353730	6.53015245	0.56045699
H	2.57187949	-2.91690768	-4.54549754
H	0.86244206	-2.45118494	-4.65699350
H	1.55703898	-2.83996013	-3.07475341
H	2.50430736	0.91660502	-5.06860284
H	1.39671775	-0.26156550	-5.80383964
H	3.14289342	-0.58546923	-5.75898430
H	4.59730868	-1.96999612	-4.17863325
H	6.63681353	-1.70963676	-2.78851304
H	6.57550024	-0.32780129	-0.72633911
H	-1.75363337	1.67656100	-2.46770504
H	3.45515012	1.30926497	0.61298563
H	-4.63128452	2.68846980	-2.84679202
H	-4.12669806	1.47114976	-1.65364489
H	-3.94267921	1.15009684	-3.38539271
H	-2.26141773	2.45303602	-4.78440048
H	-1.08996618	3.54614693	-4.01971057

H	-2.78873469	4.03379706	-4.16063809
H	4.86550449	-0.43465671	1.74892793
H	5.11954545	1.20426461	2.36991534
H	6.33173199	0.47250649	1.30510864
H	4.51786709	3.03935918	-0.88243842
H	6.12664226	2.47754164	-0.38749832
H	5.03471100	3.22050503	0.80543932
Hf	0.34147528	0.36642473	0.01529042
H	-0.17482898	-3.53196254	1.94709771
H	-1.67993518	-3.72746185	0.08342692
H	0.87232374	3.85556363	-2.38030297
H	2.77497029	2.31981028	-2.86217411
C	-2.79473062	1.32862070	1.28684346
H	-2.95511108	0.58540830	0.51255521
C	-2.36663676	0.94969657	2.54576145
H	-2.24032067	-0.11216142	2.74461531
C	-2.31013368	1.87712436	3.73003342
H	-1.34963476	1.77895867	4.24622590
H	-2.43687611	2.92051090	3.42383222
H	-3.10574560	1.62487636	4.44741703
H	-3.00264602	2.36869512	1.05837104

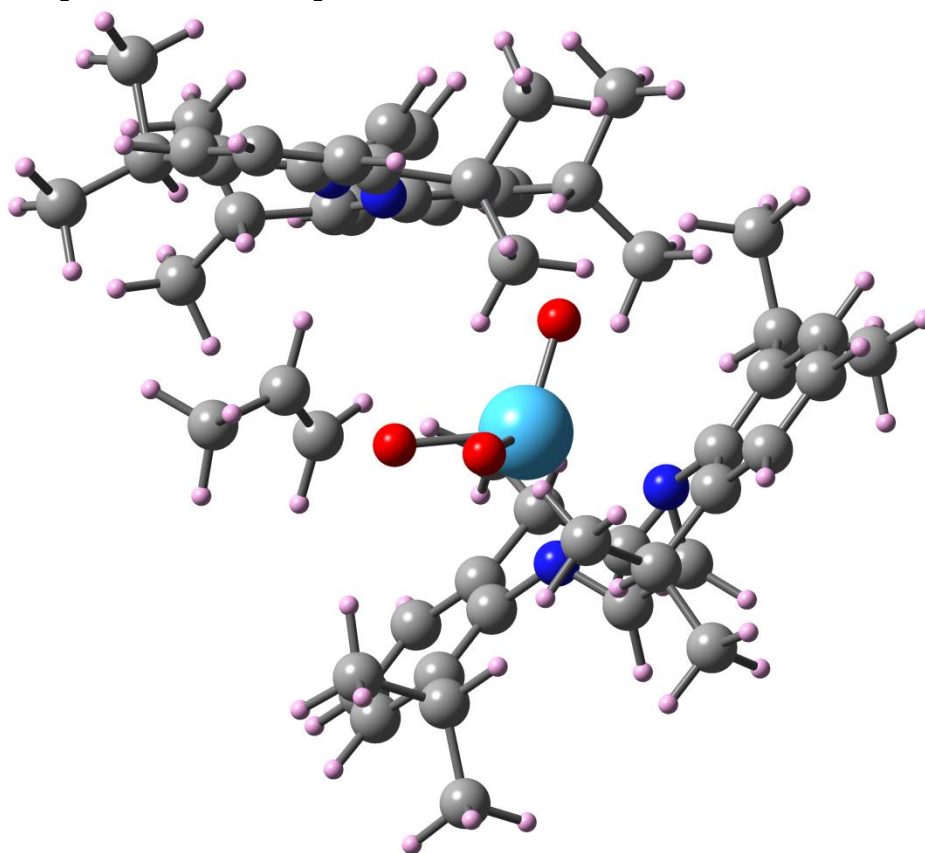
Oxo Peroxo Complex to Dioxo Complex

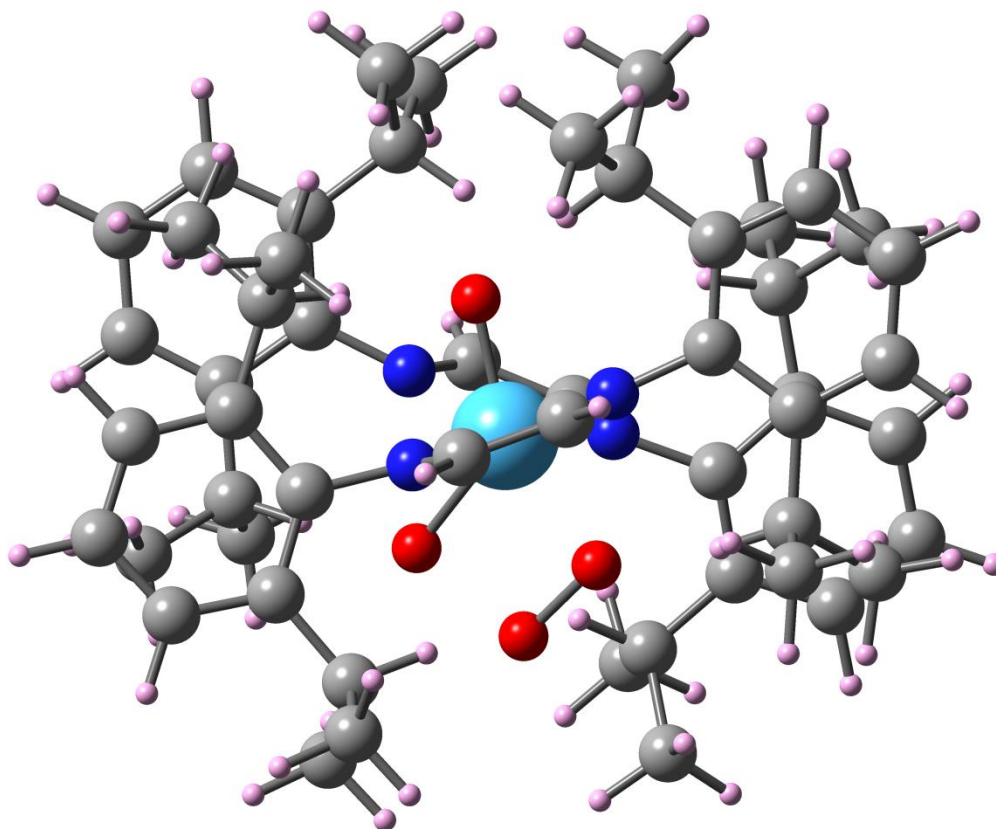
Fig. S128: NCCN Oxo Peroxo Complex to Dioxo Complex

E	E_{ZP}	H	G	<i>f</i>
-2636.0727	-2634.8514	-2634.7766	-2634.9710	-375
O	-0.28479518	0.19034779	1.38029754	
N	-2.32582372	-2.14583319	-0.71983408	
N	-3.41428929	-0.05850569	0.69653137	
N	3.06194228	2.27147155	-0.08522617	
N	3.39600778	-0.40643117	1.09757381	
C	-3.59757400	-2.16097416	-0.42473534	
C	-4.17791324	-1.05919597	0.35763149	
C	3.12523284	2.03214132	1.18485029	
C	3.37364474	0.69883684	1.76949270	
C	-1.79097860	-3.13171723	-1.64691336	
C	-2.13046659	-3.03735353	-3.02603554	
C	-1.56228493	-3.99507383	-3.89485783	
C	-0.70215412	-4.99419028	-3.41993913	
C	-0.37025671	-5.04927917	-2.05555875	
C	-0.89732571	-4.11668188	-1.14266464	
C	-2.15160692	-0.99903191	-4.54420273	
C	-2.99808504	-1.91993988	-3.62384505	
C	-4.22994137	-2.49217312	-4.37247729	

C	-4.53810773	2.98660098	-1.73580753
C	-5.11265241	1.80244375	-0.91392325
C	-6.63042032	1.61294251	-1.17701592
C	-3.99873304	1.10612281	1.34911546
C	-4.82443242	1.97957295	0.58353433
C	-5.36298440	3.10326422	1.24522324
C	-5.10179277	3.34954580	2.60017063
C	-4.27726815	2.47541793	3.32409327
C	-3.69972817	1.34139717	2.71825836
C	0.83454485	-4.75531079	0.64896174
C	-0.57750175	-4.20213639	0.35263200
C	-1.65230130	-5.04936188	1.09088064
C	-1.67977122	1.12657476	4.25742949
C	-2.84851661	0.38701953	3.56125068
C	-3.73664046	-0.37117275	4.58547540
C	2.82571063	3.57675222	-0.61068141
C	1.74666067	4.41127738	-0.17940664
C	1.61798986	5.67838066	-0.78928194
C	2.50138813	6.11361894	-1.78691339
C	3.53290967	5.26534114	-2.22557133
C	3.70406228	3.98877710	-1.66247720
C	-0.74583598	4.16455370	0.34313522
C	0.70283847	3.99192529	0.86751095
C	0.89418942	4.78148818	2.19178831
C	5.61885748	-3.08475548	-1.25563715
C	5.31070719	-1.97335232	-0.22634271
C	6.60551010	-1.19346698	0.13580937
C	3.66417000	-1.66409663	1.71453467
C	4.62379769	-2.48664856	1.04173628
C	4.96819354	-3.72706622	1.60814444
C	4.36735131	-4.16828264	2.79997124
C	3.38746552	-3.37821027	3.41851883
C	3.00079184	-2.12347904	2.89762173
C	5.17222077	3.16302540	-3.60884166
C	4.85395271	3.07709680	-2.09815060
C	6.12866329	3.37151290	-1.25849922
C	0.62621673	-2.24956387	3.83923503
C	1.86686858	-1.35311557	3.59331673
C	2.34081591	-0.74288962	4.94081657
H	-4.25787053	-2.95171853	-0.78470487
H	-5.24107679	-1.08769157	0.59908084
H	3.04688441	2.83332076	1.93175640
H	3.57777660	0.72553120	2.84798499
H	-1.79091176	-3.94686464	-4.95606667
H	-0.28145044	-5.72152130	-4.10978045
H	0.30851378	-5.81885293	-1.70257058
H	-3.37349362	-1.27606170	-2.82117205
H	-4.59460064	0.91083293	-1.28214402
H	-1.70577987	-1.56513460	-5.37298215
H	-1.35639490	-0.51029543	-3.97103471
H	-2.78824241	-0.21408483	-4.97274967
H	-3.92903190	-3.09771471	-5.23658186

H	-4.85704768	-1.67241987	-4.74564448
H	-4.84572964	-3.12744381	-3.72068314
H	-4.95587125	3.94816234	-1.40974205
H	-4.78039811	2.85532957	-2.79929760
H	-3.44755005	3.01186596	-1.64049597
H	-7.03818605	0.75563644	-0.62276783
H	-6.81083468	1.44812656	-2.24743556
H	-7.20196133	2.50055412	-0.87699786
H	-5.98650528	3.79557669	0.68616830
H	-5.53275505	4.22057417	3.08762394
H	-4.07918837	2.67252663	4.37408436
H	-0.62475536	-3.18447342	0.76864850
H	-2.38370466	-0.34981433	2.89882559
H	0.91827169	-5.81789078	0.38554624
H	1.05663778	-4.66617204	1.71789363
H	1.61094762	-4.20389995	0.10565698
H	-1.64769164	-6.08305652	0.72075213
H	-2.66305653	-4.64579391	0.94662334
H	-1.44597809	-5.07053336	2.16850818
H	-0.98037555	1.49505301	3.50039071
H	-1.13354000	0.43165509	4.90892720
H	-2.02876469	1.96188015	4.87899051
H	-4.18544450	0.31881738	5.31262530
H	-3.13431354	-1.10134852	5.14201746
H	-4.55604572	-0.91115775	4.09028755
H	0.80414382	6.33013150	-0.48221115
H	2.37952544	7.09962697	-2.22974883
H	4.20212377	5.60043438	-3.01318552
H	0.81525723	2.92521866	1.08915524
H	4.62204569	-1.25686550	-0.69024738
H	-0.97458113	5.21235512	0.10482214
H	-1.45590656	3.83585685	1.11452767
H	-0.91683003	3.54607112	-0.54434343
H	1.90455105	4.65722579	2.60512195
H	0.17116740	4.43855962	2.94414004
H	0.73476214	5.85695940	2.03407370
H	6.38747050	-3.78240657	-0.89589836
H	5.99611207	-2.63648202	-2.18443827
H	4.71923225	-3.66419597	-1.50038974
H	6.38740753	-0.35639675	0.81022331
H	7.07524778	-0.78564647	-0.76981974
H	7.33271219	-1.85081299	0.63228583
H	5.71051997	-4.35225023	1.11960771
H	4.65211728	-5.12372393	3.23503700
H	2.90729342	-3.74256846	4.32348295
H	4.54868774	2.04863445	-1.86806324
H	1.51498084	-0.54816587	2.93826657
H	5.59574698	4.13783887	-3.88579577
H	4.27365563	2.99894579	-4.21711342
H	5.91359381	2.39866183	-3.87887202
H	6.94020233	2.68338068	-1.53300077
H	5.93137236	3.25425507	-0.18576086

H	6.47829610	4.39904199	-1.42904237
H	0.26161833	-2.67006889	2.89581061
H	-0.18273274	-1.64372069	4.26521165
H	0.83502376	-3.07447977	4.53437803
H	3.21025238	-0.08524062	4.81292393
H	2.63016952	-1.53084949	5.65020504
H	1.53356364	-0.15425702	5.39732060
O	-1.68372024	1.37589135	-1.34057053
O	-0.15894213	0.28200926	-1.87228041
C	1.46178348	-1.35022896	-2.08830809
H	1.58264332	-1.77236386	-1.09232131
H	1.08550543	-1.99937047	-2.87559392
C	1.83283240	-0.04419821	-2.33513563
H	2.26095499	0.53626975	-1.51853469
C	1.88588092	0.57677777	-3.70687427
H	1.40357644	1.55984103	-3.68345535
H	2.93232010	0.72061939	-4.01587635
H	1.38196945	-0.04490185	-4.45600757
Hf	-1.21599048	-0.11353226	-0.17896598

Dioxo Complex to Oxo η^2 -Ozone ComplexFig. S129: NCCN Dioxo Complex to Oxo η^2 -Ozone Complex

E	E_{zp}	H	G	<i>f</i>
-2593.3630	-2592.2179	-2592.1487	-2592.3218	-153
O	-1.26973022	0.86731059	1.66511930	
O	1.18238871	1.79817784	0.97462837	
O	-0.44614833	-1.02871093	-1.15125368	
N	-1.16434676	1.89373944	-1.08794128	
N	1.48131744	1.12749110	-1.65878718	
N	1.24989915	-1.19624306	1.66573390	
N	-1.46150841	-1.84979380	1.16209053	
C	-0.44985781	2.54315189	-1.95431464	
C	0.92508535	2.13247360	-2.26269190	
C	0.65732493	-2.22555178	2.20910049	
C	-0.69360668	-2.64227468	1.84695744	
C	-2.57931263	2.27146286	-0.97212356	
C	-3.52072036	1.53764477	-1.74822163	
C	-4.87391087	1.92569981	-1.66441712	
C	-5.27739412	2.99830812	-0.85363727	
C	-4.32493997	3.70681524	-0.10976061	
C	-2.95598302	3.36334709	-0.14946308	
C	-4.14022686	-0.70933690	-2.83260885	

C	-3.09059648	0.41950404	-2.70743959
C	-2.79075021	1.00503478	-4.11695048
C	1.85981827	-2.50415281	-3.86566501
C	1.62293070	-0.98791311	-3.66281239
C	1.11070076	-0.34888995	-4.98303938
C	2.80615140	0.74875398	-2.15943421
C	2.87464046	-0.25562328	-3.16438264
C	4.13608693	-0.51166634	-3.74093926
C	5.28305674	0.18316275	-3.32611777
C	5.18859558	1.14658273	-2.31073135
C	3.95101763	1.45685373	-1.70545201
C	-2.32475044	4.20231416	2.17009308
C	-1.95611439	4.18859279	0.66540730
C	-1.84102681	5.63131082	0.10423706
C	4.95447804	2.38880215	0.45782120
C	3.87480675	2.55724265	-0.63942514
C	3.98789853	3.96235661	-1.29291253
C	2.62493715	-0.96312544	2.13990464
C	2.83213308	-0.17246375	3.30062995
C	4.15802326	-0.03161387	3.76335847
C	5.23017506	-0.65345476	3.10792918
C	4.99383236	-1.44077363	1.97094914
C	3.68911024	-1.61940714	1.46410979
C	1.98289436	1.90250765	4.54116321
C	1.67741161	0.45446166	4.08954613
C	1.32088608	-0.42707562	5.31935252
C	-1.71057630	-3.95425060	-2.40866742
C	-1.61902935	-4.05328243	-0.86540842
C	-1.43139286	-5.52687583	-0.41511630
C	-2.75642255	-2.34262931	0.74466112
C	-2.84058756	-3.41560798	-0.19028057
C	-4.12816803	-3.88514452	-0.52781764
C	-5.28390543	-3.32039786	0.02954781
C	-5.17394743	-2.25379793	0.93661447
C	-3.91685296	-1.74012121	1.31162605
C	4.60709805	-2.53049929	-0.75576309
C	3.44752639	-2.55072325	0.26711935
C	3.21636968	-4.01574106	0.73670806
C	-4.94455336	0.38869331	2.32654323
C	-3.80105804	-0.64852220	2.37646067
C	-3.71341996	-1.28811890	3.79090489
H	-5.61737096	1.38479585	-2.24156994
H	-6.32675323	3.27995571	-0.80623775
H	-4.64171334	4.53825084	0.51436757
H	-2.17186008	-0.03988625	-2.32198443
H	0.83659066	-0.89796059	-2.90225072
H	-5.05009412	-0.37243891	-3.34861276
H	-4.42403886	-1.10416784	-1.85155062
H	-3.72118145	-1.53671776	-3.41867227
H	-3.68948465	1.46964851	-4.54550406
H	-2.45991118	0.20780512	-4.79577886
H	-2.00272527	1.76883001	-4.08974028

H	2.57773666	-2.71542602	-4.67020448
H	0.91182576	-2.98841026	-4.13107213
H	2.22721564	-2.97192616	-2.94399180
H	0.87572857	0.71635813	-4.85522186
H	0.19666378	-0.85592567	-5.31909582
H	1.86131012	-0.43093810	-5.78167203
H	4.21897464	-1.26180611	-4.52241726
H	6.24460963	-0.02821036	-3.78802801
H	6.08226440	1.67376272	-1.98778785
H	-0.97309960	3.71697169	0.60805957
H	2.90539821	2.49767334	-0.13446122
H	-3.30235010	4.67022032	2.35147226
H	-1.57030847	4.76737131	2.73305398
H	-2.33980288	3.17814168	2.55580002
H	-2.79777320	6.16601077	0.17537741
H	-1.53776426	5.63447196	-0.95245069
H	-1.09422533	6.19983795	0.67419140
H	4.89103339	1.40154878	0.92762284
H	4.80623341	3.14412245	1.24041918
H	5.97055852	2.51823092	0.06050809
H	4.94892765	4.08136314	-1.81160140
H	3.91578591	4.74391001	-0.52521856
H	3.19030085	4.13624681	-2.02775053
H	4.34821931	0.57017165	4.64716723
H	6.24357244	-0.53008703	3.48254420
H	5.82965783	-1.92294554	1.47387919
H	0.79706256	0.51527123	3.44477242
H	-0.72836065	-3.47982716	-0.59442100
H	2.78422770	1.94353267	5.29201745
H	1.08360680	2.34368825	4.98837962
H	2.26763149	2.52167899	3.68439711
H	1.02176797	-1.44260752	5.02553466
H	0.48598672	0.02115788	5.87345539
H	2.17670796	-0.51654063	6.00242134
H	-2.59664262	-4.46670928	-2.80653775
H	-0.82351549	-4.41502095	-2.86442859
H	-1.73661151	-2.90064207	-2.70290792
H	-1.31906939	-5.61051976	0.67490422
H	-0.53634651	-5.95781434	-0.88404046
H	-2.29131351	-6.14590278	-0.70401579
H	-4.22345921	-4.69955669	-1.24148968
H	-6.26405911	-3.70480042	-0.24311020
H	-6.07285981	-1.81839909	1.36233918
H	2.53846069	-2.21837828	-0.25255640
H	-2.86368896	-0.09769455	2.20866313
H	5.50533223	-3.02037188	-0.35642436
H	4.87096984	-1.51053746	-1.04943970
H	4.31491473	-3.07736021	-1.66040018
H	3.06932342	-4.67190802	-0.13128635
H	2.33696095	-4.11621298	1.38348005
H	4.08742957	-4.38071043	1.29709846
H	-5.04508373	0.82359199	1.32563705

H	-4.72579377	1.20602645	3.02561039
H	-5.91275061	-0.04279736	2.61841446
H	-2.86696231	-1.98291301	3.86960768
H	-4.63128713	-1.84489416	4.02746553
H	-3.57908955	-0.50677834	4.55028459
O	0.19376704	2.20604472	1.92196293
H	1.43310848	2.66899741	-3.06738695
H	-0.86868985	3.37234245	-2.52754519
H	1.18207833	-2.83139554	2.94978920
H	-1.00976106	-3.63980334	2.16162417
Hf	-0.06229767	0.19069127	0.19564265

12. Transition States for NCCNO Complex

12.1 Singlet Geometries

Bisperoxo Complex to Oxo Peroxo Complex (Propene)

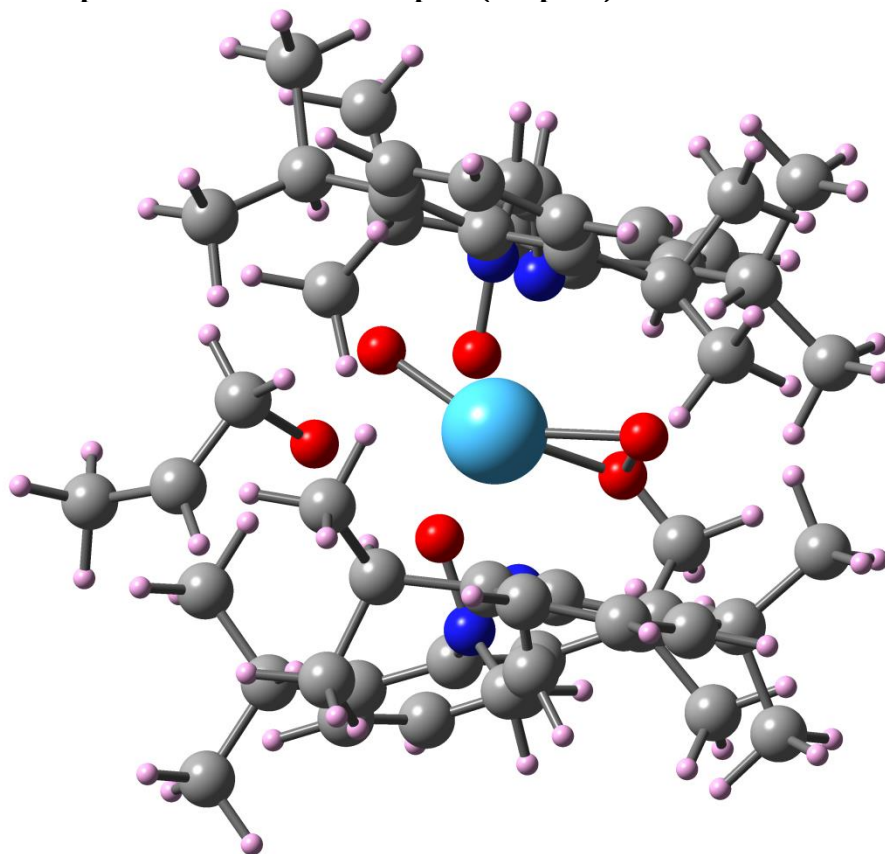


Fig. S130: NCCNO Bisperoxo Complex to Oxo Peroxo Complex (Propene)

E	E_{zp}	H	G	<i>f</i>
-2861.5971	-2860.3614	-2860.2855	-2860.4747	-356
O	2.01720289	0.14517742	0.42675041	
O	-2.12506732	-0.75477254	0.60170415	
O	-0.33593672	0.89934133	1.93453934	
N	0.03441102	-2.16257794	-0.86987062	
N	-2.91084527	-1.59380638	-0.08030576	
N	0.02460500	2.41967309	0.15676642	
N	2.85767256	1.22427315	0.52809467	
C	-1.06541098	-2.78477800	-1.24683316	
C	-2.43830336	-2.52631129	-0.89674038	
C	1.15559307	3.06160378	0.45156307	
C	2.45487294	2.50589951	0.58457490	
C	1.24334259	-2.67294818	-1.52148631	
C	1.36291287	-2.62440229	-2.94530808	
C	2.51269931	-3.20467009	-3.52269617	
C	3.51065568	-3.80284194	-2.74153073	

C	3.37666678	-3.82807727	-1.34608167
C	2.24665879	-3.27223549	-0.71356104
C	0.97840753	-0.86694551	-4.75479126
C	0.33390115	-1.97720111	-3.88601231
C	-0.34779416	-3.04040545	-4.79059156
C	-4.87891792	1.36088959	-2.25310523
C	-4.48397250	-0.12932626	-2.09496838
C	-4.88421829	-0.93712106	-3.35929120
C	-4.35328031	-1.43571401	0.14253572
C	-5.10715474	-0.74448273	-0.83679165
C	-6.49465815	-0.63292597	-0.60164025
C	-7.07844491	-1.15874289	0.56110176
C	-6.28759544	-1.80385024	1.52577367
C	-4.89825274	-1.95721326	1.34031538
C	3.36716263	-3.22069681	1.58961142
C	2.05930409	-3.43929117	0.79378579
C	1.46439251	-4.84554011	1.08907471
C	-3.85030632	-1.63024314	3.61117011
C	-4.03712062	-2.61278178	2.42309683
C	-4.61889712	-3.96756113	2.89824269
C	-1.13386231	3.28948306	-0.09702993
C	-1.94936080	3.75298140	0.97451578
C	-3.06244379	4.56352045	0.65403831
C	-3.34552502	4.93460108	-0.66601263
C	-2.49441554	4.51435377	-1.69896172
C	-1.37760473	3.69284221	-1.44411547
C	-2.84402166	2.70754798	3.11832566
C	-1.66794633	3.46562513	2.45326322
C	-1.34436276	4.77563554	3.21986046
C	4.69805789	-0.11798965	-3.09598652
C	4.22218278	0.88333896	-2.01820287
C	4.39460275	2.34089188	-2.53321584
C	4.28326158	0.90000186	0.56012837
C	4.94733433	0.70897942	-0.67935412
C	6.32652674	0.41982045	-0.63143447
C	7.00615363	0.32999047	0.59486458
C	6.32051534	0.53049887	1.80212832
C	4.93797010	0.81607112	1.81339161
C	-1.16346043	2.83649257	-3.85333601
C	-0.42555661	3.35186417	-2.59512916
C	0.45216580	4.58704362	-2.94097405
C	4.49412673	-0.04713654	4.18058325
C	4.21683500	1.06831425	3.14159742
C	4.61026301	2.45453957	3.72239188
H	-0.97132032	-3.62624922	-1.93560099
H	-3.18908120	-3.16161596	-1.34995297
H	1.12146343	4.14400927	0.58054782
H	3.27026852	3.20619083	0.72571306
H	2.62746207	-3.17950094	-4.60321299
H	4.38290767	-4.24666239	-3.21576581
H	4.14822750	-4.29825710	-0.74345843
H	-0.43019953	-1.47142653	-3.29052752

H	-3.39160692	-0.14900526	-2.01253480
H	1.78832505	-1.25254310	-5.38911909
H	1.36225422	-0.07504381	-4.10566903
H	0.21823396	-0.42391725	-5.41260202
H	0.37882271	-3.52263613	-5.45835516
H	-1.11385727	-2.56521327	-5.41770175
H	-0.83166527	-3.83572739	-4.20626202
H	-5.95806507	1.48600995	-2.41641699
H	-4.35549471	1.78861270	-3.11665430
H	-4.59055793	1.94338392	-1.37126745
H	-4.56922963	-1.98720555	-3.28925251
H	-4.41046165	-0.50124196	-4.24797067
H	-5.97186252	-0.92409925	-3.51271127
H	-7.11592082	-0.11603145	-1.32741672
H	-8.14900091	-1.05563675	0.72188979
H	-6.75092462	-2.18904932	2.42972078
H	1.32982093	-2.69425768	1.12961688
H	-3.03731166	-2.80517478	2.01720182
H	4.10560866	-4.00749275	1.38750248
H	3.16227772	-3.24034166	2.66795576
H	3.81802268	-2.25402374	1.33870233
H	2.14156200	-5.63443111	0.73546722
H	0.49650934	-4.98272758	0.58958075
H	1.31206068	-4.98972237	2.16715687
H	-3.32159801	-0.72961798	3.28290731
H	-3.25423498	-2.10358186	4.40105022
H	-4.81927173	-1.33989634	4.03938232
H	-5.58154334	-3.84114568	3.41004811
H	-3.92918492	-4.43948987	3.61004904
H	-4.77061981	-4.65951249	2.05937751
H	-3.70536102	4.91489317	1.45757091
H	-4.20772742	5.56030343	-0.88656719
H	-2.69509681	4.83096693	-2.71910833
H	-0.80732022	2.79728252	2.52514314
H	3.15241435	0.70679868	-1.86077693
H	-3.77823003	3.28611694	3.08912740
H	-2.60875478	2.49719388	4.17077243
H	-3.00547643	1.75014227	2.61160747
H	-0.49424222	5.30559777	2.76831319
H	-1.08798220	4.54763841	4.26376258
H	-2.19905307	5.46592403	3.22822809
H	5.73450170	0.07389465	-3.40565554
H	4.06601048	-0.02364377	-3.98730512
H	4.62403154	-1.15113660	-2.74111593
H	4.00690292	3.07464426	-1.81635819
H	3.84797350	2.47290471	-3.47565596
H	5.45391018	2.56830706	-2.71549865
H	6.87198286	0.26524208	-1.55726044
H	8.07053324	0.10694650	0.60777577
H	6.85963419	0.46106332	2.74286075
H	0.22651226	2.53531144	-2.27758936
H	3.13779256	1.08301315	2.95486808

H	-1.83589867	3.58999814	-4.28767138
H	-1.73612216	1.93993623	-3.59672730
H	-0.43025047	2.56324351	-4.62459273
H	1.17060057	4.33242589	-3.73259694
H	1.01831146	4.93796761	-2.06731870
H	-0.16245502	5.42547489	-3.29771190
H	4.25514085	-1.03816395	3.77815382
H	3.88070199	0.11456840	5.07634008
H	5.54509139	-0.05452288	4.49706564
H	4.37102394	3.26761660	3.02526880
H	5.68647691	2.50114313	3.93505252
H	4.06968154	2.64293762	4.65915260
O	-1.17992200	0.42769152	-1.61546501
O	0.33784030	0.37226462	-1.89460859
C	1.00600726	-0.95254868	3.37798478
H	1.95018622	-0.92478474	2.82770953
C	0.61019809	-2.25560351	3.90564969
H	0.90580269	-3.14891400	3.36396052
O	-0.13154424	-0.79122526	2.39540969
H	0.93153974	-0.12305341	4.08943985
C	-0.29996816	-2.40556965	5.08805308
H	-1.06509104	-3.17845150	4.92582473
H	0.26307531	-2.71033033	5.99077759
H	-0.80665162	-1.46140293	5.32000320
Hf	-0.12897100	0.09142188	0.11423944

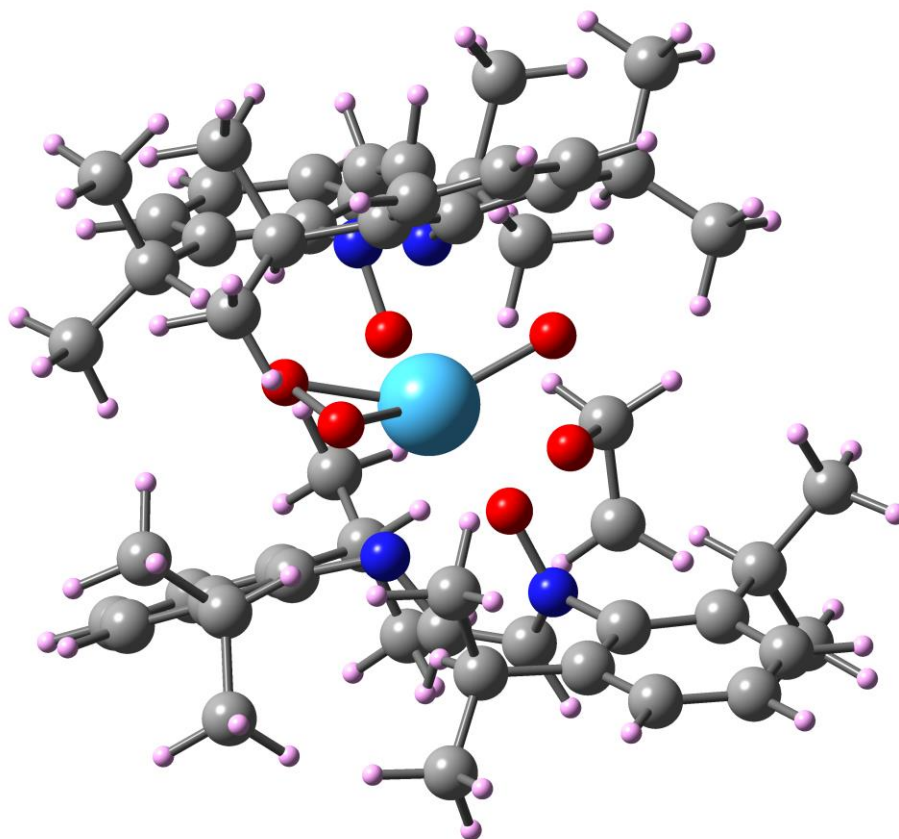
Bisperoxo Complex to Oxo Peroxo Complex (Ethylene)

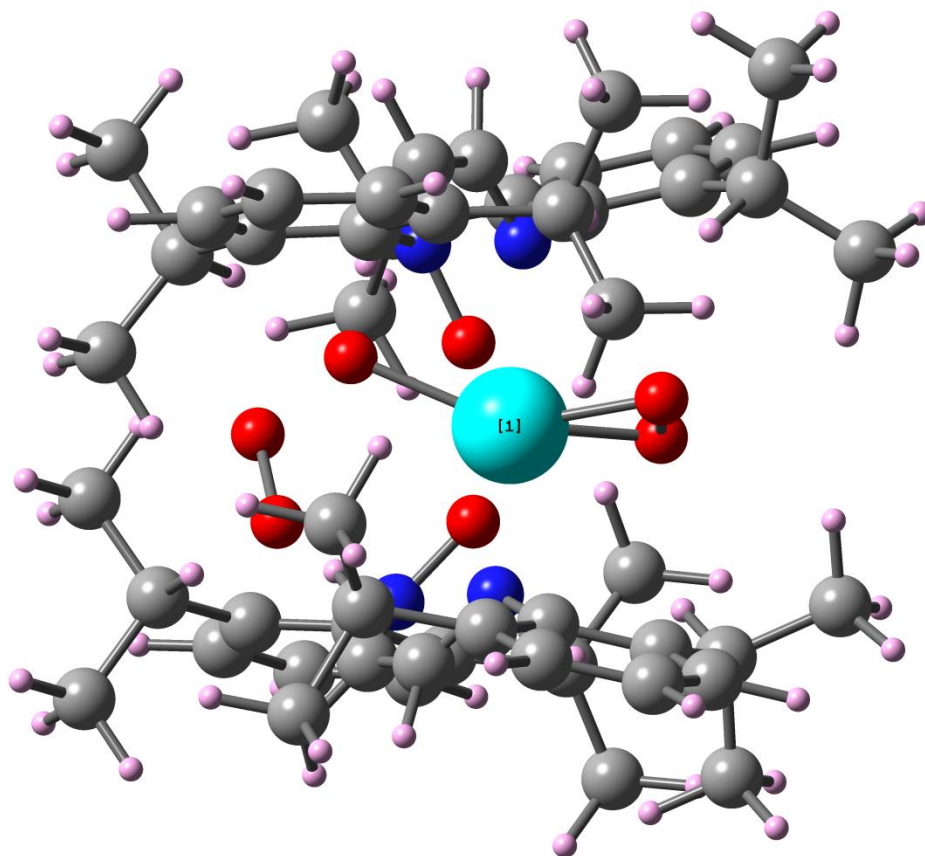
Fig. S131: NCCNO Bisperoxo Complex to Oxo Peroxo Complex (Ethylene)

E	E_{ZP}	H	G	<i>f</i>
-2822.2903	-2821.0823	-2821.0080	-2821.1933	-324
O	1.95433915	0.19690901	0.60589704	
O	-2.29466218	-0.42827203	0.03247900	
O	-0.57392304	1.43019811	1.36951610	
N	-0.07454901	-2.25164817	-0.04794500	
N	-2.90020922	-1.40811411	0.70103405	
N	0.28402502	2.51595119	-0.60009904	
N	2.89025422	1.15666009	0.40468903	
C	-0.97960208	-2.95381523	0.59690705	
C	-2.27509418	-2.52425019	1.06943808	
C	1.44028311	3.07844524	-0.32783103	
C	2.66048020	2.41622918	0.04435400	
C	0.96890207	-3.05504123	-0.71210706	
C	0.78759206	-3.36282926	-2.08904316	
C	1.74161213	-4.19730032	-2.70857021	
C	2.83652622	-4.71087536	-1.99937415	
C	2.99791323	-4.38803333	-0.64508605	
C	2.07497716	-3.55648227	0.02551800	
C	-0.00978400	-2.23414517	-4.23751033	

C	-0.42305103	-2.88335622	-2.89480722
C	-1.41906811	-4.05400431	-3.11829224
C	-4.63495936	-0.49391904	-2.51849119
C	-4.62598735	-1.76560714	-1.62599112
C	-5.38991942	-2.92982423	-2.30436818
C	-4.34850633	-1.23384909	0.89573007
C	-5.17907339	-1.43456411	-0.23624402
C	-6.56568448	-1.26711910	-0.04368200
C	-7.08667256	-0.91879507	1.21312509
C	-6.22930450	-0.71224305	2.30372817
C	-4.83077737	-0.85077907	2.16821117
C	3.73394628	-2.88059622	1.85925914
C	2.27641817	-3.27264525	1.51753012
C	1.85318014	-4.49857634	2.37449418
C	-4.17139732	0.80874706	3.98329731
C	-3.91034230	-0.58746904	3.36352626
C	-4.07683231	-1.69766613	4.43620634
C	-0.75855006	3.42480326	-1.09273808
C	-1.47932011	4.25704832	-0.19051901
C	-2.48086019	5.09509739	-0.72905805
C	-2.74460521	5.13192339	-2.10431016
C	-1.98064315	4.34354033	-2.97766423
C	-0.97069107	3.48258926	-2.50102919
C	-2.48301519	4.02310531	2.13934616
C	-1.20597909	4.31867133	1.31660610
C	-0.59605205	5.69078245	1.71081113
C	4.66800736	-1.25866409	-2.56649319
C	4.35225333	0.08930001	-1.87544714
C	4.82047137	1.27481510	-2.76487821
C	4.27436733	0.72166005	0.62936205
C	4.97966538	0.19453402	-0.48036104
C	6.31821850	-0.18965901	-0.25268602
C	6.90489255	-0.05673400	1.01683808
C	6.16731646	0.46228204	2.09320316
C	4.82444337	0.86081106	1.92501015
C	-0.86130607	2.05660215	-4.63098036
C	-0.06783101	2.75353421	-3.50187127
C	0.96655007	3.75218229	-4.09470332
C	4.07258131	0.52822304	4.34492033
C	4.03229331	1.44743411	3.09813323
C	4.54714535	2.86899722	3.45282926
H	-0.82413907	-4.03011631	0.71449805
H	-2.87870322	-3.24050025	1.61165512
H	1.55017512	4.15998632	-0.43298403
H	3.55692727	3.02602923	0.02066500
H	1.61868712	-4.44873134	-3.75847629
H	3.55679227	-5.35648039	-2.49661019
H	3.84835229	-4.78678637	-0.09872101
H	-0.92726707	-2.09091116	-2.33647118
H	-3.57841527	-2.07281216	-1.53130112
H	0.49539904	-2.94173023	-4.91011537
H	0.64571705	-1.38115311	-4.03799231

H	-0.90192307	-1.85802114	-4.75509637
H	-0.96005307	-4.86333537	-3.70277828
H	-2.30135917	-3.69999428	-3.66865128
H	-1.76170714	-4.48636034	-2.16684516
H	-5.65729141	-0.11408401	-2.65078520
H	-4.22297833	-0.72620506	-3.50876727
H	-4.01943031	0.29418802	-2.07381116
H	-5.41042440	-3.82594329	-1.67023913
H	-4.89909537	-3.19195224	-3.25019425
H	-6.42676746	-2.65678720	-2.53880719
H	-7.24074553	-1.40951411	-0.88244907
H	-8.16018661	-0.79917706	1.33852910
H	-6.64436552	-0.42486003	3.26581525
H	1.64520412	-2.41969519	1.78525914
H	-2.87188322	-0.58782804	3.01613623
H	4.42969534	-3.71401228	1.69785313
H	3.80704129	-2.59695920	2.91782322
H	4.06616931	-2.03300616	1.25368410
H	2.46053819	-5.37575742	2.11573716
H	0.80124806	-4.77060236	2.21794617
H	1.99692915	-4.29230933	3.44377626
H	-4.05891531	1.59808412	3.23306925
H	-3.44551526	1.00102808	4.78403937
H	-5.17705040	0.88363107	4.41817434
H	-5.10798039	-1.73428113	4.81215037
H	-3.41645626	-1.50439612	5.29207142
H	-3.83309829	-2.69123321	4.03607831
H	-3.05476523	5.72833843	-0.05711300
H	-3.52448327	5.78210945	-2.49469319
H	-2.16111416	4.40182134	-4.04750931
H	-0.50278504	3.52391927	1.57861512
H	3.26162325	0.14852901	-1.78878114
H	-3.27240425	4.76776837	1.96673415
H	-2.24758817	4.02344731	3.21262025
H	-2.86324622	3.03129923	1.87563515
H	0.33519403	5.89328446	1.16303909
H	-0.36958703	5.71085542	2.78599821
H	-1.28902310	6.51641348	1.49809311
H	5.73757744	-1.36607811	-2.79430821
H	4.11789331	-1.31813110	-3.51323927
H	4.35559633	-2.10640016	-1.94764715
H	4.55525435	2.24476917	-2.32460018
H	4.34088633	1.21297309	-3.74951929
H	5.90937647	1.25471310	-2.90963722
H	6.90162652	-0.59806705	-1.07252108
H	7.93848462	-0.35937803	1.16747509
H	6.63523848	0.55521704	3.06953823
H	0.47438804	1.96446515	-2.97723423
H	2.98167623	1.53966312	2.80024222
H	-1.41486211	2.76767921	-5.26091340
H	-1.55808812	1.33342910	-4.19681632
H	-0.16831401	1.50642612	-5.28207940

H	1.64969512	3.22691324	-4.77631636
H	1.57030712	4.22539332	-3.30723125
H	0.47078404	4.55358835	-4.66053335
H	3.70757428	-0.47802904	4.10822331
H	3.43813326	0.94426907	5.13810039
H	5.08917439	0.43436903	4.74792936
H	4.48211934	3.54788327	2.59279120
H	5.59539942	2.83943222	3.77810629
H	3.95026230	3.29767125	4.26815032
O	-0.71522005	0.16709601	-2.03754415
O	0.83737606	0.05306800	-1.92596215
C	0.20296902	-0.36180203	3.40569326
H	1.26224510	-0.27235602	3.14662724
C	-0.27495902	-1.71231813	3.72514529
H	0.24453902	-2.59254820	3.37195826
O	-0.64158905	-0.30684202	2.18542017
H	-0.10777301	0.43605103	4.08658031
Hf	-0.13353801	0.15929601	-0.09631201
H	-1.19545009	-1.84601014	4.28208033

Oxo Peroxo Complex to Peroxo η^2 -Ozone ComplexFig. S132: NCCNO Oxo Peroxo Complex to Peroxo η^2 -Ozone Complex

E	E_{zp}	H	G	<i>f</i>
-2818.8954	-2817.7379	-2817.6659	-2817.8471	-108
O	2.06114425	0.30874891	0.21298467	
O	-2.07488278	-0.42212396	-0.35487073	
O	-0.23759159	0.15457449	1.71471747	
N	0.18363218	-1.82114851	-1.36524658	
N	-2.54173268	-1.65226539	0.04435532	
N	-0.01346983	2.43268009	0.55175694	
N	2.61700813	0.97676102	1.22952380	
C	-0.57087117	-2.80669673	-0.91785603	
C	-1.76859778	-2.72925632	-0.12073428	
C	0.90288149	2.78847821	1.41131726	
C	2.09836840	2.06028265	1.78711431	
C	1.27593317	-2.19269068	-2.27144812	
C	1.17636803	-1.78762900	-3.63258919	
C	2.22466781	-2.14222104	-4.50513294	
C	3.32955437	-2.88070953	-4.05550303	
C	3.39524906	-3.28808610	-2.71652917	
C	2.37771422	-2.95987478	-1.79306409	
C	0.26619860	0.06753401	-5.15557201	

C	-0.06896201	-1.09063396	-4.18787232
C	-0.99470963	-2.13814177	-4.86793280
C	-4.75646292	0.78714872	-2.02387081
C	-4.55588638	-0.74565767	-1.89571776
C	-5.37085835	-1.50582421	-2.97470014
C	-3.94317142	-1.70156326	0.45302310
C	-4.90687819	-1.22822724	-0.48221030
C	-6.25675477	-1.23288640	-0.07707226
C	-6.63832242	-1.71617197	1.18383398
C	-5.66926087	-2.21282134	2.06558200
C	-4.29769874	-2.21349110	1.73004790
C	3.88172488	-3.11544641	0.26917870
C	2.50697643	-3.46984541	-0.35049820
C	2.28632423	-5.00720529	-0.28400944
C	-3.36856378	-2.03432199	4.09926749
C	-3.29448532	-2.77878911	2.74253732
C	-3.51353828	-4.30349197	2.94025683
C	-1.07076274	3.42859421	0.29822738
C	-2.19923215	3.47702818	1.16041515
C	-3.17213362	4.46783222	0.90311853
C	-3.03327869	5.37045009	-0.15960264
C	-1.90469671	5.30063917	-0.98964368
C	-0.90017125	4.33265179	-0.78497195
C	-3.77593659	1.86046880	2.35093246
C	-2.38528870	2.54291533	2.36239847
C	-2.16961098	3.31423454	3.69326188
C	5.34085834	0.53286392	-1.60316720
C	4.99852034	1.45973637	-0.40641169
C	5.93500580	2.69549647	-0.37339558
C	3.89961072	0.44010422	1.70864931
C	5.04605580	0.68434244	0.91444681
C	6.26757047	0.16955923	1.39506403
C	6.32491063	-0.54724348	2.60163395
C	5.16107257	-0.77446203	3.35252512
C	3.90679184	-0.29204353	2.92061976
C	-0.03375467	4.34694135	-3.18844371
C	0.33850149	4.32719505	-1.68598784
C	1.27480449	5.51375367	-1.32768821
C	2.44312318	-2.07797464	4.00934779
C	2.64575149	-0.56332688	3.75097848
C	2.69505552	0.22038026	5.09059361
H	-0.29930689	-3.82873211	-1.18773431
H	-2.20170044	-3.66837436	0.19792340
H	0.81009233	3.75230195	1.91739424
H	2.69488286	2.48244401	2.58653895
H	2.16873448	-1.84322101	-5.54778881
H	4.12736364	-3.14522992	-4.74584961
H	4.24746421	-3.87137900	-2.37788503
H	-0.62175063	-0.63934435	-3.36140920
H	-3.49680337	-0.93600790	-2.08632610
H	0.77491802	-0.27844269	-6.06635844
H	0.89392421	0.80605804	-4.64696556

H	-0.66059711	0.56906828	-5.46297080
H	-0.50003139	-2.60464877	-5.73108592
H	-1.91554542	-1.65582150	-5.22278816
H	-1.27724151	-2.94045108	-4.17162151
H	-5.80015307	1.07155360	-1.82983305
H	-4.49420471	1.11788220	-3.03693202
H	-4.10945907	1.32043497	-1.32041662
H	-5.23594190	-2.59240579	-2.89103001
H	-5.03786037	-1.19632631	-3.97406712
H	-6.44552796	-1.29333086	-2.90476144
H	-7.01638670	-0.86806354	-0.76285797
H	-7.68655566	-1.71301249	1.47308752
H	-5.97501911	-2.59579543	3.03540877
H	1.74762672	-2.99139594	0.27611191
H	-2.27999584	-2.63068959	2.37306401
H	4.70867674	-3.61756664	-0.25000841
H	3.91090803	-3.43229155	1.31978303
H	4.05957226	-2.03644172	0.23477727
H	3.05646028	-5.54106683	-0.85693674
H	1.31075319	-5.30382572	-0.69176525
H	2.33597583	-5.35176426	0.75726142
H	-3.16319187	-0.96673944	3.96454994
H	-2.61188898	-2.43743971	4.78456971
H	-4.35082693	-2.14273028	4.57856402
H	-4.50294355	-4.51693276	3.36611313
H	-2.75592755	-4.70619498	3.62472936
H	-3.43866472	-4.85270715	1.99123640
H	-4.04596983	4.52970565	1.54636228
H	-3.79670517	6.12406988	-0.33872117
H	-1.79994309	6.00450376	-1.81068688
H	-1.64190753	1.74228099	2.31345614
H	3.97831781	1.82127869	-0.57491909
H	-4.59462858	2.58669708	2.44256701
H	-3.85674856	1.16310962	3.19484749
H	-3.92338651	1.29045142	1.42702545
H	-1.16822549	3.76394447	3.74273403
H	-2.27666878	2.63292748	4.54793800
H	-2.90271505	4.12400360	3.81005712
H	6.35783086	0.12710310	-1.51559915
H	5.27895024	1.09644170	-2.54262943
H	4.63775520	-0.30452060	-1.66715825
H	5.69034340	3.36543583	0.46136293
H	5.83590127	3.26324511	-1.30717944
H	6.98794173	2.40242497	-0.27204694
H	7.17626195	0.33179283	0.82195616
H	7.27809338	-0.93370669	2.95443907
H	5.22169558	-1.34099788	4.27748404
H	0.88108971	3.39079907	-1.53247626
H	1.76254096	-0.22941908	3.19779331
H	-0.55295129	5.27097761	-3.47931820
H	-0.66874992	3.48641678	-3.42042085
H	0.87780700	4.27058627	-3.79595928

H	2.17670931	5.48820213	-1.95429516
H	1.59047222	5.48101479	-0.27477504
H	0.77602586	6.47873447	-1.49281228
H	2.31218721	-2.61740855	3.06594415
H	1.52976846	-2.22724442	4.59757434
H	3.28316271	-2.51820621	4.56351936
H	2.80231527	1.30194518	4.92893776
H	3.53640973	-0.10705225	5.71591255
H	1.76862938	0.05386922	5.65419112
O	-0.79286880	1.25767596	-2.03520614
O	0.77717809	1.21244353	-2.02520703
O	-0.56614564	-1.17171273	2.28518908
O	-0.03237542	-2.22167982	1.45983442
Hf	-0.06324164	0.26886446	-0.44579949

Peroxo η^2 -Ozone Complex to Peroxo η^3 -Ozone Complex

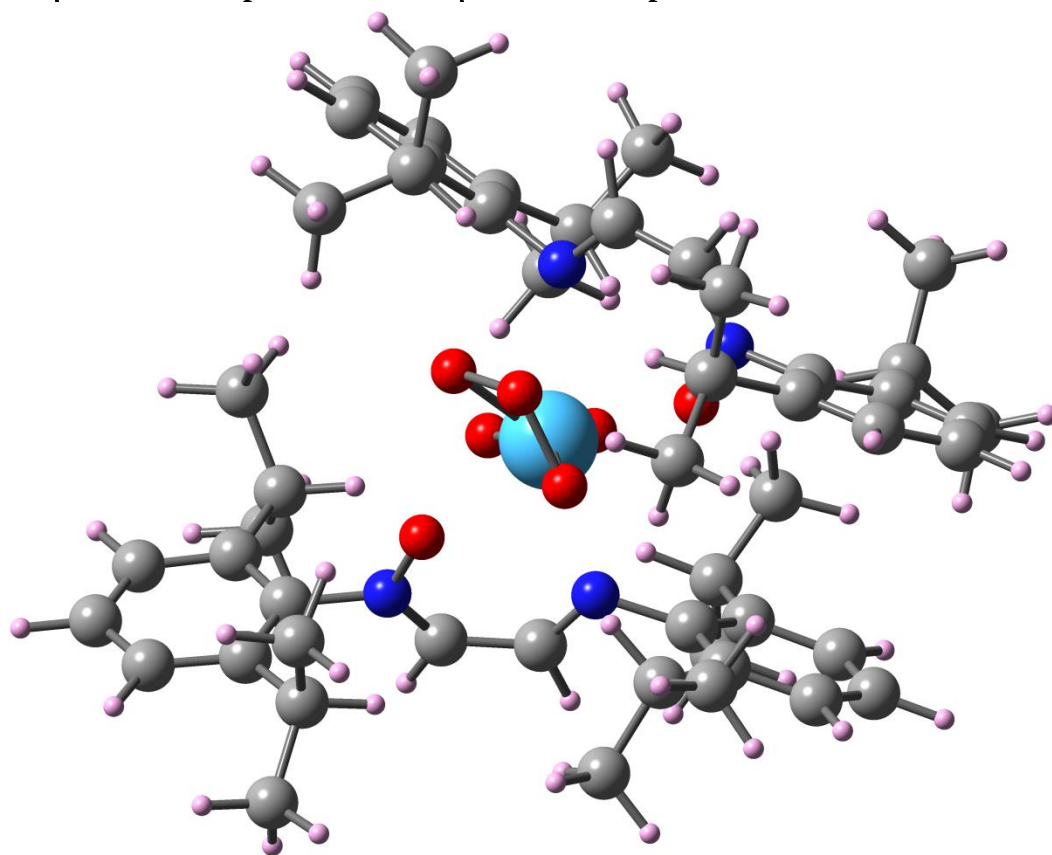


Fig. S133: NCCNO Peroxo η^2 -Ozone Complex to Peroxo η^3 -Ozone Complex

E	E_{zp}	H	G	<i>f</i>
-2818.8984	-2817.7410	-2817.6691	-2817.8509	-162
O	-1.97265579	0.47916107	0.22598299	
O	2.03907299	-1.13544758	-0.68157299	
O	1.07985940	1.13513452	-1.68360979	
N	-0.02050230	-2.08580475	0.96588372	
N	2.85644606	-1.83346127	0.11749124	
N	-0.20059429	2.65093317	-0.08063129	
N	-2.78139631	1.18467202	-0.60195633	
C	1.01976070	-2.68702452	1.49918487	
C	2.41038414	-2.49489401	1.17365734	
C	-1.25668620	3.12877803	-0.69213955	
C	-2.46441988	2.39997825	-1.00946037	
C	-1.31760899	-2.64145276	1.36275332	
C	-1.77830897	-2.52587758	2.70483643	
C	-3.02052523	-3.12105354	3.02090776	
C	-3.76987664	-3.81064407	2.06001888	
C	-3.28276310	-3.92765000	0.74822298	
C	-2.05148310	-3.35660543	0.37173379	
C	-1.84054236	-0.62287510	4.39433625	

C	-1.01363093	-1.80174847	3.82126353
C	-0.60203726	-2.78456019	4.94967303
C	5.13050820	1.37977962	1.21188362
C	4.77095655	-0.08867896	1.55840721
C	5.41485107	-0.51387481	2.90442955
C	4.27048638	-1.85417806	-0.27723263
C	5.18395968	-1.03287218	0.42423185
C	6.53339784	-1.09297622	0.01114475
C	6.92950411	-1.90840032	-1.05888298
C	5.98358549	-2.68269355	-1.75193310
C	4.62471261	-2.67320938	-1.37877321
C	-2.55978283	-3.80967855	-2.11058906
C	-1.47680505	-3.59985654	-1.02860938
C	-0.52076880	-4.82733939	-1.00937374
C	3.20360213	-2.68748717	-3.46631042
C	3.58765067	-3.46820332	-2.17814814
C	4.06113844	-4.90376608	-2.51311092
C	0.88614436	3.59571769	0.17164331
C	1.57358100	4.23333372	-0.90623793
C	2.63734170	5.10154733	-0.57439368
C	2.99408976	5.35811560	0.75542847
C	2.27168796	4.75659139	1.79669664
C	1.20929537	3.87114847	1.53280202
C	2.46367651	3.54874045	-3.20160848
C	1.24101582	4.05418558	-2.39509058
C	0.69235439	5.37622066	-2.99929495
C	-5.46935681	-0.09793860	2.55758722
C	-4.76422997	0.78144000	1.50040877
C	-5.22028803	2.26213086	1.64839814
C	-4.05608267	0.55803995	-0.97780785
C	-4.99636056	0.30786014	0.05931149
C	-6.20409015	-0.31135629	-0.31305215
C	-6.46239713	-0.65383676	-1.65169336
C	-5.52055444	-0.37108355	-2.64874695
C	-4.28565768	0.24496597	-2.34245126
C	1.17862907	2.89079255	3.90608836
C	0.34944705	3.34959115	2.68567857
C	-0.68900629	4.43299755	3.09161227
C	-2.95719070	-0.68893134	-4.32463903
C	-3.31176096	0.56340699	-3.48593229
C	-3.89661078	1.68310780	-4.39147588
H	0.85186778	-3.46924020	2.24321025
H	3.15395151	-3.02133294	1.75876889
H	-1.28218859	4.17570655	-1.00010374
H	-3.21350580	2.90462304	-1.60674012
H	-3.39772103	-3.04140693	4.03757140
H	-4.72104762	-4.26376029	2.33055252
H	-3.86167526	-4.47627187	0.01242098
H	-0.11427318	-1.34340744	3.40347439
H	3.68406858	-0.11309099	1.68587911
H	-2.78739019	-0.95994865	4.83842126
H	-2.05691542	0.10253018	3.60284793

H	-1.26453724	-0.10614639	5.17341789
H	-1.47823426	-3.21825848	5.45036913
H	-0.00872590	-2.25862736	5.70946802
H	0.00162259	-3.61841696	4.56452170
H	6.21569147	1.52607139	1.12123547
H	4.76025504	2.04710352	1.99976333
H	4.65972985	1.68566421	0.27050915
H	5.13266674	-1.53854855	3.18320515
H	5.08210347	0.15779660	3.70590870
H	6.51158077	-0.47038501	2.85992472
H	7.27175971	-0.48283841	0.52403167
H	7.97360003	-1.93350908	-1.36200543
H	6.30322918	-3.29658020	-2.58884516
H	-0.89033305	-2.72296364	-1.32578726
H	2.67244100	-3.55719662	-1.58021046
H	-3.08771308	-4.76536241	-1.98534903
H	-2.08828361	-3.82384296	-3.10117643
H	-3.29988118	-3.00150259	-2.09801453
H	-1.06554921	-5.74045257	-0.73212441
H	0.30139596	-4.69631810	-0.29521226
H	-0.08176243	-4.97863925	-2.00462733
H	2.78404430	-1.70898565	-3.21235286
H	2.44896841	-3.24600389	-4.03574202
H	4.08148602	-2.54241867	-4.11069886
H	4.90841874	-4.90244761	-3.21067002
H	3.24563965	-5.45948548	-2.99370814
H	4.36449677	-5.45237466	-1.61171915
H	3.19134635	5.58219893	-1.37637967
H	3.81792086	6.03227974	0.97868008
H	2.52859348	4.98178118	2.82763838
H	0.47800261	3.28080074	-2.50328459
H	-3.69056669	0.73424863	1.70477046
H	3.30610848	4.25198378	-3.15881400
H	2.18739790	3.42008398	-4.25712421
H	2.78438368	2.57655079	-2.81613448
H	-0.19369408	5.73905416	-2.45868805
H	0.41343281	5.22386830	-4.05067184
H	1.44514587	6.17470748	-2.96472010
H	-6.56269140	-0.00244845	2.51176473
H	-5.15679661	0.21726509	3.56109448
H	-5.20255575	-1.15358609	2.43665894
H	-4.69612546	2.92460759	0.94780412
H	-5.01429746	2.62026024	2.66529005
H	-6.29872149	2.35844811	1.46355962
H	-6.94963025	-0.52607729	0.44526642
H	-7.40174564	-1.13442407	-1.91472158
H	-5.73656856	-0.63459788	-3.68010300
H	-0.18896544	2.46371012	2.34032805
H	-2.36316972	0.91616989	-3.07572117
H	1.72589769	3.71701364	4.38193596
H	1.88738675	2.11345105	3.60262311
H	0.51008375	2.45840303	4.66230002

H	-1.34224180	4.05308534	3.88906365
H	-1.32367296	4.72294161	2.24219822
H	-0.19205936	5.34073292	3.46164038
H	-2.42588262	-1.41540178	-3.70540514
H	-2.28701759	-0.40044868	-5.14431530
H	-3.84455422	-1.16369941	-4.76458682
H	-4.13434698	2.59449295	-3.82437743
H	-4.82039117	1.35409991	-4.88546517
H	-3.17216490	1.94820359	-5.17181356
O	1.56646676	0.41456511	1.48607416
O	0.11875914	0.37657192	2.01319854
O	-0.12353178	0.65870029	-2.48688710
O	-0.51165445	-0.69824345	-1.86437343
Hf	0.21482034	0.13828142	-0.03165043

Peroxo η^3 -Ozone Complex to Bisperoxo Complex (spiro conformation) (Propene)

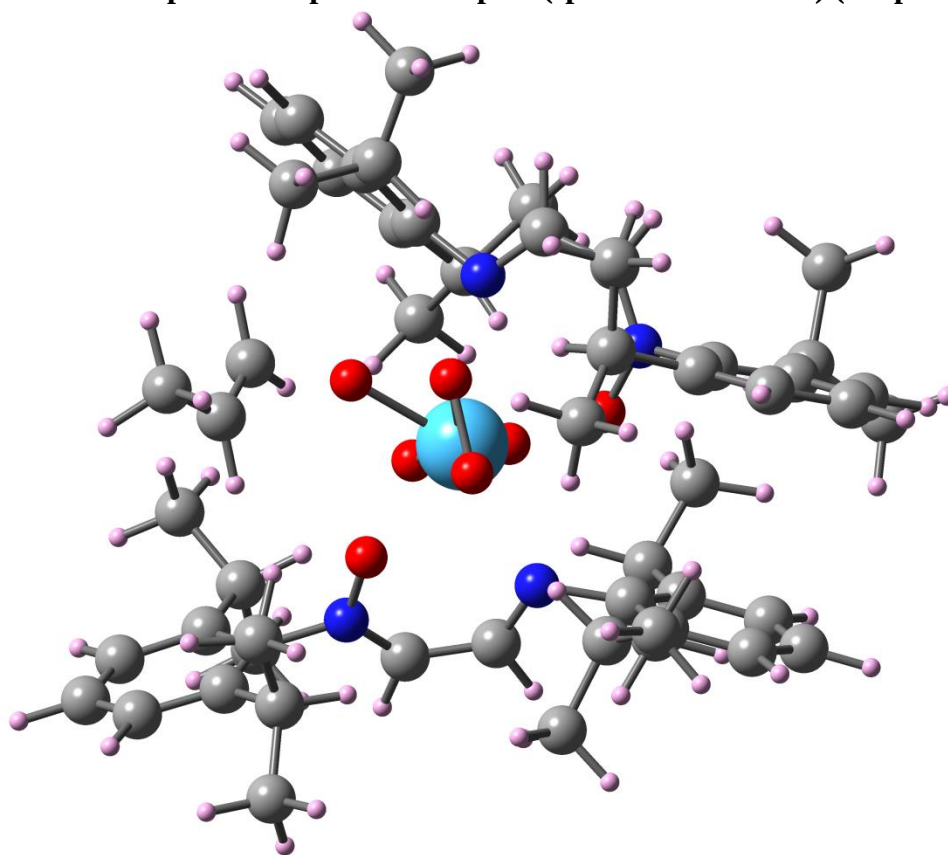


Fig. S134: NCCNO Peroxo η^3 -Ozone Complex to Bisperoxo Complex (spiro conformation) (Propene)

E	E_{ZP}	H	G	<i>f</i>
-2936.7691	-2935.5297	-2935.4525	-2935.6438	-331
O	-2.02267281	0.05144922	0.13927338	
O	2.06053974	-1.13994912	-0.71300675	
O	1.37168808	1.50601725	-1.37518829	
N	-0.05330224	-2.16868241	0.83235401	
N	2.84914931	-1.90385461	0.06599446	
N	-0.65645488	2.66561326	0.34950955	
N	-2.98981715	0.82132285	-0.37250100	
C	0.97342061	-2.79185529	1.37113751	
C	2.36420090	-2.61383953	1.07153817	
C	-1.87733248	3.00471601	0.03554772	
C	-2.95229680	2.14028946	-0.39420769	
C	-1.33497821	-2.78115818	1.18813929	
C	-1.78704847	-2.79502597	2.53869008	
C	-2.96313729	-3.52207625	2.82752191	
C	-3.66397594	-4.21017964	1.82913558	
C	-3.20320050	-4.17344016	0.50327920	
C	-2.03437437	-3.46844196	0.15403064	

C	-2.00111451	-0.97277554	4.29740882
C	-1.08103309	-2.06112452	3.68753124
C	-0.60006816	-3.04585924	4.78599565
C	5.53114074	0.68242529	2.08081466
C	4.84734972	-0.69937042	1.91792508
C	5.21816418	-1.61140838	3.12057693
C	4.26876172	-1.94601344	-0.29261191
C	5.22081877	-1.37389974	0.59012800
C	6.57479951	-1.45128880	0.19705614
C	6.94701982	-2.04341830	-1.01915452
C	5.97263522	-2.58316677	-1.87437997
C	4.60589109	-2.55512024	-1.52930059
C	-2.57416339	-3.73090352	-2.34813100
C	-1.48010818	-3.53796007	-1.27369780
C	-0.43558840	-4.68462857	-1.39441356
C	3.29511331	-2.19298863	-3.67008467
C	3.55704430	-3.15030816	-2.47540712
C	3.95169313	-4.56499665	-2.96954529
C	0.23378555	3.79598485	0.59286365
C	0.50719547	4.70960445	-0.47140114
C	1.39078629	5.77704639	-0.20254810
C	1.96879937	5.95117994	1.06307208
C	1.65647322	5.05861788	2.10006080
C	0.78549770	3.96982091	1.89290817
C	0.99950137	4.52749628	-2.98052198
C	-0.09071929	4.60259121	-1.88444122
C	-1.06165582	5.78310833	-2.16325457
C	-5.72437833	-1.07103219	2.43844766
C	-5.03399422	-0.01518051	1.54531665
C	-5.61979534	1.39053525	1.86999417
C	-4.18908874	0.12996095	-0.89210699
C	-5.15746486	-0.31293217	0.04544372
C	-6.28874513	-0.97088647	-0.47577617
C	-6.44148611	-1.16315224	-1.85974579
C	-5.47482665	-0.68380729	-2.75404968
C	-4.31691311	-0.01627413	-2.29488319
C	1.51549082	2.69883326	4.00378697
C	0.34874532	3.09938130	3.07268616
C	-0.76878566	3.82897960	3.87040572
C	-2.84677432	-0.47173744	-4.34939791
C	-3.32318006	0.56807028	-3.30663292
C	-3.95499440	1.79991021	-4.01400655
H	0.78913623	-3.59295116	2.09093181
H	3.08242070	-3.20151196	1.62840874
H	-2.16445183	4.05953205	0.044440928
H	-3.84033791	2.61811124	-0.78822039
H	-3.32732389	-3.54896656	3.85201018
H	-4.55961425	-4.77464783	2.07968709
H	-3.75218597	-4.70910843	-0.26462162
H	-0.21930780	-1.51935617	3.28993267
H	3.76592450	-0.52178356	1.94349498
H	-2.92434443	-1.39970753	4.71404649

H	-2.26528843	-0.23316522	3.53350726
H	-1.47549428	-0.44594549	5.10497601
H	-1.44125339	-3.56575293	5.26450572
H	-0.05552390	-2.50047772	5.56839826
H	0.07179143	-3.81459772	4.37923777
H	6.62053693	0.59206076	2.18588266
H	5.15006605	1.17387600	2.98511018
H	5.32079315	1.33557907	1.22709109
H	4.72109276	-2.58911424	3.07012492
H	4.92051504	-1.13149908	4.06154714
H	6.30089445	-1.79239527	3.15731779
H	7.33973702	-1.02821807	0.84184938
H	7.99618367	-2.08155580	-1.30268473
H	6.27605360	-3.03797519	-2.81293535
H	-0.97138114	-2.59197641	-1.48925178
H	2.60754234	-3.24199471	-1.93754860
H	-3.03355860	-4.72760633	-2.29210799
H	-2.12819709	-3.63449523	-3.34602814
H	-3.36644208	-2.97937837	-2.25572037
H	-0.90468353	-5.65934292	-1.20012586
H	0.39222620	-4.56043897	-0.68652353
H	-0.01287871	-4.70373092	-2.40801131
H	2.88373767	-1.24289581	-3.31592976
H	2.56368881	-2.63963785	-4.35603231
H	4.21929826	-2.00098082	-4.23278227
H	4.83746657	-4.54146262	-3.61741624
H	3.12890497	-4.99288216	-3.55663057
H	4.16213184	-5.24270692	-2.13181125
H	1.62866676	6.47941219	-0.99760913
H	2.64606745	6.78301335	1.24282919
H	2.08342875	5.21433721	3.08663872
H	-0.65039620	3.66752296	-1.97232212
H	-3.96900401	-0.01252684	1.80535499
H	1.66142680	5.40389134	-2.96991344
H	0.52806070	4.47646983	-3.97148605
H	1.59060471	3.62093970	-2.83927919
H	-1.86809149	5.84202152	-1.41888255
H	-1.51905743	5.67220029	-3.15567569
H	-0.53133176	6.74432382	-2.14446007
H	-6.81829238	-1.02680463	2.34915571
H	-5.47494762	-0.87954127	3.48967928
H	-5.39065339	-2.08252146	2.19033110
H	-5.11429561	2.19101691	1.31725871
H	-5.51062454	1.60408095	2.94110498
H	-6.68880672	1.43000938	1.62141551
H	-7.05375350	-1.33529509	0.20179901
H	-7.32108966	-1.67819722	-2.23878925
H	-5.61363487	-0.82558267	-3.82187055
H	-0.06236213	2.16420694	2.68147072
H	-2.41920868	0.89926498	-2.78892645
H	1.98345727	3.56341464	4.49567737
H	2.27474569	2.14767355	3.43892637

H	1.14030798	2.03226844	4.79141812
H	-1.12818449	3.18959624	4.68806967
H	-1.62770749	4.07394632	3.22983358
H	-0.39914635	4.76740312	4.30781232
H	-2.28525298	-1.26970594	-3.85796994
H	-2.16759096	0.01489811	-5.06041422
H	-3.67846317	-0.90804675	-4.91964225
H	-4.27647732	2.56755778	-3.29622245
H	-4.83310289	1.51331350	-4.60833060
H	-3.22132008	2.25570005	-4.69084454
O	1.54450831	0.34034932	1.53505559
O	0.08944845	0.20234876	1.97982183
O	-0.34679013	1.00686220	-1.97157528
O	-0.29973929	-0.50103576	-2.03310324
C	3.13338567	2.32568131	-0.38477032
H	2.94814184	1.90589443	0.59797667
H	3.02192863	3.40020540	-0.49542619
C	3.52436995	1.54323602	-1.44628753
H	3.63813937	0.47569292	-1.29691830
C	3.88023078	2.05440925	-2.81578742
H	3.84608658	3.14754136	-2.87134942
H	4.88908918	1.72051062	-3.09998161
H	3.17705438	1.64397935	-3.55257225
Hf	0.25955937	0.18322387	-0.09698682

Peroxo η^3 -Ozone Complex to Bisperoxo Complex (planar conformation) (Propene)

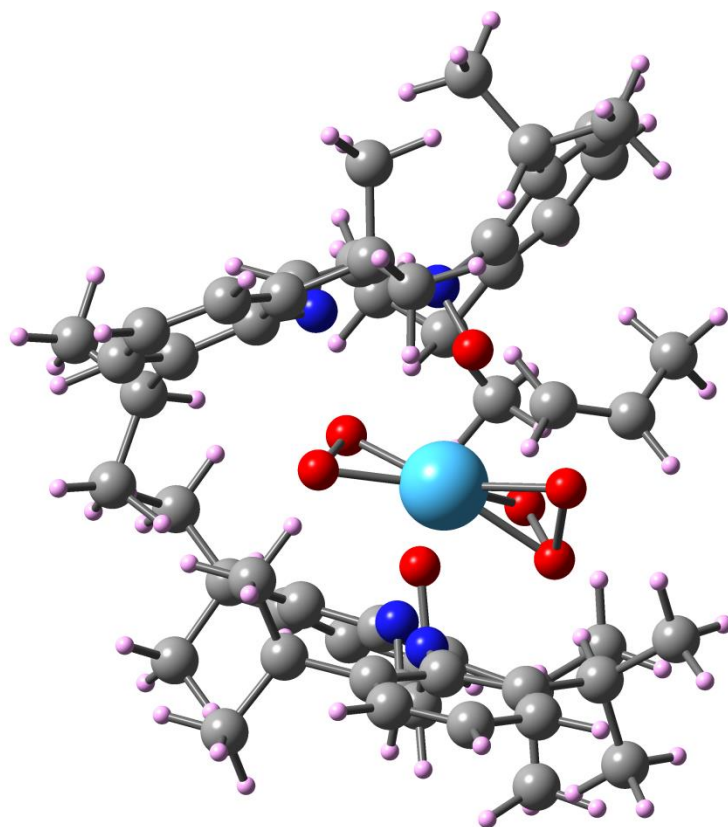


Fig. S135: NCCNO Peroxo η^3 -Ozone Complex to Bisperoxo Complex (planar conformation) (Propene)

E	E_{ZP}	H	G	<i>f</i>
-2936.7646	-2935.5260	-2935.4486	-2935.6416	-359

O	1.97923300	0.25815900	-0.48157100
O	-1.94455900	0.40695900	-0.85061500
O	-0.72914000	-2.49155800	-1.07182400
N	-1.37582700	2.70165100	1.05703200
N	-3.09477100	0.47990300	-0.11704500
N	1.46357300	-2.37333300	0.73217500
N	3.19624300	-0.26083700	-0.62763100
C	-2.28617300	2.02526600	1.69127600
C	-3.19232000	1.08853100	1.04850000
C	2.74714800	-2.42963400	0.50690700
C	3.56315300	-1.45410400	-0.18695500
C	-0.59972000	3.72853700	1.66006600
C	-0.02373800	3.65218800	2.97177500
C	0.67665600	4.78094500	3.44769400
C	0.83212900	5.93995300	2.67357800
C	0.31484200	5.97956700	1.36844800
C	-0.38762600	4.88391700	0.83618100

C	1.35650800	1.97426600	4.30192600
C	-0.06682600	2.39819800	3.85615400
C	-0.98000900	2.60857800	5.09357400
C	-3.41274200	-3.68837900	0.12758800
C	-3.83704300	-2.30184900	0.67162100
C	-4.68271100	-2.45208300	1.96620900
C	-4.27560000	-0.15872100	-0.72524400
C	-4.60681300	-1.48807600	-0.37245100
C	-5.74665800	-2.04652300	-0.99377300
C	-6.50507700	-1.31433200	-1.91699400
C	-6.15289100	0.00853500	-2.23413300
C	-5.02937500	0.61929900	-1.64349700
C	-0.06303500	5.66101400	-1.59302100
C	-0.98455900	4.95509400	-0.57087400
C	-2.38107200	5.63553300	-0.53536700
C	-4.91818000	2.48819400	-3.40913900
C	-4.69695000	2.08938700	-1.93007100
C	-5.53418000	3.01597300	-1.00312400
C	0.89403900	-3.53962400	1.41822300
C	0.77351800	-4.77535400	0.71897600
C	0.20519200	-5.86374400	1.41621000
C	-0.21044000	-5.74610800	2.74888300
C	-0.04484200	-4.52705900	3.42354200
C	0.51014400	-3.40215100	2.78065900
C	0.12076300	-5.59047900	-1.61822400
C	1.24122300	-5.00074900	-0.72585000
C	2.49844700	-5.91414500	-0.75670600
C	3.91575100	3.22081100	1.21812300
C	4.51070100	1.80520500	0.99543200
C	5.75654700	1.57513800	1.89002700
C	4.18499100	0.61630500	-1.28320500
C	4.83438800	1.58608700	-0.48550500
C	5.80530500	2.38546900	-1.12587900
C	6.09022500	2.22051800	-2.49000700
C	5.39729200	1.26579000	-3.25289900
C	4.41205300	0.44116400	-2.67021800
C	-0.34833400	-1.74454900	4.53798700
C	0.80228700	-2.13069500	3.58117700
C	2.13681900	-2.30104400	4.36110500
C	3.24967800	-0.03057500	-4.89835400
C	3.64739700	-0.58974700	-3.50983100
C	4.47873100	-1.89059200	-3.68579500
H	-2.52879100	2.19602100	2.74507600
H	-4.14217900	0.92659100	1.55122900
H	3.31672400	-3.29677300	0.84997900
H	4.60363900	-1.70204700	-0.35348300
H	1.11405600	4.74796200	4.44236900
H	1.36450200	6.79817500	3.07746500
H	0.46075100	6.86867900	0.76152800
H	-0.44137800	1.55914200	3.26522800
H	-2.92180400	-1.76883800	0.94363400
H	1.84800000	2.73703000	4.92064600

H	1.98280300	1.77310500	3.42530100
H	1.29971800	1.05099300	4.89234400
H	-0.59195300	3.40435700	5.74427400
H	-1.03839800	1.68565700	5.68613600
H	-2.00186800	2.89266400	4.80674400
H	-4.28112700	-4.31477700	-0.11967000
H	-2.82159900	-4.21605600	0.88652100
H	-2.78457600	-3.57606400	-0.76178200
H	-4.96012400	-1.47624500	2.38846500
H	-4.10550400	-2.99629300	2.72418800
H	-5.60916300	-3.01099300	1.77615800
H	-6.03417700	-3.06568200	-0.75200300
H	-7.37369800	-1.76976000	-2.38694700
H	-6.75610800	0.56603700	-2.94451200
H	-1.13447400	3.92247500	-0.90129800
H	-3.63731000	2.25469800	-1.70254900
H	0.03631400	6.73567800	-1.38887000
H	-0.48032400	5.55747300	-2.60338700
H	0.94193100	5.22030400	-1.59471600
H	-2.30259800	6.67295300	-0.18233100
H	-3.06469800	5.10061300	0.13575500
H	-2.82707200	5.65074700	-1.53969500
H	-4.38535600	1.81648100	-4.09051100
H	-4.54915500	3.50845300	-3.57676800
H	-5.98203800	2.47819900	-3.67912400
H	-6.60776400	2.88585300	-1.19366600
H	-5.27856900	4.06801100	-1.18379500
H	-5.35258800	2.80102100	0.05729400
H	0.08712500	-6.81351600	0.90138400
H	-0.64668600	-6.60023300	3.26196700
H	-0.34143000	-4.44823600	4.46537300
H	1.49880800	-4.03842200	-1.17588800
H	3.74074900	1.08927700	1.30483900
H	-0.20241000	-6.58342300	-1.27696700
H	0.48426400	-5.69391500	-2.64968100
H	-0.73697100	-4.91244100	-1.62616700
H	3.32633800	-5.49776000	-0.16497100
H	2.84819800	-6.04315800	-1.79000800
H	2.27547100	-6.90982800	-0.35044000
H	4.63052500	4.00507000	0.93582500
H	3.65874600	3.36152700	2.27481600
H	3.00150600	3.35938300	0.63039600
H	6.16958700	0.56661200	1.75595500
H	5.48752100	1.69531000	2.94712900
H	6.55246000	2.29639500	1.66366600
H	6.33420500	3.14190900	-0.55278400
H	6.84466300	2.84410500	-2.96353500
H	5.61370200	1.16840000	-4.31231500
H	0.91243800	-1.29658200	2.88273400
H	2.71130200	-0.84246200	-2.99871800
H	-0.52212600	-2.49769700	5.31921600
H	-1.26828000	-1.59578700	3.96380200

H	-0.10741800	-0.80025200	5.04413900
H	2.38331200	-1.37674600	4.90146800
H	2.97315900	-2.53106400	3.68562100
H	2.06826900	-3.11694400	5.09420600
H	2.73057900	0.93074100	-4.80746700
H	2.57473600	-0.73851200	-5.39436800
H	4.12131700	0.11025100	-5.55143700
H	4.72539100	-2.35557200	-2.72301800
H	5.42091000	-1.68665700	-4.21245000
H	3.90811900	-2.62166500	-4.27189000
O	-1.07893900	-0.76019900	1.49028700
O	0.12455200	0.21743100	1.51070300
O	0.51518800	-2.08903300	-1.86612100
O	0.18539500	-0.41168700	-2.49283000
C	-0.08110000	1.78086100	-2.86838700
H	-0.84424400	2.09062600	-2.16250100
H	0.92673700	2.15862200	-2.72225500
C	-0.37305700	0.89828500	-3.88921900
H	0.41825300	0.65165900	-4.59461200
C	-1.75405400	0.42336200	-4.26317900
H	-2.13520300	0.98634500	-5.13001000
H	-1.72040100	-0.63775800	-4.53420800
H	-2.44120100	0.53550000	-3.42211900
Hf	-0.06748900	-0.68251600	-0.31985500

Peroxo η^3 -Ozone Complex to Bisperoxo Complex (spiro conformation) (Ethylene)

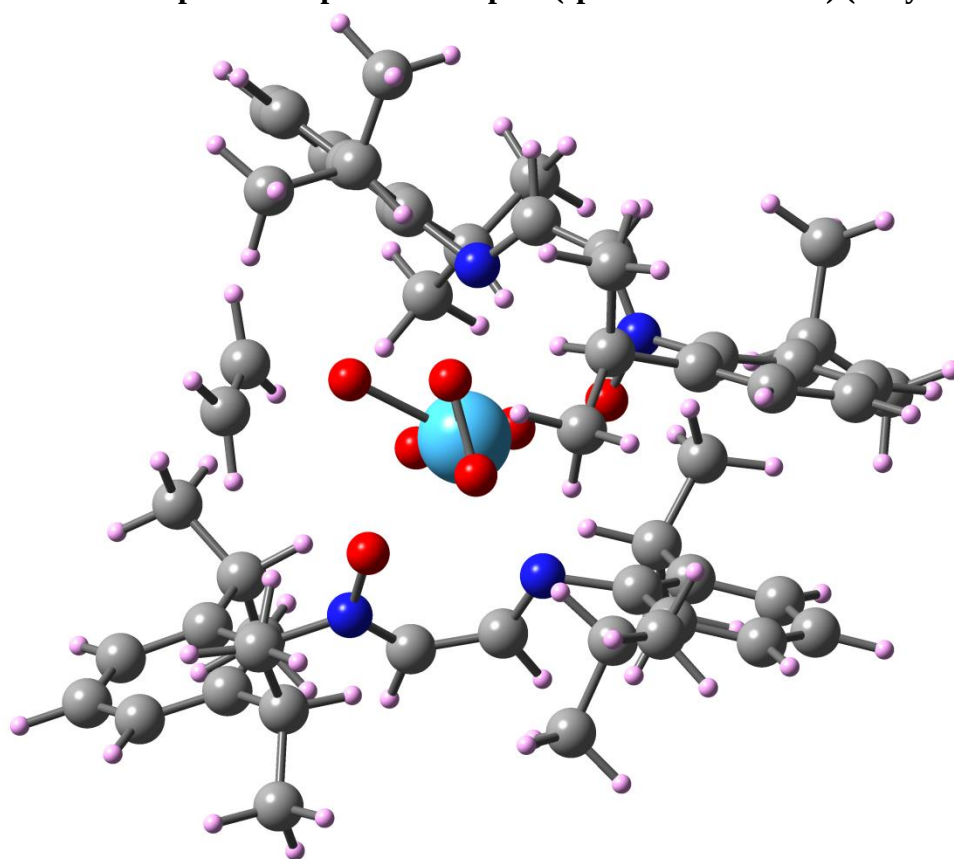


Fig. S136: NCCNO Peroxo η^3 -Ozone Complex to Bisperoxo Complex (spiro conformation) (Ethylene)

E	E_{ZP}	H	G	<i>f</i>
-2897.4557	-2896.2442	-2896.1688	-2896.3551	-361
O	-1.98289915	0.05802900	0.16259901	
O	2.12372616	-1.05102008	-0.74822306	
O	1.31066710	1.47714311	-1.54583412	
N	0.08170501	-2.09014416	0.88663907	
N	2.95573322	-1.76953913	0.02810300	
N	-0.63987405	2.68001320	0.17731401	
N	-2.96259322	0.77704406	-0.39863303	
C	1.14218109	-2.66411521	1.41594711	
C	2.51876019	-2.45913219	1.06980108	
C	-1.86206514	2.98975723	-0.16014401	
C	-2.93288322	2.09016016	-0.52564704	
C	-1.17293309	-2.72574121	1.29718310	
C	-1.59651812	-2.69274021	2.65637320	
C	-2.75140721	-3.43030126	2.99978823	
C	-3.45810426	-4.17369032	2.04629516	
C	-3.02121723	-4.18900432	0.71203906	
C	-1.87371914	-3.47745027	0.30974702	

C	-1.80755114	-0.81502606	4.35743233
C	-0.87966807	-1.90400215	3.76126128
C	-0.35070203	-2.84064222	4.87954037
C	5.67517046	0.92185107	1.87787814
C	4.99745838	-0.46836404	1.76798814
C	5.41457940	-1.34681510	2.98077723
C	4.36301233	-1.79044714	-0.38241803
C	5.33472941	-1.17097409	0.44517903
C	6.67366649	-1.22784309	0.00100900
C	7.01280454	-1.84614614	-1.21183109
C	6.01958647	-2.43420118	-2.01130715
C	4.66707736	-2.42818919	-1.61332512
C	-2.44413319	-3.87945629	-2.16747717
C	-1.33925410	-3.61014228	-1.12109209
C	-0.27528502	-4.74291736	-1.19638909
C	3.28733725	-2.18625117	-3.72973429
C	3.59983627	-3.08119223	-2.49958319
C	4.00473031	-4.51135134	-2.93871522
C	0.23621802	3.83217429	0.37860703
C	0.52928004	4.69179136	-0.72496905
C	1.38546311	5.78837343	-0.48739104
C	1.92436915	6.03854547	0.78284806
C	1.59819912	5.19463040	1.85504914
C	0.74894306	4.08248931	1.68180813
C	1.10079008	4.45092534	-3.21394325
C	-0.02133900	4.49561334	-2.14742516
C	-1.04654608	5.60863144	-2.50221919
C	-5.54826343	-1.00092408	2.61008320
C	-4.92226537	0.01569100	1.62878012
C	-5.54267342	1.42175911	1.87925414
C	-4.16132232	0.03380700	-0.83963506
C	-5.08418139	-0.38016503	0.15543201
C	-6.21216450	-1.09871809	-0.28599902
C	-6.40605748	-1.37540810	-1.65049112
C	-5.48604240	-0.92052207	-2.60459520
C	-4.33329033	-0.19513301	-2.22649017
C	1.46472511	2.89861922	3.84460029
C	0.30025402	3.26907425	2.89768422
C	-0.81147306	4.04217031	3.66129828
C	-2.91009222	-0.73475006	-4.29345933
C	-3.39444826	0.35582303	-3.30768425
C	-4.09763531	1.51061511	-4.07516631
H	1.00114708	-3.44455526	2.16741017
H	3.26777925	-3.01086623	1.62263812
H	-2.15694216	4.04059031	-0.21652402
H	-3.82680429	2.53217919	-0.94711307
H	-3.09427324	-3.42088226	4.03196031
H	-4.33824833	-4.74242236	2.33861318
H	-3.57109027	-4.77080636	-0.02079600
H	-0.04009900	-1.35835810	3.32403326
H	3.91519730	-0.30181502	1.82326814
H	-2.70729421	-1.24678510	4.81812437

H	-2.11173816	-0.11155701	3.57462227
H	-1.27091810	-0.24618602	5.12843439
H	-1.16825309	-3.36609426	5.39174540
H	0.19504901	-2.25653117	5.63262244
H	0.33260803	-3.60464428	4.48303634
H	6.76596849	0.83897806	1.97332315
H	5.30291739	1.44127611	2.77010221
H	5.45452344	1.54554812	1.00491708
H	4.92823038	-2.33093218	2.96930323
H	5.13997239	-0.84771307	3.91880730
H	6.50001348	-1.51446112	2.98829823
H	7.45235457	-0.76735206	0.60202305
H	8.05057759	-1.86689614	-1.53602712
H	6.29704347	-2.90905922	-2.94804423
H	-0.85221707	-2.66802421	-1.39462411
H	2.66798821	-3.16257624	-1.93046715
H	-2.88088222	-4.88164937	-2.05547716
H	-2.01505615	-3.82273429	-3.17574624
H	-3.25105525	-3.14120024	-2.09905316
H	-0.72495706	-5.71461543	-0.94847207
H	0.55764004	-4.56997535	-0.50466704
H	0.13722701	-4.80584337	-2.21247517
H	2.86689922	-1.22741309	-3.41142826
H	2.54597619	-2.67813021	-4.37265733
H	4.19131732	-2.00397015	-4.32718233
H	4.87423537	-4.50452734	-3.60855128
H	3.17482624	-4.97786338	-3.48502827
H	4.24602932	-5.14675539	-2.07647616
H	1.63540813	6.45158350	-1.31153710
H	2.58276120	6.89031552	0.93733707
H	1.99594715	5.40687442	2.84336522
H	-0.52082804	3.52513027	-2.20977017
H	-3.85062129	0.06824501	1.85206714
H	1.68193413	5.38205743	-3.24780325
H	0.66095305	4.29531233	-4.20817632
H	1.77031614	3.61318828	-3.00825723
H	-1.88139114	5.64970846	-1.78899714
H	-1.46197311	5.43701540	-3.50439627
H	-0.56991104	6.59789651	-2.50118919
H	-6.64517849	-0.99985007	2.55274920
H	-5.27507240	-0.73258606	3.63833028
H	-5.18571239	-2.01472915	2.41724219
H	-5.08842639	2.19549117	1.24885410
H	-5.39680042	1.71587113	2.92666622
H	-6.62171149	1.40928011	1.67519213
H	-6.94245255	-1.44350711	0.43849903
H	-7.28161357	-1.93686615	-1.96800615
H	-5.65758441	-1.12715409	-3.65704128
H	-0.11537101	2.31993718	2.54809119
H	-2.48863319	0.75475606	-2.84371922
H	1.95382915	3.78039929	4.28235933
H	2.20666517	2.30044317	3.30550025

H	1.08173508	2.28649517	4.67185936
H	-1.17917009	3.44017026	4.50321835
H	-1.66607913	4.27081332	3.00891523
H	-0.43333503	4.99343138	4.06186631
H	-2.30114818	-1.47432211	-3.76837529
H	-2.27536317	-0.27301802	-5.06017538
H	-3.74194129	-1.24081409	-4.80254837
H	-4.42965034	2.31323818	-3.40160026
H	-4.98089638	1.14812409	-4.61828535
H	-3.40517126	1.94669715	-4.80624737
O	1.59700912	0.47984504	1.45811411
O	0.15644701	0.32130802	1.93678915
O	-0.39523503	0.90066607	-2.04815216
O	-0.31996802	-0.60468205	-2.01353515
C	3.16419924	2.34667918	-0.55831904
H	3.14643424	1.86124114	0.41126603
H	2.99929223	3.41892226	-0.57586404
C	3.31776225	1.63292912	-1.72468713
H	3.53196627	0.57250804	-1.72008613
Hf	0.28532502	0.20548902	-0.13770801
H	3.35950025	2.13304916	-2.68809421

Oxo Peroxo Complex to Dioxo Complex (Propene)

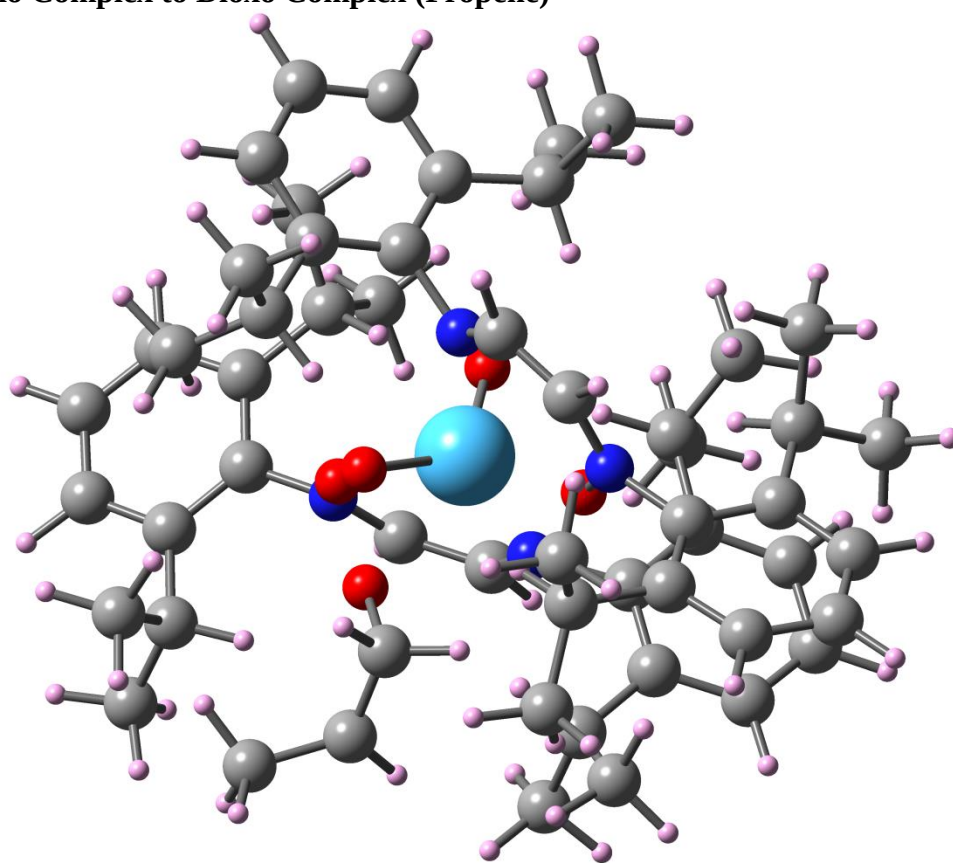


Fig. S137: NCCNO Oxo Peroxo Complex to Dioxo Complex (Propene)

E	E_{ZP}	H	G	<i>f</i>
-2786.4292	-2785.1969	-2785.1219	-2785.3095	-338
O	-1.96938597	0.15429274	-0.09359836	
O	2.24039377	-0.76521125	-0.39401323	
O	0.49435888	0.51756878	-2.05755635	
N	-0.00830140	-1.87547661	1.23559170	
N	2.95600800	-1.51129523	0.43376106	
N	-0.15126656	2.35230461	-0.65030298	
N	-2.88611304	1.00859865	-0.68503164	
C	1.05276820	-2.51617186	1.68182231	
C	2.43808064	-2.32561727	1.34970964	
C	-1.28219282	2.84338794	-1.17640367	
C	-2.54431171	2.21118277	-1.18697127	
C	-1.24073836	-2.23940939	1.94663876	
C	-1.41922383	-1.78409790	3.28410219	
C	-2.56815647	-2.23053667	3.97340757	
C	-3.50458380	-3.07886706	3.36621853	
C	-3.31329290	-3.49510259	2.03922722	
C	-2.18122060	-3.08699486	1.30641439	
C	-1.14456479	0.40426249	4.56612968	

C	-0.43154895	-0.84895299	3.99731465
C	0.32225115	-1.59189795	5.13357361
C	4.75973439	1.94809276	1.91199459
C	4.32895124	0.46864841	2.07053677
C	4.54319233	-0.00937489	3.53254749
C	4.41594187	-1.39725819	0.28360367
C	5.07719496	-0.44273259	1.09090309
C	6.48011049	-0.36849135	0.95308362
C	7.16260626	-1.18487910	0.03715293
C	6.45865786	-2.08712646	-0.77725770
C	5.05725202	-2.21253415	-0.67699775
C	-3.21530309	-3.70629496	-0.95682651
C	-1.92917597	-3.62732739	-0.10192052
C	-1.24392046	-5.02071569	-0.02657721
C	4.16068937	-2.44367784	-3.01988075
C	4.28211691	-3.12678990	-1.62951690
C	4.91049708	-4.53661437	-1.74815568
C	0.95235675	3.31417282	-0.56180328
C	1.72228570	3.65874866	-1.70936269
C	2.77047418	4.59247465	-1.54514245
C	3.03410516	5.19046966	-0.30647775
C	2.23261905	4.87142264	0.80018511
C	1.18319218	3.93637163	0.70043931
C	2.69796682	2.31432551	-3.63881413
C	1.46734826	3.09461194	-3.11178777
C	1.05735192	4.21996349	-4.09870965
C	-4.91091443	0.59795577	3.14165303
C	-4.33282638	1.18827715	1.83549402
C	-4.47938733	2.73781574	1.85321714
C	-4.27628982	0.56632615	-0.66694689
C	-4.97833796	0.61350468	0.56932571
C	-6.32236709	0.19162666	0.56873596
C	-6.94796731	-0.23943714	-0.61348717
C	-6.23965833	-0.24960309	-1.82224265
C	-4.88524173	0.14833697	-1.87862979
C	1.03803396	3.47655434	3.21930460
C	0.26181328	3.70814095	1.90294010
C	-0.73458762	4.89258812	2.04181364
C	-4.32194658	-1.17936635	-3.99586297
C	-4.16194370	0.15884348	-3.23104844
C	-4.66668173	1.33480696	-4.11291627
H	0.90869235	-3.27482335	2.45421720
H	3.16546238	-2.89857433	1.91074441
H	-1.26876618	3.84081716	-1.61683474
H	-3.37580320	2.76405842	-1.60800874
H	-2.72835634	-1.90519618	4.99805200
H	-4.37719395	-3.41432259	3.92210352
H	-4.04460445	-4.14937901	1.57336118
H	0.29820163	-0.47080476	3.27106491
H	3.25115200	0.43877166	1.86048765
H	-1.88275642	0.14757607	5.33844423
H	-1.65258678	0.95684333	3.76740051

H	-0.40356355	1.07575402	5.01740515
H	-0.36983606	-1.94990601	5.90846364
H	1.04390235	-0.91619287	5.61141830
H	0.87440862	-2.46352758	4.75682998
H	5.81195584	2.10675576	2.18661364
H	4.14295549	2.57880392	2.56277311
H	4.61117869	2.29409989	0.88278223
H	4.18816410	-1.03861512	3.67932021
H	3.98642179	0.63884567	4.22104826
H	5.60499912	0.02355824	3.81409545
H	7.03585334	0.34367211	1.55601498
H	8.24357113	-1.10742885	-0.05362239
H	6.99899588	-2.69163273	-1.50010135
H	-1.23329078	-2.94482920	-0.60235853
H	3.25941399	-3.25114202	-1.25318147
H	-3.90695122	-4.47293984	-0.58358634
H	-2.96362404	-3.97372908	-1.99162839
H	-3.74327952	-2.74595386	-0.96445606
H	-1.88999269	-5.74344623	0.48954723
H	-0.29114800	-4.97244744	0.51612597
H	-1.03873079	-5.40794060	-1.03383560
H	3.60567060	-1.50294734	-2.93823825
H	3.62080129	-3.09858450	-3.71512319
H	5.15250124	-2.23564126	-3.44335865
H	5.90133658	-4.50263692	-2.21907043
H	4.27417892	-5.17718582	-2.37241676
H	5.01969637	-5.01552386	-0.76622372
H	3.37962203	4.85565319	-2.40680897
H	3.84506293	5.90873718	-0.20650654
H	2.41934589	5.35976806	1.75300398
H	0.65917425	2.36187683	-3.05531030
H	-3.26438679	0.94793138	1.80637529
H	3.59147514	2.95046785	-3.70974739
H	2.48778234	1.91284814	-4.63999215
H	2.91063896	1.46935659	-2.97612703
H	0.16835524	4.76209977	-3.74690752
H	0.82740054	3.79188980	-5.08428565
H	1.86156925	4.95634717	-4.23388828
H	-5.94696796	0.92066618	3.31232150
H	-4.31675729	0.94664772	3.99523493
H	-4.87996342	-0.49666389	3.13463249
H	-4.02206794	3.20370175	0.97299153
H	-3.98777478	3.15241713	2.74293091
H	-5.53896134	3.02665067	1.88260418
H	-6.88702848	0.20655602	1.49509984
H	-7.98734578	-0.55868524	-0.59096624
H	-6.73730915	-0.57518569	-2.73159747
H	-0.30130440	2.79039851	1.72110720
H	-3.09234615	0.31290024	-3.05529179
H	1.67420185	4.33015223	3.49072540
H	1.64940077	2.57535896	3.11309803
H	0.33115603	3.31799156	4.04571945

H	-1.43139179	4.71069529	2.87223496
H	-1.32455866	5.03201831	1.12572901
H	-0.20513712	5.83397311	2.24418101
H	-4.01329427	-2.03309217	-3.38282029
H	-3.70292267	-1.16899963	-4.90221247
H	-5.36081837	-1.34537411	-4.30859311
H	-4.52505020	2.30519338	-3.62082236
H	-5.73645670	1.22720314	-4.33518934
H	-4.12179164	1.35672904	-5.06563837
O	0.99498953	0.70748630	1.47988659
C	-0.76505848	-1.58016895	-3.17450583
H	-1.73754445	-1.47033877	-2.68480614
C	-0.33018608	-2.96137273	-3.40809615
H	-0.64378089	-3.73128624	-2.70877603
O	0.32816638	-1.23168986	-2.21462055
H	-0.68136341	-0.91380127	-4.04087508
C	0.64337222	-3.31281979	-4.49336331
H	1.26960377	-4.17379899	-4.22525544
H	0.12253920	-3.57627792	-5.43414181
H	1.29973883	-2.46267148	-4.71991549
Hf	0.18338531	0.11701631	-0.09032500

Oxo Peroxo Complex to Dioxo Complex (Ethylene)

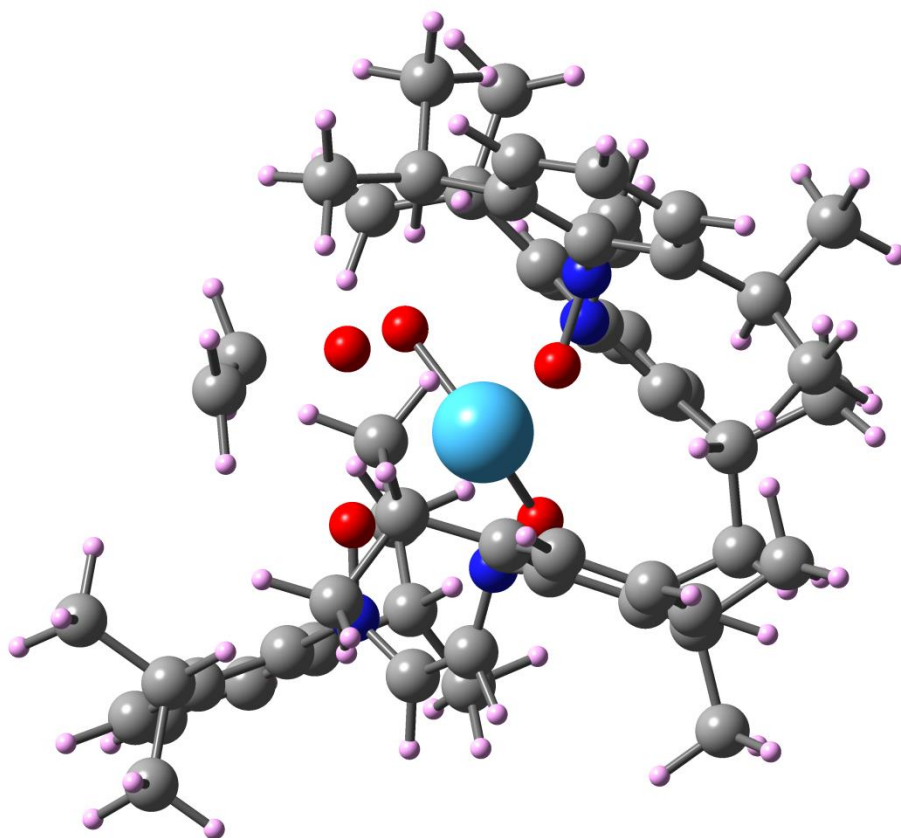


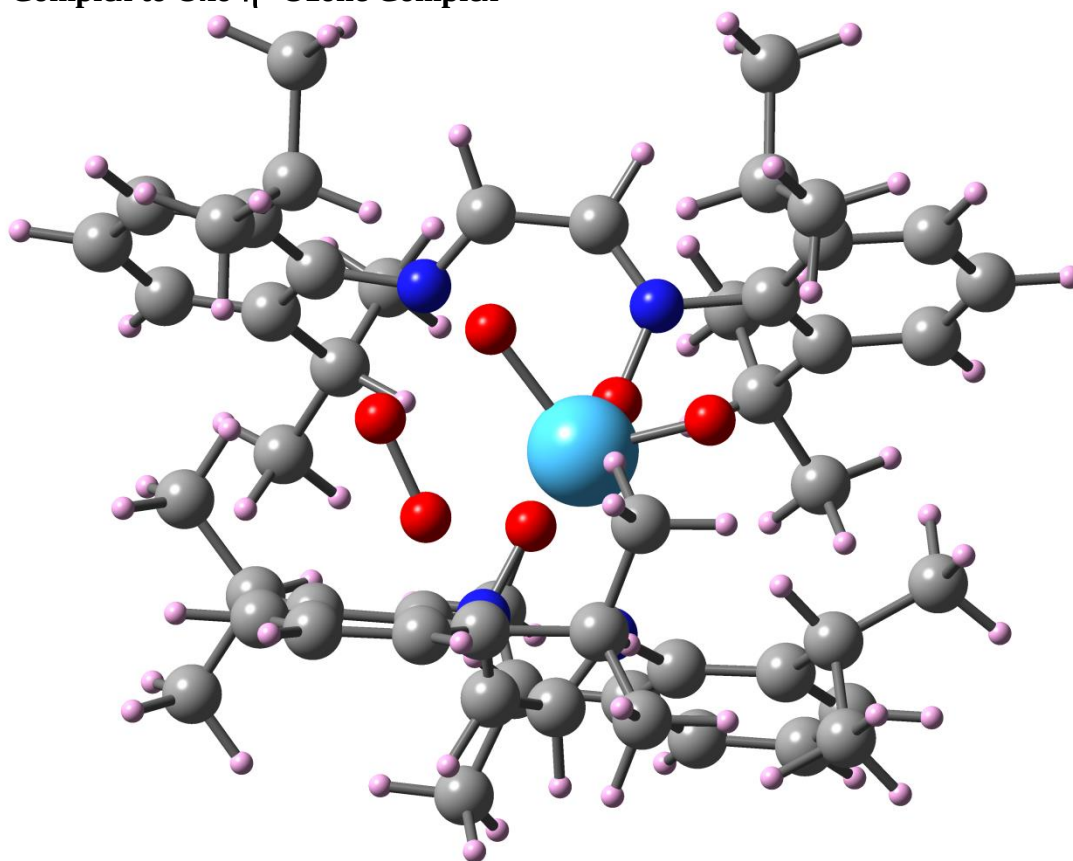
Fig. S138: NCCNO Oxo Peroxo Complex to Dioxo Complex (Ethylene)

E	E_{ZP}	H	G	<i>f</i>
-2747.1291	-2745.9248	-2745.8514	-2746.0348	-320
O	-1.89296014	0.04255600	-0.11460401	
O	2.15406416	-1.03984808	-0.54525904	
O	0.70297205	1.04502908	-1.96587015	
N	0.06250100	-1.77700314	1.26897710	
N	2.96565123	-1.49883912	0.40795203	
N	-0.46664604	2.53569820	-0.24401202	
N	-2.87343522	0.77033006	-0.73721806	
C	1.13139409	-2.21213017	1.89062314	
C	2.51662819	-1.96683315	1.56039712	
C	-1.63836513	2.91684122	-0.73902306	
C	-2.75497121	2.07387816	-1.00254308	
C	-1.19052709	-2.28328117	1.83631014	
C	-1.62072813	-1.81179514	3.10605424	
C	-2.77124721	-2.40852318	3.66713328	
C	-3.47307927	-3.41736726	2.99357923	
C	-3.04388223	-3.84044329	1.72485513	
C	-1.89904914	-3.28484425	1.12041109	
C	-1.89555815	0.48120104	4.16606332	

C	-0.91419507	-0.68336805	3.87179529
C	-0.28464102	-1.19886709	5.19348540
C	4.57226535	2.11803116	-0.08554301
C	4.47942234	0.95195607	0.93330807
C	5.11799539	1.34858510	2.28935217
C	4.40312734	-1.49261811	0.09231701
C	5.13002839	-0.30957202	0.36004003
C	6.50852350	-0.33563703	0.05514800
C	7.10864055	-1.47778611	-0.49724504
C	6.34326747	-2.62351420	-0.77070506
C	4.96213538	-2.65687720	-0.48792604
C	-2.52684319	-4.21932732	-1.18802009
C	-1.39071511	-3.80411229	-0.22601402
C	-0.41410003	-4.99584638	-0.01790900
C	4.18528432	-4.21705632	-2.34226018
C	4.13879332	-3.90516630	-0.82325506
C	4.60661835	-5.12878439	0.00824800
C	0.49724004	3.61874727	-0.04533700
C	1.05847208	4.29807433	-1.16774309
C	1.97689215	5.34073742	-0.91407307
C	2.31954218	5.71659646	0.39115303
C	1.73258413	5.05340939	1.47950511
C	0.81561106	4.00033331	1.28920910
C	1.99779315	3.60869228	-3.43793726
C	0.72547206	3.96679830	-2.62944820
C	-0.04070200	5.13740239	-3.30322625
C	-5.55917544	-0.06425501	2.44599819
C	-5.00739438	0.76556806	1.26218910
C	-5.71271743	2.14958917	1.20435709
C	-4.11124631	0.05424900	-1.05445408
C	-5.14125739	0.04027900	-0.08119101
C	-6.33873751	-0.62439305	-0.41962903
C	-6.48926250	-1.24638610	-1.66853813
C	-5.44881642	-1.21034209	-2.61074920
C	-4.23019332	-0.55613904	-2.32949418
C	1.08502608	3.02652223	3.64007128
C	0.10618701	3.39156426	2.50079419
C	-1.01247308	4.34907633	2.99785123
C	-3.03607023	-1.71417213	-4.28677032
C	-3.12362924	-0.45899404	-3.38676626
C	-3.33623925	0.79644106	-4.28072433
H	1.00783008	-2.86186222	2.76170321
H	3.27279925	-2.29322117	2.26347517
H	-1.79887014	3.96618830	-0.98907208
H	-3.62888828	2.52203519	-1.45867411
H	-3.12005624	-2.07526316	4.64154535
H	-4.35130033	-3.86852230	3.44969026
H	-3.60157228	-4.61306035	1.20405409
H	-0.11076301	-0.26797702	3.25319525
H	3.40949226	0.78345106	1.11302409
H	-2.72155521	0.16362401	4.81610537
H	-2.32320818	0.87428807	3.23599725

H	-1.36670810	1.29943710	4.66978736
H	-1.05035608	-1.59497912	5.87416544
H	0.23589802	-0.38142903	5.70927942
H	0.44278103	-2.00156315	5.01204438
H	5.61512043	2.40054318	-0.29001502
H	4.04803331	2.99560223	0.31026602
H	4.09361631	1.84582314	-1.03341708
H	5.03361939	0.53860404	3.02686523
H	4.59998135	2.22709417	2.69342521
H	6.18252147	1.60152012	2.18542516
H	7.10929853	0.54872504	0.24821402
H	8.17221962	-1.47373011	-0.72398106
H	6.81951155	-3.49410627	-1.21367709
H	-0.83309206	-2.99655923	-0.71409605
H	3.08797424	-3.71698328	-0.57281305
H	-3.04532423	-5.12487539	-0.84505307
H	-2.10666916	-4.43790934	-2.17788417
H	-3.26724525	-3.41858226	-1.29823810
H	-0.92745607	-5.83896844	0.46419304
H	0.44047903	-4.71857136	0.61299605
H	-0.02382000	-5.34187843	-0.98440407
H	3.80080429	-3.37597926	-2.93016722
H	3.56688427	-5.09573939	-2.56665020
H	5.20852840	-4.43155534	-2.67664920
H	5.64608746	-5.39306040	-0.22451902
H	3.98022030	-6.00224147	-0.21494902
H	4.54672635	-4.93071238	1.08661408
H	2.42813718	5.86126146	-1.75518213
H	3.02765223	6.52494450	0.55977705
H	1.98141415	5.36480043	2.49041619
H	0.10327101	3.06848023	-2.65653220
H	-3.94195830	0.93595407	1.45615311
H	2.71653821	4.43875534	-3.47032726
H	1.72443813	3.35850226	-4.47224234
H	2.48027219	2.73058221	-2.99774823
H	-0.96588708	5.38535140	-2.76396221
H	-0.30894302	4.87056437	-4.33467033
H	0.57082104	6.04925548	-3.34121225
H	-6.64829852	-0.18855201	2.38376218
H	-5.34163141	0.44925903	3.39148926
H	-5.09705539	-1.05584108	2.48193419
H	-5.29846140	2.78540921	0.41225703
H	-5.59264944	2.67806321	2.15908717
H	-6.78742250	2.03070116	1.01305908
H	-7.15353056	-0.65872705	0.29762002
H	-7.41901957	-1.75643813	-1.90994615
H	-5.58360644	-1.69538713	-3.57235227
H	-0.35178803	2.45379819	2.17820317
H	-2.15369816	-0.35765603	-2.88577722
H	1.63150512	3.89916630	4.02261531
H	1.79249314	2.27908617	3.26806225
H	0.53391504	2.59309920	4.48666734

H	-1.56148812	3.89568430	3.83490929
H	-1.73304613	4.57347435	2.19912117
H	-0.59281305	5.30320341	3.34520126
H	-2.93847423	-2.62881520	-3.69219428
H	-2.15353317	-1.63329612	-4.93242338
H	-3.91276330	-1.81555514	-4.94120638
H	-3.32349725	1.72488313	-3.69836728
H	-4.29564433	0.74066106	-4.81354737
H	-2.53175220	0.86265807	-5.02385938
O	1.25657510	0.79868006	1.30330310
C	1.13743208	-1.30625710	-3.35681226
H	1.01819808	-0.79603606	-4.31702033
C	0.55803104	-2.63517720	-3.26879325
H	-0.29220002	-2.91571722	-3.88240530
O	0.19926002	-0.58436404	-2.37177518
H	2.14832416	-1.19093709	-2.96171922
Hf	0.29022702	0.25176402	-0.16768301
H	0.85493706	-3.30523925	-2.46720919

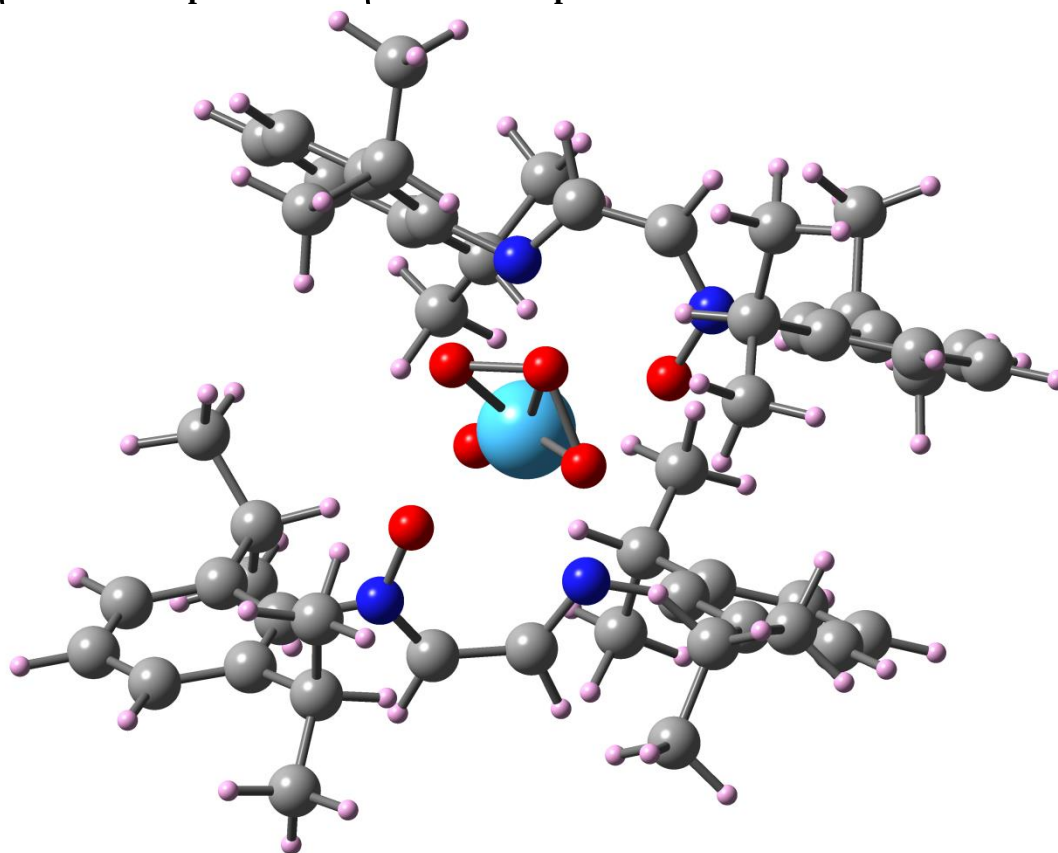
Dioxo Complex to Oxo η^2 -Ozone ComplexFig. S139: NCCNO Dioxo Complex to Oxo η^2 -Ozone Complex

E	E_{zp}	H	G	<i>f</i>
-2743.7156	-2742.5629	-2742.4911	-2742.6740	-148
O	-1.57698050	-0.65020517	-0.16962886	
O	2.75840402	-0.01006389	-0.48013199	
O	0.26086996	1.14473428	-1.75288512	
N	1.26375815	-1.34393641	1.58480248	
N	3.58929747	0.28710342	0.51490044	
N	-2.89495671	2.13533076	-0.37716679	
N	-2.45591040	-0.83481034	-1.20731142	
C	2.29863269	-0.90427868	2.25750823	
C	3.37237935	-0.06652744	1.77452429	
C	-3.03797399	1.59252638	-1.54701982	
C	-3.08427845	0.15743546	-1.79879351	
C	0.39573240	-2.27662470	2.30376439	
C	-0.41795359	-1.79906689	3.36778675	
C	-1.16962352	-2.75236802	4.08806552	
C	-1.11855044	-4.11559319	3.76501392	
C	-0.33189703	-4.55295903	2.68681104	
C	0.43670399	-3.64787855	1.92690830	
C	-2.00344577	0.17726361	3.47321591	

C	-0.55398080	-0.31289755	3.72522644
C	-0.11691432	-0.03023826	5.18608165
C	3.32271792	4.39341644	0.12064274
C	3.72305552	3.18931619	1.01034402
C	4.08854527	3.66285357	2.44280545
C	4.81149274	1.00833051	0.12710671
C	4.87672715	2.39742656	0.38405736
C	6.07486676	3.04871308	0.01836185
C	7.12332057	2.34626267	-0.59471308
C	7.00088795	0.97293621	-0.86464248
C	5.83506083	0.26441421	-0.50946106
C	0.69572261	-5.25928458	-0.05405760
C	1.34674910	-4.14655174	0.79961874
C	2.70581813	-4.62634862	1.38066722
C	5.37003997	-1.38930917	-2.36361106
C	5.68774577	-1.22115993	-0.85202191
C	6.93150387	-2.05021753	-0.44614821
C	-2.93943879	3.54012099	-0.17882324
C	-2.28844570	4.49013227	-1.03423728
C	-2.44739602	5.85754674	-0.72590453
C	-3.19982195	6.28674410	0.37715933
C	-3.79070460	5.34198167	1.23349238
C	-3.66054697	3.96474966	0.98538407
C	0.00589349	4.79863316	-2.11288081
C	-1.37836698	4.10823690	-2.21129625
C	-2.04532458	4.44699068	-3.57272621
C	-4.24612356	-3.44641121	1.71059182
C	-4.10430063	-2.42076848	0.56338496
C	-5.49086897	-1.79093642	0.24256088
C	-2.72906068	-2.22779865	-1.61456570
C	-3.49362780	-3.01501442	-0.71241684
C	-3.75861095	-4.34495483	-1.08977053
C	-3.29268281	-4.85458538	-2.31383490
C	-2.56613924	-4.03822006	-3.18955662
C	-2.25957625	-2.69668204	-2.86651070
C	-4.39643920	3.35373257	3.37327167
C	-4.33684897	2.93081736	1.88766927
C	-5.76243078	2.59927739	1.36369242
C	-0.23337041	-2.53091993	-4.42069298
C	-1.51290611	-1.83600209	-3.89420217
C	-2.45965470	-1.46572881	-5.07145985
H	2.42786464	-1.21675619	3.29746329
H	4.13568515	0.23501173	2.48034410
H	-3.26358333	2.17669785	-2.44608381
H	-3.71667679	-0.15610714	-2.62443489
H	-1.80240508	-2.41864286	4.90671250
H	-1.69625888	-4.83324123	4.34306806
H	-0.30942470	-5.60905505	2.43422552
H	0.07811603	0.28396972	3.06111496
H	2.83631472	2.55047932	1.08122994
H	-2.72993897	-0.37727503	4.08315992
H	-2.26445807	0.06169575	2.41526910

H	-2.08648646	1.24166742	3.72661471
H	-0.75645631	-0.55506061	5.90809772
H	-0.18528070	1.04465982	5.39870752
H	0.91865378	-0.34912507	5.36940147
H	4.13708502	5.12477862	0.03006632
H	2.45761362	4.90366476	0.56116005
H	3.03869782	4.05957659	-0.88306633
H	4.33787637	2.81927202	3.10111630
H	3.24064435	4.19891246	2.88727355
H	4.95108384	4.34261696	2.43080591
H	6.17703200	4.11455525	0.20116979
H	8.03382638	2.87113460	-0.87376226
H	7.81582435	0.44836646	-1.35473218
H	1.53367639	-3.31557285	0.11093970
H	4.83012767	-1.63027504	-0.30474811
H	0.54044648	-6.18891785	0.51155444
H	1.34776990	-5.49275417	-0.90509805
H	-0.26691034	-4.92579235	-0.45774303
H	2.56709605	-5.48362284	2.05427112
H	3.20891044	-3.83250375	1.95032795
H	3.37594519	-4.93641573	0.56778370
H	4.44569139	-0.86441515	-2.62571826
H	5.23711824	-2.45166853	-2.60474454
H	6.18733079	-0.99560395	-2.98296223
H	7.81933497	-1.76452235	-1.02451294
H	6.74508737	-3.11456255	-0.63804225
H	7.16876239	-1.93044772	0.61911642
H	-1.96222604	6.59839594	-1.35581181
H	-3.31127219	7.34989712	0.57843011
H	-4.34918941	5.68244527	2.10034688
H	-1.16221977	3.03640434	-2.17944227
H	-3.44405573	-1.62397584	0.92075543
H	-0.06244004	5.89098846	-2.20868476
H	0.65362380	4.42692240	-2.91711329
H	0.48401542	4.55152493	-1.16061809
H	-3.01986667	3.95345902	-3.69575785
H	-1.39561482	4.12916340	-4.39881532
H	-2.21453889	5.52811443	-3.67134078
H	-4.99541089	-4.21652995	1.48292448
H	-4.57414846	-2.93296635	2.62369039
H	-3.29176313	-3.93839771	1.92480695
H	-5.42124470	-1.01568546	-0.53074050
H	-5.91318549	-1.32668254	1.14340332
H	-6.19356450	-2.55820845	-0.10946822
H	-4.33562510	-4.98403374	-0.42924579
H	-3.50461102	-5.88599843	-2.58592653
H	-2.21814081	-4.44440424	-4.13444449
H	-3.74241219	2.01352018	1.81295949
H	-1.17682694	-0.91021181	-3.41570135
H	-5.08020418	4.19797632	3.53540859
H	-3.40585683	3.64091522	3.74810889
H	-4.76264588	2.51712596	3.98311027

H	-6.23122435	1.82538317	1.98721868
H	-5.72956813	2.23039808	0.33105597
H	-6.40475909	3.49036506	1.38552293
H	0.43635295	-2.72763194	-3.57758085
H	0.28187442	-1.86201836	-5.12349749
H	-0.45924391	-3.46414315	-4.95501887
H	-3.37092318	-0.95012668	-4.73556700
H	-2.77448646	-2.36411046	-5.61896876
H	-1.93816454	-0.80579354	-5.77648070
O	0.26639019	2.23130945	-0.07380090
O	0.67398347	1.34237596	0.93678416
O	0.78412608	-1.88728814	-1.57084695
Hf	0.56897800	-0.40031537	-0.53782748

Oxo η^2 -Ozone Complex to Oxo η^3 -Ozone ComplexFig. S140: NCCNO Oxo η^2 -Ozone Complex to Oxo η^3 -Ozone Complex

E	E_{zp}	H	G	<i>f</i>
-2743.7388	-2742.5839	-2742.5134	-2742.6904	-37
O	-1.90976315	0.43789203	0.25671202	
O	2.16337416	-0.99495507	-0.70695706	
O	1.01641108	1.01172808	-1.93285315	
N	-0.07221101	-2.10517316	0.80208606	
N	2.87284922	-1.82056614	0.05783200	
N	-0.15193901	2.56143020	-0.16668301	
N	-2.76675921	1.15753809	-0.51280204	
C	0.93716007	-2.83038522	1.21757910	
C	2.34125718	-2.64612520	0.94541007	
C	-1.22893909	3.07508324	-0.70563405	
C	-2.45805419	2.36041318	-0.96186808	
C	-1.37049711	-2.56988319	1.30321010	
C	-1.71358813	-2.29637518	2.65535621	
C	-2.93140822	-2.82592221	3.13567224	
C	-3.77374529	-3.58286927	2.30949318	
C	-3.41329726	-3.82528729	0.97386507	
C	-2.20522617	-3.33088225	0.44122003	
C	-1.59945712	-0.30101602	4.24415033	

C	-0.82116906	-1.47507111	3.59786827
C	-0.20144102	-2.37459818	4.70164936
C	4.93588738	1.36920310	1.68414913
C	4.47160834	-0.10520101	1.79282014
C	4.80116337	-0.68340805	3.19510824
C	4.32643733	-1.78576014	-0.16532801
C	5.09705539	-0.96501807	0.68825805
C	6.49188548	-0.96470307	0.46752804
C	7.05946152	-1.71988013	-0.57047005
C	6.24792450	-2.48612719	-1.42493411
C	4.85026937	-2.53524519	-1.24605310
C	-2.96310422	-3.85479830	-1.95764715
C	-1.77248613	-3.67655628	-0.98788107
C	-0.90239107	-4.96561038	-0.99894608
C	3.63969028	-2.39693718	-3.45750626
C	3.94892630	-3.29405725	-2.22486917
C	4.53935035	-4.65620336	-2.66071520
C	0.94787307	3.47940327	0.10817601
C	1.62385512	4.15385931	-0.95162007
C	2.68838721	5.01316738	-0.59864405
C	3.05591923	5.22001840	0.73676705
C	2.35208618	4.56937035	1.76236114
C	1.29102010	3.68980828	1.47638811
C	2.49530719	3.51100927	-3.26173825
C	1.27913310	4.00883931	-2.44080518
C	0.73404206	5.34451040	-3.01610523
C	-5.34943238	0.12122401	2.82573821
C	-4.65758536	0.90864107	1.69063413
C	-5.05362339	2.41187419	1.77525913
C	-4.07443531	0.54971404	-0.80018006
C	-4.96851838	0.36670303	0.28992702
C	-6.20457250	-0.24317302	0.00644400
C	-6.53586953	-0.63614205	-1.30192510
C	-5.64322942	-0.40737803	-2.35620618
C	-4.38314633	0.19621002	-2.13910016
C	1.28940810	2.67469721	3.83704729
C	0.45134103	3.09614524	2.61085220
C	-0.66510105	4.09818231	3.01841823
C	-3.18474424	-0.79746606	-4.17945532
C	-3.47733826	0.47484304	-3.34702826
C	-4.10911932	1.58168612	-4.23750232
H	0.73770206	-3.68613528	1.86728814
H	3.04538023	-3.27671325	1.47366911
H	-1.26046210	4.13289931	-0.97452207
H	-3.23549125	2.86808722	-1.51895012
H	-3.21822624	-2.64245220	4.16836032
H	-4.70460236	-3.98581931	2.70272721
H	-4.07456031	-4.41026033	0.34207303
H	-0.00777400	-1.01895508	3.02158723
H	3.37905726	-0.09244201	1.68337213
H	-2.42838918	-0.65037805	4.87499637
H	-2.00610715	0.36342103	3.47312127

H	-0.92209607	0.28858002	4.87546237
H	-0.97833808	-2.82907622	5.33187439
H	0.45603703	-1.78007414	5.34972243
H	0.39571703	-3.19147724	4.27404133
H	6.01503645	1.47838811	1.86028714
H	4.40870034	1.97616415	2.42979319
H	4.70196036	1.78245014	0.69615706
H	4.42766834	-1.71045313	3.30763325
H	4.32968233	-0.06896001	3.97259831
H	5.88418446	-0.69766405	3.38045026
H	7.13082255	-0.35750503	1.10247108
H	8.13588160	-1.70157113	-0.72470906
H	6.70334952	-3.04527523	-2.23664717
H	-1.16197709	-2.84944822	-1.37144611
H	2.98798823	-3.49691727	-1.73429913
H	-3.53840327	-4.76518636	-1.73818213
H	-2.58912620	-3.94411930	-2.98522623
H	-3.64471628	-2.99778123	-1.91791115
H	-1.47357011	-5.82452343	-0.62002704
H	-0.00293900	-4.85988137	-0.38025003
H	-0.57971405	-5.19306540	-2.02351416
H	3.13334324	-1.47562911	-3.15190424
H	2.98235223	-2.93110923	-4.15592732
H	4.56504335	-2.13429716	-3.98816730
H	5.44311242	-4.53156334	-3.27088925
H	3.80690129	-5.19682140	-3.27359925
H	4.79527136	-5.28500040	-1.79774614
H	3.23413825	5.52409744	-1.38760611
H	3.87826030	5.88964742	0.97840408
H	2.62654620	4.75130336	2.79704921
H	0.51468704	3.23792225	-2.55903320
H	-3.57786727	0.83083606	1.85083914
H	3.34542926	4.20406632	-3.20320025
H	2.21510117	3.40905526	-4.31893633
H	2.80613621	2.52565119	-2.90198622
H	-0.14623101	5.70161244	-2.46235219
H	0.44594203	5.21254140	-4.06768231
H	1.49119911	6.13868448	-2.97361323
H	-6.43851250	0.26344402	2.81939822
H	-4.98100038	0.47834704	3.79580729
H	-5.13365839	-0.94997307	2.75422821
H	-4.54149234	3.01657023	1.01635608
H	-4.78942137	2.81686921	2.76068821
H	-6.13555149	2.53591520	1.63327012
H	-6.91517251	-0.40857403	0.80926506
H	-7.49504356	-1.10971709	-1.49748912
H	-5.91867846	-0.70130106	-3.36494426
H	-0.00879700	2.17903616	2.23586717
H	-2.50167119	0.82793707	-3.00706423
H	1.79091314	3.52289127	4.32356633
H	2.03413016	1.93175215	3.53410027
H	0.63584405	2.20830217	4.58651335

H	-1.30779710	3.65777528	3.79315229
H	-1.30052110	4.36688133	2.16290816
H	-0.23615302	5.02700338	3.41959626
H	-2.58778520	-1.49760312	-3.59047228
H	-2.59342820	-0.52494904	-5.06278339
H	-4.10151531	-1.29384110	-4.52537135
H	-4.31401733	2.50281019	-3.67305328
H	-5.05874839	1.24770509	-4.67613936
H	-3.42682426	1.83191314	-5.05957539
O	1.09982608	0.28465702	1.46677211
O	-0.33019103	0.56795004	-2.50466419
O	-0.54007504	-0.86294607	-1.99386015
Hf	0.25379202	0.11143901	-0.16948401

Oxo η^3 -Ozone Complex to Oxo Peroxo Complex (Propene)

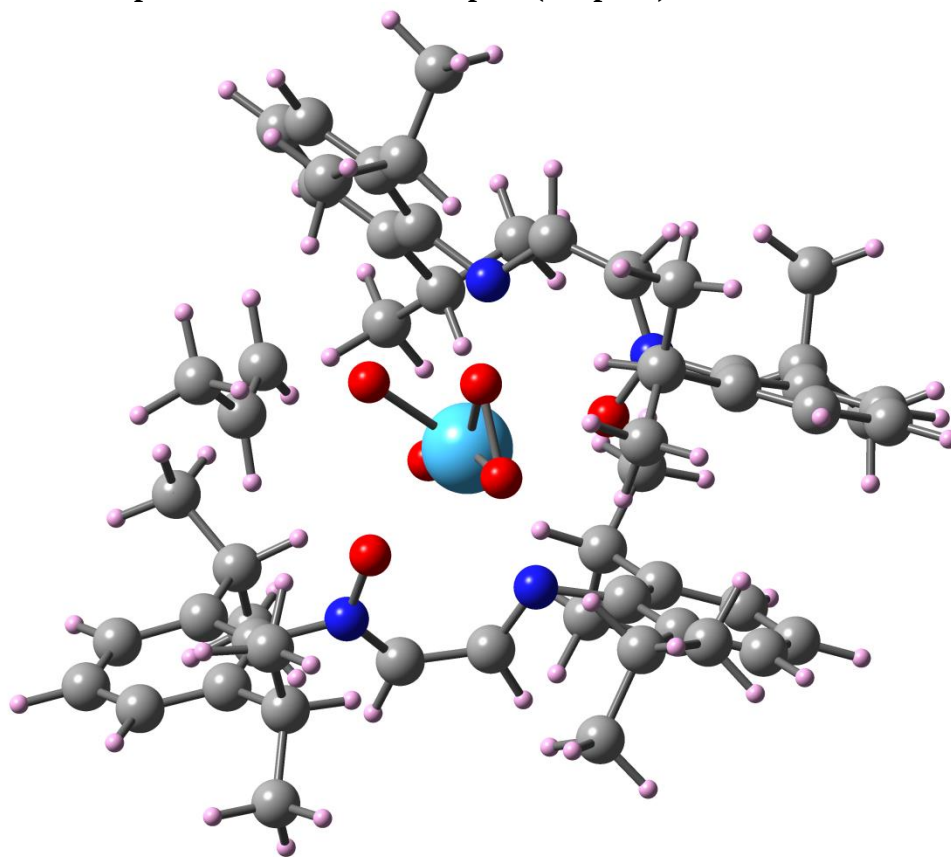


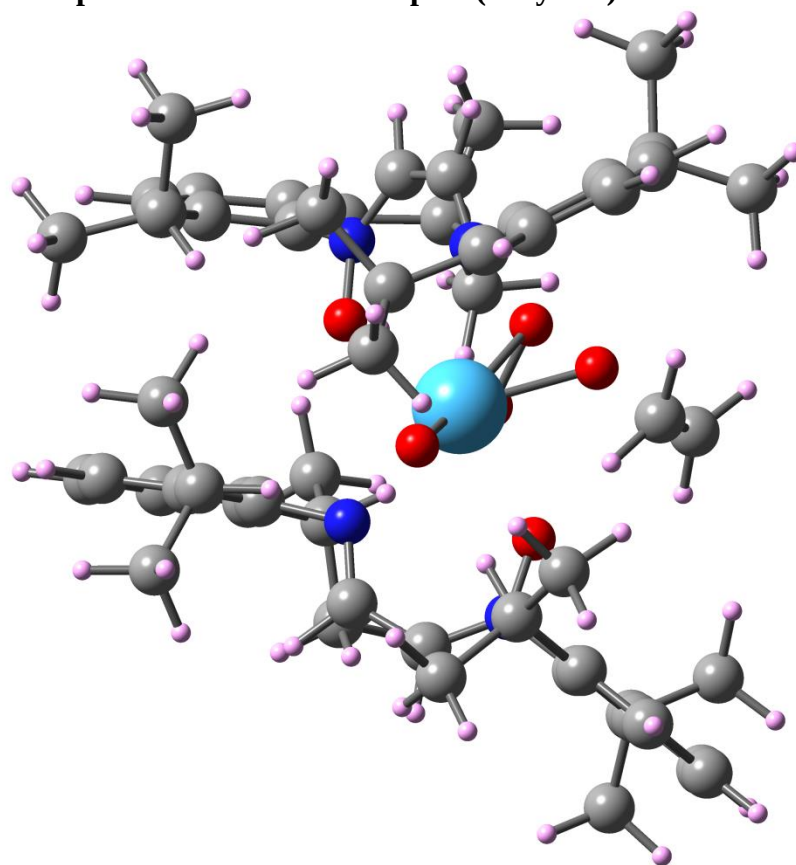
Fig. S141: NCCNO Oxo η^3 -Ozone Complex to Oxo Peroxo Complex (Propene)

E	E_{zp}	H	G	<i>f</i>
-2861.5960	-2860.3591	-2860.2831	-2860.4716	-376
O	-1.95045615	0.10721601	0.22810302	
O	2.13878917	-1.13265208	-0.70625405	
O	1.39341711	1.44663511	-1.50482312	
N	-0.11106801	-2.16376817	0.75788606	
N	2.83856722	-1.94238015	0.08902401	
N	-0.62869805	2.67161720	0.25274902	
N	-2.93058322	0.81251106	-0.36614703	
C	0.87519006	-2.88808622	1.22602709	
C	2.28501017	-2.73039321	0.99193307	
C	-1.82877814	3.01256823	-0.13175301	
C	-2.89131022	2.12055016	-0.52401604	
C	-1.40999911	-2.67701820	1.20532709	
C	-1.78862513	-2.47718119	2.55975320	
C	-2.96520223	-3.11696624	3.00592623	
C	-3.73325728	-3.91182830	2.14252316	
C	-3.34673426	-4.06842131	0.80096806	
C	-2.17755617	-3.45890026	0.30232902	
C	-1.82021314	-0.48048004	4.14957232	

C	-0.96751607	-1.61935412	3.53532927
C	-0.34864003	-2.48811819	4.66357536
C	5.21407640	0.82648706	2.26339317
C	4.54283035	-0.55376604	2.04880216
C	4.71004036	-1.41695011	3.33044825
C	4.29395533	-1.95159215	-0.12226701
C	5.11106939	-1.28450410	0.82338906
C	6.50263550	-1.32686610	0.58933905
C	7.03087955	-1.97799115	-0.53675204
C	6.18144348	-2.60714520	-1.46166211
C	4.78341737	-2.61252020	-1.27502310
C	-2.86604322	-3.93808830	-2.12803916
C	-1.70398513	-3.70138928	-1.13616809
C	-0.72866105	-4.91190537	-1.19970009
C	3.72076828	-2.38359418	-3.56436927
C	3.86013130	-3.27743825	-2.30178518
C	4.33091433	-4.70502536	-2.67604020
C	0.27269902	3.77898829	0.50721104
C	0.54966204	4.72726536	-0.52623604
C	1.45236811	5.77065546	-0.22618802
C	2.04661016	5.88731444	1.03811108
C	1.74274113	4.95367538	2.04272016
C	0.85461007	3.88709230	1.80419514
C	1.05230608	4.58994535	-3.03548923
C	-0.04310700	4.67052636	-1.94477115
C	-0.98169608	5.88134347	-2.20172517
C	-5.70733443	-0.73594906	2.64632120
C	-4.95689738	0.17802001	1.65073913
C	-5.46299239	1.63936212	1.83379814
C	-4.13987132	0.07953901	-0.80156506
C	-5.10076139	-0.26153402	0.18742801
C	-6.24858946	-0.94913007	-0.25157302
C	-6.43288248	-1.25866409	-1.61016112
C	-5.48232541	-0.86543507	-2.56056819
C	-4.30622033	-0.17575501	-2.18522217
C	1.52048212	2.73275621	4.00432331
C	0.43526203	2.93558522	2.92554822
C	-0.88324907	3.43600126	3.57957927
C	-2.89833722	-0.80026906	-4.23878633
C	-3.34555125	0.32247902	-3.27238925
C	-4.00902631	1.48688711	-4.06111131
H	0.64644205	-3.73579529	1.87738114
H	2.96688023	-3.36347126	1.54440012
H	-2.11069216	4.06703931	-0.18776501
H	-3.77090529	2.55936619	-0.97729907
H	-3.27697825	-2.99354723	4.04052031
H	-4.62832036	-4.40864934	2.51092319
H	-3.95478630	-4.67757036	0.13917701
H	-0.15294301	-1.12812908	2.98979323
H	3.46915426	-0.36988603	1.90184215
H	-2.68094921	-0.86590307	4.71347236
H	-2.18751217	0.19086601	3.36524626

H	-1.20544709	0.11379301	4.83864737
H	-1.12546208	-2.97759023	5.26711140
H	0.25601702	-1.86266114	5.33359940
H	0.30123902	-3.27662025	4.26052532
H	6.26423649	0.73148706	2.57147220
H	4.68452336	1.36785110	3.05739023
H	5.17539240	1.43696011	1.35449510
H	4.19421432	-2.38240318	3.25047425
H	4.28950333	-0.88582907	4.19357832
H	5.77018444	-1.62016112	3.53519327
H	7.17372756	-0.83232706	1.28520510
H	8.10629964	-1.98933615	-0.69779505
H	6.60606150	-3.09910624	-2.33198118
H	-1.16117209	-2.80618822	-1.46666211
H	2.85583322	-3.36584326	-1.87125614
H	-3.37113026	-4.89669738	-1.94401015
H	-2.47520419	-3.96751530	-3.15291824
H	-3.61231628	-3.13857524	-2.07302116
H	-1.23343609	-5.83379546	-0.87880707
H	0.15025601	-4.76834437	-0.56027004
H	-0.37474303	-5.05582739	-2.22924817
H	3.27418325	-1.41786211	-3.30651525
H	3.06555624	-2.86933422	-4.29875233
H	4.69763036	-2.21169417	-4.03694931
H	5.29171640	-4.69348236	-3.20652725
H	3.59529528	-5.17499940	-3.34126726
H	4.44318134	-5.33979040	-1.78731313
H	1.69467913	6.49793249	-0.99719608
H	2.73675721	6.70297650	1.24183209
H	2.19613917	5.05906239	3.02338023
H	-0.62549905	3.75227828	-2.05961316
H	-3.89276630	0.14562301	1.91016615
H	1.74800013	5.43872644	-2.99218923
H	0.58656505	4.58858235	-4.03041731
H	1.60616012	3.65640628	-2.92112722
H	-1.79011514	5.94524146	-1.45973111
H	-1.43651711	5.80409243	-3.19836724
H	-0.42701103	6.82792054	-2.15919417
H	-6.79643053	-0.62326005	2.55727220
H	-5.43460939	-0.46024804	3.67289528
H	-5.44879642	-1.78784714	2.49726519
H	-4.91761238	2.35357118	1.20702909
H	-5.33928541	1.95118615	2.87903722
H	-6.52920152	1.71129313	1.58051112
H	-7.00458155	-1.24075410	0.46961604
H	-7.32579654	-1.79328714	-1.92589015
H	-5.64791645	-1.08944408	-3.61033328
H	0.27397502	1.94916315	2.47185819
H	-2.42541519	0.69743506	-2.81682321
H	1.70622413	3.63985528	4.59758035
H	2.46234719	2.40678718	3.54804827
H	1.19934709	1.94460715	4.69762436

H	-1.21572109	2.72894421	4.35138933
H	-1.69224213	3.53315927	2.84348822
H	-0.74063805	4.41737634	4.05470831
H	-2.30093618	-1.53982212	-3.70076428
H	-2.25464917	-0.36995003	-5.01591238
H	-3.74557829	-1.29574010	-4.73371136
H	-4.31763633	2.31135518	-3.40253226
H	-4.90107738	1.14605709	-4.60450135
H	-3.29743625	1.88855315	-4.79341236
O	1.12587709	0.26679602	1.48229111
O	-0.38834403	0.91329907	-2.12582716
O	-0.33568303	-0.60035304	-2.13346516
C	3.07837923	2.19855817	-0.47987404
H	2.88704922	1.73124813	0.48003204
H	2.98397023	3.27856325	-0.54017904
C	3.45714426	1.46033211	-1.58641912
H	3.57849527	0.38917403	-1.47927611
C	3.83945429	2.03896116	-2.92178622
H	3.80091029	3.13303624	-2.92516922
H	4.85773437	1.72533813	-3.19624924
H	3.15679124	1.66109713	-3.69397128
Hf	0.29191902	0.15355701	-0.19371001

Oxo η^3 -Ozone Complex to Oxo Peroxo Complex (Ethylene)Fig. S142: NCCNO Oxo η^3 -Ozone Complex to Oxo Peroxo Complex (Ethylene)

E	E_{zp}	H	G	<i>f</i>
-2822.2838	-2821.0748	-2821.0008	-2821.1834	-399
O	-1.91279615	0.17673901	0.27258602	
O	2.20856617	-1.00324807	-0.78007306	
O	1.20826509	1.33904010	-1.79618413	
N	-0.00954100	-2.16109717	0.68712105	
N	2.93070523	-1.82110414	-0.01345900	
N	-0.50963504	2.66602920	0.06116500	
N	-2.88516422	0.85011606	-0.37426203	
C	1.00335908	-2.88174522	1.10028709	
C	2.40420318	-2.67719620	0.84281306	
C	-1.69858613	3.01578423	-0.34667603	
C	-2.79446521	2.13163417	-0.66775005	
C	-1.28736010	-2.67860721	1.18932609	
C	-1.60905712	-2.47176619	2.55815120	
C	-2.77777421	-3.09234124	3.05034323	
C	-3.59179128	-3.87572830	2.21971717	
C	-3.25582025	-4.04728431	0.86674907	
C	-2.09642016	-3.45900026	0.32151002	
C	-1.55309712	-0.49103104	4.16821532	

C	-0.73862505	-1.62995312	3.50426927
C	-0.07907201	-2.51783319	4.59407035
C	5.11507339	1.09249608	2.21112517
C	4.48895034	-0.30190102	1.95476515
C	4.60786535	-1.16241109	3.24383225
C	4.38995134	-1.75063313	-0.19201601
C	5.13931339	-1.01873808	0.76230306
C	6.53765650	-0.99277207	0.57322704
C	7.13683856	-1.64614912	-0.51625904
C	6.35259946	-2.34044718	-1.45095111
C	4.95031738	-2.40750718	-1.31204010
C	-2.87775822	-3.95944530	-2.07574816
C	-1.67797413	-3.72616829	-1.12919609
C	-0.72222706	-4.95097338	-1.20976909
C	4.26477833	-2.56033120	-3.75712429
C	4.10630631	-3.16918224	-2.33947118
C	4.45908934	-4.68015636	-2.34318718
C	0.39693703	3.76937629	0.34520503
C	0.75266106	4.70195936	-0.67791605
C	1.61608112	5.76098845	-0.32192902
C	2.10953216	5.90126546	0.98254607
C	1.73837814	4.97690838	1.97166915
C	0.87671407	3.90053930	1.68136413
C	1.44810711	4.74912936	-3.14761024
C	0.27908602	4.60696335	-2.13849416
C	-0.78838806	5.69055041	-2.46199819
C	-5.45596640	-0.57248604	2.87731722
C	-4.75340536	0.28276602	1.79925414
C	-5.20655040	1.76473614	1.95411115
C	-4.12478132	0.11634601	-0.70276206
C	-5.00568538	-0.20391402	0.36609703
C	-6.17813650	-0.90866607	0.03452700
C	-6.46447849	-1.25530709	-1.29737110
C	-5.59295441	-0.88247807	-2.32769618
C	-4.39591633	-0.17718401	-2.06295116
C	1.39759111	2.75841221	3.92565130
C	0.37470703	2.97291523	2.78956621
C	-0.96375007	3.51191627	3.36805026
C	-3.12537024	-0.87394606	-4.18314732
C	-3.52774327	0.28625202	-3.24084525
C	-4.27076133	1.40024811	-4.03096231
H	0.81151606	-3.74776329	1.73880913
H	3.11101424	-3.31025125	1.36332810
H	-1.95433215	4.07195931	-0.45234403
H	-3.66530128	2.56387520	-1.14392409
H	-3.04679623	-2.96226823	4.09597331
H	-4.48185434	-4.35427333	2.62287520
H	-3.89663030	-4.65141736	0.23185502
H	0.05271100	-1.13550309	2.92794222
H	3.41802226	-0.14661901	1.75522613
H	-2.38887218	-0.87426607	4.77004236
H	-1.95169115	0.18854701	3.40685926

H	-0.90083607	0.09316301	4.83092737
H	-0.83314506	-3.00334923	5.22908440
H	0.56470505	-1.90701314	5.24087740
H	0.54066804	-3.31092325	4.15376932
H	6.14463148	1.01936208	2.58739720
H	4.52363035	1.62084612	2.96868822
H	5.12694239	1.70687013	1.30378210
H	4.11277832	-2.13583317	3.13820824
H	4.13343132	-0.63882505	4.08316431
H	5.66007742	-1.34587110	3.50183527
H	7.15888154	-0.44510403	1.27543410
H	8.21641661	-1.60679312	-0.64073205
H	6.83009753	-2.83128521	-2.29477918
H	-1.13774509	-2.84264422	-1.49225811
H	3.04788423	-3.07249224	-2.07471216
H	-3.38441126	-4.91224138	-1.86687914
H	-2.52497019	-3.99868630	-3.11398024
H	-3.61417328	-3.15244624	-1.99886215
H	-1.22661009	-5.86120944	-0.85639506
H	0.18188801	-4.80992137	-0.60568905
H	-0.40849603	-5.11492739	-2.24930017
H	3.96907630	-1.50509012	-3.76615629
H	3.62465328	-3.09592224	-4.46956434
H	5.30097441	-2.63104520	-4.11329032
H	5.50118640	-4.84694637	-2.64577320
H	3.81395529	-5.21644540	-3.05094924
H	4.32235933	-5.12811339	-1.35015410
H	1.91262914	6.47893249	-1.08202208
H	2.77449421	6.72645351	1.22742809
H	2.11455316	5.09706939	2.98286823
H	-0.14814701	3.61364728	-2.30653618
H	-3.67581728	0.23057302	1.98681015
H	1.86045614	5.76685243	-3.15818224
H	1.08889408	4.52618535	-4.16081332
H	2.25702117	4.05287631	-2.91453222
H	-1.67277213	5.62324642	-1.81506514
H	-1.12321109	5.59389243	-3.50363227
H	-0.36947903	6.69778051	-2.33442918
H	-6.54664749	-0.44344803	2.85201622
H	-5.11427939	-0.25865202	3.87180530
H	-5.22384240	-1.63490212	2.75869121
H	-4.69137836	2.43462419	1.25620710
H	-4.99508438	2.11768916	2.97175522
H	-6.28675050	1.85684214	1.77828614
H	-6.87531752	-1.18525809	0.81814206
H	-7.37501357	-1.80305114	-1.52903312
H	-5.83771143	-1.13549509	-3.35533425
H	0.21443502	1.98569515	2.34098918
H	-2.58441620	0.69625805	-2.87141322
H	1.58067412	3.66943628	4.51359634
H	2.34971918	2.39798718	3.52036527
H	1.01942608	1.99199615	4.61473435

H	-1.35101910	2.82220021	4.13009331
H	-1.73186113	3.61838427	2.59030720
H	-0.82314006	4.49577035	3.83852030
H	-2.44629719	-1.55449512	-3.66401228
H	-2.58152420	-0.46668804	-5.04498438
H	-3.99269330	-1.43227911	-4.56212835
H	-4.55698235	2.24563017	-3.38874826
H	-5.18802440	1.01713408	-4.49838634
H	-3.62075028	1.78515214	-4.82685837
O	1.10128908	0.27815002	1.42077211
O	-0.54402704	0.74456806	-2.23102117
O	-0.48349004	-0.75205306	-2.09233016
C	3.22558625	2.06990916	-1.00804208
H	3.39532826	1.48252412	-0.11495301
H	3.11752224	3.14247424	-0.88384507
C	3.02421023	1.45514311	-2.23560017
H	3.23756825	0.40080403	-2.36170318
Hf	0.29723502	0.14329601	-0.26270002
H	2.93800423	2.03883416	-3.14720924

12.2. Triplet Geometries

Oxo Complex to Oxo Complex with Adsorbed Oxygen Molecule

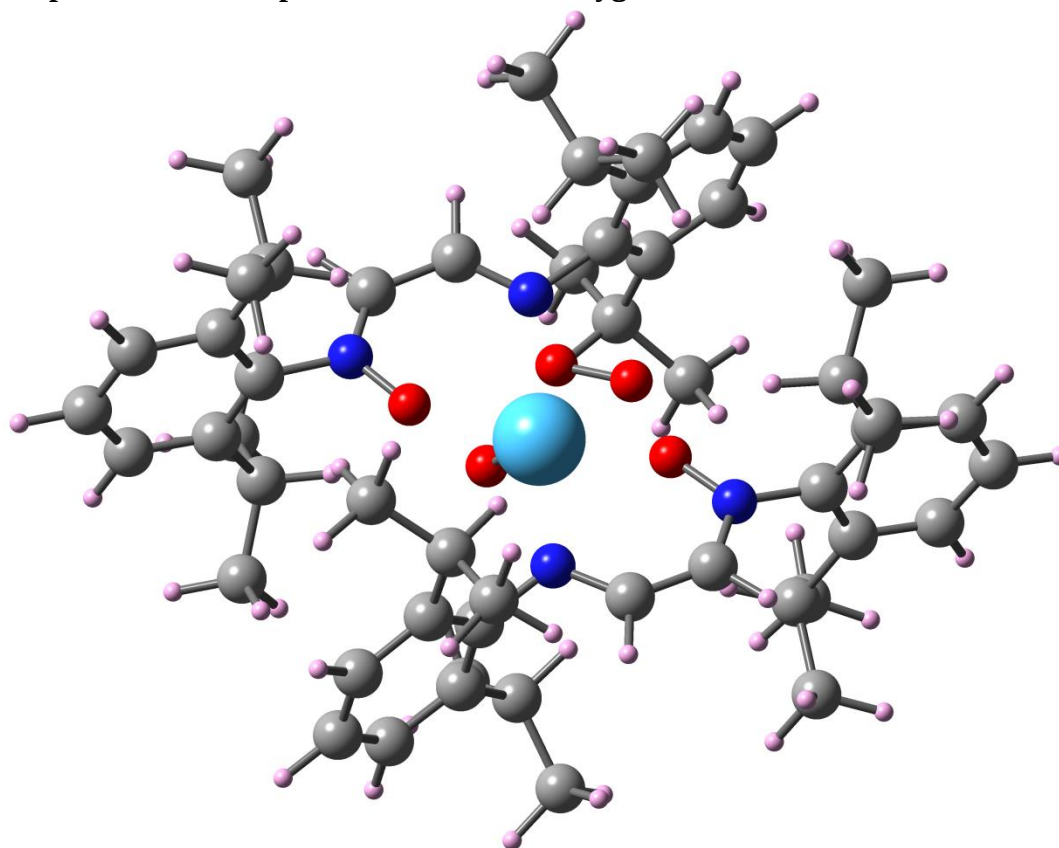


Fig. S143: NCCNO Oxo Complex to Oxo Complex with Adsorbed Oxygen Molecule

E	E_{ZP}	H	G	<i>f</i>
-2668.5941	-2667.4443	-2667.3738	-2667.5532	-117
O	-2.13362589	0.47351516	0.20809206	
O	2.03252984	-0.41074181	-0.10949394	
O	-0.54138007	-0.62952325	-1.81689034	
N	-0.03008700	-2.00076082	1.03340334	
N	2.87333914	-1.05704064	0.78992190	
N	-0.00017907	2.07620202	-0.99128552	
N	-2.90439588	1.17213640	-0.64385457	
C	1.05399210	-2.45249224	1.72588329	
C	2.37481336	-2.00055954	1.63998552	
C	-1.08075163	2.62352772	-1.50340692	
C	-2.42998557	2.12450921	-1.44121840	
C	-1.19935927	-2.87470422	1.07659370	
C	-2.18391704	-2.69062978	2.08612902	
C	-3.29874367	-3.55591415	2.09430590	
C	-3.43721054	-4.57214224	1.13653930	
C	-2.44816598	-4.74645152	0.15635084	
C	-1.31114299	-3.91241792	0.10803105	

C	-3.32258981	-0.79057487	3.36653352
C	-2.03554260	-1.62759584	3.17918065
C	-1.60639301	-2.27849808	4.52249203
C	4.67416080	2.41494848	2.37777753
C	4.27593164	0.92024059	2.43713503
C	4.55800010	0.34001880	3.85090357
C	4.30180574	-0.87213189	0.58247647
C	4.98705511	0.08645735	1.36918701
C	6.37975763	0.21223874	1.17322565
C	7.05134833	-0.57462906	0.22623412
C	6.34492883	-1.51259244	-0.54459289
C	4.95458879	-1.68297362	-0.38553868
C	-0.78210993	-4.01367044	-2.39206332
C	-0.23332177	-4.17329361	-0.95148777
C	0.41259825	-5.57004834	-0.74776805
C	4.63780956	-2.80216110	-2.67640755
C	4.20821094	-2.75457634	-1.18919481
C	4.40523844	-4.15194950	-0.53693298
C	1.23023958	2.86564945	-1.12019567
C	2.10235338	2.58203226	-2.20441227
C	3.27483750	3.35800948	-2.31825944
C	3.56683297	4.37457217	-1.39655298
C	2.67872037	4.64295563	-0.34372644
C	1.49030578	3.90013953	-0.17975016
C	2.94974301	0.55336091	-3.50344990
C	1.77364334	1.53036219	-3.26984367
C	1.35178515	2.21760033	-4.59708061
C	-5.09415460	2.62313422	2.69486928
C	-4.53323024	2.69853349	1.25317466
C	-4.76547912	4.11825163	0.66409365
C	-4.34689497	0.89295461	-0.59077535
C	-5.13173020	1.62987666	0.33028520
C	-6.51605485	1.36314126	0.33488766
C	-7.06914504	0.40455492	-0.53064047
C	-6.25217146	-0.31399614	-1.41721350
C	-4.85864218	-0.09241735	-1.46607582
C	1.21391716	4.39517717	2.32412823
C	0.51512931	4.25903270	0.94969323
C	-0.25875877	5.56166860	0.60413482
C	-4.27867232	-2.37016010	-2.46163316
C	-3.96988289	-0.85341397	-2.45548577
C	-4.12677433	-0.26185059	-3.88388757
H	0.90241216	-3.29648558	2.39940593
H	3.12118479	-2.46586258	2.27178952
H	-0.98886480	3.57125600	-2.03796215
H	-3.17622797	2.62473578	-2.04558104
H	-4.06309639	-3.43414136	2.85786009
H	-4.30477426	-5.22808550	1.15866180
H	-2.55502298	-5.54324175	-0.57648797
H	-1.24337021	-0.93376583	2.88386312
H	3.19568487	0.85876180	2.26980436
H	-4.15527578	-1.39505394	3.75177819

H	-3.62710154	-0.34522433	2.41355223
H	-3.13687662	0.01952045	4.08440205
H	-2.36595975	-2.98808444	4.87862432
H	-1.46955745	-1.50746647	5.29223113
H	-0.65965249	-2.82405420	4.41905004
H	5.73491795	2.56787495	2.61868402
H	4.08613692	2.98279539	3.10978516
H	4.48091566	2.83772082	1.38489075
H	4.23410460	-0.70579952	3.92729683
H	4.01246520	0.91562017	4.60948765
H	5.62951786	0.38155252	4.09107209
H	6.93833015	0.93318788	1.76341764
H	8.12433305	-0.46028582	0.08911218
H	6.87846877	-2.11555588	-1.27385329
H	0.55306134	-3.42206158	-0.83413681
H	3.13852706	-2.51880371	-1.16793857
H	-1.63259607	-4.68401932	-2.57844344
H	0.00312187	-4.25671899	-3.12178633
H	-1.08813921	-2.97547963	-2.55852554
H	-0.32012214	-6.37557824	-0.89069235
H	0.83253663	-5.67490809	0.26154360
H	1.22276420	-5.72283991	-1.47404038
H	4.55597760	-1.81818218	-3.14983877
H	3.99194311	-3.49927948	-3.22590456
H	5.67169948	-3.15340272	-2.79165680
H	5.46569585	-4.43775856	-0.54183868
H	3.84312845	-4.91382815	-1.09292254
H	4.05460749	-4.16455455	0.50186304
H	3.96076380	3.16381156	-3.13844149
H	4.47793106	4.95910144	-1.50131154
H	2.90861217	5.43839989	0.36008261
H	0.92797198	0.92236274	-2.93152670
H	-3.45174132	2.53232408	1.32570337
H	3.83227681	1.05712461	-3.92105703
H	2.64427134	-0.23020824	-4.20901886
H	3.23342881	0.07591622	-2.56020022
H	0.48595034	2.87832160	-4.45185429
H	1.07763955	1.45973428	-5.34264098
H	2.16907848	2.82412025	-5.01104975
H	-6.15934637	2.88570391	2.73308268
H	-4.55741913	3.33257446	3.33749721
H	-4.97100066	1.62089444	3.11813851
H	-4.32606562	4.22240279	-0.33630692
H	-4.31183808	4.87809059	1.31352040
H	-5.83859134	4.33568706	0.58290601
H	-7.16253191	1.90082199	1.02210474
H	-8.13971697	0.21475614	-0.50971713
H	-6.69570630	-1.05848249	-2.07139863
H	-0.20836842	3.44519643	1.05702984
H	-2.91631673	-0.74222084	-2.16871130
H	1.95795727	5.20284728	2.33215786
H	1.70624362	3.45807272	2.60115396

H	0.46805507	4.62090042	3.09757165
H	-0.97903192	5.79898888	1.39875174
H	-0.81117829	5.47036436	-0.34112782
H	0.42765106	6.41312210	0.50441256
H	-4.16575601	-2.80242529	-1.46087296
H	-3.57546324	-2.88196331	-3.12859963
H	-5.29446643	-2.58299542	-2.82206446
H	-3.86175224	0.80351402	-3.91347827
H	-5.15876040	-0.36411975	-4.24695426
H	-3.46201142	-0.78947469	-4.57868622
O	-0.10972616	1.15832842	1.78481168
O	0.89915635	0.96040540	2.69062844
Hf	-0.02838296	-0.11377801	-0.14069391

Oxo Complex with Adsorbed Oxygen Molecule to Dioxo Complex (Propene)

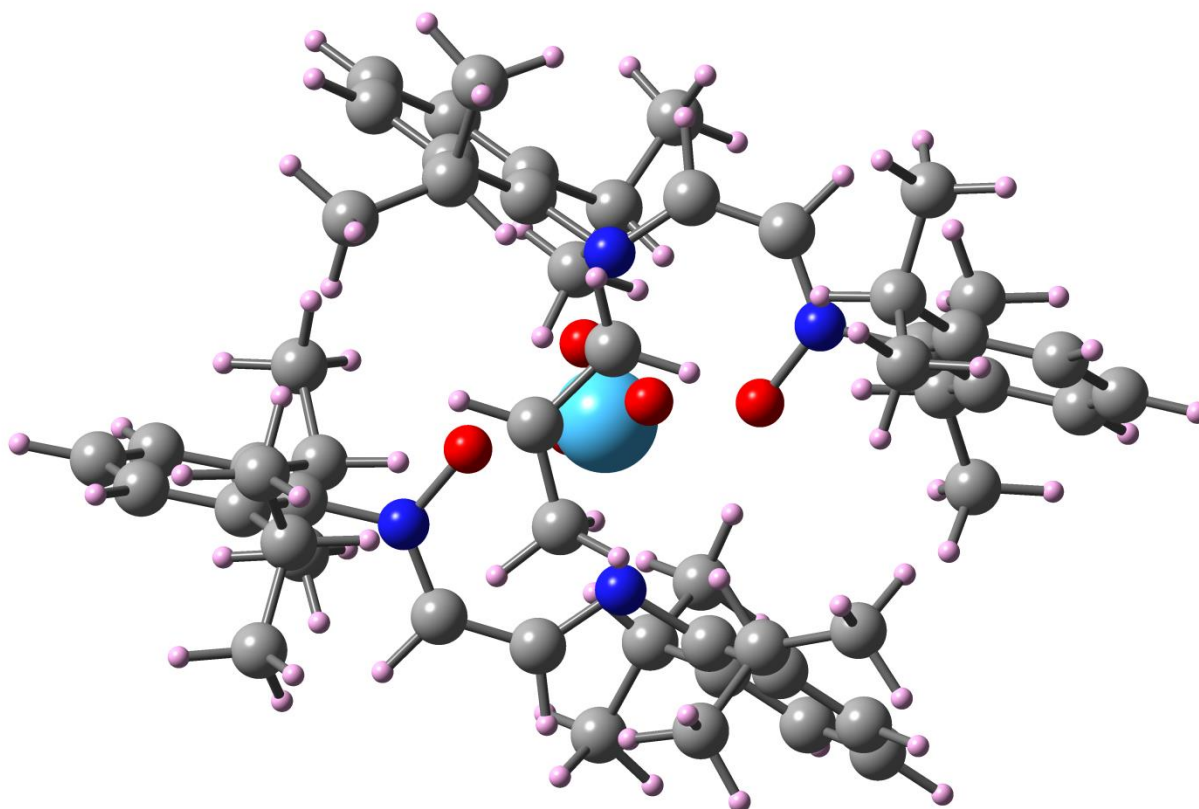


Fig. S144: NCCNO Oxo Complex with Adsorbed Oxygen Molecule to Dioxo Complex (Propene)

E	E_{zp}	H	G	<i>f</i>
-2786.4480	-2785.2156	-2785.1411	-2785.3294	-126
O	1.99571715	0.39786403	-0.07999301	
O	-1.91488815	-0.67389605	0.47149904	
O	-0.36305303	-0.05789700	3.18943224	
O	0.53928304	-0.46373804	2.13177916	
N	0.23059402	-2.08552816	-0.92793307	
N	-2.74662321	-1.53689312	-0.25647902	
N	-0.14410401	2.26808618	0.45755204	
N	2.76998521	1.29125610	0.64179005	
C	-0.85704006	-2.85924922	-1.18981209	
C	-2.21020117	-2.60060220	-0.91996007	
C	0.93528707	2.93479123	0.94480207	
C	2.25469117	2.48232419	1.06679908	
C	1.46036211	-2.56960720	-1.55295812	
C	1.63256013	-2.43054718	-2.96155423	
C	2.80971121	-2.95196922	-3.54376927	
C	3.79481129	-3.57906827	-2.77023821	
C	3.61483028	-3.69780728	-1.38287311	

C	2.45360819	-3.20528925	-0.75477606
C	1.22868809	-0.56586204	-4.65229336
C	0.60206105	-1.74923513	-3.87188630
C	-0.04201800	-2.76839621	-4.84872437
C	-4.33567433	1.54606312	-2.64868820
C	-3.97910230	0.06518601	-2.37334818
C	-4.19419332	-0.79266106	-3.65071828
C	-4.17348032	-1.29033010	-0.18188601
C	-4.78004536	-0.51610204	-1.20514509
C	-6.17798949	-0.32936903	-1.13266909
C	-6.93205151	-0.87783507	-0.08410801
C	-6.30344948	-1.62869912	0.92282807
C	-4.91080537	-1.84503414	0.89624007
C	3.53816527	-3.41662826	1.56968012
C	2.23237217	-3.42644326	0.74295506
C	1.46424811	-4.75791236	0.97738908
C	-4.62895335	-2.23584517	3.40685626
C	-4.23841132	-2.69345120	1.97880915
C	-4.56550935	-4.19894432	1.78233514
C	-1.29441410	3.12535624	0.17122601
C	-2.35667418	3.22600024	1.11161009
C	-3.43932226	4.08284331	0.82007506
C	-3.47382526	4.82927637	-0.36665103
C	-2.41514518	4.72566836	-1.28098310
C	-1.31183810	3.88026529	-1.03820408
C	-3.63096228	1.73924313	2.76230221
C	-2.31524818	2.49212819	2.45320619
C	-1.96023515	3.47761327	3.60035427
C	4.87996537	0.36127903	-2.89955922
C	4.42110734	1.32194510	-1.77671014
C	4.81719137	2.78758221	-2.11068816
C	4.17644132	0.96209407	0.77178806
C	4.97722638	0.93413507	-0.40249303
C	6.34367050	0.62209005	-0.25271702
C	6.89631051	0.36369703	1.01196408
C	6.08771947	0.41496603	2.15679916
C	4.70941236	0.70544005	2.06376816
C	-0.67903105	3.42944526	-3.47165327
C	-0.17367301	3.83579029	-2.06485116
C	0.58213104	5.19170139	-2.10756516
C	4.02508131	-0.49619604	4.21817632
C	3.86418930	0.77208406	3.34237625
C	4.21951832	2.03764816	4.17042932
H	-0.68752205	-3.79072529	-1.73246213
H	-2.94442323	-3.29820125	-1.30661910
H	0.78998706	3.97435331	1.24384409
H	2.98591123	3.15262024	1.50162112
H	2.95296323	-2.85859522	-4.61770335
H	4.69365936	-3.97187730	-3.24052725
H	4.38308934	-4.18289232	-0.78763006
H	-0.18331101	-1.30697610	-3.25442225
H	-2.91078622	0.03972000	-2.13285816

H	2.04257616	-0.88895407	-5.31729640
H	1.61512512	0.18356601	-3.95326130
H	0.45990604	-0.07890001	-5.26654640
H	0.70495905	-3.20782924	-5.52466144
H	-0.80247006	-2.27065317	-5.46572940
H	-0.52810904	-3.59240027	-4.30918633
H	-5.36830639	1.66602913	-3.00613323
H	-3.66577428	1.94282815	-3.42084726
H	-4.20508632	2.15997616	-1.75058013
H	-3.89086430	-1.83540614	-3.49034527
H	-3.59133227	-0.38977903	-4.47447634
H	-5.24849340	-0.78869306	-3.96239430
H	-6.67635153	0.25431902	-1.90136115
H	-8.00778763	-0.72002005	-0.05007200
H	-6.89923951	-2.04711215	1.73023813
H	1.60664712	-2.60230420	1.10249708
H	-3.15614224	-2.56605319	1.87210514
H	4.17293432	-4.28395932	1.34471310
H	3.30232525	-3.46338626	2.64232220
H	4.12083632	-2.50693119	1.38289511
H	2.03689816	-5.60682944	0.58018905
H	0.48682704	-4.74726136	0.48118304
H	1.30321210	-4.93433738	2.05090415
H	-4.41156634	-1.17056809	3.55237227
H	-4.07840431	-2.82008822	4.15894332
H	-5.69775442	-2.38838418	3.60285328
H	-5.64556643	-4.37927833	1.86147314
H	-4.06420731	-4.80937537	2.54660720
H	-4.23733032	-4.55161635	0.79692906
H	-4.25682832	4.17212432	1.53157712
H	-4.31441133	5.48747943	-0.57523804
H	-2.44376619	5.30871542	-2.19851117
H	-1.51835812	1.74679813	2.40583618
H	3.33043825	1.26709010	-1.73444313
H	-4.48468134	2.42262318	2.86212022
H	-3.53743527	1.19288509	3.71297328
H	-3.85628629	1.01748708	1.96995315
H	-0.99555708	3.96840930	3.41725626
H	-1.89716615	2.94693022	4.56185435
H	-2.72197221	4.26296932	3.69883928
H	5.96477948	0.41053603	-3.06661723
H	4.38927533	0.63434905	-3.84261629
H	4.60959835	-0.67462405	-2.66809721
H	4.44973634	3.48594027	-1.34762610
H	4.38662134	3.08366324	-3.07635624
H	5.90845047	2.89810422	-2.17578017
H	6.98228451	0.59154505	-1.13089009
H	7.95436862	0.12958301	1.10468208
H	6.52946648	0.21927802	3.13056724
H	0.53329504	3.06017623	-1.76159214
H	2.80999422	0.83536406	3.05336123
H	-1.44709711	4.11800331	-3.85054529

H	-1.07980108	2.41208819	-3.42605326
H	0.15723901	3.43592126	-4.18523132
H	1.42155611	5.13551239	-2.81411422
H	0.98301407	5.46051944	-1.12079408
H	-0.07767501	6.00730247	-2.43364418
H	3.73680128	-1.39595911	3.66433628
H	3.39532826	-0.41615203	5.11678539
H	5.05810038	-0.62854705	4.56375435
H	4.08634231	2.95533823	3.58466527
H	5.26432140	2.00682516	4.50689334
H	3.57940927	2.10898116	5.06061538
O	-0.59517705	0.53557804	-1.94271515
C	-0.93909407	-1.61687612	4.15344432
H	-1.98183915	-1.40462911	4.36976434
C	0.06598700	-0.61074405	4.55129435
H	-0.19335701	0.11946101	5.31571543
H	1.11641208	-0.89168807	4.52508435
C	-0.54025704	-2.77445821	3.34334726
H	-0.10732301	-2.32734518	2.40665219
H	0.28410102	-3.34354425	3.79143029
H	-1.36930910	-3.43194826	3.07987323
Hf	-0.09501901	0.10649601	-0.25052502

Oxo Complex with Adsorbed Oxygen Molecule to Dioxo Complex (Ethylene)

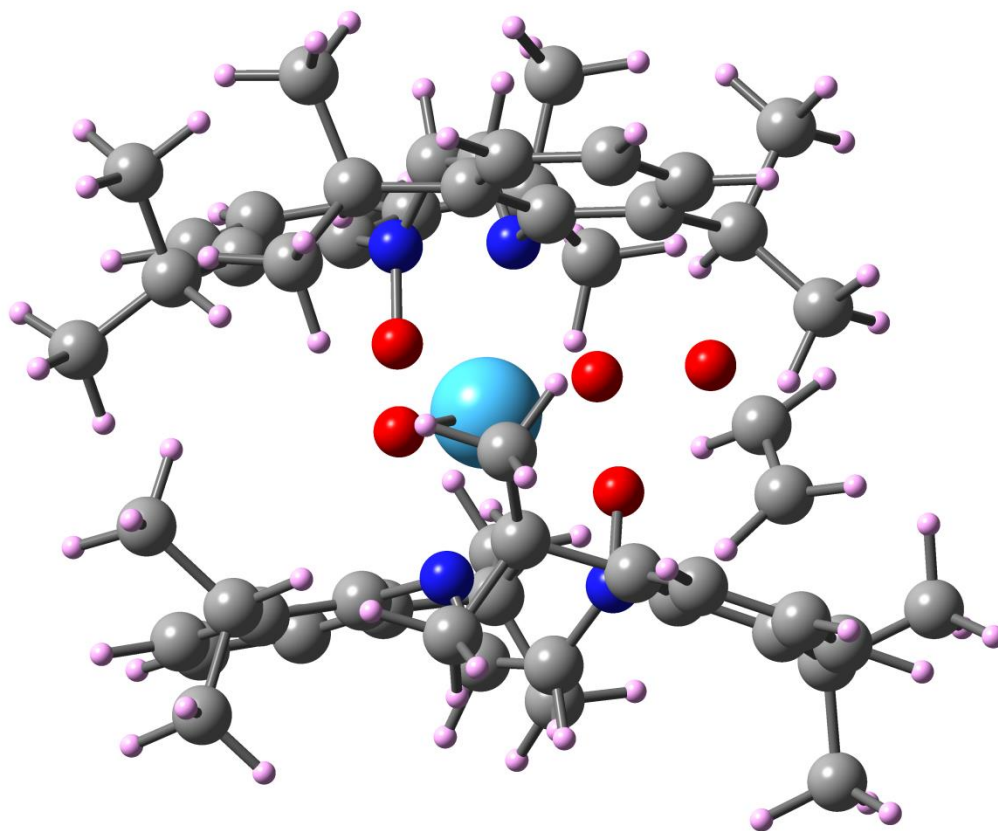


Fig. S145: NCCNO Oxo Complex with Adsorbed Oxygen Molecule to Dioxo Complex (Ethylene)

E	E_{zp}	H	G	<i>f</i>
-2747.1242	-2745.9211	-2745.8484	-2746.0321	-570

O	2.00489015	0.40576403	-0.10621901
O	-1.92371315	-0.68738605	0.55847404
O	-0.16580501	-0.20183902	3.25308725
O	0.65658205	-0.25643802	2.03895616
N	0.21180002	-2.13203816	-0.76967006
N	-2.76128221	-1.54246012	-0.17595401
N	-0.12663101	2.29559217	0.39100803
N	2.80109421	1.35416010	0.49356004
C	-0.87128606	-2.89972222	-1.04884608
C	-2.22857617	-2.61734020	-0.82109206
C	0.96072407	2.99596223	0.77494506
C	2.29428117	2.55669220	0.86998907
C	1.47110811	-2.67294120	-1.27186610
C	1.76391013	-2.58681720	-2.66266420
C	2.97056723	-3.15901524	-3.12388324
C	3.86358529	-3.78769129	-2.24609417
C	3.56235227	-3.85368929	-0.87548507
C	2.36896418	-3.30467125	-0.36562103

C	1.54443112	-0.77489206	-4.44520134
C	0.82657306	-1.90998615	-3.67198128
C	0.22704902	-2.94673723	-4.65885835
C	-4.36044833	1.49513011	-2.70046120
C	-3.95727630	0.04965400	-2.32451318
C	-4.09996032	-0.88528907	-3.55835427
C	-4.19070532	-1.28671710	-0.12312901
C	-4.77478536	-0.50257004	-1.15373209
C	-6.17039347	-0.29596902	-1.09840108
C	-6.94799552	-0.84112306	-0.06569900
C	-6.34593950	-1.61711912	0.93676107
C	-4.95597538	-1.85406514	0.92934507
C	3.25445125	-3.46173626	2.04304816
C	2.01526615	-3.43787726	1.11891109
C	1.15067609	-4.70673636	1.36444410
C	-4.72522336	-2.30330618	3.43545226
C	-4.33179233	-2.74768721	2.00397815
C	-4.71566736	-4.23491633	1.77294314
C	-1.31925110	3.10458424	0.15319501
C	-2.33436218	3.16327924	1.14737809
C	-3.46877027	3.96504530	0.90082107
C	-3.59586527	4.69381936	-0.29136702
C	-2.57991620	4.63099835	-1.25683309
C	-1.42637311	3.84266829	-1.06071208
C	-3.44335226	1.65621413	2.89855522
C	-2.18101016	2.45376019	2.49509819
C	-1.79612314	3.47379026	3.60192227
C	5.13630439	0.20894202	-2.95575323
C	4.48107634	1.09944809	-1.87538814
C	4.65664636	2.60300120	-2.23315017
C	4.19665132	1.00138107	0.68627105
C	5.01737138	0.83661907	-0.46362304
C	6.37089349	0.50765304	-0.25290702
C	6.89014353	0.36357703	1.04484808
C	6.05968948	0.53956004	2.16031716
C	4.69019836	0.85039107	2.00975116
C	-0.88346207	3.33520626	-3.50487627
C	-0.33857203	3.83143929	-2.14203116
C	0.32240402	5.23016540	-2.27518617
C	3.93419830	-0.17718701	4.22664832
C	3.81572029	1.02702908	3.25869825
C	4.17305632	2.34230718	4.00360031
H	-0.69586105	-3.84852230	-1.55835912
H	-2.96331523	-3.30881425	-1.21701409
H	0.82296706	4.05202731	1.01431908
H	3.03342823	3.25539125	1.24126510
H	3.20926325	-3.10652424	-4.18363032
H	4.78636036	-4.22344732	-2.62310120
H	4.26289732	-4.33834733	-0.20173602
H	0.00828200	-1.42702511	-3.13141124
H	-2.89589222	0.07455601	-2.05378616
H	2.39384818	-1.14751609	-5.03495138

H	1.90575415	-0.01038800	-3.74855428
H	0.83841906	-0.29017002	-5.13191339
H	1.00959707	-3.43171226	-5.25912240
H	-0.46940804	-2.45207819	-5.34933639
H	-0.32318202	-3.73601729	-4.12913232
H	-5.37793641	1.54981612	-3.11310324
H	-3.67212128	1.87495014	-3.46420627
H	-4.29847433	2.16514117	-1.83568014
H	-3.76035829	-1.90415315	-3.33285325
H	-3.48719126	-0.50335004	-4.38461234
H	-5.14386240	-0.94020607	-3.89873530
H	-6.64932153	0.29898702	-1.87017914
H	-8.02132663	-0.66601305	-0.04456300
H	-6.95991354	-2.04228516	1.72663513
H	1.41579911	-2.55969519	1.38772411
H	-3.24398825	-2.66933421	1.91406615
H	3.84360329	-4.37921634	1.91366815
H	2.94143623	-3.43189726	3.09702324
H	3.90951630	-2.60383320	1.85174414
H	1.70500313	-5.61261144	1.08352508
H	0.22528702	-4.68184636	0.77759906
H	0.87976407	-4.79468236	2.42738919
H	-4.47317834	-1.24950409	3.60719028
H	-4.20680032	-2.92049122	4.18299232
H	-5.80183146	-2.42052919	3.61126627
H	-5.80232646	-4.37501033	1.84028514
H	-4.24295232	-4.87811537	2.52771019
H	-4.39410934	-4.57966435	0.78240006
H	-4.25367533	4.02506331	1.65069313
H	-4.47636234	5.30859339	-0.46463804
H	-2.68282920	5.19927140	-2.17828917
H	-1.35632911	1.74078313	2.41471218
H	3.41036226	0.87527107	-1.87583714
H	-4.31319333	2.30923118	3.05020323
H	-3.26209425	1.12650209	3.84523930
H	-3.69324828	0.91767707	2.12935716
H	-0.86802407	4.00295931	3.34954226
H	-1.64482113	2.96015923	4.56156435
H	-2.58476120	4.22636832	3.73861429
H	6.19777945	0.45017703	-3.10352624
H	4.62967335	0.36662403	-3.91610030
H	5.04921139	-0.85347206	-2.70056520
H	4.14095532	3.25126325	-1.51381911
H	4.23954632	2.80525721	-3.22836325
H	5.71948842	2.88130322	-2.24411817
H	7.02659453	0.36976403	-1.10691708
H	7.93991562	0.11528801	1.18373109
H	6.47406850	0.42243703	3.15835424
H	0.43373003	3.11615824	-1.84826914
H	2.76817721	1.07986408	2.94756323
H	-1.72009313	3.95134030	-3.86273030
H	-1.20354109	2.29347117	-3.40293726

H	-0.08814301	3.37732126	-4.26266333
H	1.13032609	5.19822540	-3.01880523
H	0.74867406	5.56835841	-1.32072810
H	-0.40411203	5.98653046	-2.60187320
H	3.68616928	-1.11463609	3.71809529
H	3.24372925	-0.04299100	5.07119439
H	4.94525538	-0.27357802	4.64323935
H	4.05723031	3.22137124	3.35732526
H	5.21246840	2.32531718	4.35763233
H	3.51973227	2.47639819	4.87610437
O	-0.62677905	0.45528603	-1.89220215
C	-1.12932409	-1.81517214	3.61481728
H	-2.06546416	-1.55828212	4.09637431
C	0.15339801	-1.38352611	4.17908732
H	0.17807901	-1.03457308	5.21040340
H	1.06695808	-1.86514314	3.84115329
Hf	-0.09433501	0.08394201	-0.18925601
H	-1.14916109	-2.30014917	2.64661720

Propene Chemisorbed on Dioxo Complex forming Octahedral Complex to Octahedral Complex with Transferred Allylic Hydrogen

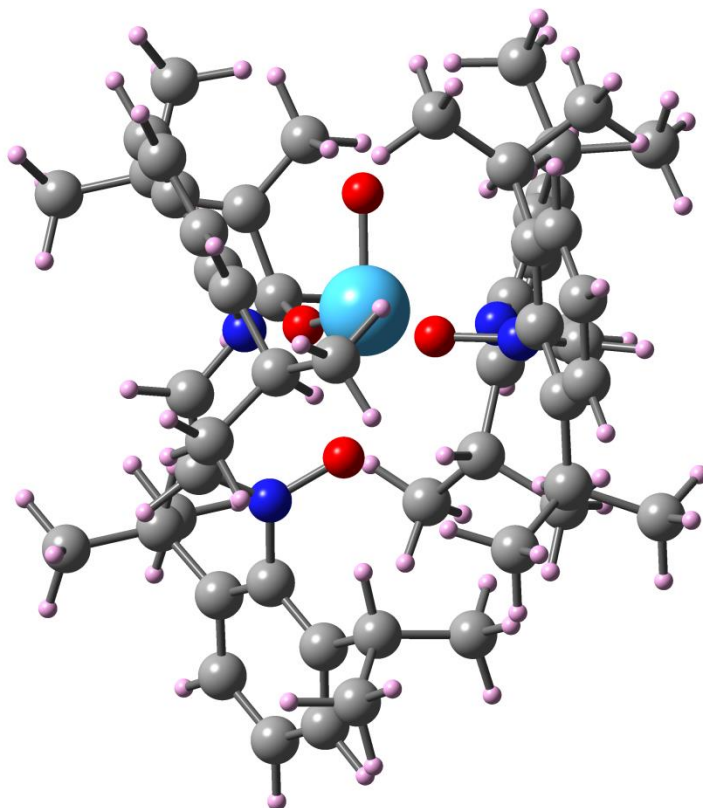


Fig. S146: NCCNO Propene Chemisorbed on Dioxo Complex forming Octahedral Complex to Octahedral Complex with Transferred Allylic Hydrogen

E	E_{ZP}	H	G	<i>f</i>
-2711.3382	-2710.1098	-2710.0368	-2710.2203	-432

N	-0.24148883	1.54501419	-1.77173042
N	0.25150687	-0.66624986	2.20925266
C	0.56318455	1.20677204	-2.81230095
C	1.68445126	0.37060066	-2.81162641
C	-0.65706928	-1.55340633	2.63361551
C	-1.80578042	-2.05677313	1.97238845
C	-1.11699253	2.67986809	-2.05407406
C	-2.48159719	2.44999474	-2.38975406
C	-3.30732415	3.56582520	-2.64348482
C	-2.80058638	4.87391035	-2.58302595
C	-1.44593666	5.08206357	-2.28449122
C	-0.57626234	4.00089014	-2.02124525
C	-4.51488511	0.88792074	-2.17472698
C	-3.02393932	1.02729548	-2.55793380
C	-2.81345928	0.54308365	-4.02043302
C	2.46313519	-4.38685256	-2.49651942

C	2.55291918	-2.93981977	-3.04391481
C	2.67987642	-2.95182456	-4.59127020
C	3.51205398	-0.90491318	-1.77059309
C	3.70497700	-2.15735290	-2.40503062
C	5.01953419	-2.66829104	-2.45263811
C	6.08800348	-1.96551835	-1.87423010
C	5.86357375	-0.73334634	-1.23837489
C	4.57108679	-0.17242168	-1.17303384
C	1.20460574	5.44386570	-0.82347592
C	0.91931213	4.27280863	-1.79518161
C	1.62001308	4.55382294	-3.15556230
C	4.88789309	1.23055276	0.93938634
C	4.35429657	1.19395049	-0.51475549
C	5.00215590	2.31650562	-1.36968922
C	1.43393828	-0.59186784	3.07695320
C	1.52004889	0.42269781	4.06751555
C	2.64371010	0.43122211	4.92049415
C	3.65239791	-0.53502622	4.80533357
C	3.54642045	-1.53495606	3.82789203
C	2.44358615	-1.59059538	2.94890635
C	0.94508358	2.88318998	4.43420296
C	0.40112577	1.44272472	4.28830009
C	-0.46206300	1.04286162	5.51674585
C	-1.60040073	-3.30777998	-2.91588875
C	-1.79174442	-3.82358631	-1.46574309
C	-1.57142513	-5.35652585	-1.38285015
C	-3.35303584	-2.49245546	0.12475721
C	-3.17106177	-3.42596992	-0.93002056
C	-4.32553358	-4.01792944	-1.48153165
C	-5.60395172	-3.71011598	-0.99184988
C	-5.75123783	-2.79694284	0.06226226
C	-4.63500484	-2.15610377	0.64144253
C	3.72618514	-3.06919144	1.28971443
C	2.35539495	-2.73101701	1.92435462
C	1.76615722	-4.01793247	2.56918734
C	-5.94437192	-0.10725475	1.45526652
C	-4.86094846	-1.16365451	1.79162601
C	-5.25294193	-1.91344777	3.09547013
H	0.36758345	1.68695445	-3.77150318
H	2.26746400	0.28524009	-3.72037593
H	-0.50672738	-1.99520874	3.62091978
H	-2.43980553	-2.73885530	2.52311615
H	-4.35190923	3.41118164	-2.89878299
H	-3.45285592	5.72168302	-2.78113348
H	-1.05498401	6.09603100	-2.26206162
H	-2.45013200	0.36559869	-1.90109103
H	1.61394088	-2.43563551	-2.78956450
H	-5.17494752	1.38166252	-2.90122794
H	-4.71171020	1.32157154	-1.18741540
H	-4.79496651	-0.17279358	-2.14395141
H	-3.33679250	1.20155467	-4.72750360
H	-3.20701820	-0.47494111	-4.14685165

H	-1.75101320	0.53097627	-4.28989184
H	3.36658793	-4.96576717	-2.72762250
H	1.61034001	-4.91003807	-2.94949950
H	2.32792551	-4.38913148	-1.40834427
H	2.70441586	-1.93351575	-4.99944351
H	1.82819720	-3.47811902	-5.04268494
H	3.59915978	-3.46165775	-4.90873596
H	5.20690720	-3.62271048	-2.93818771
H	7.09378978	-2.37719296	-1.91809853
H	6.69912928	-0.19932428	-0.79360522
H	1.36401413	3.38044540	-1.34538338
H	3.28194849	1.39754719	-0.45219160
H	0.79645621	6.39688234	-1.18681379
H	2.28990874	5.57186691	-0.71453124
H	0.79578418	5.24097163	0.16915006
H	1.22353277	5.46962230	-3.61561752
H	1.47557544	3.73333397	-3.86845489
H	2.69992567	4.68875447	-3.00588020
H	4.40963444	0.46010221	1.55401153
H	4.65608767	2.20336615	1.38976257
H	5.97660527	1.08582207	0.98243383
H	6.09064778	2.18678327	-1.44343516
H	4.80691144	3.29448031	-0.91086471
H	4.59304777	2.32967580	-2.38858610
H	2.72473788	1.19873151	5.68537326
H	4.51084777	-0.51248539	5.47284271
H	4.33109132	-2.28155810	3.74560736
H	-0.24291771	1.43225197	3.40453267
H	-1.02315414	-3.34229795	-0.85469883
H	1.60071531	2.99172356	5.30829997
H	0.11424200	3.59037279	4.56205193
H	1.50037314	3.15955574	3.53210525
H	-0.89720943	0.04181077	5.39410801
H	-1.28583039	1.75697283	5.65740883
H	0.13861747	1.03613426	6.43638801
H	-2.35222671	-3.73237977	-3.59505689
H	-0.60868114	-3.59185639	-3.29124163
H	-1.67927967	-2.21604822	-2.94775442
H	-1.70546860	-5.72432975	-0.35737577
H	-0.55123841	-5.60489122	-1.70285157
H	-2.26613576	-5.90585258	-2.03142818
H	-4.22082114	-4.73491805	-2.29137732
H	-6.48147640	-4.18189145	-1.42730553
H	-6.74648800	-2.56731836	0.43228588
H	1.69128900	-2.40780885	1.11502639
H	-3.92908910	-0.61902566	1.97601688
H	4.40895036	-3.53158140	2.01505699
H	4.21105196	-2.17799544	0.88074538
H	3.59205385	-3.78630714	0.47036539
H	1.72031782	-4.82879621	1.82883791
H	0.75377729	-3.85995757	2.95827031
H	2.39709318	-4.35571158	3.40278149

H	-5.69886558	0.43787085	0.53847281
H	-6.02321218	0.61805457	2.27602764
H	-6.93451976	-0.56251651	1.32585183
H	-4.49718203	-2.65152485	3.39220314
H	-6.20304392	-2.44833481	2.96660613
H	-5.37418290	-1.20184869	3.92265538
O	0.88244783	2.18663993	1.04874220
O	-1.89489027	1.35451127	0.92835023
O	-1.42116681	-1.10108350	-0.15184859
O	1.50392763	-0.37065696	-0.55146322
N	-2.16342582	-1.85825655	0.68649907
N	2.18456809	-0.31839138	-1.74880785
C	-2.15913497	3.28847846	2.25577323
H	-2.25488881	3.04838218	3.31631735
C	-2.85088244	2.39330157	1.26787673
H	-3.74943585	1.92953989	1.69525625
H	-3.12626592	2.93977803	0.35538420
C	-1.09179684	4.18621485	1.81171680
H	-1.33694198	4.68890492	0.86714639
H	-0.76922728	4.90467237	2.57284154
H	-0.18178550	3.52237949	1.55882035
Hf	-0.07199214	0.75038178	0.36862521

13. Transition States for ONCCNO Complex

13.1 Singlet Geometries

Bisperoxo Complex to Oxo Peroxo Complex

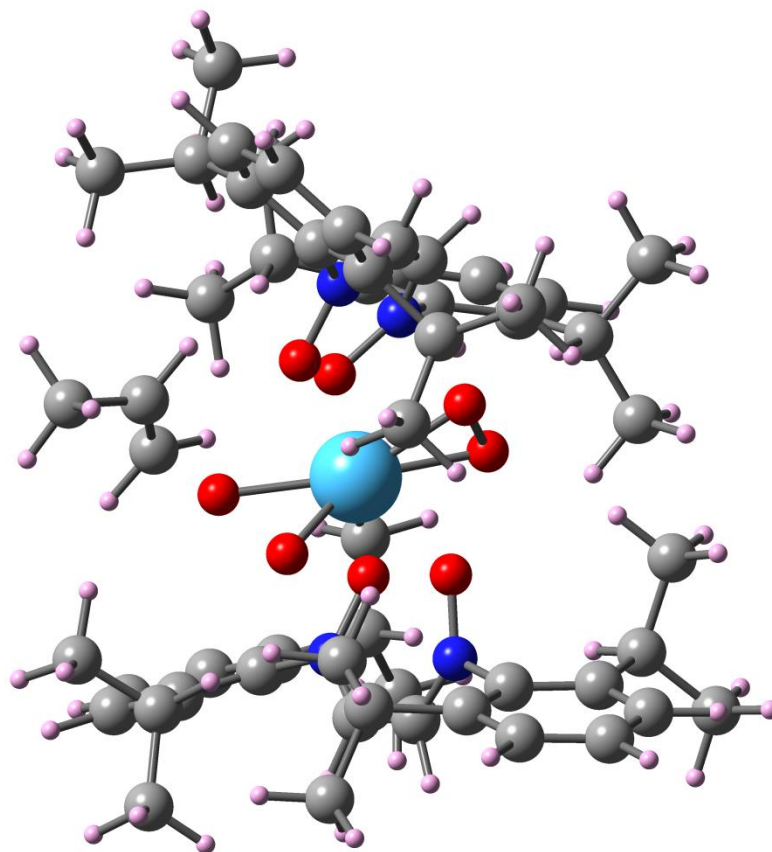


Fig. S147: ONCCNO Bisperoxo Complex to Oxo Peroxo Complex

E	E_{zp}	H	G	<i>f</i>
-3011.9477	-3010.7031	-3010.6252	-3010.8196	-479
O	-1.94198929	0.79113182	-0.05989137	
O	1.89038769	-1.05124837	-0.94168069	
O	0.37929755	1.24588548	-1.68538905	
N	-0.31996232	-3.04647000	0.67954418	
N	2.62096756	-2.05480093	-0.42496797	
N	0.37473556	3.24236456	0.50035997	
N	-2.54605050	1.95055581	-0.41636887	
C	0.93218916	-3.49425112	0.83930070	
C	2.18893562	-3.08949891	0.31536705	
C	-0.76332330	3.74619691	-0.01254404	
C	-2.01129918	3.18468673	-0.37208964	
C	-1.41134452	-3.64323238	1.45459392	
C	-1.40029976	-3.53109399	2.87401318	
C	-2.46127831	-4.14857613	3.57213800	
C	-3.48590029	-4.83126862	2.90300797	

C	-3.46564916	-4.92568013	1.50386008
C	-2.42787612	-4.34283106	0.74925807
C	-0.93022039	-1.74824124	4.63643445
C	-0.31742249	-2.80466875	3.68327709
C	0.54173366	-3.82408782	4.48159841
C	4.79918386	0.55214133	1.81506961
C	4.43166140	-0.94097219	1.61282178
C	4.99587320	-1.80818346	2.76868897
C	4.05180942	-1.96091638	-0.74046621
C	4.92141145	-1.44397507	0.25023954
C	6.29292139	-1.37724328	-0.07961620
C	6.75545893	-1.77795392	-1.34231844
C	5.85440872	-2.24438681	-2.31416875
C	4.47556744	-2.34354744	-2.03659617
C	-3.69530513	-3.95665876	-1.41938728
C	-2.41536512	-4.54395614	-0.76967738
C	-2.25356132	-6.04536175	-1.12930034
C	3.21449105	-1.59456071	-4.08786876
C	3.48806919	-2.78058881	-3.12162666
C	3.96299169	-4.03734626	-3.89121688
C	1.47770808	4.14515762	0.84949072
C	2.37493154	4.52263463	-0.17589521
C	3.42726632	5.39087358	0.18935773
C	3.57901131	5.82357271	1.51579624
C	2.68979729	5.39029910	2.51466061
C	1.61453124	4.53205773	2.20527195
C	3.54645223	3.30404943	-2.07661780
C	2.24653426	4.01165514	-1.61534983
C	1.87423403	5.16485157	-2.58429474
C	-4.32673255	-0.51351121	2.01445514
C	-4.27375119	1.01612296	1.76192500
C	-5.04021057	1.79030757	2.86570857
C	-3.98229400	1.81134481	-0.69737872
C	-4.80688087	1.34837926	0.36338269
C	-6.18399274	1.20621088	0.09517181
C	-6.71853458	1.52997122	-1.16107805
C	-5.87973128	1.99858677	-2.18233999
C	-4.48937321	2.14216804	-1.98330971
C	1.33171216	2.73300979	3.96034099
C	0.69095332	3.98678216	3.29899695
C	0.31954723	5.04999455	4.36041553
C	-3.90867112	1.90091190	-4.46611863
C	-3.62183294	2.65646626	-3.14192025
C	-3.83758868	4.17960268	-3.36537951
H	0.99688029	-4.34783206	1.50412214
H	3.00224056	-3.74900895	0.59840677
H	-0.72204427	4.82367905	-0.12358021
H	-2.73366772	3.93820205	-0.66345936
H	-2.48498982	-4.08079430	4.65592158
H	-4.29258450	-5.29177969	3.46862826
H	-4.25370776	-5.47080892	0.99134960
H	0.33165161	-2.24417618	3.00756565

H	3.33899781	-0.99236197	1.65730002
H	-1.59926673	-2.19456414	5.38580454
H	-1.47160561	-0.99749294	4.05392600
H	-0.12303096	-1.22935667	5.16958347
H	-0.06171303	-4.36407469	5.22415060
H	1.34323153	-3.29799732	5.01635484
H	1.00848569	-4.57551929	3.82875855
H	5.88655719	0.70804580	1.84206179
H	4.37877048	0.91016490	2.76303637
H	4.38036777	1.16887700	1.01146187
H	4.70769440	-2.86269848	2.66054650
H	4.60691714	-1.44836487	3.72980556
H	6.09282704	-1.76374201	2.80917515
H	6.99764483	-0.99431889	0.65374296
H	7.81603306	-1.71468156	-1.57503706
H	6.22455524	-2.53077320	-3.29462506
H	-1.55996875	-4.00593436	-1.18625916
H	2.53072152	-3.02461073	-2.64600341
H	-4.59842469	-4.46558668	-1.05805487
H	-3.66111717	-4.07545643	-2.51051516
H	-3.79405318	-2.88864145	-1.19192447
H	-3.09951673	-6.64083977	-0.76195754
H	-1.33584146	-6.46332599	-0.69532244
H	-2.20286409	-6.17008570	-2.21932036
H	2.76140836	-0.75837340	-3.54552330
H	2.51991112	-1.90566970	-4.87926937
H	4.14444939	-1.25342662	-4.56335699
H	4.86945792	-3.83955311	-4.47780816
H	3.18405811	-4.36002778	-4.59458325
H	4.17619333	-4.87194545	-3.21033149
H	4.13753530	5.71414457	-0.56686826
H	4.39899121	6.48909216	1.77642471
H	2.83462515	5.71848372	3.53970383
H	1.45727631	3.25221701	-1.66938476
H	-3.22079136	1.30302680	1.82285303
H	4.40226328	3.99250487	-2.11209727
H	3.40056985	2.88762076	-3.08099317
H	3.79570591	2.47298031	-1.40685383
H	0.92799053	5.64345305	-2.29720876
H	1.76057807	4.77514010	-3.60410319
H	2.65108423	5.94179784	-2.60188090
H	-5.35720393	-0.89197089	1.96262936
H	-3.92658725	-0.74486359	3.00947153
H	-3.71673878	-1.04562872	1.27768492
H	-5.01397188	2.87411354	2.69091575
H	-4.57957231	1.59137478	3.84200996
H	-6.09270660	1.48384467	2.92853838
H	-6.84282382	0.85134570	0.88267993
H	-7.78477583	1.41910092	-1.34346194
H	-6.30561149	2.24424322	-3.15106463
H	-0.24269066	3.65032011	2.83079484
H	-2.56636498	2.49625872	-2.89518053

H	2.30537290	2.98456387	4.40438576
H	1.46395253	1.93013359	3.22805730
H	0.67715454	2.35591137	4.75731333
H	-0.42443895	4.63581037	5.05307821
H	-0.10408528	5.95325352	3.90150685
H	1.18900640	5.34955579	4.96031084
H	-3.84722000	0.81532427	-4.33531597
H	-3.17708234	2.19717027	-5.22906161
H	-4.90585763	2.13780742	-4.85794331
H	-3.61196294	4.76958725	-2.46792082
H	-4.87908230	4.38816705	-3.64321827
H	-3.19070304	4.53950083	-4.17598277
O	1.12165070	-0.55819770	1.55614549
O	-0.32001202	-0.21377134	1.92419162
C	-1.54288534	-0.35520936	-3.18158840
H	-2.38342969	-0.05323467	-2.55269728
C	-1.43320894	-1.78334742	-3.45513614
H	-1.83491111	-2.46847431	-2.71777389
O	-0.25878492	-0.31798159	-2.37229125
H	-1.40700556	0.30749565	-4.04114068
C	-0.64589091	-2.33056752	-4.60840085
H	0.10794134	-3.06118671	-4.27955314
H	-1.30352920	-2.85933889	-5.32237423
H	-0.12976967	-1.53099885	-5.15152448
Hf	0.08674603	-0.01758138	-0.14665969
O	0.62368614	1.96302674	0.74550578
O	-0.64587370	-2.10114400	-0.25005897

Oxo Peroxo Complex to Peroxo η^2 -Ozone Complex

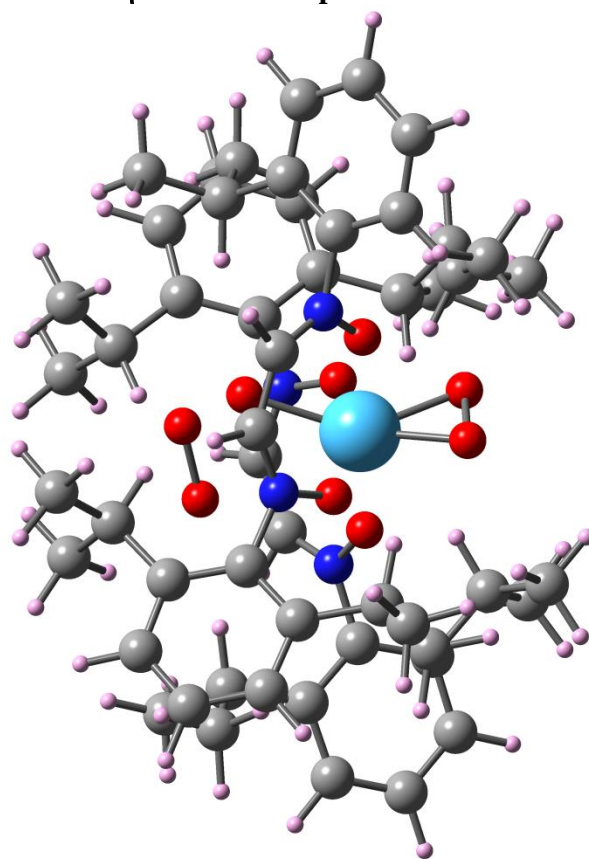


Fig. S148: ONCCNO Oxo Peroxo Complex to Peroxo η^2 -Ozone Complex

E	E_{ZP}	H	G	<i>f</i>
-2969.2298	-2968.0641	-2967.9899	-2968.1769	-82
O	-0.75253251	-1.97298711	-0.36387675	
O	0.70910822	2.01311219	-0.54786708	
O	0.80519879	-0.18798831	1.14384524	
N	-2.53217720	1.79660771	-0.43251328	
N	0.44109159	2.94331251	0.40877965	
N	2.56840658	-2.15873422	-0.21383103	
N	-0.53538391	-2.86345686	0.61711448	
C	-2.08480381	2.74092805	0.40084724	
C	-0.80663252	3.21556961	0.81439606	
C	2.00192701	-3.03221889	0.62800637	
C	0.65974481	-3.31260631	1.01000328	
C	-3.93515505	1.74924028	-0.83957183	
C	-4.23976697	2.15136840	-2.16603622	
C	-5.59354254	2.10432692	-2.55664683	
C	-6.59089195	1.68192399	-1.66239012	
C	-6.25118704	1.27490861	-0.36372942	
C	-4.90933115	1.28099451	0.07612915	
C	-2.88094898	1.44096062	-4.18203441	

C	-3.15983039	2.58084631	-3.16427723
C	-3.52066943	3.90135979	-3.88983953
C	2.84360580	3.48713289	-2.57395103
C	1.86819503	4.36292727	-1.74421420
C	1.74250628	5.78519101	-2.35153470
C	1.58380562	3.77844190	0.78727143
C	2.29400557	4.41691399	-0.27049642
C	3.43575026	5.16679039	0.07723318
C	3.83699431	5.31088992	1.41362184
C	3.09063545	4.70890196	2.43480071
C	1.95102389	3.92369226	2.15354931
C	-5.07339605	-0.67001537	1.69309277
C	-4.56669481	0.77954128	1.48249710
C	-5.14165655	1.72297982	2.57256376
C	2.10160109	2.40191807	4.19707575
C	1.18810276	3.30755291	3.33315428
C	0.53334341	4.41608468	4.20177515
C	4.01672081	-2.24897416	-0.46877588
C	4.88436358	-1.52619552	0.37993436
C	6.26682369	-1.64207797	0.11692448
C	6.73512011	-2.41439932	-0.95689096
C	5.83333698	-3.07788336	-1.80644235
C	4.44213110	-3.00744214	-1.58703758
C	4.78231149	0.85680683	1.21693689
C	4.38065750	-0.61476260	1.50366606
C	4.90399017	-1.07430947	2.88904235
C	-3.27228012	-3.45565930	-2.00785307
C	-2.33789560	-4.35765368	-1.15714065
C	-2.46421831	-5.84417300	-1.57830743
C	-1.75269693	-3.43904030	1.20591094
C	-2.61729686	-4.15766766	0.33720956
C	-3.78323060	-4.70538288	0.90938313
C	-4.06009228	-4.55755612	2.27762244
C	-3.18099623	-3.84358838	3.10366630
C	-2.00691662	-3.25073434	2.59028232
C	3.20546308	-2.69222893	-3.76833281
C	3.45262498	-3.64808915	-2.56571472
C	3.90342376	-5.04770757	-3.04881139
C	-1.86975035	-1.35198169	4.29687793
C	-1.09383698	-2.45925282	3.53867158
C	-0.39265044	-3.41376761	4.54447952
H	-2.90040084	3.33016097	0.80968090
H	-0.86045041	4.02378088	1.53299164
H	2.73260408	-3.67886083	1.09991783
H	0.58379044	-4.09244235	1.75826728
H	-5.86813245	2.40346390	-3.56414232
H	-7.63047229	1.66174475	-1.98139642
H	-7.03085796	0.93360083	0.31223531
H	-2.22348925	2.74920418	-2.62121874
H	0.88802270	3.88538883	-1.81557389
H	-3.78528264	1.19619669	-4.75677330
H	-2.52809692	0.54006023	-3.67084487

H	-2.09652617	1.74877410	-4.88464927
H	-4.40236887	3.78654579	-4.53377387
H	-2.68511750	4.21006820	-4.53103557
H	-3.72494703	4.71261143	-3.17837969
H	3.87051902	3.87618697	-2.52321738
H	2.53356939	3.47227619	-3.62655174
H	2.83225756	2.45449123	-2.21303146
H	1.06298148	6.41719407	-1.76411447
H	1.34625702	5.71400032	-3.37297502
H	2.71203812	6.29639698	-2.41078212
H	4.00558463	5.65585660	-0.70763266
H	4.71985018	5.89725551	1.65717405
H	3.39887924	4.83804191	3.46877895
H	-3.47875516	0.75365298	1.60134459
H	0.39768359	2.65807723	2.95835158
H	-6.16861496	-0.73176654	1.63943119
H	-4.76399046	-1.03513913	2.68010499
H	-4.65534302	-1.34627449	0.93819097
H	-6.23865612	1.75997707	2.53137654
H	-4.76930260	2.75001761	2.45909250
H	-4.85099782	1.36847195	3.56982449
H	2.50577702	1.58221878	3.59316621
H	1.51754069	1.95898206	5.01411650
H	2.93707312	2.95907381	4.64140181
H	1.28872252	5.07173743	4.65478886
H	-0.05111469	3.96239219	5.01287383
H	-0.14143233	5.05289620	3.61240820
H	6.97513072	-1.11179919	0.74763234
H	7.80391051	-2.48706372	-1.14413778
H	6.21240538	-3.64863706	-2.64875194
H	3.28536698	-0.63850153	1.53177889
H	-1.31463659	-4.03815642	-1.37639760
H	5.87352461	0.98050557	1.19285975
H	4.38291958	1.51591342	1.99714562
H	4.37576779	1.19257814	0.25620541
H	4.60333512	-2.10697510	3.11207163
H	4.49901736	-0.42603191	3.67671963
H	5.99970978	-1.02466286	2.94423600
H	-4.32850402	-3.70582725	-1.83660257
H	-3.05605629	-3.59207442	-3.07505534
H	-3.11508905	-2.40033574	-1.76396712
H	-1.81740211	-6.49321578	-0.97318659
H	-2.17074549	-5.95417080	-2.63018497
H	-3.49410717	-6.21182609	-1.48533607
H	-4.47276193	-5.26113787	0.28060820
H	-4.96214875	-4.99573440	2.69798003
H	-3.41323840	-3.73068122	4.15869643
H	2.48596138	-3.77308782	-2.06122257
H	-0.32383158	-1.94133128	2.95943896
H	4.14573968	-2.48480145	-4.29761636
H	2.76353099	-1.74700331	-3.43845336
H	2.50587550	-3.15520553	-4.47601032

H	3.10985046	-5.50003824	-3.65696029
H	4.11878871	-5.72121692	-2.20851279
H	4.80071784	-4.99138676	-3.67841820
H	-2.26086799	-0.61087042	3.59319668
H	-1.18476853	-0.82682412	4.97457685
H	-2.69194942	-1.76148105	4.89866964
H	0.18028443	-4.20475760	4.04023644
H	-1.12479773	-3.90593075	5.19831690
H	0.30004278	-2.84718423	5.17973826
O	0.72962905	0.50979541	-2.74164611
O	0.04742318	-0.86211037	-2.76155441
O	0.14910079	0.58113271	2.23069481
O	-1.20211344	0.91129335	1.92402211
Hf	0.10754961	-0.02787499	-0.88320748
O	1.96378547	-1.21414250	-0.91954181
O	-1.77684296	0.79421862	-0.96460200

Peroxo η^2 -Ozone Complex to Peroxo η^3 -Ozone Complex

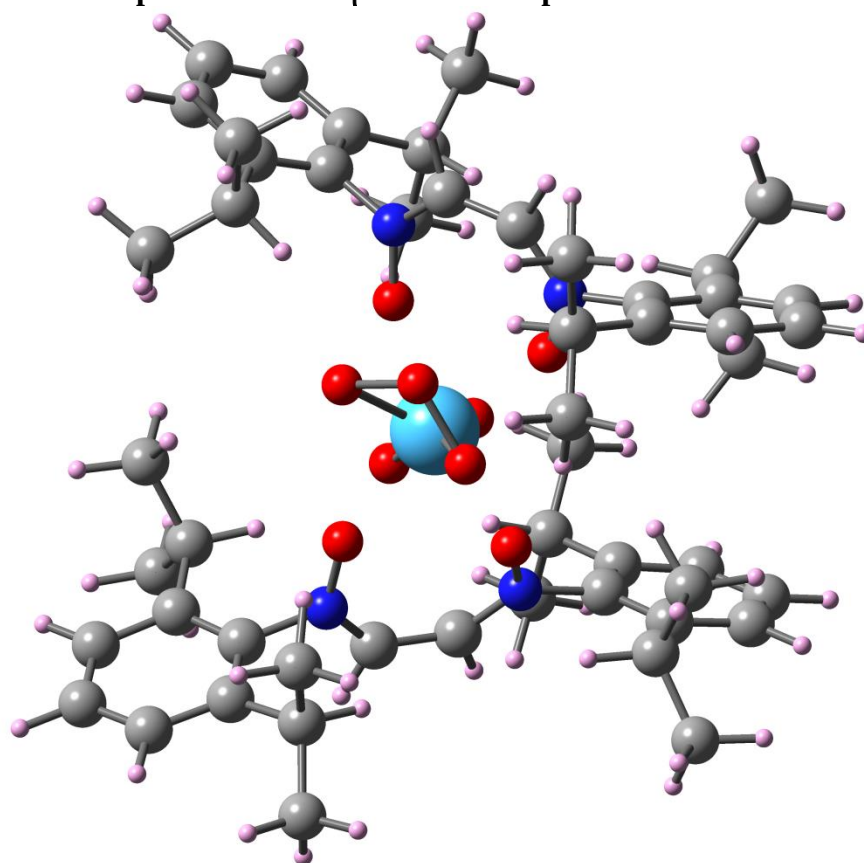


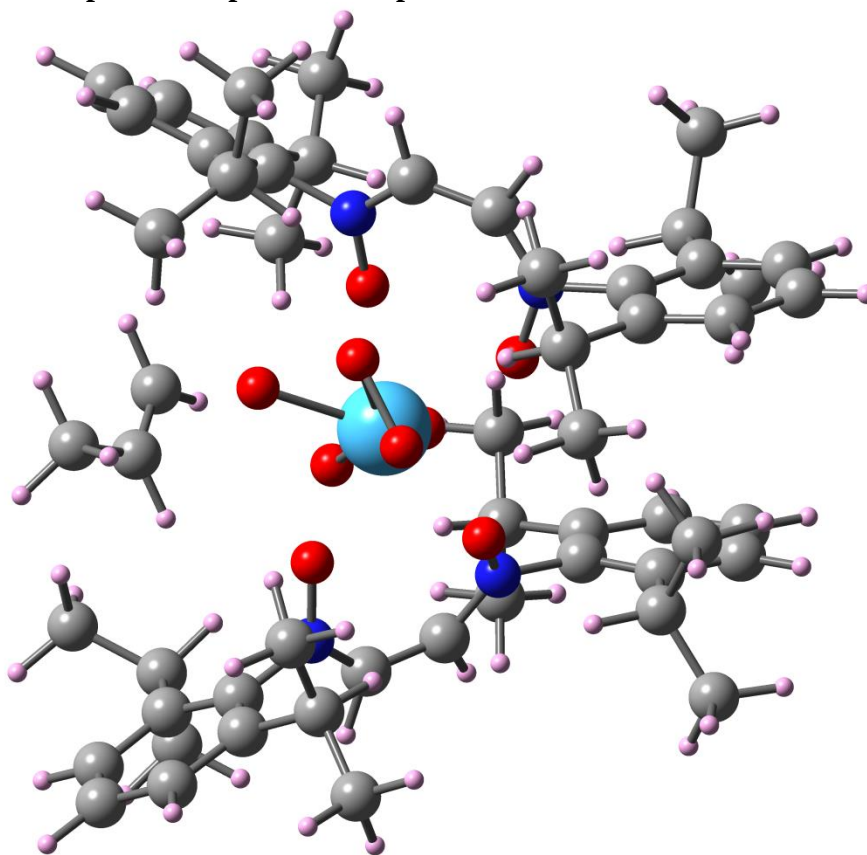
Fig. S149: ONCCNO Peroxo η^2 -Ozone Complex to Peroxo η^3 -Ozone Complex

E	E_{zp}	H	G	<i>f</i>
-2969.2356	-2968.0701	-2967.9960	-2968.1841	-142
O	-1.97621147	-0.18757064	-0.17892551	
O	2.45239865	-0.19571965	-0.75843566	
O	0.65176801	1.63301986	-1.66169939	
N	1.07422298	-2.64711870	1.08489554	
N	3.44539368	-0.78295998	-0.09783792	
N	-1.50401772	2.99315405	0.10261427	
N	-2.91240349	0.28941957	-1.03119791	
C	2.33621568	-2.48222247	1.44958392	
C	3.39231449	-1.72347293	0.85039626	
C	-2.55391746	2.76691071	-0.70880395	
C	-3.14909613	1.58626894	-1.23498979	
C	0.18098492	-3.57309235	1.78532446	
C	-0.10765940	-3.37927904	3.16365409	
C	-0.97422784	-4.31646068	3.76760554	
C	-1.53361859	-5.37491920	3.03919086	
C	-1.22361775	-5.53607161	1.68010908	
C	-0.35039276	-4.64908621	1.01947476	
C	-0.67267221	-1.44166354	4.72075798	

C	0.45663384	-2.23859787	4.02153955
C	1.46798336	-2.78776230	5.06515369
C	4.11353060	2.92315023	0.95519085
C	4.53517833	1.49401387	1.39182378
C	5.35065182	1.53185355	2.70884099
C	4.77437112	-0.27036647	-0.48556504
C	5.30452799	0.80878090	0.25754436
C	6.57526127	1.28151155	-0.13667216
C	7.25105840	0.71428543	-1.22831438
C	6.66705124	-0.32957846	-1.96588431
C	5.40283743	-0.84683927	-1.61461899
C	-1.20289207	-4.51411479	-1.36714314
C	-0.00669319	-4.89622304	-0.45562894
C	0.44196122	-6.35911189	-0.70692814
C	4.01640605	-1.23823869	-3.68686550
C	4.71607573	-1.91354159	-2.47294684
C	5.68021606	-3.03280475	-2.93323134
C	-1.29379426	4.36059761	0.61582838
C	-0.60071396	5.28636236	-0.19774089
C	-0.42885996	6.58476159	0.33043614
C	-0.89763181	6.91422194	1.61148097
C	-1.54610686	5.95122169	2.40281277
C	-1.76047947	4.64249735	1.92308580
C	1.44954491	5.30284600	-1.71122139
C	-0.04835523	4.92721210	-1.58136231
C	-0.87994375	5.60473781	-2.70341814
C	-4.03705591	-2.29177674	1.64571225
C	-4.65468574	-1.10869913	0.85526880
C	-6.07752434	-0.77261225	1.37249154
C	-3.82393992	-0.72617299	-1.57950909
C	-4.65389898	-1.40664591	-0.64858137
C	-5.51554790	-2.39650664	-1.16107318
C	-5.55371930	-2.68456141	-2.53476906
C	-4.72701472	-1.98543349	-3.42436290
C	-3.83245452	-0.98966678	-2.97221009
C	-1.35264105	2.98827517	3.79358897
C	-2.40651143	3.57503358	2.81231806
C	-3.64615024	4.10378691	3.57456288
C	-2.03381531	-1.27260800	-4.74901608
C	-2.94344286	-0.27069236	-3.99301986
C	-3.80256071	0.56268676	-4.98234132
H	2.63992353	-3.07281009	2.30585331
H	4.37269228	-1.95241075	1.25401502
H	-3.07704625	3.67859180	-0.97067820
H	-3.99348194	1.77066911	-1.88920962
H	-1.22174808	-4.20185172	4.81899138
H	-2.20641328	-6.07487851	3.52919406
H	-1.65211036	-6.36736578	1.12785149
H	0.96107444	-1.51511229	3.37814794
H	3.60732639	0.94833564	1.59357188
H	-1.25852223	-2.06317975	5.41188546
H	-1.33465718	-1.00393063	3.96787185

H	-0.23440320	-0.61622365	5.29679618
H	0.98151143	-3.47388079	5.77173334
H	1.89799700	-1.95865388	5.64182927
H	2.29620598	-3.33762151	4.59453469
H	4.98922687	3.56205523	0.77503180
H	3.50267365	3.38675537	1.73983235
H	3.51629164	2.88578766	0.03697291
H	5.63988571	0.52328663	3.03360522
H	4.74721651	1.98481275	3.50556479
H	6.26745405	2.12717923	2.60448947
H	7.02862128	2.10580802	0.40717685
H	8.22802644	1.09598844	-1.51573818
H	7.19310576	-0.73908850	-2.82317842
H	0.82108628	-4.24249150	-0.74427033
H	3.92440651	-2.38755693	-1.87937275
H	-2.09479084	-5.10804000	-1.12357319
H	-0.94758799	-4.69730543	-2.41918431
H	-1.44242740	-3.45242376	-1.25675834
H	-0.37450497	-7.07497721	-0.54668989
H	1.27549307	-6.64536212	-0.05170384
H	0.77260472	-6.46823300	-1.74818849
H	3.26249814	-0.51868286	-3.35137062
H	3.51169408	-1.99646049	-4.29963186
H	4.74938339	-0.71703242	-4.31790867
H	6.43858288	-2.65651287	-3.63176295
H	5.11537756	-3.81382085	-3.45819629
H	6.20038549	-3.49685452	-2.08479351
H	0.08979289	7.33386109	-0.26122410
H	-0.74780165	7.91907202	1.99960793
H	-1.88565952	6.21682740	3.39954631
H	-0.09766202	3.84197293	-1.72037469
H	-4.01817820	-0.23991830	1.04844352
H	1.61065827	6.38872957	-1.66629625
H	1.83395918	4.94228627	-2.67314802
H	2.04072109	4.83172410	-0.91736661
H	-1.93711381	5.30882390	-2.66185201
H	-0.48808930	5.31508650	-3.68668387
H	-0.83630395	6.70002332	-2.62783225
H	-4.62062485	-3.21199446	1.50566648
H	-4.01780584	-2.06126853	2.71897884
H	-3.00888295	-2.47769551	1.31971462
H	-6.51799953	0.06952232	0.82238295
H	-6.03251337	-0.50090680	2.43535624
H	-6.75912819	-1.62787746	1.27908589
H	-6.16551842	-2.93993480	-0.48093711
H	-6.22675318	-3.45216188	-2.90953928
H	-4.76249813	-2.21911918	-4.48473573
H	-2.74120951	2.74371824	2.17974927
H	-2.26753876	0.41180881	-3.47313893
H	-0.92940825	3.77913814	4.42835164
H	-0.54466383	2.49308388	3.24608473
H	-1.82422369	2.24023323	4.44454999

H	-4.12889997	3.27800604	4.11294041
H	-4.38452362	4.54795533	2.89395789
H	-3.37315841	4.86182470	4.32004295
H	-1.35509137	-1.76366807	-4.04494713
H	-1.41741749	-0.73133463	-5.47836044
H	-2.61657441	-2.03050309	-5.29020558
H	-4.43903288	1.29141675	-4.46013770
H	-4.46001673	-0.07828898	-5.58478751
H	-3.14860547	1.11408058	-5.66983656
O	1.30306990	0.26419176	1.54359874
O	-0.14619430	-0.11183907	1.86596668
O	-0.34895480	0.80658305	-2.47498493
O	-0.00095640	-0.64859751	-2.17827452
Hf	0.21164243	0.12348634	-0.19344046
O	-0.62587775	2.11427712	0.55250401
O	0.58934301	-2.07217884	-0.04634332

Peroxo η^3 -Ozone Complex to Bisperoxo ComplexFig. S150: ONCCNO Peroxo η^3 -Ozone Complex to Bisperoxo Complex

E	E_{zp}	H	G	<i>f</i>
-3087.1086	-3085.8607	-3085.7816	-3085.9804	-346
O	-1.98011853	-0.34095851	-0.28121081	
O	2.41351540	-0.44087813	-0.66209456	
O	1.17283178	2.08320090	-0.78240688	
N	0.60593835	-2.69115238	0.94103054	
N	3.27674461	-1.34955140	-0.20710006	
N	-1.63354821	2.91528506	0.38917271	
N	-3.03166473	0.26662052	-0.82715493	
C	1.88139957	-2.87039842	1.26908032	
C	3.05257357	-2.35686081	0.64767049	
C	-2.69620012	2.75453015	-0.39184856	
C	-3.32214553	1.56985087	-0.88185652	
C	-0.45089146	-3.45081308	1.61318602	
C	-0.63684669	-3.33570821	3.02063850	
C	-1.66852487	-4.10933689	3.59542914	
C	-2.47287228	-4.95772294	2.82269215	
C	-2.23676690	-5.07894029	1.44598894	
C	-1.21121147	-4.34861779	0.81140274	
C	-0.64252618	-1.50580206	4.80042355	

C	0.22223086	-2.47297132	3.95540193
C	1.09581768	-3.37260949	4.87349150
C	5.91509720	1.07527314	1.99724807
C	5.39741341	-0.33779803	1.62437181
C	6.04929856	-1.39934629	2.55334720
C	4.64329644	-1.16296779	-0.72479886
C	5.64941831	-0.67590584	0.14741665
C	6.94024143	-0.51220798	-0.40002770
C	7.19768521	-0.79670880	-1.74999851
C	6.16788337	-1.25388439	-2.58811160
C	4.86100388	-1.45116621	-2.09525889
C	-2.11630796	-4.13664839	-1.55119797
C	-0.93468367	-4.61775904	-0.67381812
C	-0.62450665	-6.11758147	-0.92269063
C	3.27689782	-0.76906466	-3.95043827
C	3.74328467	-1.92876429	-3.02845628
C	4.16711796	-3.16810418	-3.85676627
C	-1.15734128	4.25751433	0.73276091
C	-0.77244670	5.14530156	-0.30904984
C	-0.28943599	6.41132321	0.08697648
C	-0.18143745	6.76380633	1.43985742
C	-0.57091614	5.85847306	2.43945154
C	-1.07703024	4.58399074	2.11425228
C	0.51664445	5.02314443	-2.51348552
C	-0.84583245	4.81881331	-1.80858051
C	-1.95511068	5.66241326	-2.49501262
C	-5.13153013	-2.12113663	1.83489155
C	-5.07173491	-0.85080499	0.95103226
C	-6.27605556	0.08418630	1.24717938
C	-4.02833842	-0.66011824	-1.40888274
C	-5.00951707	-1.19425683	-0.54130802
C	-5.97000659	-2.05008260	-1.12004100
C	-5.93444614	-2.35204242	-2.49110668
C	-4.93262251	-1.81256021	-3.31339679
C	-3.94135223	-0.95414837	-2.79028136
C	-0.30068809	3.02361086	3.96403052
C	-1.52656149	3.64109125	3.23823366
C	-2.47025898	4.35242510	4.24218445
C	-2.19362694	-1.42678557	-4.59777706
C	-2.86028933	-0.35791900	-3.69810001
C	-3.44879543	0.78933184	-4.56418312
H	2.05932192	-3.57204095	2.07480592
H	3.96221508	-2.88070991	0.91778889
H	-3.18671192	3.67499009	-0.68155564
H	-4.24507893	1.75935269	-1.41743175
H	-1.84275426	-4.03819833	4.66537653
H	-3.26677453	-5.53344848	3.29303697
H	-2.83909258	-5.76546879	0.85707488
H	0.87032864	-1.83166056	3.35718305
H	4.31756329	-0.33922285	1.81335549
H	-1.34758470	-2.03592549	5.45590099
H	-1.19212197	-0.83435016	4.13438388

H	0.00851117	-0.89028761	5.43578570
H	0.47752821	-3.99520822	5.53430263
H	1.74066176	-2.74775386	5.50554290
H	1.74230050	-4.05154960	4.29819646
H	7.00681008	1.14792547	1.90666149
H	5.65195090	1.30112116	3.03864774
H	5.46391247	1.84584410	1.36324585
H	5.68648035	-2.41361957	2.34114441
H	5.82427832	-1.17259511	3.60349406
H	7.14084660	-1.40715112	2.43397131
H	7.74402151	-0.14567574	0.23230261
H	8.19906102	-0.65608465	-2.15019108
H	6.37912987	-1.46317621	-3.63285159
H	-0.06320240	-4.03801074	-0.98470574
H	2.87428749	-2.21377876	-2.42604126
H	-3.05022043	-4.65421538	-1.29174185
H	-1.90573529	-4.33461709	-2.61081014
H	-2.26626503	-3.06098319	-1.42230873
H	-1.48943363	-6.75846153	-0.70663252
H	0.21281671	-6.46355327	-0.30189732
H	-0.35355488	-6.27058683	-1.97605425
H	2.84786445	0.04344687	-3.35663255
H	2.49420280	-1.12552552	-4.63222094
H	4.11139606	-0.38351022	-4.55328744
H	4.96809548	-2.93022709	-4.56900936
H	3.31016663	-3.53266484	-4.43757898
H	4.51735464	-3.98621069	-3.21331055
H	0.01867401	7.12039496	-0.67616466
H	0.20425537	7.74254934	1.71528592
H	-0.49216903	6.14723387	3.48345214
H	-1.07449747	3.75866373	-1.94370801
H	-4.15516545	-0.31935971	1.22994807
H	0.88902239	6.05245378	-2.42157271
H	0.41275531	4.79742194	-3.58293946
H	1.24646174	4.32766146	-2.09462300
H	-2.93971794	5.52078596	-2.02628473
H	-2.03919046	5.38294761	-3.55314249
H	-1.72370641	6.73474889	-2.44710147
H	-6.05062859	-2.69590023	1.65911923
H	-5.11352774	-1.83801707	2.89529142
H	-4.27350017	-2.77431806	1.64468190
H	-6.22078707	1.01226844	0.66290409
H	-6.29598739	0.35284508	2.31144445
H	-7.22705635	-0.40794192	1.00407888
H	-6.74627400	-2.48271586	-0.49460946
H	-6.68600748	-3.01214455	-2.91803453
H	-4.91172983	-2.06514303	-4.36964683
H	-2.08005348	2.80420872	2.80155001
H	-2.05399797	0.05387016	-3.08373067
H	0.35263928	3.80739719	4.37270848
H	0.27426911	2.39278774	3.27995368
H	-0.63881146	2.39278386	4.79687015

H	-2.85655908	3.62062446	4.96362431
H	-3.32628289	4.81792715	3.73547750
H	-1.95156285	5.13215029	4.81513564
H	-1.77568750	-2.23840880	-3.99289774
H	-1.36667804	-0.96535044	-5.15037358
H	-2.89357710	-1.85614351	-5.32834531
H	-3.87401199	1.59111674	-3.94537965
H	-4.24250094	0.42184812	-5.22950556
H	-2.65767577	1.22948472	-5.18408853
O	1.33776505	0.18882312	1.71282601
O	-0.04716840	-0.38109965	1.93134692
O	-0.29686611	1.45969924	-1.75506936
O	0.10722453	0.07547943	-2.20263580
Hf	0.25076134	0.23908238	-0.07920769
O	-0.98923865	1.89411448	0.96679803
O	0.29666756	-2.01311572	-0.21586468
C	3.24981581	2.56689280	-0.28882586
H	3.59637704	1.53918952	-0.28702911
C	2.41468671	2.98039429	0.72219748
H	2.13954416	2.31497737	1.53458962
H	2.04024402	4.00088551	0.75468548
C	3.76869597	3.43653817	-1.40215982
H	3.43110677	4.47438536	-1.30585180
H	4.86913678	3.42845129	-1.41722585
H	3.42640977	3.04453783	-2.36894742

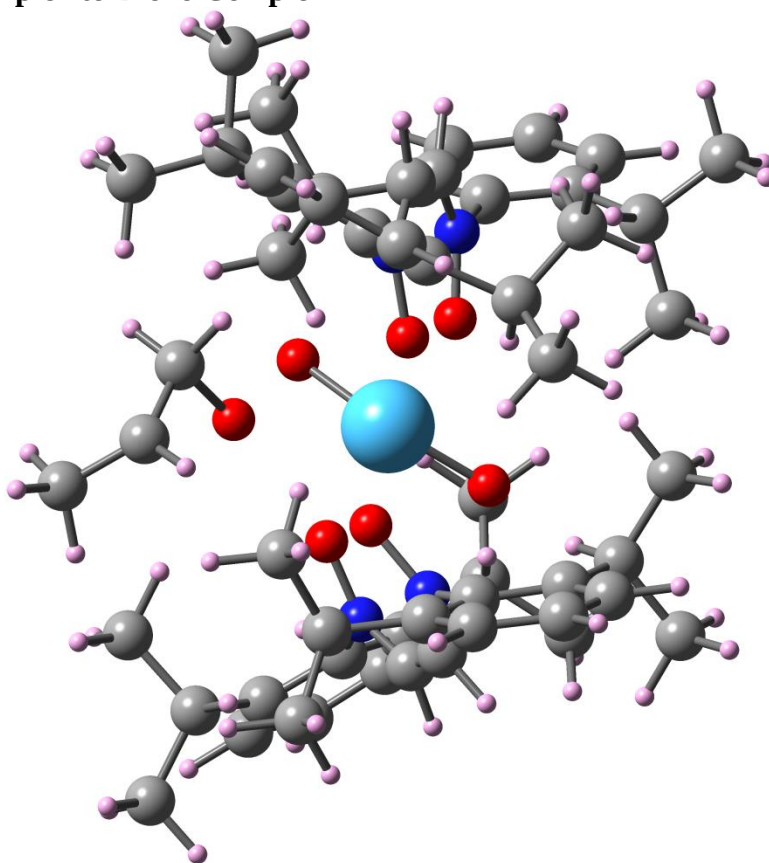
Oxo Peroxo Complex to Dioxo Complex

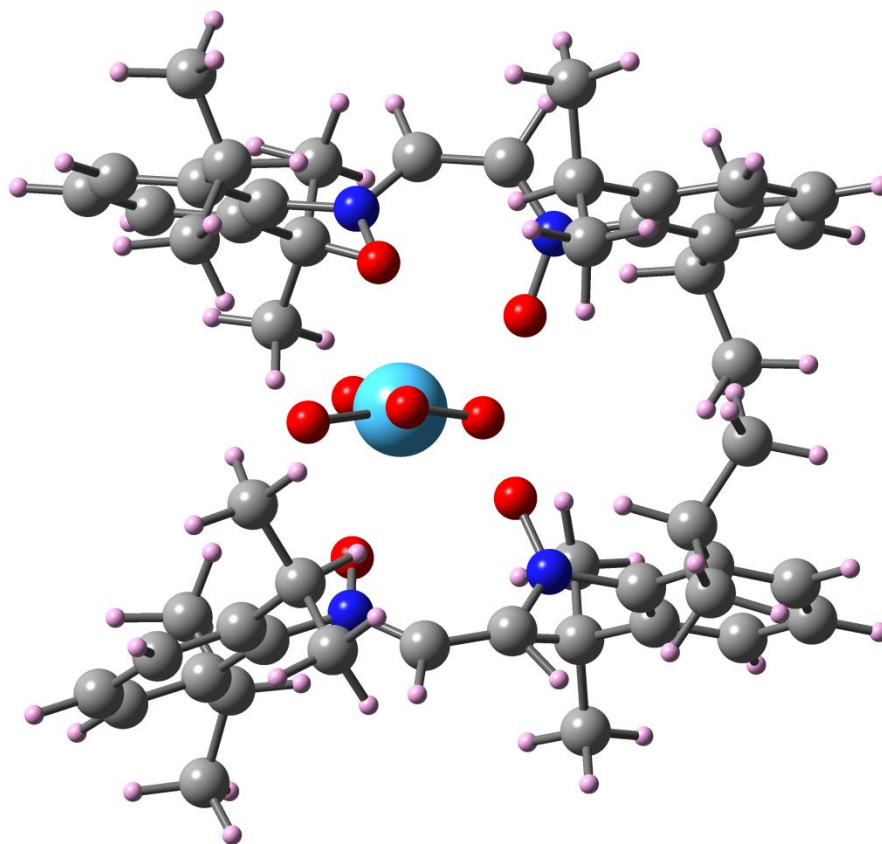
Fig. S151: ONCCNO Oxo Peroxo Complex to Dioxo Complex

E	E_{ZP}	H	G	<i>f</i>
-2936.7713	-2935.5309	-2935.4536	-2935.6492	-344
O	-1.84172711	0.35843167	-0.03807214	
O	2.21688887	-1.00519307	-0.83306760	
O	0.74601510	1.22572379	-1.73123027	
N	0.11571064	-2.92613148	0.92595747	
N	3.01094660	-1.79624664	-0.12726350	
N	-0.32245115	3.32611894	0.33620607	
N	-2.78771607	1.26744668	-0.46609016	
C	1.37883075	-3.16202742	1.26268717	
C	2.64191465	-2.70456973	0.77954381	
C	-1.60168856	3.49712454	-0.08501682	
C	-2.64458442	2.61413587	-0.40734981	
C	-0.95978379	-3.55712364	1.69977615	
C	-1.15294884	-3.15794844	3.04894616	
C	-2.16156908	-3.83537781	3.76935183	
C	-2.94738192	-4.82951014	3.16832595	
C	-2.74823377	-5.17168105	1.82091292	
C	-1.74522945	-4.54508156	1.05372292	
C	-1.26539528	-0.95390960	4.32312904	

C	-0.34085072	-2.04857509	3.73146817
C	0.57385228	-2.63293336	4.84098769
C	4.48070941	1.65878555	1.30202562
C	4.38871593	0.13484864	1.57637672
C	4.95383198	-0.21196652	2.97810862
C	4.44921727	-1.57736660	-0.36215604
C	5.11048743	-0.65239467	0.47692217
C	6.48910650	-0.45850285	0.23691741
C	7.14648853	-1.13815858	-0.79977412
C	6.44037298	-2.02095376	-1.63555947
C	5.06453726	-2.25824394	-1.43964793
C	-2.74485096	-4.45349221	-1.26849888
C	-1.54462375	-4.93925699	-0.41277200
C	-1.32302639	-6.46453257	-0.57922630
C	3.80164004	-2.29318406	-3.62288146
C	4.26392582	-3.13973558	-2.40302481
C	5.03424823	-4.40216569	-2.85749446
C	0.50456436	4.49990721	0.62570576
C	1.24782014	5.07154323	-0.43234375
C	2.02251587	6.21202797	-0.12714657
C	2.06850726	6.72477898	1.17851650
C	1.35272048	6.10098880	2.21520767
C	0.55458643	4.96581435	1.96344229
C	2.66803920	4.22042677	-2.36774083
C	1.23300243	4.48720309	-1.84840391
C	0.45738337	5.41319957	-2.82269749
C	-4.82464555	-1.42535247	2.33417496
C	-4.29179565	-0.17897764	1.59322988
C	-4.66699718	1.10777409	2.38454273
C	-4.08477010	0.69754769	-0.83437398
C	-4.79076958	-0.06018803	0.14758574
C	-6.02932667	-0.61721314	-0.22354160
C	-6.57074860	-0.41100509	-1.50325530
C	-5.87691161	0.36757401	-2.43611020
C	-4.61849627	0.93523296	-2.13299530
C	0.80943997	3.19199026	3.74597922
C	-0.15756539	4.22544720	3.09998359
C	-0.75088895	5.17482212	4.16776486
C	-3.87172562	1.07519311	-4.58366995
C	-3.93793972	1.79416025	-3.21047036
C	-4.67202142	3.15456307	-3.37571383
H	1.46956566	-3.86956428	2.07951320
H	3.48907337	-3.18723872	1.25355170
H	-1.86793646	4.54471553	-0.16636431
H	-3.56008084	3.12499031	-0.68181853
H	-2.33752087	-3.56920513	4.80813829
H	-3.71961859	-5.33217094	3.74609185
H	-3.36852095	-5.93806873	1.36407203
H	0.28677001	-1.53077612	2.99322392
H	3.31751244	-0.10706143	1.58018200
H	-1.90941473	-1.33599796	5.12794902
H	-1.89975828	-0.51846108	3.54273261

H	-0.64848961	-0.14562571	4.73504193
H	-0.01224973	-3.09953293	5.64534666
H	1.17899421	-1.83106592	5.28261106
H	1.26252355	-3.39454727	4.44917941
H	5.51826326	2.02103780	1.32583199
H	3.90773973	2.20341400	2.06240957
H	4.04864997	1.90232095	0.32444828
H	4.85951627	-1.28476727	3.19632847
H	4.39563116	0.33768567	3.74647011
H	6.01525071	0.05785814	3.07139076
H	7.04272931	0.23857199	0.86017602
H	8.20817922	-0.97155111	-0.96738814
H	6.96069297	-2.52185701	-2.44657358
H	-0.65631508	-4.42830031	-0.79669583
H	3.35480099	-3.48057966	-1.89058951
H	-3.68103428	-4.93027860	-0.94801791
H	-2.58404469	-4.70385749	-2.32577156
H	-2.86460287	-3.36779567	-1.18272363
H	-2.20474710	-7.04122581	-0.27120408
H	-0.46872230	-6.81344596	0.01555270
H	-1.12472425	-6.70119974	-1.63291754
H	3.16310059	-1.46353726	-3.30107851
H	3.23038770	-2.91928530	-4.32208725
H	4.66813300	-1.88550457	-4.16117416
H	5.89799160	-4.14987002	-3.48588704
H	4.37473895	-5.04366065	-3.45641265
H	5.39642062	-4.98693665	-2.00170681
H	2.60183549	6.68902787	-0.91322320
H	2.67359564	7.60280061	1.39371299
H	1.41912255	6.49782427	3.22401083
H	0.73918250	3.50886285	-1.83113152
H	-3.20122512	-0.24940681	1.56234198
H	3.24954040	5.14645453	-2.48044683
H	2.61728818	3.72689736	-3.34598005
H	3.20526729	3.54895933	-1.68856713
H	-0.57864605	5.56887811	-2.49259503
H	0.43062511	4.96571684	-3.82496136
H	0.93558676	6.39931777	-2.90400342
H	-5.90576600	-1.36564070	2.52182350
H	-4.32925915	-1.50988195	3.30857490
H	-4.61832429	-2.34678723	1.77621119
H	-4.24706816	2.00738324	1.91913688
H	-4.27686366	1.04776739	3.40929480
H	-5.75797352	1.22701855	2.44058851
H	-6.58442318	-1.20526022	0.49924459
H	-7.53170702	-0.84764512	-1.76479721
H	-6.30789616	0.53091587	-3.41985085
H	-0.99062261	3.65415429	2.67123817
H	-2.90868558	2.00657776	-2.90261985
H	1.69526615	3.69708743	4.15623188
H	1.12975444	2.44288968	3.01376213
H	0.30375644	2.66824100	4.56927413

H	-1.34577950	4.59719810	4.88710710
H	-1.40171697	5.93656666	3.71846652
H	0.03352950	5.69062772	4.73690235
H	-3.41709440	0.08212994	-4.49980673
H	-3.27170065	1.66918855	-5.28549501
H	-4.86896263	0.95406730	-5.02508056
H	-4.71183035	3.72251561	-2.43727457
H	-5.70585480	3.00142757	-3.71134297
H	-4.16033201	3.77370346	-4.12410600
O	1.08045501	-0.22297710	1.49629936
C	-0.87107172	-0.23218776	-3.43261915
H	-1.74149880	0.13843179	-2.88467076
C	-0.89103353	-1.66645935	-3.74785726
H	-1.34953955	-2.33179930	-3.01921685
O	0.29858883	-0.30813715	-2.50901386
H	-0.61888240	0.42496874	-4.27211623
C	-0.11219035	-2.26537529	-4.87998872
H	0.68177855	-2.93929452	-4.51924094
H	-0.76153968	-2.87465578	-5.53346817
H	0.36089530	-1.49027844	-5.49415273
Hf	0.27019588	0.02105783	-0.16549365
O	0.29883244	2.16207585	0.53379467
O	-0.27612980	-2.13703444	-0.10993045

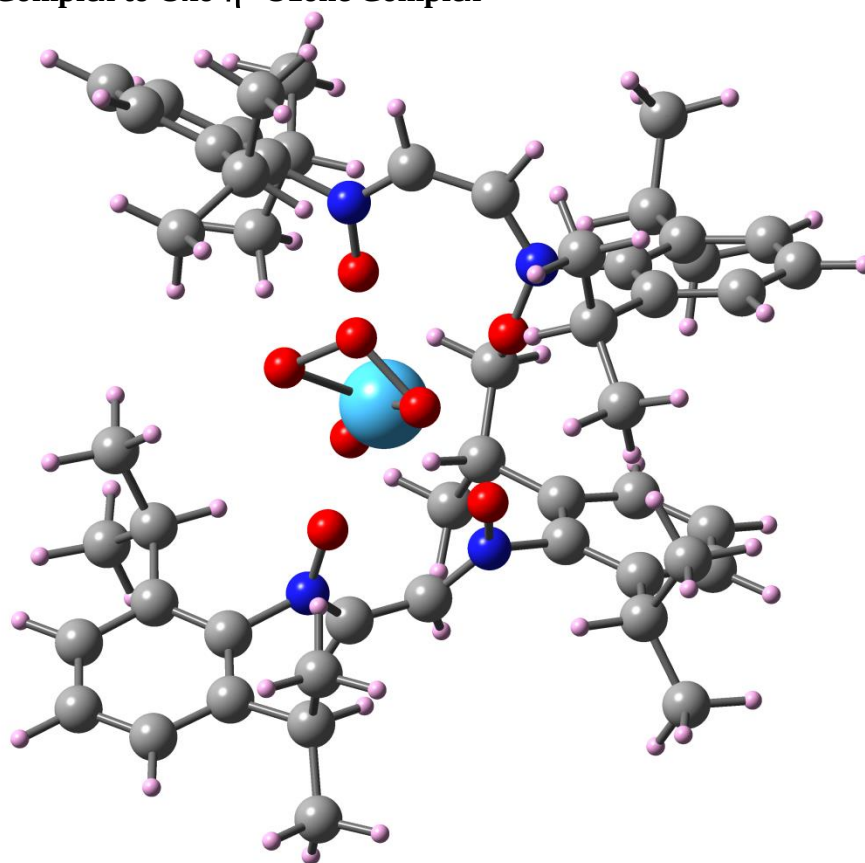
Dioxo Complex to Oxo η^2 -Ozone ComplexFig. S152: ONCCNO Dioxo Complex to Oxo η^2 -Ozone Complex

E	E_{zp}	H	G	<i>f</i>
-2894.0521	-2892.8906	-2892.8906	-2893.0043	-156
O	2.02294100	-1.51810200	0.64832700	
O	-1.77893300	0.95457900	0.32633800	
O	-0.32872800	-0.49701500	-1.90445500	
N	0.00817400	3.41642400	0.38091300	
N	-2.62014900	1.93863600	0.04985500	
N	-0.64975800	-2.85068100	0.19188700	
N	2.46827900	-2.38491600	-0.27136400	
C	-1.19830500	3.85417800	0.72607500	
C	-2.42018700	3.23319600	0.32890400	
C	0.29355500	-3.55656700	-0.44621500	
C	1.66169400	-3.31618500	-0.77508600	
C	1.23465000	4.04796100	0.86437400	
C	1.48590100	4.11241100	2.26353800	
C	2.67869500	4.75045300	2.66214500	
C	3.57837800	5.27601200	1.72392000	
C	3.29906000	5.18927600	0.35238500	
C	2.11762200	4.58104700	-0.11643100	
C	1.33435200	2.59339500	4.30593800	

C	0.56472900	3.53358300	3.34555800
C	-0.14754000	4.67121900	4.12837700
C	-4.75130000	-0.70775800	2.12548000
C	-4.70583700	0.80272700	1.77690300
C	-5.74352500	1.60023600	2.60894600
C	-3.89863900	1.54547900	-0.56700200
C	-4.90576600	1.01524300	0.27330500
C	-6.13174100	0.67833700	-0.33770900
C	-6.32452100	0.85979900	-1.71710400
C	-5.29081300	1.36735300	-2.51983500
C	-4.04108800	1.71782600	-1.96505600
C	2.82029700	3.59533100	-2.34598800
C	1.84342300	4.56310000	-1.62560400
C	1.91014700	5.99009500	-2.23128000
C	-2.56474800	1.23213100	-3.98366300
C	-2.91822400	2.24591700	-2.86490600
C	-3.29459800	3.62877200	-3.46096700
C	-1.90584500	-3.54572900	0.53214900
C	-2.87947700	-3.71311500	-0.47971400
C	-4.05506800	-4.40589500	-0.11659200
C	-4.24426100	-4.87479400	1.19275800
C	-3.26476300	-4.65797300	2.17622500
C	-2.06427000	-3.98432600	1.86905700
C	-3.90608000	-2.33654600	-2.36158400
C	-2.69416500	-3.18709200	-1.90795600
C	-2.45256200	-4.35641000	-2.90138800
C	4.46106600	-1.24856700	2.70832000
C	4.36136200	-2.60542300	1.95858900
C	5.16275400	-3.70984600	2.69368000
C	3.89485300	-2.33126100	-0.59484500
C	4.80171000	-2.43883300	0.49819500
C	6.17585500	-2.38725200	0.19384800
C	6.62454500	-2.24515100	-1.12856200
C	5.70231800	-2.13704500	-2.17750200
C	4.31028400	-2.16243800	-1.94254800
C	-1.48878900	-2.52567900	3.85325800
C	-1.02136400	-3.70440900	2.95578200
C	-0.69801600	-4.95877400	3.80442500
C	3.69022200	-0.67059200	-3.90509700
C	3.36163500	-1.97270800	-3.13209700
C	3.39848200	-3.20532600	-4.07553100
H	-1.24063400	4.78976000	1.26937400
H	-3.30187700	3.85831600	0.24804900
H	-0.06136100	-4.53792800	-0.74084700
H	2.12592200	-4.03846900	-1.43408000
H	2.91442900	4.81211500	3.72031400
H	4.49754200	5.74932600	2.06143700
H	4.00073500	5.60350000	-0.36559700
H	-0.18370600	2.89589400	2.86775000
H	-3.70887700	1.16054200	2.05659300
H	2.14030900	3.10992100	4.84520700
H	1.73454500	1.75928900	3.72206700

H	0.63980000	2.18608500	5.05426600
H	0.57825900	5.29683600	4.66512200
H	-0.83486600	4.24392400	4.87056700
H	-0.72751100	5.33556500	3.47084600
H	-5.72651700	-1.14636800	1.87563500
H	-4.57963300	-0.85206100	3.19997800
H	-3.97664000	-1.25644100	1.57929800
H	-5.70427800	2.67359600	2.38074800
H	-5.54458000	1.47210700	3.68084300
H	-6.76716200	1.25370800	2.41624100
H	-6.93723200	0.27418400	0.26956600
H	-7.27867400	0.59755500	-2.16810000
H	-5.44936500	1.48587200	-3.58819100
H	0.83641900	4.17516200	-1.80425100
H	-2.00751000	2.36986300	-2.27049800
H	3.86429600	3.90883400	-2.20214100
H	2.61329400	3.59365600	-3.42526700
H	2.69863200	2.57262100	-1.97185500
H	2.92096300	6.41421800	-2.17200100
H	1.22449700	6.68124000	-1.72186700
H	1.63216100	5.95218400	-3.29294800
H	-2.19336900	0.29982100	-3.54670800
H	-1.76365300	1.64229000	-4.61138900
H	-3.42674400	1.01701700	-4.63015700
H	-4.18064700	3.55843500	-4.10606300
H	-2.46564400	4.01322900	-4.06870000
H	-3.51070900	4.36509300	-2.67479000
H	-4.82957600	-4.56749400	-0.86126800
H	-5.15923700	-5.40337600	1.45000400
H	-3.43273300	-5.01584800	3.18809100
H	-1.82029100	-2.52621800	-1.93955700
H	3.30612700	-2.89591100	1.98242900
H	-4.82502600	-2.93440500	-2.42949600
H	-3.70847000	-1.91271000	-3.35384300
H	-4.08515800	-1.50597400	-1.67063600
H	-1.57083200	-4.95202800	-2.62894500
H	-2.29217200	-3.96324600	-3.91331900
H	-3.31585100	-5.03490700	-2.93228600
H	5.49139000	-0.86640300	2.69283800
H	4.15966400	-1.37540700	3.75708100
H	3.79770700	-0.50902600	2.25015300
H	5.13241800	-4.66430200	2.15115600
H	4.73470100	-3.86962100	3.69215200
H	6.21565600	-3.43317200	2.83328700
H	6.90054700	-2.46556400	0.99859800
H	7.69110900	-2.21077300	-1.33829400
H	6.06183500	-2.00531200	-3.19382600
H	-0.08913800	-3.38014700	2.47916200
H	2.34028600	-1.83228500	-2.77141200
H	-2.43405100	-2.76671100	4.35916900
H	-1.62574800	-1.61900000	3.25527900
H	-0.73188100	-2.31421600	4.61910400

H	0.10666300	-4.72761100	4.51404900
H	-0.37060200	-5.79840500	3.17735200
H	-1.56497900	-5.29167800	4.38962800
H	3.59559600	0.18453500	-3.22960000
H	2.96605300	-0.53798500	-4.71892400
H	4.69723500	-0.68792600	-4.34422400
H	3.13741300	-4.13821300	-3.55435800
H	4.39653200	-3.34366600	-4.51267600
H	2.68634900	-3.06626200	-4.89918600
O	0.96440100	0.87579400	1.74256500
O	0.78057100	-0.00453100	-2.62896400
O	2.10414100	0.47347600	-1.20781200
O	-0.63424900	-1.57511700	0.57626100
O	0.10976500	2.43342300	-0.53701400
Hf	0.56508600	0.27400200	0.06960600

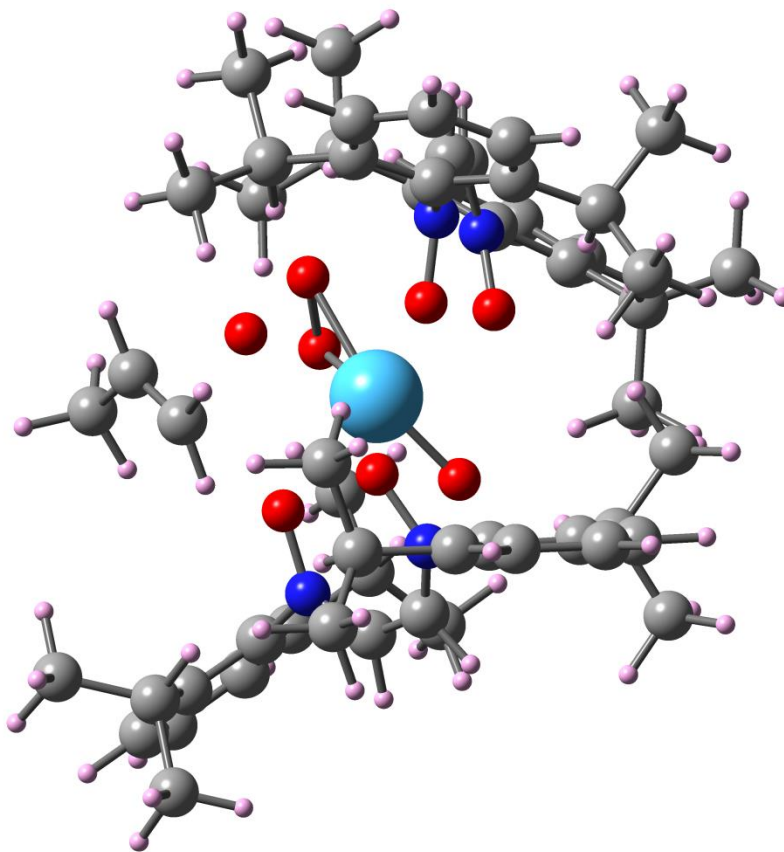
Oxo η^2 -Ozone Complex to Oxo η^3 -Ozone ComplexFig. S153: ONCCNO Oxo η^2 -Ozone Complex to Oxo η^3 -Ozone Complex

E	E_{ZP}	H	G	<i>f</i>
-2894.0767	-2892.9142	-2892.8412	-2893.0266	-118
O	-1.82783362	0.06320730	-0.29969151	
O	2.33720438	-0.96856781	-0.74700400	
O	1.57005196	1.64200685	-1.17314629	
N	0.17568490	-2.79954601	0.97854314	
N	3.09510103	-1.73387205	0.03497205	
N	-0.81018468	3.19611425	0.05824979	
N	-2.76796463	0.81712100	-0.87468375	
C	1.39959420	-2.98957562	1.44828652	
C	2.68955561	-2.55911904	0.99738608	
C	-1.90139135	3.20532669	-0.70416344	
C	-2.78047526	2.14394476	-1.06893800	
C	-0.96968568	-3.42825149	1.65162919	
C	-1.36157501	-2.95731047	2.93056552	
C	-2.45904584	-3.61062977	3.53509922	
C	-3.13473341	-4.65505258	2.88744936	
C	-2.72920181	-5.07728982	1.61068258	
C	-1.63301152	-4.47469462	0.96164128	
C	-1.68688507	-0.67080509	3.99386055	

C	-0.67364036	-1.79507287	3.65793462
C	0.04028961	-2.28890937	4.94382035
C	4.41942610	1.78537528	0.90005119
C	4.50496023	0.35955851	1.51194447
C	5.19280503	0.38750656	2.89951501
C	4.54102921	-1.57495035	-0.20436100
C	5.21964505	-0.57967206	0.53451562
C	6.60238509	-0.44139991	0.28197265
C	7.24813141	-1.24247295	-0.67205298
C	6.52504468	-2.19171614	-1.41491913
C	5.14314659	-2.37583130	-1.20433201
C	-2.24109009	-4.42466000	-1.48881794
C	-1.21932890	-4.93623912	-0.43888645
C	-1.04818583	-6.47379629	-0.52534148
C	3.88675523	-2.57510446	-3.38118386
C	4.32340064	-3.32141058	-2.08772483
C	5.06267348	-4.63739519	-2.42563945
C	-0.06257358	4.42753417	0.33565326
C	0.54897275	5.13815697	-0.73134320
C	1.26253977	6.30703169	-0.38631523
C	1.37768372	6.72926465	0.94427535
C	0.76981218	5.99324128	1.97368106
C	0.03016368	4.82646803	1.69932705
C	1.93875684	4.52941131	-2.77587981
C	0.50903024	4.71318247	-2.20498352
C	-0.30493215	5.72944483	-3.05104638
C	-5.18816513	-0.79016262	2.07640328
C	-4.92382946	0.34643589	1.05681706
C	-5.91180201	1.52419289	1.27567726
C	-3.95294268	0.05392317	-1.32539221
C	-4.99039827	-0.16092101	-0.38739578
C	-6.12707190	-0.86108048	-0.84302771
C	-6.20468659	-1.32832101	-2.16481851
C	-5.14280990	-1.11417881	-3.05759690
C	-3.97877982	-0.42186895	-2.65819528
C	0.42863608	3.22244254	3.62309355
C	-0.62824935	4.06311136	2.85602867
C	-1.39813470	5.00629115	3.81589105
C	-2.44664119	-1.46734907	-4.41792449
C	-2.83092182	-0.18326647	-3.64268141
C	-3.18867625	0.95731573	-4.63432036
H	1.43520619	-3.63336350	2.32011838
H	3.51460025	-3.00689217	1.54055747
H	-2.17913169	4.18070066	-1.08388802
H	-3.65906703	2.47032758	-1.61262559
H	-2.79093144	-3.28697824	4.51800660
H	-3.97936942	-5.13757473	3.37399306
H	-3.26501548	-5.88348388	1.11716573
H	0.07392523	-1.32853672	3.00355492
H	3.46956628	0.03078731	1.66220119
H	-2.46297599	-1.00282083	4.69802812
H	-2.17424005	-0.30808781	3.08123780

H	-1.15361695	0.17509192	4.44536384
H	-0.66872729	-2.71720057	5.66607459
H	0.55390906	-1.44919699	5.42918850
H	0.79268920	-3.05866784	4.72176453
H	5.41906269	2.19893347	0.70437656
H	3.89998411	2.45464670	1.59771882
H	3.85267886	1.77634197	-0.03827831
H	5.26222141	-0.61753621	3.33776403
H	4.61024405	1.01614819	3.58473971
H	6.20809767	0.80405266	2.84757474
H	7.16941799	0.30662764	0.82904326
H	8.31368531	-1.11729890	-0.85058232
H	7.03586291	-2.78486926	-2.16749581
H	-0.25651350	-4.47991461	-0.69159443
H	3.40377961	-3.59194343	-1.55258512
H	-3.24181308	-4.83725292	-1.30139351
H	-1.93090633	-4.72661779	-2.49800023
H	-2.30180113	-3.33205137	-1.45646216
H	-1.99852614	-7.00059224	-0.36967511
H	-0.33212659	-6.84269946	0.22076951
H	-0.67818591	-6.75161287	-1.52095234
H	3.29267759	-1.68776609	-3.13830596
H	3.27690307	-3.23574951	-4.01188436
H	4.76482473	-2.26135075	-3.96196514
H	5.93287364	-4.46109974	-3.07098258
H	4.38856951	-5.31212322	-2.96894655
H	5.40935626	-5.15386953	-1.52083208
H	1.74996825	6.87694130	-1.17189475
H	1.94402582	7.62685182	1.18119425
H	0.86519175	6.33231721	3.00083846
H	0.03643355	3.73292925	-2.29384759
H	-3.91147026	0.71730577	1.25348372
H	2.52268064	5.45890132	-2.73937776
H	1.87572378	4.20871245	-3.82372394
H	2.46030058	3.74497643	-2.21914731
H	-1.33171705	5.85324114	-2.67640610
H	-0.36218102	5.38725379	-4.09232370
H	0.16635271	6.72130662	-3.04888959
H	-6.20950115	-1.18287516	1.98903622
H	-5.06337246	-0.41166534	3.09920412
H	-4.48791769	-1.62074710	1.93301723
H	-5.70433982	2.35721496	0.59120685
H	-5.83403190	1.90053483	2.30407413
H	-6.94925946	1.20552449	1.10959584
H	-6.95067390	-1.04560054	-0.15859908
H	-7.09063170	-1.86443144	-2.49711138
H	-5.20996321	-1.49409027	-4.07291204
H	-1.35281536	3.35211800	2.44605486
H	-1.92957556	0.10865088	-3.09250119
H	1.22695712	3.86399103	4.02188282
H	0.86765005	2.46502596	2.96625380
H	-0.04606770	2.70700352	4.46967462

H	-1.94350493	4.40873117	4.55818627
H	-2.12464021	5.62927576	3.27715985
H	-0.72449064	5.67372342	4.36812327
H	-2.21792927	-2.28755207	-3.72834476
H	-1.54535878	-1.27098574	-5.01045382
H	-3.24019853	-1.79711838	-5.10326681
H	-3.41202232	1.89809242	-4.11306223
H	-4.06398623	0.69608400	-5.24566544
H	-2.34200823	1.14189009	-5.30714059
O	1.07037784	-0.15230002	1.56286395
O	0.41209188	1.52689012	-2.18758559
O	0.15711557	0.05077064	-2.36998300
O	-0.39350904	2.10906178	0.73144754
O	-0.11707419	-2.05270928	-0.10842742
Hf	0.45188745	0.18542292	-0.14916653

Oxo η^3 -Ozone Complex to Oxo Peroxo ComplexFig. S154: ONCCNO Oxo η^3 -Ozone Complex to Oxo Peroxo Complex

E	E_{zp}	H	G	<i>f</i>
-3011.9423	-3010.6981	-3010.6201	-3010.8154	-418
O	-1.89411814	-0.32123202	-0.38397003	
O	2.43550219	-0.51714304	-0.72564606	
O	1.01589008	1.99124615	-1.15422409	
N	0.67799205	-2.58177420	1.20831909	
N	3.31823825	-0.94355807	0.18716301	
N	-1.55473412	2.94741923	0.25140202	
N	-2.99493623	0.29683802	-0.82740706	
C	1.88657614	-2.38550818	1.71845713	
C	3.04740824	-1.68303913	1.25979309	
C	-2.60816420	2.80745421	-0.54517604	
C	-3.27418025	1.60242112	-0.92542707	
C	-0.29699402	-3.40705426	1.93077314	
C	-0.81511506	-2.93206222	3.16314324	
C	-1.73772014	-3.77129729	3.82677029	
C	-2.13672516	-4.99809638	3.27663425	
C	-1.62172212	-5.42069642	2.03998516	
C	-0.68612205	-4.63491635	1.33741010	
C	-1.69084813	-0.71140805	4.04058931	

C	-0.43410703	-1.58054212	3.78212029
C	0.36865803	-1.77979613	5.09524939
C	3.73956729	2.98701923	0.36959903
C	4.03489331	1.71249713	1.20425709
C	4.54496134	2.07937216	2.62208620
C	4.69618236	-0.46937504	-0.02338000
C	5.03396338	0.81298506	0.47056504
C	6.35954147	1.24637510	0.24962802
C	7.28447853	0.44006103	-0.43152603
C	6.90499754	-0.82146506	-0.91857307
C	5.59283640	-1.30392210	-0.73325206
C	-1.24743010	-4.95551838	-1.10600508
C	-0.15037101	-5.10503539	-0.01808000
C	0.39240003	-6.55538749	0.03492100
C	5.51623043	-2.81760621	-2.78879621
C	5.19195140	-2.67876620	-1.27952010
C	5.86584847	-3.81666429	-0.46611304
C	-0.96496207	4.25521533	0.54154504
C	-0.55969404	5.10420839	-0.52776904
C	0.00503700	6.34776347	-0.17139601
C	0.18254301	6.71740352	1.16783409
C	-0.21025302	5.84701346	2.19554817
C	-0.79806706	4.59782135	1.91512215
C	0.72510406	4.86241237	-2.71444821
C	-0.65742205	4.75862536	-2.02080115
C	-1.70475913	5.66080144	-2.72843321
C	-4.94784738	-1.81231714	2.16926217
C	-4.91511837	-0.60304305	1.20088209
C	-6.04991346	0.40198903	1.53752712
C	-4.06671931	-0.63635905	-1.24412609
C	-4.99726838	-1.04957008	-0.26230702
C	-6.04252244	-1.89643715	-0.68809205
C	-6.13319247	-2.31298218	-2.02495015
C	-5.17310940	-1.90186014	-2.96339822
C	-4.10424031	-1.05607508	-2.59564920
C	0.02286200	2.98090223	3.68458728
C	-1.21880409	3.70006128	3.08672424
C	-1.99067015	4.48592334	4.17838632
C	-2.66294020	-1.73971413	-4.59109635
C	-3.07276223	-0.59574105	-3.63192028
C	-3.61733028	0.60806205	-4.45102934
H	2.04148216	-2.89882822	2.66102620
H	3.90815030	-1.80832014	1.90808215
H	-3.05187323	3.72440529	-0.91059207
H	-4.23424132	1.77197513	-1.40010311
H	-2.15441417	-3.45043326	4.77768036
H	-2.85205722	-5.62249144	3.80707429
H	-1.94389215	-6.36982048	1.62053212
H	0.18314501	-1.00357607	3.08076123
H	3.08034523	1.18775909	1.32979710
H	-2.38337218	-1.17699109	4.75619237
H	-2.22637617	-0.52539304	3.10270724

H	-1.38293211	0.25998102	4.44580234
H	-0.22854102	-2.28980418	5.86422146
H	0.67633405	-0.80500506	5.49464841
H	1.27696310	-2.37693718	4.93276838
H	4.65211636	3.57336927	0.18824801
H	3.02442623	3.62177228	0.90781407
H	3.28415625	2.72593121	-0.59179305
H	4.74873436	1.18211509	3.22249824
H	3.77875229	2.66635520	3.14396824
H	5.46467740	2.67991921	2.58741220
H	6.66331350	2.22395617	0.61337205
H	8.30000661	0.79612606	-0.58908405
H	7.62864658	-1.43004511	-1.45418611
H	0.67731605	-4.45228134	-0.31426702
H	4.10641932	-2.79386721	-1.17731609
H	-2.11641816	-5.58878243	-0.88109107
H	-0.85249607	-5.25492540	-2.08603116
H	-1.58058112	-3.91418630	-1.16758409
H	-0.40148903	-7.28209957	0.25018402
H	1.16814809	-6.66653450	0.80388406
H	0.83052306	-6.82520650	-0.93497707
H	5.03384539	-2.02341415	-3.36929626
H	5.15363839	-3.78372529	-3.16382924
H	6.59659351	-2.77157821	-2.97702323
H	6.95954852	-3.76188929	-0.54467704
H	5.54817940	-4.79752037	-0.84401706
H	5.60470643	-3.75919729	0.59877005
H	0.33045403	7.02136055	-0.95871807
H	0.63120205	7.67767358	1.41123611
H	-0.06555501	6.14346449	3.22985925
H	-0.95049807	3.71288028	-2.13925916
H	-3.95771430	-0.09435001	1.36048110
H	1.14277509	5.87755244	-2.67051420
H	0.62335705	4.58546135	-3.77218629
H	1.41844411	4.15605732	-2.24823117
H	-2.70331921	5.57823942	-2.27394817
H	-1.78906413	5.37837240	-3.78590529
H	-1.41456311	6.71916049	-2.68528121
H	-5.89904344	-2.35655318	2.10578016
H	-4.83061937	-1.46564711	3.20375825
H	-4.13482332	-2.51427119	1.95233115
H	-6.01146747	1.28661310	0.88844507
H	-5.96257144	0.74007906	2.57831020
H	-7.03760454	-0.06154700	1.41393211
H	-6.78368350	-2.23286117	0.03150600
H	-6.94780353	-2.96326823	-2.33505518
H	-5.24893740	-2.24634317	-3.99016031
H	-1.88466514	2.91528422	2.71539921
H	-2.15862816	-0.27351302	-3.11880324
H	0.78793806	3.71096028	3.98559731
H	0.45193203	2.27898517	2.96067523
H	-0.27060502	2.41531918	4.58055435

H	-2.37926218	3.78353829	4.92770137
H	-2.84002222	5.04094038	3.75775528
H	-1.34768210	5.20045240	4.70798836
H	-2.31230718	-2.61809720	-4.03626431
H	-1.84611614	-1.39857511	-5.23807140
H	-3.48935527	-2.05169616	-5.24384340
H	-3.86658930	1.46162911	-3.80814129
H	-4.52068334	0.32976402	-5.01167438
H	-2.85705522	0.94548607	-5.16644839
O	0.98573007	0.21645602	1.49963912
O	-0.25409702	1.60537512	-1.90830815
O	0.16954301	-0.05224300	-2.52953119
O	-1.02029608	1.89191515	0.87861407
O	0.24050602	-2.02983116	0.05605900
C	1.06875108	-1.11552408	-3.88287330
H	0.34723803	-0.94629007	-4.68159836
C	0.82642506	-2.15315016	-3.00079323
H	-0.10701401	-2.70548921	-3.01939523
H	1.53820312	-2.40017218	-2.22052017
C	2.39405018	-0.40959903	-4.04632831
H	2.94715923	-0.81747006	-4.90778438
H	2.22432117	0.65905105	-4.21860832
H	2.99813823	-0.50706004	-3.14059024
Hf	0.32014402	0.24041802	-0.25469602

Bisperoxo Complex (butterfly conformation) to Oxo Peroxo Complex (butterfly conformation)

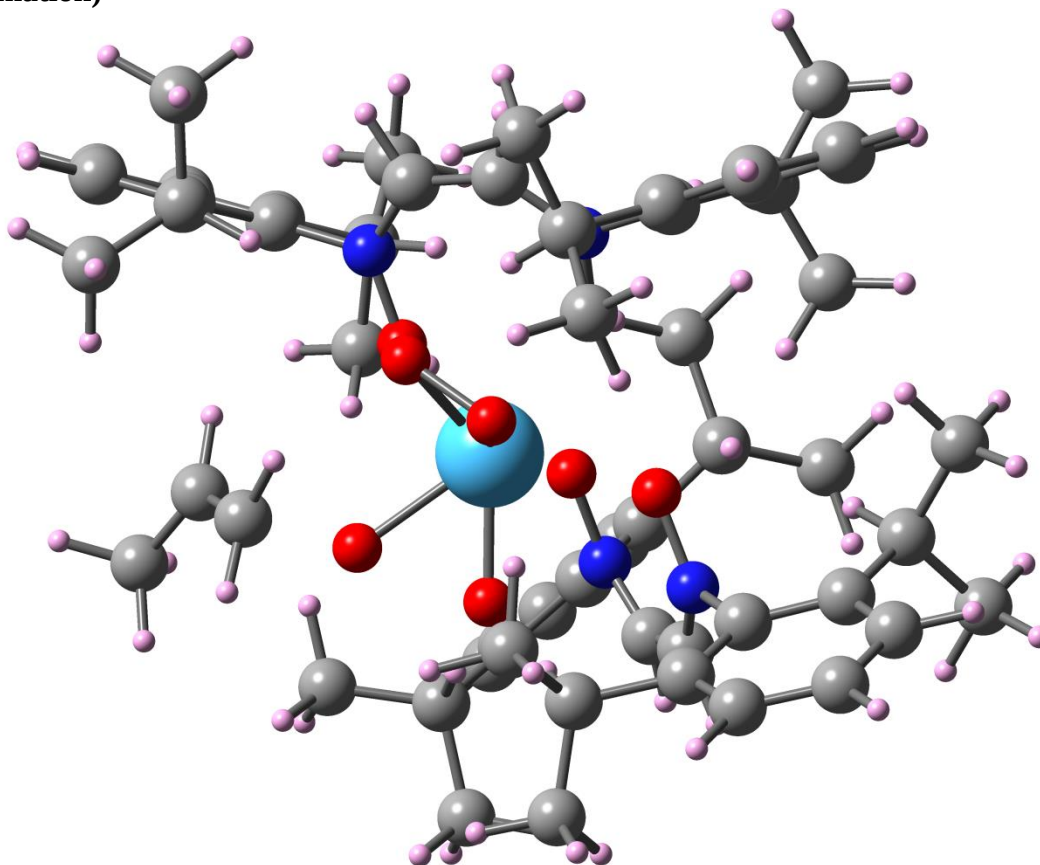


Fig. S155: ONCCNO Bisperoxo Complex (butterfly conformation) to Oxo Peroxo Complex (butterfly conformation)

E	E_{ZP}	H	G	<i>f</i>
-3011.9571	-3010.7124	-3010.6343	-3010.8285	-469
O	0.23766100	-0.97963000	1.29139200	
O	2.12035700	0.20686400	-0.23809900	
O	0.80649700	-1.82195500	-1.57808300	
N	0.25646100	2.85858500	0.34327500	
N	2.87220400	1.18618100	-0.76346000	
N	-2.76848700	-1.56140400	0.52404000	
N	0.26234500	-2.32079600	1.47014500	
C	1.38278900	3.18044100	-0.28973800	
C	2.50640600	2.46148000	-0.81695400	
C	-2.17682300	-2.65531600	1.01239300	
C	-0.83652700	-3.04729200	1.32096700	
C	-0.63875200	3.94593900	0.76953300	
C	-1.36841900	4.64428400	-0.22401000	
C	-2.19046100	5.70314600	0.22084200	
C	-2.29620900	6.02035100	1.58334800	
C	-1.58451100	5.27925900	2.54085000	

C	-0.73578900	4.22145700	2.15490600
C	-2.72966500	4.06862600	-2.28974400
C	-1.30871000	4.28999500	-1.71530500
C	-0.57048200	5.39300800	-2.52052200
C	2.79529100	-0.83592300	-4.26234700
C	3.10895100	0.55841200	-3.65786100
C	3.38356600	1.60112200	-4.77309200
C	4.18035200	0.77474000	-1.30122900
C	4.28596300	0.47667300	-2.68164300
C	5.56132200	0.08495300	-3.14733300
C	6.65904400	-0.00931300	-2.27984600
C	6.50903800	0.27922200	-0.91343000
C	5.26029900	0.67046200	-0.39002300
C	-0.98916300	2.55008700	4.03264000
C	0.01211400	3.40942900	3.21606300
C	0.86360100	4.31228500	4.14485500
C	5.63493900	-0.17332500	1.98765100
C	5.11612900	0.98701400	1.10196700
C	5.83472200	2.31722600	1.45608200
C	-4.23856600	-1.57574400	0.39500200
C	-4.85391400	-2.51468500	-0.47906200
C	-6.26272700	-2.47195700	-0.56363000
C	-7.01247700	-1.53774300	0.16552600
C	-6.36833500	-0.62050100	1.00967200
C	-4.96543500	-0.61932500	1.15029200
C	-4.54152700	-3.58960100	-2.79137700
C	-4.09101300	-3.56330200	-1.30759900
C	-4.27393700	-4.98281700	-0.69790000
C	2.09970900	-0.00235500	3.83160900
C	1.32984500	-1.33758400	4.01138800
C	1.18934700	-1.70527400	5.51002700
C	1.50994700	-2.92155500	1.95482700
C	2.01096300	-2.44368600	3.19740300
C	3.19872300	-3.02622700	3.68110000
C	3.84898100	-4.04746400	2.97061000
C	3.32419100	-4.49923200	1.75285900
C	2.14574200	-3.94568900	1.20387600
C	-4.33478700	1.81140700	1.44270500
C	-4.29751700	0.39787700	2.08208800
C	-4.93749600	0.40311100	3.49376200
C	2.74977600	-4.37780500	-1.22908000
C	1.64432600	-4.46926000	-0.14759500
C	1.12668900	-5.92757800	-0.01742300
H	1.48213200	4.25278200	-0.41963700
H	3.22930700	3.09738500	-1.31611200
H	-2.89403800	-3.43928800	1.22208200
H	-0.72299100	-4.09880500	1.55539400
H	-2.76207600	6.27165300	-0.50741400
H	-2.93912800	6.83832500	1.90019300
H	-1.68445500	5.52690400	3.59430100
H	-0.76745900	3.34640500	-1.85532100
H	2.20295400	0.87513900	-3.12889700

H	-3.32730000	4.99095600	-2.28780200
H	-3.26445100	3.30482400	-1.71401000
H	-2.65171200	3.71308000	-3.32332100
H	-1.09114600	6.35830500	-2.45104000
H	-0.51825300	5.10779100	-3.57866300
H	0.45791700	5.54319600	-2.16437900
H	3.66000100	-1.25942400	-4.79361600
H	1.96759700	-0.74417800	-4.97778600
H	2.47390300	-1.53286100	-3.48047100
H	3.59271500	2.59552100	-4.35462900
H	2.49968000	1.68712700	-5.41741100
H	4.23653200	1.31552300	-5.40486700
H	5.68697100	-0.15189300	-4.20022300
H	7.62982400	-0.31255000	-2.66532000
H	7.36507100	0.19408800	-0.24945200
H	0.68984900	2.71133500	2.71451700
H	4.05209900	1.10735200	1.33256300
H	-1.72591200	3.18119300	4.54777100
H	-0.45710000	1.96209600	4.79212500
H	-1.52004700	1.85700100	3.37088800
H	0.23803100	4.99343500	4.73634000
H	1.57304200	4.92184400	3.57010900
H	1.43724100	3.69424100	4.84811700
H	5.10362200	-1.10517300	1.76385100
H	5.47612200	0.06433600	3.04781900
H	6.70940200	-0.34577500	1.84317700
H	6.91311600	2.24800700	1.26148500
H	5.69728700	2.55497700	2.51941600
H	5.44213400	3.15531000	0.86517700
H	-6.77423300	-3.16957600	-1.22029600
H	-8.09584200	-1.52317300	0.07365300
H	-6.95915200	0.09792600	1.57070000
H	-3.02187600	-3.32180400	-1.30857900
H	0.32361100	-1.17243600	3.61473800
H	-5.58129800	-3.92510000	-2.89924200
H	-3.90836800	-4.29023400	-3.35072100
H	-4.44353500	-2.60510200	-3.25871600
H	-3.95897700	-5.03847500	0.35259600
H	-3.68439500	-5.71390900	-1.26557300
H	-5.32714200	-5.29053300	-0.73868100
H	3.13587200	-0.09537900	4.18496200
H	1.61358900	0.79616500	4.40765000
H	2.10614100	0.27973600	2.77389900
H	0.67384000	-2.66539300	5.64295800
H	0.60743200	-0.93111700	6.02798500
H	2.16284600	-1.77246100	6.01244400
H	3.61224800	-2.68670200	4.62653500
H	4.76201800	-4.48723600	3.36529100
H	3.84129900	-5.28250700	1.20606100
H	-3.24165900	0.13441800	2.19700500
H	0.83387700	-3.83364900	-0.50975000
H	-5.36836600	2.14330400	1.27273900

H	-3.80227500	1.80631500	0.48650100
H	-3.84580000	2.54091500	2.10080300
H	-4.37476300	1.07853700	4.15140500
H	-4.92870900	-0.59805800	3.94442300
H	-5.97684900	0.75554500	3.47369000
H	3.09269400	-3.34380300	-1.32995600
H	2.33611100	-4.68299100	-2.19826300
H	3.60998900	-5.02476100	-1.00597700
H	0.31414500	-6.01648800	0.71835800
H	1.92687600	-6.61321400	0.29353200
H	0.74288000	-6.27347300	-0.98583500
O	0.38786500	1.32757500	-2.06564100
O	-1.23093500	0.53080200	-2.57674400
O	-0.68505200	-2.13727800	-1.37018600
O	-2.19645400	-0.41275100	0.11897200
O	-0.20180400	1.62014100	0.60077300
C	-3.24623000	-0.19635600	-3.16646500
H	-3.61840500	-0.60825700	-2.23312500
C	-2.04989200	-0.69164300	-3.68453000
H	-1.61227800	-1.60854300	-3.29785100
H	-1.70154000	-0.34879100	-4.65651800
C	-4.04642300	0.90982700	-3.79772100
H	-3.49359800	1.38053300	-4.61900900
H	-4.99724800	0.52293000	-4.20197500
H	-4.30396400	1.68559800	-3.06621400
Hf	-0.11653100	-0.14398200	-0.85444400

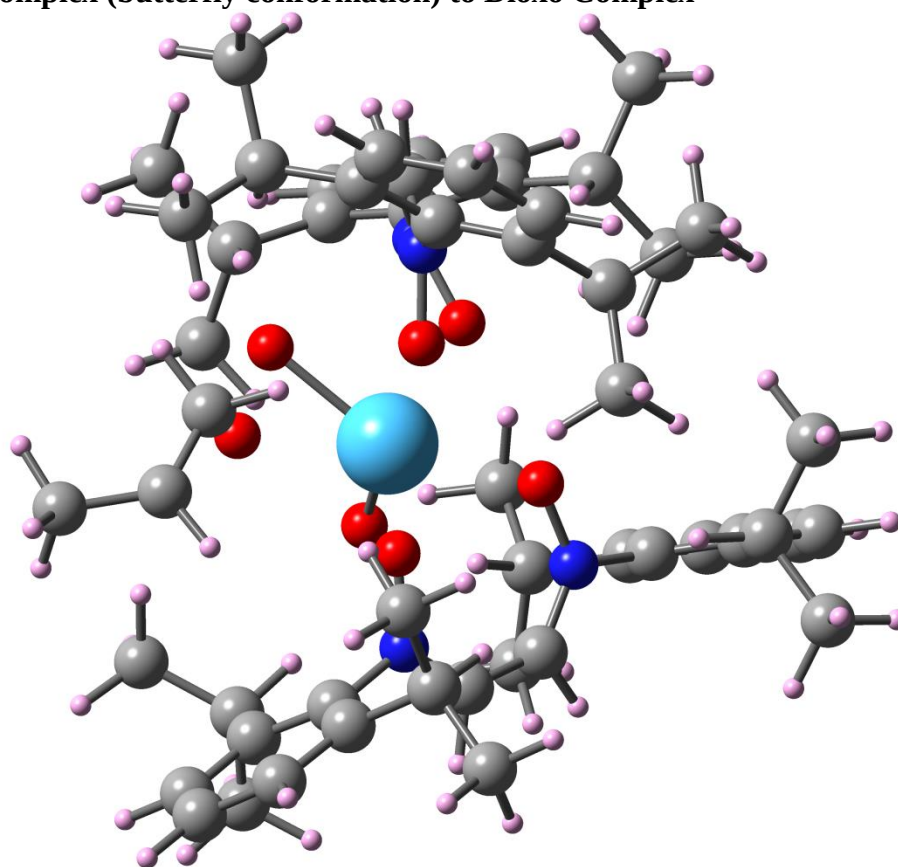
Oxo Peroxo Complex (butterfly conformation) to Dioxo Complex

Fig. S156: ONCCNO Oxo Peroxo Complex (butterfly conformation) to Dioxo Complex

E	E_{ZP}	H	G	<i>f</i>
-2936.7937	-2935.5539	-2935.4766	-2935.6726	-86
O	-0.64140463	1.71022699	0.68192218	
O	-1.97393247	-0.93058010	0.14004379	
O	-1.49081567	0.77939838	-2.17708227	
N	0.68940411	-2.61178702	1.20597539	
N	-2.35655837	-2.23464975	0.04828473	
N	2.38989644	1.77929454	-0.85027112	
N	-0.16376170	2.95838055	0.83711245	
C	-0.29799219	-3.46496247	0.89200898	
C	-1.61087402	-3.29925345	0.38251758	
C	1.95500154	3.01907162	-0.59765200	
C	0.91664727	3.50775367	0.23435813	
C	1.97012536	-3.14547049	1.68560355	
C	2.88807578	-3.65450806	0.73304215	
C	4.09290740	-4.19342106	1.23635258	
C	4.36860936	-4.20427326	2.61197776	
C	3.44562566	-3.66557466	3.52309079	
C	2.22498694	-3.11771841	3.07832406	
C	3.75660529	-2.92576285	-1.54743705	

C	2.62022426	-3.64335281	-0.77571109
C	2.42548591	-5.08763641	-1.30930316
C	-2.69376834	-2.13839367	-4.03235048
C	-2.62921154	-3.04653950	-2.77726704
C	-2.53584889	-4.54199225	-3.18194706
C	-3.70079493	-2.42374960	-0.49339371
C	-3.82927592	-2.81013519	-1.85190323
C	-5.14459001	-2.97252492	-2.34129205
C	-6.26069815	-2.73538537	-1.52456750
C	-6.09204529	-2.32674684	-0.19050047
C	-4.80354356	-2.16015488	0.35634550
C	1.88483828	-1.37828144	4.89448453
C	1.23446208	-2.53189899	4.08811395
C	0.68213087	-3.62822944	5.03729897
C	-5.07166707	-0.21761143	1.96465497
C	-4.62900408	-1.69631125	1.80575558
C	-5.38310303	-2.61362437	2.80211350
C	3.64812956	1.54562538	-1.56495592
C	3.67527458	1.50610851	-2.98129509
C	4.92328997	1.24152426	-3.58968613
C	6.07794642	1.02374569	-2.82580108
C	6.01557219	1.07003482	-1.42344402
C	4.80042093	1.33137582	-0.76028630
C	2.07157697	0.39040647	-4.59715340
C	2.43880944	1.70600961	-3.86002634
C	2.63654164	2.87328785	-4.86134329
C	-1.18023978	1.14082980	4.04048462
C	-0.19192414	2.28303182	3.68045532
C	0.68215152	2.67470653	4.89832359
C	-0.96708800	3.80303637	1.73285319
C	-0.96460541	3.47742113	3.11372702
C	-1.73669156	4.28672666	3.97179977
C	-2.47362739	5.37368442	3.47587520
C	-2.46588264	5.66130490	2.10348437
C	-1.72415240	4.87607385	1.19428574
C	5.05226569	-0.01879474	1.37759946
C	4.76729239	1.37966750	0.77159722
C	5.75408126	2.43969548	1.32746056
C	-3.24295139	5.24883076	-0.82064934
C	-1.78176173	5.21109112	-0.30232045
C	-1.07235850	6.55941733	-0.60296943
H	-0.02217083	-4.50061329	1.05520799
H	-2.13716239	-4.23415657	0.22438052
H	2.55722969	3.79241806	-1.06329923
H	0.99561830	4.56982292	0.43851307
H	4.82175421	-4.59832227	0.53970958
H	5.30376216	-4.62551478	2.97399584
H	3.67406711	-3.67007541	4.58585734
H	1.70846396	-3.07415555	-0.99429786
H	-1.69848256	-2.77310557	-2.26734672
H	4.72309285	-3.43936960	-1.44325308
H	3.87159179	-1.89241057	-1.20138748

H	3.50266494	-2.89030733	-2.61395132
H	3.33052462	-5.69670157	-1.17367922
H	2.19237166	-5.05685400	-2.38108534
H	1.59753748	-5.60034236	-0.80008178
H	-3.59527977	-2.32418253	-4.63376250
H	-1.81683117	-2.33158018	-4.66247597
H	-2.66135028	-1.08268061	-3.74256667
H	-2.45353570	-5.19777920	-2.30374119
H	-1.64744226	-4.70112499	-3.80595334
H	-3.41632111	-4.86224307	-3.75638434
H	-5.29072123	-3.27610025	-3.37450858
H	-7.26272930	-2.86254258	-1.92806276
H	-6.96550435	-2.13981208	0.42894578
H	0.38854912	-2.10303503	3.54034699
H	-3.56368821	-1.73676491	2.05807904
H	2.74209709	-1.73211150	5.48204214
H	1.15740861	-0.94505973	5.59383739
H	2.23445124	-0.58604833	4.22175505
H	1.48365740	-4.07658566	5.63899320
H	0.19468160	-4.43485121	4.47447571
H	-0.05635608	-3.19863231	5.72724869
H	-4.48464321	0.43398106	1.30830814
H	-4.92089344	0.11481299	3.00035434
H	-6.13472359	-0.09153712	1.71898784
H	-6.46901624	-2.57534428	2.64638297
H	-5.18484126	-2.29266430	3.83327522
H	-5.06640513	-3.66003762	2.70273231
H	4.98148874	1.19863873	-4.67391185
H	7.02448036	0.81662788	-3.31997084
H	6.91715549	0.90195438	-0.83986128
H	1.57828927	1.94360670	-3.22938500
H	0.47449266	1.89141117	2.90560577
H	2.88458862	0.05499486	-5.25729491
H	1.17431191	0.55035086	-5.20846375
H	1.84117721	-0.40691619	-3.88165179
H	2.87942457	3.81300195	-4.34590435
H	1.71269627	3.02834779	-5.43343795
H	3.44244824	2.66667882	-5.57876881
H	-1.89040777	1.46208549	4.81520241
H	-0.62900472	0.27137365	4.41949558
H	-1.74088518	0.82999541	3.15264651
H	1.37749598	3.48642947	4.64786981
H	1.27234934	1.80926930	5.22562794
H	0.07522781	3.00199310	5.75266301
H	-1.75635883	4.06711768	5.03565427
H	-3.05745240	5.98973807	4.15561073
H	-3.05340460	6.49550722	1.72946527
H	3.76016542	1.65973637	1.09559946
H	-1.26171002	4.42741582	-0.86278350
H	6.04523411	-0.38706002	1.08648958
H	4.30181870	-0.74305488	1.04519616
H	5.01806455	0.02962783	2.47441987

H	5.67184982	2.49348376	2.42133762
H	5.54458258	3.43720641	0.91892917
H	6.79543462	2.19087999	1.08486301
H	-3.76032532	4.30203697	-0.62884755
H	-3.25093939	5.42676746	-1.90405984
H	-3.81960107	6.05440575	-0.34842938
H	-0.02469019	6.55444333	-0.27434929
H	-1.57478819	7.39158311	-0.09281474
H	-1.08816690	6.76513028	-1.68107048
O	0.26533989	-1.64846142	-1.69852583
O	-0.11103775	1.44082746	-2.11453659
O	1.88324813	0.67784708	-0.20127657
O	0.62132258	-1.26436213	1.10943985
C	-2.68915268	1.82984170	-1.73988074
H	-2.45179121	1.98108082	-0.68173070
C	-3.96811769	1.23306938	-2.01620336
H	-4.37917580	0.53500627	-1.28894194
C	-4.69637682	1.40165549	-3.31687835
H	-4.23706127	2.18009027	-3.93915330
H	-4.69679156	0.46615792	-3.90510971
H	-5.75713726	1.65891872	-3.16036298
H	-2.42615641	2.68258292	-2.37090614
Hf	-0.09601898	-0.16251658	-0.70112872

13.2 Triplet Geometries

Oxo Complex to Oxo Complex with Adsorbed Oxygen Molecule

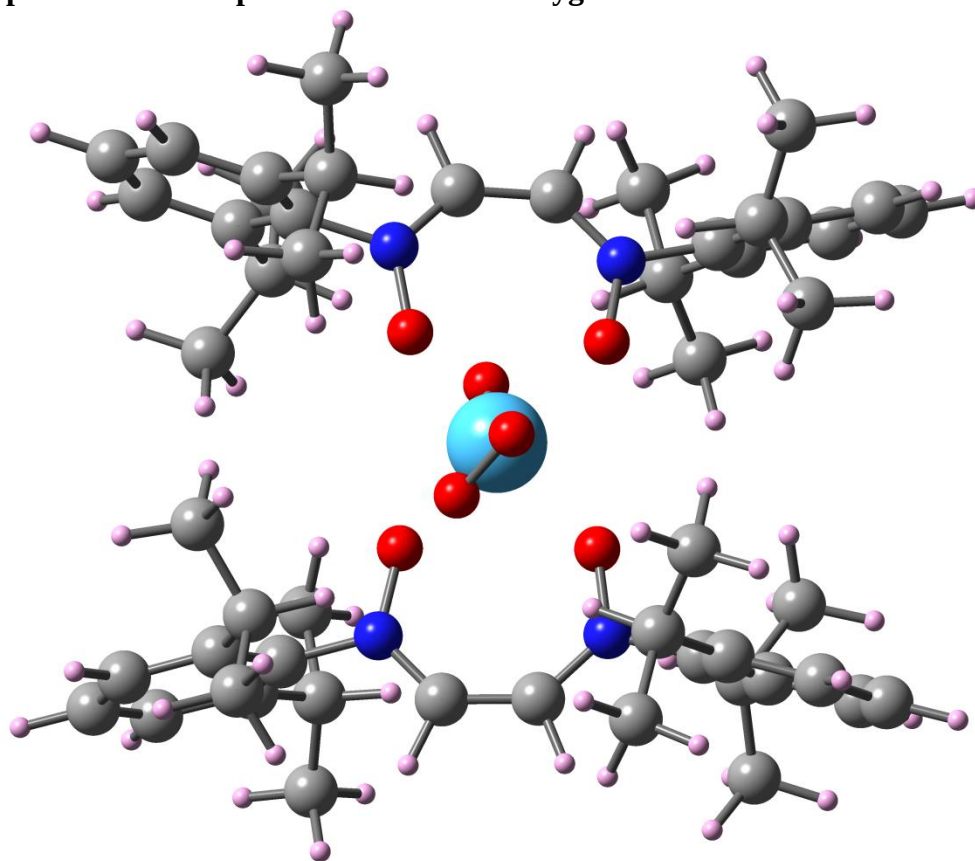


Fig. S157: ONCCNO Oxo Complex to Oxo Complex with Adsorbed Oxygen Molecule

E	E_{ZP}	H	G	<i>f</i>
-2818.9420	-2817.7847	-2817.7116	-2817.9005	-129

O	-1.41112211	-1.48245212	-0.64171705
O	1.54604612	1.46924511	0.32293202
O	0.18699301	0.14877301	2.65641321
O	-0.59807405	-0.72827506	1.96082915
N	-1.49233111	2.83080722	0.18428501
N	1.75301013	2.62644620	-0.34386403
N	1.56162012	-2.71631521	0.36770803
N	-1.71980813	-2.73392421	-0.15260901
C	-0.58417604	3.63481628	-0.37403503
C	0.82094006	3.54528727	-0.60555605
C	0.56591504	-3.63366828	0.52853004
C	-0.81497406	-3.64438828	0.30515802
C	-2.88645022	3.27880725	0.29618602
C	-3.72559828	3.11923324	-0.83175106
C	-5.05669139	3.57049027	-0.69600705
C	-5.51672542	4.11751232	0.51203204
C	-4.65958835	4.22267532	1.62043913

C	-3.31617125	3.80207529	1.53980712
C	-4.15524932	1.30533010	-2.56383520
C	-3.24405225	2.48620719	-2.14296616
C	-3.16676024	3.54772427	-3.27265125
C	2.87335822	1.22624909	-4.10986331
C	2.39819618	2.40522618	-3.22380425
C	2.06560216	3.63971728	-4.10510632
C	3.13725024	2.86301422	-0.77224006
C	3.43929326	2.76499021	-2.15478417
C	4.77789136	3.01823623	-2.52608119
C	5.75502246	3.32605625	-1.56708312
C	5.41952143	3.38649826	-0.20477602
C	4.09784831	3.15475424	0.22739002
C	-2.74305121	2.69952921	3.74083829
C	-2.40073618	3.85987530	2.76611921
C	-2.45682419	5.22998840	3.48595427
C	4.41290134	2.01334915	2.46256219
C	3.75399728	3.20500225	1.71896613
C	4.15692631	4.55696935	2.36145118
C	2.92796723	-3.03474323	0.75435206
C	3.27685425	-3.02658623	2.12998516
C	4.60565735	-3.36726026	2.46480719
C	5.54625441	-3.68373128	1.47327011
C	5.17554540	-3.66918328	0.11888901
C	3.85960029	-3.34635825	-0.26990502
C	2.79291921	-1.51371511	4.12592931
C	2.28109817	-2.67883521	3.24169125
C	1.96179715	-3.92516730	4.11075031
C	-2.76727021	-2.39762818	-3.73749228
C	-2.56425719	-3.61822128	-2.79896022
C	-2.68223121	-4.95022638	-3.58054328
C	-3.11752024	-3.10110524	-0.33158003
C	-3.53223727	-3.54407527	-1.61468212
C	-4.89234437	-3.87836129	-1.77658613
C	-5.79401245	-3.77658429	-0.70373405
C	-5.35472738	-3.32650925	0.55046004
C	-4.00560231	-2.96773123	0.76346906
C	4.29483433	-2.29171717	-2.53449819
C	3.47774126	-3.35160726	-1.75228214
C	3.65281428	-4.76088636	-2.37648318
C	-4.30765233	-1.13892709	2.50033419
C	-3.55660227	-2.44421319	2.13059116
C	-3.74108629	-3.51841727	3.23459125
H	-1.01657108	4.56921835	-0.71420705
H	1.22760309	4.41836034	-1.10276308
H	0.94517107	-4.55976235	0.94775907
H	-1.29304010	-4.58247035	0.56716904
H	-5.73819144	3.47818627	-1.53704312
H	-6.54809849	4.45243834	0.59468405
H	-5.03707038	4.63130235	2.55353920
H	-2.23947117	2.06667516	-2.00927815
H	1.47356111	2.06119116	-2.74448321

H	-5.18002840	1.63300112	-2.78612821
H	-4.19782332	0.54230304	-1.77805014
H	-3.74794729	0.83335306	-3.46619526
H	-4.15260132	3.98517930	-3.48240426
H	-2.79607922	3.08315224	-4.19492432
H	-2.48441419	4.36845034	-3.01195323
H	3.76493729	1.47876611	-4.70064036
H	2.07175316	0.95166607	-4.80665337
H	3.09903524	0.34576503	-3.49906327
H	1.68655113	4.48124434	-3.50858627
H	1.29461510	3.37529626	-4.83990437
H	2.95058222	3.99329231	-4.65198935
H	5.05703838	2.95833023	-3.57426828
H	6.77987051	3.51130127	-1.88019715
H	6.18842645	3.61620228	0.52785704
H	-1.36545611	3.70031428	2.44214319
H	2.67198320	3.08794123	1.83828514
H	-3.77878329	2.77968421	4.09821131
H	-2.07551516	2.72839221	4.61174635
H	-2.61405120	1.73115813	3.24702925
H	-3.44482627	5.41974443	3.92480330
H	-2.22706417	6.05686045	2.80107421
H	-1.72613713	5.25027340	4.30482233
H	4.08409631	1.06243008	2.02997816
H	4.12973431	2.02571615	3.52311127
H	5.50854942	2.06182916	2.40138518
H	5.24337040	4.71156936	2.33560318
H	3.84434429	4.57860035	3.41358726
H	3.68456028	5.40413439	1.84682014
H	4.90551337	-3.37463026	3.50945827
H	6.56540053	-3.93975330	1.75419413
H	5.91182948	-3.91625930	-0.64196105
H	1.34515710	-2.34102718	2.78869021
H	-1.54065712	-3.55098727	-2.41400118
H	3.71895228	-1.77819614	4.65462936
H	2.03329516	-1.25576110	4.87390837
H	2.98002923	-0.61938105	3.52181927
H	1.55751012	-4.74712536	3.50501027
H	1.21746910	-3.66985228	4.87611037
H	2.86004922	-4.29680033	4.62207736
H	-3.79187329	-2.37104418	-4.13439831
H	-2.07241416	-2.45354518	-4.58623335
H	-2.57033620	-1.46672311	-3.19674525
H	-2.55021920	-5.81795544	-2.92094222
H	-1.91119615	-4.99342338	-4.36105133
H	-3.65638228	-5.04842238	-4.07735831
H	-5.24812140	-4.22125132	-2.74438121
H	-6.83857553	-4.04370831	-0.84805307
H	-6.06441848	-3.24394125	1.36970810
H	2.42439919	-3.07069224	-1.84193514
H	-2.49329519	-2.19101317	2.08537716
H	5.36913741	-2.52069719	-2.52089419

H	4.15034532	-1.29732710	-2.09736816
H	3.96966930	-2.25926917	-3.58285927
H	3.33224526	-4.75126736	-3.42678726
H	3.05317223	-5.51039741	-1.84373814
H	4.70105036	-5.08735839	-2.34901918
H	-4.14240131	-0.36536503	1.74137214
H	-3.93792830	-0.75503106	3.45994626
H	-5.38959842	-1.30541210	2.59404820
H	-3.18991024	-4.43767434	2.99583623
H	-4.79857337	-3.78573329	3.36561226
H	-3.36820126	-3.13869724	4.19473832
O	-0.17748801	0.85251406	-1.80182214
O	-1.26324010	1.60668612	0.69731905
O	1.40973211	-1.49566512	-0.27392402
Hf	-0.02423400	0.02750400	-0.18080801

Oxo Complex with Adsorbed Oxygen Molecule to Dioxo Complex

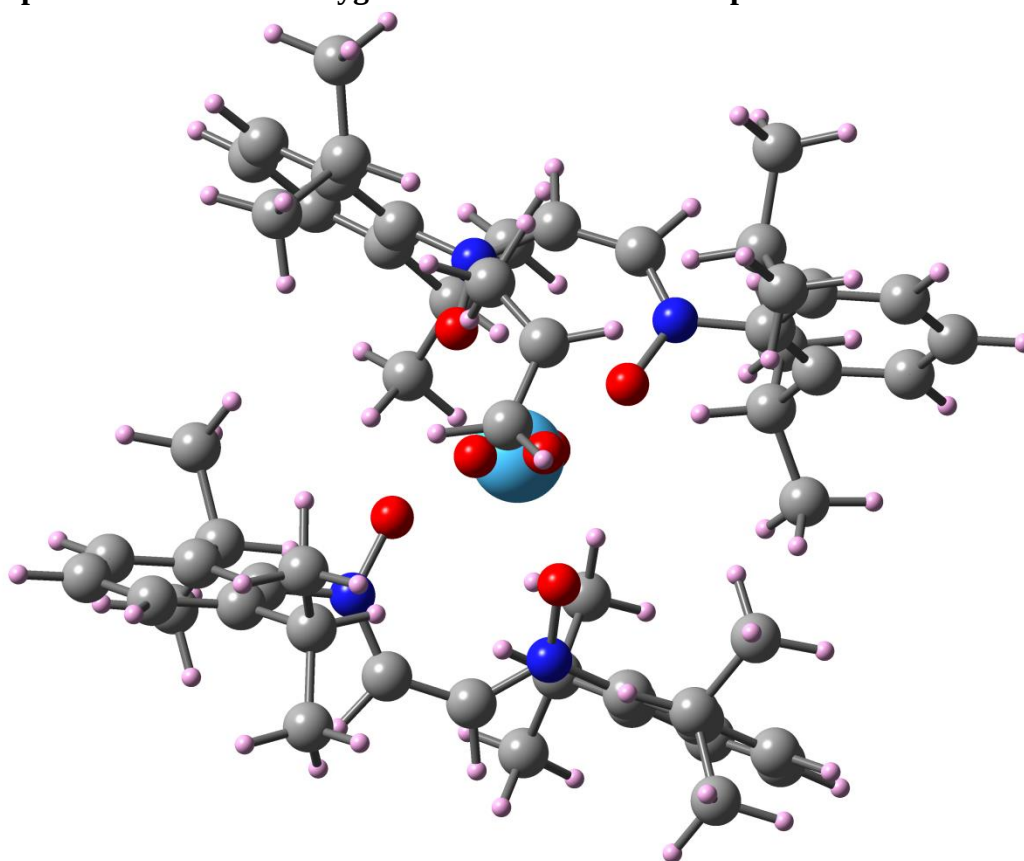


Fig. S158: ONCCNO Oxo Complex with Adsorbed Oxygen Molecule to Dioxo Complex

E	E_{zp}	H	G	<i>f</i>
-2936.8092	-2935.5688	-2935.4920	-2935.6863	-104
O	-1.87676177	-0.97603580	0.04384613	
O	1.70819544	1.05121543	0.85728365	
O	0.44204766	0.00914500	3.44009707	
O	-0.60976751	-0.04654293	2.43875652	
N	-0.62707233	2.93350704	-0.70692439	
N	2.43842637	2.02815871	0.18991259	
N	0.51746932	-3.14755371	-0.21055656	
N	-2.48357297	-2.16402455	0.37989539	
C	0.61515376	3.45817238	-0.89316668	
C	1.90408933	3.07540643	-0.50362437	
C	-0.67046671	-3.81118508	-0.24330796	
C	-1.95752664	-3.39742425	0.10702996	
C	-1.77998580	3.46335510	-1.41517094	
C	-1.92301483	3.18661796	-2.80112018	
C	-3.04300073	3.74205229	-3.45853770	
C	-3.99232338	4.50583017	-2.76352360	
C	-3.84084733	4.73627154	-1.38620982	
C	-2.73030706	4.22478151	-0.68521960	

C	-1.64072899	1.17787163	-4.34758953
C	-0.92835046	2.32341771	-3.58536387
C	-0.09620971	3.19221689	-4.56633945
C	4.40238380	-0.73904090	-2.31177131
C	3.89307175	0.68288544	-1.97290944
C	4.07216868	1.62331454	-3.19630863
C	3.88564388	1.90383784	0.30453168
C	4.59624885	1.26346879	-0.74282577
C	6.00251876	1.20222065	-0.62780661
C	6.66572915	1.73828115	0.48651995
C	5.93370625	2.34609154	1.51910340
C	4.52818679	2.43565102	1.45071753
C	-3.63226175	3.64751589	1.60763112
C	-2.58683837	4.47935121	0.81757316
C	-2.68995198	5.98520249	1.16943520
C	4.08624130	2.50784537	3.95796662
C	3.74641582	3.12028077	2.57493293
C	3.99747747	4.65226575	2.57618463
C	1.71558088	-3.67783006	-0.82434712
C	2.79663340	-4.05543029	0.01965202
C	3.96058035	-4.55920547	-0.59381811
C	4.04151192	-4.70136898	-1.98898094
C	2.95831282	-4.32839258	-2.79701319
C	1.77441360	-3.79720595	-2.23996178
C	3.66275650	-2.81358046	2.05417055
C	2.72762350	-3.94278889	1.54632307
C	3.05449993	-5.29119982	2.23831290
C	-4.87134289	0.08918120	-1.95705339
C	-4.51089645	-1.37625281	-1.60004434
C	-5.21225568	-2.37251234	-2.56044713
C	-3.86668617	-2.04525320	0.81510679
C	-4.85109678	-1.67849511	-0.13833659
C	-6.19013347	-1.60835948	0.29980557
C	-6.53369455	-1.89624122	1.63008035
C	-5.53732391	-2.24347348	2.55576865
C	-4.18070649	-2.31073600	2.17287449
C	1.07479618	-2.18353294	-4.08494969
C	0.64026148	-3.36554815	-3.17919972
C	0.12193921	-4.56477480	-4.01683208
C	-3.23053234	-1.78944748	4.47891124
C	-3.10603408	-2.66331775	3.20598096
C	-3.15669467	-4.17009775	3.57513289
H	0.59216452	4.34658481	-1.51577780
H	2.67965260	3.74190933	-0.86718089
H	-0.58710221	-4.83427540	-0.59647892
H	-2.70192003	-4.18594805	0.15127897
H	-3.17825748	3.55760803	-4.52107575
H	-4.85113737	4.91522476	-3.29095559
H	-4.58620431	5.32350381	-0.85569217
H	-0.24531145	1.82735375	-2.88810492
H	2.81851712	0.59747465	-1.77310415
H	-2.32964879	1.54985435	-5.11955162

H	-2.20077812	0.54448179	-3.65074134
H	-0.88907432	0.54587306	-4.83627851
H	-0.73469585	3.66283997	-5.32747507
H	0.64445202	2.56802529	-5.08314261
H	0.44420669	3.99188224	-4.04205440
H	5.45540658	-0.73864760	-2.62720972
H	3.80792554	-1.15360423	-3.13336080
H	4.30002609	-1.41505492	-1.45502549
H	3.66698249	2.62388805	-2.99813433
H	3.53912507	1.21181168	-4.06297281
H	5.13262583	1.73265053	-3.46461644
H	6.57954940	0.72405521	-1.41436123
H	7.74994776	1.67993515	0.55239229
H	6.45865627	2.75355627	2.37974800
H	-1.59682325	4.12988131	1.12700493
H	2.67955813	2.95380810	2.38953034
H	-4.65627562	3.92648152	1.32505605
H	-3.52404943	3.82060046	2.68809227
H	-3.49716890	2.57867184	1.40965224
H	-3.68332322	6.39013215	0.93747491
H	-1.94852591	6.57638461	0.61646834
H	-2.51595157	6.13560700	2.24380749
H	3.88034498	1.42980240	3.97012087
H	3.49849673	2.99543852	4.74977627
H	5.14391482	2.64766577	4.21349556
H	5.05710056	4.87966064	2.75188999
H	3.41162125	5.14083525	3.36718511
H	3.71254290	5.10040470	1.61618310
H	4.80440752	-4.85494052	0.02447580
H	4.94688755	-5.09786106	-2.44315238
H	3.03538181	-4.43297598	-3.87632761
H	1.70991307	-3.65683849	1.82620673
H	-3.43046632	-1.47935614	-1.73489384
H	4.71027958	-3.01148222	1.78728275
H	3.60103692	-2.73369169	3.14850906
H	3.36801736	-1.85090875	1.62330813
H	2.39188434	-6.09272110	1.88607365
H	2.92600586	-5.19485105	3.32511753
H	4.09022409	-5.60619728	2.05504840
H	-5.94631358	0.28119405	-1.83612520
H	-4.60737220	0.30122742	-3.00094765
H	-4.32052269	0.79003337	-1.31985522
H	-4.93900696	-3.41051766	-2.32922414
H	-4.91746441	-2.16579600	-3.59781411
H	-6.30581750	-2.29071859	-2.50052428
H	-6.96853167	-1.33362549	-0.40766229
H	-7.57348091	-1.84586445	1.94548047
H	-5.81457321	-2.45307412	3.58577124
H	-0.19507047	-2.99190405	-2.58126979
H	-2.12621630	-2.44931347	2.76732189
H	1.98869597	-2.41600275	-4.64933441
H	1.22547532	-1.28830902	-3.47040129

H	0.27851102	-1.96362848	-4.81036929
H	-0.72605005	-4.24963678	-4.63922823
H	-0.21286611	-5.39256165	-3.37645275
H	0.89924082	-4.95527482	-4.68715180
H	-3.21588460	-0.72497514	4.21480338
H	-2.39123198	-1.99949573	5.15677693
H	-4.15749530	-1.99244183	5.03120004
H	-3.00482586	-4.80214975	2.69162376
H	-4.12586874	-4.43678489	4.01831972
H	-2.37087144	-4.41361647	4.30294472
O	0.50994382	0.04912699	-1.66371661
O	-0.89487596	1.89897568	0.18451185
O	0.66575414	-2.00196407	0.56667855
C	0.43924177	1.68357355	4.25912566
H	1.49419765	1.87364424	4.42544195
C	-0.11636930	0.42859495	4.80462899
H	0.42606728	-0.09896151	5.58688475
H	-1.19494824	0.29851275	4.82135571
C	-0.38557290	2.60136064	3.45389753
H	-0.69966155	2.03620244	2.53969011
H	-1.31927712	2.87972512	3.95982833
H	0.16211182	3.49150981	3.13718477
Hf	0.03180095	-0.03512821	0.09348008

Adsorbed PO Octahedral Complex to Octahedral Complex with Transferred Allylic H

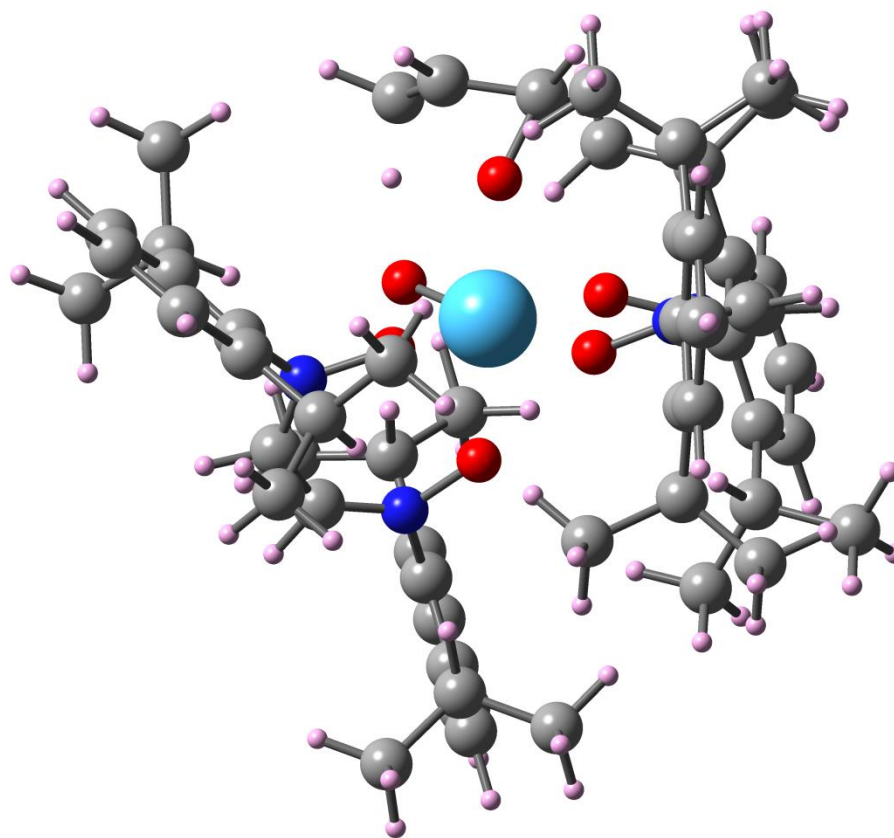


Fig. S159: ONCCNO Adsorbed PO Octahedral Complex to Octahedral Complex with Transferred Allylic H

E	E_{zp}	H	G	<i>f</i>
-2861.7041	-2860.4680	-2860.3926	-2860.5849	-464
O	0.50498604	-1.25252310	0.81980906	
O	1.69343013	0.91202807	-1.13079408	
O	0.03620800	-1.34566310	-2.10909916	
N	-0.08593701	2.95816423	0.77609706	
N	2.62186720	1.76201913	-0.54457904	
N	-2.66376320	-1.88119414	-0.11732301	
N	0.37099703	-2.61959820	0.99101707	
C	1.13926709	3.51314727	0.54096804	
C	2.31727717	2.96672323	0.02641400	
C	-2.06782716	-3.00983923	0.35941303	
C	-0.78227606	-3.32249125	0.81324606	
C	-1.14633409	3.72634829	1.41270511	
C	-1.91470115	4.63179535	0.63996005	
C	-2.92842322	5.35955041	1.30031610	
C	-3.17722824	5.17489140	2.66814820	
C	-2.41420118	4.25448533	3.40553226	
C	-1.38127310	3.51318227	2.79706921	

C	-2.97175723	4.41199734	-1.65719813
C	-1.70375813	4.82513537	-0.86450707
C	-1.28645010	6.28149450	-1.19744409
C	3.35516826	0.68347505	-4.19572932
C	3.68655928	1.89402815	-3.28336225
C	4.37060633	3.03015723	-4.08589931
C	4.00741731	1.38525610	-0.76886506
C	4.53033335	1.44540911	-2.08829516
C	5.87513447	1.07057608	-2.28131717
C	6.67646451	0.66809305	-1.20092209
C	6.13904448	0.62207605	0.09362901
C	4.79133537	0.96410507	0.33781203
C	-1.44211011	1.25217109	3.92756030
C	-0.57520304	2.50123519	3.61573128
C	-0.00014400	3.12253724	4.91340037
C	4.51312134	-0.50397404	2.40686418
C	4.23552732	0.87713207	1.76303413
C	4.80832237	2.01622515	2.64987320
C	-4.05322631	-1.89885015	-0.54277504
C	-4.38393134	-2.49545619	-1.78739014
C	-5.74844346	-2.53294619	-2.14806417
C	-6.73288550	-1.96956115	-1.32168810
C	-6.37182749	-1.35593910	-0.11132501
C	-5.02607538	-1.31176210	0.30737902
C	-3.49249227	-2.56436719	-4.17533032
C	-3.32589126	-3.08752824	-2.72605521
C	-3.37316126	-4.63974236	-2.71500521
C	1.36952510	-1.77043014	4.85507337
C	0.70987205	-2.79180421	3.89388930
C	-0.00603300	-3.91414730	4.69195636
C	1.55900412	-3.28293425	1.50517111
C	1.72675813	-3.37820026	2.90962022
C	2.87108222	-4.05213931	3.38496726
C	3.81011829	-4.59381735	2.49193119
C	3.62616528	-4.46599634	1.10559208
C	2.49740919	-3.80185329	0.57804304
C	-4.84915037	0.90026407	1.52260412
C	-4.65453236	-0.63532105	1.62919713
C	-5.45076940	-1.21922609	2.82397222
C	3.53253227	-3.06209523	-1.63288313
C	2.29757618	-3.68534528	-0.93574907
C	1.96263415	-5.07176639	-1.54880512
H	1.20513009	4.55020835	0.85284706
H	3.18635324	3.61270228	0.11005101
H	-2.74697021	-3.85556330	0.35514603
H	-0.65628705	-4.36677034	1.07997608
H	-3.53354827	6.06534549	0.73647205
H	-3.96643330	5.74126544	3.15734524
H	-2.61959820	4.11527731	4.46371634
H	-0.89268307	4.16309132	-1.18415909
H	2.73759321	2.28197117	-2.89892822
H	-3.84587829	5.00302438	-1.35520111

H	-3.19870424	3.35189126	-1.49640211
H	-2.81963621	4.57491735	-2.73380121
H	-2.07345316	6.99614954	-0.92343107
H	-1.09738208	6.38992948	-2.27407817
H	-0.37287003	6.56839948	-0.66059205
H	4.27203533	0.22459702	-4.58984235
H	2.74790821	1.00527308	-5.05387739
H	2.79832821	-0.07570801	-3.63633228
H	4.60894135	3.88763429	-3.44312926
H	3.70630828	3.37843026	-4.88861437
H	5.30338640	2.69257520	-4.55578735
H	6.30089546	1.10274608	-3.28100725
H	7.71409061	0.38856703	-1.36851711
H	6.76598151	0.30173802	0.92125507
H	0.26579102	2.15332017	3.00789223
H	3.14829124	0.99842707	1.71807213
H	-2.31945118	1.51871911	4.53389435
H	-0.85206807	0.51410704	4.48703134
H	-1.78077413	0.78692906	2.99605723
H	-0.79338306	3.42747426	5.60884142
H	0.61610705	4.00518531	4.69738136
H	0.62794905	2.38674018	5.43310340
H	4.09580631	-1.31517110	1.80091214
H	4.05064431	-0.55318304	3.40078326
H	5.58828643	-0.68729205	2.53381619
H	5.89976244	1.93333615	2.74149821
H	4.37942233	1.96617015	3.65959728
H	4.58048335	3.00556423	2.23297717
H	-6.04000345	-2.99396523	-3.08816223
H	-7.77774661	-2.00409715	-1.62225913
H	-7.14152352	-0.91567507	0.51746304
H	-2.33340518	-2.77384021	-2.38355818
H	-0.04991200	-2.24949517	3.32163825
H	-4.42830034	-2.91191722	-4.63274935
H	-2.66321720	-2.92569822	-4.79688037
H	-3.48916427	-1.46776311	-4.19967932
H	-3.20969525	-5.04228338	-1.70748913
H	-2.59261520	-5.04751338	-3.37061826
H	-4.34506633	-5.00915938	-3.07001423
H	2.15033716	-2.23808917	5.46919144
H	0.61633805	-1.35050110	5.53531341
H	1.82221114	-0.94555407	4.29262133
H	-0.50700704	-4.62331935	4.02062931
H	-0.76446106	-3.48438827	5.35982839
H	0.70466905	-4.48072134	5.30835542
H	3.03000823	-4.15096332	4.45614834
H	4.68632336	-5.11146139	2.87630322
H	4.36496633	-4.88259637	0.42588103
H	-3.59062528	-0.80707806	1.81804314
H	1.45334211	-3.01977923	-1.14433809
H	-5.89928443	1.15666109	1.32483110
H	-4.23092232	1.30652810	0.71503506

H	-4.54925035	1.38951211	2.45842719
H	-5.11388139	-0.75551906	3.76070429
H	-5.30633338	-2.30426818	2.90887922
H	-6.52819751	-1.02921908	2.72908721
H	3.76293429	-2.07516316	-1.21492809
H	3.32094225	-2.93156222	-2.70168221
H	4.42588934	-3.69552828	-1.53901112
H	1.05973208	-5.50169441	-1.09507808
H	2.78614321	-5.78576945	-1.40626611
H	1.78159914	-4.96873938	-2.62652720
O	-1.05035708	1.33376310	-2.22625117
O	-2.07016816	-0.62759305	-0.11650701
O	-0.32229202	1.61395812	0.66869005
C	-0.54072204	2.12539716	-3.35360226
H	-0.99097208	3.11684524	-3.41463026
C	-1.23981709	0.98894908	-4.00495131
H	-2.31766118	1.09557408	-4.10024531
C	-0.56838704	-0.20954802	-4.49108034
H	-0.29254202	-0.86313707	-3.53680327
H	-1.20880309	-0.82694106	-5.12536239
H	0.39970003	-0.00471700	-4.96162938
H	0.54816904	2.13645916	-3.41914426
Hf	-0.15840301	-0.04641000	-0.78925706

14. Zr_NCCN Complexes

Zr_NCCN Bisperoxo Complex to Oxo Peroxo Complex (Ethylene)

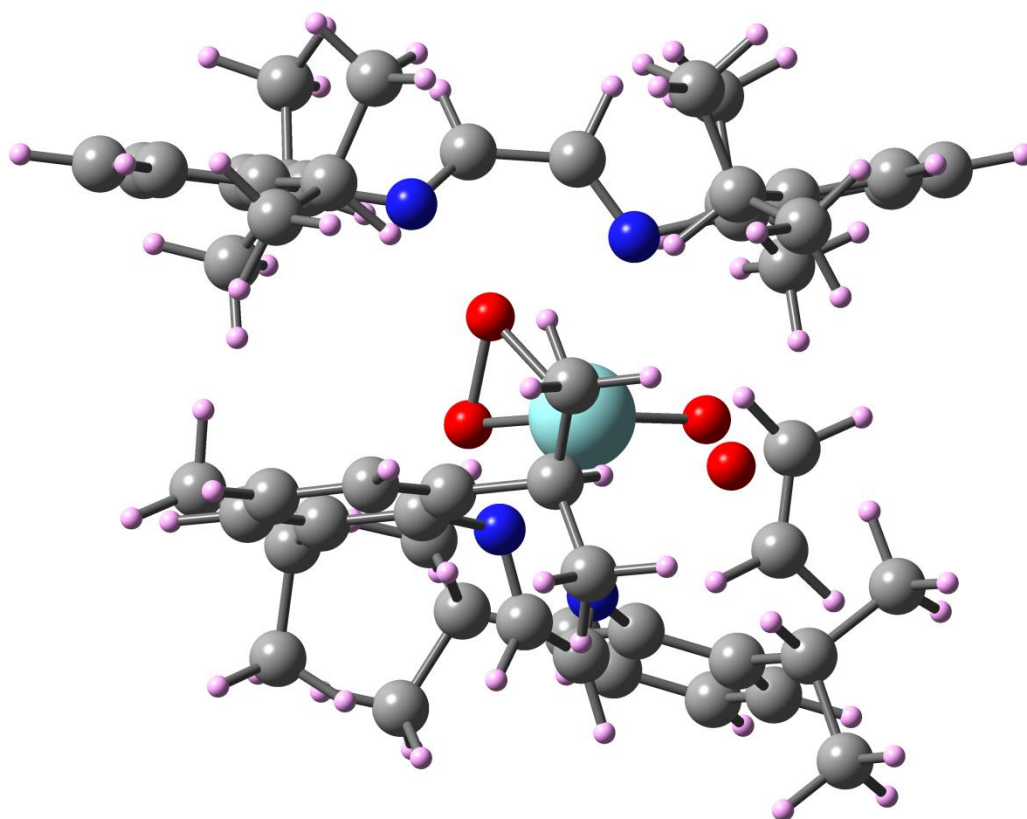


Fig. S160: Zr_NCCN Bisperoxo Complex to Oxo Peroxo Complex (Ethylene)

E	E_{ZP}	H	G	<i>f</i>
-2669.5636	-2668.3653	-2668.2923	-2668.4747	-486
Zr	0.89630491	-0.02356777	-0.22241033	
O	2.52460178	0.85655081	-0.66531527	
N	-2.93501552	0.52856201	-1.09778888	
N	-0.28330882	2.18953816	-1.00503537	
N	2.61264813	-1.60576578	0.73723820	
N	0.06049618	-1.17271667	1.87612662	
C	-2.38217431	1.24716490	-2.01919140	
C	-1.31488007	2.23867133	-1.79754044	
C	2.40033249	-1.85503803	1.99175777	
C	1.03389858	-1.74153477	2.53119705	
C	-4.01270707	-0.36560364	-1.39806858	
C	-3.97759516	-1.30069988	-2.48359701	
C	-5.08980342	-2.15817402	-2.63844876	
C	-6.19691160	-2.09990084	-1.78163382	
C	-6.21689704	-1.17198623	-0.72571708	
C	-5.13492667	-0.30090507	-0.51091709	
C	-2.32727400	-2.88731666	-3.65948557	

C	-2.81591177	-1.42765800	-3.48264944
C	-3.22217998	-0.84095257	-4.86392385
C	3.25436944	2.18288394	-3.40212172
C	1.76495591	2.52215403	-3.15562565
C	1.11103302	3.05118885	-4.46460167
C	0.54256213	3.41407828	-1.03934786
C	1.56014051	3.53858016	-2.02412012
C	2.34512936	4.71131085	-2.00572450
C	2.12281003	5.72902451	-1.06864083
C	1.07176662	5.60933181	-0.14676851
C	0.25229030	4.46139464	-0.12058770
C	-6.09590897	0.41174767	1.77404078
C	-5.18023936	0.76958329	0.58287897
C	-5.61463935	2.13754095	-0.01752016
C	-0.77902076	5.20563460	2.13213387
C	-0.96598932	4.41270148	0.81464403
C	-2.23440042	4.95591710	0.09455731
C	3.90795076	-1.89008117	0.13955140
C	5.07133718	-1.16350941	0.52335116
C	6.28930145	-1.50224838	-0.10305340
C	6.36419337	-2.51897055	-1.06420066
C	5.20566067	-3.22539769	-1.41874995
C	3.95855090	-2.92847021	-0.83453656
C	5.54543927	1.30603218	0.88522211
C	5.06775857	-0.01660775	1.53808524
C	5.91898956	-0.36910424	2.78679383
C	-2.29180784	-4.24447938	-0.01518020
C	-1.26614450	-3.61599772	0.95925407
C	-0.49608546	-4.74765067	1.69639286
C	-1.29271580	-1.45020155	2.38829434
C	-1.91911364	-2.65669476	1.96305365
C	-3.17124475	-2.97697911	2.52679915
C	-3.78315809	-2.14157073	3.47243268
C	-3.15740687	-0.94765306	3.85388054
C	-1.90805008	-0.57336408	3.31634778
C	2.52987791	-3.92711274	-2.70873409
C	2.74474473	-3.79482499	-1.18248581
C	2.87819305	-5.19170651	-0.51474051
C	-2.20549969	1.93675460	3.68143785
C	-1.24800420	0.72357959	3.78548910
C	-0.71572949	0.58017663	5.23759095
H	-2.75522093	1.26131974	-3.05013306
H	-1.43199838	3.11924644	-2.44130992
H	3.17060450	-2.26441782	2.64964795
H	0.84230342	-2.26080268	3.47449988
H	-5.08451702	-2.88277750	-3.44838705
H	-7.03972268	-2.77016999	-1.93480780
H	-7.08036280	-1.13023395	-0.06915217
H	-1.94544762	-0.88320295	-3.10667420
H	1.26976775	1.58422865	-2.89025732
H	-3.10429727	-3.54663303	-4.06992660
H	-1.98193608	-3.29891847	-2.70716269

H	-1.47508042	-2.90147795	-4.35068129
H	-4.04059711	-1.42000596	-5.31362989
H	-2.36718829	-0.87108020	-5.55221856
H	-3.56425064	0.20070602	-4.79035688
H	3.82346460	3.04997107	-3.76558238
H	3.33094341	1.39632992	-4.16498465
H	3.70554666	1.81055106	-2.47836694
H	0.03636581	3.24441100	-4.34139741
H	1.23150874	2.31375760	-5.26916657
H	1.58156465	3.98966555	-4.78831990
H	3.13902480	4.82570840	-2.73811783
H	2.74888562	6.61833915	-1.06915294
H	0.88328934	6.42010158	0.55061831
H	-4.15405400	0.88602872	0.95582784
H	-1.16161642	3.36230596	1.07105429
H	-7.15687046	0.41414014	1.48904068
H	-5.97326214	1.15604900	2.57228250
H	-5.84977662	-0.57298210	2.18623753
H	-6.63406995	2.07459524	-0.42185726
H	-4.94715986	2.45233156	-0.82786426
H	-5.60279838	2.91806937	0.75592274
H	0.14784029	4.94081058	2.65284857
H	-1.62180608	5.00801973	2.80682669
H	-0.76312485	6.28720914	1.94778849
H	-2.07599224	5.99469800	-0.22369730
H	-3.09880013	4.93265716	0.77199499
H	-2.49082116	4.36899460	-0.79394352
H	7.18739102	-0.95040368	0.16212093
H	7.31597458	-2.75954311	-1.53199268
H	5.26774157	-4.02173925	-2.15514260
H	4.04058084	0.17636389	1.85151462
H	-0.55401462	-3.05206850	0.34499179
H	6.57037892	1.22865828	0.49739355
H	5.52751233	2.11830754	1.62577033
H	4.86629201	1.57262799	0.06996342
H	5.56594483	-1.28822397	3.27643030
H	5.87598470	0.44773368	3.52063797
H	6.97414995	-0.52216192	2.52417838
H	-2.95812264	-4.95557817	0.49163334
H	-1.75968062	-4.79714647	-0.79919101
H	-2.90863587	-3.47809908	-0.49639870
H	0.29558971	-4.35924944	2.35034116
H	-0.02682463	-5.42184860	0.96892997
H	-1.18072461	-5.33878401	2.31973704
H	-3.67128834	-3.88958503	2.21835685
H	-4.74210293	-2.41760376	3.90399523
H	-3.64092644	-0.29754495	4.57817515
H	1.84657051	-3.31078901	-0.79108289
H	-0.39399795	0.92378126	3.13052657
H	3.36950821	-4.43220528	-3.20583734
H	2.38881612	-2.93797786	-3.15499988
H	1.62187397	-4.51190699	-2.90553535

H	1.99159445	-5.80321897	-0.73109053
H	2.98099534	-5.11070251	0.57657036
H	3.75898816	-5.72823572	-0.89269491
H	-2.60221362	2.04179542	2.66419889
H	-1.67457914	2.85975302	3.94536343
H	-3.05602684	1.83849182	4.36735625
H	-0.00005010	-0.24814017	5.32764975
H	-1.54042811	0.37902889	5.93345441
H	-0.21518290	1.50195629	5.56043266
O	-0.13027603	-0.45046778	-1.95903775
O	0.64114620	-1.67577456	-1.43467716
C	2.25717719	1.72788845	3.30488549
H	1.63978000	1.01374857	3.83738036
C	1.72596902	2.62145237	2.38517407
H	0.65200278	2.73836975	2.29238188
O	2.15784635	1.32202842	1.13174400
H	2.32156521	3.43572843	1.98673416
H	3.32466929	1.70117391	3.49722526

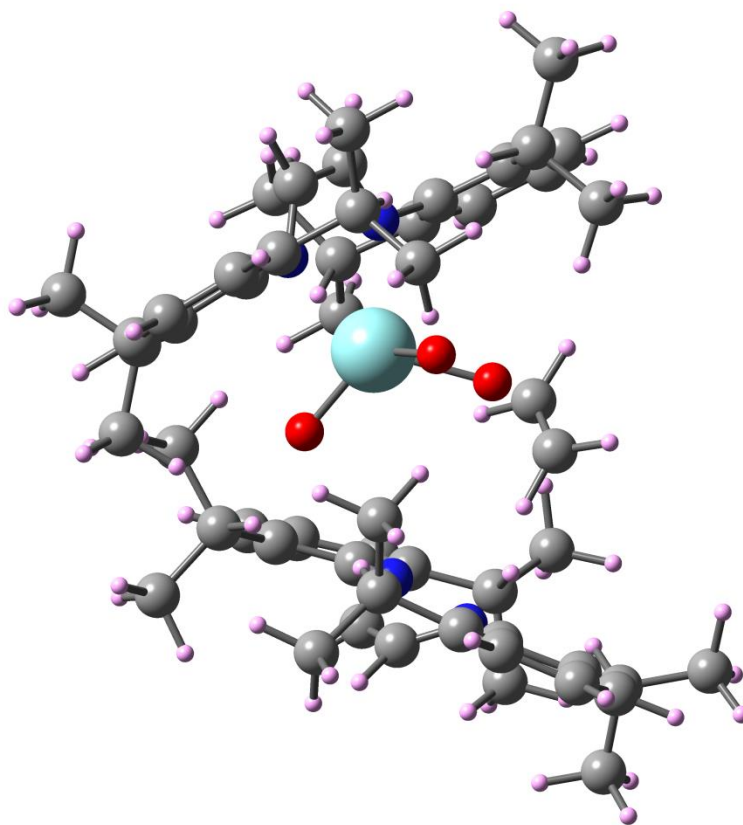
Zr_NCCN Oxo Peroxo Complex to Dioxo Complex (Ethylene)

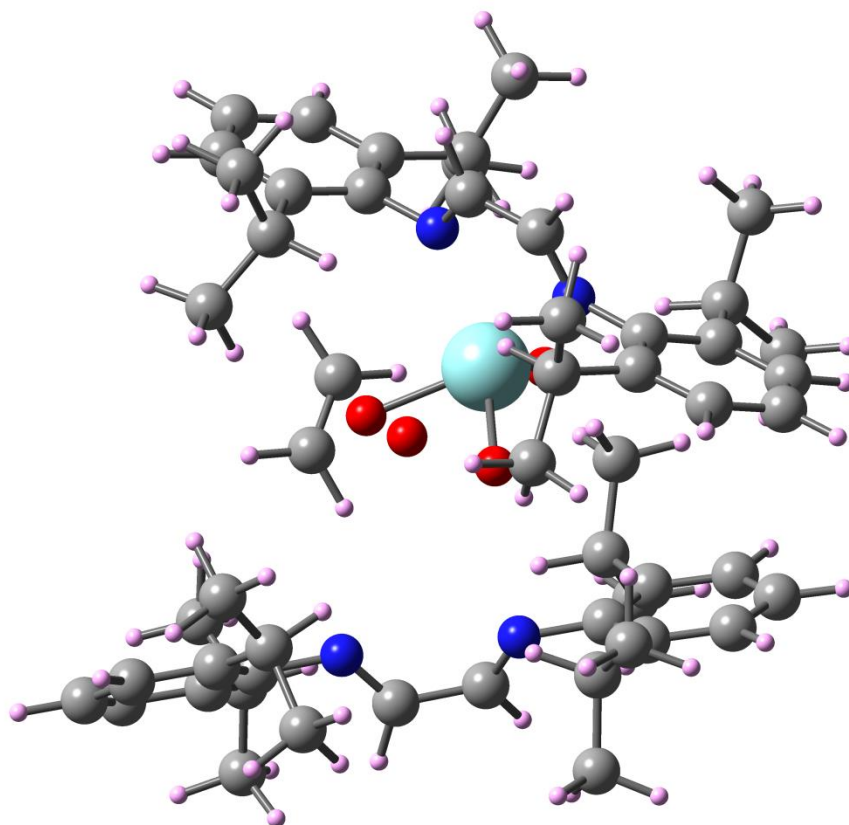
Fig. S161: Zr_NCCN Oxo Peroxo Complex to Dioxo Complex (Ethylene)

E	E_{ZP}	H	G	<i>f</i>
-2594.4128	-2593.2197	-2593.1465	-2593.3369	-431
Zr	-1.25137302	-0.13051273	-0.14589788	
O	-0.35198296	0.20981353	1.43091863	
N	-2.35972963	-2.20142582	-0.83084630	
N	-3.56110168	-0.16195451	0.61774036	
N	3.00231108	2.33290518	-0.14598667	
N	3.38174127	-0.32777604	1.04042932	
C	-3.65101206	-2.19746953	-0.64982179	
C	-4.28903534	-1.12807185	0.13491886	
C	3.10290885	2.10901177	1.12410520	
C	3.37482875	0.77963262	1.70933310	
C	-1.75497560	-3.14485330	-1.74968532	
C	-2.03588051	-3.04290688	-3.14351728	
C	-1.38031514	-3.95430031	-4.00036975	
C	-0.49319061	-4.91875882	-3.50403063	
C	-0.22034322	-4.98331320	-2.12692152	
C	-0.83411091	-4.09570205	-1.22417261	
C	-2.06209478	-0.95934224	-4.59755360	
C	-2.92057296	-1.95419015	-3.76938901	

C	-4.06412641	-2.56398292	-4.62134543
C	-4.64236109	2.95370746	-1.74921868
C	-5.23838657	1.73216091	-1.00031088
C	-6.74193633	1.53986331	-1.33305433
C	-4.19361513	0.96671446	1.27672996
C	-5.01109993	1.85235642	0.51350499
C	-5.58815826	2.94503727	1.19423107
C	-5.37188543	3.15326190	2.56348071
C	-4.55050423	2.27332615	3.28444418
C	-3.93567429	1.17011144	2.66061636
C	0.82981816	-4.71573084	0.63888483
C	-0.58196014	-4.19842807	0.28322272
C	-1.66641649	-5.08834967	0.95441711
C	-1.96427239	0.92932471	4.26363701
C	-3.09455027	0.20058406	3.49618439
C	-4.00371067	-0.61421502	4.45708875
C	2.74677425	3.62447597	-0.69314747
C	1.68273127	4.46978096	-0.24670042
C	1.52975785	5.71916715	-0.88641412
C	2.37558062	6.12660913	-1.92743260
C	3.39088887	5.26648607	-2.38064509
C	3.58415883	4.00611600	-1.78925415
C	-0.79005776	4.22278331	0.36091011
C	0.67570810	4.07715439	0.84496038
C	0.90488293	4.90743931	2.13783004
C	5.58513063	-2.97037435	-1.36966423
C	5.28799049	-1.86644244	-0.32909488
C	6.58266562	-1.07482847	0.00733110
C	3.68071571	-1.58295080	1.64853999
C	4.63482512	-2.39192240	0.95180696
C	5.00599291	-3.62990290	1.50653189
C	4.43646684	-4.08182850	2.70978983
C	3.46187110	-3.30491334	3.35272914
C	3.04999396	-2.05296103	2.84469586
C	4.96479806	3.11573959	-3.77045862
C	4.71523763	3.08078697	-2.24492759
C	6.02533535	3.40392475	-1.47320666
C	0.69468301	-2.20436550	3.82881619
C	1.92370857	-1.29670242	3.56692715
C	2.41785293	-0.68960602	4.90842150
H	-4.29387213	-2.95633305	-1.10104805
H	-5.37259987	-1.15813633	0.26263316
H	3.04449871	2.91667723	1.86601586
H	3.61289524	0.81151546	2.78102563
H	-1.56186367	-3.89655474	-5.07014876
H	-0.00584605	-5.61070418	-4.18633228
H	0.47977951	-5.72459741	-1.75593065
H	-3.38943316	-1.35893588	-2.97847847
H	-4.69662698	0.86113329	-1.38340968
H	-1.52676172	-1.47333632	-5.40723658
H	-1.33681120	-0.44813910	-3.95450722
H	-2.70844209	-0.19555802	-5.04942865

H	-3.67263205	-3.11335151	-5.48670604
H	-4.71309963	-1.76589083	-5.00400390
H	-4.68183030	-3.26065530	-4.03783694
H	-5.08547807	3.89719394	-1.40444225
H	-4.83626128	2.86214990	-2.82667253
H	-3.55724487	2.98660377	-1.60501959
H	-7.16356069	0.65847172	-0.82918742
H	-6.87661607	1.41498907	-2.41551623
H	-7.33438270	2.41027555	-1.02345131
H	-6.20497145	3.64600810	0.63857617
H	-5.83385420	4.00058138	3.06416831
H	-4.38584466	2.44226269	4.34500054
H	-0.68060422	-3.19042883	0.71442889
H	-2.59756557	-0.50454308	2.82182259
H	0.95752866	-5.77034716	0.36180688
H	0.99572771	-4.64061973	1.71907893
H	1.61554594	-4.13204715	0.14475548
H	-1.61488402	-6.11426046	0.56664375
H	-2.67948892	-4.70880580	0.76862913
H	-1.51096105	-5.12448981	2.04018100
H	-1.23708940	1.33186708	3.55104540
H	-1.43812547	0.21901679	4.91511197
H	-2.34897093	1.73943045	4.89717928
H	-4.48595694	0.03933752	5.19614586
H	-3.40804416	-1.35776309	5.00287399
H	-4.79756979	-1.14394642	3.91215249
H	0.72596490	6.37836098	-0.56883371
H	2.23601407	7.09971238	-2.39300578
H	4.02914651	5.57924433	-3.20246561
H	0.80299952	3.01860742	1.09499371
H	4.58238044	-1.15483281	-0.77493301
H	-1.03408377	5.26071399	0.09605576
H	-1.47282272	3.91434271	1.16468926
H	-0.98365605	3.57474206	-0.50061675
H	1.92770767	4.79660190	2.52364062
H	0.20540291	4.58784778	2.92191842
H	0.73916474	5.97730738	1.95144877
H	6.37018561	-3.65985159	-1.03040964
H	5.93510036	-2.51408726	-2.30514254
H	4.68728505	-3.56018222	-1.59568179
H	6.37162238	-0.24259714	0.68993561
H	7.02772734	-0.65873527	-0.90690713
H	7.32724653	-1.72681733	0.48469981
H	5.74476790	-4.24504086	1.00012406
H	4.74146992	-5.03540672	3.13508795
H	3.00607203	-3.67771307	4.26684862
H	4.42245006	2.06032949	-1.96810422
H	1.55470445	-0.48949588	2.92481172
H	5.37360996	4.08080660	-4.09910184
H	4.04008345	2.92991123	-4.33150671
H	5.69422655	2.34254854	-4.04730672
H	6.82425504	2.70505909	-1.75748096

H	5.87536985	3.32660115	-0.38915694
H	6.36695583	4.42397078	-1.69675579
H	0.31450779	-2.61932141	2.88873719
H	-0.11001171	-1.60790881	4.27506601
H	0.92382658	-3.03367233	4.51219766
H	3.27850179	-0.02313442	4.76685795
H	2.72813861	-1.47869695	5.60757441
H	1.61381838	-0.11150218	5.38357374
O	-1.74815838	1.39332615	-1.28021893
O	-0.20228731	0.37449535	-1.87971953
C	1.45291382	-1.20096083	-2.23623520
H	1.68156907	-1.67714266	-1.28407365
H	1.05704518	-1.82437774	-3.03349443
C	1.66874584	0.15537118	-2.40026931
H	2.15478618	0.73929654	-1.62296548
H	1.55926977	0.62230965	-3.37500965

Zr_NCCN Oxo η^3 -Ozone Complex to Oxo Peroxo Complex (Ethylene)Fig. S162: Zr_NCCN Oxo η^3 -Ozone Complex to Oxo Peroxo Complex (Ethylene)

E	E_{ZP}	H	G	<i>f</i>
-2669.5841	-2668.3886	-2668.3138	-2668.5088	-344

Zr	1.32746366	-0.41937285	0.16059716
O	-0.27965365	-1.57333742	-0.55541869
N	-2.57967389	2.49692887	0.27854292
N	-4.36941706	0.29606403	-0.36571037
N	2.74987279	-2.33784202	0.51767330
N	3.64840707	0.11492189	-0.37152361
C	-3.84459693	2.49498512	0.54500728
C	-4.77057091	1.45703625	0.03300447
C	3.93091947	-2.23803691	-0.01923277
C	4.40104916	-0.93648633	-0.52350569
C	-1.70337513	3.51573971	0.75763842
C	-1.52135700	3.77299906	2.14853759
C	-0.64650191	4.81830243	2.51399908
C	0.03487482	5.57506589	1.54979720
C	-0.11212696	5.26588300	0.18543131
C	-0.96191898	4.22695402	-0.23446407
C	-1.02162858	2.17364481	4.05214522
C	-2.13597840	2.90131175	3.25106564

C	-3.06402254	3.71530186	4.18926462
C	-6.86485907	-1.90438828	2.18637937
C	-6.80144432	-0.71850279	1.18753839
C	-8.15044435	0.04818327	1.16438591
C	-5.23333358	-0.70500893	-0.90016887
C	-6.39033425	-1.18711329	-0.21562490
C	-7.15266233	-2.19743394	-0.84196716
C	-6.78920763	-2.72482952	-2.08934161
C	-5.62191580	-2.26942332	-2.72804423
C	-4.81897261	-1.27161259	-2.14723922
C	0.13934616	4.02589314	-2.54833651
C	-1.15422085	3.89011750	-1.71464305
C	-2.29392106	4.75238480	-2.32629427
C	-2.79572710	-1.83087481	-3.63887164
C	-3.56200345	-0.74708850	-2.84669092
C	-3.91620359	0.45093622	-3.77143415
C	2.28679875	-3.61806206	1.02567486
C	1.97267373	-4.66380474	0.11547917
C	1.52540701	-5.88494441	0.66595282
C	1.39297299	-6.05655443	2.05077861
C	1.68909220	-4.99562034	2.92394327
C	2.13242629	-3.75200653	2.43454627
C	0.61841267	-4.67676756	-2.03673133
C	2.02888917	-4.51170320	-1.41078859
C	3.04447378	-5.49951853	-2.04309134
C	3.42594657	3.41580311	2.36352441
C	3.98824819	2.19139896	1.60683760
C	5.30257167	1.69451560	2.27287747
C	4.08261533	1.40964228	-0.85008016
C	4.21883738	2.45044965	0.11511719
C	4.66003319	3.70677304	-0.34074495
C	4.93782353	3.93104766	-1.69922363
C	4.76122457	2.90009013	-2.63241273
C	4.32640788	1.61704852	-2.23902460
C	1.61760985	-2.56191453	4.65744501
C	2.49914673	-2.60931676	3.38813792
C	4.00149859	-2.69371799	3.77931120
C	2.98656549	1.06448198	-4.32836954
C	4.05996998	0.56549371	-3.32517547
C	5.36673034	0.16002758	-4.05772626
H	-4.32514227	3.30247119	1.11964943
H	-5.82628734	1.76588037	-0.01283094
H	4.60648461	-3.09321501	-0.08619283
H	5.39143794	-0.88445823	-0.97868361
H	-0.48927166	5.03137015	3.56899579
H	0.69041014	6.38684268	1.85780227
H	0.44569825	5.83304731	-0.55459623
H	-2.74367263	2.11790709	2.78550493
H	-6.03862389	-0.03165029	1.57018054
H	-0.39579704	2.89064724	4.60188622
H	-0.37290076	1.59337957	3.38399553
H	-1.47233335	1.49237247	4.78866463

H	-2.50828799	4.50601577	4.71060679
H	-3.50613128	3.06032347	4.95260977
H	-3.88010698	4.19606683	3.63255238
H	-7.64543722	-2.62462659	1.91037578
H	-7.09060598	-1.53861679	3.19738170
H	-5.90823350	-2.44020401	2.22113200
H	-8.10680310	0.91911847	0.49727479
H	-8.41297791	0.39848493	2.17191637
H	-8.96432012	-0.59753628	0.80972731
H	-8.03861612	-2.58039016	-0.34046696
H	-7.40066972	-3.49518668	-2.55366164
H	-5.32958882	-2.69991608	-3.68153363
H	-1.46867339	2.84023670	-1.76066890
H	-2.89015208	-0.36273504	-2.07085568
H	0.48807482	5.06649019	-2.60912169
H	-0.04557130	3.67989191	-3.57410117
H	0.94087655	3.40777113	-2.12837591
H	-2.03120147	5.81939920	-2.30558698
H	-3.23336089	4.62586168	-1.77275991
H	-2.47384892	4.46487878	-3.37124584
H	-2.59881966	-2.71505137	-3.01919187
H	-1.82597862	-1.42999382	-3.95665838
H	-3.34308999	-2.15273403	-4.53641042
H	-4.60346652	0.13985745	-4.57077599
H	-3.00529670	0.85147328	-4.23520728
H	-4.39358106	1.26236058	-3.20762191
H	1.26890520	-6.70292671	-0.00198439
H	1.05007363	-7.00794924	2.44990796
H	1.56948925	-5.13573053	3.99375567
H	2.34991360	-3.49596834	-1.66460804
H	3.23810454	1.39910584	1.71047854
H	0.19683191	-5.66883583	-1.82742193
H	0.67696764	-4.55636469	-3.12628605
H	-0.05789666	-3.90810164	-1.64851677
H	4.05418041	-5.36862855	-1.62925280
H	3.09571095	-5.34500576	-3.12857318
H	2.74946690	-6.54226320	-1.86882008
H	4.15761002	4.23257577	2.43668731
H	3.15918734	3.11906079	3.38553270
H	2.51841871	3.79736000	1.88268298
H	5.69031154	0.78879239	1.78659154
H	5.12549784	1.46178472	3.33111554
H	6.08380568	2.46491579	2.21864871
H	4.78236465	4.51708406	0.37076321
H	5.27543262	4.91034555	-2.02979063
H	4.94369056	3.09588161	-3.68564233
H	2.34090809	-1.65799213	2.86532213
H	3.63778296	-0.33442941	-2.86576284
H	1.80782021	-3.41223415	5.32594104
H	0.55129139	-2.55285282	4.40248893
H	1.83408435	-1.64504088	5.21918120
H	4.27397196	-1.84903782	4.42523463

H	4.65622674	-2.66996452	2.89785357
H	4.20925557	-3.62372977	4.32544747
H	2.05101525	1.27439830	-3.80084866
H	2.78966374	0.28862881	-5.08024329
H	3.31383624	1.97021775	-4.85542683
H	6.12411258	-0.23053900	-3.36312468
H	5.81178571	1.01693127	-4.57973968
H	5.15597253	-0.61395973	-4.80722989
O	0.98994035	0.37062407	1.78030730
O	0.69483091	-0.83944761	-2.01794897
O	0.93536522	0.60239189	-1.61922751
C	-1.18659488	-2.30085335	1.48640537
H	-0.92646776	-1.53950032	2.21812553
H	-0.79450441	-3.30370001	1.63500777
C	-1.95268414	-1.98514261	0.37890648
H	-2.43460775	-1.01744858	0.27328629
H	-2.28683380	-2.76286436	-0.30237512

15. Zr_NCCNO Complexes

15.1 Ground States

Zr_NCCNO Propene Chemisorbed on Dioxo Complex forming Octahedral Complex

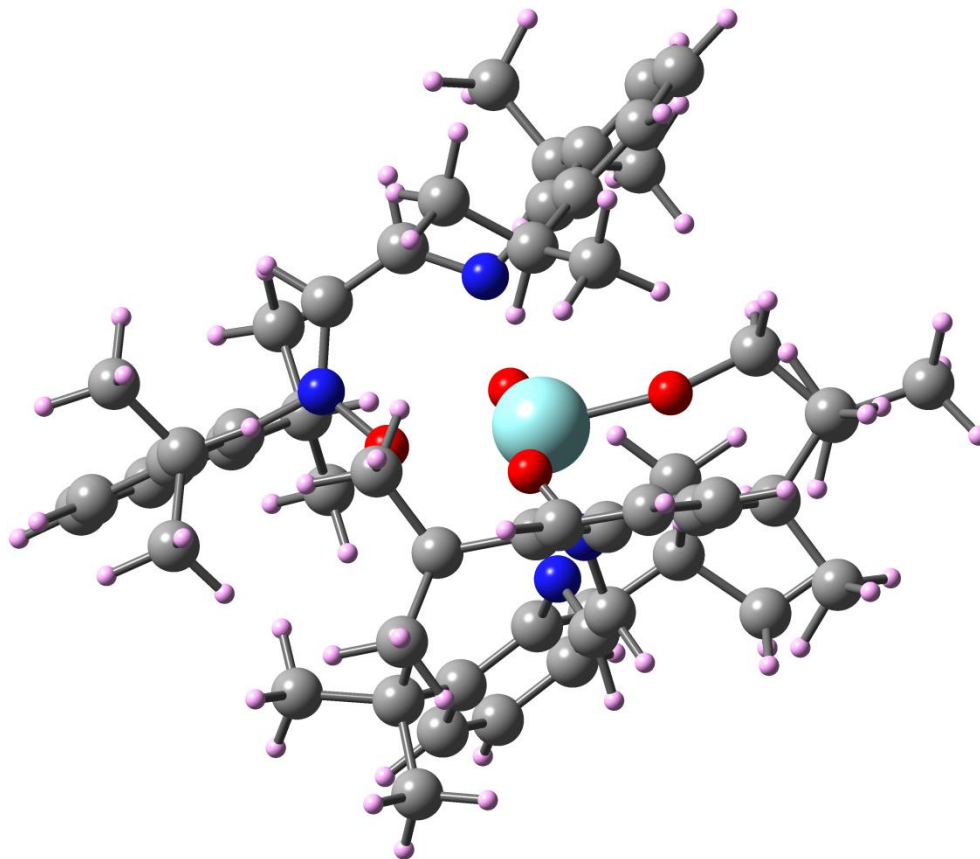


Fig. S163: Zr_NCCNO Propene Chemisorbed on Dioxo Complex forming Octahedral Complex

E	E _{ZP}	H	G
-2708.9995	-2707.7710	-2707.6962	-2707.8856

N	0.38701100	-0.75638100	-2.31612000
N	-0.45013900	-0.31014200	2.26797400
C	-0.58436400	-0.49277900	-3.15908700
C	-1.88914100	0.03507900	-2.85624000
C	0.35210800	0.46705100	3.04053000
C	1.42629100	1.28796500	2.66254300
C	1.56991000	-1.39746500	-2.89014700
C	2.73184200	-0.60820000	-3.11080000
C	3.86478300	-1.24534800	-3.65533100
C	3.84476900	-2.61317500	-3.97516700
C	2.68284100	-3.36654500	-3.75660000
C	1.51849900	-2.78375200	-3.20851900
C	4.10281100	1.47120700	-2.45526800
C	2.72091500	0.90133000	-2.84655200
C	2.17977700	1.65902600	-4.09277200

C	-2.92144500	4.52894400	-0.99249900
C	-2.91216200	3.39799600	-2.05337700
C	-3.07505200	3.97784300	-3.48346000
C	-3.70542100	0.98341500	-1.56219700
C	-3.99297800	2.35494000	-1.75422200
C	-5.34707300	2.73978000	-1.66738300
C	-6.34859500	1.79582100	-1.38870700
C	-6.01752200	0.44793000	-1.17899100
C	-4.67966300	0.00278900	-1.25196500
C	0.55931000	-4.98304100	-2.29132100
C	0.26023400	-3.64343600	-3.00912100
C	-0.43050900	-3.92189500	-4.37329600
C	-4.98204500	-2.02587900	0.27123000
C	-4.33299200	-1.47274100	-1.02191700
C	-4.75848100	-2.32583600	-2.24796000
C	-1.60925000	-0.86141900	2.96163300
C	-1.62461400	-2.23412200	3.33652300
C	-2.75538000	-2.73251400	4.01715800
C	-3.84075100	-1.90339900	4.33445200
C	-3.80918700	-0.55012100	3.96556900
C	-2.70749100	-0.00421200	3.27321500
C	-0.85896900	-4.40169100	2.22794700
C	-0.44329700	-3.17326300	3.07646100
C	0.22030900	-3.60883600	4.41041000
C	1.19214900	4.61463600	-1.13122700
C	1.34401100	4.31186700	0.38199500
C	1.00854800	5.56147900	1.23679200
C	2.98421000	2.47459900	1.18064800
C	2.74954100	3.78465100	0.68684200
C	3.86779000	4.62037700	0.48851700
C	5.16633100	4.17461600	0.78269400
C	5.36962600	2.87442400	1.26868500
C	4.28823100	1.98913600	1.46708900
C	-4.04985800	1.91825800	2.23350700
C	-2.72113800	1.48512800	2.90141800
C	-2.44836300	2.37485600	4.14597700
C	5.63624000	-0.16210500	1.14143400
C	4.55724200	0.56881000	1.97971000
C	4.97334600	0.59036600	3.47584900
H	-0.44605000	-0.72565800	-4.21760900
H	-2.62486700	0.03681900	-3.65047900
H	0.15394800	0.47308100	4.11414600
H	1.99408000	1.76598700	3.45148800
H	4.76707300	-0.66843300	-3.83427700
H	4.72905600	-3.08630200	-4.39607000
H	2.67637200	-4.42335400	-4.01023700
H	2.04206000	1.09265400	-2.00643300
H	-1.92936700	2.91679400	-1.99514500
H	4.80831100	1.45619000	-3.29749900
H	4.54546300	0.91046200	-1.62534400
H	3.99801100	2.51404700	-2.13173500
H	2.82601800	1.48242600	-4.96340200

H	2.15417500	2.74033300	-3.90170600
H	1.16419000	1.33988200	-4.35835400
H	-3.87458800	5.07322600	-0.98963000
H	-2.12540800	5.25381000	-1.20512200
H	-2.75734100	4.12161100	0.01185000
H	-3.04001800	3.18679000	-4.24385400
H	-2.27035100	4.69292900	-3.69862900
H	-4.03220000	4.50423600	-3.59242500
H	-5.61767900	3.78189900	-1.81544500
H	-7.38701700	2.11284200	-1.32748200
H	-6.80108500	-0.26712100	-0.94622000
H	-0.44139200	-3.10762900	-2.36059800
H	-3.25001700	-1.59105900	-0.88922500
H	1.23177100	-5.62821700	-2.87271700
H	-0.37841700	-5.53178200	-2.13492800
H	1.00812000	-4.80906300	-1.30752300
H	0.22917500	-4.49306900	-5.04094500
H	-0.70202400	-2.99367900	-4.89387600
H	-1.34762100	-4.50629000	-4.22085400
H	-4.69564600	-1.43194400	1.14614800
H	-4.62849800	-3.05001700	0.44018400
H	-6.07929600	-2.05232300	0.21039200
H	-5.84479700	-2.28317400	-2.40942000
H	-4.47685300	-3.37336600	-2.08384200
H	-4.26811100	-1.98706000	-3.17087400
H	-2.77914400	-3.77990700	4.30892500
H	-4.70068700	-2.30556900	4.86552800
H	-4.65275000	0.08932900	4.21415500
H	0.31220600	-2.62775400	2.50331600
H	0.61870600	3.53019000	0.62403300
H	-1.61951300	-5.00828400	2.73904200
H	0.01384600	-5.04489100	2.04609900
H	-1.25373400	-4.06850700	1.26188500
H	0.54818100	-2.73975400	4.99702800
H	1.09825400	-4.23789400	4.20894500
H	-0.47439900	-4.18921500	5.03263300
H	1.90080500	5.38637100	-1.46129900
H	0.17809100	4.97482100	-1.34840200
H	1.36739000	3.70836000	-1.72185600
H	1.09962000	5.34500000	2.30887100
H	-0.02218800	5.88686400	1.04172000
H	1.67436600	6.40347100	1.00560100
H	3.71958300	5.63004700	0.11337200
H	6.01568800	4.83693900	0.63188300
H	6.37971500	2.53659800	1.48429400
H	-1.92207100	1.66067200	2.17380000
H	3.63833400	-0.01866800	1.89099000
H	-4.89866600	1.84737600	2.92652100
H	-4.27361100	1.30252000	1.35657600
H	-3.98133600	2.96499300	1.90653000
H	-2.44153900	3.43725600	3.86494400
H	-1.48224100	2.14024700	4.60876700

H	-3.22767500	2.23052900	4.90664800
H	5.36181200	-0.19225500	0.08075600
H	5.73244700	-1.19670600	1.49364000
H	6.62055900	0.31724600	1.22752300
H	4.20744400	1.06236000	4.10410700
H	5.91013100	1.14647000	3.61622800
H	5.12746800	-0.43350200	3.84077800
O	-1.18552100	-2.14742200	-0.28552900
O	1.78199700	-1.80442900	0.43711900
O	1.13585400	1.21595000	0.28641600
O	-1.52501700	0.68123800	-0.62301900
N	1.83993100	1.60501200	1.40198500
N	-2.30930700	0.53611600	-1.69775800
C	3.36266200	-3.07481000	1.80251600
H	2.87917400	-2.60936200	2.65962400
C	2.76967100	-2.83215200	0.43916900
H	3.57136600	-2.56665900	-0.27724900
H	2.32669400	-3.77463800	0.05424200
C	4.41003200	-4.13969000	1.99322100
H	5.14716600	-4.13074000	1.17484100
H	4.95116300	-4.01284600	2.93939700
H	3.97357200	-5.15621100	2.00612500
Zr	0.07264700	-0.84727600	0.10192500

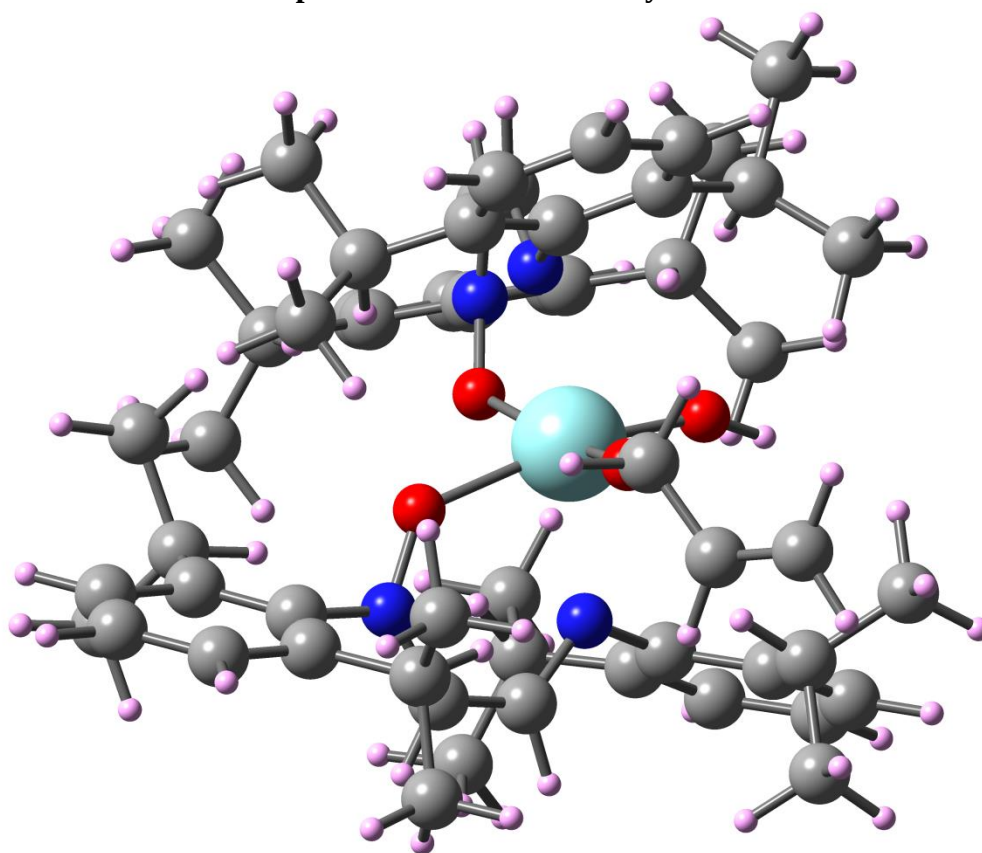
Zr_NCCNO Octahedral Complex with Transferred Allylic H

Fig. S164: Zr_NCCNO Octahedral Complex with Transferred Allylic H

E	E_{zp}	H	G
-2709.0852	-2707.8549	-2707.7806	-2707.9683

N	0.20866770	-0.79221973	-2.28372547
N	-0.27540202	-0.32687712	2.29824052
C	-0.76883476	-0.42007175	-3.15351900
C	-1.99004399	0.19741712	-2.86434936
C	0.54309148	0.43139823	3.07517547
C	1.59222861	1.26779912	2.67754074
C	1.33600829	-1.46970658	-2.91421368
C	2.47849341	-0.71384126	-3.30138021
C	3.54926121	-1.39010202	-3.92366217
C	3.49552299	-2.77262856	-4.16358407
C	2.35952338	-3.50112451	-3.78021958
C	1.26401781	-2.87141606	-3.15004543
C	3.92149552	1.32259503	-2.67669525
C	2.53023749	0.80663365	-3.11374300
C	2.07986803	1.52644447	-4.41575035
C	-2.87633679	4.54919132	-0.38870911
C	-2.89848220	3.53100061	-1.55695891
C	-3.03280922	4.25980141	-2.92107972

C	-3.76056359	1.10372092	-1.41286630
C	-4.01409896	2.49828542	-1.37964105
C	-5.34973185	2.91684485	-1.20874861
C	-6.38817589	1.98164574	-1.07262037
C	-6.10729226	0.60683856	-1.09212471
C	-4.78683010	0.13553418	-1.25290110
C	0.40742941	-4.90085630	-1.85041107
C	0.03621472	-3.70567092	-2.76465768
C	-0.71749111	-4.19618490	-4.03019413
C	-5.02160466	-2.04919165	0.04242278
C	-4.50781020	-1.37123171	-1.25410195
C	-5.12143435	-2.04934523	-2.50783429
C	-1.35013900	-0.98909167	3.02937658
C	-1.18404140	-2.33851227	3.45352473
C	-2.23687860	-2.95545854	4.16300977
C	-3.42116414	-2.26218053	4.45553270
C	-3.56501559	-0.92911534	4.04185566
C	-2.54393885	-0.26816695	3.32493992
C	-0.09633026	-4.52322440	2.64923311
C	0.12408184	-3.10345102	3.22573186
C	0.94179594	-3.17340583	4.54478023
C	1.11499505	4.43378004	-1.23334384
C	1.32908450	4.19649989	0.28427812
C	0.97773783	5.46527944	1.10458472
C	3.06701734	2.45409496	1.08907152
C	2.76285539	3.73598479	0.55984052
C	3.83843762	4.60870460	0.29507223
C	5.16327788	4.22841400	0.55953377
C	5.43779112	2.95497653	1.07972393
C	4.40125758	2.03390807	1.34180240
C	-4.14441794	1.51849675	2.40182652
C	-2.72356341	1.20318935	2.92799375
C	-2.39359448	2.13900101	4.12483148
C	5.84610794	-0.05227183	1.03303272
C	4.75015509	0.64209110	1.88209875
C	5.19771363	0.71421464	3.36755796
H	-0.61874277	-0.65449915	-4.20853845
H	-2.70537647	0.33674222	-3.66593560
H	0.38111149	0.40215015	4.15379879
H	2.16606505	1.77580844	3.44256689
H	4.42982395	-0.83058272	-4.22816067
H	4.32923063	-3.27525358	-4.64895729
H	2.31955509	-4.57073889	-3.97367821
H	1.82134039	1.07293082	-2.32245613
H	-1.93899396	3.00419117	-1.54744071
H	4.67445304	1.19885621	-3.46678419
H	4.27552780	0.79938276	-1.78082130
H	3.86653411	2.39251625	-2.43845441
H	2.74799496	1.27470007	-5.25089617
H	2.10003616	2.61668478	-4.27970217
H	1.06015607	1.23911975	-4.69924198
H	-3.81044128	5.12322628	-0.33090183

H	-2.05694127	5.26654475	-0.52640329
H	-2.72768012	4.03991051	0.57103039
H	-3.01474616	3.54740939	-3.75566546
H	-2.20382432	4.96655632	-3.06055099
H	-3.97256419	4.82508716	-2.98062537
H	-5.57986569	3.97898048	-1.18694287
H	-7.41296341	2.32380460	-0.94755611
H	-6.91827301	-0.10717903	-0.97340694
H	-0.64679525	-3.07367710	-2.19028598
H	-3.42544491	-1.52584140	-1.28278838
H	1.09467798	-5.59992045	-2.34630557
H	-0.49773153	-5.46065608	-1.57812373
H	0.87655084	-4.54938958	-0.92461817
H	-0.08597427	-4.85543625	-4.64135171
H	-1.02928827	-3.35344253	-4.66118153
H	-1.61686540	-4.75948864	-3.74575176
H	-4.56392253	-1.60299511	0.93335771
H	-4.77189605	-3.11903788	0.02839382
H	-6.11195643	-1.96709831	0.14320453
H	-6.21417437	-1.93994130	-2.52778208
H	-4.88956122	-3.12262189	-2.51093183
H	-4.72277038	-1.61372697	-3.43300456
H	-2.12308007	-3.98401278	4.49668021
H	-4.22059419	-2.75278931	5.00632209
H	-4.48183558	-0.39543600	4.27781861
H	0.72129268	-2.55145246	2.49525885
H	0.64181336	3.39981167	0.58170484
H	-0.65734352	-5.16808356	3.33905252
H	0.87307047	-5.00047692	2.45708947
H	-0.63833474	-4.47925199	1.69662647
H	1.15615405	-2.16956287	4.93450520
H	1.89785329	-3.68711500	4.37496089
H	0.39378199	-3.72395656	5.32153993
H	1.77956028	5.22007856	-1.61634526
H	0.08045433	4.74340410	-1.42752956
H	1.30603506	3.51341649	-1.79642845
H	1.11885621	5.29504529	2.17970243
H	-0.07145347	5.74284852	0.93979406
H	1.60001671	6.32242832	0.81500920
H	3.63587483	5.59758487	-0.10831272
H	5.97816698	4.91978876	0.35804585
H	6.46818082	2.66647919	1.26979938
H	-2.01980980	1.42223467	2.11744329
H	3.85115784	0.01861634	1.83217546
H	-4.90418633	1.42505824	3.18930916
H	-4.42214443	0.85723419	1.57485370
H	-4.18479557	2.55099422	2.03183709
H	-2.51469587	3.19131041	3.83264772
H	-1.36428695	2.00181010	4.47606227
H	-3.06798052	1.94130993	4.96944308
H	5.58153725	-0.06500434	-0.03104275
H	5.97609297	-1.09028089	1.36469624

H	6.81591076	0.45224440	1.13218963
H	4.41879113	1.14954938	4.00567960
H	6.10066400	1.32978836	3.47450043
H	5.42590294	-0.29043017	3.74743449
O	-1.31195987	-2.12706778	0.17458288
O	1.67142173	-1.78207903	0.16618863
O	1.23275122	1.07744915	0.32736094
O	-1.52428745	0.69986247	-0.57395854
N	1.97316118	1.55225927	1.39802340
N	-2.40463446	0.64339724	-1.64482510
C	3.42159969	-3.07632352	1.25827912
H	3.31740977	-2.49913924	2.17949578
C	2.96457785	-2.37309896	-0.00230938
H	3.68272430	-1.57744391	-0.25930256
H	2.94447998	-3.07756188	-0.84471475
C	3.94655424	-4.31767696	1.29411104
H	4.04826304	-4.92035655	0.39241540
H	4.29149273	-4.76806908	2.22236467
H	-1.94896999	-2.66996878	0.66020742
Zr	0.03962255	-0.69293936	0.01614831

15.2 Transition States

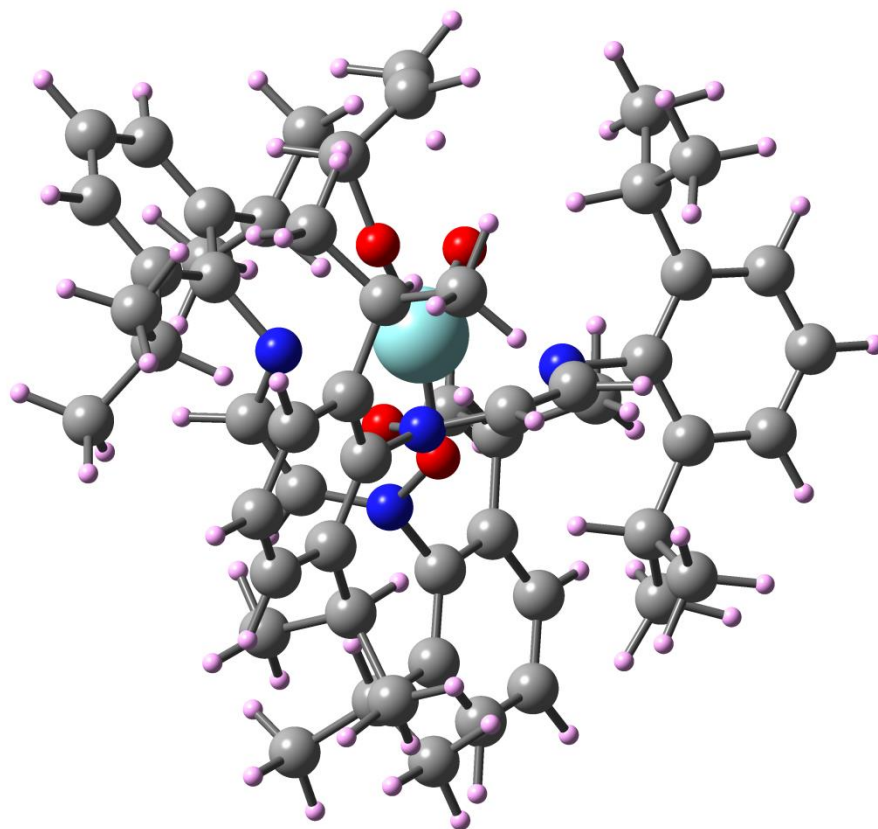
Zr_NCCNO Propene Chemisorbed on Dioxo Complex forming Octahedral Complex to Octahedral Complex with Transferred Allylic Hydrogen

Fig. S165: Zr_NCCNO Propene Chemisorbed on Dioxo Complex forming Octahedral Complex to Octahedral Complex with Transferred Allylic Hydrogen

E	E_{ZP}	H	G	<i>f</i>
-2708.9864	-2707.7582	-2707.6853	-2707.8683	-573

N	-0.12322400	1.76110100	-1.65985400
N	0.14895300	-0.81418900	2.22241400
C	0.69313600	1.46469100	-2.70529100
C	1.78408100	0.59164200	-2.74101900
C	-0.77693900	-1.72853200	2.54411800
C	-1.91049700	-2.16433000	1.81574800
C	-0.96552900	2.92965100	-1.88579100
C	-2.32000700	2.75333000	-2.28900200
C	-3.11414200	3.90143300	-2.49534000
C	-2.58728400	5.19108700	-2.31943100
C	-1.24365000	5.34928500	-1.94779200
C	-0.40565900	4.23357700	-1.72995000
C	-4.37908100	1.21506700	-2.20226000
C	-2.88413100	1.35678000	-2.56914700

C	-2.67079300	0.97842400	-4.06181800
C	2.42285700	-4.19117700	-2.67463700
C	2.56654600	-2.72386900	-3.15284800
C	2.71949400	-2.66782900	-4.69666700
C	3.56326600	-0.79224900	-1.75410200
C	3.73098500	-2.01018700	-2.45885000
C	5.03204900	-2.55322400	-2.52382900
C	6.11249100	-1.91526100	-1.89514800
C	5.91338000	-0.71706700	-1.18969100
C	4.63560600	-0.12637800	-1.10438400
C	1.33845500	5.53398700	-0.33564200
C	1.08163100	4.45427600	-1.41518800
C	1.85278300	4.82719400	-2.71333200
C	4.94734000	1.12677200	1.09964200
C	4.44843000	1.20277200	-0.36542200
C	5.15411500	2.35461700	-1.13070700
C	1.30072600	-0.80675900	3.12956500
C	1.34749900	0.12123800	4.20510900
C	2.45115400	0.07481500	5.08233400
C	3.47943600	-0.86199100	4.90919800
C	3.41238300	-1.77771100	3.84920700
C	2.33039300	-1.77527900	2.94302500
C	0.70984200	2.52354500	4.80727800
C	0.20300800	1.09886800	4.48233400
C	-0.70568000	0.56050700	5.62217600
C	-1.61127000	-3.08739500	-3.13197000
C	-1.83393100	-3.67748300	-1.71489700
C	-1.61742300	-5.21304100	-1.70622800
C	-3.42380300	-2.42816300	-0.09110700
C	-3.22361000	-3.30343400	-1.19062300
C	-4.36886400	-3.85301700	-1.80234100
C	-5.65660600	-3.55697100	-1.32978800
C	-5.82301600	-2.69462700	-0.23610000
C	-4.71515500	-2.09837400	0.40365300
C	3.66482500	-3.10292400	1.19691400
C	2.27826900	-2.82816400	1.82712700
C	1.68578900	-4.16658900	2.35336300
C	-6.01502100	-0.06590200	1.26086300
C	-4.95405800	-1.14858600	1.58609600
C	-5.38649500	-1.93718400	2.85315300
H	0.53048100	2.00918800	-3.63667800
H	2.37243700	0.53544300	-3.64875000
H	-0.65706800	-2.25249700	3.49534500
H	-2.56114800	-2.88685800	2.29076500
H	-4.14999100	3.78740700	-2.80309900
H	-3.21515000	6.06418600	-2.48343000
H	-0.83687400	6.35093500	-1.83352300
H	-2.32647500	0.63844300	-1.95969600
H	1.63967500	-2.20238100	-2.88927600
H	-5.02736600	1.77974000	-2.88649300
H	-4.56883600	1.56919900	-1.18256900
H	-4.67852800	0.16075900	-2.25935200

H	-3.18070500	1.69338700	-4.72232300
H	-3.07667200	-0.02245700	-4.26390700
H	-1.60674200	0.97179300	-4.32539000
H	3.31424600	-4.78568800	-2.91293400
H	1.56574000	-4.66757700	-3.16910700
H	2.26309200	-4.23866300	-1.59078500
H	2.78842000	-1.63295600	-5.05521100
H	1.85695800	-3.13976000	-5.18591000
H	3.62468600	-3.19628500	-5.02410100
H	5.19902900	-3.48214800	-3.06337600
H	7.10747200	-2.35062900	-1.95383700
H	6.75789700	-0.23248800	-0.70654500
H	1.48967600	3.51722200	-1.02515400
H	3.38105600	1.43529900	-0.31790500
H	0.97474600	6.52426500	-0.64186800
H	2.41803800	5.62218200	-0.15484100
H	0.86630700	5.26442700	0.61271000
H	1.48943700	5.78011800	-3.12241300
H	1.73515000	4.06293600	-3.49073500
H	2.92527900	4.93472300	-2.50128600
H	4.42550400	0.33923400	1.65439600
H	4.74646000	2.07813800	1.60779600
H	6.02792400	0.93411200	1.15485800
H	6.23963200	2.19418600	-1.18315200
H	4.97713500	3.30895800	-0.61762900
H	4.77493500	2.44311800	-2.15722100
H	2.50326400	0.77480200	5.91181700
H	4.32258700	-0.88214300	5.59605100
H	4.21146800	-2.50282800	3.72358700
H	-0.40251400	1.17130100	3.57419400
H	-1.07910100	-3.22937900	-1.06265700
H	1.30843800	2.54954800	5.72719400
H	-0.14137200	3.20220900	4.95667800
H	1.31484800	2.90214800	3.97704200
H	-1.12558900	-0.42249700	5.37122800
H	-1.54117100	1.25043400	5.80744600
H	-0.14135700	0.45460500	6.55853000
H	-2.34194800	-3.48333700	-3.85040300
H	-0.60772200	-3.34301900	-3.49602300
H	-1.70050700	-1.99585600	-3.11050600
H	-1.76795600	-5.63118700	-0.70257700
H	-0.59303800	-5.44820700	-2.02289200
H	-2.30378500	-5.72686900	-2.39182000
H	-4.24994200	-4.52656200	-2.64697000
H	-6.52690900	-3.99636200	-1.81131100
H	-6.82559900	-2.46905900	0.11645800
H	1.62788200	-2.44536500	1.03279400
H	-4.01803600	-0.62576400	1.80965200
H	4.33935900	-3.61148900	1.89860800
H	4.14583600	-2.17794400	0.86592200
H	3.55478200	-3.75704100	0.32303200
H	1.66020900	-4.91491300	1.54895400

H	0.66514800	-4.04469900	2.73387200
H	2.30322100	-4.56679000	3.16919800
H	-5.75060900	0.49235700	0.35705600
H	-6.09115700	0.64338900	2.09587800
H	-7.01112000	-0.50204200	1.11164800
H	-4.64283700	-2.68881700	3.14540300
H	-6.33664300	-2.46008400	2.68175700
H	-5.52498500	-1.25188200	3.69973200
O	0.80769500	2.15175600	1.34896700
O	-1.96274900	1.40626100	0.94028000
O	-1.48176000	-1.02762100	-0.21298700
O	1.56666500	-0.25138300	-0.51776900
N	-2.24339600	-1.84891900	0.54434500
N	2.25153100	-0.17258500	-1.71283400
C	-2.22855500	3.19541400	2.39741300
H	-2.39323800	2.80747900	3.40447200
C	-2.89595500	2.47413800	1.26473900
H	-3.86008300	2.03845300	1.55639000
H	-3.03643500	3.12045300	0.38900400
C	-1.11342700	4.10054500	2.15269100
H	-1.26040600	4.72664100	1.26416900
H	-0.81533300	4.69289600	3.02384900
H	-0.20499200	3.42103500	1.88479600
Zr	-0.07801800	0.77494200	0.45381300

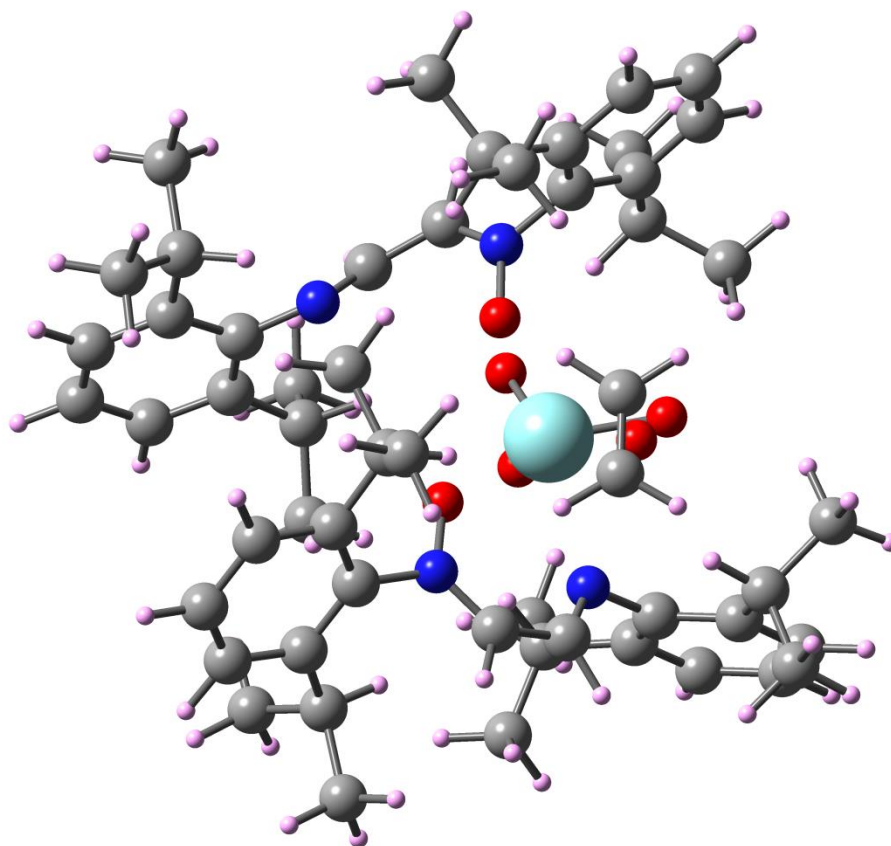
Zr_NCCNO Bisperoxo Complex to Oxo Peroxo Complex (Ethylene)

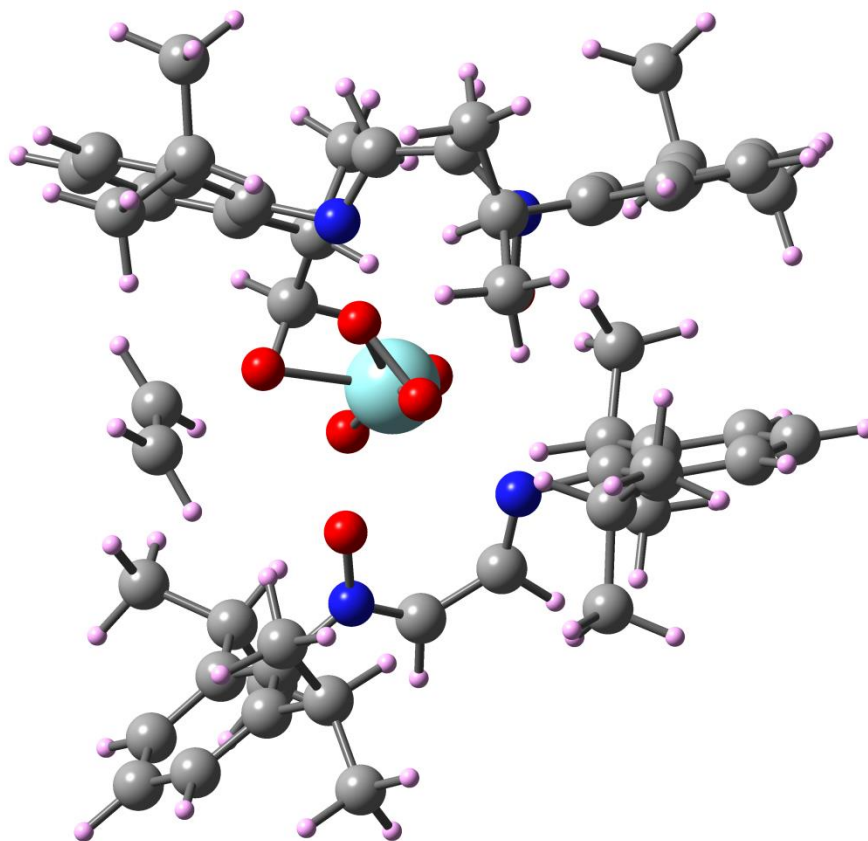
Fig. S166: Zr_NCCNO Bisperoxo Complex to Oxo Peroxo Complex (Ethylene)

E	E_{ZP}	H	G	<i>f</i>
-2819.9440	-2818.7373	-2818.6623	-2818.8508	-478
Zr	1.13093808	0.57279404	-0.21148402	
O	0.04799800	-1.19827009	0.74526206	
O	-0.73374806	1.77228013	0.33340403	
O	2.50039519	1.88420614	0.09916401	
N	-3.01021023	0.36337303	-1.31289210	
N	-1.18061009	2.74880121	-0.51381204	
N	2.90394622	-1.08780509	0.30463002	
N	0.38692803	-2.17048417	1.60502212	
C	-2.46717319	1.25803909	-2.07676016	
C	-1.90202115	2.51727119	-1.58579112	
C	2.84100822	-1.92787215	1.30151810	
C	1.64091813	-2.42399119	1.95018715	
C	-3.65852128	-0.79271706	-1.84413614	
C	-3.06978724	-1.63808112	-2.83694821	
C	-3.81597529	-2.75706321	-3.26838825	
C	-5.08613639	-3.04507923	-2.74989921	
C	-5.63766645	-2.21963417	-1.75470613	
C	-4.93843737	-1.09660509	-1.27920310	

C	-0.77509206	-2.68764620	-3.20869924
C	-1.66150213	-1.43328611	-3.41323826
C	-1.71534713	-1.05540108	-4.91808038
C	2.41251418	4.43073734	-1.95744015
C	0.87423607	4.29985533	-2.09733216
C	0.37703903	5.01473838	-3.38448726
C	-0.83435707	4.13359331	-0.12989501
C	0.14089801	4.84913737	-0.86788806
C	0.40982903	6.16921145	-0.43928703
C	-0.25181602	6.73356851	0.65879205
C	-1.21646409	5.99218943	1.36122910
C	-1.52947312	4.67216836	0.98443608
C	-6.40539749	-0.89362107	0.82556207
C	-5.56408541	-0.15927301	-0.24374302
C	-6.41617947	0.93375007	-0.94788507
C	-2.50998119	3.99866431	3.25411725
C	-2.63925520	3.90472430	1.71350313
C	-4.03417831	4.41329034	1.25429810
C	4.22637932	-0.89327507	-0.29659102
C	5.23793040	-0.18474101	0.40894103
C	6.49266649	-0.04956300	-0.22442402
C	6.73735350	-0.59021705	-1.49344411
C	5.72166942	-1.29155010	-2.16176616
C	4.44875734	-1.45922411	-1.58293812
C	5.34840742	1.96535815	1.76789113
C	5.03522339	0.44757203	1.79089914
C	5.88865347	-0.28114802	2.86435622
C	-0.44319903	-5.68378541	-0.50367004
C	0.26661602	-5.00924138	0.69977605
C	1.18050109	-6.03117747	1.42875711
C	-0.71725606	-3.01854023	2.08483416
C	-0.74523106	-4.37771334	1.66693213
C	-1.80205914	-5.17246439	2.15775616
C	-2.79221122	-4.63249435	2.99120423
C	-2.75392721	-3.27647625	3.34654325
C	-1.71633013	-2.43158519	2.90186922
C	3.34125225	-2.11500716	-3.80541529
C	3.39181326	-2.32526318	-2.27543817
C	3.62321928	-3.82369429	-1.93207515
C	-2.87281822	-0.20516102	2.59052620
C	-1.72261713	-0.95739407	3.31017825
C	-1.81534614	-0.78800906	4.84869437
H	-2.51439019	1.21325009	-3.17063924
H	-2.09873316	3.39863926	-2.19045417
H	3.75584329	-2.39876418	1.67055413
H	1.76598414	-3.17562224	2.71953121
H	-3.38880026	-3.41346226	-4.02251730
H	-5.63985444	-3.90840330	-3.11203624
H	-6.61733451	-2.45388919	-1.34812910
H	-1.14867809	-0.62091605	-2.89284622
H	0.66953405	3.22999825	-2.20689317
H	-1.15314809	-3.55878727	-3.76190129

H	-0.71808906	-2.94867622	-2.14479916
H	0.24080802	-2.46765919	-3.55423627
H	-2.15665516	-1.86264314	-5.51911841
H	-0.70086005	-0.86433307	-5.28930340
H	-2.31561018	-0.15135101	-5.08968839
H	2.73441221	5.47921840	-1.88477314
H	2.89477122	3.99294530	-2.84131322
H	2.76166421	3.87908230	-1.07828808
H	-0.70934505	4.91439038	-3.52218927
H	0.86964206	4.57934635	-4.26302833
H	0.60981705	6.08812048	-3.36142426
H	1.15510009	6.75223851	-0.97215708
H	-0.01976200	7.75029559	0.96700907
H	-1.73094513	6.44419851	2.20449917
H	-4.73749636	0.35224703	0.26248602
H	-2.56333420	2.84582922	1.44845911
H	-7.31474456	-1.33993410	0.40118303
H	-6.72390451	-0.18504801	1.60206712
H	-5.82734246	-1.69304413	1.30658110
H	-7.26022957	0.48393404	-1.48828011
H	-5.81610745	1.49960112	-1.67167013
H	-6.82069352	1.64261512	-0.21212702
H	-1.52097611	3.66787528	3.59187727
H	-3.26780825	3.36416826	3.73293428
H	-2.66654920	5.02304538	3.61569028
H	-4.16857732	5.47388641	1.50471512
H	-4.83067437	3.84210729	1.74961313
H	-4.16430132	4.30482633	0.16967701
H	7.28105354	0.49928404	0.28387402
H	7.71199861	-0.46682804	-1.96005115
H	5.92054243	-1.71414913	-3.14209324
H	3.98000230	0.38032703	2.06741416
H	0.90739607	-4.22522432	0.28090802
H	6.39094550	2.17132916	1.48809611
H	5.17659239	2.39460618	2.76468821
H	4.67296736	2.45884419	1.06303608
H	5.64839345	-1.35296911	2.92561522
H	5.71301843	0.16369801	3.85328229
H	6.96217953	-0.19859602	2.64678720
H	-1.02747508	-6.55858652	-0.19243701
H	0.30479302	-6.02535244	-1.23058909
H	-1.11813709	-4.98554438	-1.01023808
H	1.73421513	-5.57196745	2.25847117
H	1.90950815	-6.45695549	0.72766206
H	0.58949305	-6.85728454	1.84426214
H	-1.86059614	-6.21716750	1.86698414
H	-3.59949928	-5.26500540	3.35172725
H	-3.53482527	-2.86613422	3.97995930
H	2.40769918	-2.03303016	-1.89503514
H	-0.79154506	-0.49254604	2.97902723
H	4.26874032	-2.42966918	-4.30290233
H	3.14712324	-1.06210308	-4.03227831

H	2.52300719	-2.70906821	-4.23375332
H	2.84055522	-4.44528234	-2.38904418
H	3.61089527	-3.99914631	-0.84648107
H	4.59544035	-4.16765132	-2.31052417
H	-2.72775021	-0.21329002	1.50541612
H	-2.89283622	0.84057806	2.92263322
H	-3.84745229	-0.65434605	2.82449022
H	-1.02295108	-1.34301310	5.36743140
H	-2.78141321	-1.13441009	5.23847440
H	-1.71018213	0.27161202	5.11138439
O	0.38383303	1.02971008	-2.10559116
O	1.40051111	-0.12764401	-2.14836116
C	1.51828311	0.79907606	3.94017430
H	1.01543708	-0.16121801	3.98613831
C	0.98104008	1.88307314	3.25016625
H	-0.04376200	1.86546114	2.88730922
O	1.92303915	1.34266710	1.78056313
H	1.41403811	2.87241122	3.36816826
H	2.49741419	0.86839307	4.40491934

Zr_NCCNO Peroxo η^3 -Ozone Complex to Bisperoxo Complex (Ethylene)Fig. S167: Zr_NCCNO Peroxo η^3 -Ozone Complex to Bisperoxo Complex (Ethylene)

E	E_{zp}	H	G	<i>f</i>
-2895.1078	-2893.8964	-2893.8210	-2894.0072	-362

Zr	0.29374902	0.22613602	-0.14042901
O	-2.00473215	0.04923400	0.17701201
O	2.19475417	-1.01611208	-0.78068906
O	1.30290010	1.52920412	-1.57482212
N	0.15323701	-2.13095516	0.84385307
N	3.02885623	-1.72600913	-0.00301100
N	-0.68770605	2.70687321	0.19823602
N	-2.99402523	0.76611306	-0.36827603
C	1.22536109	-2.68867721	1.36093111
C	2.59968420	-2.44204219	1.02411508
C	-1.91875315	2.99551623	-0.12452401
C	-2.98103023	2.08141616	-0.48176304
C	-1.09138008	-2.78978021	1.24092409
C	-1.52037212	-2.78113321	2.59863020
C	-2.67032021	-3.53366927	2.92565022
C	-3.36786126	-4.26633533	1.95708815
C	-2.92729922	-4.25498833	0.62385305
C	-1.78431214	-3.52764727	0.23776502

C	-1.76212313	-0.93068807	4.32451033
C	-0.81716506	-1.99821615	3.71622628
C	-0.27817402	-2.94284422	4.82288937
C	5.64864841	1.03501508	1.88487315
C	5.01029338	-0.37287703	1.76571814
C	5.43234943	-1.24019109	2.98469123
C	4.44377934	-1.71044213	-0.39328803
C	5.38613442	-1.06585208	0.44834003
C	6.73250549	-1.08790508	0.02364100
C	7.10517053	-1.69801413	-1.18346309
C	6.13941046	-2.31177018	-1.99727415
C	4.78141137	-2.33994218	-1.61941712
C	-2.34665918	-3.88005630	-2.24836517
C	-1.24592809	-3.62491727	-1.19421409
C	-0.17100201	-4.74551536	-1.29191410
C	3.42495026	-2.12489216	-3.75284229
C	3.74317429	-3.01687123	-2.52200619
C	4.18947232	-4.43458934	-2.96121023
C	0.17519901	3.86867630	0.39133303
C	0.44448903	4.73664936	-0.71148506
C	1.29104310	5.84196744	-0.47892904
C	1.84323314	6.09186245	0.78560806
C	1.54281912	5.23728940	1.85725314
C	0.70534505	4.11602032	1.68840013
C	0.99625608	4.49536234	-3.20408625
C	-0.11790701	4.53817635	-2.12886616
C	-1.15132609	5.64620843	-2.47446619
C	-5.51441143	-1.11182509	2.62708020
C	-4.92758238	-0.06063200	1.65805913
C	-5.58295645	1.32381610	1.93730215
C	-4.18492732	0.01295200	-0.81415706
C	-5.09308339	-0.43466803	0.17963501
C	-6.21123950	-1.16556709	-0.26654402
C	-6.40876247	-1.42353511	-1.63421612
C	-5.50262544	-0.93751907	-2.58635320
C	-4.36060433	-0.19790602	-2.20339417
C	1.46250711	2.94158423	3.84315230
C	0.28540302	3.28351025	2.90137522
C	-0.84595406	4.01969131	3.67275828
C	-2.93713423	-0.68747205	-4.28198533
C	-3.43553026	0.38274203	-3.28099025
C	-4.16022532	1.53551712	-4.03118031
H	1.10414508	-3.48941226	2.09529916
H	3.35850426	-2.98251623	1.57481512
H	-2.23193217	4.04180031	-0.17567301
H	-3.88509530	2.51516119	-0.89027107
H	-3.01713023	-3.54379327	3.95646330
H	-4.24460432	-4.84661337	2.23664617
H	-3.47130426	-4.82731337	-0.12080101
H	0.01629800	-1.43491311	3.28965825
H	3.92339430	-0.23525202	1.80556514
H	-2.65560620	-1.38206711	4.77857237

H	-2.07622816	-0.22253702	3.54988327
H	-1.23478909	-0.36327703	5.10282839
H	-1.09004608	-3.48741727	5.32404140
H	0.25602102	-2.36171218	5.58647241
H	0.41768203	-3.69095128	4.41796034
H	6.73983851	0.98184008	1.99589115
H	5.24951940	1.54370812	2.77161721
H	5.42338342	1.65279612	1.00881608
H	4.96874938	-2.23515917	2.96776823
H	5.13341939	-0.74677005	3.91825230
H	6.52122851	-1.38245110	3.00694523
H	7.49022260	-0.60743404	0.63571205
H	8.14782460	-1.69232613	-1.49225911
H	6.44291250	-2.77937521	-2.92953022
H	-0.76590206	-2.67294821	-1.44548611
H	2.80609321	-3.12459124	-1.96565315
H	-2.77237721	-4.88945537	-2.16156217
H	-1.91759414	-3.79284529	-3.25446125
H	-3.16170524	-3.15265424	-2.16176816
H	-0.61114405	-5.72646445	-1.06429608
H	0.65963105	-4.57822335	-0.59591205
H	0.24285802	-4.78331437	-2.30866117
H	2.98200723	-1.17558509	-3.43619926
H	2.70105921	-2.62994720	-4.40542634
H	4.33129933	-1.92162815	-4.33975033
H	5.06722438	-4.40290434	-3.61943228
H	3.37890326	-4.91965138	-3.52023227
H	4.43554234	-5.06723639	-2.09830916
H	1.52298411	6.51192748	-1.30288510
H	2.49327619	6.95070051	0.93622507
H	1.95276715	5.44763943	2.84092122
H	-0.61486905	3.56607527	-2.18657917
H	-3.85582930	0.01767900	1.87257514
H	1.57932412	5.42531243	-3.23784225
H	0.54866004	4.34518533	-4.19575232
H	1.66408513	3.65412928	-3.00625623
H	-1.97934515	5.68276145	-1.75299513
H	-1.57528812	5.47230242	-3.47264327
H	-0.67975305	6.63786452	-2.47826319
H	-6.61118849	-1.14468909	2.57743120
H	-5.24230540	-0.85129507	3.65767528
H	-5.12141239	-2.11058016	2.41517418
H	-5.15709539	2.11814016	1.31244410
H	-5.43240441	1.60672312	2.98713823
H	-6.66362053	1.28508110	1.74553813
H	-6.93058855	-1.53533212	0.45667603
H	-7.27614256	-1.99537715	-1.95559615
H	-5.67661442	-1.13109609	-3.64087828
H	-0.10474601	2.32514218	2.54723920
H	-2.53457519	0.79077606	-2.81522421
H	1.92176115	3.83434329	4.29091533
H	2.22480517	2.37515918	3.29794325

H	1.10104508	2.30708518	4.66300736
H	-1.19386809	3.40302226	4.51248535
H	-1.70868013	4.22675332	3.02392523
H	-0.49380404	4.97937438	4.07697931
H	-2.31520318	-1.42406711	-3.76810729
H	-2.31142818	-0.20655502	-5.04424939
H	-3.76277029	-1.19960409	-4.79507937
H	-4.50272534	2.32394718	-3.34624725
H	-5.03945038	1.16532509	-4.57557835
H	-3.47777126	1.99176715	-4.75931036
O	1.62880412	0.48911704	1.46917811
O	0.19925602	0.31078902	1.95841215
O	-0.39557803	0.93309907	-2.06581016
O	-0.31011202	-0.56389004	-2.05981315
C	3.12974424	2.42706019	-0.58374004
H	3.11070024	1.93653715	0.38360803
H	2.94004523	3.49525327	-0.59861605
C	3.32074425	1.72340013	-1.74985613
H	3.55207127	0.66633605	-1.74584113
H	3.35792326	2.22785017	-2.71133921

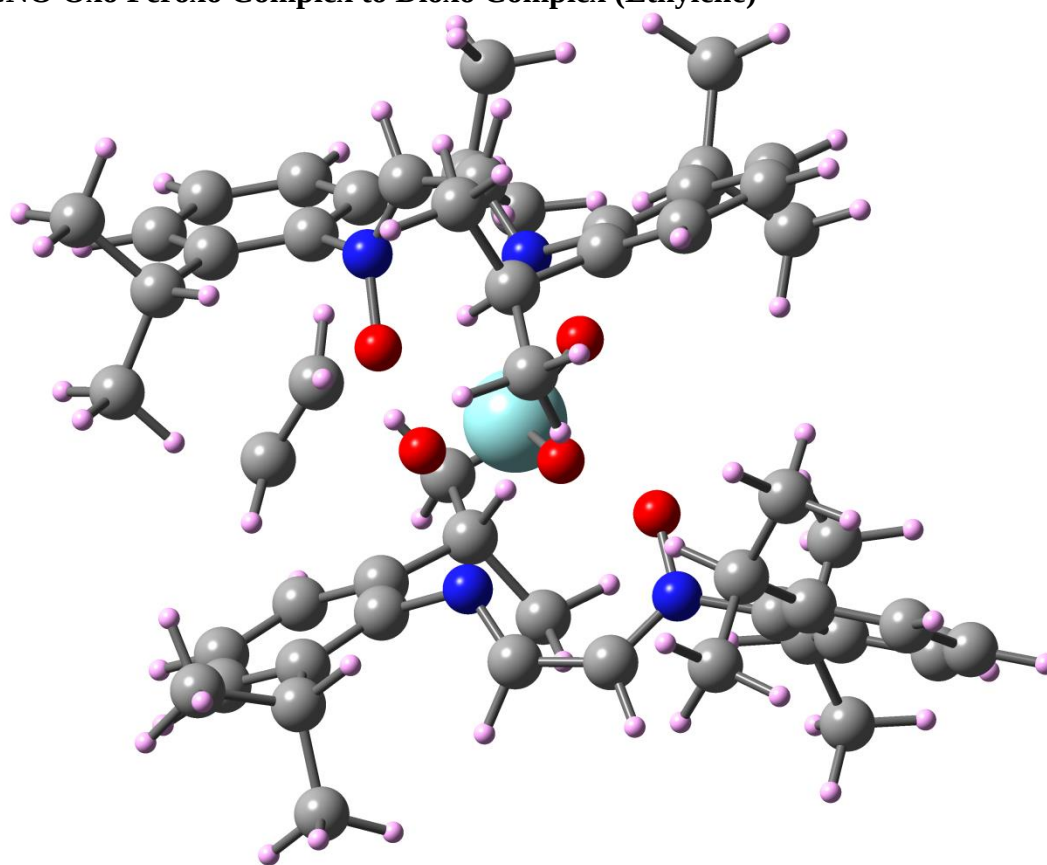
Zr_NCCNO Oxo Peroxo Complex to Dioxo Complex (Ethylene)

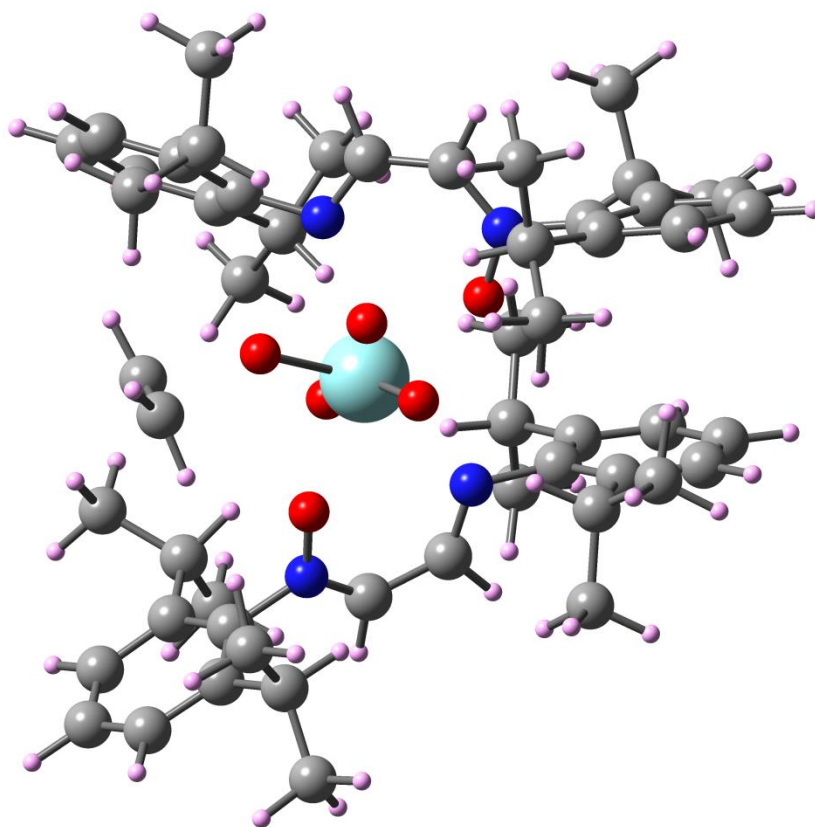
Fig. S168: Zr_NCCNO Oxo Peroxo Complex to Dioxo Complex (Ethylene)

E	E_{ZP}	H	G	<i>f</i>
-2744.7598	-2743.5548	-2743.4815	-2743.6652	-485
Zr	-0.10774997	0.11202604	-0.23784999	
O	2.17920521	0.43068805	-0.32690900	
O	-1.96846012	-0.84974302	0.95002310	
O	0.02380705	0.97866511	1.43853014	
N	0.01566703	-2.42605215	-0.34024900	
N	-2.83905519	-1.68388208	0.38644806	
N	0.04937106	2.58842723	-0.63768502	
N	2.85820426	1.51940513	0.08427203	
C	-1.08936806	-3.07804720	-0.62204502	
C	-2.45555316	-2.65515616	-0.43420701	
C	1.13224415	3.28254928	-0.39106800	
C	2.43983624	2.77232823	-0.05190598	
C	1.25275012	-3.20242222	-0.34953700	
C	1.69659115	-3.94597228	-1.48816609	
C	2.90471923	-4.66866634	-1.36717908	
C	3.64938529	-4.67198935	-0.18206899	
C	3.18564726	-3.95445729	0.93055610	
C	1.98576617	-3.21961922	0.87792110	

C	1.91466016	-3.92670328	-4.05016428
C	0.95291009	-4.02502528	-2.83334819
C	0.16605802	-5.36223038	-2.97467620
C	-5.26978135	1.02148514	-1.75437310
C	-4.72846933	-0.40973297	-1.51076909
C	-5.19787436	-1.36375504	-2.64252618
C	-4.25012030	-1.53033006	0.77848609
C	-5.15315736	-0.94106501	-0.13754098
C	-6.50041248	-0.84964799	0.27877105
C	-6.90302350	-1.29182802	1.54721615
C	-5.96549043	-1.83464607	2.44160021
C	-4.61042133	-1.96838509	2.07826218
C	2.50079522	-2.20785915	3.19156927
C	1.42330813	-2.57563317	2.15009319
C	0.38081305	-3.52713524	2.80432424
C	-3.17255921	-1.39498305	4.07515034
C	-3.58648025	-2.51333014	3.07869426
C	-4.09109030	-3.77049623	3.82862132
C	-1.18875003	3.36975230	-0.71821803
C	-1.73207907	3.94842135	0.46720206
C	-2.91820415	4.70578741	0.34008905
C	-3.54231520	4.89632343	-0.89950404
C	-2.98495316	4.31929238	-2.05065013
C	-1.81080307	3.54530431	-1.98435713
C	-2.14126111	3.10719628	2.83142324
C	-1.12804402	3.77513833	1.86663617
C	-0.63193498	5.13107743	2.43485522
C	5.27108044	-1.03084308	-1.80338111
C	5.13306743	0.48349604	-1.49951609
C	6.19798652	1.30232110	-2.27657315
C	4.13664836	1.25923310	0.76607009
C	5.21586444	0.74595506	0.00632003
C	6.42202254	0.49320703	0.69263208
C	6.53831755	0.74765705	2.06742318
C	5.44871948	1.26120510	2.78776024
C	4.21175837	1.52738312	2.16181319
C	-2.19044311	2.23306222	-4.14857229
C	-1.18263803	3.00331627	-3.26518322
C	-0.49370297	4.14926135	-4.05600128
C	2.89325427	1.41162312	4.36489736
C	3.04644629	2.10076718	2.98580726
C	3.23612131	3.62808429	3.21341927
H	-1.02269506	-4.11589828	-0.94971804
H	-3.24363823	-3.27526020	-0.84100903
H	1.07547215	4.37284836	-0.33691500
H	3.17886330	3.51309028	0.22627504
H	3.26849126	-5.23150139	-2.22173714
H	4.57819835	-5.23423640	-0.12223398
H	3.75835830	-3.97460529	1.85141617
H	0.25024004	-3.18575921	-2.89978619
H	-3.63366124	-0.33080997	-1.55543709
H	2.46341120	-4.86497435	-4.20276529

H	2.64764922	-3.12464722	-3.93274427
H	1.33721212	-3.73674326	-4.96437935
H	0.85753807	-6.21452743	-2.94243220
H	-0.36039802	-5.38966240	-3.93801128
H	-0.57551404	-5.52022540	-2.18239114
H	-6.36660943	1.04809415	-1.82033311
H	-4.86668932	1.40639617	-2.69816518
H	-4.95086833	1.70401620	-0.95848104
H	-4.78889634	-2.37652212	-2.52260417
H	-4.86038734	-0.98128401	-3.61410525
H	-6.29371045	-1.44639104	-2.66879217
H	-7.23212751	-0.41039295	-0.39283000
H	-7.94529556	-1.20384501	1.84504017
H	-6.28911047	-2.15771909	3.42671529
H	0.90171810	-1.64730210	1.88908517
H	-2.67953818	-2.80049516	2.53401722
H	2.98008325	-3.09708222	3.62322130
H	2.02774218	-1.66297111	4.01660534
H	3.27964628	-1.56851911	2.75907724
H	0.86322208	-4.45764231	3.13418227
H	-0.42471102	-3.79133625	2.10941119
H	-0.07315999	-3.04350820	3.67884431
H	-2.72593517	-0.55025899	3.54080430
H	-2.43390816	-1.77993509	4.79132839
H	-4.04195028	-1.03574002	4.64236338
H	-4.93227436	-3.53897421	4.49437837
H	-3.28514024	-4.17843126	4.45254537
H	-4.41602133	-4.55489129	3.13259027
H	-3.35492518	5.14783045	1.23227612
H	-4.45166627	5.48933748	-0.96880404
H	-3.46374220	4.47261740	-3.01444920
H	-0.29609596	3.06634027	1.81089317
H	4.15246336	0.80316307	-1.86579112
H	-3.05943317	3.69937733	2.95033825
H	-1.68457107	2.98423427	3.82310632
H	-2.39976513	2.11078721	2.45892221
H	0.12052308	5.59611847	1.78194017
H	-0.17940894	4.98390242	3.42550029
H	-1.45659103	5.84824946	2.54845122
H	6.25673853	-1.40792011	-1.49905009
H	5.15930243	-1.21049809	-2.88034719
H	4.50752937	-1.61131612	-1.27357907
H	6.09906652	2.37781318	-2.07984813
H	6.07892449	1.14014008	-3.35563123
H	7.21833561	1.00314306	-2.00450413
H	7.27490360	0.10202200	0.14459404
H	7.47736459	0.54753403	2.57798523
H	5.55375349	1.44781911	3.85223632
H	-0.43181398	2.27312821	-2.96769920
H	2.10295121	1.92940417	2.45199321
H	-3.03694917	2.85845427	-4.46598131
H	-2.55372715	1.36651515	-3.58846824

H	-1.69083408	1.86813719	-5.05735536
H	0.00819206	3.75330432	-4.95012535
H	0.25769009	4.66872939	-3.44450423
H	-1.22741102	4.89776942	-4.38578731
H	2.82741826	0.32586804	4.26332235
H	1.96851620	1.76193515	4.83946740
H	3.72499433	1.64831814	5.04253041
H	3.31862932	4.19169333	2.27601320
H	4.14574338	3.82327330	3.79770232
H	2.38017225	4.03086632	3.76945331
O	-1.59337108	0.25843906	-1.52149909
O	0.04953504	0.01476103	-2.51026917
C	1.86979918	-0.56349502	-3.50200424
H	2.52574323	-0.93427605	-2.72290318
C	1.39150915	0.74385108	-3.49175624
H	1.83372219	1.48863013	-2.83553619
H	0.85925111	1.13168011	-4.35551431
H	1.52946415	-1.25503707	-4.26231830

Zr_NCCNO Oxo η^3 -Ozone Complex to Oxo Peroxo Complex (Ethylene)Fig. S169: Zr_NCCNO Oxo η^3 -Ozone Complex to Oxo Peroxo Complex (Ethylene)

E	E_{zp}	H	G	<i>f</i>
-2819.9380	-2818.7299	-2818.6552	-2818.8413	-407
Zr	0.32785202	0.20923102	-0.25575802	
O	-1.93801815	0.11327301	0.24407902	
O	2.28128917	-1.00067608	-0.80860306	
O	1.26513010	1.44434411	-1.77126814	
N	0.10252001	-2.14705216	0.75564806	
N	3.03058723	-1.75877313	-0.01212600	
N	-0.64649205	2.68621320	0.07477401	
N	-2.93290023	0.75970106	-0.38967803	
C	1.14379509	-2.81219621	1.18327409	
C	2.53756619	-2.57382319	0.90297107	
C	-1.85258814	2.98211523	-0.32746102	
C	-2.90726722	2.05208716	-0.65233105	
C	-1.15674309	-2.70178821	1.25715110	
C	-1.50059412	-2.48549019	2.61843220	
C	-2.64819320	-3.14359924	3.11145624	
C	-3.42509026	-3.96826830	2.28518817	
C	-3.07535523	-4.13983032	0.93536707	
C	-1.93450915	-3.51582727	0.39137503	

C	-1.55092112	-0.46150104	4.17043832
C	-0.67865505	-1.58332112	3.55173927
C	0.00570600	-2.40874318	4.67435036
C	5.28218640	1.18221709	2.09853316
C	4.66945936	-0.22736302	1.89841615
C	4.87057937	-1.06455908	3.19271124
C	4.48461034	-1.68833913	-0.23701402
C	5.26919240	-0.95065107	0.68388005
C	6.65863251	-0.91768907	0.43745503
C	7.21553155	-1.56645612	-0.67642105
C	6.39694251	-2.26735917	-1.57634412
C	5.00283138	-2.34805818	-1.37685011
C	-2.68512020	-4.06180031	-2.00564315
C	-1.50009011	-3.77067429	-1.05674408
C	-0.48967704	-4.95154138	-1.12992909
C	4.03730831	-2.34070818	-3.72299928
C	4.12002231	-3.10558024	-2.37465918
C	4.61144835	-4.56011535	-2.58938920
C	0.22484602	3.82292029	0.31886202
C	0.51494204	4.75098736	-0.72875606
C	1.36343610	5.83604145	-0.41931503
C	1.90226314	6.00593746	0.86366807
C	1.59407612	5.08550939	1.87827414
C	0.75223606	3.98309530	1.63327212
C	1.12709209	4.67598436	-3.21806125
C	-0.01192600	4.62787936	-2.16872217
C	-1.05342308	5.73881646	-2.47970719
C	-5.45981542	-0.74582506	2.81587022
C	-4.84621337	0.16937101	1.73239613
C	-5.46026242	1.59510012	1.85815714
C	-4.13436831	-0.02520000	-0.74339506
C	-5.03206638	-0.36029703	0.30476702
C	-6.16698848	-1.11576609	-0.04679500
C	-6.39836049	-1.49703311	-1.37977910
C	-5.51115440	-1.10859508	-2.39171418
C	-4.35091633	-0.35260503	-2.10497816
C	1.40422711	2.85302322	3.84922229
C	0.31946102	3.05466123	2.76948521
C	-0.99440907	3.58141227	3.41202026
C	-3.01245123	-1.01082708	-4.19693032
C	-3.46396526	0.13378701	-3.25880525
C	-4.21270032	1.23432710	-4.06273931
H	0.99005708	-3.66974128	1.84507914
H	3.26628525	-3.16310024	1.44416511
H	-2.15298317	4.02667731	-0.43868503
H	-3.79627829	2.44796218	-1.12639209
H	-2.93154323	-3.00778223	4.15259732
H	-4.29910633	-4.47555434	2.68815020
H	-3.69115228	-4.77125936	0.30235102
H	0.10101901	-1.07626508	2.97176323
H	3.58902827	-0.09282301	1.74786814
H	-2.36364218	-0.86466807	4.79017337

H	-1.98945515	0.16262901	3.38354926
H	-0.93065907	0.18388801	4.80664837
H	-0.73421205	-2.91711522	5.30782942
H	0.60518005	-1.75015613	5.31683739
H	0.67265005	-3.17884324	4.26355832
H	6.32780947	1.13272608	2.43163818
H	4.71490136	1.71875113	2.86935522
H	5.24432240	1.77361314	1.17705309
H	4.39526033	-2.05142616	3.12705624
H	4.42786734	-0.53875004	4.04802831
H	5.93833745	-1.21999209	3.39976226
H	7.30498257	-0.36590403	1.11339709
H	8.28841562	-1.51906212	-0.84720907
H	6.84193654	-2.75616721	-2.43858118
H	-0.99780807	-2.86521422	-1.42126211
H	3.09837924	-3.15622124	-1.98219315
H	-3.15123624	-5.03363938	-1.79059214
H	-2.32683418	-4.09440431	-3.04214823
H	-3.45542026	-3.28610525	-1.93796315
H	-0.95648107	-5.88355643	-0.78163906
H	0.40202903	-4.77168536	-0.51785804
H	-0.16025901	-5.10004539	-2.16689917
H	3.59688727	-1.34815810	-3.58074427
H	3.40247826	-2.89064222	-4.42934934
H	5.03095339	-2.22278517	-4.17590532
H	5.60338841	-4.58826735	-3.05848623
H	3.91751530	-5.09402539	-3.25121725
H	4.67137335	-5.11024339	-1.64117913
H	1.61094513	6.55240049	-1.19846209
H	2.55374519	6.85142353	1.07278708
H	2.00517215	5.23026840	2.87261122
H	-0.48633004	3.65036428	-2.29538318
H	-3.77147029	0.23982702	1.93215615
H	1.66128013	5.63531044	-3.20852324
H	0.70896806	4.53580835	-4.22368932
H	1.84034514	3.86937230	-3.03696323
H	-1.90003314	5.72831245	-1.77958014
H	-1.44990811	5.61414944	-3.49627926
H	-0.59407304	6.73433052	-2.41759018
H	-6.55741852	-0.74551106	2.77496021
H	-5.17154040	-0.38103503	3.81001329
H	-5.10419039	-1.77513914	2.71464421
H	-5.01445838	2.30411718	1.15053109
H	-5.29890739	1.98644815	2.87099122
H	-6.54207349	1.56590212	1.67156913
H	-6.87713350	-1.40376510	0.72137906
H	-7.27953856	-2.08410516	-1.62813613
H	-5.71524045	-1.38915011	-3.42097026
H	0.14197901	2.06541216	2.33462918
H	-2.54043019	0.56516904	-2.86386522
H	1.61374412	3.76979029	4.41866534
H	2.33312618	2.49256219	3.39348226

H	1.06853608	2.09043516	4.56417735
H	-1.33827510	2.89053222	4.19367332
H	-1.79919214	3.67852128	2.67078420
H	-0.84087306	4.56800835	3.87211030
H	-2.34292518	-1.68873813	-3.66230728
H	-2.44236419	-0.58687005	-5.03306839
H	-3.85806329	-1.57561612	-4.61377935
H	-4.53337635	2.06996616	-3.42415726
H	-5.10935539	0.83220507	-4.55389335
H	-3.55159327	1.63743713	-4.84016937
O	1.22147109	0.39511003	1.38400311
O	-0.46986604	0.77120006	-2.28081017
O	-0.37161503	-0.71598705	-2.14474117
C	3.13688124	2.31283718	-0.84111007
H	3.19951925	1.79277614	0.10746801
H	2.97341423	3.38504426	-0.80915006
C	3.12061224	1.61802313	-2.04227116
H	3.38469726	0.56878104	-2.07812216
H	3.11974624	2.14647416	-2.99157323

**Zr_NCCNO Oxo Complex with Adsorbed Oxygen Molecule to Dioxo Complex (triplet)
(Ethylene)**

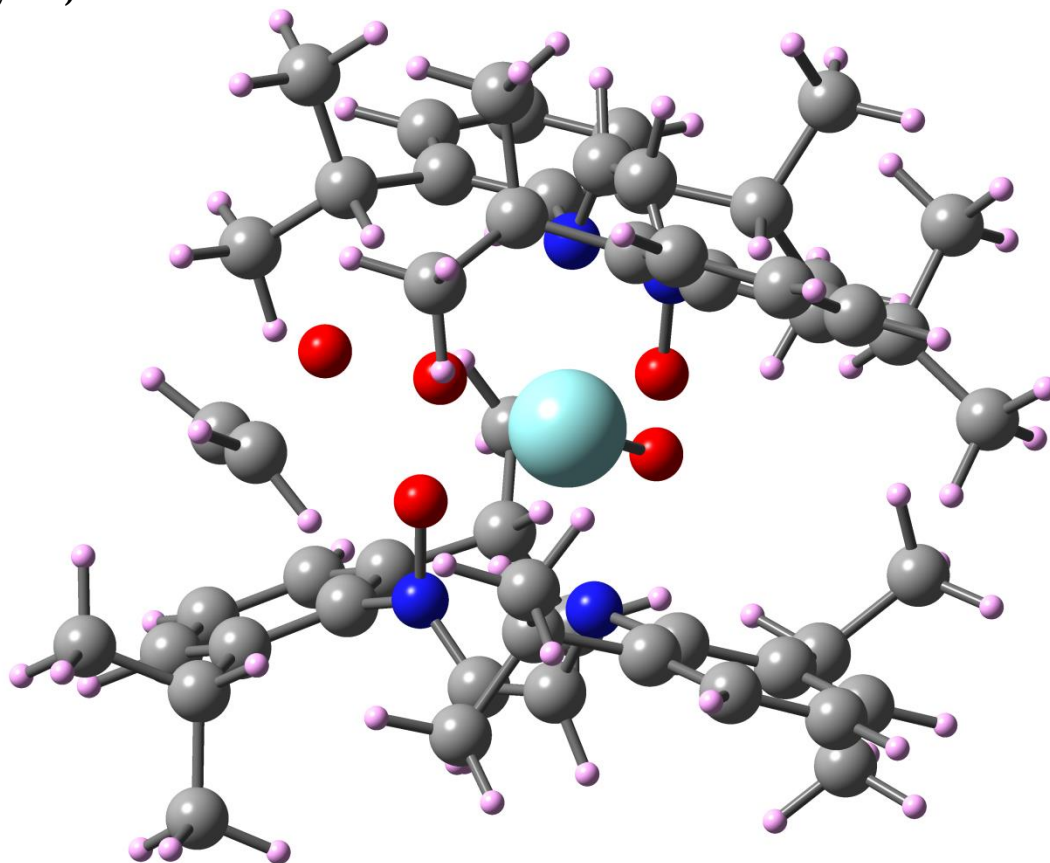


Fig. S170: NCCNO Oxo Complex with Adsorbed Oxygen Molecule to Dioxo Complex (triplet) (Ethylene)

E	E_{ZP}	H	G	<i>f</i>
-2744.7775	-2743.5737	-2743.5004	-2743.6850	-558

Zr	0.14295601	0.15150301	0.20211402
O	-2.01097515	0.35786603	0.05667400
O	2.00117515	-0.72263805	-0.49607504
O	0.14123701	-0.31823902	-3.40609426
O	-0.46525004	-0.25829902	-2.08553016
N	-0.17209501	-2.05182716	0.96583707
N	2.82128021	-1.54650812	0.29868502
N	-0.00626300	2.39048918	-0.41941403
N	-2.84020922	1.21890909	-0.62588905
C	0.91396107	-2.77821321	1.32825510
C	2.27060718	-2.52765119	1.06753908
C	-1.12219709	2.98953123	-0.88496207
C	-2.40991318	2.44202519	-1.02778708
C	-1.43176211	-2.56733420	1.48773912
C	-1.74792413	-2.38446018	2.86398122
C	-2.94380523	-2.95545623	3.35304025

C	-3.80796629	-3.67051328	2.51305219
C	-3.49091026	-3.82026329	1.15263209
C	-2.30565918	-3.27760225	0.61745305
C	-1.61764712	-0.42499403	4.48989435
C	-0.84900107	-1.59717112	3.82751629
C	-0.23674002	-2.52531719	4.91008838
C	4.52580134	1.89094714	2.04237516
C	4.14080032	0.39286903	2.03636016
C	4.37885734	-0.23424002	3.43846626
C	4.25450132	-1.37042711	0.15493301
C	4.89933737	-0.40662203	0.97440507
C	6.29527147	-0.25744902	0.82696606
C	7.01600654	-1.03519208	-0.09235901
C	6.35582348	-1.99055715	-0.88114607
C	4.96143238	-2.17683517	-0.77728406
C	-3.16574624	-3.58887428	-1.78480814
C	-1.93623315	-3.49624326	-0.85279307
C	-1.05537708	-4.76734536	-1.01310008
C	4.66147336	-3.19464024	-3.11030424
C	4.27376033	-3.26354825	-1.61160912
C	4.59223035	-4.67388536	-1.04271908
C	1.10522708	3.30135525	-0.16268001
C	2.12564016	3.45997227	-1.14070409
C	3.15989224	4.38643834	-0.88785107
C	3.19246224	5.13181639	0.29963302
C	2.18384117	4.95520938	1.25833709
C	1.12629009	4.04459931	1.05287008
C	3.45117527	2.04989916	-2.81222321
C	2.09109716	2.71007221	-2.47631319
C	1.64362413	3.65719528	-3.62303928
C	-5.33399739	0.14257501	2.74548721
C	-4.64750535	0.98464308	1.64604612
C	-4.91354237	2.49892119	1.88389414
C	-4.19287332	0.75173206	-0.88038807
C	-5.07363239	0.59738805	0.22547702
C	-6.38247051	0.15248001	-0.04441100
C	-6.80141654	-0.11565401	-1.35890210
C	-5.91410647	0.05381900	-2.43066018
C	-4.58444635	0.48147704	-2.21858117
C	0.63183205	3.50780427	3.49776327
C	0.03844300	3.91108630	2.12436416
C	-0.79594306	5.21586640	2.23050417
C	-3.60554928	-0.60099205	-4.32242533
C	-3.64686628	0.65796805	-3.42086926
C	-4.05699331	1.89849315	-4.26105933
H	0.74269806	-3.66797628	1.93711515
H	2.99944223	-3.17661524	1.53959012
H	-1.05467808	4.04362831	-1.16204009
H	-3.17938124	3.06251023	-1.47001411
H	-3.19858424	-2.83345022	4.40330834
H	-4.72228036	-4.10558632	2.91088722
H	-4.17257832	-4.36574133	0.50646104

H	-0.03187000	-1.14063109	3.26235825
H	3.06572523	0.33767503	1.83849514
H	-2.45396619	-0.77841706	5.10929339
H	-2.01199015	0.25577202	3.72648229
H	-0.93772307	0.15045401	5.13152539
H	-1.01618508	-2.98726723	5.53179343
H	0.42648203	-1.95113715	5.57102345
H	0.35240703	-3.33501325	4.45899634
H	5.56805641	2.05072715	2.35338918
H	3.88112230	2.42908518	2.74714921
H	4.38563834	2.34560318	1.05506508
H	4.05635731	-1.28306510	3.46778727
H	3.80135729	0.31547002	4.19220032
H	5.44081542	-0.19467101	3.71951128
H	6.81925050	0.47101704	1.43907711
H	8.09139563	-0.90339707	-0.18878001
H	6.92860451	-2.59469620	-1.57999712
H	-1.34303810	-2.62923120	-1.16881609
H	3.18940124	-3.11943524	-1.53947912
H	-3.74928228	-4.50132335	-1.60277512
H	-2.83987822	-3.62095228	-2.83376222
H	-3.82909929	-2.72567621	-1.65612313
H	-1.60120912	-5.66029846	-0.67915205
H	-0.13330701	-4.69403436	-0.42503103
H	-0.77873506	-4.91901837	-2.06750116
H	4.48152534	-2.19527617	-3.52625927
H	4.07461131	-3.92206130	-3.68725428
H	5.72149643	-3.43220126	-3.26523425
H	5.66989546	-4.87892337	-1.08597508
H	4.07422931	-5.44947943	-1.62274612
H	4.27564833	-4.76417836	0.00338000
H	3.94135030	4.53259435	-1.62960013
H	3.99619330	5.84320445	0.47595504
H	2.21475817	5.53336540	2.17890117
H	1.34178410	1.91481215	-2.40291718
H	-3.56991927	0.81365906	1.72952713
H	4.25391032	2.79211621	-2.90629222
H	3.38794826	1.52071912	-3.77341029
H	3.74136928	1.33190810	-2.03579015
H	0.65901805	4.09428731	-3.41408126
H	1.57688412	3.10879924	-4.57283135
H	2.35703718	4.48218334	-3.75386229
H	-6.41128448	0.34837703	2.81068422
H	-4.89562937	0.38787003	3.72118328
H	-5.19057940	-0.93003307	2.57289920
H	-4.38423333	3.12196424	1.15267909
H	-4.57076335	2.79022221	2.88558022
H	-5.98674446	2.72321921	1.81174314
H	-7.08092156	0.01860000	0.77548906
H	-7.81805462	-0.45481803	-1.54457912
H	-6.25055250	-0.15927401	-3.44187226
H	-0.63322105	3.09978924	1.83272214

H	-2.62855320	0.81159906	-3.05300523
H	1.36636010	4.24002032	3.86082630
H	1.10331809	2.52358819	3.41135926
H	-0.17011901	3.43991126	4.24640232
H	-1.60115512	5.09363939	2.96772423
H	-1.25210910	5.48040539	1.26686810
H	-0.17408701	6.06347247	2.54934420
H	-3.29839525	-1.48143911	-3.74948629
H	-2.88245122	-0.44775003	-5.13494839
H	-4.58014235	-0.81288606	-4.78179436
H	-4.05681631	2.81680221	-3.66036228
H	-5.06461339	1.77610813	-4.68061336
H	-3.35695126	2.04003315	-5.09516539
O	0.73183206	0.62563405	1.86547614
C	1.89270114	-1.10110708	-3.54492827
H	2.40400618	-0.60024804	-4.36107533
C	0.59280805	-1.74264213	-3.77580629
H	0.28448602	-1.96026815	-4.79725937
H	0.21960302	-2.44041619	-3.03039623
H	2.26745817	-1.02619108	-2.52535819