

*Electronic Supplementary Information*

**Selective Oxidation Passing through  $\eta^3$ -Ozone Intermediates: Applications to Direct Propene Epoxidation Using Molecular Oxygen Oxidant**

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Energies are in Hartrees. DFT calculations performed with B3LYP functional. LANL2DZ basis sets were used for Sections 1 – 11. For Section 12, 6-311++G\*\* basis sets were used on all atoms except the SDD basis set (with relativistic effective core potential for 28 core electrons) was used on Zr. Enthalpy (H) and Gibbs Free Energy (G) were computed at 298.15 Kelvin and 1 atmosphere pressure.

## 1. Constrained Geometry Optimization Curves

This section contains constrained geometry optimization curves for situations that do not have a regular transition state. When O<sub>2</sub> adsorbs on the dioxo complexes, the energy barrier is defined by the singlet-triplet crossing point, because there is no regular transition state. This singlet-triplet crossing point was located by a series of constrained geometry optimizations. The relevant crossing point occurs where the triplet energy (T.E.) at the singlet optimized geometry (S.G.) equals the singlet energy (S.E.) at the singlet optimized geometry (S.G.).

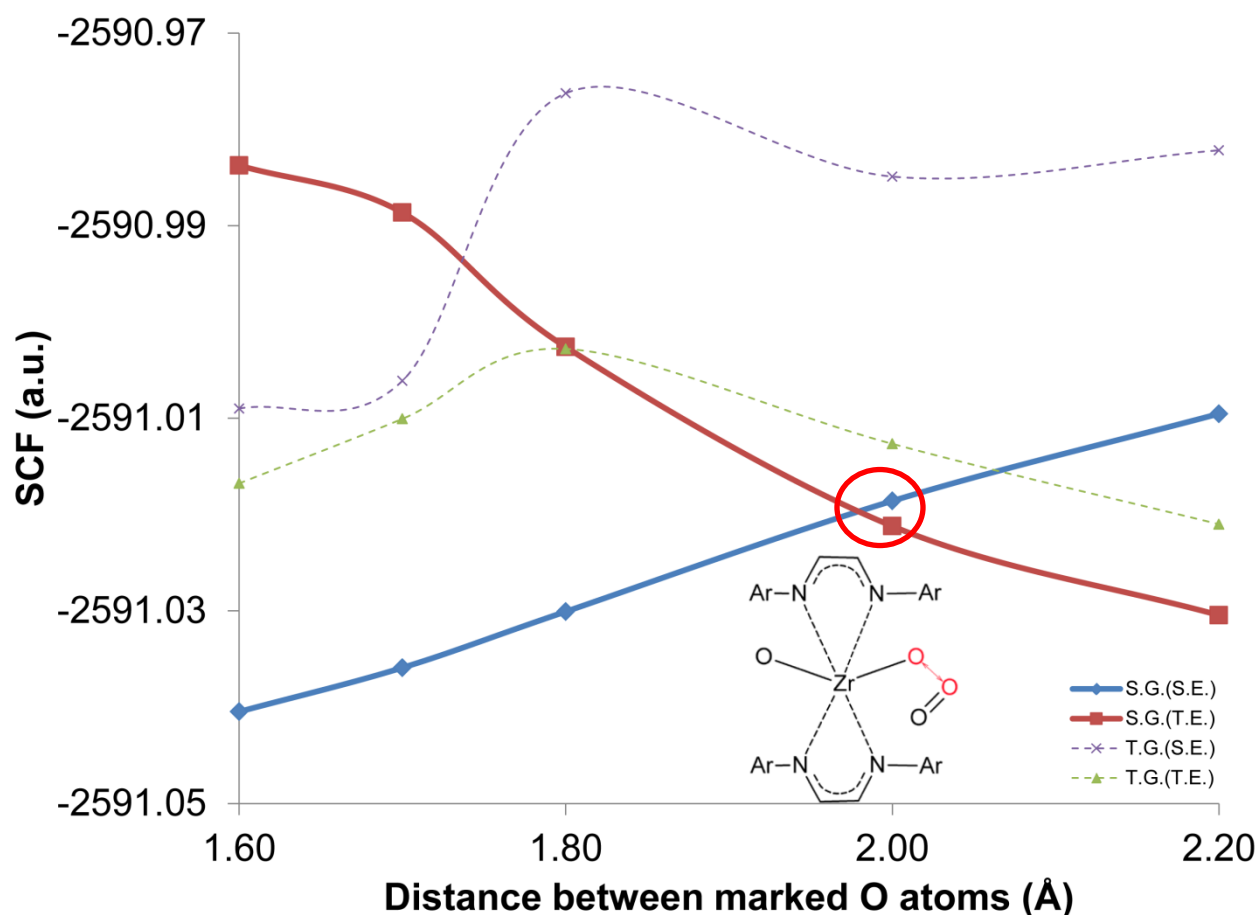


Fig. S1: O<sub>2</sub> adsorption to the Zr\_NCCN dioxo complex. Legend: S.G. = singlet geometry, S.E. = singlet energy, T.G. = triplet geometry, T.E. = triplet energy. The energy barrier was estimated near the singlet-triplet crossing point circled in red.

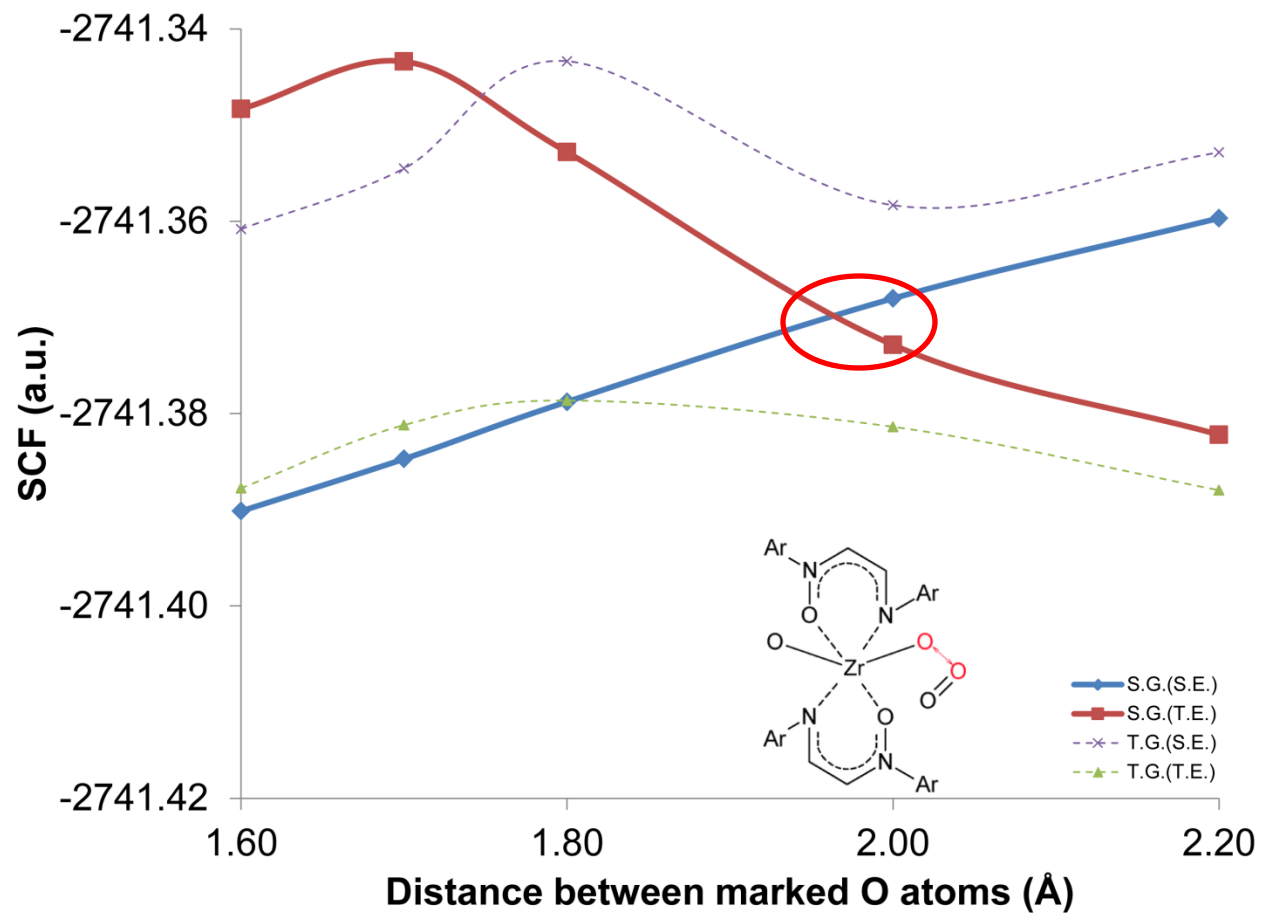


Fig. S2: O<sub>2</sub> adsorption to the Zr\_NCCNO dioxo complex. Legend: S.G. = singlet geometry, S.E. = singlet energy, T.G. = triplet geometry, T.E. = triplet energy. The energy barrier was estimated near the singlet-triplet crossing point circled in red.

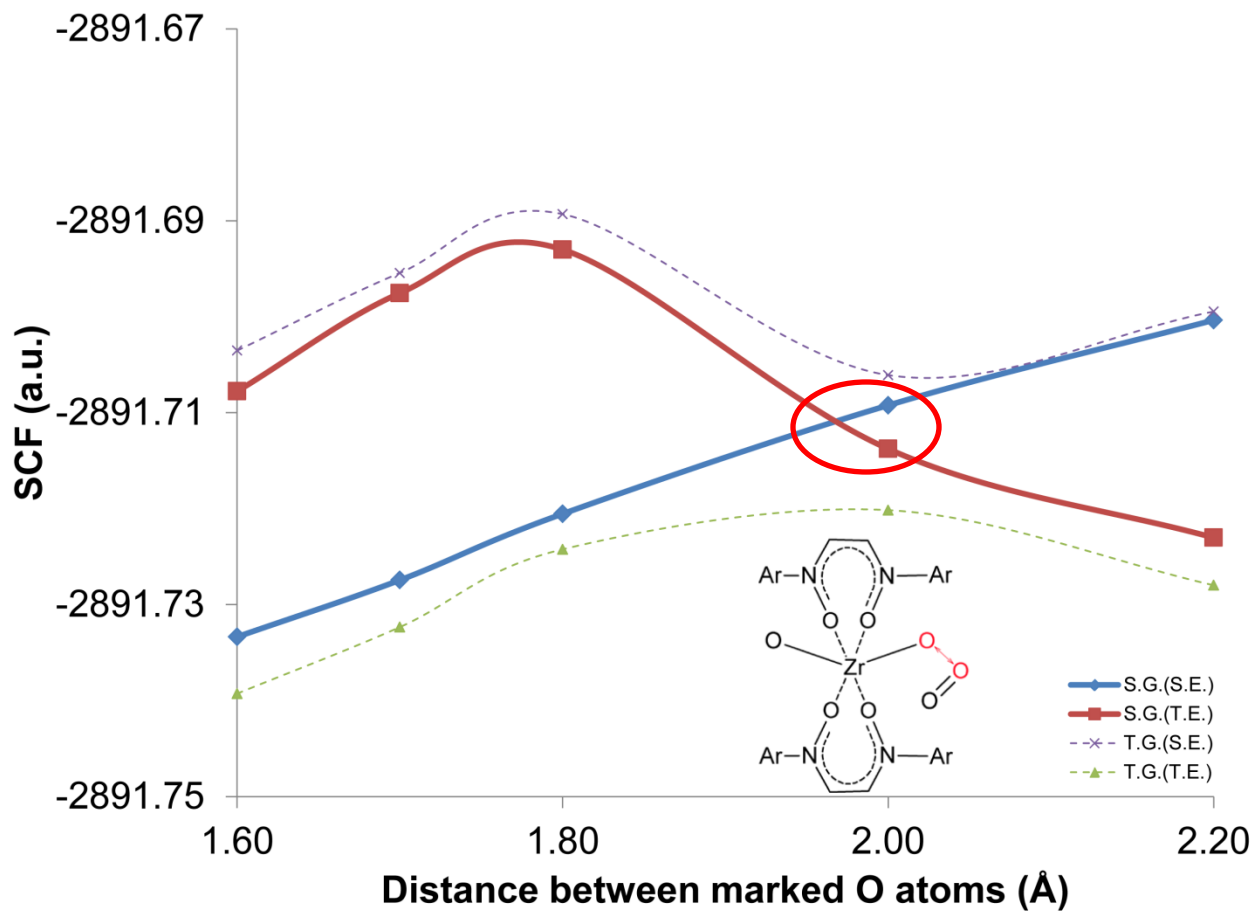


Fig. S3: O<sub>2</sub> adsorption to the Zr\_ONCCNO dioxo complex. Legend: S.G. = singlet geometry, S.E. = singlet energy, T.G. = triplet geometry, T.E. = triplet energy. The energy barrier was estimated near the singlet-triplet crossing point circled in red.



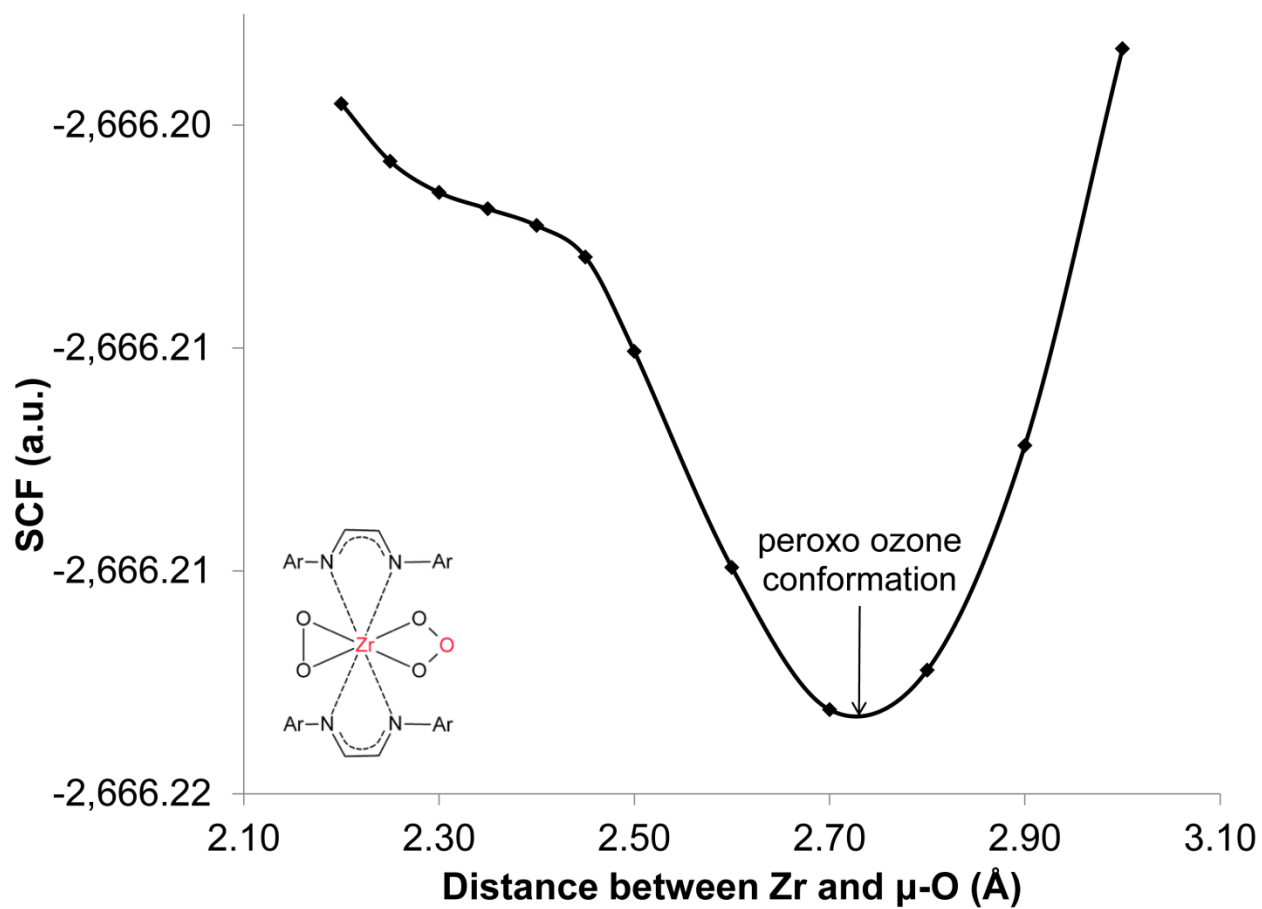


Fig. S4: Zr\_NCCN constrained geometry optimization that shows the peroxo  $\eta^3$ -ozone state does not exist. The single minimum corresponds to the peroxo  $\eta^2$ -ozone state.

## 2. NCCN Singlet Ground States

### 2.1 Structures with zero oxygen atoms

#### Bare Complex (puckered conformation)

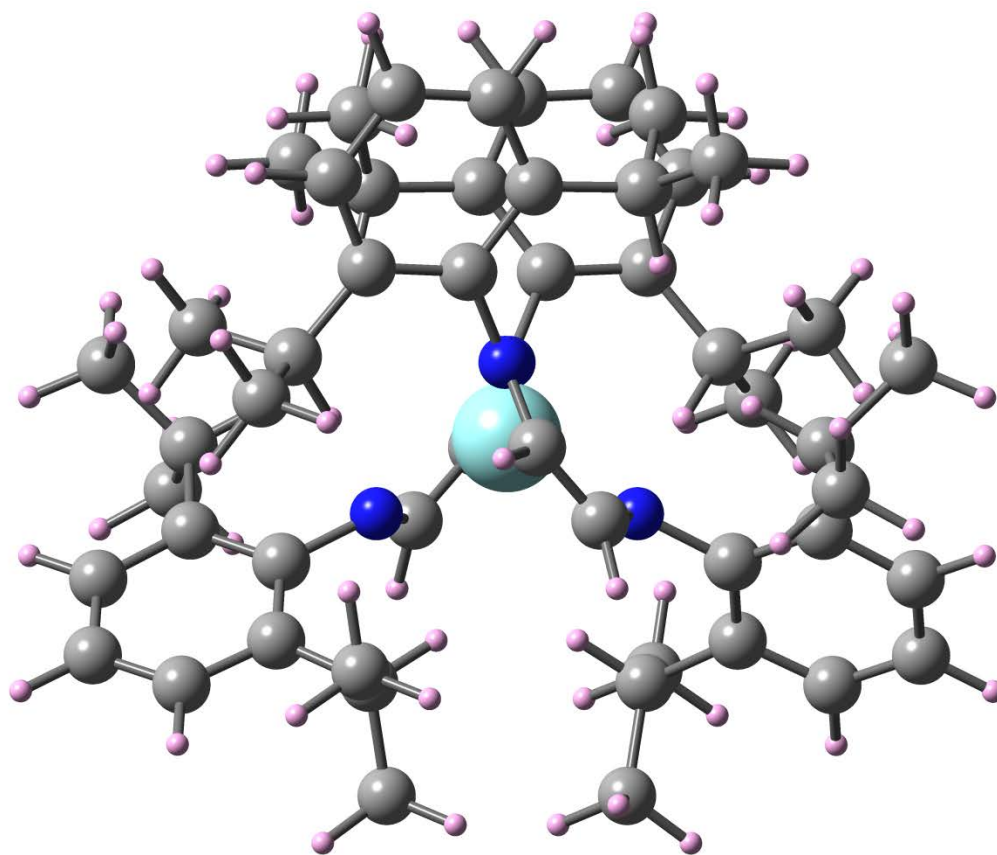


Fig. S5: NCCN Bare Complex (puckered conformation)

SCF	$E_{ZP}$	H	G
-2290.280002	-2289.146590	-2289.082898	-2289.245676

Zr	-0.00078008	-0.27548711	0.00036288
N	-1.72237594	-1.28271076	-0.73272856
N	0.02816742	0.70993814	-1.82794405
N	-0.02728034	0.71088120	1.82812529
N	1.72175107	-1.28298739	0.73102626
C	-1.23282540	-1.37201041	-2.07087655
C	-0.39397405	-0.40989550	-2.60721818
C	0.39525190	-0.40937671	2.60692924
C	1.23301660	-1.37183882	2.06961399
C	-2.97918846	-1.91690462	-0.41481778
C	-4.17687077	-1.50310092	-1.08547527
C	-5.39382776	-2.14038253	-0.76926160
C	-5.46577740	-3.14542947	0.20534200

C	-4.29599725	-3.53498271	0.86853000
C	-3.04535618	-2.95036598	0.57157175
C	-4.40968667	-0.96314750	-3.56385120
C	-4.20188068	-0.38594457	-2.13711167
C	-5.29049710	0.67706485	-1.83470377
C	0.51333620	1.90340378	-2.48275539
C	1.85331961	1.95845051	-2.97062806
C	2.30115236	3.14665975	-3.58565104
C	1.46139115	4.26225865	-3.71344686
C	0.14695118	4.19748713	-3.22909308
C	-0.35271373	3.02722831	-2.61938101
C	-1.58829701	-4.99857599	0.92867463
C	-1.81856987	-3.50912331	1.30002802
C	-1.93375842	-3.35795217	2.83906264
C	-0.51171143	1.90431160	2.48353420
C	0.35387379	3.02880853	2.61737864
C	-0.14541785	4.19935708	3.22687709
C	-1.45889627	4.26362788	3.71386120
C	-2.29808459	3.14723336	3.58898382
C	-1.85072678	1.95879222	2.97408696
C	1.99089286	3.96993938	0.90955129
C	1.80027647	3.01284149	2.11628440
C	2.80061109	3.35814787	3.24963453
C	2.97800738	-1.91848298	0.41340493
C	3.04311393	-2.95237193	-0.57260094
C	4.29304368	-3.53885254	-0.86891421
C	5.46310553	-3.15068539	-0.20543380
C	5.39218530	-2.14512953	0.76873129
C	4.17604922	-1.50596110	1.08427008
C	-4.08056994	1.17375103	2.02434778
C	-2.82696815	0.78508822	2.84970926
C	-3.24097434	0.23737240	4.24085639
C	3.24719763	0.23707335	-4.23341776
C	2.83018915	0.78553401	-2.84346137
C	4.08188808	1.17601330	-2.01617340
C	1.93103875	-3.35659807	-2.84032936
C	1.81572412	-3.50942297	-1.30141212
C	1.58409550	-4.99912651	-0.93193510
C	4.40495608	-0.96636346	3.56304608
C	4.20212139	-0.38866390	2.13574644
C	5.29464412	0.67116500	1.83619436
C	-2.79854408	3.35676739	-3.25531356
C	-1.79992361	3.01090830	-2.12069319
C	-1.99233756	3.96749774	-0.91374154
H	-1.45082997	-2.26973643	-2.64747906
H	0.04581886	-0.56169272	-3.59096698
H	-0.04383455	-0.56105428	3.59095486
H	1.45120054	-2.26948392	2.64628616
H	-6.30125863	-1.83480183	-1.28417162
H	-6.41664102	-3.61705429	0.44144615
H	-4.34756218	-4.32029200	1.61910543
H	-3.23412773	0.12208263	-2.12249583

H	-3.61898427	-1.67643035	-3.82469868
H	-4.40221317	-0.15702415	-4.31004741
H	-5.37271867	-1.48616181	-3.63834539
H	-6.30155032	0.25511666	-1.89953143
H	-5.22935529	1.49404941	-2.56487147
H	-5.16747153	1.10112847	-0.83114378
H	3.32077313	3.20009873	-3.96037037
H	1.82743107	5.17180005	-4.18398879
H	-0.50191465	5.06424310	-3.32989137
H	-0.93395371	-2.95169615	0.97471169
H	-2.43143153	-5.62136292	1.25407899
H	-0.68067312	-5.38122477	1.41380027
H	-1.47778198	-5.12472377	-0.15486883
H	-2.08565135	-2.31235767	3.12858004
H	-1.01964670	-3.72044199	3.32850911
H	-2.77635005	-3.94102657	3.23313174
H	0.50297459	5.06676183	3.32525749
H	-1.82478618	5.17341000	4.18407336
H	-3.31693611	3.20033994	3.96584642
H	2.02396044	1.99785955	1.77249876
H	1.77699837	5.00987595	1.19086090
H	1.32804276	3.70538748	0.07671844
H	3.02601871	3.92624018	0.54465867
H	3.83089020	3.30686107	2.87491447
H	2.70397238	2.65970243	4.09075083
H	2.63957348	4.37312533	3.63580111
H	4.34372958	-4.32450997	-1.61919462
H	6.41344955	-3.62362091	-0.44098506
H	6.29986923	-1.84069393	1.28386596
H	-2.32686915	-0.02578197	2.30936144
H	-4.68108289	1.93280887	2.54284379
H	-4.71443325	0.29397948	1.85591881
H	-3.79417924	1.58135829	1.04711948
H	-2.36661245	-0.07898671	4.82483536
H	-3.91100484	-0.62529900	4.12833338
H	-3.77078344	1.00078550	4.82557565
H	2.32968977	-0.02521449	-2.30333387
H	2.37414046	-0.08028223	-4.81878294
H	3.91757906	-0.62506011	-4.11901422
H	3.77762779	1.00044392	-4.81765092
H	4.68274276	1.93504295	-2.53428604
H	4.71615639	0.29693240	-1.84569556
H	3.79335002	1.58436335	-1.03985820
H	0.93171896	-2.95149018	-0.97530194
H	2.08290121	-2.31074553	-3.12881287
H	1.01707192	-3.71874420	-3.33031747
H	2.77382406	-3.93918079	-3.23472165
H	2.42612109	-5.62244186	-1.25917709
H	0.67554581	-5.37999385	-1.41675294
H	1.47450546	-5.12678865	0.15152758
H	3.23597550	0.12238226	2.11878737
H	3.61186889	-1.67761360	3.82217851

H	4.39788495	-0.16018505	4.30917530
H	5.36650301	-1.49184540	3.63970267
H	6.30430188	0.24637331	1.90373619
H	5.23380580	1.48825167	2.56630033
H	5.17545506	1.09562489	0.83237712
H	-2.02407765	1.99580898	-1.77751680
H	-2.63759058	4.37236876	-3.63993904
H	-3.82945313	3.30436812	-2.88253007
H	-2.69998629	2.65947820	-4.09715764
H	-1.33091870	3.70234268	-0.07998099
H	-3.02810778	3.92383184	-0.55071292
H	-1.77767935	5.00749065	-1.19421730

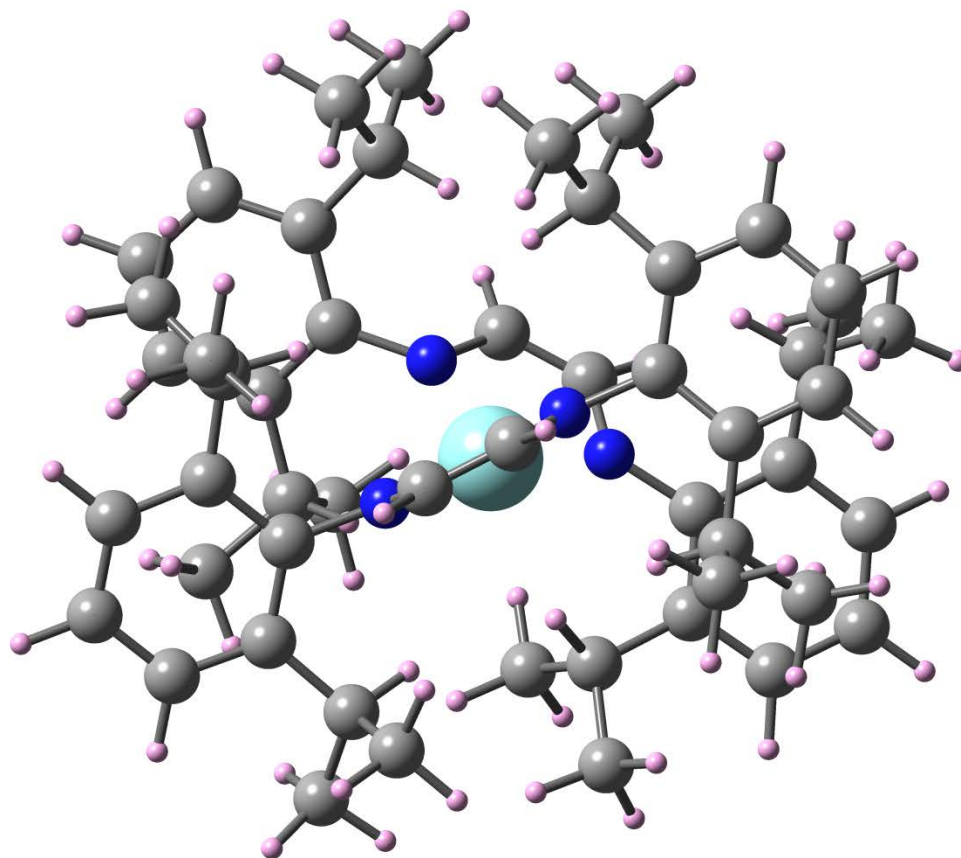
**Bare Complex (unpuckered conformation)**

Fig. S6: NCCN Bare Complex (unpuckered conformation)

SCF	$E_{ZP}$	H	G
-2290.248247	-2289.115592	-2289.052106	-2289.212566

Zr	-0.04653722	-0.26796936	-0.06762492
N	-0.85987632	1.07929780	-1.47235864
N	1.58579505	-0.20951289	-1.52898783
N	0.97566845	0.35917977	1.67395281
N	-1.49628752	-0.88307755	1.40463085
C	0.11145547	1.45989771	-2.44719426
C	1.31285986	0.81675034	-2.47523458
C	0.25464159	-0.06274716	2.84531867
C	-0.94888802	-0.67822817	2.71485743
C	-2.20857913	1.54856055	-1.74439347
C	-3.16734057	0.62944392	-2.27074161
C	-4.45502587	1.10262211	-2.59506736
C	-4.79654005	2.45404123	-2.43104292
C	-3.84542842	3.35025584	-1.92730800
C	-2.54911335	2.92097007	-1.57011158
C	-3.96878587	-1.81921239	-2.44521510
C	-2.79795203	-0.82221541	-2.59952891

C	-2.20456860	-0.90181959	-4.03367490
C	1.54330972	-4.48221632	-0.70816176
C	1.37929647	-3.08929738	-1.35748932
C	0.46934938	-3.16804316	-2.61081300
C	2.78810264	-0.97130470	-1.74530425
C	2.70567408	-2.39733781	-1.68195079
C	3.84013207	-3.17670985	-1.97486805
C	5.05965958	-2.57714364	-2.32476996
C	5.15490896	-1.17992340	-2.32651836
C	4.05235461	-0.35377013	-2.01771000
C	-2.08912622	4.61532809	0.27393910
C	-1.55907100	3.95349904	-1.02433532
C	-1.22835752	5.03610367	-2.08646436
C	5.41623942	1.48407238	-0.89643771
C	4.30820667	1.16043835	-1.93279508
C	4.68362604	1.76673200	-3.31203279
C	2.27470841	0.93150393	1.99464209
C	2.46563219	2.34275162	1.99207365
C	3.70709278	2.86389779	2.41763324
C	4.74166205	2.02425116	2.85039264
C	4.54790267	0.63551426	2.84692404
C	3.33050468	0.06479826	2.42076599
C	1.81374596	4.35943172	0.56697030
C	1.34966429	3.32050525	1.61905026
C	0.80246788	4.02450066	2.89063681
C	-2.37655981	-4.93586413	-0.11855172
C	-1.96180993	-3.75014463	0.78480153
C	-1.33920674	-4.27753961	2.10807790
C	-2.85273027	-1.40535647	1.41164827
C	-3.10505025	-2.77541865	1.09096471
C	-4.42975344	-3.25659264	1.14075520
C	-5.49489432	-2.42358846	1.51399936
C	-5.23887603	-1.08746005	1.84654711
C	-3.93240926	-0.55394054	1.80293880
C	4.33498038	-2.18169490	1.71604295
C	3.18660901	-1.46195356	2.46848070
C	3.11138041	-1.97807817	3.93178002
C	-4.69934885	1.86456374	1.47663403
C	-3.72980142	0.90877567	2.21607521
C	-3.89282836	1.08179704	3.75177627
H	-0.14438199	2.23544744	-3.16170610
H	2.04118248	1.04301806	-3.24404936
H	0.70961653	0.11380403	3.81424746
H	-1.51361239	-1.02294355	3.57559389
H	-5.19597076	0.41461275	-2.99057269
H	-5.79263473	2.80128263	-2.69473002
H	-4.11223335	4.39745510	-1.80515829
H	-2.00434892	-1.14637912	-1.90477529
H	0.85069321	-2.47808689	-0.58556200
H	-4.73711799	-1.65848368	-3.21242188
H	-4.44080677	-1.74392197	-1.46003480
H	-3.60152477	-2.84616511	-2.57165028

H	-2.94628931	-0.55824730	-4.76697815
H	-1.93097932	-1.93519880	-4.28507885
H	-1.31239048	-0.27323695	-4.12946413
H	1.92675527	-5.21153923	-1.43229271
H	0.57549423	-4.85340174	-0.35666404
H	2.23245350	-4.44932372	0.14386876
H	0.32414390	-2.17966392	-3.05735370
H	-0.51185213	-3.59751610	-2.36695615
H	0.94251366	-3.81184832	-3.36337591
H	3.77749382	-4.25983525	-1.93767667
H	5.92400987	-3.18995285	-2.56756937
H	6.11185445	-0.71568349	-2.55309977
H	-0.62878155	3.43430487	-0.77716192
H	3.39768985	1.65313285	-1.57978352
H	-3.03380292	5.14593469	0.09779005
H	-1.36429096	5.34646539	0.65522013
H	-2.26416946	3.86629357	1.05556498
H	-2.12197555	5.61355935	-2.35831509
H	-0.82892814	4.58797537	-3.00495319
H	-0.47955291	5.73962022	-1.69837028
H	5.16599069	1.07942901	0.08905056
H	5.53043476	2.57190227	-0.79590251
H	6.38833687	1.07328194	-1.19993333
H	5.62243350	1.33750828	-3.68686382
H	4.82266576	2.85291465	-3.22742976
H	3.91326586	1.57974830	-4.07125314
H	3.85678060	3.94076312	2.42835841
H	5.68651580	2.44496985	3.18641069
H	5.35223877	-0.01500594	3.18155059
H	0.52618528	2.74379749	1.18507946
H	-1.17325368	-3.19237009	0.25971908
H	2.62675236	4.99003220	0.94963668
H	0.98536364	5.02451644	0.29347472
H	2.17060840	3.86467157	-0.34540028
H	0.43029918	3.28915473	3.61495475
H	-0.02324259	4.70079228	2.63417915
H	1.58670487	4.61556668	3.38247640
H	-3.05441235	-5.62257627	0.40381495
H	-1.49472664	-5.52069954	-0.40938276
H	-2.87839884	-4.59539123	-1.03290776
H	-0.95752367	-3.45408271	2.72114758
H	-0.50843136	-4.96676601	1.90330166
H	-2.09492039	-4.81882933	2.69277924
H	-4.63442745	-4.29405753	0.89546592
H	-6.50883502	-2.81495910	1.55111255
H	-6.06408192	-0.44558765	2.14417477
H	2.24423498	-1.73060043	1.97654678
H	-2.70647035	1.19887355	1.95428212
H	5.30273000	-2.01647833	2.20756700
H	4.41778320	-1.83751957	0.68040630
H	4.15639311	-3.26602626	1.70310035
H	2.98100631	-3.06892191	3.94649694



H	2.27284180	-1.52858874	4.47549012
H	4.03441273	-1.74171990	4.47804021
H	-4.62066787	1.75548738	0.39069580
H	-4.46878217	2.90711081	1.73264335
H	-5.74362207	1.68180449	1.76320733
H	-3.18580950	0.45487339	4.30662390
H	-4.90868954	0.81109416	4.07075752
H	-3.71627953	2.12754088	4.03826706

## 2.2 Structures with one oxygen atom

### Oxo Complex

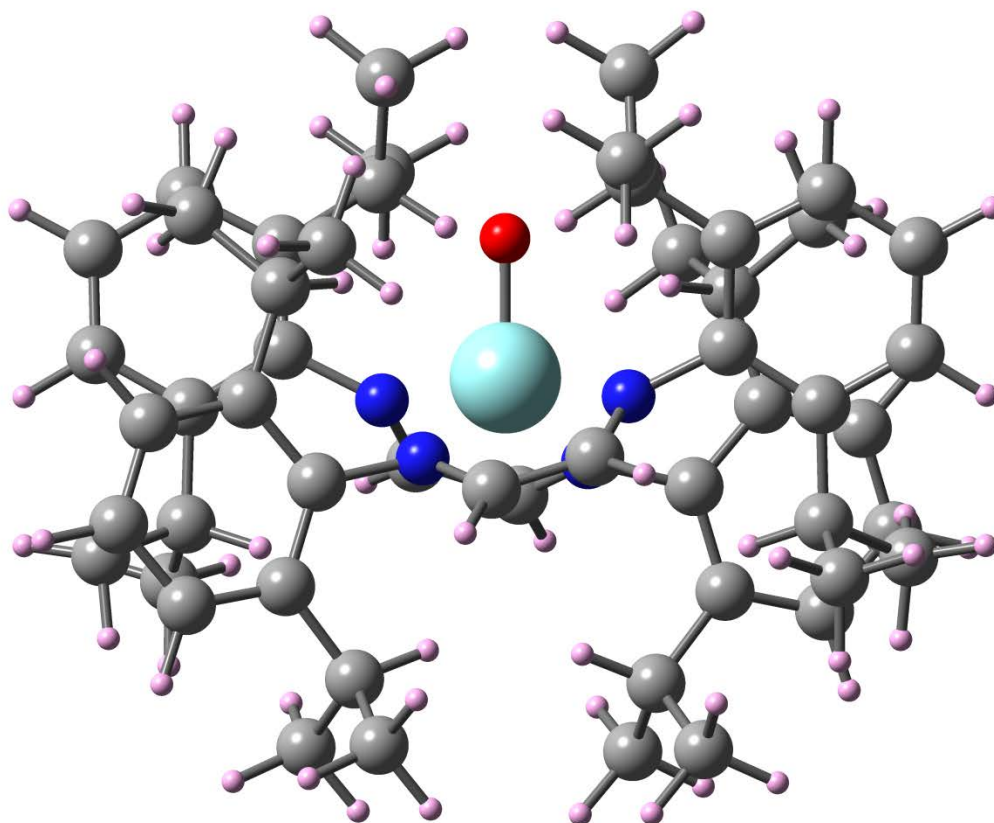


Fig. S7: NCCN Oxo Complex

SCF	E <sub>ZP</sub>	H	G
-2365.516270	-2364.379334	-2364.314910	-2364.477478

O	-0.00454120	2.23222503	-0.03247605
N	-1.07609622	-0.62799101	1.75965015
N	1.60388931	0.18059594	1.65446249
N	1.07469985	-0.67668525	-1.74413926
N	-1.60577739	0.12886817	-1.65069233
C	-0.18035878	-1.02633209	2.70477302
C	1.16293907	-0.60448053	2.66518135
C	0.17610028	-1.10348982	-2.67472663
C	-1.16742332	-0.68342609	-2.64158733
C	-2.45690802	-0.93436971	2.09555839
C	-3.35879127	0.14278481	2.34150037
C	-4.64193600	-0.16169877	2.84056716
C	-5.03339267	-1.48607229	3.09273043
C	-4.15181220	-2.53661754	2.80217797
C	-2.86031435	-2.29110694	2.29136924

C	-4.05623617	2.53481561	1.68539768
C	-2.92555775	1.60354658	2.18095149
C	-2.32612190	2.13355650	3.51272653
C	1.60677376	4.38024977	1.78155278
C	1.66454203	3.02704324	2.52921566
C	1.56430973	3.23597354	4.06630079
C	2.89727404	0.83025774	1.86197163
C	2.92499693	2.21744361	2.20257526
C	4.17944102	2.84225886	2.36879652
C	5.37770749	2.12804377	2.24000494
C	5.33330740	0.75267092	1.97522404
C	4.10865857	0.07495833	1.79359573
C	-2.59465391	-4.38307732	0.84911950
C	-1.96332748	-3.49295758	1.95269304
C	-1.64378203	-4.35267853	3.20481691
C	5.25060617	-1.90746580	0.62787724
C	4.14185173	-1.44777300	1.60467341
C	4.35053266	-2.17008984	2.96759081
C	2.45474033	-0.99139955	-2.07298885
C	2.85819506	-2.35202406	-2.23921140
C	4.15386613	-2.60897763	-2.73389481
C	5.03822616	-1.56557672	-3.04030250
C	4.64507048	-0.23569694	-2.82075648
C	3.35927681	0.07992546	-2.33613232
C	2.57911245	-4.40973382	-0.75398759
C	1.95893282	-3.54794588	-1.88571159
C	1.65763053	-4.43425049	-3.12388060
C	-1.56650352	4.32223234	-1.94150731
C	-1.64801275	2.93991898	-2.63206630
C	-1.56358806	3.08603435	-4.17745084
C	-2.89507346	0.78122691	-1.87630952
C	-2.91270566	2.15679388	-2.26132045
C	-4.16258899	2.78864052	-2.43516664
C	-5.36632123	2.08999931	-2.27564808
C	-5.33241918	0.72233004	-1.97247313
C	-4.11245529	0.03926221	-1.77864572
C	4.06434212	2.49095090	-1.76278473
C	2.92552269	1.54362646	-2.20571810
C	2.29288352	2.03849727	-3.53569692
C	-5.26586413	-1.90200233	-0.55665608
C	-4.15585484	-1.47700157	-1.54748473
C	-4.37027748	-2.23568548	-2.88960655
H	-5.33541956	0.64723761	3.04974289
H	-6.02067049	-1.69619500	3.49679960
H	-4.47170589	-3.56252832	2.96998278
H	-2.12776238	1.65827259	1.43186183
H	0.79027530	2.46118179	2.20694265
H	-4.84054922	2.67149150	2.44227255
H	-4.52094961	2.15154126	0.76961442
H	-3.64107251	3.52587906	1.46276460
H	-3.08566643	2.13117083	4.30649561
H	-1.96546993	3.16228915	3.38370006

H	-1.48273157	1.51690960	3.84648961
H	2.44556020	5.03841733	2.04665478
H	0.67705148	4.90658057	2.03585413
H	1.60532562	4.21352034	0.70008437
H	1.56860136	2.27687817	4.60170662
H	0.63358159	3.76220189	4.31763886
H	2.40497335	3.83397090	4.44376777
H	4.21217335	3.89825162	2.62344198
H	6.33349648	2.63042142	2.36925771
H	6.26276295	0.19410751	1.91201861
H	-1.01368778	-3.12085410	1.55378671
H	3.17703884	-1.76508009	1.19096391
H	-3.54423763	-4.82272342	1.18074016
H	-1.91524324	-5.20819086	0.59542177
H	-2.78890386	-3.80708575	-0.06297992
H	-2.55770984	-4.78506191	3.63211621
H	-1.15863079	-3.76246844	3.99249538
H	-0.97372742	-5.18152747	2.93959375
H	5.20130668	-1.36741927	-0.32028058
H	5.14549672	-2.97881708	0.41618046
H	6.25017139	-1.75840893	1.05722657
H	5.31670653	-1.88495140	3.40451651
H	4.35145585	-3.25962409	2.82577670
H	3.57314540	-1.92383828	3.69967381
H	4.47451970	-3.63860472	-2.87569991
H	6.02883580	-1.78479310	-3.43115634
H	5.34054316	0.56817789	-3.04238845
H	1.00227139	-3.17077397	-1.50923117
H	-0.77574889	2.37822457	-2.29670256
H	3.54170086	-4.84028771	-1.05851185
H	1.90717927	-5.24025799	-0.49750975
H	2.74691883	-3.81411128	0.15099459
H	1.19504889	-3.85703732	-3.93451123
H	0.97414732	-5.25027052	-2.85384696
H	2.57567806	-4.88471574	-3.52269215
H	-2.40213196	4.97840962	-2.22140236
H	-0.63568863	4.82762758	-2.23160270
H	-1.55022928	4.19970596	-0.85426953
H	-1.58441055	2.10682200	-4.67487615
H	-0.63068894	3.59233420	-4.46001172
H	-2.40242802	3.67789560	-4.56851327
H	-4.18781679	3.83711012	-2.71972382
H	-6.31844816	2.59756496	-2.41147182
H	-6.26664192	0.17473577	-1.88762412
H	2.14556759	1.61651042	-1.43936534
H	-3.19206700	-1.78849584	-1.12718958
H	4.82898258	2.60895101	-2.54245207
H	4.55226662	2.13338179	-0.84855378
H	3.65139194	3.48647575	-1.55688266
H	1.94265434	3.07304543	-3.42578499
H	1.43599113	1.41985412	-3.82854795
H	3.03038864	2.00871492	-4.34948688

H	-5.21287250	-1.33374072	0.37465880
H	-5.16612180	-2.96687368	-0.31254931
H	-6.26476546	-1.76124520	-0.99002925
H	-3.59127079	-2.01550443	-3.62816695
H	-5.33455308	-1.95673164	-3.33470379
H	-4.37858319	-3.32073062	-2.71693267
H	-0.52151068	-1.59918339	3.56413774
H	1.80720721	-0.83569636	3.50967769
H	0.51520019	-1.69799521	-3.52010733
H	-1.81418495	-0.93839665	-3.47731662
Zr	0.00001620	0.42190928	-0.00626239

## 2.3 Structures with two oxygen atoms

### Peroxo Complex

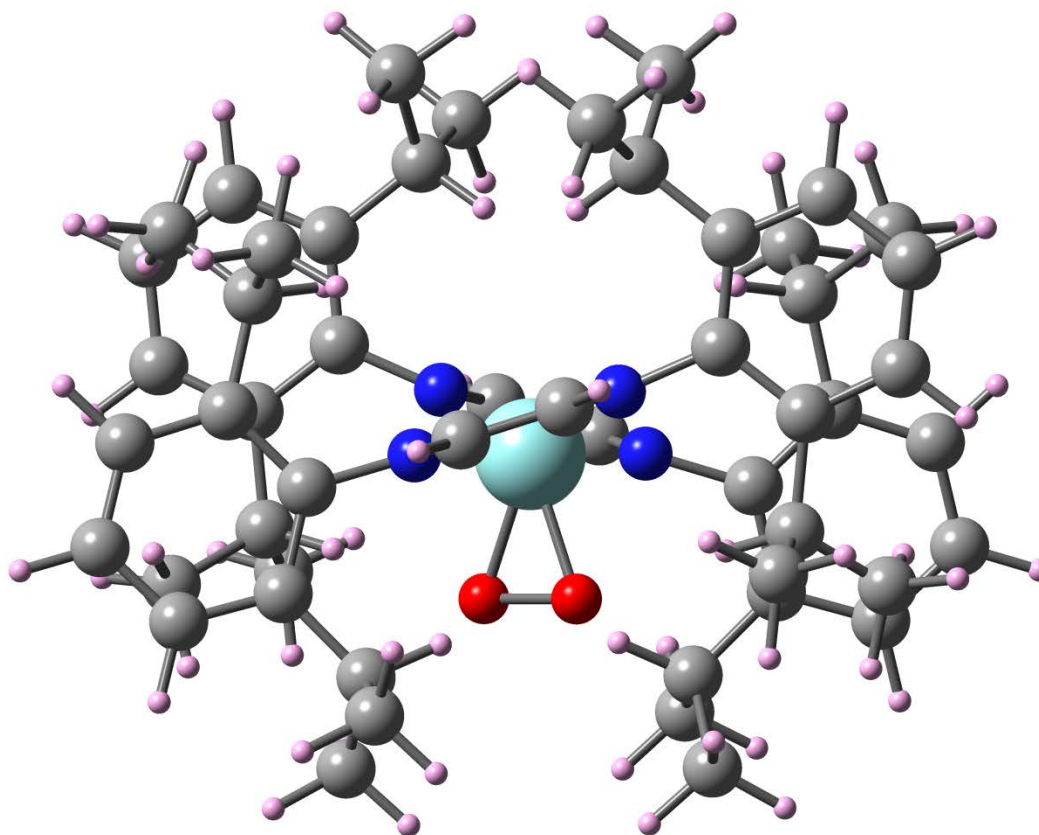


Fig. S8: NCCN Peroxo Complex

SCF	E <sub>ZP</sub>	H	G
-2440.656571	-2439.517461	-2439.450805	-2439.619454

Zr	0.00086511	-0.39787451	-0.00321126
N	1.50082720	-0.39062785	-1.74621763
N	-1.15526639	0.43662187	-1.84761596
N	-1.50073489	-0.41387862	1.73850943
N	1.15534350	0.41456447	1.85159137
C	0.90183622	-0.15962965	-2.94017772
C	-0.44190222	0.26619449	-2.98729574
C	-0.89788422	-0.21099563	2.93546986
C	0.44572743	0.21479724	2.98885648
C	2.89892841	-0.80724498	-1.84960580
C	3.92658643	0.18090043	-1.83166774
C	5.26244841	-0.24233906	-1.99426812
C	5.57848803	-1.59569294	-2.18878710
C	4.55269394	-2.54905875	-2.22986408
C	3.19856672	-2.18253024	-2.06746148

C	4.70983618	2.48643232	-0.99796890
C	3.61072269	1.67867138	-1.72680349
C	3.37538422	2.29507418	-3.13576540
C	-1.74420098	4.53349502	-0.94484900
C	-1.41374621	3.37481121	-1.91857482
C	-0.88916022	3.93748024	-3.26760136
C	-2.47500632	1.01919766	-2.06084654
C	-2.60442383	2.43459234	-2.14322890
C	-3.85951910	2.97381013	-2.49527160
C	-4.95912782	2.14113481	-2.74934820
C	-4.81950974	0.74852811	-2.64360779
C	-3.58361720	0.15796936	-2.30422115
C	2.36802546	-4.46329205	-1.25674591
C	2.11723545	-3.26137128	-2.20049691
C	2.00881915	-3.73777402	-3.67552397
C	-4.65715862	-2.08489961	-1.65586499
C	-3.44008887	-1.36860104	-2.28782843
C	-3.19989614	-1.91136759	-3.72511042
C	-2.90029658	-0.82642894	1.83674581
C	-3.20588789	-2.20362787	2.03344064
C	-4.56144186	-2.56616126	2.19277408
C	-5.58275473	-1.60739143	2.16836983
C	-5.26078016	-0.25264944	1.99402984
C	-3.92321523	0.16672654	1.83585606
C	-2.38883505	-4.47555860	1.18502488
C	-2.12933877	-3.28963508	2.14638906
C	-2.01825923	-3.78963740	3.61338182
C	1.76233057	4.52437505	0.98180281
C	1.41745679	3.34826091	1.92923373
C	0.86416235	3.88730690	3.27657012
C	2.47496239	0.99320677	2.07660853
C	2.60628080	2.40813433	2.16306020
C	3.85855445	2.94401521	2.52909333
C	4.95408371	2.10836606	2.79217428
C	4.81306181	0.71649075	2.68102330
C	3.57930604	0.12924529	2.32766292
C	-4.69723193	2.49084819	1.04530545
C	-3.59920119	1.66427805	1.75420748
C	-3.35205352	2.25557148	3.17188181
C	4.64138454	-2.10487609	1.63776743
C	3.43600052	-1.39728373	2.30175216
C	3.22586010	-1.95239862	3.73882561
H	1.45547498	-0.29195148	-3.86706570
H	-0.89414643	0.49840318	-3.94985500
H	-1.44926059	-0.36418400	3.86050031
H	0.90041511	0.42381753	3.95555808
H	6.06219609	0.49168154	-1.97491188
H	6.61478615	-1.90054860	-2.31503497
H	4.80050358	-3.59416316	-2.39598658
H	2.67794095	1.78669597	-1.15569392
H	-0.59897569	2.79089202	-1.47104341
H	5.62098652	2.56330464	-1.60621739

H	4.97286239	2.03691988	-0.03622716
H	4.36039152	3.50955353	-0.80956909
H	4.27038748	2.17100072	-3.75999534
H	3.16598591	3.37064156	-3.05212712
H	2.53281463	1.82561145	-3.65453598
H	-2.53002512	5.18759548	-1.34336118
H	-0.85319280	5.15290995	-0.78130850
H	-2.08345948	4.15446262	0.02727325
H	-0.59184116	3.12990705	-3.94757246
H	-0.01680180	4.58452782	-3.10426525
H	-1.66445853	4.53105513	-3.76983176
H	-3.97656727	4.05176716	-2.57501189
H	-5.91791740	2.57322547	-3.02605403
H	-5.67682694	0.11049366	-2.83825978
H	1.15299706	-2.83909647	-1.91218502
H	-2.55934968	-1.62726087	-1.69006674
H	3.30958618	-4.98251779	-1.48410771
H	1.55100361	-5.18967470	-1.35881524
H	2.38562750	-4.12868371	-0.21467213
H	2.94275016	-4.20588583	-4.01623448
H	1.78666920	-2.90280223	-4.35370349
H	1.20339553	-4.47776079	-3.77347223
H	-4.88977048	-1.68647162	-0.66324588
H	-4.43779105	-3.15464513	-1.54699983
H	-5.55474702	-1.99733166	-2.28349039
H	-4.04791669	-1.66904772	-4.38064091
H	-3.08679935	-3.00301753	-3.69986431
H	-2.29163934	-1.49194862	-4.17386722
H	-4.81397490	-3.61252673	2.34319479
H	-6.62023144	-1.90932617	2.29196026
H	-6.05713313	0.48526402	1.98756614
H	-1.16405631	-2.86759912	1.86142158
H	0.61417996	2.76803368	1.45623625
H	-3.33213209	-4.99390643	1.40714301
H	-1.57489182	-5.20714690	1.27327158
H	-2.40805501	-4.12505759	0.14820861
H	-1.78676671	-2.96701988	4.30345342
H	-1.21788846	-4.53693307	3.69613694
H	-2.95415427	-4.25607456	3.95092940
H	2.53239520	5.17816010	1.41031380
H	0.87063083	5.13939856	0.80629883
H	2.12848385	4.16389412	0.01241598
H	0.55521080	3.06825524	3.93730428
H	-0.00622782	4.53530076	3.10638466
H	1.62833042	4.47407695	3.80337097
H	3.97719732	4.02142119	2.61290536
H	5.91078049	2.53797809	3.07976830
H	5.66722094	0.07600880	2.88208668
H	-2.66881532	1.77601326	1.17981253
H	2.54424095	-1.65201542	1.71902471
H	-5.60493826	2.56179987	1.65937749
H	-4.96715372	2.05997357	0.07697153



H	-4.34317975	3.51533767	0.87368095
H	-3.13687590	3.33114617	3.10481195
H	-2.50902465	1.77288604	3.67763591
H	-4.24403888	2.12628104	3.79939046
H	4.84702487	-1.70123287	0.64138442
H	4.42565577	-3.17555029	1.53025830
H	5.55375291	-2.01353545	2.24310512
H	2.32810988	-1.53506135	4.21053818
H	4.08763884	-1.71699433	4.37867857
H	3.11063082	-3.04366520	3.70684283
O	0.60424173	-2.27439207	0.48027692
O	-0.59902356	-2.27106440	-0.50858608

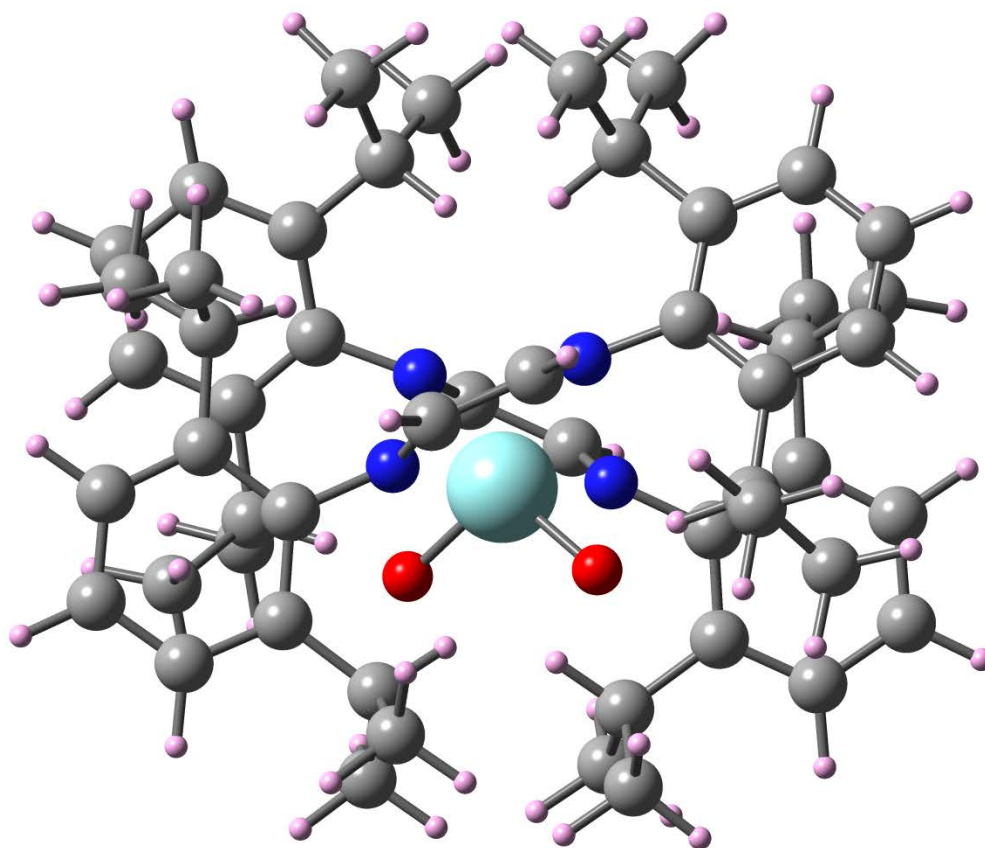
**Dioxo Complex (conformation 1 lower energy)**

Fig. S9: NCCN Dioxo Complex (conformation 1 lower energy)

SCF	$E_{ZP}$	H	G
-2440.716550	-2439.577285	-2439.509610	-2439.681936

Zr	0.00191600	-0.68426200	0.03332400
N	1.42110600	-0.62325400	-1.97598000
N	-1.06898500	0.76919000	-2.05414000
N	-1.42184900	-0.40991500	2.02707000
N	1.07332900	0.98171900	1.96011700
C	0.91337300	-0.16305500	-3.08382400
C	-0.41821100	0.44364000	-3.13517100
C	-0.91620600	0.17144900	3.07755600
C	0.41840600	0.77293500	3.06729700
C	2.74538400	-1.24288300	-2.05400300
C	3.89696900	-0.41854800	-2.18613300
C	5.15204300	-1.05529800	-2.28841200
C	5.26205200	-2.45291300	-2.26220500
C	4.10940600	-3.24058900	-2.12966800
C	2.82867400	-2.66030800	-2.01935900
C	4.88593500	1.77481400	-1.31170100
C	3.82998300	1.11458400	-2.23192500

C	3.99341700	1.64118000	-3.68496400
C	-1.96895500	4.62266600	-0.49859900
C	-1.52653100	3.58003700	-1.55259200
C	-0.91689300	4.28614700	-2.79608000
C	-2.42454300	1.26640300	-2.23574500
C	-2.66196500	2.64656700	-1.98044900
C	-3.94752400	3.16272100	-2.23283600
C	-4.97840800	2.33472100	-2.70374300
C	-4.73211300	0.97205400	-2.91965800
C	-3.45905700	0.39974900	-2.69961000
C	1.70797100	-4.57703500	-0.76960300
C	1.59656400	-3.56641100	-1.93732300
C	1.36318700	-4.28883700	-3.29243800
C	-4.29499600	-1.94692700	-2.16396200
C	-3.26691500	-1.09997700	-2.95650700
C	-3.34956700	-1.42202100	-4.47286600
C	-2.75214800	-1.00344700	2.16426900
C	-2.85158200	-2.41861000	2.24610800
C	-4.13777000	-2.97412700	2.40514100
C	-5.28158500	-2.16573200	2.47675900
C	-5.15605000	-0.77196200	2.39359700
C	-3.89471900	-0.15841000	2.23785700
C	-1.75672900	-4.47636700	1.21106600
C	-1.62757000	-3.33902200	2.25269100
C	-1.38633400	-3.90153900	3.68079300
C	2.01281000	4.60289700	-0.03095600
C	1.55787900	3.72381400	1.15854800
C	0.97696200	4.60399300	2.30052800
C	2.43097300	1.48829600	2.09616500
C	2.67923200	2.83200600	1.69824500
C	3.96541100	3.36577400	1.90870900
C	4.98686900	2.58774300	2.47469200
C	4.73088100	1.25626200	2.82960700
C	3.45647800	0.67047200	2.65914400
C	-4.84976200	1.96218900	1.17032800
C	-3.81819600	1.37345500	2.16424800
C	-4.01304300	2.01330800	3.56711700
C	4.28493400	-1.72216300	2.37978500
C	3.25385300	-0.79320000	3.06967900
C	3.32013000	-0.95590900	4.61209300
H	1.44525000	-0.26707100	-4.03245600
H	-0.85468000	0.57637900	-4.12879000
H	-1.45347400	0.18042300	4.02879900
H	0.85315100	1.00739800	4.04272500
H	6.05026500	-0.45143400	-2.38417800
H	6.23884800	-2.92384000	-2.34431400
H	4.20024200	-4.32320000	-2.11199700
H	2.84438600	1.43225900	-1.86762200
H	-0.73573800	2.96376500	-1.10411200
H	5.90558300	1.60230400	-1.67926200
H	4.82104600	1.38868600	-0.28962400
H	4.73045800	2.86086800	-1.27536500

H	4.96649500	1.34116300	-4.09517700
H	3.93960300	2.73823800	-3.70712100
H	3.21852200	1.24797600	-4.35540500
H	-2.69988300	5.33182200	-0.90735300
H	-1.10612900	5.20842600	-0.15872800
H	-2.42034900	4.13811200	0.37631900
H	-0.55243300	3.55656800	-3.53049000
H	-0.07523100	4.92899600	-2.50708100
H	-1.67051800	4.91159000	-3.29241700
H	-4.14445900	4.21774800	-2.06529000
H	-5.96547600	2.74814200	-2.89659900
H	-5.53866800	0.33390600	-3.27025600
H	0.70967100	-2.96047000	-1.72956200
H	-2.29298300	-1.41049200	-2.56416800
H	2.57466200	-5.24457800	-0.87761300
H	0.80521900	-5.20078300	-0.73666800
H	1.78316100	-4.02625500	0.17418700
H	2.20140000	-4.95344700	-3.54397400
H	1.24453800	-3.57302300	-4.11851600
H	0.45141500	-4.89779100	-3.23771300
H	-4.19374100	-1.76081900	-1.08998800
H	-4.09471300	-3.01278500	-2.33158300
H	-5.33173600	-1.74446300	-2.46831900
H	-4.33734200	-1.17209500	-4.88477300
H	-3.17819700	-2.49394300	-4.63725100
H	-2.60014900	-0.86638100	-5.05407700
H	-4.24019600	-4.05341600	2.47595700
H	-6.26314400	-2.61786800	2.59823300
H	-6.04706000	-0.15216300	2.44646500
H	-0.73892700	-2.76708500	1.97036000
H	0.74829800	3.07224000	0.80421600
H	-2.62252200	-5.12445600	1.40713300
H	-0.85591200	-5.10318900	1.23733200
H	-1.84298000	-4.03770700	0.21123200
H	-1.25421200	-3.09557800	4.41693900
H	-0.47976000	-4.52045900	3.68968100
H	-2.22790800	-4.52432000	4.01477500
H	2.77710800	5.33092000	0.26840400
H	1.16389800	5.17076800	-0.43057000
H	2.42840200	3.99108800	-0.84157900
H	0.60955800	3.98725000	3.13094400
H	0.14193200	5.21676200	1.93639000
H	1.74638200	5.27754600	2.70050200
H	4.16933200	4.39700300	1.63469800
H	5.97416400	3.01474600	2.63369900
H	5.53070500	0.65433100	3.25241000
H	-2.82342200	1.65982900	1.79967600
H	2.28193500	-1.13896600	2.70275000
H	-5.87880600	1.81122400	1.52058700
H	-4.75623800	1.50484000	0.18054100
H	-4.69619600	3.04393900	1.06178000
H	-3.95220300	3.10832300	3.50367100

H	-3.25742000	1.67035100	4.28559300
H	-4.99761600	1.75168900	3.97590400
H	4.19470500	-1.64732200	1.29143700
H	4.07763300	-2.76420000	2.65447200
H	5.31966900	-1.49332500	2.67227700
H	2.57097300	-0.33655000	5.12539700
H	4.30658400	-0.67305500	5.00554000
H	3.13740600	-2.00344100	4.88565400
O	-1.22794200	-1.84423900	-0.74723600
O	1.23813900	-1.75862200	0.91858000

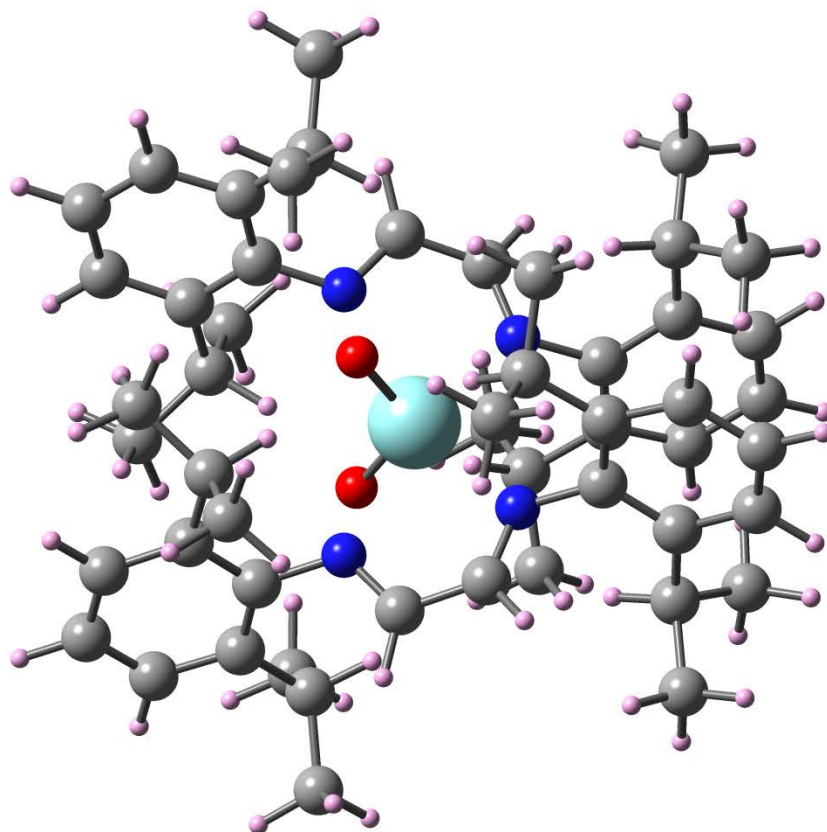
**Dioxo Complex (conformation 2 higher energy)**

Fig. S10: NCCN Dioxo Complex (conformation 2 higher energy)

SCF	$E_{ZP}$	H	G
-2440.712444	-2439.573186	-2439.505748	-2439.677515

O	-1.07422719	-1.00615282	-1.32332999
O	-1.06653830	1.01012141	1.32667533
N	1.42229077	1.31371494	-1.39163001
N	-1.26999153	2.05391051	-1.05802049
N	-1.27169971	-2.05256463	1.05826899
N	1.42090831	-1.31530292	1.39265313
C	0.94103474	2.44496771	-1.84377895
C	-0.40274534	2.90817182	-1.52566166
C	-0.40652037	-2.90621598	1.53100843
C	0.93712705	-2.44336376	1.85003875
C	2.73869527	0.94522508	-1.92262819
C	3.89614543	1.65597351	-1.49570143
C	5.12448995	1.34432445	-2.11772583
C	5.20521485	0.37405204	-3.12686694
C	4.05138565	-0.31904070	-3.52258734
C	2.79692492	-0.05566345	-2.93325572
C	4.95665312	2.55956565	0.65172024

C	3.86068534	2.75663462	-0.42489167
C	4.00354672	4.16769644	-1.06084945
C	-2.07315168	3.87601548	2.53615785
C	-1.79890180	4.16702314	1.03823549
C	-1.66879370	5.68929123	0.76908417
C	-2.62028481	2.49274657	-0.79008118
C	-2.87813361	3.52565132	0.15712063
C	-4.21974804	3.92063732	0.34197319
C	-5.26490422	3.32191131	-0.37576659
C	-4.98627504	2.29501626	-1.29219552
C	-3.66731060	1.85454138	-1.51713822
C	1.75118756	-2.28249079	-3.66630599
C	1.54323990	-0.76265520	-3.45978229
C	1.07065039	-0.09701948	-4.78186049
C	-4.47319924	-0.26260392	-2.73163040
C	-3.35745955	0.79510383	-2.57651416
C	-3.06992746	1.47665040	-3.94420190
C	-2.62164060	-2.49206754	0.78829924
C	-2.87728184	-3.52590853	-0.15820476
C	-4.21848262	-3.92149225	-0.34531548
C	-5.26517309	-3.32212331	0.36958496
C	-4.98854631	-2.29405164	1.28538808
C	-3.67011821	-1.85318269	1.51242389
C	-2.06765933	-3.87966075	-2.53535052
C	-1.79605670	-4.16790188	-1.03641460
C	-1.66560514	-5.68976612	-0.76487519
C	1.74440003	2.27461492	3.66909558
C	1.54060779	0.75307447	3.47081433
C	1.07828066	0.09157687	4.79849320
C	2.73710298	-0.94630295	1.92446810
C	2.79444889	0.04940624	2.93998487
C	4.04931759	0.31264981	3.52877658
C	5.20399221	-0.37579782	3.12782474
C	5.12392921	-1.34118069	2.11378228
C	3.89540381	-1.65226405	1.49198842
C	-4.47889035	0.26567017	2.72183609
C	-3.36230934	-0.79163760	2.57019875
C	-3.07622657	-1.47026287	3.93966513
C	4.96260183	-2.55755238	-0.65238295
C	3.85858690	-2.74860376	0.41688734
C	3.98706616	-4.16310320	1.04858735
H	6.02365553	1.87244926	-1.81219952
H	6.15975531	0.16021788	-3.60160097
H	4.11998886	-1.06726601	-4.30707051
H	2.89237394	2.71488887	0.08858226
H	-0.83716806	3.69218941	0.82270843
H	5.96228123	2.69716258	0.23346750
H	4.90492657	1.56239975	1.09761315
H	4.83048730	3.29884320	1.45373044
H	4.96132641	4.25912332	-1.58965106
H	3.97157242	4.94130217	-0.28234351
H	3.20673343	4.38189138	-1.78408576

H	-3.03725644	4.28681604	2.86454926
H	-1.28622034	4.32748253	3.15778325
H	-2.06320400	2.79168110	2.68568000
H	-1.43380971	5.89922088	-0.28418999
H	-0.87168824	6.11993446	1.39046864
H	-2.60044065	6.21841313	1.00885991
H	-4.44756773	4.69636736	1.06896537
H	-6.29067133	3.64719004	-0.21682765
H	-5.80127170	1.82984379	-1.83799525
H	0.72349820	-0.66029980	-2.73983813
H	-2.45584620	0.25204665	-2.26228103
H	2.45097185	-2.50338049	-4.48400286
H	0.78939758	-2.74837973	-3.91197920
H	2.13073580	-2.75954726	-2.75322788
H	1.83435889	-0.18600174	-5.56705886
H	0.85528756	0.97055414	-4.64053847
H	0.15128618	-0.57968530	-5.13648530
H	-4.71594515	-0.72529986	-1.76760317
H	-4.12710971	-1.05841034	-3.40369259
H	-5.39460671	0.15524713	-3.16284627
H	-3.95441000	2.01713671	-4.31098951
H	-2.79645597	0.72063428	-4.69283675
H	-2.24198693	2.19500479	-3.87344317
H	-4.44460193	-4.69807335	-1.07192740
H	-6.29059047	-3.64767857	0.20897774
H	-5.80474935	-1.82823260	1.82884898
H	-0.83489681	-3.69254032	-0.81961997
H	0.71779975	0.64472817	2.75535523
H	-3.03013588	-4.29319610	-2.86511608
H	-1.27847669	-4.33045890	-3.15460551
H	-2.06022888	-2.79562634	-2.68706598
H	-1.43240095	-5.89801419	0.28911153
H	-0.86716401	-6.12087428	-1.38422371
H	-2.59655900	-6.21968210	-1.00557318
H	2.44959376	2.50141261	4.48052447
H	0.78278974	2.73835770	3.91945149
H	2.11544983	2.74868259	2.75102602
H	0.86645284	-0.97753662	4.66329625
H	0.15913479	0.57228678	5.15640279
H	1.84594137	0.18689773	5.57907901
H	4.11735835	1.05719073	4.31686793
H	6.15891514	-0.16169806	3.60166947
H	6.02387916	-1.86550767	1.80420606
H	-2.46033151	-0.24900031	2.25639849
H	2.89343582	-2.69735744	-0.10187346
H	-5.40037691	-0.15204097	3.15300700
H	-4.72114861	0.72604392	1.75658428
H	-4.13409641	1.06319525	3.39249821
H	-2.80396306	-0.71261749	4.68708230
H	-2.24794995	-2.18845842	3.87140966
H	-3.96099658	-2.01032124	4.30637314
H	4.92492682	-1.55766600	-1.09360548



H	4.83268452	-3.29114037	-1.45899188
H	5.96431465	-2.70905332	-0.22948142
H	3.18320045	-4.37520613	1.76446837
H	4.94006842	-4.26236112	1.58457815
H	3.95639993	-4.93345566	0.26680370
H	1.53294374	3.06659406	-2.51939628
H	-0.65363468	3.94773168	-1.74654864
H	-0.65903370	-3.94478487	1.75460740
H	1.52672916	-3.06216854	2.53022131
Zr	-0.17930832	-0.00014668	0.00062684

## 2.4 Structures with three oxygen atoms

### Oxo Peroxo Complex (planar conformation)

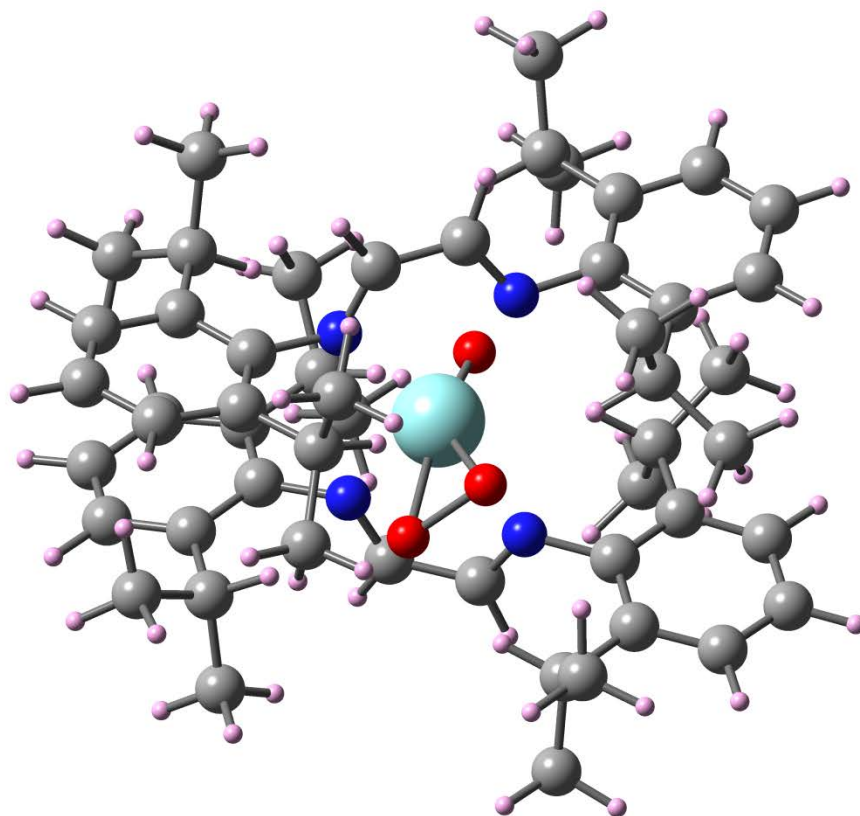


Fig. S11: NCCN Oxo Peroxo Complex (planar conformation)

SCF	E <sub>ZP</sub>	H	G
-2515.884790	-2514.740946	-2514.672895	-2514.842534

O	0.61628800	1.00286600	-1.40796500
O	0.78666300	-1.03914000	1.74053500
O	-0.40424600	-1.84307800	1.15878900
N	-1.32878300	-1.24229100	-1.56708800
N	1.38720700	-1.80498700	-1.06289100
N	1.26075400	1.88130200	1.10291800
N	-1.46312500	1.29353600	1.45724100
C	-0.69526900	-2.19126000	-2.19234000
C	0.70307000	-2.51906300	-1.89933100
C	0.47391100	2.71345600	1.72274400
C	-0.90170200	2.32672800	2.02320400
C	-2.70303300	-1.00506500	-2.01409900
C	-3.75044100	-1.74963500	-1.41048200
C	-5.04715700	-1.59132900	-1.94390700
C	-5.28521800	-0.73593500	-3.03204600
C	-4.23074000	0.00200500	-3.59257200

C	-2.91535900	-0.10515700	-3.09229700
C	-4.59068600	-2.72343400	0.80965000
C	-3.48021800	-2.73684100	-0.26750800
C	-3.30253900	-4.18078900	-0.81543900
C	2.28118800	-3.98748900	2.37619100
C	2.00471500	-3.99599300	0.85189700
C	1.87916900	-5.44941200	0.32005600
C	2.78004200	-2.17444300	-0.82956500
C	3.07990700	-3.22739100	0.07476200
C	4.43980100	-3.57418200	0.23327000
C	5.45231300	-2.90428500	-0.46806600
C	5.12297400	-1.86428100	-1.35295800
C	3.78307800	-1.47591000	-1.55747700
C	-2.11800000	2.17813700	-3.93697100
C	-1.76533000	0.68417900	-3.73189900
C	-1.34726300	0.04273300	-5.08315400
C	4.47309400	0.72553000	-2.68907000
C	3.41792600	-0.39960100	-2.58701100
C	3.20713000	-1.04256300	-3.98753700
C	2.61347500	2.32450800	0.81252600
C	2.83218000	3.38419800	-0.11300100
C	4.16520700	3.80152800	-0.31649600
C	5.23267700	3.20149400	0.36571800
C	4.98801700	2.15416200	1.26871300
C	3.67962100	1.69200600	1.51292200
C	1.91878900	3.86411900	-2.43979300
C	1.71519500	4.06336000	-0.91611800
C	1.59766700	5.56839700	-0.55568700
C	-1.98331100	-1.96557800	4.12066900
C	-1.78149300	-0.46155400	3.81606400
C	-1.50547800	0.33058800	5.12396900
C	-2.82032200	0.98258200	1.92593100
C	-2.97214500	0.15009300	3.06737600
C	-4.28384500	-0.05484700	3.54809300
C	-5.39229100	0.53474200	2.92405400
C	-5.21091800	1.34944400	1.79542000
C	-3.92385400	1.59790900	1.27461000
C	4.53030600	-0.43070000	2.68970300
C	3.40893300	0.62693800	2.57972900
C	3.17789400	1.30390600	3.96099200
C	-4.89131700	2.48022200	-0.93642000
C	-3.73722600	2.55642200	0.09046700
C	-3.58397200	4.02583400	0.57711800
H	-5.87312300	-2.14729000	-1.50974200
H	-6.28984100	-0.64137300	-3.43770300
H	-4.42903500	0.66958000	-4.42692200
H	-2.54274200	-2.45026700	0.22591100
H	1.04247600	-3.48912300	0.72949800
H	-5.53377400	-3.14021400	0.43033100
H	-4.78391900	-1.71004300	1.17549300
H	-4.28101300	-3.33789900	1.66458000
H	-4.21007100	-4.51530900	-1.33646500

H	-3.10518700	-4.87483900	0.01158000
H	-2.46475500	-4.25454600	-1.52007300
H	3.24336700	-4.45350500	2.63127400
H	1.48931700	-4.54186000	2.89752100
H	2.26542700	-2.95660800	2.74297100
H	1.64268500	-5.47174300	-0.75333800
H	1.07994700	-5.97971600	0.85508600
H	2.81227300	-6.01165500	0.46383500
H	4.70276300	-4.37594700	0.91845800
H	6.49244700	-3.18985500	-0.32793200
H	5.91316900	-1.35136500	-1.89298100
H	-0.89858700	0.66487000	-3.05877500
H	2.47189600	0.06805100	-2.28129800
H	-2.93632900	2.32175200	-4.65592300
H	-1.23853000	2.71192200	-4.31890000
H	-2.40672500	2.64739800	-2.98846900
H	-2.17686700	0.05415800	-5.80380200
H	-1.03138100	-1.00156000	-4.95624700
H	-0.50652600	0.59703100	-5.52017400
H	4.69526700	1.15634200	-1.70705900
H	4.08993300	1.52985800	-3.32961000
H	5.41381600	0.37153200	-3.13414000
H	4.13000400	-1.52353200	-4.34084300
H	2.92010100	-0.27324400	-4.71680600
H	2.41662600	-1.80402000	-3.97621700
H	4.36592800	4.60157000	-1.02453700
H	6.25016600	3.54459300	0.19342200
H	5.82018300	1.69405100	1.79229500
H	0.76455000	3.57364200	-0.68738400
H	-0.88910000	-0.40766000	3.18683000
H	2.88547600	4.25811200	-2.78131600
H	1.12661500	4.38738500	-2.99386500
H	1.85003800	2.79651600	-2.66944300
H	1.42065400	5.71940000	0.51862000
H	0.76578600	6.02660000	-1.10729800
H	2.51262000	6.11597500	-0.81755100
H	-2.84442800	-2.15204000	4.77771600
H	-1.08824500	-2.35781300	4.61988900
H	-2.10734000	-2.52310800	3.18714700
H	-1.30344600	1.39255200	4.92456000
H	-0.63035500	-0.08825800	5.63742000
H	-2.36112100	0.27971600	5.81154400
H	-4.43262800	-0.68287400	4.42188500
H	-6.39263700	0.36194800	3.31382300
H	-6.07587300	1.79961200	1.31825500
H	2.48785700	0.09371800	2.31893000
H	-2.81068500	2.27865900	-0.43085900
H	5.45728600	-0.00873400	3.10286800
H	4.75652000	-0.87846700	1.71567400
H	4.20806300	-1.23579300	3.36170100
H	2.93855000	0.54471500	4.71688900
H	2.34662000	2.02049200	3.92972400

H	4.07737900	1.84418900	4.28741300
H	-5.08626700	1.44978300	-1.24705600
H	-4.63284500	3.06103900	-1.83076200
H	-5.82014300	2.90344300	-0.53131200
H	-2.71397200	4.16179000	1.23043300
H	-4.47493100	4.33982600	1.13687700
H	-3.46581200	4.69891600	-0.28230100
H	-1.18640700	-2.76668300	-2.97993700
H	1.14021200	-3.37259500	-2.42200200
H	0.81162700	3.69883800	2.04892200
H	-1.44470800	2.92514500	2.75737500
Zr	0.05612000	-0.04910500	0.06681400

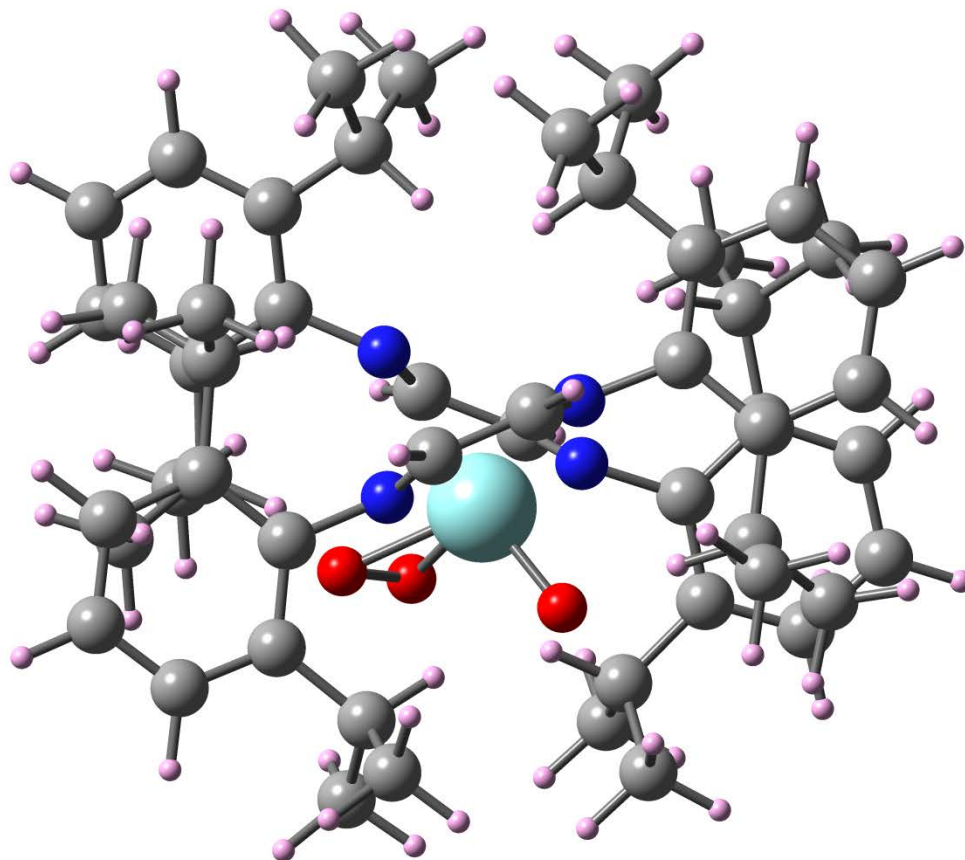
**Oxo Peroxo Complex (butterfly conformation)**

Fig. S12: NCCN Oxo Peroxo Complex (butterfly conformation)

SCF	E <sub>ZP</sub>	H	G
-2515.882348	-2514.738734	-2514.670412	-2514.842441

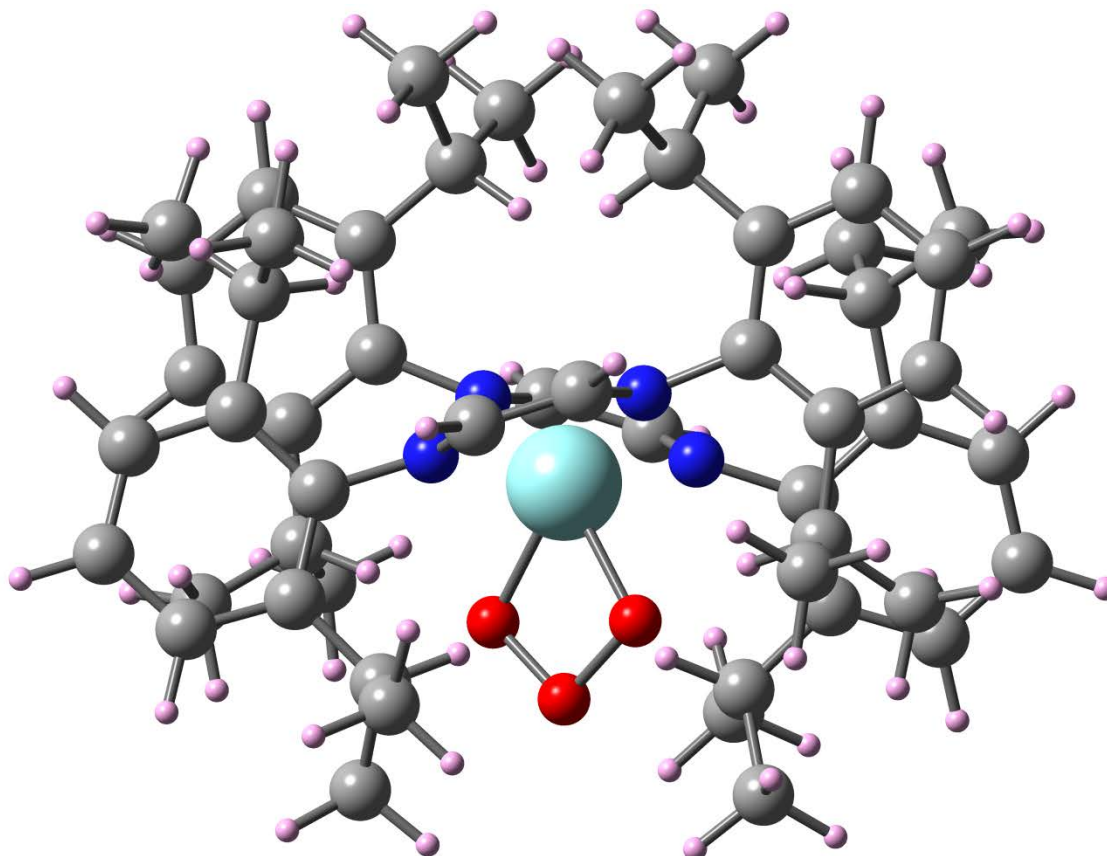
O	-1.74120866	-1.49663916	-1.16507875
N	1.08496702	-0.09293372	2.01133714
N	-1.42903586	-1.36909515	1.62547674
N	1.52686401	0.28945892	-1.82838656
N	-1.12299797	1.64720721	-1.43929737
C	0.39287642	-0.58286887	2.99934033
C	-0.94075115	-1.16618903	2.81231056
C	0.87900815	0.99385107	-2.71218150
C	-0.50499773	1.47952915	-2.57579655
C	2.42960975	0.37918705	2.38036145
C	3.50251425	-0.55228158	2.46250781
C	4.74744389	-0.06766471	2.92338700
C	4.92307980	1.26922659	3.30319873
C	3.84796517	2.16531480	3.21080485
C	2.58683632	1.74541578	2.74209818
C	4.47074738	-2.53058362	1.16749513

C	3.36057715	-2.04186167	2.13161027
C	3.36148674	-2.88938832	3.43346673
C	-1.77166092	-4.83664773	-0.62787195
C	-1.64648839	-4.18880638	0.77340722
C	-1.42964181	-5.26570883	1.87155913
C	-2.76021970	-1.97066321	1.53316740
C	-2.86362289	-3.32192965	1.10665832
C	-4.15144518	-3.89438115	1.06192859
C	-5.29183239	-3.16036893	1.41653810
C	-5.16233409	-1.82555392	1.82579609
C	-3.90049129	-1.19871788	1.89404687
C	1.82305811	4.12854096	2.18643280
C	1.41502490	2.73369816	2.71855210
C	0.78380867	2.86589089	4.13311772
C	-4.83910553	1.15883554	1.57677374
C	-3.82648785	0.26908744	2.34014678
C	-4.05076444	0.40346211	3.87180131
C	2.92775549	-0.03710194	-2.12519144
C	3.24088483	-1.28198291	-2.73950404
C	4.60141963	-1.55748811	-3.00036643
C	5.61267515	-0.64465600	-2.67685874
C	5.27670546	0.58504228	-2.09178516
C	3.93619313	0.91870506	-1.80779192
C	2.45151526	-3.71100702	-2.62132391
C	2.18984032	-2.29794496	-3.19946499
C	2.12275484	-2.33170323	-4.75139945
C	-2.04128714	4.42178576	1.60271111
C	-1.54696254	3.96995980	0.20679380
C	-0.87207435	5.15053720	-0.54627837
C	-2.44936865	2.22616279	-1.46838130
C	-2.66805043	3.37361252	-0.64741036
C	-3.91579637	4.02300633	-0.70598350
C	-4.94229561	3.54586198	-1.53434692
C	-4.72820342	2.39660975	-2.30610765
C	-3.49438906	1.70954096	-2.30086824
C	4.70282865	2.82351231	-0.26208424
C	3.60777792	2.29998604	-1.22212347
C	3.38408332	3.34834729	-2.35002007
C	-4.45522810	-0.60678133	-2.73885824
C	-3.38394972	0.43599398	-3.15199255
C	-3.49838230	0.75894581	-4.66657046
H	0.79795933	-0.60814635	4.01405678
H	-1.48427982	-1.46413157	3.71109490
H	1.36359304	1.26093965	-3.65583907
H	-0.95730637	1.79522223	-3.52047753
H	5.58333497	-0.75783154	2.99492270
H	5.88802714	1.61142502	3.66920245
H	3.99119099	3.20000916	3.50764325
H	2.41760941	-2.21250910	1.60339585
H	-0.74892055	-3.56582463	0.74286265
H	5.47055127	-2.49060480	1.62244869
H	4.48358042	-1.93439216	0.24812771

H	4.27250221	-3.57209817	0.88491513
H	4.30621748	-2.77915405	3.98412020
H	3.23226840	-3.95141783	3.18796926
H	2.54590353	-2.59937101	4.11107277
H	-2.60914823	-5.54679364	-0.68238604
H	-0.84994015	-5.38455637	-0.86295716
H	-1.91273724	-4.05813405	-1.38432121
H	-1.29592964	-4.81167177	2.86392154
H	-0.53131092	-5.85423192	1.64400666
H	-2.28234107	-5.95599519	1.93202187
H	-4.25655139	-4.92811945	0.74413232
H	-6.27495371	-3.62296248	1.37231676
H	-6.05212908	-1.26018152	2.08866666
H	0.64365005	2.33708110	2.04510483
H	-2.82711741	0.65922984	2.10985821
H	2.55413971	4.61733799	2.84208767
H	0.94701738	4.78446442	2.13376408
H	2.25874705	4.05916393	1.18333671
H	1.51940649	3.25560815	4.84885972
H	0.43233922	1.89837531	4.51361088
H	-0.07172249	3.55306626	4.11230286
H	-4.71144030	1.06791752	0.49336612
H	-4.69555376	2.21259379	1.84652295
H	-5.87527169	0.89409924	1.82290036
H	-5.04242929	0.02492248	4.15130174
H	-3.99159955	1.45625424	4.17969377
H	-3.30898632	-0.16375640	4.44960381
H	4.86308660	-2.50205956	-3.46922160
H	6.65300497	-0.88351938	-2.88481481
H	6.06532199	1.29106418	-1.85183924
H	1.20318009	-1.99845217	-2.84138469
H	-0.78613553	3.19266029	0.34694123
H	3.42448337	-4.11629629	-2.93344347
H	1.67249416	-4.39965487	-2.97475032
H	2.40053487	-3.67860330	-1.52831537
H	1.89596692	-1.34000497	-5.16707541
H	1.33160775	-3.02086580	-5.07340712
H	3.07127386	-2.67081818	-5.19080961
H	-2.76627975	5.24263351	1.53497596
H	-1.20165840	4.78561793	2.20746547
H	-2.51962409	3.59394844	2.14196991
H	-0.48452204	4.82755219	-1.52089185
H	-0.03542939	5.55873569	0.03568534
H	-1.59230913	5.96024470	-0.72366784
H	-4.08588401	4.91220059	-0.10571229
H	-5.89988399	4.05978120	-1.57200471
H	-5.53385272	2.01677163	-2.92866600
H	2.67428729	2.21488778	-0.64870082
H	-2.42236788	-0.04855146	-2.97680312
H	5.62191633	3.08165483	-0.80395396
H	4.95006676	2.08668088	0.50788099
H	4.35792556	3.73684015	0.23852504



H	3.16860949	4.33541312	-1.91846080
H	2.55147215	3.08094644	-3.01041733
H	4.28511556	3.43733212	-2.97115970
H	-4.33656863	-0.87742990	-1.68517202
H	-4.31898910	-1.52285807	-3.32746713
H	-5.47849358	-0.24192120	-2.90633048
H	-2.73013186	1.47322210	-4.99581300
H	-4.47701052	1.19130705	-4.91668051
H	-3.37739946	-0.16140598	-5.25245268
O	1.04293765	-2.33596420	0.06225664
O	-0.70721191	-1.22910520	-2.24055695
Zr	0.02743171	-0.85789707	-0.28392100

$\eta^2$ -Ozone ComplexFig. S13: NCCN  $\eta^2$ -Ozone Complex

SCF	E <sub>ZP</sub>	H	G
-2515.816724	-2514.672824	-2514.605650	-2514.773407

O	0.89747800	-2.32894500	0.78278300
O	-0.88037300	-2.34582100	-0.70797100
N	1.66073400	-0.31474800	-1.61352600
N	-1.00337600	0.45318200	-1.74606200
N	-1.65647400	-0.26168500	1.62102400
N	1.00113900	0.51646000	1.74699200
C	1.11215000	0.03065800	-2.79695500
C	-0.22997200	0.45106000	-2.86479000
C	-1.11613100	0.11548000	2.79898000
C	0.22460200	0.53994700	2.86329500
C	3.05654200	-0.76522300	-1.70906500
C	4.10378400	0.20190400	-1.64600800
C	5.43534000	-0.24732700	-1.77383700
C	5.73372800	-1.60149500	-1.98073900
C	4.69090000	-2.52924200	-2.08852800
C	3.33973100	-2.13750500	-1.96826400

C	4.95359800	2.46778100	-0.78012400
C	3.83007600	1.70653300	-1.52312000
C	3.63417600	2.35745300	-2.92338300
C	-1.81322400	4.47865200	-0.72375300
C	-1.34497000	3.38691400	-1.72016300
C	-0.73930900	4.04931400	-2.98808000
C	-2.34075700	1.00133200	-2.02962700
C	-2.47879800	2.42014400	-2.09042500
C	-3.69319300	2.95554400	-2.56647300
C	-4.75075200	2.12374400	-2.95850900
C	-4.60579100	0.73318100	-2.86918600
C	-3.40520300	0.13923700	-2.41906600
C	2.49798600	-4.50504100	-1.44965700
C	2.25199200	-3.18602200	-2.22195400
C	2.12876200	-3.46820100	-3.74607800
C	-4.53258100	-2.11664100	-1.93561100
C	-3.27726600	-1.38648600	-2.47540400
C	-2.97344200	-1.84750600	-3.92879300
C	-3.05791100	-0.69412700	1.71654700
C	-3.35955300	-2.05929100	1.99196700
C	-4.71603100	-2.43306700	2.10960200
C	-5.74685800	-1.49395900	1.98580200
C	-5.43068000	-0.14604000	1.76495300
C	-4.09310500	0.28527900	1.63788500
C	-2.54003500	-4.44354900	1.51527800
C	-2.28637100	-3.11651100	2.27090700
C	-2.18101000	-3.37644400	3.80030100
C	1.87758400	4.50041600	0.56298500
C	1.38621800	3.44035400	1.58184300
C	0.75995000	4.14289600	2.81790600
C	2.34136600	1.06185500	2.02082500
C	2.50478100	2.47864500	2.00628100
C	3.72544000	3.01517600	2.46457300
C	4.76458100	2.18588700	2.91005300
C	4.59343100	0.79550600	2.89819600
C	3.38348000	0.20366900	2.47205400
C	-4.90553300	2.54785300	0.72655800
C	-3.80262200	1.78563800	1.49927900
C	-3.62622600	2.45408800	2.89389800
C	4.39125000	-2.09573500	1.96219800
C	3.21890200	-1.31303900	2.60288200
C	3.04845600	-1.71405700	4.09426800
H	6.24728000	0.47010800	-1.71420000
H	6.76779600	-1.92541700	-2.07222100
H	4.92245000	-3.57343400	-2.27814300
H	2.89885600	1.83242600	-0.95669700
H	-0.54722800	2.81572100	-1.23216300
H	5.86215400	2.53921800	-1.39313000
H	5.21059700	1.98639400	0.16734800
H	4.63003600	3.49262100	-0.56206600
H	4.52316500	2.19548100	-3.54751000
H	3.48585500	3.44142600	-2.82046000

H	2.76801400	1.95038000	-3.45473400
H	-2.61285200	5.09890500	-1.14753200
H	-0.97914800	5.14638900	-0.47545700
H	-2.18599800	4.03593000	0.20700900
H	-0.35075700	3.29789800	-3.68585100
H	0.08687200	4.71883400	-2.71357800
H	-1.49483000	4.64263900	-3.51977300
H	-3.80972800	4.03390700	-2.63657000
H	-5.67725300	2.55474900	-3.33025000
H	-5.42687100	0.09184000	-3.17558100
H	1.29046700	-2.79831400	-1.88417800
H	-2.44288400	-1.71990700	-1.85451600
H	3.39902300	-5.02636000	-1.80076000
H	1.64419900	-5.17869800	-1.59085700
H	2.59670700	-4.31237600	-0.37632000
H	3.06356400	-3.88126400	-4.14881400
H	1.89560600	-2.55544400	-4.31051600
H	1.32647300	-4.19483400	-3.93046200
H	-4.79171800	-1.77477900	-0.92733300
H	-4.33233400	-3.19469000	-1.88522600
H	-5.40809100	-1.97609300	-2.58414300
H	-3.78602400	-1.56403000	-4.61233400
H	-2.86348700	-2.93927600	-3.96017700
H	-2.04241100	-1.40538700	-4.30557200
H	-4.96135500	-3.47177400	2.31162900
H	-6.78528200	-1.80382300	2.07672900
H	-6.23342100	0.58076500	1.69368000
H	-1.31688800	-2.74492200	1.93774600
H	0.59514300	2.85679700	1.09681600
H	-3.45313600	-4.94682200	1.86144800
H	-1.69780800	-5.12677000	1.67809200
H	-2.62132300	-4.26530100	0.43789000
H	-1.94151400	-2.45749900	4.35193800
H	-1.38966600	-4.10995900	4.00365500
H	-3.12461600	-3.77116700	4.20080500
H	2.66951500	5.13237900	0.98401500
H	1.05018000	5.16204000	0.27874500
H	2.26768900	4.03078500	-0.34725900
H	0.35476200	3.41414200	3.53005400
H	-0.05760000	4.80782000	2.50835200
H	1.50889500	4.74818100	3.34559600
H	3.86269100	4.09325200	2.47857400
H	5.69639700	2.62005800	3.26451500
H	5.39810200	0.15454200	3.24806600
H	-2.86067000	1.89548600	0.94760900
H	2.31207600	-1.62396400	2.08079800
H	-5.82352900	2.63707900	1.32289800
H	-5.15199300	2.05637000	-0.21831100
H	-4.56765700	3.56656000	0.50076000
H	-3.46357400	3.53470400	2.77864200
H	-2.77562700	2.04483300	3.44813900
H	-4.52902400	2.31072100	3.50256300

H	4.52907900	-1.81717300	0.91190600
H	4.17841600	-3.17178900	2.00086700
H	5.33946800	-1.92548400	2.49052900
H	2.18213200	-1.21514500	4.54802200
H	3.93754700	-1.44929200	4.68306700
H	2.89512700	-2.79802100	4.17603900
O	0.00690000	-3.30769800	0.05084200
H	-0.64865000	0.76622900	-3.81709800
H	1.69738200	-0.03591900	-3.71146500
H	-1.70772600	0.07328100	3.71076400
H	0.64003200	0.87689000	3.80966300
Zr	0.00684600	-0.60308000	0.01479300

## 2.5 Structures with four oxygen atoms

### Bisperoxo Complex (spiro conformation)

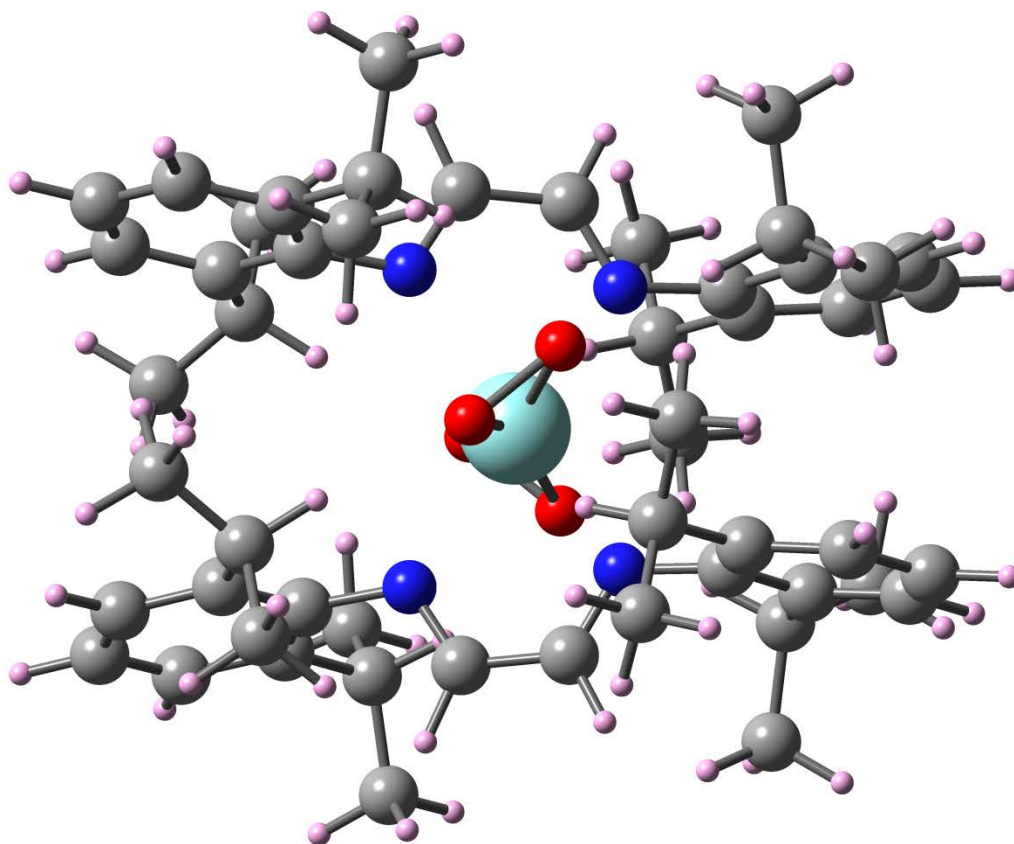


Fig. S14: NCCN Bisperoxo Complex (spiro conformation)

	<b>SCF</b>	<b>E<sub>ZP</sub></b>	<b>H</b>	<b>G</b>
	-2591.070000	-2589.922304	-2589.853400	-2590.024327
Zr	-0.00199902	0.00004265	-0.00034077	
O	-0.58471854	0.10989537	2.00325607	
O	0.58746591	1.06256560	1.69868255	
O	0.58747253	-1.06257207	-1.69925567	
O	-0.58452142	-0.10972233	-2.00398624	
N	-1.36244369	2.04611983	-0.25295198	
N	1.36106585	1.82040696	-0.96941426	
N	1.36073561	-1.82035787	0.96939627	
N	-1.36272036	-2.04584644	0.25274063	
C	-0.69785078	3.05547602	-0.72425627	
C	0.70076202	2.92209970	-1.14977661	
C	0.70003324	-2.92164440	1.15073762	
C	-0.69858556	-3.05495440	0.72520485	
C	-2.74048131	2.30806457	0.16509761	
C	-3.78629654	2.03523097	-0.75819510	

C	-5.10181039	2.35158919	-0.36097552
C	-5.36465544	2.92247965	0.89493957
C	-4.31047182	3.18004976	1.78304607
C	-2.97335429	2.87691335	1.44551817
C	-4.60166460	0.56109746	-2.70021932
C	-3.49553960	1.49979302	-2.16567172
C	-3.28466840	2.67590033	-3.16137336
C	2.11393409	-0.11427433	-4.60904986
C	1.84606758	1.19154759	-3.82066857
C	1.62142482	2.38289683	-4.79167266
C	2.74003250	1.79444201	-1.46049219
C	2.97447017	1.50952944	-2.83191327
C	4.31130363	1.56276735	-3.28296065
C	5.36440757	1.87559255	-2.41126989
C	5.10016357	2.14528014	-1.05869694
C	3.78440881	2.11664129	-0.55180800
C	-2.10882975	2.57326187	3.83087984
C	-1.84583590	3.19359138	2.43622566
C	-1.63240213	4.72796415	2.54841611
C	4.58774477	2.02438897	1.88759650
C	3.49429858	2.50213176	0.90403343
C	3.31284978	4.04130780	1.03291591
C	2.73961523	-1.79450686	1.46067844
C	2.97380035	-1.50995448	2.83221457
C	4.31048631	-1.56384782	3.28361845
C	5.36368498	-1.87700607	2.41216275
C	5.09969276	-2.14627545	1.05945053
C	3.78409899	-2.11687209	0.55218666
C	2.11353141	0.11434266	4.60899690
C	1.84528457	-1.19143720	3.82068565
C	1.61988745	-2.38257824	4.79177367
C	-2.10879957	-2.57419104	-3.83150317
C	-1.84584329	-3.19325831	-2.43629053
C	-1.63182220	-4.72764872	-2.54723792
C	-2.74079615	-2.30775522	-0.16536541
C	-2.97358244	-2.87631702	-1.44592547
C	-4.31068322	-3.17925733	-1.78367274
C	-5.36493643	-2.92181212	-0.89560707
C	-5.10216376	-2.35130112	0.36048811
C	-3.78665864	-2.03513352	0.75791950
C	4.58843693	-2.02528052	-1.88695898
C	3.49416391	-2.50195854	-0.90379380
C	3.31111358	-4.04093702	-1.03272514
C	-4.60165264	-0.56031102	2.69954779
C	-3.49611358	-1.50004613	2.16558103
C	-3.28683747	-2.67641164	3.16131757
H	-1.15557100	4.04264230	-0.81682622
H	1.16058196	3.78796034	-1.63086756
H	1.15951313	-3.78720411	1.63269396
H	-1.15664396	-4.04188018	0.81865940
H	-5.92470637	2.15486152	-1.04136143
H	-6.38632324	3.16468468	1.17819453

H	-4.52347944	3.61942383	2.75392745
H	-2.56449325	0.92060717	-2.13466102
H	0.92085837	1.01524404	-3.26427043
H	-5.53352013	1.10390892	-2.91043882
H	-4.82211811	-0.24425299	-1.99208428
H	-4.27113199	0.10221980	-3.64046523
H	-4.18963180	3.29509740	-3.22994403
H	-3.05751566	2.28608363	-4.16210316
H	-2.45463895	3.32784894	-2.86088253
H	3.02982428	-0.05911005	-5.21374020
H	1.27413289	-0.31224725	-5.28806902
H	2.18732153	-0.95847824	-3.91643285
H	1.38010377	3.30943054	-4.25174416
H	0.78984685	2.16208498	-5.47385413
H	2.51556849	2.57848803	-5.39947107
H	4.52435333	1.35394973	-4.32789061
H	6.38608744	1.91009133	-2.78232550
H	5.92189384	2.38577391	-0.39086158
H	-0.91687736	2.73730125	2.08167399
H	2.55336236	2.03009136	1.21126936
H	-3.02873024	2.95707562	4.29327035
H	-1.27165762	2.80789110	4.50137334
H	-2.17246406	1.48388316	3.74711933
H	-2.53018215	5.23090479	2.93327994
H	-1.39333967	5.17880437	1.57484482
H	-0.80302074	4.94437846	3.23471374
H	4.78595487	0.95323809	1.77823312
H	4.25797049	2.20278989	2.91883337
H	5.53186476	2.56845137	1.74725106
H	4.22810115	4.56805592	0.73008081
H	3.09030489	4.30879631	2.07407357
H	2.49031355	4.41347195	0.40878630
H	4.52334995	-1.35523487	4.32862781
H	6.38524573	-1.91202963	2.78349454
H	5.92149913	-2.38701586	0.39179972
H	0.92027054	-1.01477932	3.26406950
H	-0.91712132	-2.73636611	-2.08189993
H	3.02922643	0.05879609	5.21394953
H	1.27364202	0.31279246	5.28776896
H	2.18752449	0.95845620	3.91632899
H	1.37817289	-3.30904572	4.25191187
H	0.78832760	-2.16126296	5.47381518
H	2.51384584	-2.57856174	5.39971798
H	-3.02829936	-2.95893390	-4.29391229
H	-1.27126559	-2.80883099	-4.50153478
H	-2.17316457	-1.48478380	-3.74868182
H	-1.39266765	-5.17762310	-1.57328754
H	-0.80229180	-4.94430784	-3.23328059
H	-2.52939481	-5.23121491	-2.93177246
H	-4.52362946	-3.61841531	-2.75466262
H	-6.38659519	-3.16386496	-1.17902547
H	-5.92511055	-2.15469823	1.04085387



H	2.55383452	-2.02894758	-1.21137033
H	-2.56453572	-0.92170582	2.13509550
H	5.53200330	-2.57019314	-1.74620893
H	4.78757080	-0.95429359	-1.77759547
H	4.25890532	-2.20344780	-2.91831237
H	3.08856492	-4.30818858	-2.07394153
H	2.48798817	-4.41218911	-0.40881638
H	4.22570160	-4.56868497	-0.72962644
H	-4.82090849	0.24525358	1.99129129
H	-4.27122274	-0.10177237	3.63999685
H	-5.53415715	-1.10222393	2.90919969
H	-2.45714020	-3.32899778	2.86127838
H	-4.19232157	-3.29491219	3.22925345
H	-3.06001852	-2.28688537	4.16223703

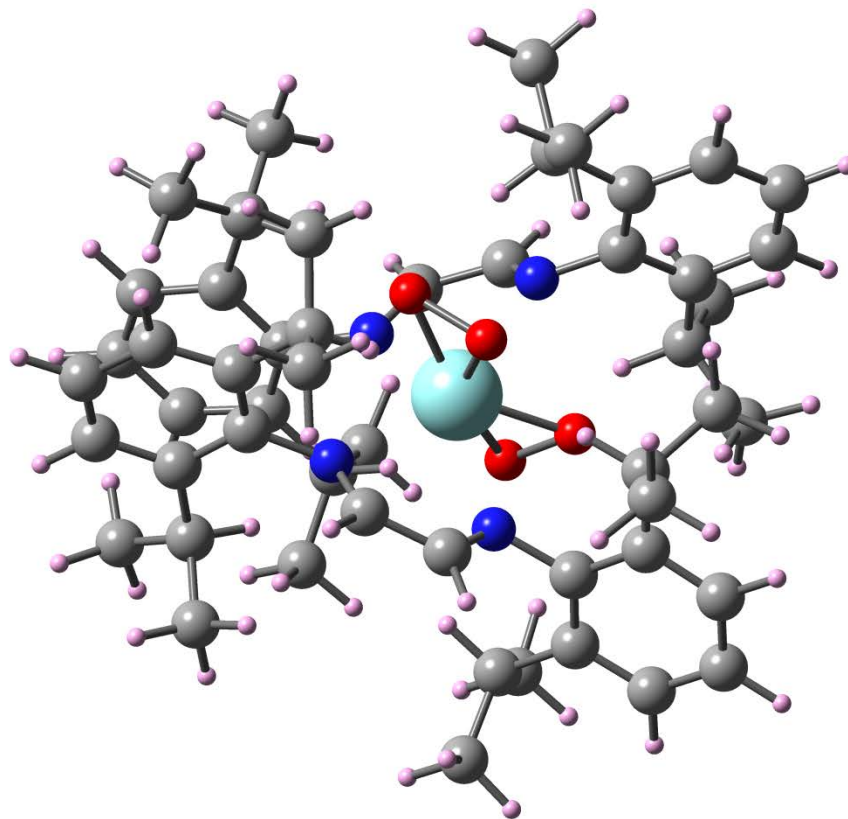
**Bisperoxo Complex (planar conformation)**

Fig. S15: NCCN Bisperoxo Complex (planar conformation)

SCF	$E_{ZP}$	H	G
-2591.041198	-2589.895299	-2589.825726	-2590.001244

O	2.15655016	-0.57238240	-0.64070206
N	-1.68607456	-0.99600991	1.57614442
N	0.87511703	-2.07537111	1.22010669
N	1.55739746	1.88316542	-1.07288772
N	-1.05178296	1.00246930	-1.78321228
C	-1.16358631	-1.80143621	2.45179862
C	0.14067263	-2.43389500	2.22475043
C	1.06444804	2.11434913	-2.25469976
C	-0.31079652	1.73026046	-2.57251982
C	-3.01715654	-0.49108627	1.90869180
C	-3.18782090	0.45615895	2.95713930
C	-4.51045156	0.84616912	3.26617976
C	-5.61286645	0.31816507	2.58207100
C	-5.41694048	-0.63397137	1.56836494
C	-4.12262665	-1.06533526	1.21819435
C	-2.04649804	2.58622112	3.78904891
C	-2.03379667	1.03730849	3.78582218
C	-2.07890653	0.49281461	5.24082862

C	4.40339466	-0.16593109	2.32648014
C	3.27231902	-1.16111229	2.68961349
C	3.37156665	-1.58554796	4.17947546
C	2.13595047	-2.79606809	1.03058215
C	3.27786124	-2.38335025	1.76401840
C	4.45703915	-3.14120022	1.61336857
C	4.50448865	-4.25439859	0.76006784
C	3.36523423	-4.62205721	0.02941282
C	2.15895319	-3.89960721	0.14372724
C	-5.03065346	-2.29411769	-0.85643432
C	-3.92312122	-2.21030425	0.21776290
C	-3.83439738	-3.57390178	0.96282527
C	1.25635315	-4.32158604	-2.19422512
C	0.93861283	-4.32744692	-0.67757279
C	0.40382533	-5.70929593	-0.21667446
C	2.90119380	2.34057341	-0.76785909
C	4.01737725	1.87470203	-1.52706851
C	5.29137564	2.37195329	-1.17845199
C	5.46235976	3.29488907	-0.13696178
C	4.34714183	3.74608159	0.58436827
C	3.04939688	3.28201980	0.29055544
C	4.81988707	-0.37940541	-2.41700383
C	3.92462661	0.85906754	-2.67550931
C	4.28684127	1.52122662	-4.03317162
C	-4.19212160	3.17277493	0.22194291
C	-3.05347594	2.86521622	-0.77794057
C	-2.65928075	4.16522681	-1.53465766
C	-2.43535967	0.82826833	-2.23052601
C	-3.41185201	1.75153688	-1.77007844
C	-4.70793602	1.65354597	-2.31780566
C	-5.01494726	0.68700271	-3.28977670
C	-4.03335007	-0.22170014	-3.71348842
C	-2.72415619	-0.17990349	-3.18792834
C	2.04343841	3.95025365	2.55183461
C	1.84288049	3.87633941	1.02039387
C	1.51402932	5.27950778	0.43720133
C	-2.15631371	-2.63290736	-3.65257005
C	-1.65819045	-1.16632026	-3.68448527
C	-1.18125075	-0.79618280	-5.11516958
H	-1.69304443	-2.06853456	3.36920808
H	0.44831010	-3.22312921	2.91420289
H	1.62121321	2.65541494	-3.02147285
H	-0.72236163	2.12591176	-3.50428874
H	-4.67223532	1.57265185	4.05784024
H	-6.61950636	0.63718367	2.84156470
H	-6.27772348	-1.05171915	1.05619034
H	-1.08030008	0.75202426	3.33554513
H	2.33174236	-0.61614011	2.56268028
H	-2.96490344	2.99549088	4.23219416
H	-1.93475090	2.95846950	2.76678397
H	-1.19535105	2.95841332	4.37421081
H	-2.99938362	0.79912550	5.75626327

H	-1.22672003	0.88268238	5.81278956
H	-2.03409918	-0.60510963	5.27286942
H	5.39835471	-0.59793190	2.50010989
H	4.31693780	0.73828597	2.94259105
H	4.33642647	0.13437019	1.27552301
H	2.54172274	-2.24486073	4.47050224
H	3.34617683	-0.70076413	4.82913019
H	4.30768500	-2.12523678	4.37687846
H	5.34816866	-2.85036230	2.16377086
H	5.42452867	-4.82540145	0.65966192
H	3.41125483	-5.47776692	-0.63972356
H	-2.96478461	-2.04593106	-0.29605745
H	0.14410907	-3.58829703	-0.52439837
H	-5.98710526	-2.61415439	-0.42198076
H	-4.75675219	-3.03646398	-1.61678470
H	-5.18006207	-1.33418483	-1.35873559
H	-4.77396264	-3.77902637	1.49277239
H	-3.02358021	-3.59474920	1.70025463
H	-3.66071153	-4.38919443	0.24790110
H	1.56061335	-3.31549843	-2.50100075
H	0.36509086	-4.61208068	-2.76789950
H	2.05749976	-5.02989384	-2.44330753
H	1.15605776	-6.49517257	-0.36565196
H	-0.49019301	-5.98704821	-0.79163154
H	0.13793205	-5.70383832	0.84946788
H	6.16104635	2.02305220	-1.72924194
H	6.45659306	3.66189772	0.10769525
H	4.48218939	4.47130318	1.38182236
H	2.90402824	0.47284762	-2.73575585
H	-2.18354323	2.54057475	-0.19327146
H	5.88268303	-0.11343604	-2.33714846
H	4.71478349	-1.09310935	-3.24573246
H	4.50161186	-0.87970920	-1.49789685
H	3.64465516	2.38544106	-4.25578509
H	4.17620158	0.79486379	-4.84965270
H	5.32583933	1.87688268	-4.03930615
H	-5.05572486	3.63942670	-0.27175004
H	-3.83202014	3.87548534	0.98394295
H	-4.53361758	2.26748775	0.73299639
H	-1.80491788	4.01087898	-2.20554345
H	-2.38378341	4.94905931	-0.81740845
H	-3.49925841	4.53292881	-2.13970431
H	-5.47868864	2.34488358	-1.99009045
H	-6.01611137	0.64095778	-3.71185679
H	-4.28459943	-0.97111884	-4.45952483
H	0.97797273	3.22924516	0.85476199
H	-0.78594469	-1.10935092	-3.02381701
H	2.85936788	4.62832522	2.83947336
H	2.24617052	2.95148274	2.95242560
H	1.12297084	4.31839204	3.02407959
H	0.61896801	5.69075843	0.92348607
H	1.32187636	5.23108491	-0.64392785

H	2.34293035	5.98306668	0.59806584
H	-2.48723286	-2.91828737	-2.64640027
H	-1.34181818	-3.30654668	-3.94567614
H	-2.99223305	-2.79871312	-4.34477290
H	-0.75560492	0.21486754	-5.15107353
H	-2.01284221	-0.83415854	-5.83174437
H	-0.40682406	-1.49802153	-5.44986964
O	0.75667193	0.91352852	1.84567051
O	-0.44675049	1.64082792	1.16085780
O	1.05768391	-0.98466162	-1.62710814
Zr	0.29155636	0.04225162	0.04539441

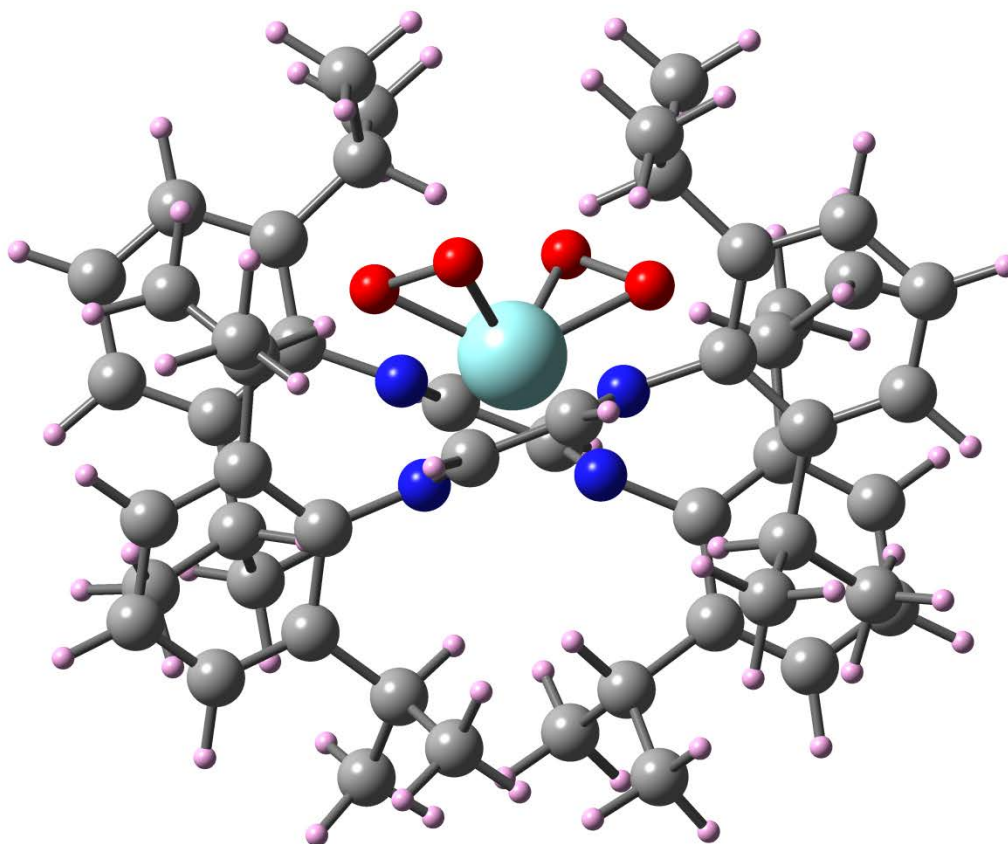
**Bisperoxo Complex (butterfly conformation)**

Fig. S16: NCCN Bisperoxo Complex (butterfly conformation)

SCF	E <sub>ZP</sub>	H	G
-2591.026897	-2589.880877	-2589.811271	-2589.986149

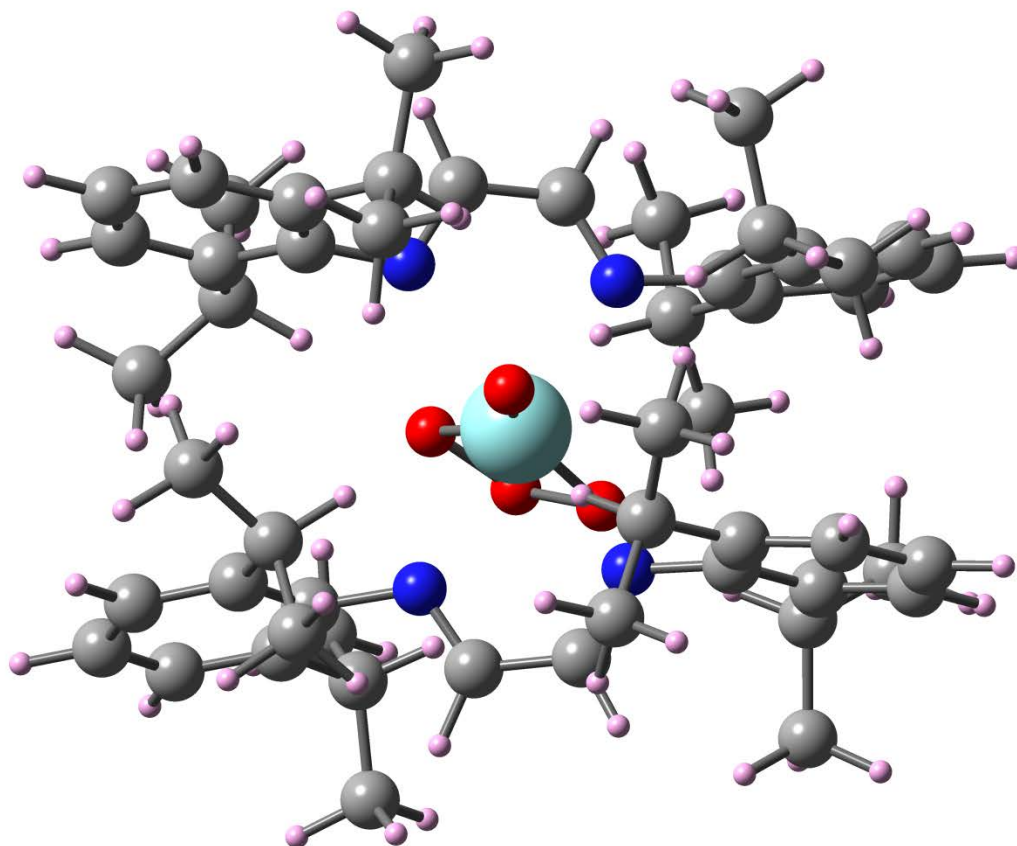
O	-1.82084248	1.74427437	0.48594436
N	1.16402782	-0.70599531	-1.96860924
N	-1.46449883	0.53293066	-1.96245097
N	1.46539443	0.39792080	1.98650043
N	-1.16225229	-0.84058643	1.91979611
C	0.56117052	-0.28171207	-3.04104941
C	-0.81237699	0.24747607	-3.04617677
C	0.81448196	0.04522453	3.05105380
C	-0.55864822	-0.48303231	3.01573088
C	2.50093565	-1.25514550	-2.17309411
C	3.56186894	-0.44152096	-2.67200959
C	4.79802054	-1.07485310	-2.93292481
C	4.98124815	-2.44894098	-2.73461808
C	3.92275287	-3.22774074	-2.24271773
C	2.67382634	-2.65086564	-1.94433712
C	4.50196552	1.85992156	-2.12273340

C	3.44944377	1.06585482	-2.93812359
C	3.58931376	1.37707613	-4.45347701
C	-2.18160701	4.56082749	-1.31231209
C	-1.98087029	3.46000474	-2.38443385
C	-1.89546336	4.07407957	-3.80800969
C	-2.84366316	1.01416065	-2.11924789
C	-3.08465283	2.40042522	-2.31278019
C	-4.42590870	2.81214422	-2.47329087
C	-5.48368889	1.89563612	-2.44731658
C	-5.21646314	0.53005736	-2.26716767
C	-3.89793609	0.05958628	-2.10256671
C	1.93765989	-4.68998518	-0.56771348
C	1.50443112	-3.53599601	-1.50267728
C	0.76241703	-4.10224540	-2.74687402
C	-4.77366500	-2.19909819	-1.25216580
C	-3.63046914	-1.44549019	-1.97075672
C	-3.38785183	-2.09326471	-3.36420123
C	2.84557269	0.86535269	2.17589553
C	3.08796462	2.23527384	2.46168161
C	4.42880126	2.63203398	2.65887506
C	5.48482778	1.71652157	2.57859310
C	5.21645532	0.36700786	2.30352768
C	3.89795521	-0.08827674	2.09990898
C	2.20166676	4.47236506	1.62486663
C	1.98404305	3.28783725	2.59968439
C	1.87531820	3.78269728	4.06744284
C	-1.92640736	-4.69580619	0.22397439
C	-1.49621412	-3.63169348	1.26127065
C	-0.76931514	-4.30886465	2.45767503
C	-2.49695121	-1.40520468	2.08954152
C	-2.66632611	-2.78238676	1.76623437
C	-3.91268796	-3.38257951	2.02803438
C	-4.97256504	-2.64206011	2.57311808
C	-4.79336452	-1.28374861	2.86323394
C	-3.55946970	-0.63054447	2.64437064
C	4.77576656	-2.28636327	1.10530215
C	3.62731498	-1.57970593	1.86227100
C	3.36730626	-2.32214209	3.20403715
C	-4.50886612	1.69991002	2.25583486
C	-3.45096681	0.85573769	3.01171311
C	-3.58658660	1.06173541	4.54530010
H	1.04174131	-0.34699290	-4.02082793
H	-1.26459722	0.39050073	-4.03097856
H	1.26860315	0.12591931	4.04202613
H	-1.03712384	-0.60947042	3.99051803
H	5.62411607	-0.47535571	-3.30541106
H	5.93958006	-2.91065235	-2.95983318
H	4.07126759	-4.29283326	-2.09417719
H	2.47756639	1.42974927	-2.59996648
H	-1.01421988	3.00197539	-2.16836733
H	5.53091139	1.59961573	-2.40845256
H	4.36791309	1.67931658	-1.05226814

H	4.36356196	2.93484039	-2.29553976
H	4.57533147	1.08357077	-4.83874841
H	3.46964181	2.45490755	-4.62290095
H	2.83182624	0.85431254	-5.05485866
H	-3.10805450	5.12961661	-1.47533766
H	-1.34136189	5.26665184	-1.34657785
H	-2.21108805	4.10591192	-0.31734076
H	-1.70627435	3.30559520	-4.57111850
H	-1.07530136	4.80253365	-3.85003304
H	-2.82383736	4.59372327	-4.08185086
H	-4.63596118	3.86873754	-2.61574521
H	-6.50840353	2.23897197	-2.56822924
H	-6.04187976	-0.17427753	-2.25121288
H	0.79186971	-2.90495469	-0.95464775
H	-2.71754143	-1.57683897	-1.37214136
H	2.58763829	-5.40889836	-1.08187508
H	1.05980485	-5.24556560	-0.21867947
H	2.47494321	-4.31423766	0.31118591
H	1.43239967	-4.74224057	-3.33610998
H	0.40555287	-3.29819525	-3.40262171
H	-0.10497298	-4.70233415	-2.44285256
H	-5.01587937	-1.73858869	-0.28921964
H	-4.48090671	-3.23893447	-1.06475439
H	-5.68480445	-2.22556764	-1.86403364
H	-4.26943955	-1.95970649	-4.00479629
H	-3.20210091	-3.17120921	-3.26070446
H	-2.52976468	-1.65206535	-3.88529319
H	4.64008670	3.67584736	2.87488302
H	6.50930096	2.04819444	2.73027860
H	6.04097248	-0.33609941	2.24398049
H	1.02168773	2.85082387	2.32834133
H	-0.77482922	-2.95932752	0.77811286
H	3.12539244	5.02574593	1.84614383
H	1.36131832	5.17463835	1.70381222
H	2.24471273	4.10014962	0.59653391
H	1.67773831	2.95350290	4.76179597
H	1.05248439	4.50357933	4.15784671
H	2.79869738	4.27909869	4.39625499
H	-2.58126302	-5.45654252	0.66726666
H	-1.04800204	-5.22017014	-0.16882477
H	-2.45795395	-4.24115229	-0.62045699
H	-0.41306299	-3.56644680	3.18288343
H	0.09641290	-4.88729198	2.10955914
H	-1.44887100	-4.99196762	2.98396738
H	-4.05841743	-4.43603571	1.80902839
H	-5.92894619	-3.12098753	2.76879543
H	-5.62099461	-0.71310862	3.27580165
H	2.72087602	-1.66496552	1.24557353
H	-2.48160769	1.24527616	2.69568804
H	5.67952707	-2.36055871	1.72417153
H	5.03108754	-1.76061458	0.17992151
H	4.48055138	-3.30886074	0.84169343



H	3.17601357	-3.38877128	3.02280082
H	2.50677900	-1.91272629	3.74628072
H	4.24327491	-2.24001211	3.86088960
H	-4.38121387	1.58995088	1.17497718
H	-4.37055327	2.76147749	2.49733817
H	-5.53579808	1.42013416	2.53013639
H	-2.82791512	0.49788268	5.10681155
H	-4.57181389	0.74243855	4.91189518
H	-3.46577831	2.12506502	4.78945749
O	0.70706293	2.20368193	-1.36002624
O	1.81079676	1.79282040	-0.36455411
O	-0.71865586	2.09972973	1.50413992
Zr	-0.00158747	0.87055710	0.02702683

Oxo  $\eta^2$ -Ozone ComplexFig. S17: NCCN Oxo  $\eta^2$ -Ozone Complex

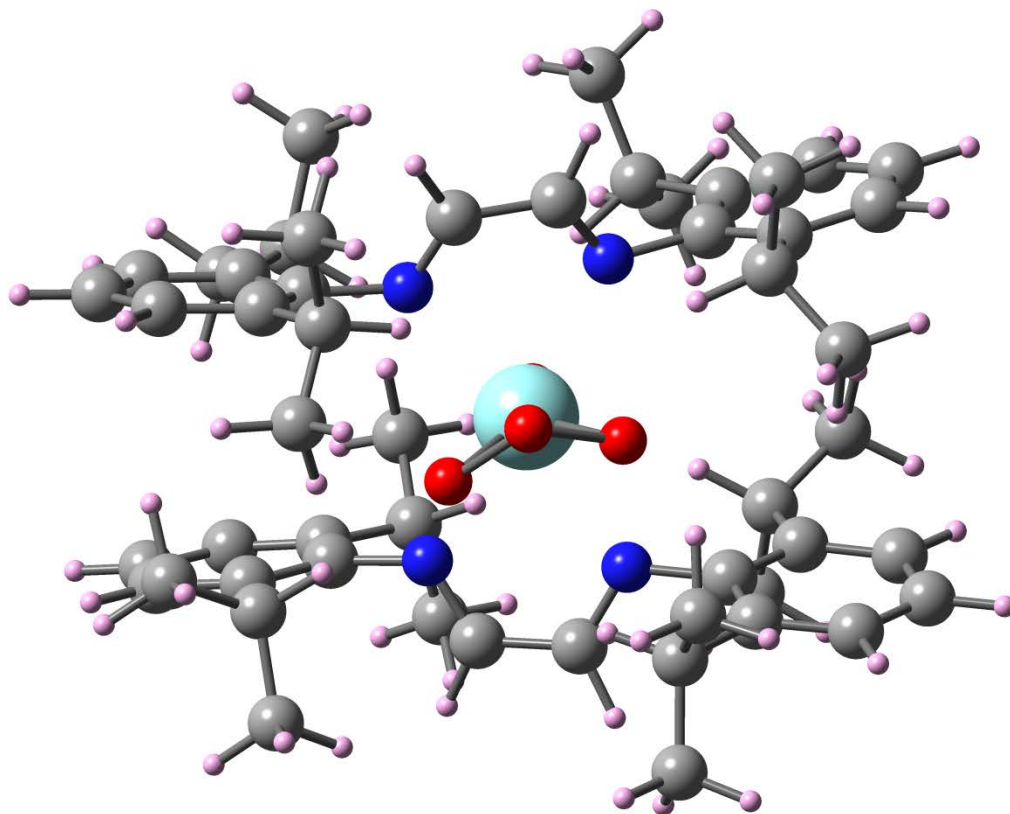
SCF	E <sub>ZP</sub>	H	G
-2591.041807	-2589.895510	-2589.826724	-2589.998526

O	-1.12899390	-0.08104716	-2.01040667
O	1.08121303	-1.04373914	-1.72954601
O	-0.11518967	0.46506235	1.64343635
N	-1.27401738	-2.11394623	0.17438477
N	1.43189926	-1.86604143	0.88891293
N	1.28687888	1.87058730	-0.96024495
N	-1.42396143	2.08686783	-0.27512493
C	-0.57211890	-3.14789314	0.53238928
C	0.82236952	-3.00895468	0.96199077
C	0.61439758	2.96113837	-1.19157037
C	-0.77558601	3.10386666	-0.75442004
C	-2.68968590	-2.34758837	-0.11892672
C	-3.62710407	-2.02653599	0.90182050
C	-4.98648859	-2.30039058	0.64770600
C	-5.39691980	-2.87832822	-0.56445127
C	-4.44859708	-3.18930981	-1.54852989
C	-3.07397404	-2.93097938	-1.35444445

C	-4.20851570	-0.55769838	2.93109486
C	-3.17441867	-1.49661236	2.26871413
C	-2.86328816	-2.68138595	3.22778540
C	1.87979793	-0.03163292	4.71381869
C	1.65950688	-1.21284672	3.73825612
C	1.25327165	-2.48732538	4.52873512
C	2.77254211	-1.80040415	1.47370832
C	2.88523613	-1.49565326	2.85943022
C	4.17804976	-1.51590620	3.42384945
C	5.30952512	-1.81246770	2.64837984
C	5.16672770	-2.09894371	1.28234951
C	3.89838921	-2.10564700	0.66271407
C	-2.47413802	-2.70253953	-3.82527793
C	-2.07470468	-3.30384833	-2.45512899
C	-1.91781643	-4.84560889	-2.55796646
C	4.85706031	-1.88993385	-1.70789704
C	3.75661226	-2.50435784	-0.81069108
C	3.75762578	-4.05232739	-0.95462810
C	2.69952528	1.88972590	-1.35307527
C	3.05890222	1.70052264	-2.71272891
C	4.42737318	1.81142838	-3.04224773
C	5.39386052	2.09102720	-2.06659192
C	5.00862834	2.26887315	-0.72823517
C	3.65598424	2.17869312	-0.34070304
C	2.42935323	0.16494610	-4.65066773
C	2.03831779	1.41110146	-3.81869483
C	1.85475965	2.64981695	-4.73749193
C	-1.76335043	2.54114898	3.88025357
C	-1.62430181	3.16884494	2.47185880
C	-1.36021769	4.69564886	2.57537343
C	-2.75232593	2.35280435	0.27528474
C	-2.84869086	2.88820161	1.59027590
C	-4.13947481	3.19366945	2.07277566
C	-5.28338903	2.97414093	1.29166188
C	-5.15642084	2.44151373	-0.00081507
C	-3.89308673	2.12211051	-0.54103933
C	4.28933361	2.04944038	2.14829134
C	3.23369680	2.47869210	1.10382484
C	2.92577949	3.99393354	1.27580100
C	-4.88097625	0.65637099	-2.40604910
C	-3.76351117	1.64093984	-1.98971931
C	-3.73861385	2.85809381	-2.95725001
H	-5.72786312	-2.06512551	1.40479976
H	-6.45028093	-3.08500671	-0.73861815
H	-4.77472842	-3.63400158	-2.48488906
H	-2.24714335	-0.92382959	2.13494497
H	0.83252915	-0.90866561	3.08744149
H	-5.11182361	-1.09975612	3.24294327
H	-4.50684221	0.25335061	2.25903320
H	-3.77328112	-0.10638049	3.83146801
H	-3.76232090	-3.29007731	3.39460096
H	-2.52009552	-2.30174654	4.19914318

H	-2.08137110	-3.34098749	2.83069764
H	2.65761826	-0.24098042	5.46102698
H	0.94676463	0.17505757	5.25391923
H	2.15523387	0.87619164	4.16606933
H	1.03206275	-3.33057687	3.86053451
H	0.35645882	-2.29141425	5.13176146
H	2.05769077	-2.80473957	5.20676250
H	4.29803006	-1.29403356	4.48061761
H	6.29594548	-1.82137206	3.10625590
H	6.04710411	-2.32832976	0.68896350
H	-1.10035562	-2.87032790	-2.21714382
H	2.79620432	-2.13487963	-1.18763720
H	-3.43305634	-3.09729047	-4.18893936
H	-1.70610724	-2.94333156	-4.57138003
H	-2.53947712	-1.61275195	-3.75059273
H	-2.86858741	-5.32499567	-2.82787311
H	-1.58259088	-5.28857441	-1.60950959
H	-1.17962113	-5.09909321	-3.33011137
H	4.90101367	-0.80157158	-1.59492743
H	4.63741656	-2.11031691	-2.76051907
H	5.85140542	-2.30178160	-1.48576914
H	4.70096121	-4.48205428	-0.58997738
H	3.63806686	-4.33302511	-2.00931015
H	2.93889126	-4.51634836	-0.38885680
H	4.73520116	1.67223953	-4.07508710
H	6.44198232	2.17030045	-2.34535304
H	5.76494035	2.48535608	0.01949250
H	1.07396281	1.17146938	-3.36432771
H	-0.75435491	2.67926547	2.02551272
H	3.37374493	0.30777611	-5.19380623
H	1.64458632	-0.04643877	-5.38791410
H	2.51823266	-0.70729534	-3.99592577
H	1.51583429	3.53138203	-4.17511409
H	1.10823859	2.43614774	-5.51362942
H	2.79546892	2.91885498	-5.23696375
H	-2.61807066	2.94608666	4.43903335
H	-0.85540570	2.74103102	4.46479147
H	-1.87190462	1.45566372	3.79385490
H	-1.20858424	5.15168844	1.58716932
H	-0.46244504	4.88624167	3.17885369
H	-2.20316361	5.21495772	3.05148134
H	-4.24578174	3.60555039	3.07282228
H	-6.26710712	3.21863470	1.68564078
H	-6.04582991	2.27822130	-0.60228175
H	2.31015721	1.92507172	1.32053260
H	-2.81215025	1.10903546	-2.10238057
H	5.19500032	2.66810428	2.08919532
H	4.57761868	1.00084183	2.02469301
H	3.87995830	2.17058452	3.15897828
H	2.60145906	4.20012226	2.30428294
H	2.13269989	4.33612606	0.59939262
H	3.82203241	4.59506178	1.07139646

H	-4.94847716	-0.18719556	-1.71073207
H	-4.66051400	0.25339209	-3.40290565
H	-5.86533332	1.14244536	-2.45860122
H	-2.91047012	3.54277404	-2.73063169
H	-4.67438959	3.43047063	-2.89296157
H	-3.61607042	2.51422507	-3.99264292
O	-0.02736942	-0.83209236	-2.74939219
H	1.30220489	-3.89128472	1.39117196
H	-1.01636827	-4.14426392	0.57669486
H	1.08346026	3.81951908	-1.67620962
H	-1.21867168	4.10091770	-0.80266765
Zr	-0.02639707	-0.03253754	-0.15053552

Oxo  $\eta^3$ -Ozone ComplexFig. S18: NCCN Oxo  $\eta^3$ -Ozone Complex

SCF	E <sub>ZP</sub>	H	G
-2591.039977	-2589.893496	-2589.823926	-2589.999310

N	1.37133800	-2.07582400	0.39575000
N	-1.36066900	-2.06555600	-0.19807300
N	-1.42758900	2.06523000	0.06753300
N	1.32566800	2.13034300	-0.44492800
C	0.78733600	-3.15120900	-0.03859100
C	-0.63358100	-3.12867500	-0.39515000
C	-0.81781100	3.17958900	-0.19733100
C	0.59652800	3.19586600	-0.57641400
C	2.72785800	-2.19042000	0.92298600
C	3.83097800	-2.40687000	0.05078500
C	5.10863400	-2.53758500	0.63974100
C	5.28598000	-2.47645500	2.02820500
C	4.17571900	-2.28774500	2.86695500
C	2.87741000	-2.14095300	2.34006100
C	4.66099800	-1.58060900	-2.22001200
C	3.69869300	-2.53574500	-1.47190600
C	3.93299300	-4.00372700	-1.92165200
C	-2.73168700	-1.73006500	-4.13967900
C	-2.36562500	-2.70661600	-2.99366400

C	-2.42292000	-4.17749200	-3.48970100
C	-2.78601200	-2.18264100	-0.46099000
C	-3.26446700	-2.50759700	-1.76374300
C	-4.65990500	-2.65537000	-1.92281400
C	-5.54310600	-2.49435400	-0.84742100
C	-5.04444000	-2.18633600	0.42877300
C	-3.66265700	-2.03357000	0.65311600
C	1.91873700	-1.22083500	4.54640500
C	1.66326800	-2.05647800	3.27175700
C	1.19692400	-3.48926200	3.65557700
C	-4.09968400	-1.14662100	3.03052800
C	-3.11181500	-1.84782400	2.07184800
C	-2.71093600	-3.22825500	2.66834800
C	-2.78892300	2.18714800	0.58896400
C	-2.95951300	2.47046600	1.97287800
C	-4.28072000	2.63951300	2.44037000
C	-5.38056300	2.52872000	1.57701700
C	-5.17894200	2.25624400	0.21445700
C	-3.88206300	2.08871500	-0.31407100
C	-1.95084400	1.87017500	4.25744900
C	-1.77606700	2.65243300	2.93343800
C	-1.54426400	4.16000000	3.22924500
C	2.52474000	1.33411100	-4.40408400
C	2.15179100	2.37690500	-3.32081400
C	2.05402500	3.79710200	-3.94304700
C	2.73920000	2.23399100	-0.78700800
C	3.13751100	2.36128800	-2.14560600
C	4.51981900	2.48577600	-2.40365200
C	5.46156100	2.48271500	-1.36516900
C	5.03710000	2.36243800	-0.03180500
C	3.67026100	2.24054800	0.28823700
C	-4.79897100	1.11981200	-2.51216900
C	-3.66270500	1.90794400	-1.82094400
C	-3.50331400	3.29110300	-2.51541700
C	4.20944400	1.58170100	2.71666200
C	3.19491300	2.22815300	1.74673000
C	2.87962400	3.67732300	2.21753700
H	1.30169200	-4.11359200	-0.07620200
H	-1.07529800	-4.06411700	-0.74330200
H	-1.31810500	4.14541800	-0.09695400
H	1.02005200	4.14096900	-0.92189800
H	5.97144600	-2.69131500	-0.00285400
H	6.28009400	-2.58376400	2.45604200
H	4.31748800	-2.25877400	3.94327700
H	2.69114500	-2.23115300	-1.76441600
H	-1.33108600	-2.47443300	-2.72982900
H	5.71529800	-1.82035200	-2.02567900
H	4.48063300	-0.54126900	-1.92838200
H	4.49505500	-1.66036600	-3.30258800
H	4.95099500	-4.33736200	-1.67898900
H	3.79869400	-4.09275100	-3.00793400
H	3.23483300	-4.69886800	-1.43492500

H	-3.77083200	-1.85454100	-4.47306200
H	-2.07695500	-1.90997800	-5.00283400
H	-2.57729900	-0.69912600	-3.80900500
H	-2.13965800	-4.89009800	-2.70220700
H	-1.73879600	-4.31606800	-4.33717200
H	-3.43277200	-4.44684700	-3.82615800
H	-5.05519400	-2.89555600	-2.90645100
H	-6.61343400	-2.61232000	-0.99945000
H	-5.73575200	-2.07464800	1.25737800
H	0.85637000	-1.54778000	2.73466200
H	-2.20202200	-1.23517500	2.01638600
H	2.65864700	-1.68332000	5.21465300
H	0.98227800	-1.12066800	5.11028900
H	2.25968800	-0.21304300	4.28747200
H	1.97810100	-4.01948500	4.21794600
H	0.95760900	-4.09245100	2.76928400
H	0.29730600	-3.44116600	4.28333700
H	-4.45380100	-0.19408300	2.62294200
H	-3.60208700	-0.94175200	3.98645900
H	-4.97122100	-1.77863400	3.24942300
H	-3.59024000	-3.88148100	2.75157500
H	-2.28503100	-3.09687300	3.67154300
H	-1.96379400	-3.74258000	2.05248300
H	-4.44570300	2.86015000	3.49162700
H	-6.38944000	2.66067600	1.96130700
H	-6.03658900	2.18056700	-0.44667600
H	-0.88099800	2.22915200	2.46750600
H	1.16244000	2.08595700	-2.95657700
H	-2.82617900	2.20097200	4.83322800
H	-1.06301600	2.01478100	4.88677900
H	-2.04320400	0.79881600	4.05586100
H	-1.37093200	4.73818000	2.31129400
H	-0.66905800	4.28854000	3.88025400
H	-2.41245500	4.60211000	3.73734500
H	3.49740900	1.54927600	-4.86734000
H	1.76754500	1.33912600	-5.19934200
H	2.54938400	0.33519600	-3.96021700
H	1.74382200	4.55049300	-3.20541100
H	1.32290200	3.80235800	-4.76244000
H	3.02143700	4.11767100	-4.35241300
H	4.85875200	2.57635600	-3.43217200
H	6.52124300	2.57508600	-1.59167700
H	5.77389100	2.36658000	0.76514800
H	-2.73078300	1.34873700	-1.97385800
H	2.26230700	1.65080600	1.80656500
H	-5.73721100	1.69130300	-2.53516100
H	-4.98692400	0.16433300	-2.01258600
H	-4.52053700	0.90974200	-3.55224500
H	-3.33292500	3.15442900	-3.59127900
H	-2.65717500	3.86091700	-2.11276400
H	-4.40983000	3.89780600	-2.38474500
H	4.48847400	0.57261200	2.39518700



H	3.76565500	1.50784500	3.71759800
H	5.12431800	2.18238300	2.81212700
H	2.12087700	4.15893500	1.58811700
H	3.78466900	4.29940100	2.18873200
H	2.50264500	3.66639400	3.24873600
O	-0.90304500	0.09937500	-1.99643200
O	0.28136100	-0.77282100	-2.42275300
O	1.50913100	-0.23518100	-1.71189400
Zr	0.09729400	-0.00119200	-0.05195600
O	0.08694100	0.29128100	1.77353100

## 2.6 Structures with five oxygen atoms

### Peroxo Ozone Complex (conformation 1 lowest energy)

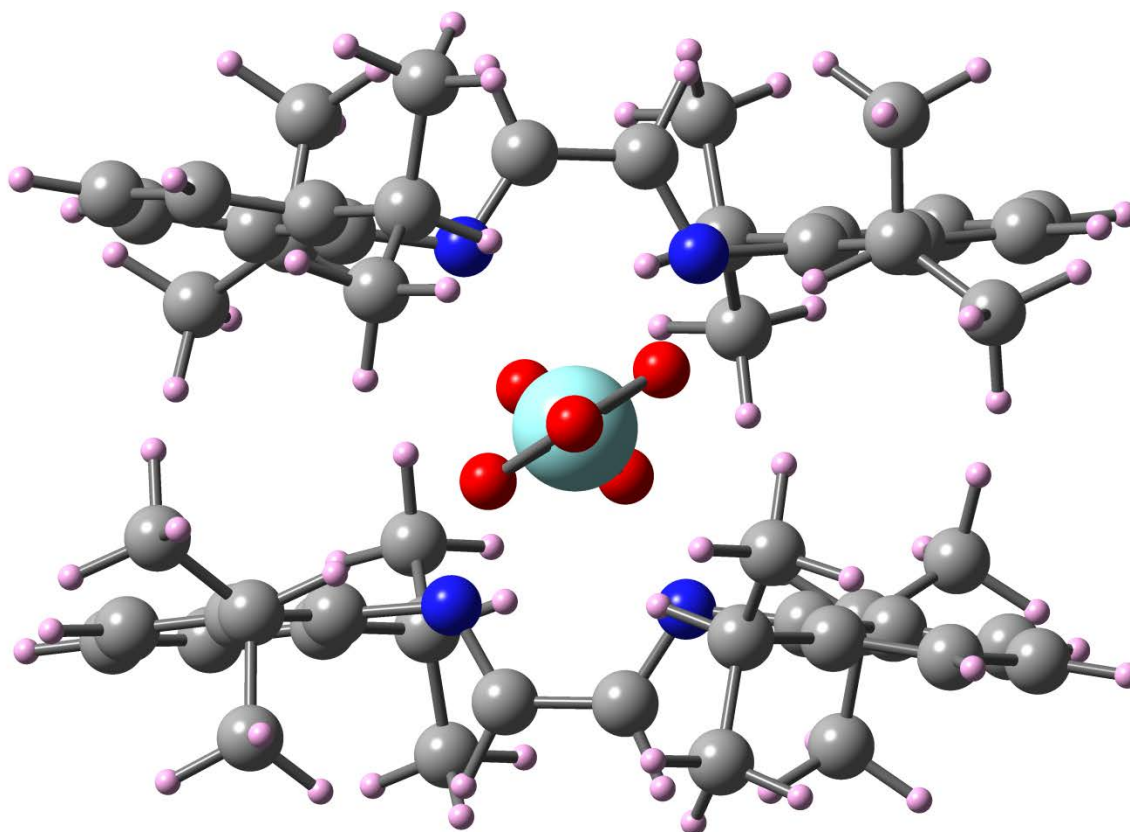


Fig. S19: NCCN Peroxo Ozone Complex (conformation 1 higher energy)

SCF	$E_{ZP}$	H	G
-2666.214636	-2665.064315	-2664.994039	-2665.168520

O	-0.97629000	0.89741300	-1.79560500
O	0.98752800	-0.43280700	-1.95864500
O	0.58779400	0.26195900	1.86174300
O	-0.60095100	-0.71272600	1.73718400
N	-1.33562300	-1.98045200	-0.71285600
N	1.37029400	-2.09738300	0.13229400
N	1.33988800	2.09141400	-0.20626400
N	-1.37017700	2.00157600	0.63746300
C	-0.66646700	-3.09311500	-0.70322200
C	0.72341900	-3.16012900	-0.23111300
C	0.66863500	3.16794000	0.07064100
C	-0.72089000	3.11925000	0.54517600
C	-2.73911500	-2.06142800	-1.13602600
C	-3.73329200	-2.19528000	-0.12685800
C	-5.07463600	-2.31246300	-0.54574400

C	-5.41577700	-2.31021400	-1.90728800
C	-4.41244000	-2.19265200	-2.87865200
C	-3.05268100	-2.06480000	-2.52070600
C	-4.41782600	-1.65530900	2.29326400
C	-3.37269400	-2.30828500	1.35933700
C	-3.17816600	-3.80021800	1.75316300
C	1.83588000	-1.84488000	4.29443300
C	1.64668100	-2.69026200	3.01081100
C	1.36772300	-4.17592100	3.36895900
C	2.71736900	-2.29594000	0.67843300
C	2.84817700	-2.58509400	2.06413000
C	4.14820600	-2.83037100	2.55599900
C	5.26898200	-2.78494700	1.71443000
C	5.10767300	-2.49750700	0.35032900
C	3.83286200	-2.25191900	-0.20205800
C	-2.31335500	-0.87889900	-4.65805500
C	-1.98892600	-1.98108800	-3.62003700
C	-1.81283600	-3.35782200	-4.31695400
C	4.78809000	-1.15223600	-2.31915900
C	3.67215700	-2.03365400	-1.71037100
C	3.61456800	-3.40132000	-2.44765500
C	2.74237600	2.27911000	-0.59750500
C	3.05431200	2.63271400	-1.93643800
C	4.41262300	2.85825800	-2.24966500
C	5.41635500	2.73627800	-1.27948100
C	5.07731100	2.38903500	0.03769500
C	3.73758700	2.15858400	0.41238200
C	2.33146700	1.99642700	-4.29920600
C	1.99226800	2.81096400	-3.02660100
C	1.80413900	4.31410500	-3.36925100
C	-1.84181500	0.71905400	4.59914300
C	-1.65277400	1.86509700	3.57487800
C	-1.38375700	3.21154700	4.30178500
C	-2.71730600	2.06328600	1.21402900
C	-2.85137600	1.99922900	2.62785200
C	-4.15255400	2.11375600	3.16248000
C	-5.27173800	2.27903900	2.33397100
C	-5.10718500	2.34146000	0.94185900
C	-3.83084400	2.24193900	0.34834400
C	4.43522600	1.03309300	2.61784400
C	3.37802200	1.88530000	1.87807800
C	3.16098700	3.22424300	2.63878500
C	-4.77134600	1.69024200	-1.97749300
C	-3.66904200	2.41178100	-1.16648300
C	-3.63893100	3.92155900	-1.53723700
H	-5.85707800	-2.41232700	0.20016400
H	-6.45672800	-2.40458000	-2.20741100
H	-4.68309600	-2.19782000	-3.93104800
H	-2.42214800	-1.79213900	1.53304200
H	0.76326300	-2.28040700	2.51390600
H	-5.36666900	-2.20901800	2.30045200
H	-4.62350200	-0.61953700	2.00429500

H	-4.03630200	-1.64796200	3.32207400
H	-4.10623600	-4.36787800	1.60041000
H	-2.89791800	-3.87801500	2.81177000
H	-2.39025400	-4.28347000	1.16090800
H	2.69091700	-2.18153400	4.89703200
H	0.93624000	-1.91899100	4.91958900
H	1.97477900	-0.79115900	4.03188300
H	1.18211900	-4.78343800	2.47193000
H	0.48425200	-4.25042900	4.01704500
H	2.21747700	-4.62483600	3.90131000
H	4.27895300	-3.05838800	3.61049000
H	6.26095800	-2.97623100	2.11702900
H	5.97889300	-2.46971800	-0.29753200
H	-1.03379900	-1.69731300	-3.17275500
H	2.72475000	-1.51649600	-1.89594700
H	-3.23468900	-1.09317100	-5.21711600
H	-1.49164600	-0.79905100	-5.38086000
H	-2.41620700	0.09053300	-4.15992700
H	-2.74349200	-3.68035100	-4.80313000
H	-1.52355100	-4.14250900	-3.60376200
H	-1.03196500	-3.29481000	-5.08618000
H	4.88247400	-0.20104400	-1.78419800
H	4.54581100	-0.92647800	-3.36573000
H	5.76574200	-1.65386800	-2.30954300
H	4.54272400	-3.96956500	-2.29594800
H	3.48025400	-3.24358300	-3.52585500
H	2.78112000	-4.02247800	-2.09311000
H	4.68124400	3.13019700	-3.26676700
H	6.45590300	2.91337500	-1.54505400
H	5.85984300	2.30198200	0.78517400
H	1.03867600	2.41880600	-2.66621700
H	-0.76559900	1.60041600	2.99339500
H	3.25502000	2.34609400	-4.78049000
H	1.51526600	2.08992100	-5.02661700
H	2.43889700	0.93556800	-4.05090900
H	1.50599800	4.89952800	-2.48799500
H	1.02520900	4.43267100	-4.13390000
H	2.73202700	4.75408500	-3.75914700
H	-2.70941500	0.88115400	5.25336900
H	-0.95059900	0.64396100	5.23613300
H	-1.95974400	-0.23464300	4.07501800
H	-1.19998300	4.02897300	3.59020000
H	-0.50200500	3.12234200	4.95035400
H	-2.23681900	3.50524500	4.92867700
H	-4.28568500	2.07153300	4.24012200
H	-6.26476800	2.36319300	2.76927700
H	-5.97719200	2.47549500	0.30562900
H	2.43560000	1.32754200	1.91305500
H	-2.71334000	1.97496100	-1.47437400
H	5.37515400	1.58203500	2.76709100
H	4.65739900	0.10779200	2.07640900
H	4.05613400	0.75904000	3.61044800

H	2.88124300	3.02447500	3.68136700
H	2.36437200	3.83018700	2.18813600
H	4.07975000	3.82655900	2.63838600
H	-4.84543000	0.63377500	-1.69808600
H	-4.53069500	1.73944600	-3.04739300
H	-5.75817700	2.15416900	-1.84129800
H	-2.81339600	4.44902000	-1.04056100
H	-4.57498900	4.41722100	-1.24508500
H	-3.51002200	4.04164300	-2.62092400
O	0.00580100	0.34823700	-2.81672400
H	1.17467600	-4.15256500	-0.16413100
H	-1.12739000	-4.03104000	-1.02008100
H	1.12851400	4.15505500	-0.01147500
H	-1.17091200	4.06573800	0.85304500
Zr	0.00065300	0.01063000	-0.10865000

## Peroxo Ozone Complex (conformation 2 higher energy)

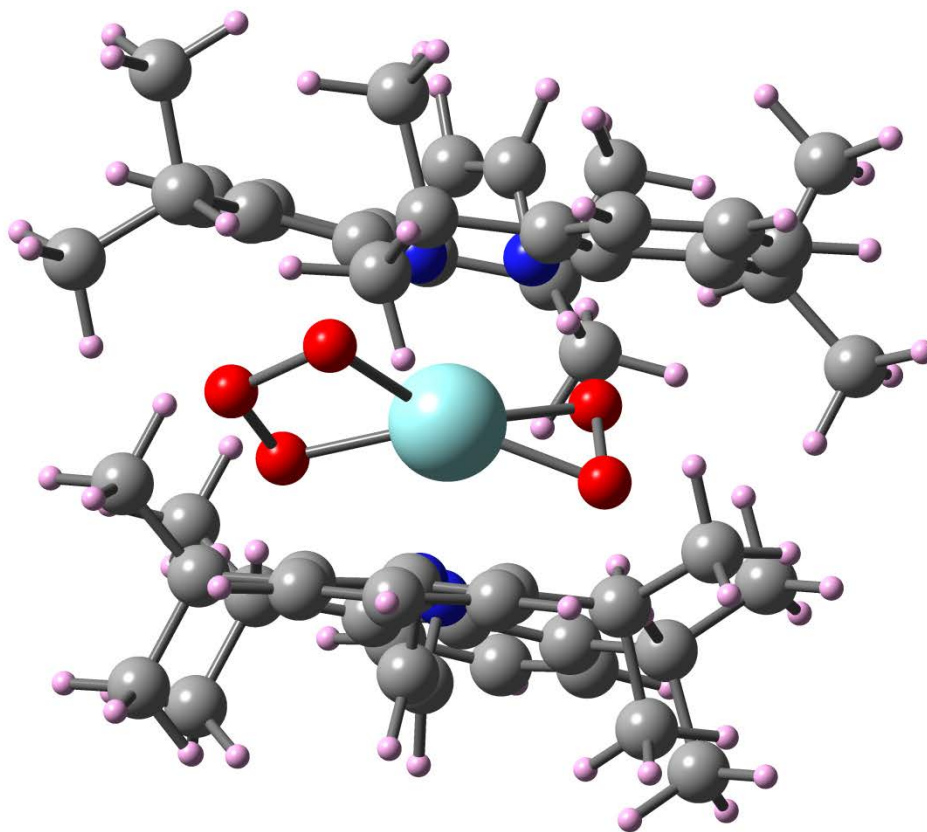


Fig. S20: NCCN Peroxo Ozone Complex (conformation 2 higher energy)

SCF	$E_{ZP}$	H	G
-2666.214634	-2665.064355	-2664.994055	-2665.168672

O	-0.97713112	0.90063902	-1.78965953
O	0.98955242	-0.42523193	-1.95586288
O	0.58905001	0.25635190	1.86598542
O	-0.59881260	-0.71913702	1.73838189
N	-1.33259968	-1.97859554	-0.72103025
N	1.37290564	-2.09817242	0.12527255
N	1.33624100	2.09446054	-0.19747126
N	-1.37364316	1.99705945	0.64641065
C	-0.66135226	-3.09001496	-0.72078254
C	0.72819499	-3.15869239	-0.24813393
C	0.66349166	3.16888730	0.08368024
C	-0.72589583	3.11606447	0.55844941
C	-2.73585525	-2.05897885	-1.14464142
C	-3.72969578	-2.19769041	-0.13574011
C	-5.07099071	-2.31546124	-0.55448924
C	-5.41264959	-2.30893998	-1.91592636

C	-4.40981978	-2.18604971	-2.88708896
C	-3.05007136	-2.05761406	-2.52916901
C	-4.41447010	-1.66919660	2.28683800
C	-3.36818424	-2.31581159	1.34983606
C	-3.17015921	-3.80898918	1.73749832
C	1.83938296	-1.85611994	4.28575822
C	1.65134124	-2.69990409	3.00106012
C	1.37498474	-4.18667814	3.35685469
C	2.72040461	-2.29897794	0.66938977
C	2.85238426	-2.59150215	2.05426997
C	4.15267608	-2.83810782	2.54455604
C	5.27281935	-2.79093300	1.70216908
C	5.11043493	-2.50011026	0.33900363
C	3.83516208	-2.25288898	-0.21191454
C	-2.31538187	-0.85943324	-4.66111335
C	-1.98748666	-1.96629558	-3.62913548
C	-1.80936796	-3.33890298	-4.33370572
C	4.78263785	-1.13335093	-2.32168877
C	3.67453057	-2.02938791	-1.71963675
C	3.63192831	-3.39380098	-2.46367759
C	2.73802530	2.28495922	-0.58964610
C	3.04801689	2.64474122	-1.92749960
C	4.40579735	2.87191218	-2.24166529
C	5.41098099	2.74588370	-1.27347724
C	5.07387026	2.39327818	0.04272757
C	3.73474667	2.16078161	0.41830734
C	2.32127830	2.02400335	-4.29391040
C	1.98412819	2.82909887	-3.01482608
C	1.79418392	4.33440046	-3.34712018
C	-1.84451714	0.70170578	4.60382881
C	-1.65709731	1.85098686	3.58291321
C	-1.38989106	3.19580940	4.31334720
C	-2.72117133	2.05479197	1.22261252
C	-2.85566998	1.98601188	2.63610330
C	-4.15718356	2.09756145	3.17054059
C	-5.27623771	2.26401326	2.34205090
C	-5.11128188	2.33068766	0.95016212
C	-3.83458800	2.23434651	0.35692475
C	4.43575036	1.02681397	2.61831315
C	3.37736273	1.88163238	1.88341344
C	3.16108735	3.21772855	2.64941012
C	-4.77482632	1.69066595	-1.97095176
C	-3.67179305	2.40802053	-1.15733365
C	-3.63846170	3.91853256	-1.52428012
H	-5.85293501	-2.41910943	0.19144029
H	-6.45352986	-2.40394856	-2.21607702
H	-4.68070360	-2.18720945	-3.93941531
H	-2.41867353	-1.79835193	1.52516643
H	0.76707595	-2.29121292	2.50474305
H	-5.36139814	-2.22622537	2.29314643
H	-4.62405395	-0.63318748	2.00137438
H	-4.03196000	-1.66375876	3.31527196

H	-4.09694864	-4.37799395	1.58208867
H	-2.88997636	-3.89048917	2.79584411
H	-2.38086576	-4.28803236	1.14364815
H	2.69526287	-2.19212387	4.88746113
H	0.94010009	-1.93274032	4.91111013
H	1.97620177	-0.80176193	4.02469287
H	1.18860468	-4.79248281	2.45879966
H	0.49265165	-4.26347537	4.00622684
H	2.22614603	-4.63566180	3.88691924
H	4.28418305	-3.06882468	3.59835262
H	6.26509831	-2.98347557	2.10341815
H	5.98120361	-2.47093783	-0.30943742
H	-1.03251192	-1.68275887	-3.18143222
H	2.72267791	-1.52031215	-1.90454857
H	-3.23847057	-1.07145813	-5.21811885
H	-1.49596638	-0.77630427	-5.38616893
H	-2.41688926	0.10777099	-4.15844016
H	-2.73969427	-3.66039701	-4.82122834
H	-1.51823385	-4.12709772	-3.62517141
H	-1.02910732	-3.27012840	-5.10305549
H	4.86383808	-0.18285799	-1.78341220
H	4.54177295	-0.90718223	-3.36850272
H	5.76610930	-1.62341038	-2.30967223
H	4.56576227	-3.95324791	-2.31418038
H	3.49684157	-3.23222419	-3.54120402
H	2.80485505	-4.02545078	-2.11269718
H	4.67289840	3.14826019	-3.25796605
H	6.45012291	2.92421714	-1.53980479
H	5.85746863	2.30346743	0.78875318
H	1.03169046	2.43354876	-2.65521114
H	-0.76954289	1.58906562	3.00074243
H	3.24393652	2.37722909	-4.77441994
H	1.50379316	2.12312830	-5.01914184
H	2.42909323	0.96126243	-4.05409932
H	1.49704495	4.91384896	-2.46162793
H	1.01390790	4.45740113	-4.10970551
H	2.72120077	4.77743787	-3.73564356
H	-2.70998969	0.86225120	5.26125502
H	-0.95158286	0.62347781	5.23804863
H	-1.96496328	-0.25007863	4.07675093
H	-1.20596009	4.01502304	3.60387402
H	-0.50882277	3.10558661	4.96268921
H	-2.24393379	3.48743968	4.93990238
H	-4.29077015	2.05222900	4.24801852
H	-6.26948196	2.34590919	2.77730538
H	-5.98115291	2.46592700	0.31401625
H	2.43520349	1.32343854	1.91743102
H	-2.71654685	1.97031744	-1.46567666
H	5.37555146	1.57552722	2.76912137
H	4.65772206	0.10410757	2.07236352
H	4.05770698	0.74809624	3.61000758
H	2.88394811	3.01417154	3.69195634



H	2.36295794	3.82469589	2.20281117
H	4.07947890	3.82059296	2.64880942
H	-4.85005090	0.63326933	-1.69546864
H	-4.53392307	1.74345406	-3.04061292
H	-5.76113715	2.15520427	-1.83318634
H	-2.81387821	4.44355627	-1.02352337
H	-4.57478103	4.41502080	-1.23430237
H	-3.50563384	4.04095973	-2.60724140
O	0.00791800	0.35828923	-2.81173518
H	1.18131783	-4.15082892	-0.18983726
H	-1.12048883	-4.02605429	-1.04570062
H	1.12171009	4.15704049	0.00494605
H	-1.17727640	4.06078891	0.86970813
Zr	0.00156855	0.01071502	-0.10490546

## Catalyst Deformation Product with Oxygen Added to Ligand

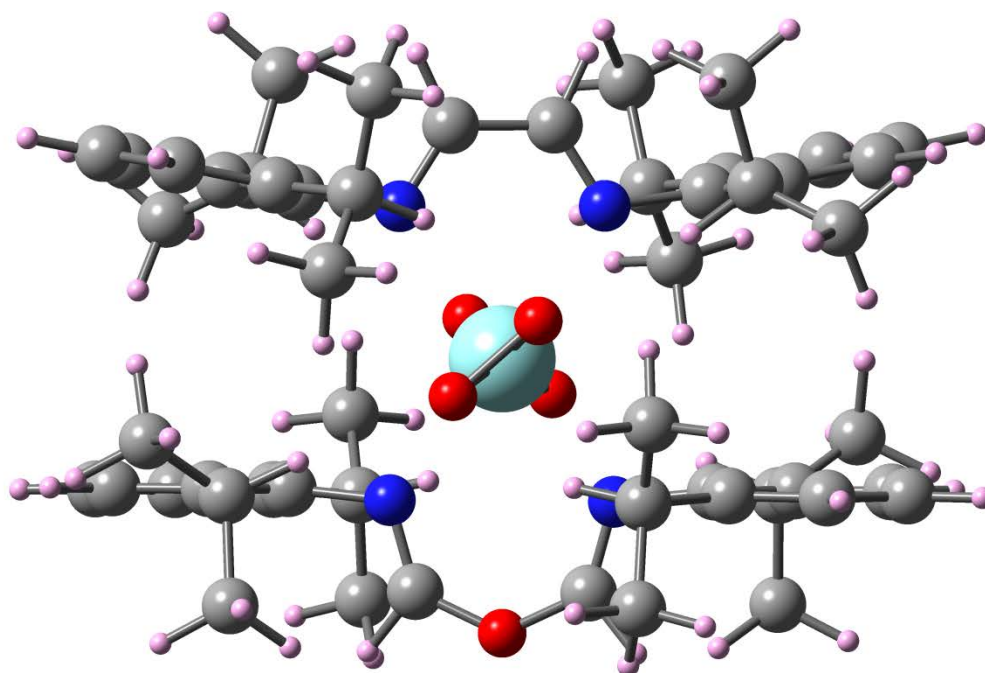


Fig. S21: NCCN Catalyst Deformation Product with Oxygen Added to Ligand

SCF	$E_{ZP}$	H	G
-2666.2672403	-2665.114415	-2665.044749	-2665.216971

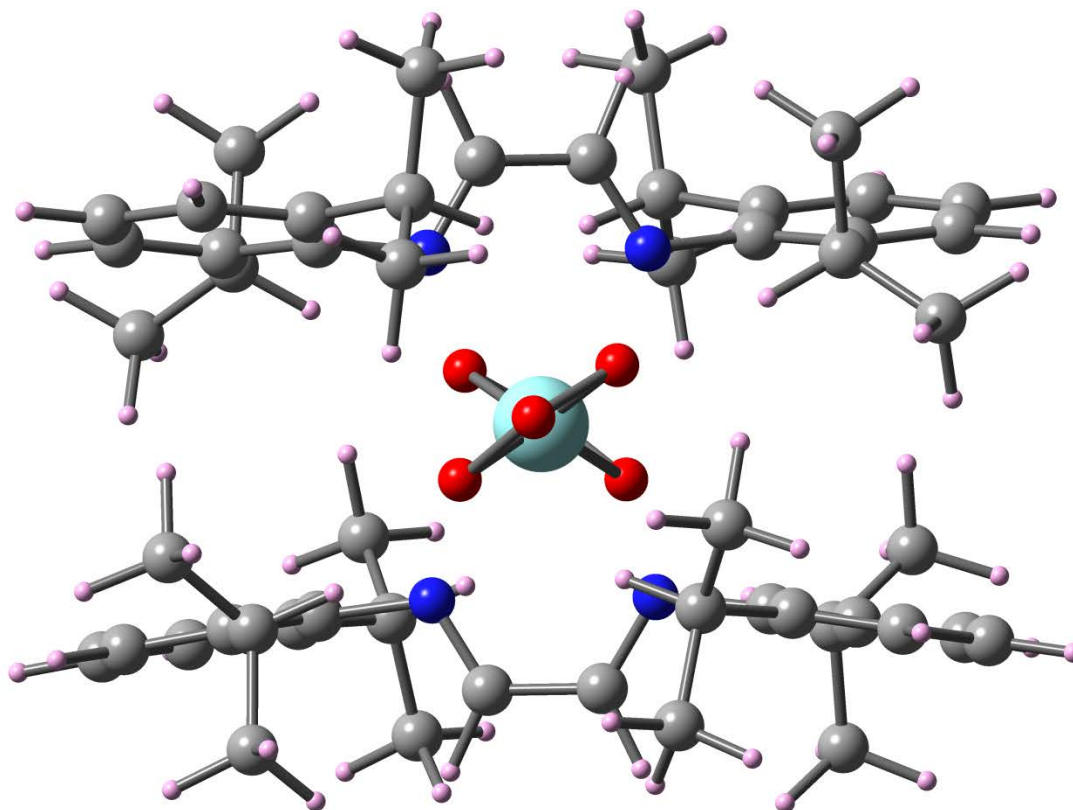
Zr	0.00310500	-0.01525500	-0.16368700
O	-0.62524800	1.94140100	0.17165100
O	0.53600100	1.87980600	-0.84424500
O	0.63640600	-1.86317500	0.55619300
O	-0.51470100	-2.01204600	-0.46236400
N	-1.54404800	0.18247700	-2.11587400
N	1.55706500	-0.57882100	-2.04031600
N	1.35583000	0.61451700	1.85602700
N	-1.36575100	-0.24932300	1.93081200
C	-1.19422100	0.06119700	-3.34444800
C	1.21820600	-0.65898000	-3.27520300
C	0.68168700	0.52976200	2.96031300
C	-0.69013200	0.01832700	3.00447500
C	-2.95751200	0.61668700	-2.01458900
C	-3.95717800	-0.38814500	-1.91085100
C	-5.30379700	0.03136100	-1.95235800
C	-5.63925900	1.38470500	-2.11568700
C	-4.62846700	2.35022700	-2.22544400
C	-3.26282800	1.99434100	-2.17666500
C	-4.62052500	-2.70258700	-1.01360100
C	-3.60763800	-1.88142600	-1.84557800
C	-3.51549700	-2.49129000	-3.27422500
C	2.36240100	-4.46048200	-0.56289400

C	2.17875900	-3.47228300	-1.74069300
C	2.15742800	-4.23595300	-3.09373900
C	2.96668200	-0.99848100	-1.85538600
C	3.26026000	-2.38442800	-1.75469200
C	4.62260900	-2.75512000	-1.73547000
C	5.64186200	-1.79492500	-1.80803000
C	5.31829600	-0.43222300	-1.90167400
C	3.97520800	-0.00085000	-1.94140800
C	-2.38875800	4.26798800	-1.39806800
C	-2.19141400	3.07602200	-2.36635800
C	-2.17179400	3.57150400	-3.83920000
C	4.63666600	2.43639200	-1.46992800
C	3.64072800	1.48047400	-2.16710100
C	3.59944800	1.80955100	-3.68739400
C	2.70890200	1.16293100	1.99878600
C	2.88066300	2.57212200	1.99122300
C	4.18226300	3.06564900	2.22843600
C	5.26068900	2.19962100	2.45896300
C	5.05707700	0.81001800	2.46296100
C	3.77795200	0.25810100	2.24314900
C	1.99974200	4.59148900	0.68923800
C	1.71531500	3.55023000	1.79935200
C	1.37866900	4.25912000	3.14026300
C	-2.02585200	-4.35926400	1.49963700
C	-1.74856800	-3.14615200	2.42114400
C	-1.44616500	-3.61516100	3.87094400
C	-2.72278000	-0.75382700	2.16346100
C	-2.90527400	-2.13855500	2.41716700
C	-4.21279200	-2.57092400	2.72992200
C	-5.28632200	-1.67078800	2.78397200
C	-5.07186600	-0.30570300	2.53220000
C	-3.78650900	0.18766600	2.22713600
C	4.75798400	-2.08727900	1.86347400
C	3.54651200	-1.25629800	2.34595900
C	3.20489200	-1.66763000	3.80686200
C	-4.74632200	2.44151100	1.44349600
C	-3.54067900	1.69376800	2.05805100
C	-3.18683800	2.35349400	3.42240400
H	-1.85822600	0.26408200	-4.18144100
H	1.88678700	-1.00150600	-4.06155600
H	1.11477400	0.84742900	3.91124600
H	-1.12444600	-0.12995500	3.99549500
H	-6.09439500	-0.70784000	-1.86970700
H	-6.68410500	1.68326700	-2.16027000
H	-4.89823600	3.39473300	-2.35640500
H	-2.62515200	-1.98920500	-1.36981900
H	1.20329900	-3.00342900	-1.58832200
H	-5.58940700	-2.79193300	-1.52409400
H	-4.78848800	-2.25835000	-0.02811100
H	-4.23560200	-3.71896800	-0.86448900
H	-4.47249900	-2.38617300	-3.80345700
H	-3.27551900	-3.56053300	-3.20894400

H	-2.73884300	-2.01671100	-3.88595700
H	3.31865400	-4.99977200	-0.61284500
H	1.55578500	-5.20520200	-0.58040500
H	2.29690700	-3.92169000	0.38709200
H	1.97361200	-3.56338600	-3.94346500
H	1.36106000	-4.99176400	-3.08590800
H	3.11076300	-4.74964000	-3.27919400
H	4.88304200	-3.80794800	-1.66771900
H	6.68402100	-2.10569000	-1.79523000
H	6.11546500	0.30242100	-1.95997000
H	-1.21173200	2.65534100	-2.12576700
H	2.64576800	1.68278400	-1.75259700
H	-3.34467400	4.78582400	-1.55878800
H	-1.58280600	4.99865600	-1.54713100
H	-2.33399900	3.92001500	-0.36228000
H	-3.13021500	4.02866000	-4.12142000
H	-1.97493700	2.75371700	-4.54664800
H	-1.38483200	4.32560000	-3.97148800
H	4.75822300	2.19029800	-0.41102700
H	4.26574100	3.46675800	-1.53732500
H	5.62600200	2.41409300	-1.94727400
H	4.56983800	1.59843600	-4.15702500
H	3.37185300	2.87347700	-3.83363900
H	2.83520300	1.23241500	-4.22207600
H	4.34719300	4.13987900	2.23177500
H	6.25449100	2.60331300	2.63818200
H	5.89756800	0.14754500	2.64538300
H	0.83186000	2.99635600	1.46940400
H	-0.85150700	-2.66751600	2.01817600
H	2.87809100	5.21317400	0.91224800
H	1.13428600	5.25844400	0.58184100
H	2.14901700	4.08575900	-0.26966300
H	1.12729900	3.53796900	3.93081200
H	0.51828500	4.92821800	3.00726100
H	2.22447100	4.86154800	3.49944200
H	-2.93270500	-4.90872000	1.78847500
H	-1.17971000	-5.05753800	1.54685200
H	-2.11999100	-4.02449800	0.46220900
H	-1.19937400	-2.77020500	4.52923000
H	-0.59294300	-4.30622000	3.87267800
H	-2.30612900	-4.13745600	4.31226000
H	-4.38576400	-3.62430900	2.93436300
H	-6.28468100	-2.02792800	3.02575200
H	-5.90895100	0.38371500	2.58154600
H	2.68967500	-1.52060400	1.71231600
H	-2.68440000	1.83199900	1.38480200
H	5.60437800	-2.01487000	2.56055800
H	5.09526100	-1.76853600	0.87363000
H	4.47646400	-3.14583100	1.79971000
H	3.05172800	-2.75312000	3.86426200
H	2.29299000	-1.18379400	4.17599300
H	4.02557300	-1.40009300	4.48637000

H	-5.09427000	1.95934200	0.52602100
H	-4.45371200	3.46938800	1.19488500
H	-5.58782400	2.50219700	2.14743300
H	-2.27490600	1.93803400	3.86716900
H	-4.00533700	2.21463200	4.14186300
H	-3.02781100	3.43128400	3.28718500
O	0.01570800	-0.33906700	-3.86290400

## 2.7 Structures with six oxygen atoms

Bis- $\eta^2$ -ozone ComplexFig. S22: NCCN Bis- $\eta^2$ -ozone Complex

SCF	$E_{ZP}$	H	G
-2741.352682	-2740.199416	-2740.128868	-2740.303245

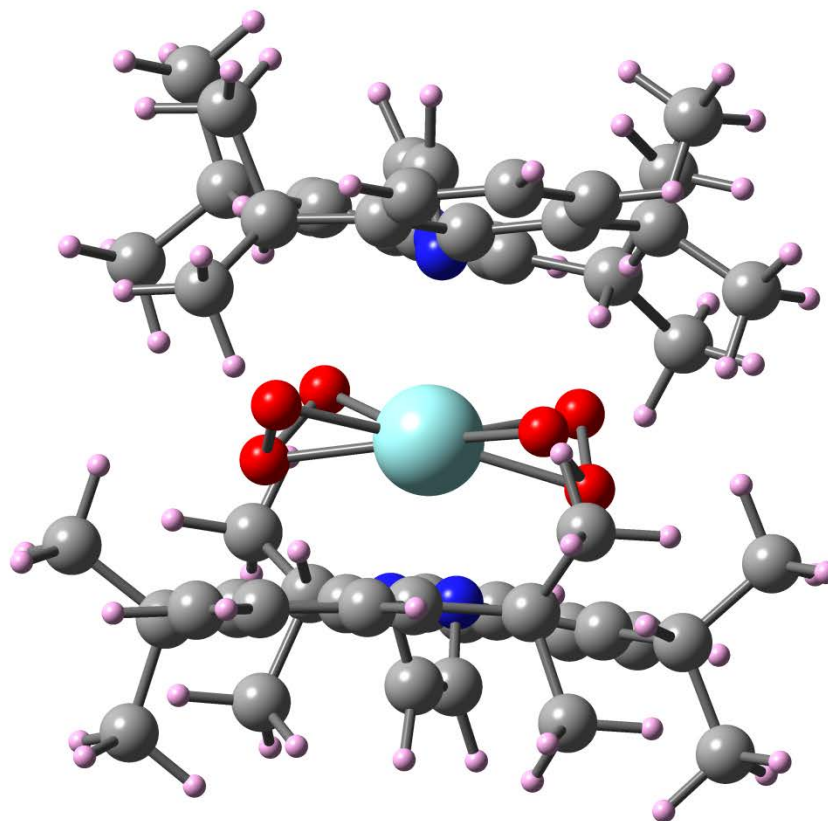
Zr	0.00041000	0.00320200	0.00858800
O	0.85881600	0.55550600	1.87893700
O	-1.05787700	-0.79271700	1.66486100
O	-0.84054300	0.80442300	-1.78205300
O	1.09141000	-0.53887200	-1.72149000
N	1.34054500	-2.13737400	0.38613200
N	-1.32438600	-2.06178800	-0.65999800
N	-1.36768500	2.04620700	0.61366200
N	1.33817800	2.14053200	-0.31231600
C	0.69092500	-3.21079400	0.05558600
C	-0.67636700	-3.17168200	-0.47851400
C	-0.71033000	3.15896500	0.48917200
C	0.65810100	3.21116400	-0.03588200
C	2.71267300	-2.33677500	0.88032600
C	3.77848300	-2.43362700	-0.05804300

C	5.07366000	-2.67589200	0.44931900
C	5.30601600	-2.82901300	1.82325100
C	4.23323000	-2.74978400	2.72233800
C	2.91709600	-2.50559700	2.27696700
C	4.56178300	-1.38631200	-2.26130700
C	3.57338000	-2.36134600	-1.57578400
C	3.68608600	-3.77852800	-2.20270100
C	-1.97884000	-0.96602200	-4.67433000
C	-1.70856600	-2.03590600	-3.58938700
C	-1.38444300	-3.40910300	-4.23967800
C	-2.68934600	-2.19316200	-1.19546400
C	-2.87279700	-2.17386500	-2.60457000
C	-4.18085400	-2.36520500	-3.09761500
C	-5.26466500	-2.57081200	-2.23244600
C	-5.05319300	-2.59629300	-0.84645500
C	-3.76720200	-2.41472400	-0.29310300
C	2.04692300	-1.60637500	4.50816500
C	1.76705500	-2.51581100	3.28791600
C	1.46117200	-3.96937000	3.74315500
C	-4.61785200	-1.72186600	2.02549500
C	-3.57591900	-2.53897900	1.22314700
C	-3.61997100	-4.03271800	1.64992300
C	-2.71684100	2.14137200	1.18338600
C	-2.87258800	2.33441000	2.58427100
C	-4.18975000	2.43506500	3.08422500
C	-5.30332300	2.36121300	2.23757000
C	-5.11893800	2.20073600	0.85575600
C	-3.82953500	2.09364700	0.29663700
C	-1.85127400	1.57051200	4.80273500
C	-1.69814000	2.48288500	3.56057300
C	-1.53864600	3.96512100	4.00000800
C	1.78025300	2.31596200	-4.53289400
C	1.63434500	3.02401100	-3.16291800
C	1.46366300	4.55517300	-3.36842900
C	2.67956200	2.33526300	-0.87244400
C	2.81937200	2.73559000	-2.23102500
C	4.13049400	2.91312500	-2.72513100
C	5.25408700	2.71612900	-1.91211200
C	5.08568700	2.35448300	-0.56671200
C	3.80292000	2.16386700	-0.01484100
C	-4.77451200	1.29374700	-1.96074400
C	-3.64646100	2.04963700	-1.22325300
C	-3.52782000	3.49440800	-1.78731200
C	4.77276700	1.05857700	2.09960100
C	3.63803600	1.90911600	1.48607500
C	3.52852400	3.26437100	2.24205100
H	1.14401100	-4.19918800	0.16185800
H	-1.13035000	-4.13402100	-0.72575600
H	-1.15939500	4.11205200	0.77590000
H	1.08382700	4.20513200	-0.18806000
H	5.90444700	-2.75467500	-0.24649500
H	6.31240100	-3.01859600	2.18898800

H	4.41383700	-2.88584200	3.78510500
H	2.57383000	-1.97333900	-1.78496600
H	-0.82227200	-1.70008300	-3.04808900
H	5.60405900	-1.72422200	-2.17919500
H	4.48919500	-0.38319800	-1.82778300
H	4.32089000	-1.30844200	-3.32948800
H	4.68492100	-4.20717200	-2.04285100
H	3.50712600	-3.72838100	-3.28497700
H	2.95431700	-4.47485300	-1.76985000
H	-2.82597600	-1.23326200	-5.32086900
H	-1.09221500	-0.85482500	-5.31100300
H	-2.18018400	0.00479000	-4.20915800
H	-1.13021100	-4.16628200	-3.48471800
H	-0.53012700	-3.31182800	-4.92250300
H	-2.23911100	-3.78951000	-4.81550900
H	-4.34609800	-2.35820300	-4.17147800
H	-6.26435700	-2.71729100	-2.63458100
H	-5.89358700	-2.76756000	-0.17947700
H	0.87127000	-2.11430700	2.81173300
H	-2.59734400	-2.13458700	1.49461200
H	2.90322100	-1.95620600	5.10113700
H	1.16818400	-1.58935200	5.16520400
H	2.23902400	-0.57900400	4.18087900
H	2.32727500	-4.41967000	4.24685200
H	1.19984400	-4.61473800	2.89280800
H	0.61728000	-3.97568600	4.44546800
H	-4.61393700	-0.66928700	1.72279700
H	-4.37291800	-1.76451700	3.09469600
H	-5.63728100	-2.11356200	1.90388000
H	-4.59003600	-4.48616500	1.40420100
H	-3.46643800	-4.12147800	2.73357500
H	-2.84144700	-4.62473200	1.14890700
H	-4.33892000	2.57232900	4.15155100
H	-6.30720700	2.43835500	2.64846200
H	-5.98430300	2.16509100	0.20143400
H	-0.77777100	2.16806200	3.06345000
H	0.72049700	2.63073300	-2.71187200
H	-2.70497800	1.86350800	5.42903700
H	-0.94698600	1.63392900	5.42206600
H	-1.97698900	0.52713400	4.49814800
H	-1.37422700	4.63340200	3.14339800
H	-0.68265900	4.06882500	4.68003200
H	-2.43463900	4.32052300	4.52637700
H	2.62191800	2.71335200	-5.11607000
H	0.86709100	2.46373400	-5.12426200
H	1.92109900	1.23986100	-4.39460200
H	1.30168300	5.08326300	-2.41859200
H	0.60288900	4.75626800	-4.02005200
H	2.35435600	4.99228300	-3.83929800
H	4.26703100	3.20891500	-3.76157900
H	6.25307900	2.85453500	-2.31882200
H	5.95856800	2.22640200	0.06572100



H	-2.70696300	1.53638900	-1.45470800
H	2.70061900	1.36993500	1.65769600
H	-5.72812100	1.83901800	-1.92705300
H	-4.93234500	0.29487500	-1.54061800
H	-4.50440700	1.17379500	-3.01743400
H	-3.36404900	3.46169500	-2.87223500
H	-2.68909300	4.04294600	-1.33957000
H	-4.44576600	4.06655500	-1.59369600
H	4.92369100	0.12672000	1.54441600
H	4.51378400	0.79422800	3.13259000
H	5.72710500	1.60261400	2.13079500
H	2.68179800	3.86503900	1.88505800
H	4.44267500	3.85966400	2.11096000
H	3.38329100	3.08579400	3.31537100
O	-0.19835100	-0.13220500	2.72207800
O	0.24916000	0.26352300	-2.68996800

Bis- $\eta^3$ -ozone ComplexFig. S23: NCCN Bis- $\eta^3$ -ozone Complex

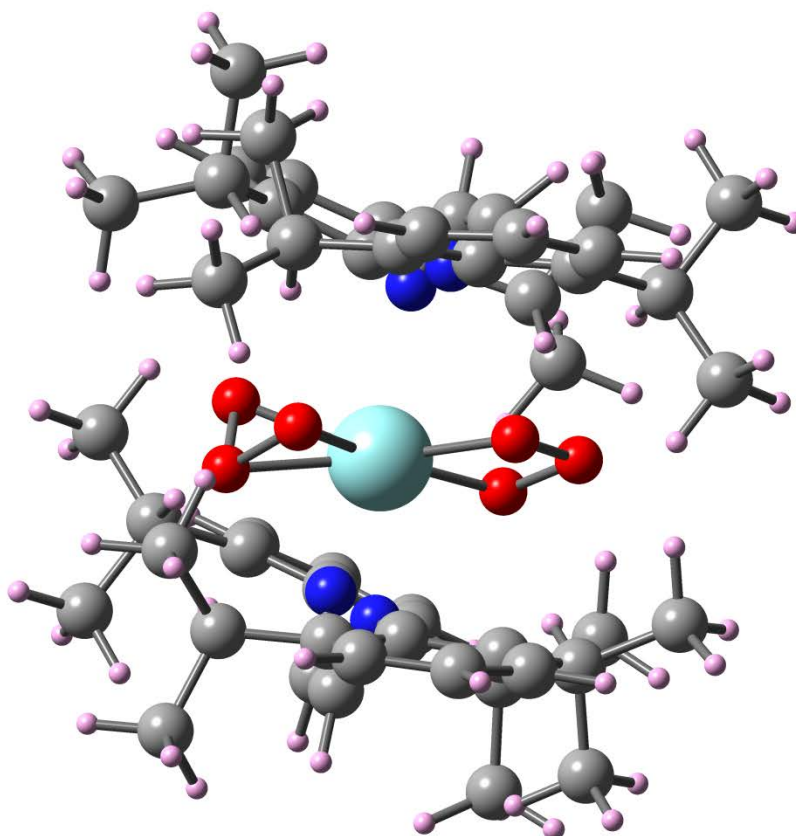
SCF	$E_{ZP}$	H	G
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N	2.04885781	-1.95006928	0.46789565
N	0.63925263	2.32071278	-0.41377451
N	-2.32458496	2.04097152	-0.01090457
C	0.21948550	-3.44153769	0.00493964
C	1.63184165	-3.16682392	0.31875649
C	-0.23265439	3.26750794	-0.22452830
C	-1.63718729	3.12024069	0.17793291
C	-2.03034780	-2.84740930	-0.35420047
C	-2.99235940	-2.83641155	0.69415634
C	-4.31030625	-3.22008407	0.37933615
C	-4.66255601	-3.61172824	-0.92185525
C	-3.69193198	-3.63130760	-1.93137782
C	-2.35408521	-3.25714214	-1.67857503
C	-3.71067235	-1.87165361	2.96534396
C	-2.58965735	-2.54287924	2.14176490

C	-2.12667076	-3.85198030	2.84291121
C	2.75491434	-0.84084435	4.47090155
C	2.70600756	-1.89984882	3.34393861
C	2.87583533	-3.33150236	3.92597615
C	3.44742857	-1.73837033	0.85964528
C	3.74904286	-1.65404030	2.24740136
C	5.09236200	-1.42552203	2.60885600
C	6.09796196	-1.29966172	1.63911089
C	5.77717657	-1.43195665	0.28139280
C	4.45074734	-1.66238257	-0.14405805
C	-1.79349684	-2.43455510	-4.02966257
C	-1.34850798	-3.31870372	-2.83650585
C	-1.11771088	-4.78490685	-3.29396768
C	4.78916802	-0.79737208	-2.53108378
C	4.17701057	-1.89992013	-1.63387855
C	4.69370514	-3.30337249	-2.05623675
C	1.94453221	2.78642108	-0.92312352
C	2.12199811	2.85876869	-2.33373297
C	3.36189576	3.32582253	-2.81427999
C	4.38656803	3.71240115	-1.93651400
C	4.17490919	3.65889086	-0.55245107
C	2.95133907	3.20420853	-0.01213408
C	1.48238715	1.69169215	-4.52673962
C	0.99612044	2.52891433	-3.32008450
C	0.30954602	3.83537003	-3.80830177
C	-3.24463583	1.86157467	4.11353155
C	-3.16301155	2.74476061	2.84291711
C	-3.44283596	4.23084639	3.19682835
C	-3.68079912	1.92621434	0.40777408
C	-4.10661992	2.25342946	1.73427140
C	-5.47125925	2.06756427	2.04340768
C	-6.38301631	1.58604282	1.09308109
C	-5.94111430	1.25303580	-0.19964794
C	-4.59158175	1.40403935	-0.56342904
C	3.90863724	2.61277289	2.29042859
C	2.74014301	3.25795380	1.50558316
C	2.52391712	4.72540373	1.96849260
C	-4.92420046	0.02310926	-2.71038188
C	-4.10045415	1.10716417	-1.98202957
C	-4.07477379	2.41173056	-2.82899034
H	-0.06358766	-4.47996404	-0.17768303
H	2.29868526	-4.02195994	0.44511613
H	0.07742366	4.30679820	-0.37809382
H	-2.08218363	4.03578156	0.58675191
H	-5.06491775	-3.21772625	1.15923323
H	-5.68580163	-3.90470903	-1.14419627
H	-3.97169971	-3.93774601	-2.93584977
H	-1.74673327	-1.84643647	2.12435939
H	1.70745023	-1.83312079	2.90465934
H	-4.55302665	-2.55298976	3.14713126
H	-4.08955396	-0.97521293	2.46242417
H	-3.31740112	-1.57277855	3.94509146

H	-2.94679970	-4.58141365	2.88680943
H	-1.80389113	-3.63725587	3.87008699
H	-1.28610923	-4.32614594	2.31844904
H	3.70618031	-0.86281322	5.01934796
H	1.95142473	-1.03196038	5.19441596
H	2.60555903	0.15837547	4.05178574
H	2.79327272	-4.10219128	3.14648694
H	2.10543409	-3.52833819	4.68336586
H	3.85827057	-3.44894133	4.40216434
H	5.35118883	-1.34962768	3.66111665
H	7.12628967	-1.11591926	1.94090283
H	6.56454908	-1.36074598	-0.46380270
H	-0.38744369	-2.91531050	-2.50760837
H	3.09942188	-1.86289759	-1.80521056
H	-2.74888418	-2.77122625	-4.45373463
H	-1.03852787	-2.47738168	-4.82586193
H	-1.88992157	-1.39311597	-3.70840700
H	-2.04289308	-5.23359448	-3.67832520
H	-0.76181020	-5.42051846	-2.47077036
H	-0.37047697	-4.81668936	-4.09781935
H	4.40324151	0.18724717	-2.24934076
H	4.51487960	-0.97833269	-3.57878264
H	5.88581348	-0.77863913	-2.47267312
H	5.78054864	-3.38388439	-1.92113369
H	4.46960581	-3.48645714	-3.11554545
H	4.22794794	-4.10511859	-1.46557906
H	3.52546396	3.38724277	-3.88660365
H	5.33733878	4.06529835	-2.32976146
H	4.96333883	3.98109228	0.12231350
H	0.24970706	1.92087570	-2.80225814
H	-2.12952726	2.66060781	2.49477989
H	2.17342042	2.25234632	-5.17134912
H	0.62251485	1.39751341	-5.14339128
H	1.98082609	0.78309668	-4.17531459
H	-0.09940845	4.41982472	-2.97260888
H	-0.51809130	3.59752137	-4.49001481
H	1.02032872	4.47805598	-4.34583528
H	-4.24600203	1.87186099	4.56358188
H	-2.53568202	2.22921299	4.86753551
H	-2.97822778	0.82824922	3.87381342
H	-3.35323972	4.88621121	2.31974510
H	-2.73562844	4.58162847	3.96048204
H	-4.45844918	4.35615724	3.59514024
H	-5.82263247	2.30097632	3.04556747
H	-7.43079932	1.46462238	1.35861510
H	-6.65274224	0.86964713	-0.92431868
H	1.84431489	2.68512501	1.75930847
H	-3.06479205	0.75260926	-1.90024285
H	4.84776446	3.16842740	2.16361545
H	4.07308524	1.57821148	1.97056818
H	3.67222858	2.60028133	3.36268113
H	2.34128956	4.75950795	3.05107323

H	1.66466767	5.18830316	1.46423946
H	3.40638503	5.34323762	1.75316679
H	-4.99308389	-0.89461177	-2.11534614
H	-4.43909240	-0.22813865	-3.66243420
H	-5.94203978	0.36639410	-2.94297113
H	-3.44644261	3.18162760	-2.36517043
H	-5.08814932	2.82107733	-2.94392225
H	-3.67222751	2.20582767	-3.82972386
O	1.33950130	0.58780944	1.83068934
O	-0.68327711	-0.12376964	-1.84244591
O	0.62961686	-0.90639988	-2.06684707
O	0.16474546	-0.30815551	2.20250238
O	-1.04393364	0.35547354	1.50400916
Zr	0.40434263	-0.15618505	0.00897817
O	1.74499287	0.06766855	-1.68187396

$\eta^2$ -Ozone  $\eta^3$ -Ozone ComplexFig. S24: NCCN  $\eta^2$ -Ozone- $\eta^3$ -Ozone Complex

SCF	E <sub>ZP</sub>	H	G
-2741.334467	-2740.182259	-2740.110561	-2740.290254

N	2.44673302	-1.54304147	-0.66254095
N	-0.15941061	-2.50340799	-0.75087785
N	-2.70399251	1.75907660	0.51766562
N	0.34773580	2.13375306	0.67075832
C	2.19448248	-2.73458587	-1.11730321
C	0.81252669	-3.21682056	-1.23170112
C	-2.03894402	2.42111421	1.40709130
C	-0.62101167	2.78367781	1.25197733
C	3.83824592	-1.24009719	-0.31764478
C	4.60459709	-0.40507775	-1.17701922
C	5.92849697	-0.11070738	-0.79417112
C	6.47866335	-0.63368626	0.38604518
C	5.71645581	-1.48972631	1.19248834
C	4.38547003	-1.82591614	0.86245488
C	4.55410608	1.45956170	-2.95057503
C	4.06782550	0.05244529	-2.53536026

C	4.44163472	-0.99100849	-3.62632077
C	-2.61997880	-1.64058491	-4.04060131
C	-1.69581575	-2.66074747	-3.33244622
C	-1.43848122	-3.89392969	-4.24254052
C	-1.50944738	-3.05653374	-0.76438807
C	-2.25229329	-3.10430758	-1.97367006
C	-3.56331774	-3.62425437	-1.90419775
C	-4.10287189	-4.08873260	-0.69706130
C	-3.32722373	-4.06779051	0.47357955
C	-2.01485732	-3.55842607	0.46711807
C	3.67245705	-2.44530775	3.25177324
C	3.63651910	-2.82981016	1.75261566
C	4.20601212	-4.26130286	1.54642211
C	-1.85878406	-3.42559615	3.03547457
C	-1.11874911	-3.67366155	1.70433879
C	-0.42599753	-5.06644017	1.72081949
C	-4.10660505	1.54215420	0.58868964
C	-4.79394648	1.14174138	1.77947017
C	-6.19729869	1.01566820	1.71419257
C	-6.90441264	1.25561499	0.52697643
C	-6.20893922	1.58849638	-0.64776245
C	-4.80895165	1.72031971	-0.64750422
C	-4.53269682	-0.63339758	3.58911398
C	-4.08293389	0.76328414	3.08672245
C	-4.31791306	1.82333773	4.19687575
C	1.00392387	3.92766536	-3.12475643
C	0.55217969	3.95929571	-1.64549256
C	-0.16043955	5.30457858	-1.32785933
C	1.59144857	2.90939294	0.49689036
C	1.70660782	3.73706301	-0.65794467
C	2.90755440	4.45821594	-0.82502867
C	3.94335272	4.38205590	0.11750230
C	3.78120670	3.60286088	1.27177847
C	2.60207531	2.85991100	1.49667769
C	-4.71452710	1.60509357	-3.21368187
C	-4.04630360	2.11116354	-1.91510172
C	-3.85534948	3.65250562	-1.98131837
C	3.68762773	1.44139849	3.34265916
C	2.40343279	2.13688257	2.83409420
C	1.88874010	3.13702097	3.90823160
H	2.99614970	-3.43905091	-1.34467631
H	0.64644722	-4.20984752	-1.65214992
H	-2.51469249	2.90073927	2.27175663
H	-0.39454323	3.77530713	1.66155067
H	6.53436349	0.52753679	-1.42985426
H	7.50009921	-0.38815983	0.66677628
H	6.15829441	-1.90797941	2.09270109
H	2.97776456	0.10651537	-2.47320402
H	-0.74094190	-2.14905654	-3.18107807
H	5.63193794	1.48204132	-3.16326640
H	4.33621904	2.19899596	-2.17197948
H	4.03300009	1.77049684	-3.86500740

H	5.53183073	-1.07764244	-3.73153777
H	4.02627424	-0.68842030	-4.59648061
H	4.04847631	-1.98907650	-3.38901201
H	-3.60643990	-2.06727120	-4.26625904
H	-2.16778755	-1.32494535	-4.99035543
H	-2.74823505	-0.75532391	-3.41212153
H	-0.74650683	-4.61008942	-3.77707501
H	-1.00750970	-3.57549500	-5.20105014
H	-2.37270539	-4.43049185	-4.45383352
H	-4.16586715	-3.66031950	-2.80781171
H	-5.11872114	-4.47574888	-0.66921483
H	-3.74394549	-4.45554624	1.39836525
H	2.57873097	-2.83143410	1.47668771
H	-0.34142889	-2.90728249	1.63984997
H	4.69615782	-2.40478501	3.64671721
H	3.12011272	-3.19177383	3.83810730
H	3.19273198	-1.47505659	3.40134760
H	5.25754078	-4.31592962	1.85758250
H	4.15919205	-4.57720481	0.49497980
H	3.63893542	-4.98579633	2.14595741
H	-2.32833070	-2.43883836	3.02913377
H	-1.14065116	-3.45112347	3.86483258
H	-2.62499538	-4.18688863	3.23675891
H	-1.16911974	-5.87150358	1.79847540
H	0.25221253	-5.14309634	2.58119115
H	0.16035694	-5.24513364	0.80856265
H	-6.74339316	0.71302900	2.60403384
H	-7.98810166	1.16358363	0.51190667
H	-6.76055141	1.73737352	-1.57090229
H	-3.00771852	0.68688875	2.89467549
H	-0.16953195	3.14740733	-1.52688765
H	-5.58149598	-0.63382789	3.91361712
H	-3.91945304	-0.93675179	4.44795890
H	-4.41790316	-1.38646500	2.80155683
H	-3.98093106	2.82341090	3.89338440
H	-3.77862061	1.54445516	5.11206676
H	-5.38532394	1.90035398	4.44335038
H	1.69596713	4.74568351	-3.36756325
H	0.12850119	4.03371431	-3.77948318
H	1.48332397	2.97035037	-3.34874615
H	-0.53688926	5.33678949	-0.29631914
H	-1.01345900	5.44917049	-2.00349469
H	0.52503337	6.15317743	-1.45658151
H	3.02637915	5.09257135	-1.69877820
H	4.86206221	4.94358004	-0.03612121
H	4.57368903	3.57686131	2.01364065
H	-3.05057518	1.65765039	-1.84277297
H	1.64786738	1.35783242	2.70545960
H	-5.65525900	2.13089776	-3.42971971
H	-4.92577614	0.52987327	-3.16343609
H	-4.04155930	1.77747399	-4.06371330
H	-3.27664934	3.92561579	-2.87426428



H	-3.31766631	4.02658802	-1.10185119
H	-4.82583143	4.16592121	-2.03236860
H	4.10439497	0.77151191	2.58314309
H	3.45477453	0.84477476	4.23391060
H	4.46240702	2.16614726	3.62792520
H	0.93827199	3.60111070	3.61544030
H	2.61671464	3.94301551	4.07365207
H	1.72911898	2.61741124	4.86227714
O	-1.14114745	0.11495554	-1.60006589
O	-1.02770158	-0.41771917	1.40724323
O	1.28191576	-0.68700607	1.68222571
O	0.17366917	-0.09082043	-2.37809164
O	1.10862878	0.99564801	-1.84374606
Zr	0.40344923	-0.17536138	-0.16074367
O	0.00501497	-0.62794935	2.49001154

### 3. NCCN Triplet Ground States

#### 3.1 Structures with zero oxygen atoms

##### Bare complex

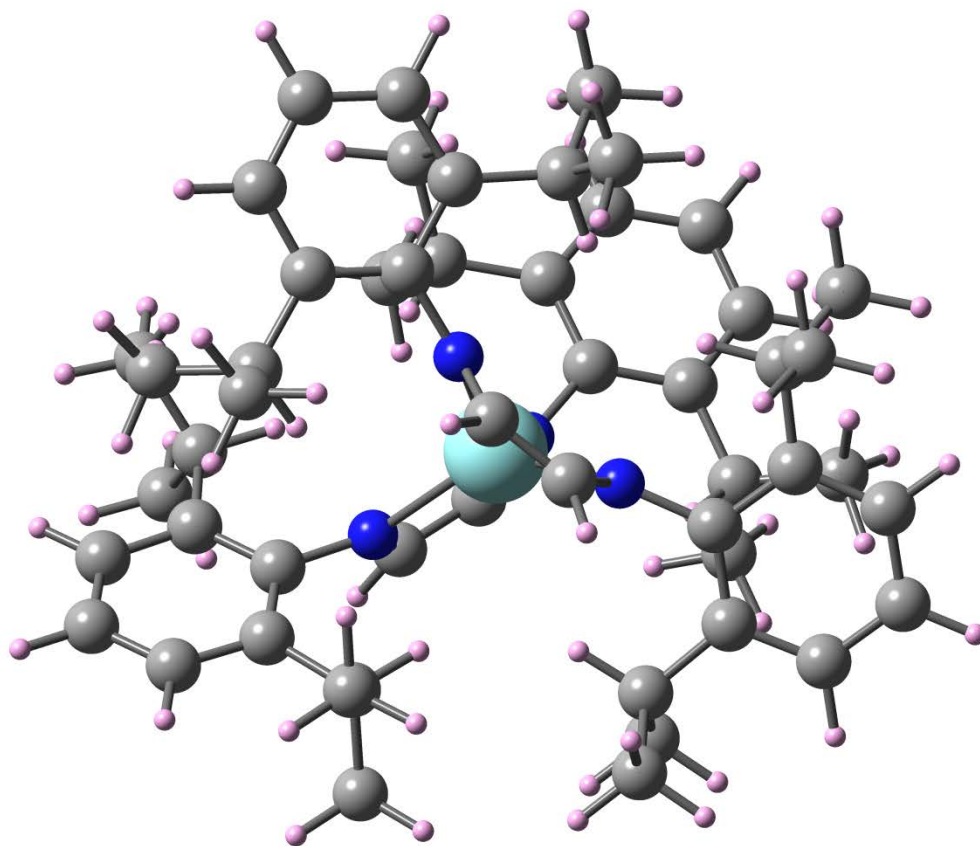


Fig. S25: NCCN Bare Complex

SCF	E <sub>ZP</sub>	H	G
-2290.229159	-2289.096443	-2289.033099	-2289.195301

Zr	-0.01113913	-0.26297665	0.11883555
N	-1.71511356	-1.42133557	-1.04163466
N	0.45643862	-0.06104666	-2.08651191
N	-0.52829488	1.05149645	1.66079716
N	1.71113040	-0.70775533	1.26084187
C	-1.34772097	-1.62299857	-2.33361134
C	-0.24527878	-0.92220104	-2.87461060
C	-0.07258006	0.18313145	2.69629964
C	1.00623682	-0.66244497	2.49806602
C	-3.03778771	-1.86891811	-0.65037268
C	-4.19216277	-1.30611199	-1.28715657
C	-5.46775176	-1.74106019	-0.87004741

C	-5.62472605	-2.69168431	0.14773522
C	-4.48786188	-3.23758144	0.76038954
C	-3.18861599	-2.84959950	0.37420537
C	-4.60436651	-0.85917351	-3.75957909
C	-4.12341150	-0.25739795	-2.41029610
C	-4.93183919	1.02444248	-2.08301020
C	1.30470764	0.91600938	-2.75280115
C	2.68790654	0.65531847	-2.96487497
C	3.46697980	1.64933108	-3.59451816
C	2.90034243	2.86178547	-4.01567982
C	1.53023900	3.09403546	-3.82309666
C	0.70883410	2.13474996	-3.19550903
C	-1.89108699	-5.01601815	0.43611981
C	-1.98977307	-3.57046141	0.99493432
C	-2.02544371	-3.57835592	2.54302599
C	-1.24991822	2.25565283	2.00164713
C	-0.57532710	3.51221464	1.92734676
C	-1.30117232	4.69188925	2.19483026
C	-2.65563123	4.64734253	2.55661352
C	-3.29705713	3.40643699	2.67784269
C	-2.61846686	2.19814085	2.40936847
C	1.35460809	4.72198197	0.70781273
C	0.93429581	3.59948368	1.68612252
C	1.65606475	3.78533558	3.05070256
C	3.03205469	-1.29158695	1.26877288
C	3.23136378	-2.66061204	0.91506125
C	4.54466130	-3.17895127	0.90279764
C	5.64511462	-2.38599322	1.25627236
C	5.43705731	-1.05378969	1.64234382
C	4.14581828	-0.48707299	1.65757734
C	-4.76999436	0.85420512	1.98888044
C	-3.35924407	0.87343883	2.62623644
C	-3.47601325	0.55188255	4.14353578
C	3.22717958	-1.67887731	-3.79160238
C	3.31589296	-0.69123958	-2.59362652
C	4.78369755	-0.58210200	-2.11986543
C	2.16018738	-4.24750593	-0.79353917
C	2.07147384	-3.61633636	0.61943486
C	1.98544592	-4.72312143	1.70472926
C	4.33290320	1.08285584	3.63696394
C	3.97758892	0.95948072	2.13045112
C	4.81605755	1.95381205	1.28667169
C	-1.49962580	2.14110062	-4.43816911
C	-0.79866160	2.39315728	-3.07410995
C	-1.14445496	3.80793214	-2.55088637
H	-1.93220309	-2.27724583	-2.97900127
H	-0.02276027	-1.00840418	-3.93690885
H	-0.63371733	0.11333449	3.62531643
H	1.25425368	-1.39370365	3.26745733
H	-6.35123106	-1.32317157	-1.34652281
H	-6.61891839	-3.00890725	0.45293317
H	-4.60984696	-3.99000573	1.53553022

H	-3.08330206	0.05292167	-2.54242764
H	-4.02954084	-1.75362487	-4.03150247
H	-4.49692540	-0.12379216	-4.56824142
H	-5.66171485	-1.15023754	-3.70695720
H	-5.99677692	0.80992558	-1.92857877
H	-4.85462079	1.73837387	-2.91438396
H	-4.55171249	1.51566306	-1.18030661
H	4.52612125	1.47240566	-3.75748475
H	3.51949745	3.61520556	-4.49707910
H	1.09474042	4.02960055	-4.16454184
H	-1.08120348	-3.03635691	0.69224657
H	-2.78555244	-5.59820787	0.69431861
H	-1.01830517	-5.53404661	0.85417927
H	-1.79857187	-5.01238671	-0.65760069
H	-2.08521498	-2.55792799	2.94108234
H	-1.11471086	-4.04612304	2.93938941
H	-2.88282665	-4.14507449	2.92880855
H	-0.79745033	5.65333512	2.13239039
H	-3.19996429	5.56712146	2.75861325
H	-4.33986848	3.37469891	2.98381072
H	1.26057849	2.64457287	1.26150504
H	1.14104031	5.72082665	1.11130123
H	0.84312283	4.62946509	-0.25687084
H	2.43537341	4.66766354	0.52076014
H	2.74318450	3.84045278	2.90811973
H	1.44016658	2.95102794	3.72913809
H	1.32914515	4.71380092	3.53831181
H	4.70375247	-4.22037951	0.63085161
H	6.64903244	-2.80414550	1.24507501
H	6.28891801	-0.44530093	1.93747860
H	-2.77669236	0.07277031	2.15570267
H	-5.45422710	1.54455471	2.49969894
H	-5.20074657	-0.15270622	2.05560045
H	-4.73411738	1.13471306	0.93140603
H	-2.49713447	0.53950573	4.63831561
H	-3.94995657	-0.42783815	4.29369972
H	-4.09046688	1.30775839	4.65088507
H	2.73436938	-1.11773029	-1.76697565
H	2.18916905	-1.86028070	-4.09455039
H	3.67833335	-2.64430030	-3.52606940
H	3.76730838	-1.27841742	-4.66011957
H	5.46027269	-0.33070214	-2.94782401
H	5.11140920	-1.54160513	-1.70321016
H	4.89942102	0.17499148	-1.33717964
H	1.13921020	-3.04118781	0.66730677
H	2.17473418	-3.47728512	-1.57364036
H	1.29650368	-4.90141621	-0.97541632
H	3.06791843	-4.85506712	-0.90502823
H	2.89254025	-5.34133190	1.71397091
H	1.13078602	-5.38530330	1.51394499
H	1.86922726	-4.28838953	2.70572943
H	2.92550541	1.23018681	2.01162677

H	3.70697741	0.41628177	4.24366591
H	4.17528308	2.11099480	3.98741749
H	5.38312388	0.81946544	3.82088699
H	5.89070546	1.73741419	1.35185453
H	4.66280413	2.98066904	1.64522005
H	4.52642250	1.91891481	0.22903364
H	-1.20863698	1.67602622	-2.35283560
H	-1.12714660	2.83825213	-5.20068243
H	-2.58457191	2.28687247	-4.34540288
H	-1.31910188	1.12147075	-4.80046338
H	-0.67884656	3.99641102	-1.57787499
H	-2.23113903	3.90685713	-2.42721186
H	-0.81921511	4.59394321	-3.24453148

### 3.2 Structures with one oxygen atom

#### Oxo Complex

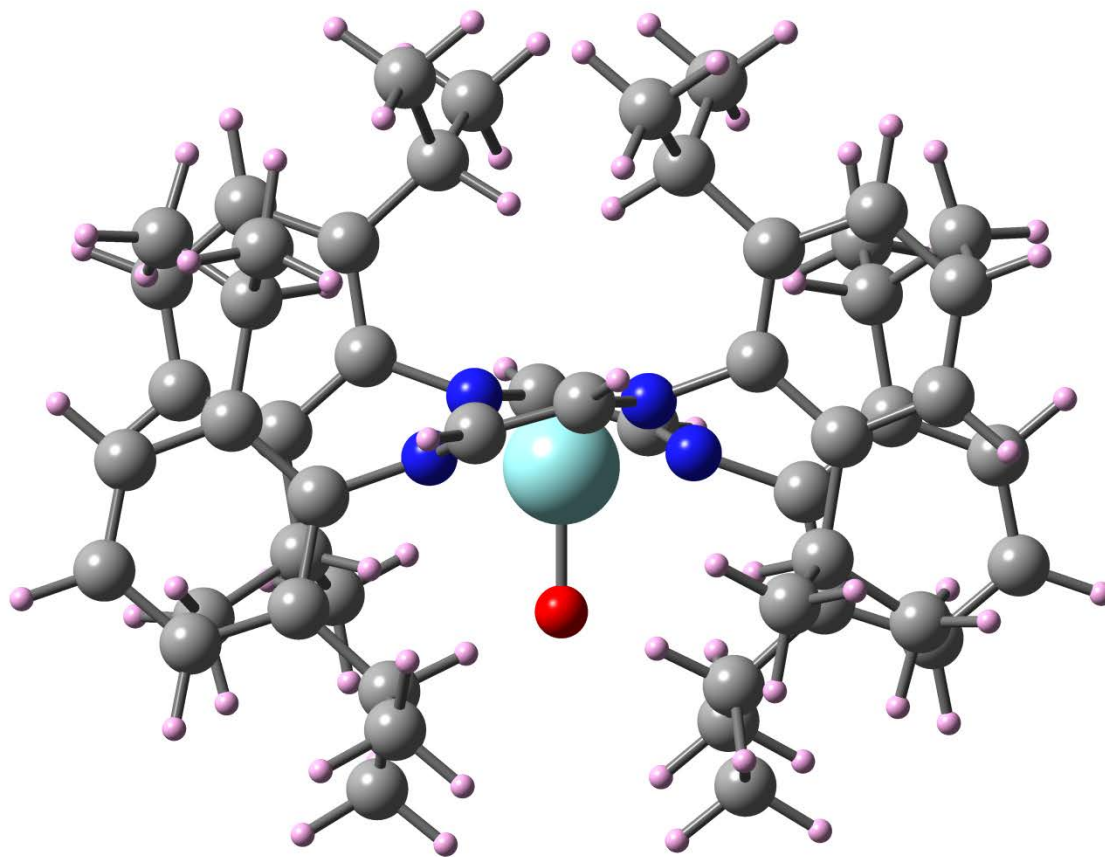


Fig. S26: NCCN Oxo Complex

SCF	E <sub>ZP</sub>	H	G
-2365.536429	-2364.399072	-2364.333753	-2364.500378

O	-0.00136808	-2.23437050	-0.03359683
N	-1.07934441	0.43860784	-1.84128857
N	1.63753911	-0.26692107	-1.69298835
N	1.07940790	0.37589277	1.85584098
N	-1.63706059	-0.32270330	1.68786923
C	-0.27900949	0.45785572	-2.94820624
C	1.07199633	0.07836718	-2.87710391
C	0.28193500	0.35494609	2.96481288
C	-1.06935173	-0.02120278	2.88282942
C	-2.42709647	0.93213429	-2.09055076
C	-3.47332564	0.00183491	-2.35173446
C	-4.73351458	0.50913662	-2.73319571
C	-4.95354513	1.88929046	-2.86747913
C	-3.91583368	2.79170158	-2.59269228

C	-2.64168315	2.33668163	-2.19353993
C	-4.43523578	-2.31625789	-1.78520990
C	-3.22684703	-1.51094421	-2.31749417
C	-2.82372786	-2.02638225	-3.72773337
C	2.27953668	-4.38773024	-1.31676121
C	2.13469099	-3.15273298	-2.23979441
C	2.06772139	-3.58500824	-3.73031789
C	3.01437877	-0.74749356	-1.78956956
C	3.25836805	-2.13068419	-2.03268840
C	4.59758707	-2.56009482	-2.16165940
C	5.66601373	-1.65856608	-2.07097535
C	5.40743492	-0.29505276	-1.86354810
C	4.08916657	0.18885745	-1.72881097
C	-1.93936472	4.38255776	-0.82604163
C	-1.53151524	3.35908109	-1.91701541
C	-1.10588340	4.09728610	-3.21452076
C	4.94315649	2.42899695	-0.79612089
C	3.84557326	1.69814195	-1.60487337
C	3.72619830	2.35910139	-3.00819333
C	2.42570069	0.86653070	2.11819601
C	2.63425646	2.26811919	2.26400336
C	3.90714324	2.71655889	2.67446815
C	4.94928838	1.81076044	2.91977031
C	4.73500110	0.43433525	2.74369802
C	3.47642310	-0.06668816	2.34888750
C	1.91947477	4.34548894	0.95357187
C	1.51925300	3.29325994	2.01985876
C	1.09676997	3.99524666	3.33821271
C	-2.28397438	-4.43120901	1.19324072
C	-2.13444523	-3.22239552	2.14959591
C	-2.06176210	-3.69563762	3.62724326
C	-3.01391232	-0.80565654	1.76900728
C	-3.25840343	-2.19479687	1.97424478
C	-4.59782828	-2.62697512	2.09135171
C	-5.66574184	-1.72272971	2.02462578
C	-5.40661919	-0.35433625	1.85246599
C	-4.08818924	0.13232709	1.73075437
C	4.44877501	-2.36306208	1.71447815
C	3.23622367	-1.57876257	2.26799588
C	2.83232694	-2.13852443	3.66100188
C	-4.94749449	2.39695348	0.86490080
C	-3.84217293	1.64372882	1.64165319
C	-3.70334756	2.27027162	3.05889389
H	-5.54545213	-0.18176754	-2.94091277
H	-5.92799325	2.25722750	-3.18003915
H	-4.09619464	3.85979239	-2.69010105
H	-2.37993951	-1.70828210	-1.64893603
H	1.18186955	-2.69064733	-1.97713546
H	-5.28262073	-2.29008968	-2.48378634
H	-4.77574404	-1.94055954	-0.81463886
H	-4.15016569	-3.36871823	-1.65924842
H	-3.62962458	-1.84431701	-4.45190495

H	-2.62997179	-3.10663547	-3.69478676
H	-1.91704329	-1.53123010	-4.09428885
H	3.20413228	-4.94830118	-1.51287908
H	1.43298620	-5.06864630	-1.47379851
H	2.26687969	-4.08356982	-0.26458310
H	1.91619844	-2.72119172	-4.39139711
H	1.23335435	-4.28244645	-3.88496593
H	2.99232882	-4.08832090	-4.04465583
H	4.79990604	-3.61233629	-2.34494699
H	6.69005791	-2.01042185	-2.17291010
H	6.23913285	0.40102653	-1.81134061
H	-0.65387042	2.81807283	-1.54496144
H	2.88901897	1.84078532	-1.08537003
H	-2.80028832	4.98708351	-1.13983328
H	-1.10711543	5.07000072	-0.62250141
H	-2.20557178	3.88030769	0.11192222
H	-1.94343005	4.66801953	-3.63697756
H	-0.76190166	3.39174151	-3.98068966
H	-0.28852552	4.80068173	-3.00617682
H	5.12861955	1.94201160	0.16511424
H	4.63577130	3.46391630	-0.59900051
H	5.88949994	2.47327408	-1.35182953
H	4.64664664	2.19932528	-3.58571325
H	3.57283566	3.44245765	-2.90690876
H	2.88941979	1.95187102	-3.58509928
H	4.08287295	3.78201597	2.80399903
H	5.92275524	2.17322973	3.24163790
H	5.55034913	-0.25894436	2.92885046
H	0.64165716	2.75934061	1.63759185
H	-1.18284750	-2.75311833	1.89523717
H	2.77933828	4.94502877	1.27959478
H	1.08407567	5.03451165	0.76929266
H	2.18479990	3.86685149	0.00303921
H	0.76217359	3.26776591	4.08792136
H	0.27339624	4.69811789	3.15317016
H	1.93287335	4.56069767	3.77053362
H	-3.20794328	-4.99654755	1.37813032
H	-1.43704903	-5.11670012	1.32689784
H	-2.27634626	-4.09773255	0.14988524
H	-1.90837570	-2.85029299	4.31135257
H	-1.22650020	-4.39651920	3.75965209
H	-2.98504633	-4.20796392	3.93079005
H	-4.80070878	-3.68370913	2.24576827
H	-6.68998838	-2.07661382	2.11711750
H	-6.23810800	0.34296057	1.81737949
H	2.39166748	-1.75874459	1.59156172
H	-2.89131235	1.79528393	1.11384949
H	5.29482288	-2.35401850	2.41508194
H	4.78912479	-1.95788327	0.75580912
H	4.16821610	-3.41251693	1.55718079
H	2.64358762	-3.21817060	3.59494659
H	1.92255995	-1.65906461	4.04050894



H	3.63597770	-1.97490850	4.39207746
H	-5.14551994	1.93454138	-0.10597101
H	-4.64023865	3.43584337	0.69022180
H	-5.88696386	2.42913708	1.43302758
H	-2.85978785	1.84827749	3.61478676
H	-4.61662315	2.09827259	3.64425529
H	-3.54927319	3.35554006	2.98171490
H	-0.69468454	0.77233245	-3.90361986
H	1.65721764	0.03316483	-3.79366767
H	0.69954482	0.63554413	3.92987564
H	-1.65332526	-0.09844308	3.79807746
Zr	-0.00149591	-0.43114047	-0.00582820

### 3.3 Structures with two oxygen atoms

#### Dioxo Complex

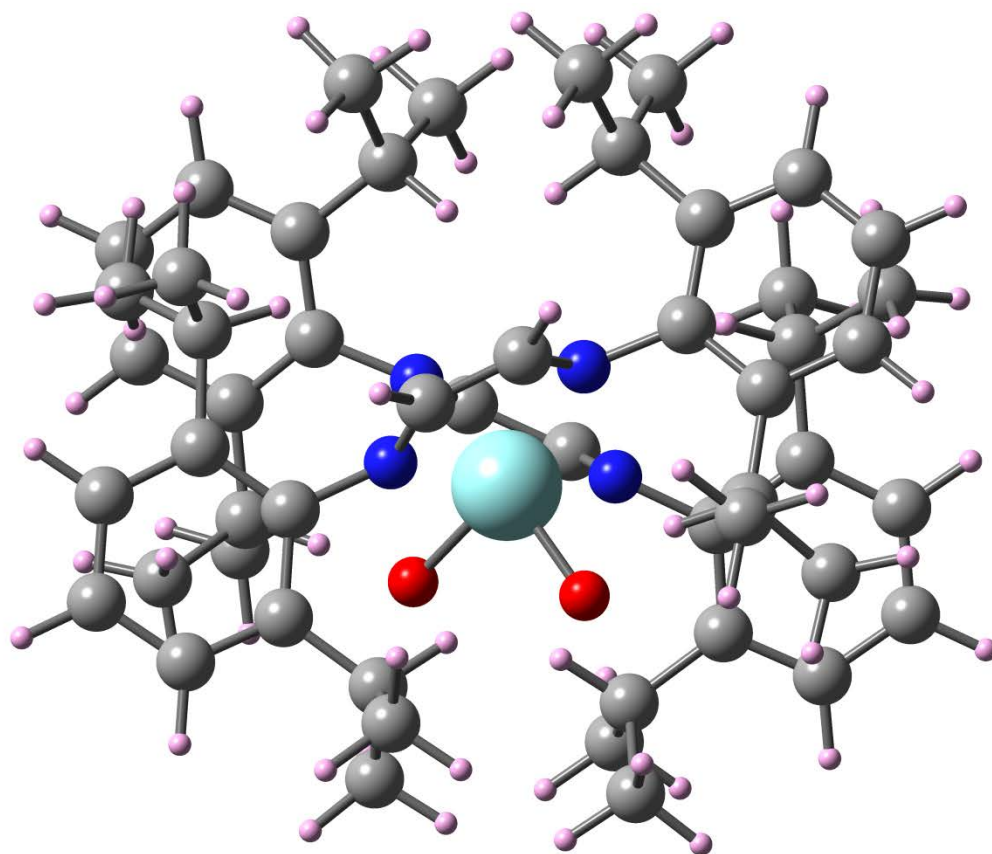


Fig. S27: NCCN Dioxo Complex

SCF	$E_{ZP}$	H	G
-2440.697568	-2439.559690	-2439.491870	-2439.664886

Zr	0.06761693	-0.67608137	0.20113344
N	1.48423033	-0.56264104	-1.85190438
N	-1.10451560	0.69033303	-1.96954563
N	-1.44542228	-0.37867515	1.92481189
N	1.07311158	0.86976669	1.77298505
C	0.90829005	-0.23408806	-2.96902810
C	-0.42891174	0.37496588	-3.03275259
C	-0.98747230	0.39761134	2.93939741
C	0.27646652	1.01618580	2.86546593
C	2.81018174	-1.18901357	-1.96171263
C	3.95809790	-0.35140727	-1.95119061
C	5.21936258	-0.97044939	-2.07038173
C	5.33465622	-2.36272513	-2.20295649
C	4.18293740	-3.16076290	-2.22583450
C	2.89354727	-2.59864809	-2.10668594

C	5.02672616	1.83459304	-1.12247163
C	3.84757773	1.17704581	-1.87525177
C	3.73537501	1.79841922	-3.29661319
C	-1.93384207	4.56071660	-0.46128655
C	-1.48248244	3.53502809	-1.52863486
C	-0.83534875	4.25377472	-2.74519723
C	-2.43878644	1.23867366	-2.19852775
C	-2.62684841	2.63285086	-1.99630434
C	-3.87680032	3.18959412	-2.32971034
C	-4.91701687	2.38863926	-2.82489600
C	-4.72157017	1.00915934	-2.97756474
C	-3.48567183	0.39687329	-2.67353799
C	1.74969128	-4.69489519	-1.19863795
C	1.66533634	-3.51184281	-2.19441629
C	1.47200269	-4.01985119	-3.64997479
C	-4.42064055	-1.88737644	-2.03751861
C	-3.34593482	-1.12056448	-2.85144240
C	-3.40981868	-1.51857651	-4.35038540
C	-2.75283834	-0.99267995	2.10858983
C	-2.84185911	-2.40147781	2.31175270
C	-4.11799549	-2.97919303	2.47742251
C	-5.28261281	-2.19927923	2.46721578
C	-5.18008345	-0.81153778	2.29924672
C	-3.92947754	-0.18228007	2.11842105
C	-1.65456532	-4.50414528	1.46883841
C	-1.60953108	-3.30057185	2.44270711
C	-1.44226120	-3.77753438	3.91125870
C	2.03431077	4.56033627	-0.03888599
C	1.56053898	3.74174622	1.18884905
C	1.06823750	4.69172545	2.31484706
C	2.41418713	1.41838482	1.95126554
C	2.65375402	2.80201022	1.70823997
C	3.92498866	3.33579312	2.00888028
C	4.94686325	2.52978441	2.52967081
C	4.70505148	1.16611291	2.74940430
C	3.44743448	0.58502656	2.47620866
C	-4.91784402	1.85259430	0.91880771
C	-3.90080927	1.34549723	1.97065116
C	-4.17093593	2.04417097	3.33257571
C	4.29518550	-1.81316290	2.19339084
C	3.22238992	-0.89021176	2.82323826
C	3.16522297	-1.08593737	4.36288428
H	1.39550276	-0.42866586	-3.92739015
H	-0.83355627	0.53893731	-4.03566485
H	-1.58047320	0.51805650	3.84401249
H	0.63391888	1.57953277	3.72730954
H	6.11710342	-0.36051414	-2.05630956
H	6.31690677	-2.82081802	-2.29030300
H	4.28029014	-4.23738382	-2.33435320
H	2.92978848	1.42431189	-1.32304335
H	-0.71330276	2.89913482	-1.07086455
H	5.96243316	1.75539672	-1.69159372

H	5.17682583	1.38216375	-0.13779636
H	4.82481524	2.90161418	-0.97186266
H	4.62599436	1.55593771	-3.89116464
H	3.65844412	2.89205858	-3.23019716
H	2.86021007	1.43090944	-3.84654493
H	-2.64887381	5.28683490	-0.86855456
H	-1.07057229	5.12637648	-0.09143919
H	-2.40641812	4.06152274	0.39342310
H	-0.46449054	3.53304059	-3.48605899
H	0.00827306	4.87777055	-2.42511670
H	-1.56754205	4.89966234	-3.24725131
H	-4.03732579	4.25669678	-2.20452553
H	-5.87503710	2.83494747	-3.07958948
H	-5.53867035	0.39111081	-3.33950334
H	0.77293693	-2.94536666	-1.91593197
H	-2.38324827	-1.45057712	-2.44807556
H	2.60080989	-5.35568980	-1.41274165
H	0.83397070	-5.29744993	-1.26207370
H	1.83547755	-4.30989784	-0.17787111
H	2.32789985	-4.62490575	-3.97824138
H	1.36179336	-3.18879163	-4.36152145
H	0.57098220	-4.64367245	-3.71429400
H	-4.36448616	-1.63176287	-0.97384168
H	-4.24877212	-2.96719276	-2.12844975
H	-5.43775799	-1.67534389	-2.39455256
H	-4.37385819	-1.24041869	-4.79716823
H	-3.29013522	-2.60452315	-4.45647504
H	-2.62030174	-1.03051822	-4.93900429
H	-4.19513737	-4.05272560	2.63098385
H	-6.25668042	-2.66455287	2.60044978
H	-6.08369974	-0.20710034	2.30703258
H	-0.71913978	-2.72442063	2.18765413
H	0.70682332	3.12803481	0.87812728
H	-2.49282748	-5.17990651	1.68940219
H	-0.72478524	-5.08241922	1.54991171
H	-1.74770001	-4.14925050	0.43664304
H	-1.36161441	-2.92564005	4.59995671
H	-0.53100449	-4.38289581	4.00944285
H	-2.29467101	-4.39111350	4.23401289
H	2.87710187	5.21585446	0.21420659
H	1.22423509	5.20122887	-0.40976477
H	2.35451046	3.90265449	-0.85736411
H	0.68003508	4.12439912	3.16943525
H	0.26658910	5.34833439	1.95038926
H	1.88747123	5.32617732	2.67808063
H	4.11297545	4.39428703	1.84410077
H	5.91812801	2.95941585	2.76396886
H	5.49583996	0.54236130	3.15855667
H	-2.90116094	1.64271181	1.63253950
H	2.26288763	-1.20912142	2.41142387
H	-5.95258401	1.68208942	1.24331384
H	-4.77907251	1.35314903	-0.04497153

H	-4.79726999	2.93293639	0.76375021
H	-4.13062051	3.13667039	3.22084668
H	-3.43932776	1.75232976	4.09546527
H	-5.16711516	1.77899300	3.71074130
H	4.32046742	-1.69824470	1.10355942
H	4.05300819	-2.86119435	2.41088329
H	5.30082073	-1.61068901	2.58801393
H	2.36665726	-0.48157835	4.81284673
H	4.11360399	-0.80032566	4.83917439
H	2.96851360	-2.13966819	4.60154838
O	-1.15287758	-1.93491896	-0.75353710
O	1.08162191	-2.11459865	0.74552719

## Peroxo Complex

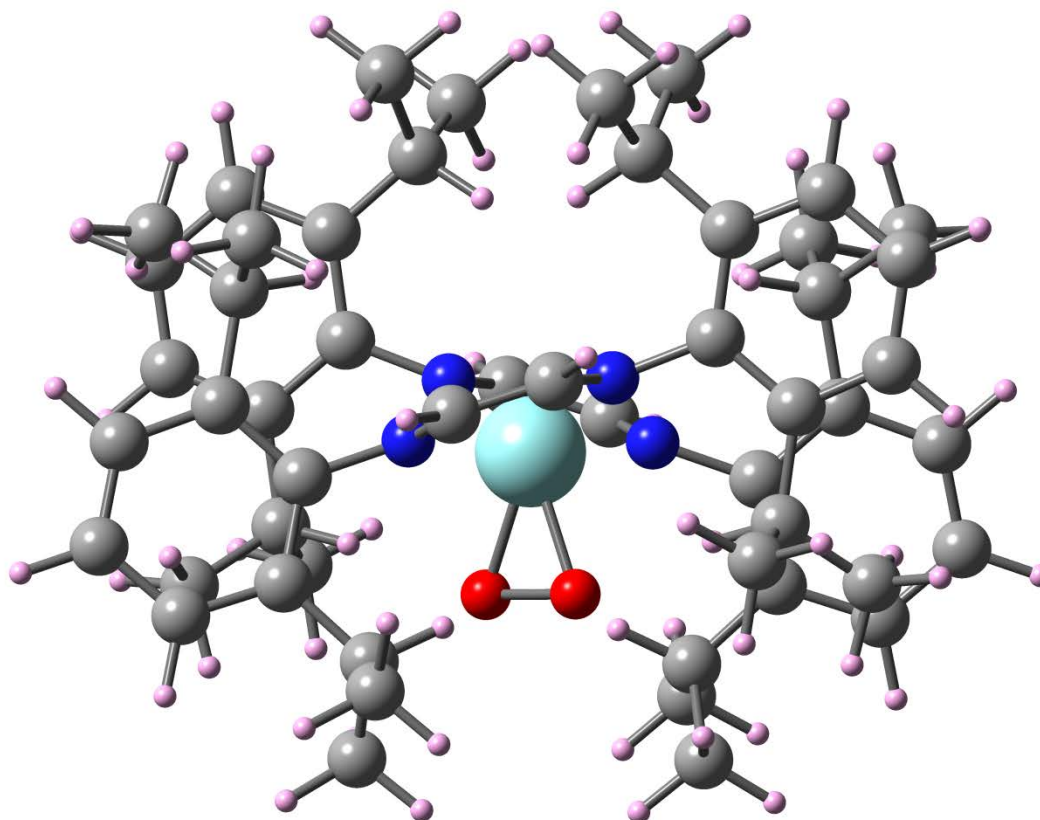


Fig. S28: NCCN Peroxo Complex

SCF	E <sub>ZP</sub>	H	G
-2440.687177	-2439.546756	-2439.480415	-2439.648548

Zr	0.00013805	-0.45950495	0.00345695
N	-1.59456007	-0.31456293	1.68943008
N	1.06972114	0.50341211	1.80616309
N	1.59437917	-0.34107496	-1.68504718
N	-1.06914603	0.47402413	-1.81451718
C	-1.03326403	0.02919009	2.87528518
C	0.30408208	0.45939712	2.93241818
C	1.03211113	-0.02084793	-2.87694027
C	-0.30544197	0.40788212	-2.94096327
C	-2.97607618	-0.79143095	1.78745009
C	-4.04641226	0.14988513	1.73041909
C	-5.36606638	-0.33041590	1.86593009
C	-5.62857037	-1.69308300	2.07220911
C	-4.56307732	-2.59744408	2.16504812
C	-3.22231621	-2.17278206	2.03594611
C	-4.91947430	2.40110531	0.84152902

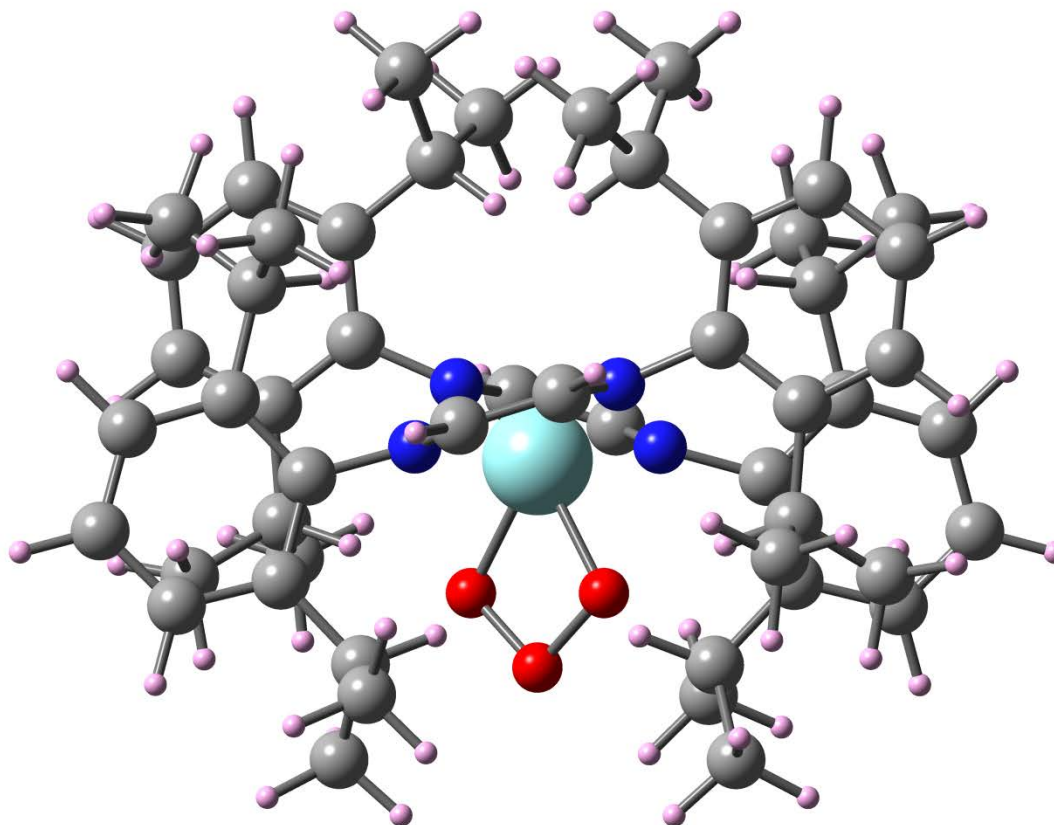
C	-3.80050522	1.65971624	1.61027208
C	-3.64046421	2.31167829	3.01411618
C	1.89096923	4.46821741	0.72368601
C	1.47256319	3.43029333	1.79617609
C	0.98063716	4.15042339	3.08059519
C	2.41163125	1.02772214	2.05190411
C	2.59876727	2.43803225	2.11239012
C	3.85633437	2.92935127	2.52105415
C	4.90358744	2.05612120	2.84863617
C	4.70928142	0.66911509	2.75938617
C	3.46657932	0.12538106	2.36940313
C	-2.26607216	-4.46082324	1.38091306
C	-2.10336914	-3.19624614	2.25972313
C	-2.02673613	-3.58184917	3.76358124
C	4.45561338	-2.17713112	1.79910709
C	3.25786829	-1.39335005	2.38671914
C	2.95585026	-1.88326808	3.83079624
C	2.97572827	-0.81983400	-1.77405718
C	3.22204928	-2.20427511	-2.00423420
C	4.56308538	-2.63101216	-2.12401521
C	5.62859746	-1.72588510	-2.04001621
C	5.36601844	-0.36048699	-1.85204719
C	4.04624536	0.12183806	-1.72625818
C	2.26030619	-4.47918828	-1.31431315
C	2.10367719	-3.23078618	-2.21702822
C	2.03657218	-3.64364721	-3.71412933
C	-1.89657705	4.46534244	-0.80151711
C	-1.47273103	3.39991736	-1.84451019
C	-0.96782599	4.08641140	-3.14236729
C	-2.41124713	0.99416718	-2.06774620
C	-2.59914213	2.40353629	-2.14693221
C	-3.85643822	2.88858034	-2.56364424
C	-4.90313830	2.01049228	-2.88010527
C	-4.70829631	0.62498317	-2.77196826
C	-3.46544021	0.08721812	-2.37407523
C	4.92207945	2.38717822	-0.87564011
C	3.79932335	1.63294018	-1.62602617
C	3.62900135	2.26511823	-3.03773028
C	-4.44977631	-2.20631305	-1.76247818
C	-3.25665921	-1.43162000	-2.37125923
C	-2.96678919	-1.94217504	-3.81067134
H	-1.61035707	-0.04562291	3.79438224
H	0.72857211	0.76539714	3.88644025
H	1.60858317	-0.11321094	-3.79485434
H	-0.73151900	0.69452414	-3.90025035
H	-6.19591040	0.36747616	1.81432309
H	-6.65376746	-2.04196802	2.17250212
H	-4.76854334	-3.64848116	2.35011213
H	-2.85953715	1.80403025	1.06303103
H	0.62356212	2.86579130	1.39280406
H	-5.84785036	2.44358732	1.42685206
H	-5.13648533	1.92395527	-0.11794006

H	-4.61501827	3.43670138	0.64466200
H	-4.54288128	2.14492129	3.61738323
H	-3.49422819	3.39628237	2.91533218
H	-2.78558514	1.90518625	3.56403723
H	2.72482530	5.09363545	1.06764804
H	1.04954317	5.13539147	0.49498299
H	2.20086526	3.97654937	-0.20634506
H	0.62433913	3.43213134	3.82912325
H	0.15573010	4.83626645	2.84524017
H	1.78891823	4.73667043	3.53729422
H	4.01539339	4.00299336	2.58779115
H	5.86433053	2.45232222	3.16891520
H	5.52634946	-0.00102096	3.01124418
H	-1.14647106	-2.75172112	1.98251211
H	2.38233322	-1.63337906	1.77490609
H	-3.18751824	-5.01367827	1.61093208
H	-1.41859410	-5.13786330	1.55013707
H	-2.26699716	-4.18875822	0.32063198
H	-2.95200721	-4.06980920	4.09944127
H	-1.86464611	-2.70011611	4.39821329
H	-1.19497408	-4.27902923	3.93168825
H	4.71713640	-1.82121110	0.79711001
H	4.19641335	-3.24081820	1.72229308
H	5.34722646	-2.10226412	2.43657214
H	3.79768033	-1.66498008	4.50236730
H	2.78751124	-2.96804517	3.83273424
H	2.05957220	-1.40265904	4.24145028
H	4.76858338	-3.68446124	-2.29486222
H	6.65395056	-2.07633813	-2.13298021
H	6.19592955	0.33774206	-1.80730919
H	1.14514811	-2.78023014	-1.95512220
H	-0.62896697	2.84276831	-1.42028116
H	3.18365025	-5.03530033	-1.52835116
H	1.41431812	-5.15971132	-1.47705716
H	2.25377619	-4.18799725	-0.25920707
H	1.87909417	-2.77336514	-4.36555138
H	1.20543911	-4.34330526	-3.87482734
H	2.96350425	-4.13814526	-4.03548635
H	-2.72765712	5.08251350	-1.16623713
H	-1.05621999	5.13792449	-0.58487709
H	-2.21247609	3.99777541	0.13889096
H	-0.60874997	3.34836934	-3.86999034
H	-0.14179192	4.77450545	-2.91791627
H	-1.77051104	4.66408546	-3.61937432
H	-4.01601722	3.96106642	-2.64535425
H	-5.86379537	2.40193832	-3.20642329
H	-5.52495540	-0.04894687	-3.01503728
H	2.86174229	1.78344420	-1.07454813
H	-2.37610714	-1.66301702	-1.76338118
H	5.84635750	2.42285322	-1.46791116
H	5.14642246	1.92439019	0.08919596
H	4.61687543	3.42488731	-0.69162610



H	3.48265834	3.35090731	-2.95286627
H	2.77056428	1.85081820	-3.57602832
H	4.52743441	2.09073720	-3.64479032
H	-4.70107732	-1.83740602	-0.76256911
H	-4.19135130	-3.26937213	-1.67478718
H	-5.34737838	-2.13795303	-2.39218523
H	-2.07399512	-1.46764301	-4.23587637
H	-3.81420326	-1.73339602	-4.47820139
H	-2.79850719	-3.02691912	-3.79865334
O	-0.58216801	-2.32525009	-0.50532609
O	0.58518308	-2.31710310	0.53798599

## 3.4 Structures with three oxygen atoms

 $\eta^2$ -ozone ComplexFig. S29: NCCN  $\eta^2$ -ozone Complex

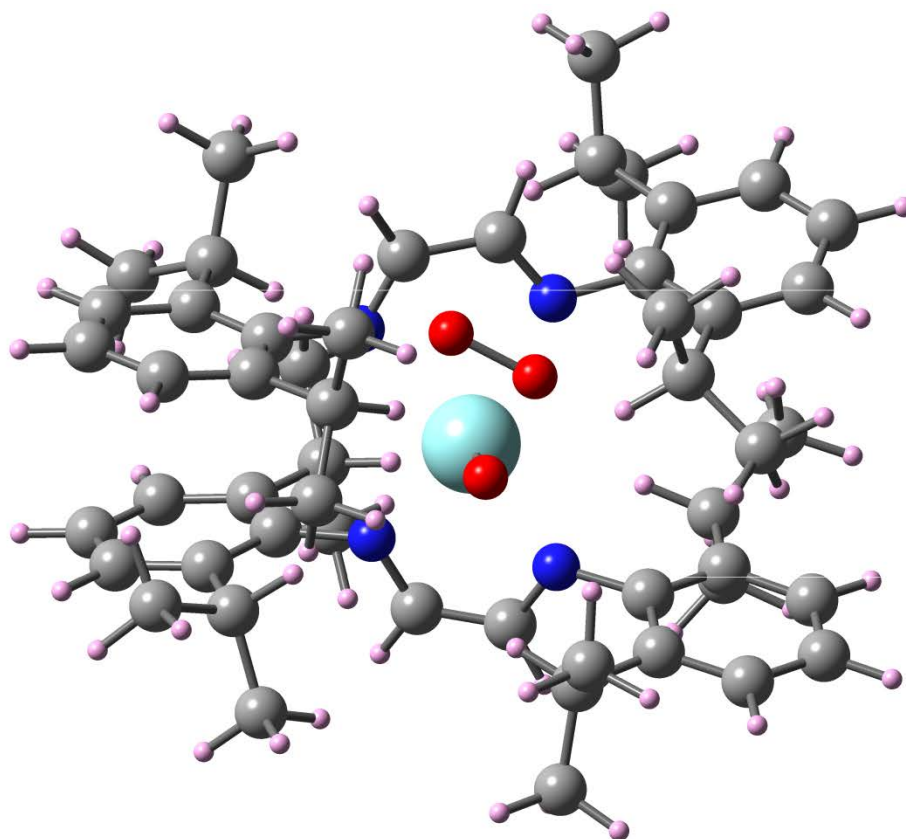
SCF	E <sub>ZP</sub>	H	G
-2515.829639	-2514.685509	-2514.618323	-2514.787493

O	0.87026413	-2.27262098	0.75443148
O	-0.87171535	-2.27291955	-0.74974142
N	1.60736552	-0.36371700	-1.66917471
N	-1.05971864	0.45557016	-1.78677822
N	-1.60718734	-0.35884163	1.67041796
N	1.05967941	0.46080621	1.78531910
C	1.02619716	-0.08787138	-2.86164894
C	-0.31479011	0.33130199	-2.92211927
C	-1.02633183	-0.07847347	2.86200168
C	0.31461816	0.34088759	2.92106027
C	3.01939637	-0.74852432	-1.76217225
C	4.02153683	0.26568815	-1.71204675
C	5.37100038	-0.12248878	-1.84885514
C	5.72826165	-1.46347597	-2.05278265

C	4.72852387	-2.43976341	-2.13942098
C	3.36223289	-2.10923075	-2.00480606
C	4.76618100	2.58110065	-0.87430421
C	3.67537359	1.75637550	-1.59740995
C	3.42680254	2.37944877	-3.00164771
C	-1.74885263	4.55831194	-0.84182638
C	-1.33537954	3.39474191	-1.77715688
C	-0.70616456	3.95759950	-3.08171167
C	-2.38225112	1.03558459	-2.05209783
C	-2.50466174	2.45530845	-2.09924329
C	-3.72826165	3.00972868	-2.52849210
C	-4.80910564	2.19336118	-2.89060641
C	-4.67699185	0.79974907	-2.82503079
C	-3.46877576	0.19096083	-2.41975961
C	2.60082817	-4.45626535	-1.32531395
C	2.31988881	-3.21361646	-2.20524601
C	2.24073819	-3.61505591	-3.70457539
C	-4.55442263	-2.05478512	-1.82391637
C	-3.35084831	-1.33506446	-2.48008171
C	-3.18051885	-1.80944201	-3.95051315
C	-3.01902001	-0.74414217	1.76461273
C	-3.36109777	-2.10443258	2.01086395
C	-4.72714699	-2.43540454	2.14628092
C	-5.72745528	-1.45986600	2.05720673
C	-5.37096170	-0.11923453	1.84992528
C	-4.02168178	0.26936360	1.71194336
C	-2.59878690	-4.45395808	1.34045475
C	-2.31789711	-3.20735067	2.21468707
C	-2.23726747	-3.60258527	3.71566432
C	1.74776343	4.56149784	0.83224430
C	1.33496656	3.40040214	1.77096796
C	0.70738498	3.96686318	3.07477235
C	2.38225606	1.04165398	2.04880933
C	2.50436356	2.46144635	2.09396144
C	3.72820475	3.01666792	2.52161264
C	4.80940767	2.20100067	2.88413101
C	4.67757293	0.80723513	2.82037945
C	3.46927930	0.19771343	2.41661535
C	-4.76753803	2.58187526	0.86728493
C	-3.67654564	1.75998914	1.59336784
C	-3.42922008	2.38714936	2.99601523
C	4.55676337	-2.04933285	1.82809033
C	3.35102997	-1.32815394	2.47867325
C	3.17534042	-1.80061388	3.94905424
H	6.15073242	0.63079890	-1.80040330
H	6.77506754	-1.73980678	-2.15505909
H	5.00595375	-3.47446667	-2.32116786
H	2.74536571	1.84356512	-1.01996508
H	-0.55970719	2.81495269	-1.26210104
H	5.66742230	2.68276571	-1.49357379
H	5.04983487	2.12973805	0.08053129
H	4.39783158	3.59466137	-0.67359587

H	4.31971277	2.26767806	-3.63119380
H	3.20957347	3.45263917	-2.90865592
H	2.58509542	1.90993934	-3.52078962
H	-2.51630778	5.19453954	-1.29945962
H	-0.88285445	5.19610142	-0.62843795
H	-2.14391727	4.18442793	0.11030471
H	-0.35955988	3.15159737	-3.73944526
H	0.15327456	4.60088056	-2.84956835
H	-1.43874952	4.55550437	-3.63997883
H	-3.83559223	4.08961879	-2.58606142
H	-5.74318630	2.63949548	-3.22369526
H	-5.51474053	0.16996111	-3.11118926
H	1.33858110	-2.83657704	-1.91522044
H	-2.45750319	-1.64841630	-1.93549453
H	3.54234411	-4.95097478	-1.60067303
H	1.78977578	-5.18530374	-1.44399187
H	2.64607305	-4.17628877	-0.26769901
H	3.19556580	-4.02832356	-4.05716379
H	1.99311813	-2.75481934	-4.34077800
H	1.46516609	-4.37868741	-3.84932890
H	-4.71176657	-1.71492034	-0.79492138
H	-4.36530768	-3.13577570	-1.79765313
H	-5.48601467	-1.89691789	-2.38467747
H	-4.05169823	-1.53316584	-4.56060315
H	-3.07336933	-2.90158170	-3.98181557
H	-2.28842472	-1.37161070	-4.41632759
H	-5.00403718	-3.46980121	2.33056718
H	-6.77409068	-1.73657172	2.16021861
H	-6.15109829	0.63351211	1.79968293
H	-1.33710961	-2.83084771	1.92226478
H	0.55851321	2.81964552	1.25822158
H	-3.53940431	-4.94846796	1.61925328
H	-1.78685679	-5.18167342	1.46119867
H	-2.64583130	-4.17873601	0.28165309
H	-1.98983681	-2.73961343	4.34820509
H	-1.46103893	-4.36506138	3.86298061
H	-3.19161310	-4.01506529	4.07047102
H	2.51608258	5.19852867	1.28732343
H	0.88167814	5.19902550	0.61844080
H	2.14143133	4.18512212	-0.11947367
H	0.36139016	3.16270768	3.73508201
H	-0.15220567	4.60967160	2.84189143
H	1.44072192	4.56612632	3.63057989
H	3.83542007	4.09666877	2.57748734
H	5.74358334	2.64774176	3.21614220
H	5.51565490	0.17801709	3.10676866
H	-2.74625655	1.84632550	1.01624637
H	2.45935555	-1.64177201	1.93140247
H	-5.66919668	2.68472730	1.48574819
H	-5.05035645	2.12748708	-0.08636017
H	-4.39977658	3.59508733	0.66378213
H	-3.21295967	3.46029052	2.90021416

H	-2.58730012	1.91983833	3.51681018
H	-4.32230021	2.27623933	3.62546957
H	4.71976964	-1.70944831	0.79996910
H	4.36616897	-3.13002478	1.80062049
H	5.48574585	-1.89314445	2.39364075
H	2.28132199	-1.36272419	4.41102039
H	4.04424962	-1.52308237	4.56185686
H	3.06855108	-2.89275345	3.98137911
O	-0.00122216	-3.24747436	0.00281939
H	-0.75465769	0.58005173	-3.88526335
H	1.59612234	-0.19095646	-3.78237105
H	-1.59635061	-0.17834577	3.78300849
H	0.75436882	0.59337878	3.88328484
Zr	-0.00007131	-0.52922965	0.00061249

**Oxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation)**Fig. S30: NCCN Oxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation)

SCF	E <sub>ZP</sub>	H	G
-2515.882611	-2514.739447	-2514.671079	-2514.843141

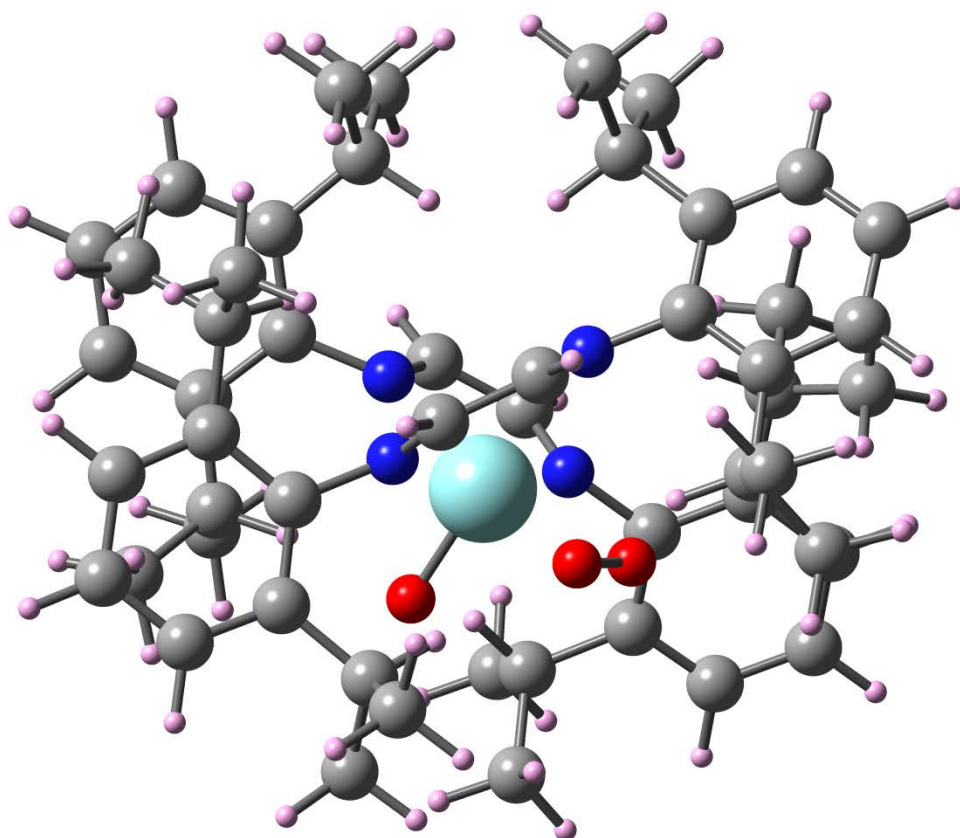
O	0.33839006	-0.63519398	1.72199613
O	1.05881207	0.83376115	-1.92615116
O	-0.16587005	1.46813716	-1.73809214
N	-1.48379415	1.52960612	1.09278808
N	1.32119205	1.97540625	0.67480404
N	1.36964518	-1.94777305	-0.73947507
N	-1.32568704	-1.52238011	-1.21362410
C	-0.86225514	2.59124622	1.51223911
C	0.54877596	2.86342029	1.21848508
C	0.69663615	-2.78633914	-1.56037913
C	-0.66452496	-2.55274616	-1.81902315
C	-2.85593125	1.38789707	1.59416412
C	-3.92497335	1.85442907	0.78219105
C	-5.22832044	1.77801002	1.31354809
C	-5.45803247	1.27640998	2.60484819
C	-4.38167335	0.83669198	3.38804325

C	-3.05480425	0.87811102	2.90668821
C	-4.81940643	2.29794208	-1.58831213
C	-3.66876435	2.51333313	-0.57892305
C	-3.41665538	4.03966625	-0.41091604
C	2.33307707	3.77319341	-2.96618224
C	2.01641504	3.98705242	-1.46396912
C	1.92007199	5.50137155	-1.13284110
C	2.71553815	2.34477531	0.44743603
C	3.04638014	3.29498540	-0.55975305
C	4.41171923	3.61841547	-0.72058906
C	5.40167932	3.03858945	0.08334400
C	5.04355333	2.12021737	1.08330307
C	3.69908624	1.75599430	1.29269609
C	-2.13895112	-0.97507209	4.42230233
C	-1.90130115	0.43007903	3.81574929
C	-1.66595316	1.46893511	4.94659737
C	4.36419435	-0.20744783	2.81512320
C	3.30254124	0.86083722	2.47143918
C	3.01512019	1.73841028	3.72406028
C	2.70877629	-2.35219004	-0.34425203
C	2.86684733	-3.18429010	0.80206905
C	4.16790845	-3.61128909	1.14119208
C	5.28202152	-3.23335603	0.37607502
C	5.10683348	-2.42242197	-0.75526007
C	3.82582336	-1.97249798	-1.14186810
C	1.83299426	-3.38979615	3.13762123
C	1.67161726	-3.67824518	1.62497912
C	1.42759628	-5.19064730	1.37069310
C	-2.31788219	1.01439606	-4.37062334
C	-2.02504613	-0.43274804	-3.89992930
C	-1.92261109	-1.38570112	-5.12179440
C	-2.72699015	-1.42499914	-1.59859313
C	-3.06932619	-0.93746511	-2.89431123
C	-4.42679829	-0.96194916	-3.28173326
C	-5.42139234	-1.44324723	-2.42014719
C	-5.06878131	-1.91938526	-1.14706810
C	-3.72573221	-1.93534621	-0.71678206
C	4.65746937	0.01884820	-2.52872820
C	3.66623933	-1.16615092	-2.43564519
C	3.81443137	-2.09319699	-3.67371429
C	-4.47631125	-2.51249728	1.67894412
C	-3.34981816	-2.58294425	0.62228804
C	-2.93765409	-4.06847135	0.41336902
H	-6.06811854	2.11982502	0.71697705
H	-6.47082650	1.23290094	2.99827222
H	-4.56904735	0.45466994	4.38811332
H	-2.75927926	2.07074713	-1.00696608
H	1.03128198	3.54211435	-1.29856911
H	-5.72225951	2.85049009	-1.29495111
H	-5.07510042	1.23934699	-1.68718014
H	-4.51886342	2.66769712	-2.57654021
H	-4.29492246	4.52785726	0.03231299

H	-3.22604638	4.49979229	-1.38921412
H	-2.55492332	4.25255330	0.23295101
H	3.29987113	4.21124748	-3.24698525
H	1.55824600	4.24894643	-3.58182428
H	2.34647311	2.70437633	-3.20224025
H	1.64866396	5.67359155	-0.08192701
H	1.16031091	5.98037555	-1.76452414
H	2.87621805	6.00999360	-1.31240011
H	4.69775524	4.33205353	-1.48860912
H	6.44599538	3.30353751	-0.06319401
H	5.81486838	1.68602537	1.71116812
H	-0.98709107	0.34036105	3.22051924
H	2.37107019	0.33694215	2.22348116
H	-3.02677219	-1.00928112	5.06831238
H	-1.27073905	-1.26361009	5.02838937
H	-2.25443411	-1.72308315	3.63100627
H	-2.54804223	1.55833009	5.59528739
H	-1.44866518	2.46886319	4.54624134
H	-0.81587808	1.16273312	5.57045041
H	4.63333539	-0.80600486	1.93867114
H	3.96494434	-0.89056989	3.57477426
H	5.27995341	0.23937824	3.22686924
H	3.91731224	2.28337135	4.03453730
H	2.69083819	1.10471222	4.55951134
H	2.22405010	2.47641931	3.53691226
H	4.30778848	-4.25109714	2.00922414
H	6.27649160	-3.57549202	0.65388704
H	5.97151056	-2.14470392	-1.35292311
H	0.78505817	-3.12736216	1.30273409
H	-1.04768805	-0.41500601	-3.41143527
H	2.72710434	-3.86872016	3.55997526
H	0.95981221	-3.77125020	3.68458327
H	1.88782023	-2.30971606	3.30710825
H	1.26897128	-5.39619832	0.30381701
H	0.53872523	-5.53116736	1.91924514
H	2.28293237	-5.79406732	1.70430112
H	-3.28635127	1.08845303	-4.88367138
H	-1.53938215	1.34439811	-5.07102740
H	-2.31726222	1.70720411	-3.52234028
H	-1.67355904	-2.40945018	-4.81463638
H	-1.14109504	-1.03774606	-5.81051246
H	-2.86909216	-1.42522915	-5.67761446
H	-4.70372933	-0.60189914	-4.26974333
H	-6.46161146	-1.45515026	-2.73763922
H	-5.84513436	-2.29803931	-0.48973305
H	2.65646424	-0.74793692	-2.45963119
H	-2.47350511	-2.05561918	1.02262607
H	5.69890548	-0.32333979	-2.60052621
H	4.57547534	0.67623425	-1.65653114
H	4.44300033	0.61554724	-3.42535927
H	3.67096434	-1.51939495	-4.59933136
H	3.07448734	-2.90361307	-3.65751429



H	4.81274346	-2.55031599	-3.70725329
H	-4.84805931	-1.49117122	1.81088113
H	-4.09919721	-2.86449429	2.64732819
H	-5.32289330	-3.15855135	1.40932810
H	-2.07850102	-4.16190033	-0.25846003
H	-3.77255713	-4.64208942	-0.01220701
H	-2.66499405	-4.52429437	1.37488510
H	-1.36876519	3.32064526	2.14866216
H	0.93241296	3.84114437	1.51946611
H	1.18942822	-3.65944419	-1.98440916
H	-1.20414698	-3.21198023	-2.49612320
Zr	0.12715903	-0.15021095	-0.03078601

**Oxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)**Fig. S31: Oxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)

SCF	E <sub>ZP</sub>	H	G
-2515.880514	-2514.737713	-2514.670084	-2514.841005

O	1.92222643	-0.93755290	1.57527623
N	-1.12504524	-0.73570461	-1.67821995
N	1.28123169	-1.96615475	-0.99492076
N	-1.35127496	1.17476159	1.51546020
N	1.29082724	2.16059554	0.56406027
C	-0.42580173	-1.47535429	-2.58989370
C	0.78554140	-2.10072024	-2.24692488
C	-0.77526333	2.28630627	1.87394385
C	0.57077937	2.73272413	1.47958046
C	-2.46201086	-0.38363291	-2.16580002
C	-3.57937024	-1.18958220	-1.78883711
C	-4.82936684	-0.93252873	-2.39345776
C	-4.98572199	0.06896526	-3.36187140
C	-3.88182361	0.85091257	-3.72539065
C	-2.61400734	0.64786187	-3.13944026
C	-4.58694031	-2.46625288	0.19957921

C	-3.44928200	-2.39083400	-0.84813937
C	-3.38304635	-3.70686128	-1.67234029
C	0.53479930	-5.13687338	1.57214228
C	0.75628157	-4.65998861	0.11456087
C	0.45834759	-5.80263872	-0.89316344
C	2.41390618	-2.80947979	-0.63846798
C	2.16877251	-4.10430832	-0.09856172
C	3.27827594	-4.91684619	0.21970526
C	4.59137677	-4.47251353	0.01295661
C	4.81515137	-3.19432808	-0.52061727
C	3.74070868	-2.34330063	-0.85274236
C	-1.75420015	3.02614880	-3.47942120
C	-1.44508362	1.51421774	-3.62309870
C	-1.07725706	1.18347765	-5.09568539
C	5.20769449	-0.23971715	-0.80386217
C	4.02203876	-0.97261734	-1.47448591
C	4.27276618	-1.10493656	-3.00267926
C	-2.71814260	0.98285706	2.03846854
C	-2.91223910	0.14200239	3.16922467
C	-4.22969101	-0.01691477	3.64769287
C	-5.31222048	0.63769517	3.04536882
C	-5.08939492	1.49147314	1.95639309
C	-3.79447184	1.69397436	1.43315115
C	-1.99220193	-1.98428212	4.27224003
C	-1.75873400	-0.48806817	3.95675240
C	-1.50192203	0.32518519	5.25651366
C	2.38193701	2.66602213	-3.43247299
C	1.90031938	3.20212127	-2.06357699
C	1.44307332	4.68464925	-2.17811710
C	2.63599780	2.64496160	0.34266863
C	2.96428345	3.09138452	-0.97062582
C	4.26537508	3.56885940	-1.21464647
C	5.22896260	3.59790289	-0.19505794
C	4.89364195	3.14913885	1.08863825
C	3.60227435	2.67086006	1.39880584
C	-4.75224895	2.63603390	-0.75497735
C	-3.60551659	2.69426295	0.28230123
C	-3.49005996	4.15221213	0.81452049
C	4.30963530	1.03585741	3.22909544
C	3.34776199	2.18726857	2.83495847
C	3.45336492	3.36160917	3.84561864
H	-0.84392284	-1.64242022	-3.58110361
H	1.28830992	-2.73622449	-2.97420098
H	-1.29207804	2.96445093	2.55720742
H	0.93196826	3.61176547	2.02390447
H	-5.68244516	-1.54725581	-2.11933156
H	-5.95332274	0.23408559	-3.83008524
H	-4.00293992	1.62384946	-4.48077159
H	-2.51617023	-2.30802954	-0.29027368
H	0.03355162	-3.85983757	-0.05821945
H	-5.56401963	-2.67660988	-0.25776763
H	-4.66744719	-1.53238616	0.76851880

H	-4.37400516	-3.27457043	0.91091592
H	-4.30377325	-3.86130762	-2.25251229
H	-3.25397508	-4.56585856	-1.00022701
H	-2.53792974	-3.69579714	-2.37260548
H	1.20421819	-5.96535459	1.84155072
H	-0.49940689	-5.48314791	1.69873660
H	0.69893269	-4.31211834	2.27447024
H	0.57128475	-5.45973298	-1.93030655
H	-0.57045480	-6.16550419	-0.76409126
H	1.13852016	-6.65282426	-0.74570255
H	3.10752399	-5.90875660	0.63092637
H	5.43269562	-5.11484287	0.26354471
H	5.83529642	-2.85437634	-0.67745769
H	-0.57015145	1.28968860	-3.00257516
H	3.12822743	-0.35121824	-1.33615563
H	-2.63503979	3.31567372	-4.06590763
H	-0.90912664	3.62423955	-3.84138368
H	-1.94346785	3.29666759	-2.43281986
H	-1.92194708	1.38630235	-5.76708299
H	-0.80407883	0.12791047	-5.21286054
H	-0.22676761	1.79261867	-5.43038502
H	5.07769215	-0.18943481	0.28299347
H	5.28113518	0.78526206	-1.18568678
H	6.16373515	-0.73868916	-1.01074771
H	5.13632163	-1.75524915	-3.19667628
H	4.48176638	-0.12207730	-3.44765375
H	3.40524936	-1.53638518	-3.51675936
H	-4.40268055	-0.65563993	4.50883615
H	-6.31966802	0.49436166	3.42831419
H	-5.93086038	2.00686624	1.50404437
H	-0.84900151	-0.44097241	3.35687853
H	1.03138901	2.60708605	-1.75700258
H	-2.87521028	-2.14555919	4.90565457
H	-1.12254210	-2.38671186	4.80861261
H	-2.10266084	-2.54458289	3.33913697
H	-1.28234853	1.38029220	5.03967262
H	-0.64448768	-0.09519587	5.79774071
H	-2.37431759	0.29682272	5.92346042
H	3.20956627	3.26227337	-3.83749824
H	1.56399836	2.70509004	-4.16232872
H	2.71832831	1.62537052	-3.35497081
H	1.03756763	5.05158665	-1.22587643
H	0.66739679	4.79724415	-2.94431274
H	2.28803980	5.32987669	-2.45160224
H	4.52387471	3.93284380	-2.20511626
H	6.23040392	3.96850307	-0.39902612
H	5.64757810	3.16589917	1.87097594
H	-2.67558124	2.44714769	-0.24557138
H	2.34228311	1.76807599	2.91246246
H	-5.68419986	3.04974417	-0.34741938
H	-4.94274481	1.61278466	-1.08743978
H	-4.48855412	3.23395218	-1.63578292

H	-3.38936318	4.85416038	-0.02419096
H	-2.63042590	4.29693809	1.47970412
H	-4.39217087	4.42494313	1.37766324
H	4.17299510	0.17328126	2.56830681
H	4.09381854	0.70685735	4.25391886
H	5.36173697	1.34722602	3.19011038
H	2.75573014	4.17539185	3.60288769
H	4.46425940	3.78939348	3.85886264
H	3.22667672	3.00746612	4.85973331
O	-0.97118671	-1.98383446	1.20095239
O	1.11221247	-0.10595900	2.33058229
Zr	-0.00178159	-0.68518074	0.41893618

### 3.5 Structures with four oxygen atoms

#### Peroxo Complex with adsorbed O<sub>2</sub> molecule (spiro conformation)

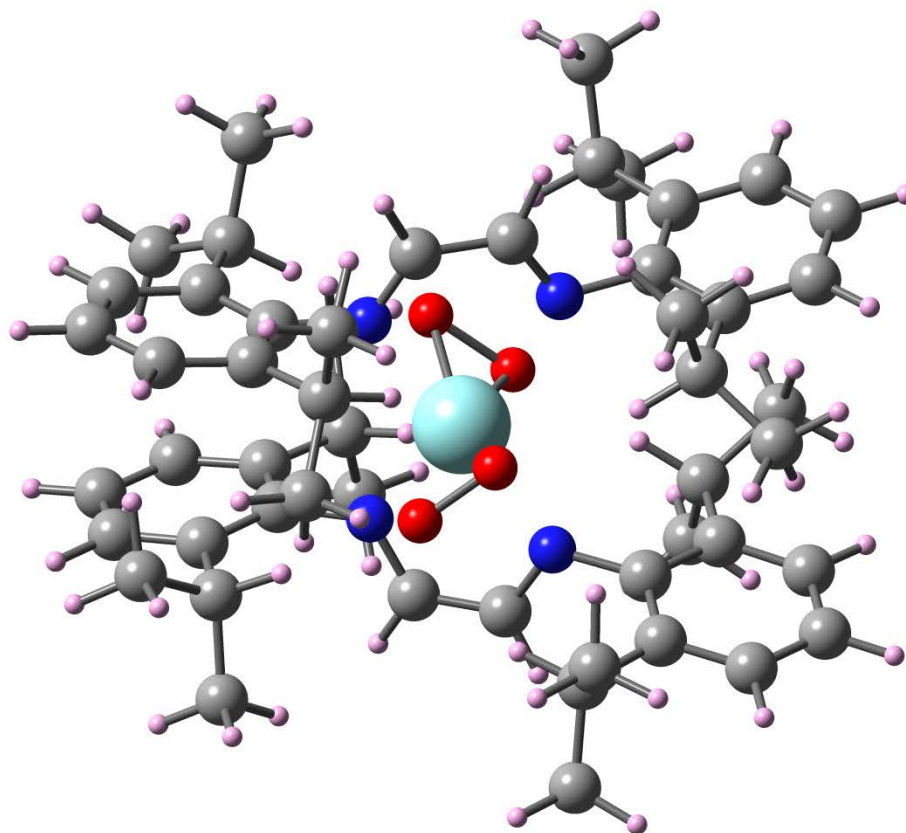


Fig. S32: NCCN Peroxo Complex with adsorbed O<sub>2</sub> molecule (spiro conformation)

SCF	E <sub>ZP</sub>	H	G
-2591.047482	-2589.901060	-2589.831764	-2590.004766

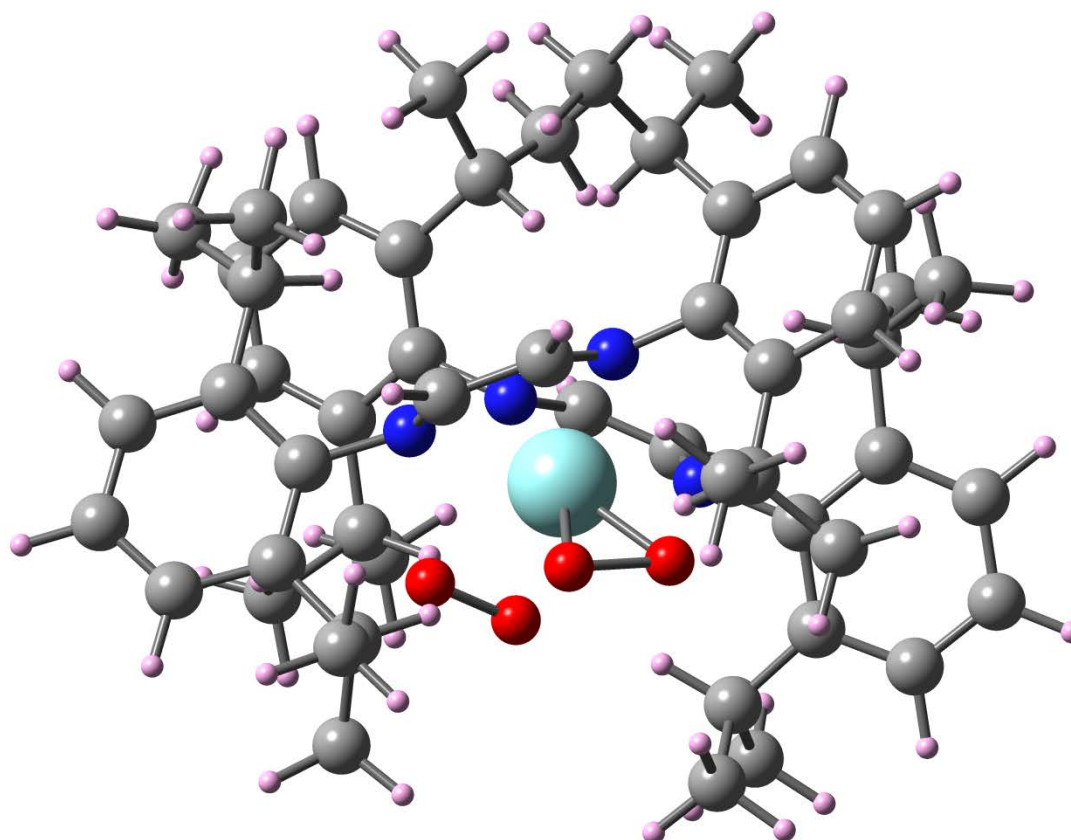
Zr	-0.01983603	-0.12989405	-0.12307007
O	0.53380301	0.18099398	2.04861610
O	-0.56444507	-0.66936110	2.08646410
O	-0.51629408	0.82748602	-1.85772320
O	0.68116302	-0.12033404	-2.04491622
N	1.32067509	-2.01914718	0.10324795
N	-1.37201211	-1.88926020	-0.61873811
N	-1.36930616	1.88325609	0.64761399
N	1.42140706	1.99580313	-0.04677506
C	0.62491705	-3.15143027	-0.17690007
C	-0.72575706	-3.08547428	-0.55705710
C	-0.67738911	2.98155218	0.66828999
C	0.72925799	3.05121520	0.24775496
C	2.69540320	-2.22315718	0.53691398

C	3.75306028	-2.08611616	-0.41135009
C	5.07227838	-2.34438316	0.01627494
C	5.34731642	-2.74823519	1.33249304
C	4.29528133	-2.90146421	2.24539711
C	2.95704522	-2.64733721	1.87304108
C	4.57741533	-0.94252106	-2.56743426
C	3.46986425	-1.77870314	-1.88586421
C	3.24981525	-3.10108224	-2.67398227
C	-2.02214918	-0.68912312	-4.55973441
C	-1.81287215	-1.83932020	-3.54379133
C	-1.62352712	-3.19402930	-4.27960839
C	-2.73728922	-1.94964921	-1.12364015
C	-2.95944024	-1.93560222	-2.53054925
C	-4.28429034	-2.07644624	-2.99728429
C	-5.35867341	-2.22710127	-2.10848622
C	-5.12060340	-2.24948127	-0.72518012
C	-3.81456730	-2.12195324	-0.20640308
C	2.05373715	-2.03200417	4.18534426
C	1.84916314	-2.88453324	2.90716016
C	1.74161315	-4.39085636	3.26850719
C	-4.65207337	-1.57437321	2.16498411
C	-3.57262528	-2.26770825	1.30074604
C	-3.47380826	-3.76979336	1.69040407
C	-2.75532526	1.99425908	1.11866202
C	-3.01655628	2.05632509	2.51527613
C	-4.36194439	2.20791209	2.91665516
C	-5.39810748	2.30335608	1.97851909
C	-5.10688645	2.26114208	0.60573499
C	-3.78393634	2.11480108	0.14256495
C	-2.17435921	0.88318701	4.62713630
C	-1.92387720	2.00975509	3.59271121
C	-1.79487320	3.38542720	4.30264227
C	2.17804911	2.06490414	-4.15598538
C	1.91464709	2.86652320	-2.85609228
C	1.72746406	4.37578531	-3.17214030
C	2.79811716	2.23077716	-0.49055610
C	3.03150917	2.66366020	-1.82383720
C	4.36843827	2.93504423	-2.18897323
C	5.42189035	2.78360323	-1.27712816
C	5.15863434	2.35615919	0.03433094
C	3.84475424	2.07509616	0.45916197
C	-4.57401140	1.61334503	-2.25437623
C	-3.46656432	2.20680409	-1.35463116
C	-3.20885831	3.68812521	-1.75529919
C	4.67083232	0.87945208	2.58306414
C	3.55205622	1.71435013	1.91983709
C	3.29466519	3.00042322	2.75558215
H	1.11381809	-4.12111434	-0.10152007
H	-1.25410508	-3.99746136	-0.82728212
H	-1.12779916	3.91897725	1.00297901
H	1.16724702	4.05042128	0.18782195
H	5.89045442	-2.24402915	-0.69085911

H	6.37116750	-2.95125620	1.63853307
H	4.51111435	-3.22891224	3.25977119
H	2.53941117	-1.20614810	-1.94799221
H	-0.88743508	-1.61488317	-3.00864629
H	5.50881740	-1.51319110	-2.68690727
H	4.80199733	-0.03121899	-2.00267621
H	4.24789830	-0.64544204	-3.57141333
H	4.14982033	-3.73095528	-2.63928326
H	3.02483023	-2.88031023	-3.72594534
H	2.41248919	-3.67777130	-2.26493823
H	-2.93381825	-0.82417113	-5.15836146
H	-1.16977111	-0.64531910	-5.25059546
H	-2.07747219	0.27112696	-4.03643237
H	-1.42791010	-4.01032536	-3.57170133
H	-0.77241006	-3.13331729	-4.97118544
H	-2.51531319	-3.46230833	-4.86282443
H	-4.47200735	-2.07315824	-4.06824137
H	-6.37186548	-2.33568628	-2.48918225
H	-5.95549247	-2.38044429	-0.04221906
H	0.89293407	-2.58141823	2.47386213
H	-2.60847021	-1.80595121	1.53677806
H	2.99414322	-2.28061918	4.69553630
H	1.23154009	-2.21058419	4.89128332
H	2.06217414	-0.96420609	3.93956124
H	2.66484022	-4.75612038	3.73787123
H	1.55497814	-5.00419541	2.37747112
H	0.91627809	-4.55500038	3.97449824
H	-4.79002239	-0.52767813	1.87535608
H	-4.35476735	-1.59969421	3.22187219
H	-5.62355043	-2.08133426	2.08833710
H	-4.40795732	-4.29542742	1.44955005
H	-3.29124124	-3.87235037	2.76876715
H	-2.65607119	-4.27099839	1.16002803
H	-4.59509141	2.25230308	3.97713924
H	-6.42639053	2.41716808	2.31277511
H	-5.91423549	2.35050108	-0.11388307
H	-0.96178212	1.78712109	3.12396918
H	0.97510102	2.47824116	-2.45398725
H	-3.11365928	1.03224301	5.17564634
H	-1.35739514	0.86316501	5.36018336
H	-2.20691820	-0.09327407	4.13298126
H	-1.57242320	4.19216727	3.59062721
H	-0.98703214	3.35409121	5.04546933
H	-2.72258327	3.65326121	4.82465431
H	3.10621618	2.37581317	-4.65432142
H	1.34972305	2.22081115	-4.85952643
H	2.23006513	0.99487606	-3.93313036
H	1.49467003	4.95805036	-2.26921223
H	0.90408899	4.51249932	-3.88555836
H	2.63422712	4.80709335	-3.61715433
H	4.58139428	3.26500426	-3.20227631
H	6.44280042	2.99731526	-1.58433618



H	5.98018642	2.24406720	0.73495200
H	-2.54530524	1.64825706	-1.55710318
H	2.63602716	1.11317708	1.94820309
H	-5.48784150	2.22301808	-2.23403123
H	-4.82972341	0.59138996	-1.95864921
H	-4.22531837	1.58406404	-3.29395631
H	-2.95641330	3.74900222	-2.82152227
H	-2.37998025	4.13327825	-1.19010515
H	-4.10361439	4.30007725	-1.57711318
H	4.92139734	-0.00348199	1.98721609
H	4.33793029	0.53575904	3.57059721
H	5.58486736	1.46983313	2.73398415
H	2.45842312	3.59109326	2.36011412
H	4.18507225	3.64349728	2.75982315
H	3.05816018	2.73527720	3.79426623

Peroxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)Fig. S33: Peroxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)

SCF	E <sub>ZP</sub>	H	G
-2591.014790	-2589.868427	-2589.799229	-2589.973499

O	-1.71295445	-2.08128511	0.41002262
N	1.02892329	1.42470920	1.37281255
N	-1.66813903	0.41988329	1.76857367
N	1.59873035	-1.16168300	-1.48526831
N	-0.99408583	-0.21131483	-1.92401199
C	0.31184807	1.66453579	2.43331524
C	-1.05470794	1.16406282	2.63565158
C	1.08352173	-1.13236002	-2.73371036
C	-0.21939475	-0.64591124	-2.95410596
C	2.36016352	2.05838324	1.40848656
C	3.35875452	1.56611244	2.29851033
C	4.57173771	2.28670085	2.37689475
C	4.78375372	3.45889414	1.64084722
C	3.77751689	3.93171020	0.78708188
C	2.55632891	3.24324616	0.64762024
C	4.29438218	-0.71945852	2.92649667

C	3.19096836	0.33457124	3.19813864
C	3.18526705	0.74337255	4.69691416
C	-2.41728854	-3.47630909	3.35450229
C	-2.18492083	-1.95689961	3.54512808
C	-2.04006860	-1.61612714	5.05447870
C	-3.05043671	0.03508470	2.10111407
C	-3.29287080	-1.10687158	2.91448676
C	-4.63705843	-1.42671157	3.20648772
C	-5.69851283	-0.64964033	2.72847295
C	-5.43095812	0.49054699	1.95670291
C	-4.11023420	0.86285670	1.63344160
C	1.95925261	4.37535172	-1.57351800
C	1.44427250	3.85419511	-0.20962890
C	0.73767552	4.99345570	0.57842478
C	-5.00327700	2.55026445	-0.08655972
C	-3.84995211	2.16744135	0.86952677
C	-3.60355092	3.34872343	1.85229986
C	2.96768092	-1.67350087	-1.37831172
C	3.19441648	-3.04230346	-1.05646023
C	4.52604470	-3.49837215	-0.95167096
C	5.61165014	-2.64613216	-1.18500157
C	5.37398817	-1.31410952	-1.55189713
C	4.06326241	-0.80307942	-1.66054531
C	2.09116240	-4.72717605	0.51450257
C	2.06982473	-4.06571586	-0.88629821
C	2.12644417	-5.13758455	-2.00884045
C	-1.87714652	3.98585867	-2.10096591
C	-1.40228364	2.62249555	-2.66058828
C	-0.75856802	2.81803167	-4.06261814
C	-2.32162648	0.21679205	-2.38453508
C	-2.52624432	1.58364136	-2.73978762
C	-3.76647532	1.96678233	-3.28980634
C	-4.79586415	1.03604105	-3.48530846
C	-4.57780599	-0.30668534	-3.15446028
C	-3.34359848	-0.74949148	-2.62761405
C	4.95009784	1.60465344	-1.58122494
C	3.87204732	0.64352321	-2.13616623
C	3.87731830	0.72895566	-3.68986367
C	-4.20425117	-2.86321046	-1.47465274
C	-3.15099441	-2.25818339	-2.43667777
C	-3.17773853	-2.99169088	-3.80610738
H	0.70766507	2.28707749	3.23927997
H	-1.53819329	1.46385840	3.56820636
H	1.66530722	-1.49979674	-3.57620308
H	-0.61302816	-0.63990526	-3.96957867
H	5.35149205	1.92450127	3.04105766
H	5.72132598	4.00130420	1.73398831
H	3.93965444	4.84831908	0.22788317
H	2.24223811	-0.15595156	2.97861087
H	-1.23048995	-1.73251307	3.06616662
H	5.29736357	-0.33806923	3.16443343
H	4.27419986	-1.03767318	1.87993460

H	4.11452095	-1.60736639	3.54597875
H	4.13864370	1.19794059	4.99835533
H	3.02241137	-0.14348016	5.32288578
H	2.38844147	1.46647239	4.92268372
H	-3.29468342	-3.83686209	3.90881090
H	-1.54255479	-4.02796032	3.72212752
H	-2.54977587	-3.71678528	2.29436876
H	-1.80719783	-0.55356758	5.21097299
H	-1.22740902	-2.20754680	5.49553833
H	-2.96437941	-1.83879658	5.60506368
H	-4.84626791	-2.29843488	3.81990011
H	-6.72497906	-0.92153419	2.96236718
H	-6.25754812	1.09732198	1.60256547
H	0.69595519	3.07781849	-0.41134232
H	-2.94411841	2.02949375	0.26298562
H	2.67105965	5.20118890	-1.45178295
H	1.12513889	4.75445448	-2.17509389
H	2.45586485	3.57979828	-2.14126125
H	1.44710273	5.79789237	0.81202983
H	0.32417673	4.62870581	1.52803110
H	-0.08484488	5.42166778	-0.00756020
H	-5.27716740	1.71801807	-0.74135920
H	-4.69921127	3.38993754	-0.72228547
H	-5.89500682	2.86920821	0.46934601
H	-4.47776729	3.49211491	2.50081922
H	-3.43804846	4.28071837	1.29492642
H	-2.73359156	3.18527288	2.49891610
H	4.70765726	-4.53869251	-0.69324186
H	6.63055135	-3.01637386	-1.09726254
H	6.21858892	-0.66254707	-1.75447559
H	1.11412205	-3.55409255	-0.98457339
H	-0.62444717	2.23157164	-1.99398176
H	3.00760648	-5.31344516	0.67118695
H	1.23465059	-5.40620733	0.62231064
H	2.02725528	-3.95981841	1.29221400
H	2.07124459	-4.67797274	-3.00516816
H	1.28320611	-5.83400332	-1.90691930
H	3.05444357	-5.72310222	-1.96178454
H	-2.63290931	4.44891284	-2.74736481
H	-1.03532326	4.68508433	-2.04048132
H	-2.30807354	3.88177970	-1.09819624
H	-0.35953224	1.87422249	-4.45194670
H	0.06546950	3.54198483	-4.01592390
H	-1.50136754	3.19126021	-4.78012733
H	-3.92692184	3.00192856	-3.57831038
H	-5.74750957	1.35103525	-3.90682755
H	-5.36536956	-1.03456003	-3.33291970
H	2.89250294	0.99094722	-1.78185482
H	-2.16966249	-2.43779122	-1.99939750
H	5.93446016	1.40202656	-2.02329143
H	5.03975861	1.52635632	-0.49369174
H	4.69384240	2.64210273	-1.82837576

H	3.76419217	1.77266029	-4.01552082
H	3.06736341	0.14547916	-4.14029989
H	4.82764201	0.35057186	-4.08971770
H	-4.16256497	-2.37880216	-0.49345954
H	-4.00792394	-3.93372136	-1.32996532
H	-5.22341566	-2.75897205	-1.87137301
H	-2.40897056	-2.60087541	-4.48581658
H	-4.15061409	-2.88380848	-4.30376410
H	-2.98983644	-4.06382433	-3.66117105
O	0.49425365	-1.29912304	2.14470306
O	1.67231224	-1.47372002	1.18131044
O	-0.69831743	-2.76839549	-0.24789783
Zr	0.06704800	-0.72274221	0.19535682

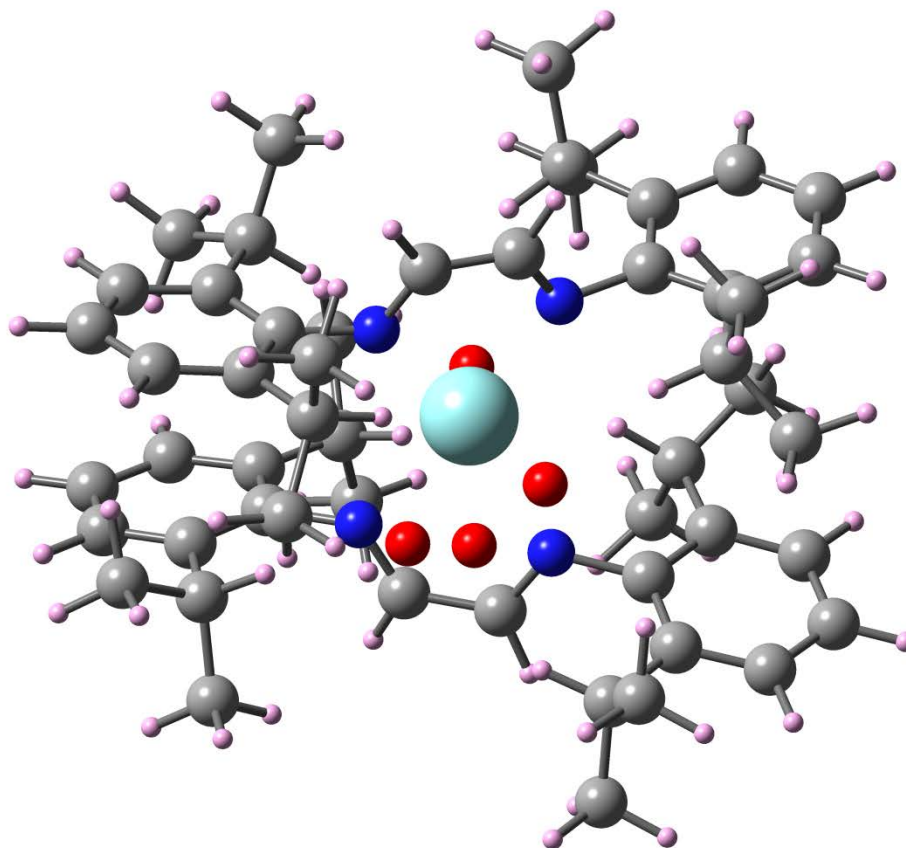
**Oxo Complex with adsorbed ozone group (conformation 1 lower energy)**

Fig. S34: NCCN Oxo Complex with adsorbed ozone group (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G
-2591.025929	-2589.880099	-2589.810367	-2589.986059

O	1.20992635	-0.42361870	2.22465534
O	-0.80145383	-1.42580029	1.69295521
O	0.13571525	0.49028624	-1.70935150
N	1.29968469	-2.00188458	-0.39124021
N	-1.51801915	-1.69717089	-0.95641003
N	-1.26365026	1.66225786	1.15398508
N	1.42102287	1.95744219	0.54165613
C	0.55394530	-2.96279814	-0.84923506
C	-0.85478841	-2.78063406	-1.21875709
C	-0.53930929	2.68178836	1.69616937
C	0.81925690	2.84520370	1.37024935
C	2.71759721	-2.32129314	-0.19202436
C	3.63739082	-1.83925819	-1.16682517
C	4.99645077	-2.17429803	-1.00338169
C	5.42698463	-2.96803410	0.07146592
C	4.49675668	-3.44900298	1.00176566

C	3.12208063	-3.14410354	0.89453630
C	4.21288094	-0.09960123	-2.97435863
C	3.16359863	-1.08736518	-2.41689097
C	2.76527236	-2.10153192	-3.52830730
C	-1.92998918	0.33905153	-4.61822644
C	-1.77754952	-0.98518568	-3.83003565
C	-1.54730152	-2.17038190	-4.80758151
C	-2.85667704	-1.60784408	-1.54176669
C	-2.98058427	-1.26559785	-2.91817486
C	-4.28417365	-1.22619359	-3.45941113
C	-5.41132564	-1.51280144	-2.67694162
C	-5.25592028	-1.86099004	-1.32582871
C	-3.98025126	-1.92417946	-0.72961231
C	2.57925582	-3.37808076	3.37980956
C	2.15456187	-3.72978276	1.93088307
C	2.02777928	-5.26916547	1.76300910
C	-4.97217023	-2.01563198	1.64248240
C	-3.81154037	-2.42673001	0.70816065
C	-3.65426716	-3.97452254	0.72164044
C	-2.68457764	1.68030668	1.46669025
C	-3.13388683	1.37212948	2.78414357
C	-4.51359697	1.48274507	3.06290347
C	-5.42716492	1.87957791	2.07772371
C	-4.96875919	2.18427660	0.78600312
C	-3.59988622	2.10580240	0.45734337
C	-2.57791166	-0.41823167	4.52065319
C	-2.18888716	0.95645534	3.91890384
C	-2.14001197	2.03763025	5.03286274
C	1.59876127	3.06962740	-3.50101171
C	1.52803832	3.44079811	-2.00008102
C	1.26032754	4.96048072	-1.82021406
C	2.72542690	2.33707538	0.01693214
C	2.78720671	3.03585292	-1.22520265
C	4.05181390	3.43943530	-1.70211508
C	5.22397261	3.17318134	-0.97838668
C	5.14337339	2.50617424	0.25257863
C	3.90279160	2.08375093	0.77846959
C	-4.14772260	2.39235982	-2.04543937
C	-3.10669281	2.57494686	-0.91732018
C	-2.67551645	4.06817411	-0.84826165
C	4.87538352	0.29526015	2.33825252
C	3.85813512	1.45024753	2.17322915
C	4.09083838	2.52998244	3.26641583
H	5.72213769	-1.81634352	-1.72625638
H	6.48082424	-3.21310874	0.17861013
H	4.83785177	-4.06777180	1.82728869
H	2.26468745	-0.50963411	-2.16847046
H	-0.88554826	-0.85151696	-3.21180100
H	5.07613095	-0.62201109	-3.40939342
H	4.57360563	0.58669170	-2.20192678
H	3.76082370	0.50315265	-3.77128398
H	3.62819821	-2.71398939	-3.82369987

H	2.40613819	-1.56296063	-4.41469300
H	1.96627969	-2.78091602	-3.20485291
H	-2.79096262	0.32486083	-5.30023578
H	-1.02875252	0.51463202	-5.21981027
H	-2.04014779	1.18298224	-3.93006937
H	-1.37989764	-3.11586199	-4.27339363
H	-0.66893142	-1.97689927	-5.43769010
H	-2.41286908	-2.31491138	-5.46830935
H	-4.41314730	-0.96649608	-4.50681813
H	-6.40462626	-1.47278964	-3.11768377
H	-6.13316347	-2.09348204	-0.73023766
H	1.16130901	-3.29905600	1.77925497
H	-2.88853334	-2.00182267	1.11886096
H	3.53478912	-3.84806365	3.64699743
H	1.82136535	-3.73570765	4.08876969
H	2.67729726	-2.29484736	3.50318882
H	2.99394937	-5.76637347	1.91890276
H	1.67360543	-5.54392921	0.75995450
H	1.31786037	-5.67269608	2.49687305
H	-5.14628070	-0.93552853	1.61371409
H	-4.72837826	-2.29106279	2.67638708
H	-5.90851021	-2.52777606	1.38139667
H	-4.55203705	-4.45964790	0.31498671
H	-3.50736941	-4.32947239	1.75002926
H	-2.79426350	-4.30717736	0.12687890
H	-4.87271346	1.25434259	4.06369352
H	-6.48610125	1.95783877	2.31321719
H	-5.68231186	2.50026725	0.03159727
H	-1.17810503	0.85535167	3.51564218
H	0.68006895	2.88977752	-1.58831456
H	-3.57821325	-0.39366901	4.97325205
H	-1.86188109	-0.70238338	5.30333554
H	-2.56330856	-1.19545983	3.74964357
H	-1.82682529	3.01253136	4.63725723
H	-1.42849444	1.74358398	5.81601595
H	-3.12348231	2.17011802	5.50317547
H	2.43064345	3.56891744	-4.01651374
H	0.66887032	3.37083618	-4.00207548
H	1.70477468	1.98607995	-3.61915345
H	1.16194186	5.22518607	-0.75929378
H	0.33095041	5.24791317	-2.33049182
H	2.07876438	5.56061088	-2.24112111
H	4.11729662	3.97733810	-2.64460316
H	6.18895219	3.49532699	-1.36338916
H	6.05129276	2.32138345	0.82130390
H	-2.21653402	1.99250233	-1.18562095
H	2.86244356	1.02979160	2.33384643
H	-5.00701849	3.06452882	-1.91767655
H	-4.51802488	1.36262806	-2.09527769
H	-3.69029968	2.63601563	-3.01272319
H	-2.29764987	4.39961433	-1.82495382
H	-1.88339455	4.22771436	-0.10869183



H	-3.53069307	4.70316888	-0.57851343
H	4.73300971	-0.47372730	1.57175523
H	4.74726007	-0.17698029	3.32152089
H	5.91287952	0.65108184	2.27489662
H	3.34222013	3.33040586	3.20743142
H	5.08260371	2.99066085	3.16144901
H	4.02809399	2.07908277	4.26597712
O	0.17105660	-1.23357669	2.71292193
H	-1.30471516	-3.59630362	-1.79079387
H	0.98076538	-3.94879244	-1.04760565
H	-1.02787655	3.40443589	2.34686419
H	1.36148557	3.71705036	1.73172476
Zr	0.09770390	0.14158700	0.08012623

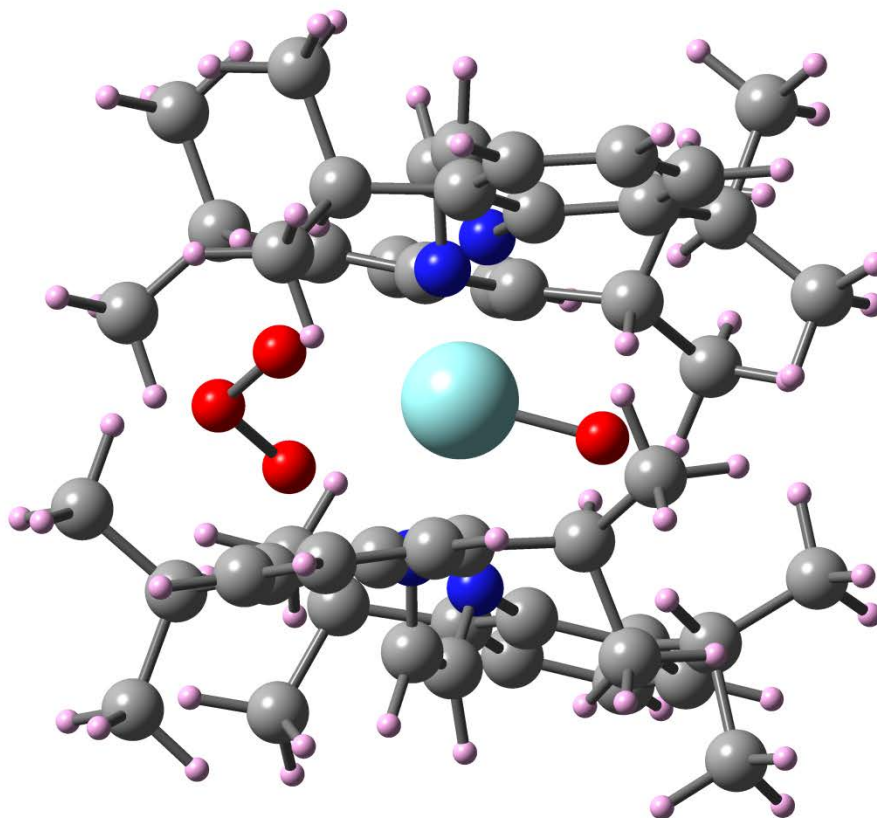
**Oxo Complex with adsorbed ozone group (conformation 2 higher energy)**

Fig. S35: NCCN Oxo Complex with adsorbed ozone group (conformation 2 higher energy)

SCF	E <sub>ZP</sub>	H	G
-2591.025873	-2589.880054	-2589.810336	-2589.985832

N	1.41889432	-1.97135803	-0.49230602
N	-1.26652999	-1.67899265	-1.11247280
N	-1.51937485	1.71108427	0.91864149
N	1.29911400	2.01294577	0.34628533
C	0.81265943	-2.87533511	-1.29954656
C	-0.54472893	-2.71338866	-1.63012503
C	-0.85989220	2.80447070	1.14927709
C	0.54859196	2.98285354	0.77668403
C	2.72174975	-2.34617307	0.03981605
C	3.90015508	-2.11139231	-0.72567628
C	5.13846986	-2.53227768	-0.19320430
C	5.21562463	-3.18019027	1.04817822
C	4.04230358	-3.42706085	1.77690227
C	2.78014828	-3.02314419	1.29391791
C	4.88973972	-0.36191613	-2.32039992
C	3.85738621	-1.49949192	-2.13007268

C	4.06798948	-2.59982431	-3.20717826
C	-2.55651285	0.30882929	-4.54114686
C	-2.17066116	-1.05115297	-3.90446487
C	-2.11563160	-2.15897081	-4.99160558
C	-2.68529071	-1.70032062	-1.43407053
C	-3.12324833	-1.43724036	-2.76524089
C	-4.49978158	-1.56249477	-3.05318510
C	-5.42141187	-1.92938489	-2.06405589
C	-4.97498521	-2.18412886	-0.75742783
C	-3.60971285	-2.08847915	-0.41813562
C	1.60460117	-3.02670847	3.57616241
C	1.51812752	-3.40112476	2.07701749
C	1.22058728	-4.91628386	1.90620409
C	-4.18809656	-2.28915049	2.08609878
C	-3.12957107	-2.50035252	0.97947593
C	-2.67876114	-3.98917710	0.97393433
C	-2.85626650	1.63658922	1.51108893
C	-2.97357933	1.34340667	2.89932993
C	-4.27402035	1.32813232	3.44922926
C	-5.40478872	1.58911900	2.66315253
C	-5.25644789	1.88238100	1.29822346
C	-3.98411396	1.92002384	0.69271827
C	-1.92411545	-0.21286825	4.64329765
C	-1.76673534	1.08471525	3.81258294
C	-1.52084545	2.29822502	4.75056862
C	2.57283929	3.30774677	-3.45153698
C	2.15318902	3.69705331	-2.01061702
C	2.03636455	5.24085042	-1.88025478
C	2.71630451	2.32922060	0.13967069
C	3.12020037	3.13087904	-0.96294095
C	4.49520845	3.43148074	-1.07816023
C	5.42629093	2.96752390	-0.14021188
C	4.99640945	2.19523883	0.95043040
C	3.63733891	1.86459042	1.12196108
C	-5.00159826	1.92703946	-1.67032526
C	-3.82260151	2.35548992	-0.76747218
C	-3.63531436	3.89736513	-0.85561947
C	4.21145135	0.15639416	2.95977033
C	3.16446321	1.13741767	2.38656874
C	2.77204184	2.17362246	3.47954109
H	1.35065388	-3.75788735	-1.64082343
H	-1.03540438	-3.44876684	-2.26470380
H	-1.31361651	3.63446021	1.69711505
H	0.97070308	3.97555317	0.95009382
H	6.04731885	-2.36125593	-0.76467678
H	6.17883988	-3.50198646	1.43787469
H	4.10497601	-3.94893029	2.72852658
H	2.86677578	-1.06717242	-2.29177430
H	-1.16179552	-0.94042071	-3.49884248
H	5.92263072	-0.73151277	-2.26105220
H	4.76500888	0.42032406	-1.56423696
H	4.75955877	0.09737917	-3.30948337

H	5.05398103	-3.07247367	-3.10061439
H	4.00525501	-2.16435229	-4.21359836
H	3.30872572	-3.38862845	-3.13112363
H	-3.55301543	0.27190112	-5.00130776
H	-1.83436150	0.57609458	-5.32413417
H	-2.54939676	1.10401557	-3.78834566
H	-1.80453240	-3.12384488	-4.57054543
H	-1.39980673	-1.88421010	-5.77783079
H	-3.09638826	-2.30314679	-5.46396084
H	-4.85019752	-1.36999143	-4.06454395
H	-6.47745190	-2.02156497	-2.30732776
H	-5.69494941	-2.47456843	0.00103542
H	0.67934482	-2.83502757	1.66677988
H	-2.25094690	-1.89587478	1.23796872
H	2.41006592	-3.56447793	4.09510594
H	0.66059319	-3.27997479	4.07719074
H	1.76509065	-1.94958332	3.69291038
H	2.03292673	-5.52900641	2.32086652
H	1.10576010	-5.18357536	0.84763105
H	0.29170701	-5.18499427	2.42746708
H	-4.57178692	-1.26323747	2.09328148
H	-3.74030143	-2.49116270	3.06738864
H	-5.03716338	-2.97671992	1.97222917
H	-3.52131900	-4.64460223	0.71350249
H	-2.31485692	-4.27871614	1.96903144
H	-1.87134485	-4.16632904	0.25551224
H	-4.39757511	1.10679322	4.50599444
H	-6.39562544	1.56927525	3.11070761
H	-6.13677045	2.09111619	0.69851768
H	-0.87955579	0.92484556	3.19346866
H	1.15759568	3.27632946	-1.84693378
H	-2.77895081	-0.16945829	5.33177766
H	-1.01925446	-0.37797394	5.24236454
H	-2.04850502	-1.07739717	3.98340230
H	-1.35353982	3.22585597	4.18585806
H	-0.63743083	2.11962521	5.37803362
H	-2.37898081	2.46852229	5.41497056
H	3.53091902	3.76504076	-3.73111626
H	1.81604461	3.65300754	-4.16777442
H	2.66387824	2.22129486	-3.54898660
H	1.69348737	5.54298552	-0.88116460
H	1.32214282	5.63007386	-2.61765787
H	3.00388374	5.72807146	-2.05778969
H	4.83588898	4.03357741	-1.91609418
H	6.48025548	3.20917369	-0.25370035
H	5.72264136	1.85061069	1.67922950
H	-2.91344686	1.89229252	-1.16792340
H	2.26300908	0.55853394	2.15119822
H	-5.92381878	2.47151367	-1.42466793
H	-5.19834783	0.85354191	-1.59044341
H	-4.76202272	2.14934578	-2.71788118
H	-3.49874138	4.20017241	-1.90187560

H	-2.75910583	4.24078495	-0.29185087
H	-4.51714757	4.41863707	-0.45881887
H	4.56774758	-0.54565862	2.19949157
H	3.75852191	-0.42909485	3.76899540
H	5.07779838	0.68313457	3.38325421
H	1.97553522	2.85034133	3.14438040
H	3.63798671	2.78768578	3.76258999
H	2.41159628	1.65311807	4.37611153
O	-0.79330060	1.39666591	-1.72421276
O	0.18225269	1.17938584	-2.73397617
O	1.21394335	0.37073666	-2.22556246
Zr	0.10159461	-0.13991286	-0.07311959
O	0.15222488	-0.44759457	1.72384268

### 3.6 Structures with five oxygen atoms

#### Peroxo Complex with adsorbed ozone group

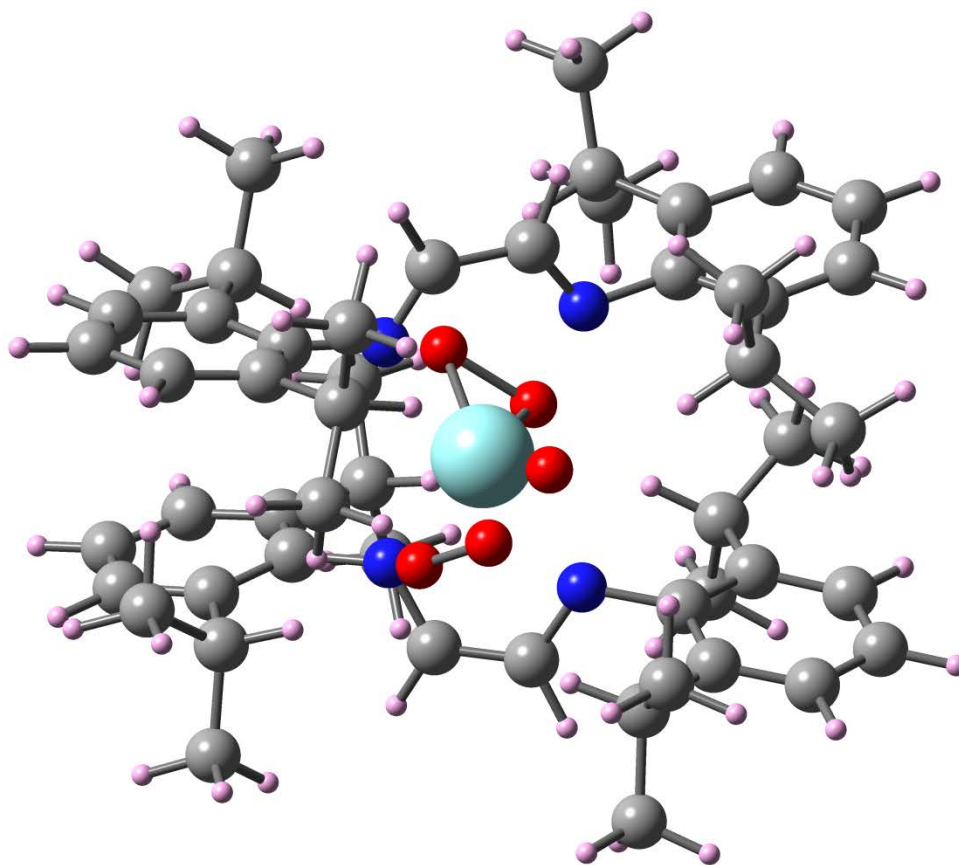


Fig. S36: NCCN Peroxo Complex with adsorbed ozone group

SCF	E <sub>ZP</sub>	H	G
-2666.185522	-2665.036398	-2664.965883	-2665.142607

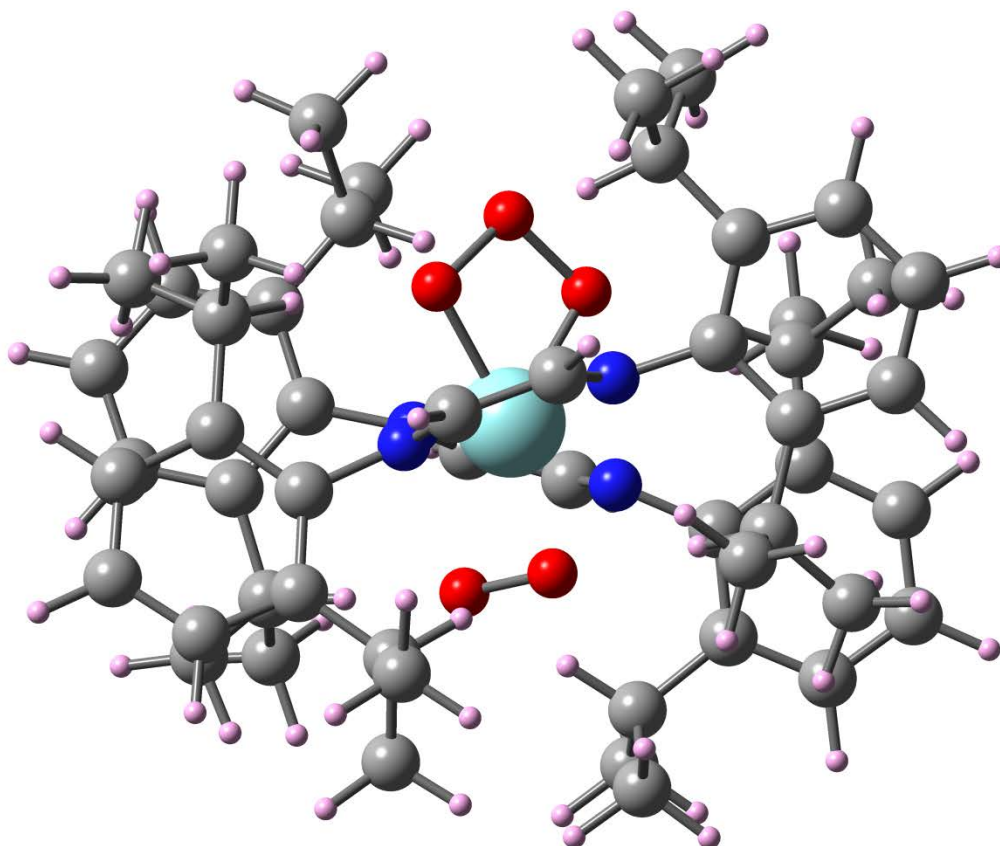
O	0.84574202	0.61197605	1.99707017
O	-0.98422814	-0.74949004	2.14066918
O	-0.50375309	0.62147906	-1.85288512
O	0.73603100	-0.29286202	-1.91265513
N	1.31632002	-1.99678716	0.42337305
N	-1.35067018	-1.95794913	-0.41107601
N	-1.38550514	1.92559317	0.52263806
N	1.41041307	2.02847915	-0.24543800
C	0.60423196	-3.14902224	0.32803505
C	-0.73555614	-3.13176722	-0.09662499
C	-0.70185508	3.02683925	0.42378605
C	0.69551103	3.08706823	-0.03167098
C	2.72212113	-2.15488619	0.78211208
C	3.70575021	-2.14995820	-0.25225100

C	5.05615930	-2.34728622	0.10551603
C	5.43477132	-2.56778324	1.43838313
C	4.45390426	-2.60543224	2.43806721
C	3.08898816	-2.40722621	2.13644919
C	4.33147526	-1.24769213	-2.58228818
C	3.32377318	-2.05644919	-1.73312411
C	3.15538915	-3.48532129	-2.32376416
C	-1.69094820	-1.13734206	-4.50511432
C	-1.54979320	-2.16563814	-3.35577723
C	-1.27735319	-3.58689225	-3.92134828
C	-2.67345228	-2.09634012	-1.01687406
C	-2.77556229	-2.18857513	-2.43611517
C	-4.05211439	-2.39071213	-3.00276021
C	-5.19707248	-2.50964713	-2.20174915
C	-5.07612347	-2.44342913	-0.80629204
C	-3.82242137	-2.24806112	-0.18654899
C	2.37580911	-1.55030713	4.43726536
C	2.06628908	-2.52464921	3.27240927
C	1.98530306	-3.98448932	3.79713431
C	-4.77908044	-1.38906905	2.03503818
C	-3.73446436	-2.29735113	1.34264512
C	-3.88213039	-3.76012624	1.84668016
C	-2.79103425	2.09147320	0.92770909
C	-3.11087227	2.32911122	2.29202020
C	-4.47014337	2.53000725	2.61808322
C	-5.46814944	2.50795726	1.63595015
C	-5.12132842	2.29520224	0.29279004
C	-3.78169732	2.09099421	-0.09540099
C	-2.38039422	1.42515014	4.56666837
C	-2.06750118	2.41233522	3.41301928
C	-1.95475316	3.86340333	3.95655232
C	1.83733311	1.69567612	-4.38048931
C	1.68624010	2.63664819	-3.15876922
C	1.49411810	4.10840831	-3.61691126
C	2.74782318	2.23536815	-0.80855004
C	2.87589919	2.52193817	-2.19641615
C	4.17925029	2.73306917	-2.69731419
C	5.30489736	2.66702116	-1.86592212
C	5.14653737	2.39878814	-0.49741902
C	3.87138826	2.18470113	0.06295203
C	-4.50370838	1.30233816	-2.43641417
C	-3.41469429	1.98779920	-1.58038610
C	-3.11305125	3.40009730	-2.15871914
C	4.86522833	1.24499605	2.24395019
C	3.70709325	2.02148112	1.57681114
C	3.54917325	3.41589523	2.24831219
H	5.81650835	-2.34280224	-0.67016603
H	6.48114238	-2.72274327	1.69153515
H	4.74741028	-2.79635726	3.46747628
H	2.35595311	-1.55628814	-1.81480212
H	-0.67651413	-1.86527513	-2.77423219
H	5.29415331	-1.76717418	-2.68606319

H	4.51892729	-0.25873806	-2.15019314
H	3.92779723	-1.10396712	-3.59295525
H	4.09817321	-4.04651334	-2.26190715
H	2.85819813	-3.42713328	-3.37953224
H	2.38550308	-4.05310033	-1.78703912
H	-2.53547726	-1.36923807	-5.16874337
H	-0.77753812	-1.13376307	-5.11467837
H	-1.82402320	-0.12963898	-4.09732529
H	-1.12482719	-4.31522831	-3.11387622
H	-0.37390212	-3.57900226	-4.54621633
H	-2.11434926	-3.94060627	-4.53915633
H	-4.14573140	-2.46753713	-4.08311229
H	-6.17111553	-2.66803713	-2.65930318
H	-5.96188255	-2.56085712	-0.18705599
H	1.08026500	-2.26643417	2.88075524
H	-2.74577828	-1.94589311	1.64570514
H	3.32624218	-1.79758916	4.92884740
H	1.58342405	-1.60415713	5.19567842
H	2.43374612	-0.51692006	4.07783033
H	2.94687813	-4.31182935	4.21423934
H	1.71376803	-4.68412637	2.99614525
H	1.22824700	-4.06308132	4.58901937
H	-4.71076242	-0.35704397	1.67633115
H	-4.60961642	-1.38493605	3.12027526
H	-5.80532250	-1.74125407	1.86344116
H	-4.86272447	-4.17294626	1.57350514
H	-3.78902038	-3.79764724	2.94053124
H	-3.11193634	-4.41337829	1.41797213
H	-4.74398539	2.70610327	3.65478230
H	-6.50847354	2.66138628	1.91186016
H	-5.89843547	2.29227825	-0.46463602
H	-1.08766511	2.13679818	3.01512025
H	0.77615703	2.31049118	-2.64957718
H	-3.31838029	1.68202817	5.07599441
H	-1.57584216	1.45395614	5.31263440
H	-2.46133624	0.39923006	4.19248934
H	-1.68156514	4.57517138	3.16550626
H	-1.18869410	3.91589132	4.74131138
H	-2.90546923	4.20002936	4.38972936
H	2.73023917	1.92740713	-4.97677336
H	0.96131104	1.79642713	-5.03494337
H	1.88889810	0.65581304	-4.04402329
H	1.34216210	4.78535336	-2.76413519
H	0.61876204	4.18847732	-4.27508931
H	2.36808218	4.47250233	-4.17353830
H	4.30750630	2.94745119	-3.75495126
H	6.29803647	2.82851316	-2.27810915
H	6.02111140	2.36024912	0.14446903
H	-2.50124523	1.39149614	-1.67955811
H	2.78685918	1.46160209	1.76977615
H	-5.39671247	1.93332821	-2.54444717
H	-4.80559542	0.34010909	-2.01152313



H	-4.11238836	1.11450914	-3.44360224
H	-2.83356424	3.31858029	-3.21676722
H	-2.28781319	3.89783333	-1.63365111
H	-3.99764232	4.04719136	-2.08445514
H	5.04039233	0.28287898	1.75190515
H	4.61708331	1.04538004	3.29437227
H	5.80324839	1.81694609	2.23427119
H	2.68734719	3.96721428	1.84998816
H	4.44496733	4.02982927	2.08375418
H	3.40494324	3.30098822	3.33060528
O	-0.03542706	-0.05532600	2.89819524
H	-1.27122620	-4.07116029	-0.21652600
H	1.08022199	-4.10113532	0.55613106
H	-1.17066010	3.98864733	0.64576907
H	1.09259107	4.08815231	-0.21835700
Zr	-0.03037706	-0.14745400	-0.02845798

$\eta^2$ -ozone Complex with adsorbed O<sub>2</sub> moleculeFig. S37: NCCN  $\eta^2$ -ozone Complex with adsorbed O<sub>2</sub> molecule

SCF	E <sub>ZP</sub>	H	G
-2666.184038	-2665.034724	-2664.964258	-2665.140264

O	-0.87215607	0.67602805	-1.96309015
O	1.00863508	-0.68424805	-2.00928115
O	0.51267204	0.42994803	1.86780514
O	-0.69785205	-0.24421002	1.97623315
N	-1.41304611	-1.95540315	-0.48177604
N	1.21916209	-2.03315915	0.37573203
N	1.49034411	1.91659415	-0.47523804
N	-1.27825910	2.05589116	0.31094902
C	-0.78151406	-3.14782224	-0.32414202
C	0.55257504	-3.18786024	0.11337501
C	0.83834407	3.03497123	-0.38074803
C	-0.55374904	3.10741124	0.08506601
C	-2.82521622	-2.04268316	-0.84217207
C	-3.80012229	-2.09270316	0.19695402
C	-5.15762440	-2.23286117	-0.16292701
C	-5.54595442	-2.34486518	-1.50603812

C	-4.57089935	-2.32819018	-2.51356819
C	-3.20060624	-2.18121717	-2.20926517
C	-4.27857233	-1.15733509	2.54325020
C	-3.41470526	-2.10792616	1.68055413
C	-3.49013927	-3.55740927	2.23748417
C	1.47680211	-1.44100511	4.49576234
C	1.38461711	-2.44032319	3.31550625
C	1.16138209	-3.88573030	3.83937529
C	2.53342119	-2.20373017	0.99165708
C	2.61739220	-2.38423418	2.40491018
C	3.88865330	-2.59871120	2.98002423
C	5.04575638	-2.65304320	2.19115616
C	4.94249238	-2.51271419	0.79926606
C	3.69675128	-2.29990718	0.17043001
C	-2.48797419	-1.25004709	-4.48341734
C	-2.17511517	-2.25118117	-3.34446425
C	-2.07839216	-3.69842328	-3.90092230
C	4.77479836	-1.52039911	-2.03304416
C	3.61840828	-2.29611818	-1.35959410
C	3.58173727	-3.75686929	-1.89188315
C	2.90376222	2.03133116	-0.86194306
C	3.25491725	2.22775417	-2.22403217
C	4.62565436	2.38453618	-2.52565319
C	5.60456144	2.35439418	-1.52412912
C	5.22725440	2.17479716	-0.18418101
C	3.87479029	2.01594916	0.17868601
C	2.55476419	1.31739810	-4.50297834
C	2.22973317	2.31091918	-3.35985726
C	2.12979916	3.76159729	-3.90597030
C	-1.60834512	1.79303414	4.47637334
C	-1.48248612	2.70469120	3.22953425
C	-1.27323310	4.18479832	3.65339728
C	-2.60166920	2.29096517	0.90240807
C	-2.69366420	2.57922719	2.29421217
C	-3.98130830	2.80592721	2.82795622
C	-5.12571939	2.76437121	2.02149716
C	-5.00169038	2.51312819	0.64637505
C	-3.74437829	2.28107618	0.05324300
C	4.48579534	1.16939309	2.53270819
C	3.47528926	1.94480415	1.65701013
C	3.27787725	3.37834826	2.22814517
C	-4.82669037	1.44689911	-2.12723216
C	-3.61772527	2.14702316	-1.46702211
C	-3.41032926	3.54970227	-2.10788716
H	-5.91360243	-2.27239418	0.61704605
H	-6.59652753	-2.45915619	-1.76352113
H	-4.87359737	-2.43806019	-3.55184727
H	-2.37650218	-1.78007314	1.77187013
H	0.50402604	-2.16707617	2.72988921
H	-5.32774739	-1.47991611	2.58206920
H	-4.25251233	-0.13297001	2.15753316
H	-3.90117030	-1.14277509	3.57458127

H	-4.51352434	-3.95086730	2.17177216
H	-3.18405824	-3.57747828	3.29237225
H	-2.83252721	-4.23551232	1.67924713
H	2.32272518	-1.66978113	5.15760639
H	0.55991604	-1.48463812	5.09884139
H	1.59131912	-0.41624703	4.12548532
H	1.04523908	-4.59659935	3.01106123
H	0.25456202	-3.93141630	4.45760434
H	2.00719815	-4.22285432	4.45323434
H	3.96801230	-2.73856921	4.05538831
H	6.01586546	-2.82149522	2.65333920
H	5.83806444	-2.58539120	0.18859401
H	-1.19464809	-1.98001115	-2.94990323
H	2.68487620	-1.81684114	-1.66430813
H	-3.44617527	-1.46946311	-4.97466738
H	-1.70001713	-1.29762910	-5.24585940
H	-2.51726819	-0.22604902	-4.09581831
H	-3.03469123	-4.02626431	-4.33120733
H	-1.80216714	-4.41366634	-3.11481124
H	-1.31550810	-3.74989229	-4.68925936
H	4.86072237	-0.50295304	-1.63757812
H	4.58853935	-1.44858411	-3.11270424
H	5.74315846	-2.02322815	-1.90170015
H	4.49439934	-4.30201833	-1.61298513
H	3.50297027	-3.75701229	-2.98726823
H	2.72189221	-4.30877533	-1.49327911
H	4.92318838	2.53025419	-3.56035327
H	6.65374148	2.47432319	-1.78289913
H	5.98945248	2.16249017	0.58877604
H	1.24737909	2.02167916	-2.98165923
H	-0.58195604	2.37892718	2.70267321
H	3.51013427	1.55029112	-4.99263738
H	1.76594714	1.35880210	-5.26449840
H	2.59546120	0.29363602	-4.11760331
H	1.84664514	4.47617234	-3.12023624
H	1.37359011	3.81366929	-4.70016836
H	3.08678123	4.09688231	-4.32778133
H	-2.46789619	2.06948716	5.10093939
H	-0.70540005	1.88010614	5.09506239
H	-1.71503013	0.74575606	4.17594332
H	-1.13584709	4.84229237	2.78384721
H	-0.38564203	4.27548533	4.29350733
H	-2.13604416	4.56193735	4.21748432
H	-4.08247231	3.01940223	3.88861230
H	-6.10654649	2.93759722	2.45752819
H	-5.89007246	2.50342719	0.02313400
H	2.51581819	1.42403511	1.73373213
H	-2.72753921	1.55288812	-1.69782313
H	5.43674541	1.70943413	2.63551320
H	4.69345536	0.17627901	2.12308116
H	4.07445831	1.03827908	3.54164027
H	2.96864922	3.32834326	3.28047625

H	2.51342819	3.94249330	1.67775513
H	4.21527932	3.94764830	2.17287617
H	-5.04544139	0.48598604	-1.65083913
H	-4.60431435	1.25321510	-3.18395124
H	-5.73245945	2.06838116	-2.09298516
H	-2.51175719	4.05005631	-1.72422413
H	-4.27117333	4.20255832	-1.90809315
H	-3.29744925	3.45103926	-3.19513825
O	0.06563600	0.02612200	-2.95628723
H	1.03631408	-4.14716032	0.28515402
H	-1.31752810	-4.07387131	-0.52104604
H	1.32137510	3.98857730	-0.60694505
H	-0.94407607	4.11009031	0.27541702
Zr	-0.01175900	-0.16996601	-0.24313102

### 3.7 Structures with six oxygen atoms

#### $\eta^2$ -ozone Complex with adsorbed ozone group

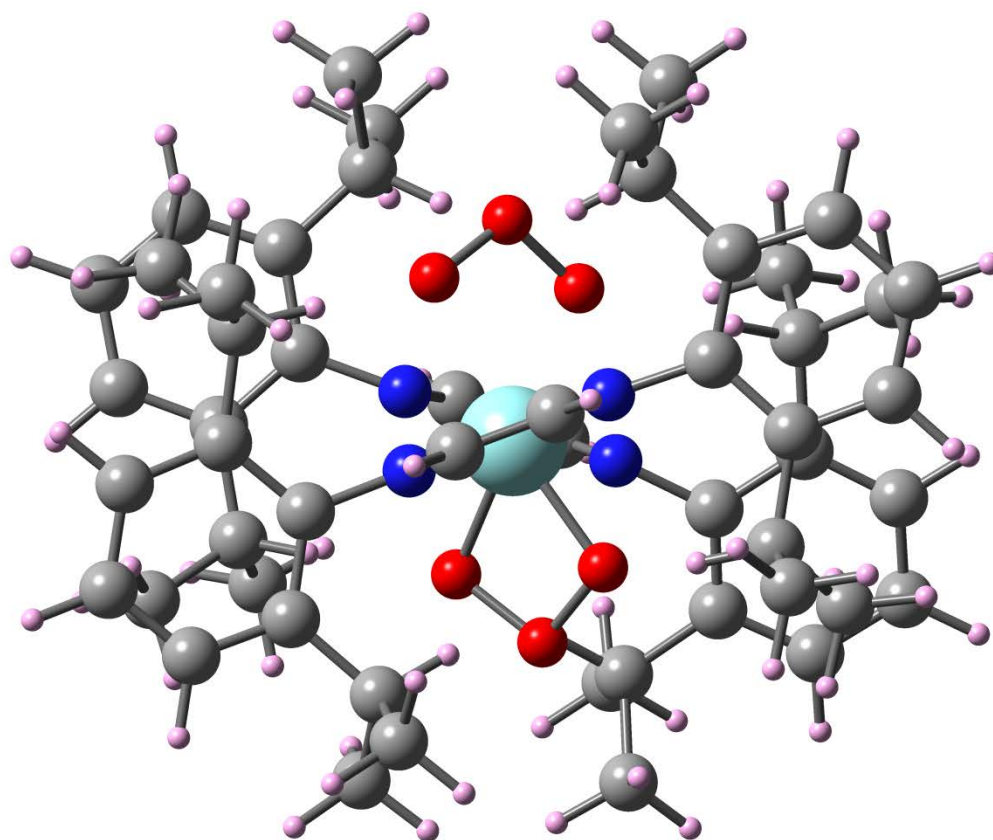


Fig. S38: NCCN  $\eta^2$ -ozone Complex with adsorbed ozone group

SCF	$E_{ZP}$	H	G
-2741.319046	-2740.166505	-2740.095068	-2740.274636

Zr	0.04618909	0.09431848	0.16929740
O	0.87957945	0.45677625	-1.97008282
O	-0.99014092	1.63104788	-1.38851762
O	-0.70086607	-1.57870579	1.20505098
O	1.26009317	-0.46813704	1.76032978
N	1.34959379	1.99736648	0.61681710
N	-1.25909861	1.42776514	1.46816939
N	-1.42864896	-1.31670317	-1.44680718
N	1.34232483	-1.97933403	-0.82094369
C	0.68483938	2.84824741	1.44047337
C	-0.62495672	2.56788209	1.85988776
C	-0.78669493	-2.33002141	-1.94990558
C	0.58374477	-2.70367822	-1.58500281
C	2.72319358	2.40580093	0.30471833

C	3.78600205	2.05720075	1.19162160
C	5.09056072	2.50315900	0.88396110
C	5.35016619	3.29327602	-0.24345055
C	4.28753156	3.67673912	-1.07256952
C	2.96461775	3.26061699	-0.81182477
C	4.47083044	0.05134966	2.62951832
C	3.57139977	1.30595606	2.51009771
C	3.79883907	2.25913215	3.71558739
C	-1.87316334	-1.48055887	4.45380345
C	-1.62151064	-0.00922048	4.04382634
C	-1.31921778	0.86393961	5.29300547
C	-2.60829817	1.27838974	2.01729176
C	-2.78823837	0.58689836	3.25052748
C	-4.08523872	0.53285165	3.80422261
C	-5.17565267	1.14976278	3.17499341
C	-4.97670968	1.85244770	1.97831961
C	-3.69936080	1.94389515	1.38370842
C	2.08089168	3.61893838	-3.19114409
C	1.83895494	3.83616165	-1.67663867
C	1.64129067	5.34711713	-1.37118271
C	-4.53599971	2.48994610	-0.98028989
C	-3.52654996	2.82819161	0.14320441
C	-3.63579128	4.32985794	0.52844839
C	-2.81368422	-1.15548828	-1.92274427
C	-3.06058188	-0.65600878	-3.23257359
C	-4.40604997	-0.54467055	-3.64782890
C	-5.46372710	-0.93064751	-2.81598142
C	-5.19124169	-1.46350290	-1.54717040
C	-3.87012778	-1.59960103	-1.07542317
C	-2.14694854	1.16021676	-4.78482530
C	-1.96244478	-0.27765516	-4.23590372
C	-1.91164994	-1.29871448	-5.40637556
C	1.53831319	-4.61422420	2.51356766
C	1.44690273	-4.39781721	0.98162313
C	1.23536545	-5.76334488	0.26844524
C	2.63605340	-2.54850571	-0.44709789
C	2.68398347	-3.67969489	0.42019081
C	3.95937860	-4.18067043	0.76309830
C	5.13433417	-3.60575508	0.26401106
C	5.05749387	-2.51494147	-0.61571958
C	3.81672239	-1.96817588	-0.99470403
C	-4.72085819	-2.14261162	1.29409357
C	-3.59917392	-2.32322859	0.24726879
C	-3.37630974	-3.84096786	-0.01390709
C	4.99661896	0.03071608	-2.11572504
C	3.74525158	-0.87169390	-2.06068078
C	3.49680747	-1.50328038	-3.46059222
H	1.17329537	3.75664494	1.78767313
H	-1.13424068	3.26122077	2.52549610
H	-1.27924824	-2.99182173	-2.66638468
H	0.93067577	-3.66125589	-1.97956253
H	5.90728035	2.23928748	1.55114033

H	6.36300563	3.62503438	-0.46017017
H	4.48060906	4.32536575	-1.92347046
H	2.54108628	0.95226504	2.55280853
H	-0.72925042	-0.00447678	3.41710204
H	5.53928562	0.30886171	2.64418289
H	4.29167949	-0.63856673	1.79808036
H	4.24293044	-0.48253371	3.56162219
H	4.83222300	2.63098160	3.74735685
H	3.60098151	1.72937705	4.65721567
H	3.13173188	3.13036641	3.66960638
H	-2.73849023	-1.58142324	5.12348541
H	-0.99414951	-1.87485183	4.97944471
H	-2.03879571	-2.10140439	3.56665850
H	-1.08537599	1.89878694	5.01032470
H	-0.45666432	0.45741082	5.83765168
H	-2.17563003	0.88847574	5.98065676
H	-4.23675455	0.01318257	4.74672585
H	-6.16622657	1.09808594	3.62118633
H	-5.81800000	2.35356206	1.50610389
H	0.90783422	3.33456135	-1.41098652
H	-2.52682788	2.66792587	-0.26454113
H	2.95867197	4.17592539	-3.54519056
H	1.21264906	3.96784913	-3.76570880
H	2.23489889	2.55769142	-3.41674524
H	2.54431014	5.92390027	-1.61119017
H	1.41079353	5.51176465	-0.31065830
H	0.81123396	5.75088921	-1.96668160
H	-4.47085364	1.43649949	-1.27030260
H	-4.32441868	3.10078914	-1.86819326
H	-5.57134038	2.69589455	-0.67635229
H	-4.62735486	4.56272950	0.93960745
H	-3.47783903	4.96145691	-0.35626799
H	-2.88726746	4.60800671	1.28121954
H	-4.62126898	-0.15315144	-4.63835772
H	-6.49128994	-0.83044041	-3.15663145
H	-6.01300700	-1.78520797	-0.91611881
H	-0.99036982	-0.30645035	-3.73825530
H	0.56221653	-3.77831686	0.81283367
H	-3.05835462	1.24823732	-5.39018909
H	-1.29573246	1.42994986	-5.42323033
H	-2.20607974	1.88767086	-3.96861485
H	-1.73119978	-2.32152047	-5.04843191
H	-1.10607319	-1.03490684	-6.10419742
H	-2.85499451	-1.30800491	-5.96736975
H	2.34349389	-5.31021723	2.78347584
H	0.59593222	-5.03958404	2.88353832
H	1.70527453	-3.66343859	3.02765650
H	1.11665405	-5.65183310	-0.81817858
H	0.33704432	-6.25929176	0.65970247
H	2.09001439	-6.43192234	0.43665879
H	4.02674193	-5.03214401	1.43426159
H	6.10295364	-4.00920451	0.54913651



H	5.97070029	-2.08728160	-1.01600010
H	-2.67454099	-1.93477709	0.68613814
H	2.88704555	-0.22828703	-1.84173453
H	-5.63778048	-2.67797321	1.01049110
H	-4.96643103	-1.08726934	1.44669733
H	-4.38983820	-2.55042063	2.25695975
H	-3.16501951	-4.35461480	0.93253969
H	-2.53100509	-4.02706528	-0.68840893
H	-4.27148034	-4.29484231	-0.46094560
H	5.23942037	0.44534215	-1.13212919
H	4.81145609	0.87270267	-2.79369043
H	5.87477802	-0.50878347	-2.49654558
H	2.57204467	-2.09254051	-3.48925437
H	4.32937591	-2.16367521	-3.73934672
H	3.41367447	-0.71445901	-4.21921563
O	-0.05905924	1.43165955	-2.41454320
O	0.45201758	-1.66704126	2.18523095

## 4. NCCN Singlet Transition States

## Spiro Bisperoxo Complex to Oxo Peroxo Complex

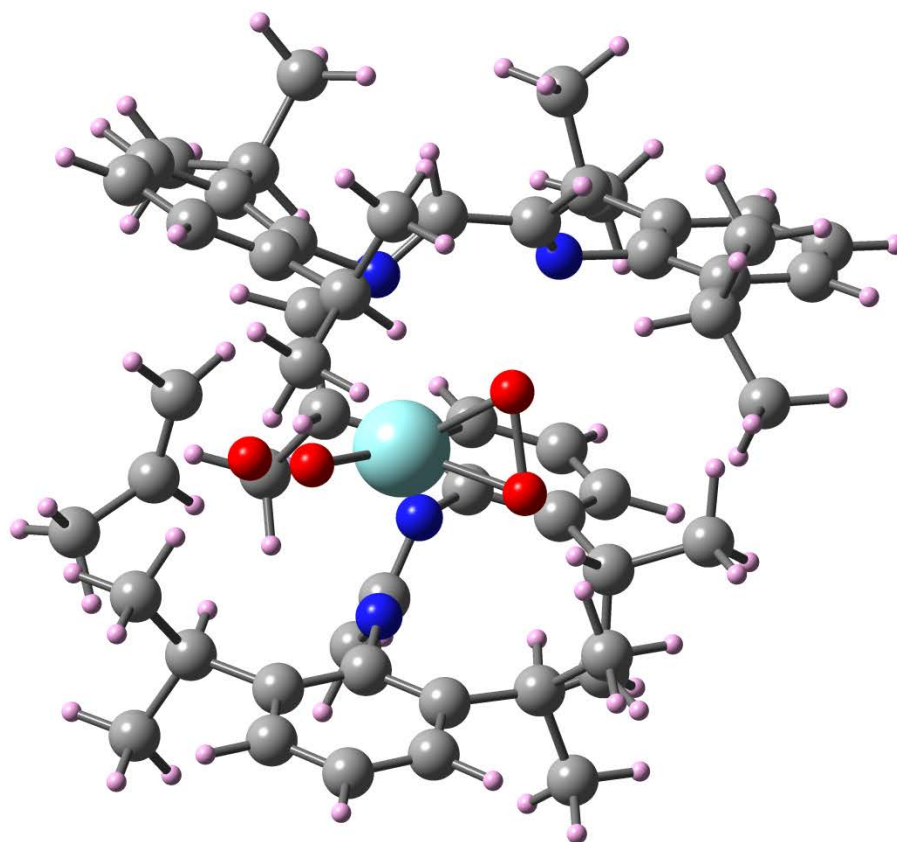


Fig. S39: NCCN Spiro Bisperoxo Complex to Oxo Peroxo Complex

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2708.874771	-2707.647817	-2707.573331	-2707.758703	-477

Zr	0.86751388	-0.05151127	-0.29104538
O	2.55778663	0.67904627	-0.77096074
N	-2.95035238	0.47938398	-1.11796693
N	-0.27303250	2.11710207	-1.20162699
N	2.49114772	-1.67803467	0.72678059
N	0.00989836	-1.02951770	1.91921352
C	-2.39581301	1.11130585	-2.10015345
C	-1.32207808	2.11292555	-1.97202423
C	2.32749540	-1.79808661	2.00692989
C	0.98969931	-1.57169178	2.58714379
C	-4.04887062	-0.41369901	-1.34261091
C	-4.04158521	-1.42771249	-2.35520448
C	-5.17748531	-2.26291357	-2.44711926
C	-6.27992935	-2.11245347	-1.59556097

C	-6.27013666	-1.11114275	-0.60891562
C	-5.16541755	-0.25458762	-0.46045088
C	-2.43170793	-3.14605619	-3.39269024
C	-2.88288817	-1.66469535	-3.33857503
C	-3.27506168	-1.18635854	-4.76516542
C	3.27541898	1.91916817	-3.58273724
C	1.78405794	2.26240599	-3.35778185
C	1.11204970	2.65847997	-4.70370263
C	0.55111906	3.33562481	-1.33634819
C	1.57343849	3.37608421	-2.32342742
C	2.35192233	4.55034959	-2.40797258
C	2.11797358	5.64825878	-1.56898464
C	1.06421609	5.60528535	-0.64361636
C	0.25204071	4.45914694	-0.51546960
C	-6.10194259	0.63736687	1.77054585
C	-5.18095733	0.89058299	0.55630647
C	-5.58438481	2.22415227	-0.13550799
C	-0.75834100	5.35288183	1.69024924
C	-0.96712287	4.49133892	0.41978489
C	-2.22217289	5.02085015	-0.33249871
C	3.71950699	-2.11763029	0.08225557
C	4.95333825	-1.44260518	0.30054024
C	6.09333664	-1.92829292	-0.37503622
C	6.02779269	-3.03778051	-1.22699464
C	4.80319849	-3.69366262	-1.41587126
C	3.62832926	-3.25203598	-0.77602598
C	5.67175075	0.99489931	0.40685476
C	5.11706235	-0.21475428	1.20212060
C	6.02668179	-0.55270242	2.41494466
C	-2.48196513	-4.16731769	0.33228657
C	-1.41844528	-3.48887408	1.22886410
C	-0.66942023	-4.57552260	2.05070506
C	-1.33491611	-1.22285989	2.49149332
C	-2.01769783	-2.42941521	2.16244483
C	-3.26867591	-2.66148795	2.77016501
C	-3.82734174	-1.74369223	3.67093902
C	-3.14406037	-0.55743242	3.96562709
C	-1.89308344	-0.27011309	3.38054666
C	2.00439162	-4.33651051	-2.43017943
C	2.34302818	-4.06761326	-0.94472337
C	2.45040736	-5.39879192	-0.14989013
C	-2.07027234	2.26900331	3.60121987
C	-1.16998759	1.01960396	3.76483751
C	-0.62241988	0.93575018	5.21571991
H	-2.77823635	1.04427092	-3.12556165
H	-1.45298738	2.94634450	-2.67349954
H	3.10321101	-2.19399301	2.66709225
H	0.81879086	-2.00145204	3.57867875
H	-5.19312744	-3.04404023	-3.20257694
H	-7.14112839	-2.76885275	-1.69823370
H	-7.12846772	-0.99973568	0.04601320
H	-1.99944423	-1.10973790	-3.01094740

H	1.30198591	1.34719228	-3.00476001
H	-3.22623902	-3.81675911	-3.74750597
H	-2.09655167	-3.48539196	-2.40896618
H	-1.58050932	-3.23902411	-4.07886778
H	-4.10903001	-1.77943817	-5.16544627
H	-2.42146787	-1.29724927	-5.44670146
H	-3.58883359	-0.13337964	-4.77986556
H	3.83442607	2.75590808	-4.02456519
H	3.35642984	1.06830100	-4.27237840
H	3.73500972	1.63205389	-2.63300203
H	0.03599243	2.84817858	-4.58738105
H	1.23372533	1.84883869	-5.43519101
H	1.56619950	3.56774946	-5.12113284
H	3.14775220	4.60253544	-3.14522362
H	2.73746710	6.53859013	-1.64886361
H	0.86642696	6.47395182	-0.02285072
H	-4.15164303	1.00839135	0.91974464
H	-1.18673947	3.46285785	0.73682425
H	-7.16348872	0.64674539	1.48755150
H	-5.95851524	1.43067093	2.51644509
H	-5.87916749	-0.32279615	2.24861338
H	-6.60483534	2.15736778	-0.53657748
H	-4.90895142	2.46849382	-0.96332906
H	-5.55521492	3.05441027	0.58382510
H	0.15440134	5.08142729	2.23163765
H	-1.61156236	5.22641087	2.36900641
H	-0.69934612	6.42073389	1.44435923
H	-2.04187540	6.03687237	-0.70753330
H	-3.08800782	5.05315822	0.34267558
H	-2.48898958	4.39148005	-1.18863736
H	7.04321525	-1.41929182	-0.23513799
H	6.92169229	-3.38946188	-1.73670580
H	4.75538653	-4.56222541	-2.06676360
H	4.13484412	0.10258112	1.56164264
H	-0.70297748	-3.00155576	0.55572410
H	6.65482005	0.78441321	-0.03564837
H	5.78330428	1.86224234	1.07180550
H	4.96466956	1.25935691	-0.38437419
H	5.60984564	-1.36750186	3.02499679
H	6.15445047	0.32789607	3.05813093
H	7.02571816	-0.86870657	2.08731451
H	-3.15417796	-4.81530122	0.91050447
H	-1.98236643	-4.79898844	-0.41239714
H	-3.08952530	-3.42787291	-0.19995303
H	0.15373585	-4.15738869	2.64450163
H	-0.24674228	-5.33439460	1.38108084
H	-1.35801935	-5.07569348	2.74508237
H	-3.81110545	-3.57156485	2.53404231
H	-4.78720344	-1.95234325	4.13690578
H	-3.58280917	0.15529411	4.65887960
H	1.50752681	-3.48987968	-0.54154838
H	-0.31899242	1.13936929	3.08924344

H	2.77181670	-4.94493650	-2.92809991
H	1.88924913	-3.38854641	-2.96356764
H	1.05082255	-4.87657654	-2.50109757
H	1.52186532	-5.97713365	-0.24889354
H	2.63172411	-5.22013030	0.91930268
H	3.27467354	-6.01862332	-0.52747032
H	-2.47939285	2.33196729	2.58531334
H	-1.49109375	3.17926880	3.79964736
H	-2.91311419	2.25440158	4.30359812
H	0.06547439	0.08858592	5.34101518
H	-1.44295800	0.80197413	5.93233192
H	-0.08618982	1.85578992	5.48144306
O	-0.11937803	-0.51119243	-2.04429368
O	0.49790210	-1.76284286	-1.39432296
C	2.24564160	2.05514356	3.13430511
H	1.66636473	1.33257143	3.70373606
C	1.63885029	2.75014616	2.10238097
H	0.56229862	2.73312041	1.97879712
O	2.16756750	1.34049965	0.96503079
H	2.15614989	3.56256121	1.60244723
C	3.68019961	2.24925935	3.54128874
H	4.18888563	1.29242598	3.70721109
H	4.23369513	2.80607336	2.77816671
H	3.73917214	2.81183967	4.48774471

## Oxo Peroxo Complex to Dioxo Complex (conformation 1 higher energy)

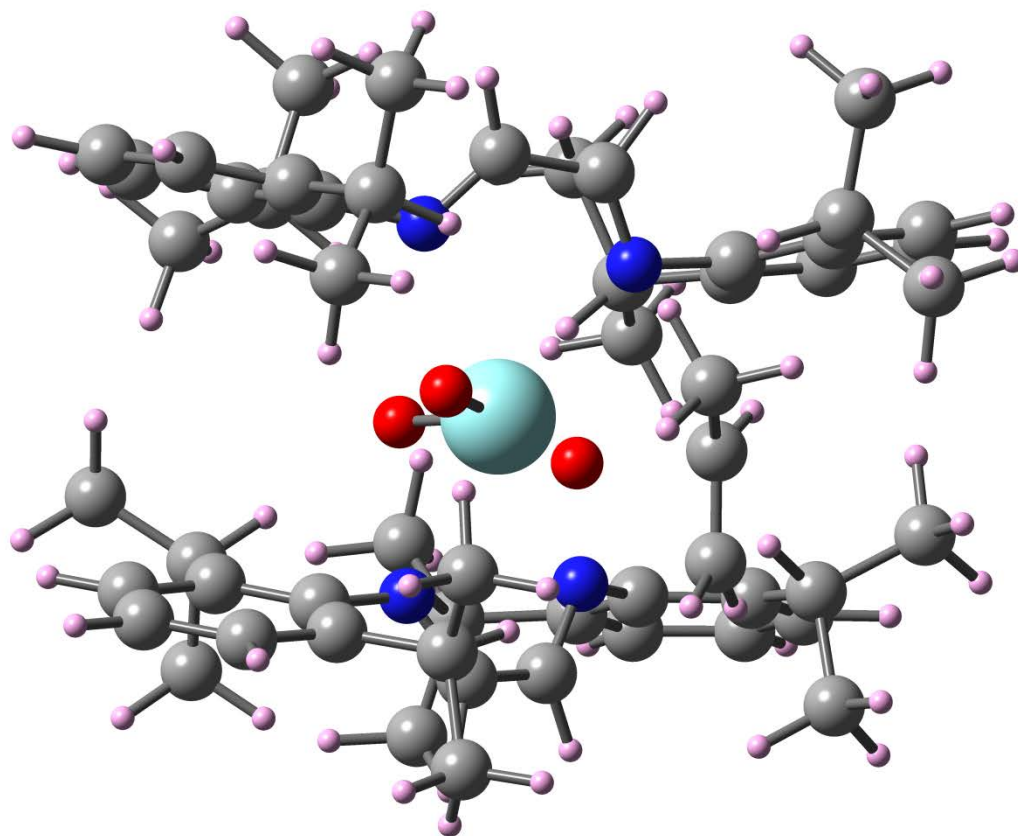


Fig. S40: NCCN Oxo Peroxo Complex to Dioxo Complex (conformation 1 higher energy)

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2633.71649206	-2632.491787	-2632.419069	-2632.598800	-498

Zr	-0.12997200	-0.00694400	-0.05016100
O	-0.44239300	-0.60689600	-1.77987800
N	1.59518900	1.94195200	-0.15510500
N	-1.11586300	2.26369100	-0.90012600
N	-1.55939700	-2.11096000	0.71185500
N	1.25715500	-2.10119100	0.28945900
C	1.01842700	3.11124200	-0.28045200
C	-0.40704200	3.28831500	-0.52317900
C	-0.80261400	-3.04219700	1.20369200
C	0.61169500	-3.10072400	0.82432900
C	3.06126900	1.98512400	-0.11846300
C	3.75134700	2.61108200	0.96207300
C	5.16064800	2.67815300	0.89287700
C	5.86649400	2.15319800	-0.19588100
C	5.16651400	1.56101500	-1.25823200
C	3.75966800	1.47849800	-1.25519200

C	3.67154600	2.77353600	3.52113600
C	3.06127600	3.25201600	2.17715600
C	3.13712800	4.80377100	2.11128000
C	-4.14807900	2.50602900	2.01024600
C	-3.20423400	3.28725900	1.06299100
C	-3.31615400	4.81643100	1.30857400
C	-2.48947600	2.44772600	-1.30557700
C	-3.47774700	2.94224400	-0.40577400
C	-4.79091000	3.09128400	-0.90189000
C	-5.11589900	2.77981000	-2.22903300
C	-4.12004500	2.31128100	-3.10211000
C	-2.79385400	2.13557500	-2.66506000
C	3.83827500	0.02047900	-3.37789400
C	3.01461700	0.99338700	-2.50520900
C	2.59300800	2.21374300	-3.37376100
C	-2.14555400	0.84001100	-4.79856600
C	-1.68072100	1.75709600	-3.64660800
C	-1.04511300	3.05086000	-4.23200700
C	-2.98480300	-2.13492600	0.94557000
C	-3.82292600	-2.21698400	-0.20738800
C	-5.21573600	-2.26071700	-0.01025300
C	-5.77235600	-2.22378200	1.27835900
C	-4.93204500	-2.14321100	2.39552400
C	-3.52760900	-2.09772800	2.26255800
C	-4.14143500	-1.85327000	-2.73331900
C	-3.22307500	-2.37447600	-1.60640800
C	-2.88196400	-3.86993800	-1.86911700
C	4.99979700	-0.89904700	2.18201300
C	3.75367800	-1.74296800	1.83028300
C	3.63218300	-2.92764500	2.83142900
C	2.54124000	-2.46297200	-0.32580000
C	3.75217600	-2.26788700	0.39176300
C	4.95594500	-2.68027200	-0.21534700
C	4.95983300	-3.28459300	-1.48204000
C	3.75072400	-3.48461000	-2.16233500
C	2.51572900	-3.08202600	-1.60882200
C	-3.08927000	-0.70793700	4.34550500
C	-2.68179100	-1.96268400	3.53310700
C	-2.76863300	-3.24135400	4.40874700
C	1.24757200	-2.83797600	-3.82541500
C	1.21933300	-3.38113300	-2.37563400
C	0.93496400	-4.90842900	-2.37039900
H	1.62119400	4.02237600	-0.28617800
H	-0.80967200	4.30175100	-0.46553700
H	-1.19324900	-3.87033400	1.80089100
H	1.08876100	-4.08131500	0.91324100
H	5.70867900	3.14819900	1.70488000
H	6.95163200	2.21440800	-0.22375800
H	5.71876800	1.17451100	-2.10790000
H	2.00247300	2.97101900	2.17755000
H	-2.19533300	2.95174200	1.31779900
H	4.69584700	3.14449600	3.65128500

H	3.69957300	1.68094300	3.59116100
H	3.07482900	3.15410300	4.35977200
H	4.18102400	5.14244600	2.12532300
H	2.62616200	5.24691100	2.97621300
H	2.67481700	5.20664100	1.20148400
H	-5.20307800	2.76909200	1.85394000
H	-3.89901500	2.73191700	3.05655900
H	-4.01655100	1.43224200	1.85015700
H	-2.62927300	5.38791000	0.66807700
H	-3.08219600	5.05170000	2.35599500
H	-4.33237300	5.17920400	1.10339600
H	-5.56939400	3.44827600	-0.23270200
H	-6.13688800	2.90385900	-2.58312400
H	-4.37531800	2.08389200	-4.13262300
H	2.09583400	0.47446700	-2.20098000
H	-0.92376900	1.19801900	-3.08380100
H	4.67302500	0.53193300	-3.87671900
H	3.19788700	-0.39581400	-4.16394600
H	4.23850300	-0.81371900	-2.79415300
H	3.47974600	2.76800100	-3.71062700
H	1.94114800	2.90721700	-2.83173500
H	2.04547100	1.86920600	-4.25946400
H	-2.63421700	-0.05754700	-4.40932900
H	-1.27405000	0.51980400	-5.38478900
H	-2.83576700	1.34770700	-5.48725100
H	-1.79172500	3.62856700	-4.79471000
H	-0.22424600	2.79842700	-4.91633500
H	-0.64118700	3.70186300	-3.44565500
H	-5.87339300	-2.32522800	-0.87088700
H	-6.85188100	-2.25531300	1.40767400
H	-5.36895300	-2.10304200	3.38999100
H	-2.28669600	-1.80255500	-1.65207400
H	2.87046200	-1.10332600	1.95512800
H	-5.05813800	-2.45120400	-2.83473100
H	-3.60909600	-1.91515500	-3.69072500
H	-4.42367400	-0.80673300	-2.56781300
H	-2.19498400	-4.27197900	-1.11364500
H	-2.40326700	-3.97926400	-2.85158100
H	-3.79221800	-4.48633400	-1.86042200
H	5.90756700	-1.51550400	2.22015300
H	4.87499000	-0.44961600	3.17583000
H	5.16114600	-0.09389300	1.45909300
H	2.71168900	-3.50413500	2.67899000
H	3.63406500	-2.55902100	3.86551000
H	4.48007700	-3.61496400	2.71249100
H	5.89467300	-2.54083600	0.31207400
H	5.89746800	-3.60484700	-1.93007300
H	3.75929400	-3.96397000	-3.13759400
H	-1.64155200	-1.79649600	3.24693000
H	0.38894900	-2.85678300	-1.89530800
H	-4.13606500	-0.74900300	4.67473500
H	-2.94120600	0.18709300	3.73446100



H	-2.46258600	-0.62299700	5.24483300
H	-2.12863300	-3.14161000	5.29652000
H	-2.45056100	-4.13788300	3.85792900
H	-3.79522100	-3.41883200	4.75621500
H	1.30053900	-1.74543800	-3.81239300
H	0.31679100	-3.11377400	-4.33767600
H	2.08641700	-3.23817000	-4.41137900
H	0.87306300	-5.31114300	-1.34980600
H	1.72479200	-5.46256200	-2.89580800
H	-0.01762300	-5.11723000	-2.87344800
O	-1.64712000	0.65867800	0.99995000
O	-0.39199900	0.10975400	2.29902400
C	0.81263300	0.64986500	3.57225400
H	1.64769000	0.97691300	2.95683600
C	0.79572700	-0.68578500	3.96939300
H	1.47390100	-1.41822100	3.55118100
H	0.06368900	-1.03697400	4.68999500
C	0.08601600	1.74314000	4.32458100
H	-0.79318400	1.33658100	4.83427800
H	0.74129500	2.20850600	5.07640600
H	-0.25858500	2.52045700	3.63313900

## Oxo Peroxo Complex to Dioxo Complex (conformation 2 lower energy)

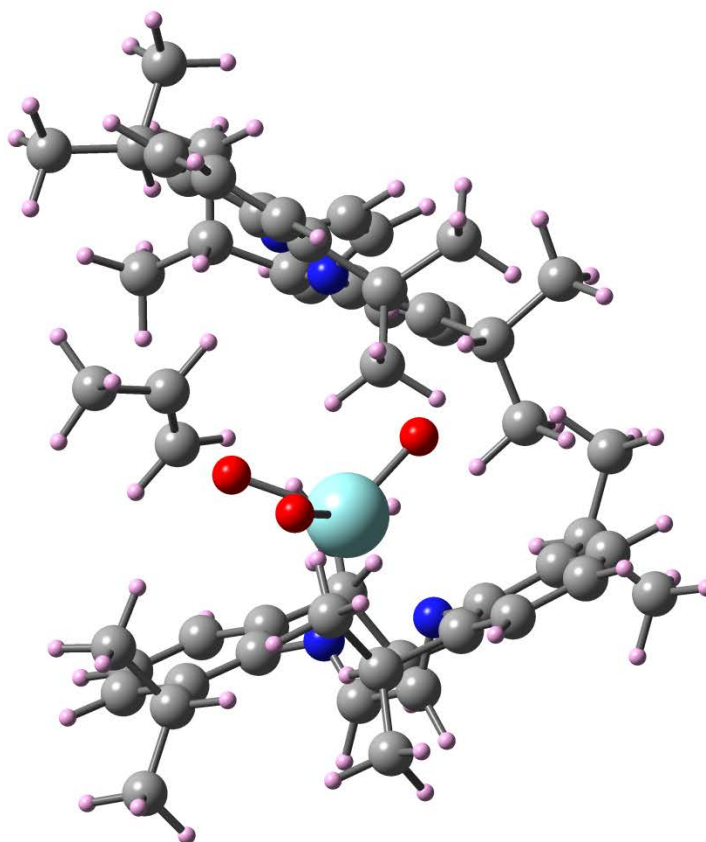


Fig. S41: NCCN Oxo Peroxo Complex to Dioxo Complex (conformation 2 lower energy)

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2633.728137	-2632.506419	-2632.431876	-2632.623680	-413

Zr	-1.26965387	-0.12826453	-0.12417774
O	-0.36157478	0.22940871	1.44631941
N	-2.48672777	-2.15253851	-0.76616501
N	-3.57570080	-0.03288912	0.65639504
N	3.05567243	2.23317179	-0.06659976
N	3.32361019	-0.45603067	1.10513519
C	-3.77423620	-2.08492134	-0.57100605
C	-4.35269345	-0.97424484	0.20275148
C	3.10548931	1.98716557	1.20285219
C	3.33133310	0.64694351	1.78128867
C	-1.93960392	-3.13420899	-1.68110366
C	-2.23531780	-3.03644935	-3.07223302
C	-1.63703488	-3.98944367	-3.92571859
C	-0.79005960	-4.98904845	-3.42879729
C	-0.49943325	-5.04815707	-2.05511801
C	-1.05637912	-4.12015316	-1.15623642

C	-2.17137744	-0.96285037	-4.53739644
C	-3.07223435	-1.91160954	-3.69993302
C	-4.24773332	-2.47067819	-4.54279816
C	-4.50025498	3.07482467	-1.76705705
C	-5.16753700	1.91031811	-0.98770421
C	-6.68268144	1.80775207	-1.30704583
C	-4.14618025	1.13829737	1.29771287
C	-4.92134890	2.05011405	0.52153624
C	-5.43270689	3.18713731	1.18211484
C	-5.19502271	3.41195136	2.54513231
C	-4.41851208	2.50295642	3.27982413
C	-3.86862332	1.35542179	2.67556450
C	0.61056227	-4.78234133	0.68932097
C	-0.78475547	-4.21313012	0.34820285
C	-1.89351199	-5.04812928	1.04945249
C	-1.91007620	1.04065593	4.28120035
C	-3.07601992	0.35787290	3.52542791
C	-4.02431340	-0.39629154	4.49764258
C	2.84341723	3.54417521	-0.58810485
C	1.77304742	4.39250038	-0.16228069
C	1.66865622	5.66439916	-0.76691636
C	2.56727064	6.09125057	-1.75446938
C	3.59002490	5.22984184	-2.18819723
C	3.73730506	3.94821453	-1.62994768
C	-0.72705835	4.17281001	0.33165468
C	0.71338197	3.98385142	0.87275819
C	0.89918261	4.76972397	2.19993123
C	5.47668290	-3.16920447	-1.27611669
C	5.19554685	-2.05531227	-0.24176354
C	6.50637525	-1.29838726	0.11156926
C	3.57262617	-1.72152078	1.71488301
C	4.51002515	-2.55994411	1.03056559
C	4.83453960	-3.80920950	1.58924478
C	4.23485081	-4.24361375	2.78421307
C	3.27598371	-3.43704114	3.41413856
C	2.91022931	-2.17262907	2.90153764
C	5.21468544	3.11384778	-3.56580041
C	4.87765663	3.02180299	-2.05956911
C	6.14714190	3.28935799	-1.20316646
C	0.53891358	-2.25574260	3.85566416
C	1.79668265	-1.38376643	3.60913255
C	2.28985297	-0.79126876	4.95753741
H	-4.45744423	-2.81838362	-1.00463557
H	-5.43481196	-0.95270747	0.34448282
H	3.03380612	2.78563423	1.95334562
H	3.54587073	0.66530519	2.85802084
H	-1.83090337	-3.93684148	-4.99362571
H	-0.34695091	-5.71276099	-4.10833820
H	0.17042859	-5.81717734	-1.68449365
H	-3.50724715	-1.29026557	-2.91006393
H	-4.68645881	0.99763681	-1.35446292
H	-1.66074549	-1.50769740	-5.34298589

H	-1.42327440	-0.47912341	-3.89943040
H	-2.78405222	-0.17519083	-4.99527225
H	-3.88684019	-3.04285611	-5.40651426
H	-4.85886065	-1.64422815	-4.92764086
H	-4.89585749	-3.13323354	-3.95260535
H	-4.87910275	4.05158622	-1.43851968
H	-4.70896424	2.97370380	-2.84084855
H	-3.41402031	3.04085988	-1.63145850
H	-7.15624132	0.96723746	-0.78014402
H	-6.83284819	1.66692836	-2.38550806
H	-7.21542942	2.72158602	-1.01470427
H	-6.01488791	3.90852731	0.61516728
H	-5.60577976	4.29388951	3.03042835
H	-4.23738587	2.68429863	4.33566320
H	-0.83559047	-3.19591752	0.76614164
H	-2.61482067	-0.38044233	2.86101899
H	0.69117575	-5.84507017	0.42593099
H	0.79730206	-4.69876391	1.76549249
H	1.41098285	-4.23834971	0.17383039
H	-1.88909441	-6.08105872	0.67721013
H	-2.89328520	-4.63097792	0.87242322
H	-1.72299689	-5.07405676	2.13326772
H	-1.16932154	1.40233994	3.56060361
H	-1.41375540	0.31279884	4.93694028
H	-2.25379318	1.87328948	4.90932041
H	-4.47910973	0.29234024	5.22220822
H	-3.46541166	-1.15609232	5.05982706
H	-4.83974260	-0.89921419	3.95915043
H	0.86195705	6.32664946	-0.46347710
H	2.46414374	7.08114784	-2.19337053
H	4.27123070	5.55871235	-2.96806344
H	0.81075178	2.91601837	1.09522086
H	4.51570935	-1.32600168	-0.69864482
H	-0.93987679	5.22229650	0.08587428
H	-1.44962018	3.85613614	1.09630807
H	-0.89593308	3.55183087	-0.55453060
H	1.90412432	4.63454747	2.62302646
H	0.16534436	4.43246570	2.94423996
H	0.75199044	5.84701278	2.04264870
H	6.23622640	-3.88050818	-0.92401361
H	5.85418112	-2.72480862	-2.20665341
H	4.56549161	-3.73266976	-1.51528572
H	6.30806227	-0.45853426	0.78862085
H	6.97605038	-0.89743579	-0.79713570
H	7.22589052	-1.96890868	0.60153358
H	5.56025253	-4.44689023	1.09202776
H	4.50420620	-5.20639242	3.21283648
H	2.79588004	-3.79565279	4.32145421
H	4.55355381	1.99663160	-1.84079593
H	1.45854932	-0.56652809	2.96237829
H	5.65662814	4.08378559	-3.83079098
H	4.32075533	2.96839855	-4.18548676

H	5.94694594	2.33980657	-3.83305068
H	6.95090536	2.59086792	-1.47434753
H	5.93584253	3.16628251	-0.13376139
H	6.51484600	4.31263764	-1.36078860
H	0.16253558	-2.66591392	2.91196555
H	-0.25587219	-1.63505878	4.28663610
H	0.73377641	-3.08758389	4.54656205
H	3.16849119	-0.14630376	4.82771264
H	2.57199863	-1.58877722	5.65903616
H	1.49502552	-0.19363432	5.42396705
O	-1.68992474	1.36780263	-1.32272296
O	-0.18544770	0.26665487	-1.85813111
C	1.38030387	-1.35509860	-2.16944193
H	1.48945428	-1.84613695	-1.20413244
H	0.99051433	-1.94473179	-2.99583915
C	1.77826934	-0.04246594	-2.33303643
H	2.22432881	0.47708420	-1.48568554
C	1.84675055	0.65780393	-3.66564924
H	1.40271809	1.65522366	-3.58056912
H	2.89588262	0.77918557	-3.97526262
H	1.31378742	0.10108063	-4.44503673

## Dioxo Complex to Oxo Ozone Complex

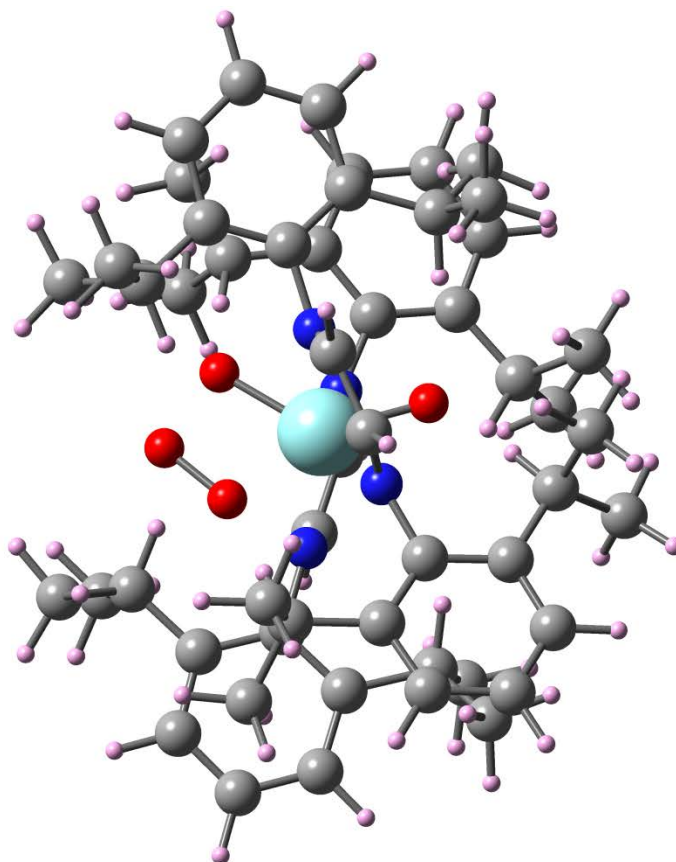


Fig. S42: NCCN Dioxo Complex to Oxo Ozone Complex

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2591.018581	-2589.874273	-2589.804646	-2589.979601	-152

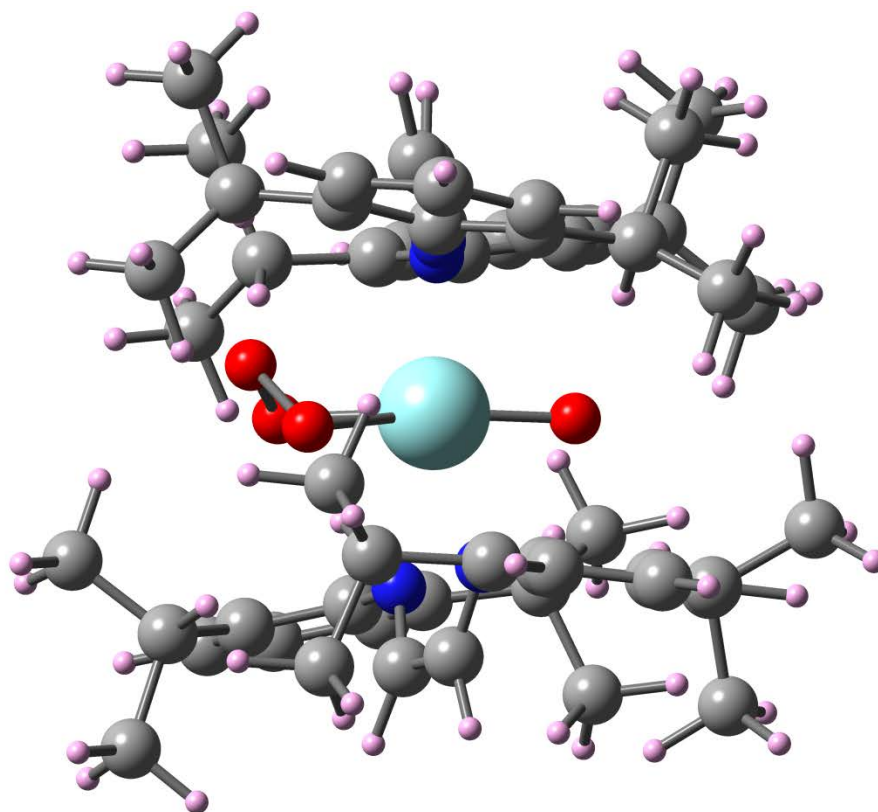
O	-1.31959010	0.54361904	1.79240514
O	1.19089909	1.53904612	1.39135810
O	-0.49124204	-0.76034206	-1.34938310
N	-1.18234709	2.14001316	-0.67574505
N	1.47757211	1.51528411	-1.39242911
N	1.26164010	-1.57738412	1.40935911
N	-1.46555011	-2.10582816	0.79828306
C	-0.45097503	2.97278423	-1.34676210
C	0.92901907	2.64035720	-1.73065813
C	0.66412205	-2.68882221	1.73691513
C	-0.69518005	-3.01778323	1.30455310
C	-2.59295220	2.48077519	-0.47496504
C	-3.53626527	1.92066314	-1.38172310
C	-4.89205337	2.26449817	-1.20528109
C	-5.29599442	3.13215124	-0.17808701
C	-4.34183933	3.67506428	0.69294005

C	-2.97015022	3.36377626	0.56880004
C	-4.11424431	-0.07066701	-2.90334322
C	-3.10053524	1.04666408	-2.56450520
C	-2.85394122	1.93122715	-3.81990629
C	1.86181914	-1.52670512	-4.36722733
C	1.62583313	-0.10586201	-3.80103829
C	1.09637408	0.83079406	-4.92206038
C	2.80472021	1.25792909	-1.95401815
C	2.87904322	0.49269404	-3.15102924
C	4.14421432	0.35829203	-3.75881328
C	5.29043740	0.93987607	-3.19346824
C	5.19121740	1.66027712	-1.99390515
C	3.94950930	1.83891414	-1.34516710
C	-2.34342018	3.71062528	3.01305823
C	-1.96680015	3.99540030	1.53785112
C	-1.83250414	5.52051645	1.28025810
C	4.94119238	2.24585317	0.97920108
C	3.86724430	2.66474820	-0.05533000
C	3.98177430	4.18363532	-0.36018503
C	2.64016420	-1.44240111	1.90322815
C	2.86456022	-0.89314407	3.19288724
C	4.19666432	-0.84545007	3.65618828
C	5.25915840	-1.32351010	2.87565722
C	5.00706338	-1.86515414	1.60623712
C	3.69527228	-1.94084815	1.09219408
C	2.04188615	0.90323907	4.82451237
C	1.72074613	-0.42475103	4.09860231
C	1.35802910	-1.52902512	5.13028639
C	-1.68651213	-3.38848926	-3.11392024
C	-1.63123513	-3.85248529	-1.63610712
C	-1.49456211	-5.39528639	-1.53940512
C	-2.76175821	-2.49576719	0.28829602
C	-2.84935622	-3.34992726	-0.84939307
C	-4.13936331	-3.71572828	-1.29099510
C	-5.29370938	-3.25922325	-0.64034705
C	-5.18010240	-2.40802718	0.47123104
C	-3.92103430	-2.00499315	0.95722107
C	4.55646435	-2.33153818	-1.29586310
C	3.43600226	-2.60687520	-0.26615502
C	3.25640525	-4.14359332	-0.10583401
C	-4.94640038	-0.13252201	2.39455418
C	-3.80120029	-1.15462609	2.22290117
C	-3.70376328	-2.06943916	3.47656026
H	-5.63639341	1.85173914	-1.87943215
H	-6.34732748	3.38477126	-0.06107500
H	-4.66071035	4.34695033	1.48547712
H	-2.15847317	0.54930004	-2.30496418
H	0.84781206	-0.20329402	-3.03364223
H	-5.05628239	0.33081403	-3.30179625
H	-4.34265533	-0.68247405	-2.02412315
H	-3.69009528	-0.73144105	-3.67005028
H	-3.77955029	2.43549919	-4.13002531

H	-2.50314619	1.31335610	-4.65729236
H	-2.09903016	2.70723021	-3.63547128
H	2.55931120	-1.53080512	-5.21621440
H	0.90895607	-1.94236615	-4.71826636
H	2.25566417	-2.19862417	-3.59485628
H	0.85598806	1.83099114	-4.53772135
H	0.18239801	0.41330603	-5.36480239
H	1.84087014	0.95064207	-5.72148246
H	4.23229132	-0.20761402	-4.68201436
H	6.25534949	0.82680006	-3.68212728
H	6.08491346	2.09635516	-1.55560812
H	-0.98901407	3.53153427	1.38926311
H	2.89537522	2.48602719	0.41572703
H	-3.30834125	4.15949832	3.28624425
H	-1.57700612	4.12728031	3.67971728
H	-2.38920619	2.62998920	3.18057225
H	-2.78706421	6.03933648	1.44195711
H	-1.51202312	5.73304842	0.25036102
H	-1.09155908	5.95612844	1.96376515
H	4.88050937	1.17546109	1.20312309
H	4.78399536	2.79549722	1.91625615
H	5.95896044	2.46877319	0.63085905
H	4.94295638	4.42016434	-0.83667406
H	3.91136530	4.76190136	0.57039504
H	3.18398224	4.52755635	-1.03205408
H	4.40049734	-0.42930403	4.63852635
H	6.27753250	-1.27631510	3.25407825
H	5.83575945	-2.23367317	1.00964008
H	0.83858806	-0.22830502	3.48322727
H	-0.72811205	-3.39417126	-1.22371909
H	2.85035922	0.79162106	5.56026745
H	1.15007809	1.25282209	5.35910040
H	2.32344218	1.67679613	4.10290231
H	1.05250408	-2.46392219	4.64085535
H	0.52646204	-1.19456109	5.76414743
H	2.21323617	-1.75886214	5.78068845
H	-2.58731220	-3.75130929	-3.62658128
H	-0.81199906	-3.77091929	-3.65858228
H	-1.66087513	-2.29507417	-3.14928824
H	-1.41722211	-5.73275044	-0.49640804
H	-0.59736905	-5.73253745	-2.07593616
H	-2.36047718	-5.90254644	-1.98504315
H	-4.23660932	-4.36010733	-2.16117616
H	-6.27571048	-3.55942927	-0.99857707
H	-6.07828445	-2.05438316	0.96802307
H	2.50098719	-2.20257817	-0.67740105
H	-2.86664522	-0.57717904	2.16442217
H	5.48928340	-2.84332122	-1.02409208
H	4.76499936	-1.26191009	-1.39050611
H	4.25621032	-2.70643521	-2.28222317
H	3.08070124	-4.60908635	-1.08465508
H	2.41155618	-4.40003833	0.54462904



H	4.15940632	-4.59235135	0.32901003
H	-5.05706039	0.49615704	1.50346411
H	-4.72024136	0.52656304	3.24231725
H	-5.91115044	-0.61692404	2.60289020
H	-2.85811322	-2.76623221	3.40712126
H	-4.62095235	-2.66238920	3.60167628
H	-3.56297327	-1.45905111	4.37816433
O	0.16981501	1.75405013	2.35501618
H	1.44811511	3.36041726	-2.36863918
H	-0.85333807	3.92295930	-1.70603513
H	1.18436609	-3.43828126	2.33742218
H	-1.01229807	-4.05825831	1.41781811
Zr	-0.08542301	0.13118201	0.23002902

Oxo  $\eta^2$ -Ozone Complex to Oxo  $\eta^3$ -Ozone ComplexFig. S43: NCCN Oxo  $\eta^2$ -Ozone Complex to Oxo  $\eta^3$ -Ozone Complex

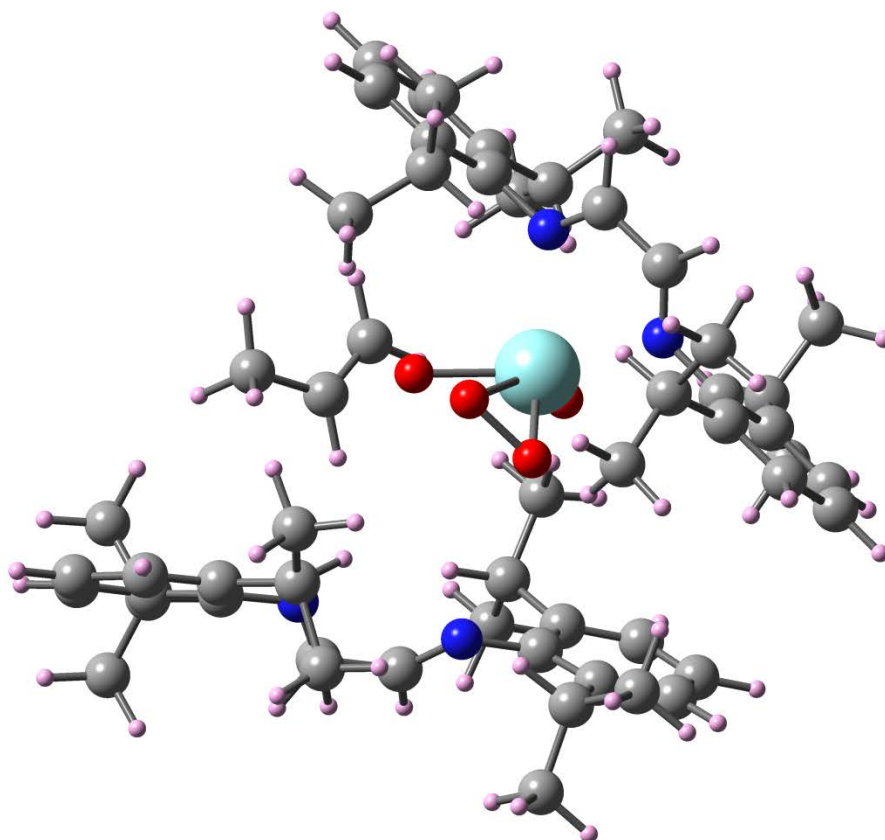
SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
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Zr	-0.08402101	0.02010300	-0.11093801
O	-1.39496510	0.12999401	-1.87134114
N	1.35126210	2.06452016	0.39531403
N	-1.39165611	2.14362716	-0.14051301
N	-1.33017810	-2.13281816	0.01965100
N	1.42381411	-2.01565115	-0.49874804
C	0.73318605	3.19333024	0.22806602
C	-0.68146505	3.23109925	-0.14725901
C	-0.67194305	-3.19030824	-0.33957403
C	0.74420106	-3.10239224	-0.71295605
C	2.70947120	2.15326616	0.93660307
C	2.86374522	2.19195617	2.35092118
C	4.17042932	2.36153718	2.85507822
C	5.27454040	2.48016819	1.99650015
C	5.08999039	2.43456518	0.60626105
C	3.80575129	2.27672417	0.04223300
C	1.93223215	1.25077109	4.55598235
C	1.66276413	2.11900216	3.30406525

C	1.22590509	3.54530527	3.74087629
C	-4.18970932	0.91858607	2.90435522
C	-3.21199725	1.75605413	2.05015616
C	-2.91781722	3.10415024	2.77013121
C	-2.81101322	2.25863717	-0.44344303
C	-3.71906128	2.02387816	0.62803805
C	-5.09549839	2.15955617	0.36216003
C	-5.55494043	2.52313820	-0.91427807
C	-4.63851035	2.76047321	-1.94768215
C	-3.24662025	2.63778320	-1.74414313
C	4.72434136	1.57464612	-2.25028617
C	3.61076428	2.31971518	-1.47805011
C	3.52254827	3.79037029	-1.97577515
C	-2.65076120	2.05684316	-4.15732731
C	-2.29896118	2.91792222	-2.91827822
C	-2.29950017	4.42722734	-3.28571425
C	-2.66834120	-2.34556518	0.57979704
C	-3.80143229	-2.32031118	-0.27788202
C	-5.06185638	-2.57676120	0.30214402
C	-5.19224539	-2.86060222	1.67019813
C	-4.05370831	-2.89546522	2.48858519
C	-2.76713021	-2.63858020	1.96894515
C	-4.81151737	-1.25673810	-2.38744218
C	-3.67126928	-2.11483616	-1.79065214
C	-3.60400227	-3.48798727	-2.51650419
C	4.21998632	-1.43808511	2.75715621
C	3.22793025	-2.04838216	1.74250913
C	2.88380522	-3.50315427	2.17658317
C	2.84792322	-2.06340116	-0.80439306
C	3.74773429	-2.03927316	0.29961502
C	5.12624939	-2.12866816	0.02520800
C	5.59793640	-2.25391817	-1.29189910
C	4.69043736	-2.29639717	-2.35811718
C	3.29668625	-2.20668917	-2.14723716
C	-1.70025213	-1.93254515	4.19189332
C	-1.54169112	-2.74753221	2.88577022
C	-1.23459410	-4.23728433	3.20098125
C	2.67878721	-1.15621809	-4.39162834
C	2.36495018	-2.27423017	-3.36487726
C	2.43322719	-3.67249428	-4.03772931
H	1.22649609	4.14919832	0.41704403
H	-1.12421508	4.20372232	-0.36943003
H	-1.11949009	-4.18609032	-0.30484802
H	1.21883309	-4.00614231	-1.10109909
H	4.32281433	2.39921818	3.93007330
H	6.27253246	2.61024120	2.40882218
H	5.94987843	2.52826719	-0.05047800
H	0.83575706	1.63132812	2.77629521
H	-2.26566917	1.20234609	1.98739415
H	2.70044121	1.68272013	5.21242940
H	2.24381817	0.24090002	4.27085832
H	1.00840408	1.16132309	5.14210439

H	2.03157816	4.05404531	4.28835533
H	0.34970803	3.48736027	4.40042634
H	0.95942308	4.17646532	2.88285822
H	-5.10552639	1.47655011	3.14391324
H	-3.71241328	0.65369805	3.85600630
H	-4.47178434	-0.01160600	2.39998818
H	-2.18770217	3.71310728	2.22245117
H	-2.51261419	2.91608022	3.77315129
H	-3.83773729	3.69543228	2.87645922
H	-5.81206242	1.98623515	1.15853109
H	-6.62182950	2.62346020	-1.09988308
H	-5.00502238	3.03856423	-2.93219823
H	2.66387920	1.82488114	-1.72387913
H	-1.28475310	2.62595520	-2.63220220
H	5.69681746	2.07817616	-2.16092017
H	4.47019434	1.53926712	-3.31729125
H	4.83310437	0.54502104	-1.89538215
H	4.44839734	4.33721333	-1.74972814
H	2.69117021	4.33516533	-1.50999511
H	3.36891926	3.81120529	-3.06270923
H	-2.60437020	0.99716808	-3.89131730
H	-1.92278815	2.24316417	-4.95830238
H	-3.64905928	2.29065717	-4.55180135
H	-3.29269625	4.75282136	-3.62280828
H	-1.58871912	4.61841735	-4.10063731
H	-2.01862016	5.06107939	-2.43285218
H	-5.94650143	-2.56084020	-0.32761603
H	-6.17379349	-3.06014324	2.09389816
H	-4.16050232	-3.12593324	3.54521727
H	-2.74116021	-1.57107512	-1.98201315
H	2.29933018	-1.46280211	1.78297814
H	-5.78208246	-1.77123614	-2.35330018
H	-4.59226635	-1.03907008	-3.44080226
H	-4.90619537	-0.30101602	-1.86073214
H	-2.75813821	-4.09550231	-2.16780017
H	-3.48666327	-3.33851425	-3.59801827
H	-4.52240034	-4.06756631	-2.34843218
H	5.12218039	-2.05531816	2.86566522
H	3.74800828	-1.38270910	3.74580529
H	4.52269534	-0.42627103	2.46917619
H	2.14466617	-3.96997430	1.51443911
H	2.47111619	-3.50597727	3.19399824
H	3.78570529	-4.13020331	2.17019017
H	5.83621343	-2.10888616	0.84535407
H	6.66629251	-2.32295618	-1.48256611
H	5.06320938	-2.39704018	-3.37401126
H	-0.68359505	-2.30322017	2.37475118
H	1.33494110	-2.10057216	-3.04395823
H	-2.56172020	-2.25732017	4.79130237
H	-1.80507614	-0.86967007	3.95477830
H	-0.80004406	-2.04908616	4.80992337
H	-0.32863203	-4.31724233	3.81679229

H	-1.07562008	-4.82437437	2.28555017
H	-2.06143816	-4.70511836	3.75261228
H	2.53452319	-0.17644501	-3.92733230
H	1.99096815	-1.23287410	-5.24407840
H	3.70452828	-1.22835010	-4.77811736
H	2.17625517	-4.47923934	-3.33669326
H	3.43939626	-3.88212029	-4.42429634
H	1.73296113	-3.71908229	-4.88215137
O	-0.12503601	-0.09131401	1.73863113
O	-0.11798801	-0.37676203	-2.52005419
O	1.02646308	0.47007704	-1.93954115

Oxo  $\eta^3$ -Ozone Complex to Oxo Peroxo Complex (conformation 1 lower energy)Fig. S44: NCCN Oxo  $\eta^3$ -Ozone Complex to Oxo Peroxo Complex (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2708.897571	-2707.673475	-2707.597426	-2707.794180	-326

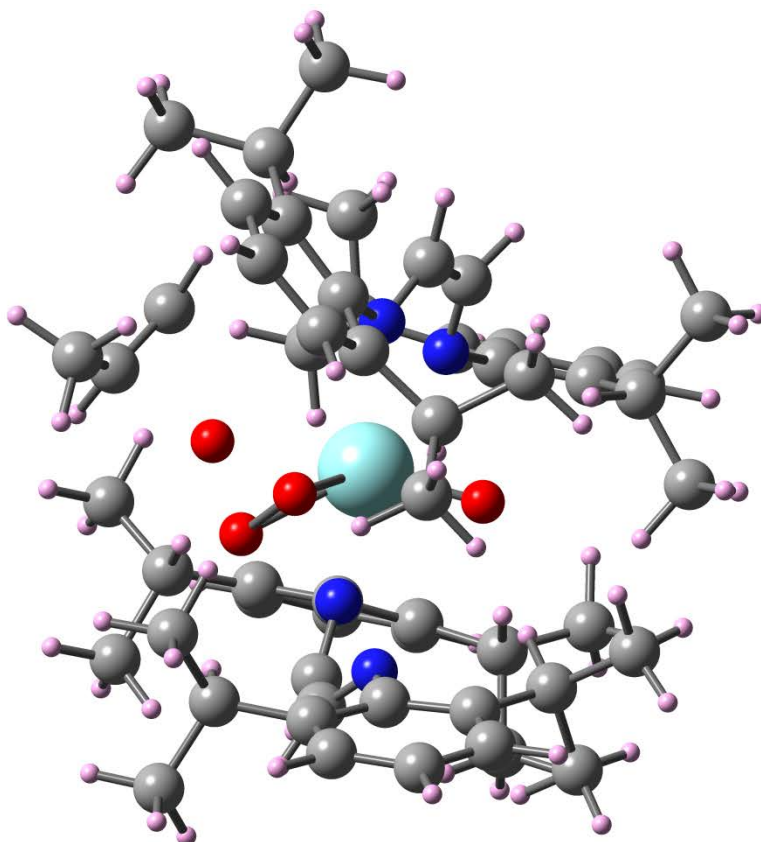
Zr	1.36580329	0.37789739	-0.11658474
O	-0.14795035	1.73523140	0.41224407
N	-2.72544167	-2.44821398	-0.45899147
N	-4.26219410	-0.10262565	0.36267883
N	3.01284269	2.10454326	-0.52062609
N	3.58962541	-0.38203322	0.52832225
C	-3.96460440	-2.24497067	-0.76624034
C	-4.77723368	-1.17259546	-0.14507004
C	4.15643746	1.89864493	0.06611326
C	4.45712280	0.58037205	0.65074423
C	-1.96042647	-3.50540483	-1.03361378
C	-1.76586841	-3.63628983	-2.44071029
C	-1.00812264	-4.73527429	-2.89898880
C	-0.44989653	-5.66463025	-2.00948329
C	-0.60094331	-5.48347621	-0.62282515

C	-1.33628859	-4.39975601	-0.11078876
C	-1.01451539	-1.92288759	-4.15204949
C	-2.23465622	-2.58659880	-3.45696344
C	-3.22136058	-3.17946013	-4.49611345
C	-6.50627015	2.60026818	-1.90567341
C	-6.57910394	1.30946715	-1.04760152
C	-8.00183391	0.69300170	-1.10801905
C	-5.03316327	0.90503977	1.01724034
C	-6.13480350	1.56976836	0.39912379
C	-6.80503670	2.56520696	1.14415640
C	-6.40552677	2.90147259	2.44526138
C	-5.29185552	2.26446847	3.02202117
C	-4.57890404	1.27455410	2.32266821
C	-0.28192932	-4.57922235	2.22660195
C	-1.52604292	-4.19490214	1.39377398
C	-2.77700126	-4.96717687	1.89872691
C	-2.55207467	1.44362191	3.90545202
C	-3.37446969	0.55966376	2.94111289
C	-3.82456166	-0.74332610	3.65990982
C	2.71503047	3.40253153	-1.09841492
C	2.54680432	4.53201382	-0.24991575
C	2.25156187	5.76608840	-0.86992743
C	2.12901299	5.87401071	-2.26176214
C	2.28077297	4.73598213	-3.07269256
C	2.56618610	3.47613136	-2.51318809
C	1.17754027	4.75861905	1.87426356
C	2.58216575	4.46437964	1.28325855
C	3.65617856	5.41259810	1.87695287
C	3.15969268	-3.75492071	-2.09571758
C	3.79942038	-2.56586473	-1.34505447
C	5.19642315	-2.23446811	-1.94296789
C	3.85221595	-1.69359852	1.08115825
C	3.91406656	-2.78590402	0.16671962
C	4.17670783	-4.06319601	0.69615946
C	4.35646984	-4.25515163	2.07609699
C	4.26220274	-3.16785971	2.95563764
C	4.00422100	-1.86200707	2.48770449
C	1.91397417	2.24946681	-4.68086271
C	2.78146730	2.24546259	-3.40115516
C	4.28480593	2.10350968	-3.77190711
C	2.66962389	-1.04563088	4.49426429
C	3.82861408	-0.73251722	3.51153773
C	5.15040876	-0.44930248	4.27443315
H	-4.51500980	-2.90401795	-1.45610797
H	-5.85901446	-1.37727683	-0.11592508
H	4.92421731	2.67330297	0.11599933
H	5.42179499	0.43804261	1.14064532
H	-0.84214588	-4.85417471	-3.96727225
H	0.11708985	-6.51113229	-2.39080831
H	-0.13556301	-6.18625773	0.06281383
H	-2.75894335	-1.78619461	-2.92379743
H	-5.89018433	0.59247330	-1.50736478

H	-0.45526356	-2.65322907	-4.75343571
H	-0.33097415	-1.48800682	-3.41179781
H	-1.35637546	-1.12645230	-4.82965560
H	-2.74688022	-3.97471254	-5.08594877
H	-3.55420855	-2.39982629	-5.19483720
H	-4.10876333	-3.61045805	-4.01241160
H	-7.19795271	3.36964582	-1.53963955
H	-6.77289648	2.37960223	-2.94829225
H	-5.49404695	3.02383579	-1.89403952
H	-8.05707885	-0.24487112	-0.53993794
H	-8.28899126	0.48399626	-2.14758261
H	-8.74711699	1.37874927	-0.68443585
H	-7.64745693	3.08707321	0.69544551
H	-6.94657240	3.66400760	3.00092675
H	-4.97014921	2.54835588	4.01984482
H	-1.71421155	-3.12446048	1.54407458
H	-2.71500575	0.25960830	2.11777824
H	-0.08578506	-5.66042001	2.20231540
H	-0.43784056	-4.29768250	3.27648994
H	0.61281413	-4.05676366	1.86759078
H	-2.64417167	-6.05060557	1.77068263
H	-3.67959669	-4.67067712	1.34936722
H	-2.94768139	-4.76701326	2.96539636
H	-2.28415310	2.40227355	3.44414191
H	-1.61524926	0.93215520	4.15481656
H	-3.09093365	1.64695817	4.84218201
H	-4.50206667	-0.51595597	4.49514963
H	-2.94967838	-1.27271385	4.05963749
H	-4.34452648	-1.42174348	2.97224381
H	2.10612176	6.64703554	-0.25033480
H	1.90620469	6.83702631	-2.71458497
H	2.17215219	4.82901252	-4.14869142
H	2.83142069	3.44652778	1.60052994
H	3.14249068	-1.70617585	-1.52091689
H	0.83491093	5.76817913	1.61029824
H	1.20916417	4.68559009	2.96910923
H	0.45148568	4.02685700	1.50563973
H	4.65974898	5.18617198	1.49056717
H	3.67925631	5.31670674	2.97014972
H	3.44070696	6.46250116	1.64110496
H	3.80155989	-4.64698024	-2.08788187
H	2.99597014	-3.47576916	-3.14406083
H	2.18536149	-4.01750463	-1.66940175
H	5.64779479	-1.35221590	-1.46852679
H	5.10899258	-2.03231550	-3.01863679
H	5.88797607	-3.07747696	-1.80903427
H	4.23714535	-4.91420866	0.02545467
H	4.55650781	-5.25102650	2.46406078
H	4.37110041	-3.33420806	4.02400176
H	2.49239670	1.35198793	-2.83351384
H	3.53499664	0.18606053	2.99283291
H	2.22497375	3.02775066	-5.39067577



H	0.85383235	2.39992307	-4.44508339
H	2.00915496	1.28209859	-5.18875929
H	4.44323049	1.19806473	-4.37184475
H	4.92135314	2.03293486	-2.87989751
H	4.62454653	2.96746687	-4.35876420
H	1.73608984	-1.17905237	3.93857033
H	2.53586057	-0.20793999	5.19181271
H	2.87099056	-1.94804118	5.08657526
H	5.97219214	-0.19064831	3.59142874
H	5.46953509	-1.32516532	4.85393311
H	5.01242942	0.38327241	4.97663280
O	1.00050357	-0.50230246	-1.68595638
O	0.71087788	1.04988931	1.98146325
O	0.80772717	-0.44167752	1.72019823
C	-0.91802609	2.31617916	-1.67336414
H	-0.65755371	1.44601627	-2.27019495
H	-0.44581234	3.26473252	-1.91997070
C	-1.82278967	2.22481654	-0.63078834
H	-2.32946131	1.27784366	-0.44933706
C	-2.34311703	3.41827972	0.12895221
H	-1.74976291	4.31705787	-0.07532476
H	-3.39000826	3.61563160	-0.14468141
H	-2.32191659	3.21477120	1.20415949

Oxo  $\eta^3$ -Ozone Complex to Oxo Peroxo Complex (conformation 2 higher energy)Fig. S45: NCCN Oxo  $\eta^3$ -Ozone Complex to Oxo Peroxo Complex (conformation 2 higher energy)

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2708.87386484	-2707.646249	-2707.572297	-2707.754730	-434

O	2.02158200	0.31223800	0.86322200
N	-1.66249700	1.50653100	-1.23161100
N	0.98862400	2.45430700	-0.87194800
N	1.63063800	-2.61318300	0.38858300
N	-1.14471600	-1.76769900	1.17311000
C	-1.19550100	2.54154300	-1.87437800
C	0.13193800	3.08330100	-1.62492200
C	0.99645700	-3.03050200	1.43333600
C	-0.43126700	-2.75286000	1.64694000
C	-2.95162100	1.02678400	-1.73260300
C	-3.01970100	0.44974900	-3.03439300
C	-4.29762700	0.08442400	-3.51192500
C	-5.45332000	0.28233500	-2.74420400
C	-5.35726800	0.86322400	-1.46948400
C	-4.11162000	1.25714600	-0.94286300

C	-1.65533000	-1.25287900	-4.37021300
C	-1.79817400	0.22788600	-3.93930700
C	-1.85833900	1.15150900	-5.18673600
C	4.60364400	0.14526500	-1.55677200
C	3.38846000	1.07304800	-1.76204600
C	3.23710400	1.43030900	-3.26941500
C	2.26800700	3.08981800	-0.61420400
C	3.45114000	2.35942000	-0.93698200
C	4.69439800	2.93072000	-0.61038000
C	4.78126200	4.19170300	-0.00198300
C	3.61438400	4.92283200	0.25092100
C	2.33600100	4.41003500	-0.05832800
C	-5.12910600	1.65845900	1.38917800
C	-4.02381100	2.03047300	0.37595100
C	-4.06829600	3.56193800	0.10293300
C	1.16158700	6.05980500	1.55400000
C	1.12785600	5.33315200	0.18436600
C	1.02851500	6.40591300	-0.94012000
C	2.97876200	-2.95237200	0.10198200
C	4.03208000	-2.86664900	1.06586100
C	5.32053400	-3.27339300	0.65947800
C	5.56984300	-3.74224000	-0.63909300
C	4.53228200	-3.76849100	-1.58751900
C	3.23175300	-3.35500000	-1.24791000
C	4.76652900	-1.04444100	2.68803500
C	3.85513000	-2.28148400	2.47464700
C	4.10798100	-3.35204700	3.56935700
C	-3.72624200	-3.25030200	-1.99303500
C	-2.75211000	-3.20858700	-0.79272800
C	-2.25455300	-4.65624500	-0.50934200
C	-2.58605800	-1.91938800	1.44392100
C	-3.37365700	-2.60289700	0.47372300
C	-4.74036200	-2.80484600	0.75726700
C	-5.30219300	-2.38082400	1.97050300
C	-4.49737600	-1.74592400	2.92640700
C	-3.12658500	-1.49857200	2.69106500
C	2.53656800	-3.07282300	-3.70761000
C	2.08617900	-3.38624700	-2.26256400
C	1.36461800	-4.76220300	-2.21814100
C	-3.00341600	0.25518000	4.56163800
C	-2.26747300	-0.87524400	3.80056400
C	-1.81802700	-1.95933900	4.82143400
H	-1.78292700	3.02294800	-2.65810300
H	0.38764800	4.00848600	-2.13978500
H	1.43657100	-3.71462300	2.17008200
H	-0.93173400	-3.51359100	2.25587000
H	-4.38280100	-0.36165800	-4.49936500
H	-6.42443700	-0.00842100	-3.13774700
H	-6.25842600	1.02311900	-0.88623800
H	-0.88817700	0.44186300	-3.37174500
H	2.49589100	0.50856000	-1.47753200
H	-2.53693600	-1.61816200	-4.91446100

H	-1.48520200	-1.87894700	-3.49021100
H	-0.78300000	-1.36042400	-5.02842600
H	-2.72746700	0.91785600	-5.81631100
H	-0.95612600	1.01653200	-5.79766400
H	-1.92774300	2.21365000	-4.91341400
H	5.52865600	0.57791400	-1.96353800
H	4.43373900	-0.80523000	-2.07342200
H	4.75508600	-0.07950900	-0.49586700
H	2.35006200	2.05003100	-3.45460300
H	3.13099800	0.51254700	-3.86157800
H	4.11807300	1.97789000	-3.63252500
H	5.60418900	2.38638300	-0.83786400
H	5.75210500	4.60942400	0.25372600
H	3.69457800	5.91056400	0.69538100
H	-3.05262500	1.80560800	0.83588800
H	0.20780300	4.73664800	0.16591200
H	-6.11778800	1.99725000	1.05154200
H	-4.93324900	2.15173900	2.35034500
H	-5.17205000	0.57886100	1.56259100
H	-5.02304000	3.83979100	-0.36319000
H	-3.26037500	3.88571900	-0.56413400
H	-3.97225100	4.11953200	1.04370600
H	1.28990600	5.36102900	2.38389400
H	0.21952100	6.60266400	1.70786800
H	1.97238000	6.79733800	1.60029000
H	1.90441900	7.06657100	-0.91254800
H	0.13230300	7.02536000	-0.80069600
H	0.99006000	5.96699400	-1.94512100
H	6.14188200	-3.21422100	1.36970500
H	6.57061700	-4.06543600	-0.91719100
H	4.74166300	-4.10180200	-2.59990000
H	2.83368600	-1.90890200	2.58654300
H	-1.88395100	-2.60063700	-1.07874500
H	5.83059900	-1.28848700	2.56852200
H	4.62300200	-0.64774100	3.70230800
H	4.49759200	-0.25426200	1.97898400
H	3.44430800	-4.22004600	3.45129000
H	3.93847700	-2.92411600	4.56655900
H	5.14122000	-3.72269000	3.53409700
H	-4.53993100	-3.97008300	-1.82934500
H	-3.18793400	-3.57130700	-2.89315900
H	-4.16650400	-2.26931500	-2.19220800
H	-1.48853400	-4.69041300	0.27329000
H	-1.81904700	-5.08883600	-1.41887000
H	-3.09057400	-5.29368200	-0.19085600
H	-5.36582500	-3.31102200	0.02887400
H	-6.35605100	-2.55570700	2.17457500
H	-4.93709400	-1.44097900	3.87137800
H	1.36591100	-2.61398600	-1.96348800
H	-1.37322400	-0.43385300	3.34648600
H	3.17147700	-3.86367300	-4.13174800
H	3.08807000	-2.12532000	-3.75769200

H	1.65265700	-2.97920100	-4.35222000
H	0.51366400	-4.76902900	-2.91335700
H	0.98282900	-4.98122800	-1.21338600
H	2.04801800	-5.57361500	-2.50661100
H	-3.35199000	1.03837700	3.87927100
H	-2.32486300	0.71321500	5.29214700
H	-3.86982900	-0.11974000	5.12221400
H	-1.21636500	-2.74641900	4.35191100
H	-2.68738900	-2.43872500	5.29212500
H	-1.20829200	-1.50317900	5.61260200
O	0.14073100	-0.63070600	-1.56473500
O	1.13983000	-0.20096000	1.96371600
O	-0.01675800	1.13758800	2.26200600
Zr	0.07412500	0.21198300	0.07212300
C	-0.31246400	2.50523700	3.51653100
H	-0.73869200	1.90009700	4.31476800
C	-1.20485500	3.10448800	2.63822000
H	-2.26281100	2.86608300	2.66873700
H	-0.87026000	3.81042200	1.88386400
C	1.11298400	2.95059700	3.75773900
H	1.14993200	3.76103900	4.50238500
H	1.70567200	2.10819400	4.12915300
H	1.57998500	3.29064900	2.82966200

## 5. NCCNO Single Ground States

### 5.1 Structures with two oxygen atoms

#### Bare Complex

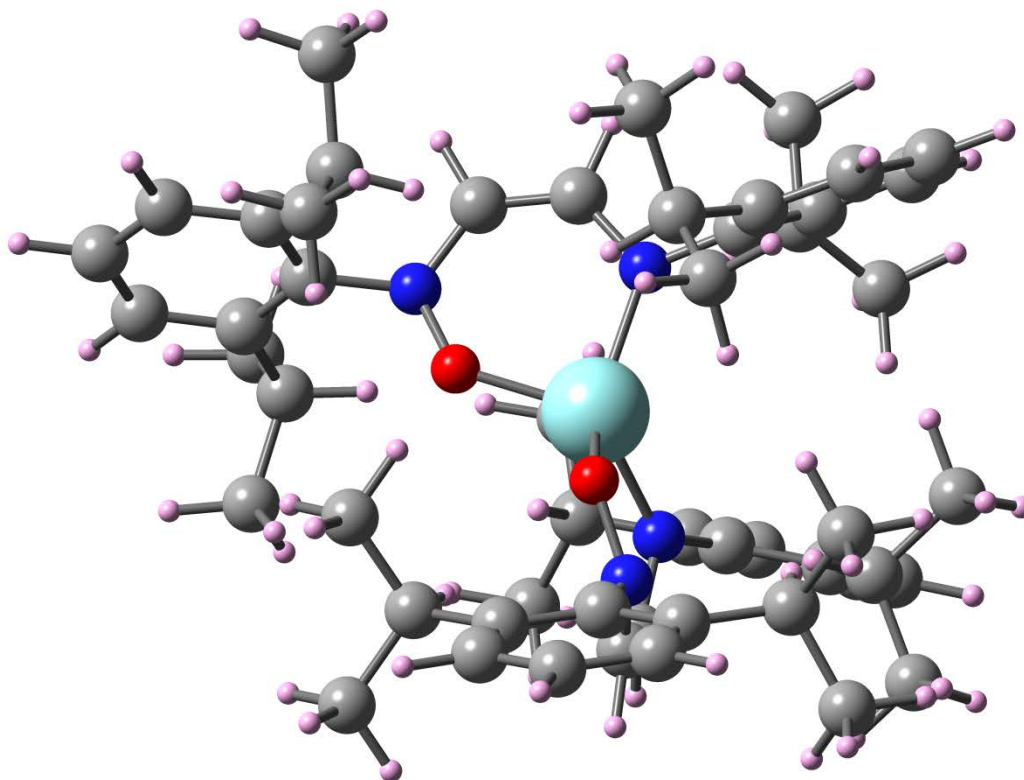


Fig. S46: NCCNO Bare Complex

SCF	E <sub>ZP</sub>	H	G
-2440.6540158	-2439.514239	-2439.447419	-2439.621007

Zr	0.05429200	-0.11155300	-0.01368400
O	-1.13919000	1.51880000	-0.04615700
O	1.94553900	0.50997500	-0.15696700
N	0.60899500	-1.33292500	1.58871000
N	3.19667800	-0.06356200	0.28972300
N	-0.93688600	-0.93175000	-1.65036500
N	-2.20756300	1.82349300	-0.96469600
C	1.98130500	-1.49626900	1.95593500
C	3.09182300	-0.92442300	1.40267300
C	-1.55236600	0.01185400	-2.54794300
C	-2.12183700	1.21207100	-2.22926000
C	-0.35838200	-1.86982400	2.53428600
C	-1.03736400	-0.98085200	3.42309300

C	-2.00443700	-1.51244600	4.30361300
C	-2.27957600	-2.88661800	4.33591300
C	-1.57385100	-3.75700300	3.49075100
C	-0.60902700	-3.27574000	2.58175700
C	-1.92996500	1.43186800	3.42673600
C	-0.68988200	0.51075100	3.52529200
C	0.10335800	0.78569600	4.83196900
C	3.09334000	3.45654300	2.43750600
C	3.69130800	2.02583400	2.39661900
C	4.46524300	1.71626300	3.70483700
C	4.30437900	0.86450900	0.15298100
C	4.57648400	1.83467500	1.15937200
C	5.69970900	2.67112000	0.98869900
C	6.50931700	2.57558500	-0.15347400
C	6.20058400	1.64343700	-1.15552600
C	5.09601300	0.77624500	-1.02395600
C	-0.75296200	-5.24009100	0.93840200
C	0.17129800	-4.27540200	1.72123700
C	1.16960900	-5.08824300	2.59201500
C	4.39170900	0.53853200	-3.44896600
C	4.76965500	-0.21101000	-2.14403100
C	5.93275200	-1.20553500	-2.39246900
C	-1.18624400	-2.31725600	-2.01755200
C	-2.49174400	-2.86689000	-1.82156200
C	-2.74111700	-4.18978000	-2.23957500
C	-1.73369500	-4.97039800	-2.82718200
C	-0.45331600	-4.42836900	-3.00079200
C	-0.15599200	-3.10343900	-2.61158100
C	-4.14918300	-2.75382500	0.11880900
C	-3.63055900	-2.06997900	-1.17397700
C	-4.79378400	-1.83858900	-2.17389700
C	0.53541000	4.66038300	-0.64620000
C	-0.48920000	4.13782000	-1.68675800
C	-0.29892200	4.84243700	-3.05467500
C	-2.72117000	3.16645800	-0.80559000
C	-1.91834500	4.28759400	-1.15767800
C	-2.46898500	5.57534000	-0.99489600
C	-3.77491900	5.74801100	-0.50858400
C	-4.55284500	4.63112400	-0.16889800
C	-4.03993900	3.32248200	-0.29945700
C	2.32635300	-3.37907200	-2.10783800
C	1.25260200	-2.56263600	-2.87426800
C	1.56790700	-2.53020800	-4.39332500
C	-5.49048000	2.24014400	1.50507300
C	-4.91358000	2.12211300	0.07148100
C	-6.05448100	1.92946300	-0.96323600
H	2.15983600	-2.16453000	2.79484600
H	4.05949300	-1.18072400	1.82049500
H	-1.61056500	-0.29711000	-3.59031000
H	-2.61375100	1.77568100	-3.01645000
H	-2.53442400	-0.84635100	4.97988300
H	-3.02685100	-3.27821800	5.02216200

H	-1.77671900	-4.82417000	3.53619700
H	-0.01864400	0.77327800	2.69648400
H	2.85243700	1.32659200	2.34006400
H	-2.63349900	1.25049200	4.24968900
H	-2.45854400	1.28213300	2.47889600
H	-1.62360000	2.48486300	3.47386100
H	-0.50750500	0.56197800	5.71657800
H	0.40175300	1.84164800	4.88351100
H	1.00847800	0.16766300	4.88044300
H	3.87664500	4.21941200	2.53613200
H	2.41669300	3.55921300	3.29692400
H	2.52537000	3.67013900	1.52478800
H	4.85359000	0.69000000	3.70507600
H	3.80462600	1.83059600	4.57465000
H	5.31586100	2.39775300	3.83686000
H	5.93491100	3.41156300	1.74944800
H	7.36941800	3.23180000	-0.26630200
H	6.82202300	1.58740100	-2.04593300
H	0.75295800	-3.70699200	0.98792700
H	3.89656300	-0.78642800	-1.82290800
H	-1.33743200	-5.87901000	1.61396700
H	-0.15278000	-5.89833000	0.29675200
H	-1.45021900	-4.69433800	0.29502500
H	0.63650300	-5.70535000	3.32785600
H	1.85755100	-4.43357900	3.14112700
H	1.76806400	-5.75784900	1.95984700
H	3.54558800	1.21577700	-3.27966500
H	4.10735500	-0.17747400	-4.23193600
H	5.23315800	1.13329700	-3.82933500
H	6.84293400	-0.68835400	-2.72404700
H	5.65739600	-1.92741100	-3.17335600
H	6.17709600	-1.76522200	-1.48055900
H	-3.73273600	-4.61400500	-2.09969700
H	-1.94462100	-5.98946800	-3.14295100
H	0.32517900	-5.03518000	-3.45788100
H	-3.24302700	-1.08681900	-0.89168400
H	-0.28228200	3.07396900	-1.83438300
H	-4.57760900	-3.74280000	-0.09219300
H	-4.93589000	-2.14180900	0.58088500
H	-3.34616000	-2.88525400	0.85466100
H	-4.44009000	-1.32060600	-3.07354200
H	-5.57914100	-1.22503600	-1.71260900
H	-5.24796900	-2.78889300	-2.48505500
H	0.40251800	5.73506100	-0.46102600
H	1.56031000	4.50018200	-1.00619700
H	0.41745000	4.12989300	0.30548700
H	-1.00927300	4.46423800	-3.80122900
H	0.71760400	4.66513100	-3.43024000
H	-0.43954400	5.92850100	-2.97647200
H	-1.87519800	6.44834000	-1.25470300
H	-4.18378000	6.74969400	-0.39539500
H	-5.56261700	4.77663200	0.20694700



H	1.29409800	-1.52785700	-2.51546800
H	-4.27652100	1.23187800	0.03621200
H	2.32035900	-4.43263600	-2.41660900
H	2.15579900	-3.34498100	-1.02424500
H	3.32876700	-2.97879000	-2.30434600
H	2.55739000	-2.08713100	-4.56872400
H	0.82544100	-1.93399000	-4.93892100
H	1.57054500	-3.54011100	-4.82463600
H	-4.69214500	2.38427600	2.24298500
H	-6.03901600	1.32559600	1.76789400
H	-6.18925800	3.08237700	1.59490400
H	-5.65274100	1.77903200	-1.97310100
H	-6.71620600	2.80570700	-0.98987300
H	-6.66448800	1.05342500	-0.70414300

## 5.2 Structures with three oxygen atoms

## Oxo Complex

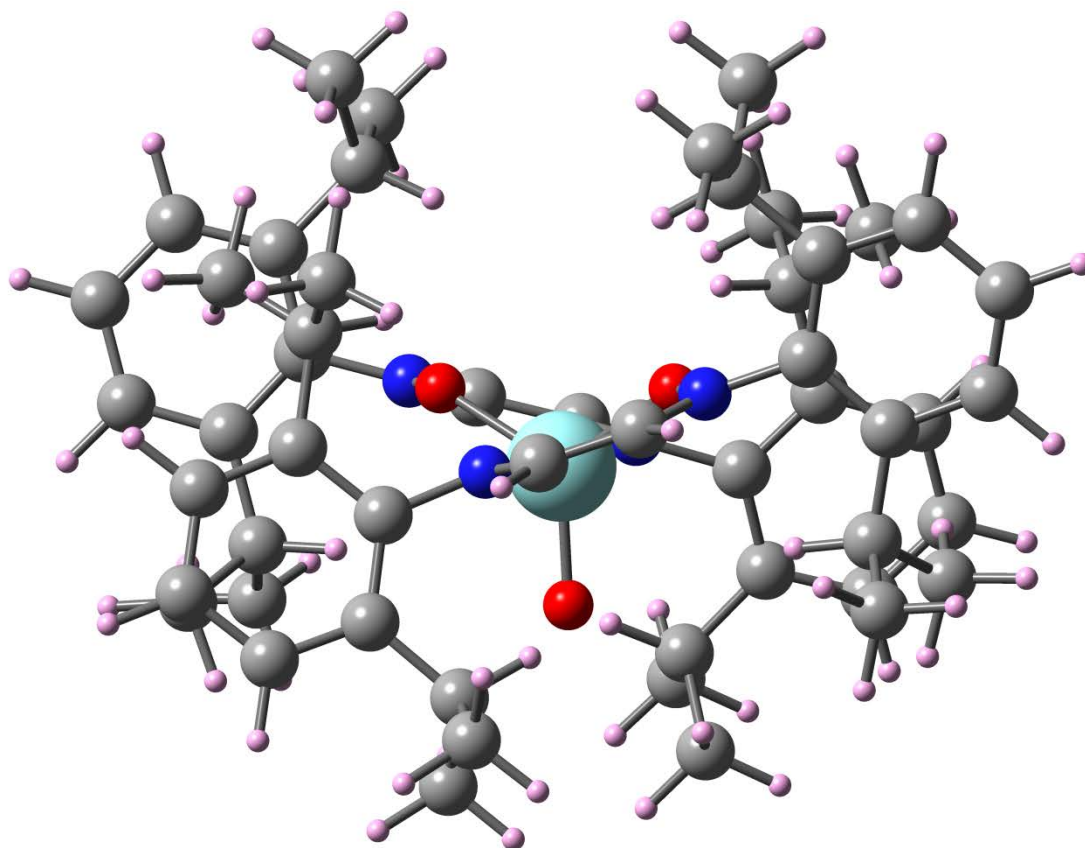


Fig. S47: NCCNO Oxo Complex

SCF	$E_{ZP}$	H	G
-2515.9011979	-2514.757357	-2514.689200	-2514.864027

Zr	-0.00004700	0.00007200	-0.47343900
N	0.21232900	2.30512400	-0.33340400
N	-0.21252000	-2.30490800	-0.33351400
C	-0.84704800	3.13907700	-0.16436000
C	-2.15587300	2.81274300	0.22385000
C	0.84675600	-3.13894900	-0.16398100
C	2.15560000	-2.81276600	0.22424500
C	1.42512700	2.95533600	-0.81502100
C	2.47142800	3.21110800	0.12051400
C	3.63070800	3.87210700	-0.33311300
C	3.76039700	4.27191500	-1.67327200
C	2.72483900	4.01126300	-2.58053100
C	1.53997900	3.35515900	-2.17859900
C	3.62614600	2.46391500	2.29641000
C	2.30401700	2.86562300	1.60413000

C	1.64584800	4.05311200	2.36163000
C	-3.23676000	0.98996100	4.58058800
C	-3.30275600	1.97197600	3.38350300
C	-3.58963800	3.41626800	3.87532000
C	-4.00092700	1.34807100	0.97512400
C	-4.33622700	1.53513700	2.34069300
C	-5.68021900	1.32612200	2.71504600
C	-6.63972800	0.93424600	1.76803000
C	-6.27698500	0.74683800	0.42402000
C	-4.94802600	0.94850600	-0.00319300
C	0.95086700	2.32404700	-4.43984000
C	0.43506900	3.12338000	-3.21655500
C	-0.19481000	4.47059400	-3.66399300
C	-5.10029900	-0.51781200	-2.09900200
C	-4.57065500	0.79812000	-1.47995200
C	-5.07034300	2.02615000	-2.29026100
C	-1.42516700	-2.95524600	-0.81535100
C	-1.53967800	-3.35504600	-2.17895200
C	-2.72441600	-4.01120000	-2.58119800
C	-3.76015400	-4.27196800	-1.67419400
C	-3.63078300	-3.87222500	-0.33397900
C	-2.47167900	-3.21112700	0.11993300
C	-0.94979600	-2.32373900	-4.43994100
C	-0.43448400	-3.12334200	-3.21662300
C	0.19525100	-4.47065500	-3.66398200
C	3.23720700	-0.99098700	4.58050200
C	3.30330400	-1.97285800	3.38328700
C	3.59057800	-3.41712900	3.87492100
C	4.00093100	-1.34806500	0.97496500
C	4.33651000	-1.53559300	2.34039000
C	5.68055800	-1.32655300	2.71456200
C	6.63982800	-0.93417200	1.76752500
C	6.27680500	-0.74630800	0.42364600
C	4.94781000	-0.94804200	-0.00339500
C	-3.62714200	-2.46470500	2.29570100
C	-2.30466700	-2.86551500	1.60355100
C	-1.64582900	-4.05253800	2.36123900
C	5.10000300	0.51822700	-2.09931300
C	4.57015400	-0.79752100	-1.48007300
C	5.06930300	-2.02573900	-2.29045000
H	-0.69638300	4.19720800	-0.38296000
H	-2.89553500	3.60327200	0.25781200
H	0.69595400	-4.19712900	-0.38225500
H	2.89509200	-3.60344100	0.25851200
H	4.43583900	4.08195600	0.36510400
H	4.66141400	4.78334100	-2.00476500
H	2.83189800	4.32200900	-3.61702200
H	1.62296900	2.00895500	1.67142500
H	-2.31476800	1.97115300	2.91031600
H	4.32693700	3.30686900	2.36395700
H	4.12215900	1.64319800	1.76651200
H	3.42194900	2.13300400	3.32320900

H	2.28457200	4.94561700	2.31172600
H	1.49757500	3.79836100	3.42024800
H	0.66958900	4.31046800	1.93406300
H	-4.18377700	0.96039800	5.13545200
H	-2.45051700	1.30277300	5.28037300
H	-3.00928800	-0.02716500	4.24182600
H	-3.58751000	4.13063400	3.04227400
H	-2.82497900	3.73264900	4.59690100
H	-4.56809800	3.47946800	4.36966600
H	-5.97648900	1.46514900	3.75175700
H	-7.67029700	0.77480500	2.07694900
H	-7.03136200	0.44330100	-0.29666600
H	-0.34670400	2.50854800	-2.76356300
H	-3.47829500	0.77275800	-1.55764000
H	1.77056500	2.84190500	-4.95689600
H	0.13555100	2.18037500	-5.16185800
H	1.28924100	1.33339300	-4.12108200
H	0.54482800	5.11113900	-4.16339200
H	-0.59916700	5.03275800	-2.81135700
H	-1.01465900	4.28907400	-4.37209000
H	-4.75211200	-1.39125600	-1.53734800
H	-4.73696300	-0.61514200	-3.12991500
H	-6.19797100	-0.54088700	-2.13103000
H	-6.16568100	2.10059700	-2.25656900
H	-4.76670200	1.93469300	-3.34112200
H	-4.65527500	2.96312400	-1.89720900
H	-2.83121900	-4.32188300	-3.61773300
H	-4.66106300	-4.78344200	-2.00590600
H	-4.43604300	-4.08217900	0.36405400
H	0.34732700	-2.50875500	-2.76335900
H	2.31525000	-1.97223000	2.91024200
H	-1.76961600	-2.84124200	-4.95714700
H	-0.13431900	-2.18037500	-5.16184300
H	-1.28779700	-1.33299000	-4.12108700
H	0.59922400	-5.03296500	-2.81126200
H	1.01534700	-4.28928500	-4.37183500
H	-0.54438200	-5.11100700	-4.16363900
H	4.18432100	-0.96120500	5.13518800
H	2.45118800	-1.30413100	5.28039100
H	3.00936100	0.02611000	4.24191300
H	3.58844800	-4.13143800	3.04182600
H	2.82612700	-3.73373500	4.59662600
H	4.56914200	-3.48017100	4.36907600
H	5.97703200	-1.46594200	3.75116700
H	7.67043800	-0.77471700	2.07630200
H	7.03101500	-0.44243700	-0.29707100
H	-1.62419400	-2.00839600	1.67087900
H	3.47778800	-0.77185600	-1.55750400
H	-4.32722700	-3.30823600	2.36341900
H	-4.12386100	-1.64452200	1.76562800
H	-3.42324400	-2.13339000	3.32242200
H	-1.49793100	-3.79761200	3.41986500

H	-0.66931600	-4.30926700	1.93388200
H	-2.28396800	-4.94545800	2.31125400
H	4.75215600	1.39180200	-1.53764000
H	4.73646600	0.61558000	-3.13015200
H	6.19767400	0.54103300	-2.13160100
H	4.65403100	-2.96256300	-1.89725800
H	6.16462600	-2.10050700	-2.25698000
H	4.76546600	-1.93423900	-3.34125000
O	-0.00062100	0.00042000	-2.29356100
O	1.79829000	-0.47432100	0.54722600
O	-1.79817800	0.47441300	0.54765400
N	2.63336000	-1.58229500	0.56040600
N	-2.63338400	1.58229800	0.56045400

### 5.3 Structures with four oxygen atoms

#### Dioxo Complex (lower energy conformation)

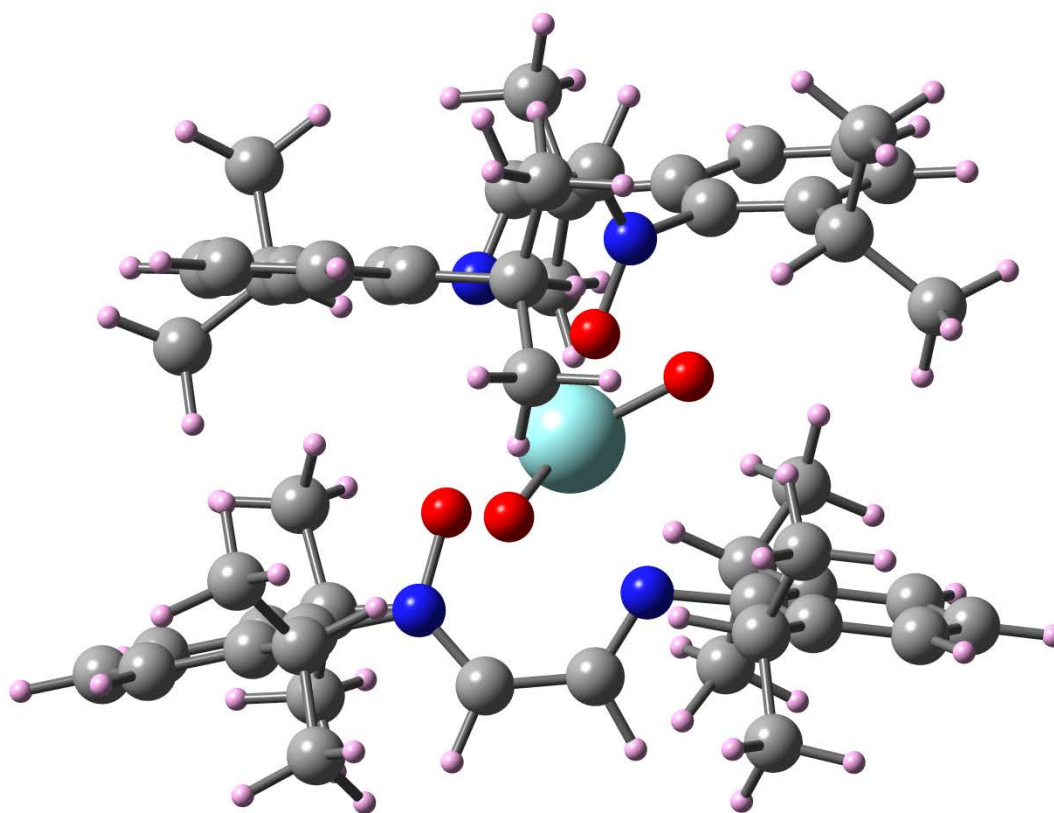


Fig. S48: NCCNO Dioxo Complex (lower energy conformation)

SCF	$E_{ZP}$	H	G
-2591.0884943	-2589.940153	-2589.870749	-2590.046750

Zr	-0.00255200	0.15159300	0.92558000
N	-0.58162400	2.42042800	0.26000300
N	0.58320800	-2.20818000	1.00943100
C	0.30580900	3.26773600	-0.18828800
C	1.62371100	2.95094600	-0.69567200
C	-0.30218900	-3.15597300	0.85463100
C	-1.62271000	-3.01862300	0.27808000
C	-1.87448100	2.98472400	0.65356700
C	-2.89731600	3.06145800	-0.33012400
C	-4.12712500	3.63699700	0.04843800
C	-4.33493600	4.10411700	1.35660900
C	-3.31443600	3.99072400	2.31153500
C	-2.06167900	3.42484100	1.98833600
C	-3.88663300	1.80946000	-2.34440100
C	-2.67040800	2.57274400	-1.76680200

C	-2.29404400	3.75620100	-2.70109800
C	2.03861400	0.12720200	-4.55809000
C	2.32306800	1.54867000	-4.00184300
C	2.50133800	2.57190200	-5.15136900
C	3.40515500	1.60811100	-1.65096300
C	3.53025500	1.51941200	-3.05883000
C	4.83430000	1.37044100	-3.57254700
C	5.94494100	1.31545500	-2.71373600
C	5.77469600	1.39690800	-1.32327600
C	4.49215600	1.53553400	-0.74590900
C	-1.47157200	2.39351500	4.22993200
C	-0.98268100	3.29994900	3.06959900
C	-0.53868900	4.69452400	3.58429900
C	5.12728900	0.51740600	1.51156200
C	4.32295000	1.61749500	0.77595700
C	4.74271500	3.02099100	1.29251000
C	1.88071900	-2.61701800	1.55167200
C	2.08253300	-2.59898700	2.95515800
C	3.33492900	-3.04380300	3.43224300
C	4.34193300	-3.47360000	2.55621400
C	4.12188700	-3.45229100	1.16930300
C	2.89143800	-3.01732900	0.63620900
C	1.52920700	-0.90120800	4.75969700
C	1.01726600	-2.12008600	3.94788200
C	0.56089200	-3.27431900	4.87899200
C	-2.07202700	-1.55741400	-4.30255200
C	-2.32410200	-2.72054900	-3.30581500
C	-2.48104400	-4.06920600	-4.05270100
C	-3.40820700	-2.05177800	-1.05155000
C	-3.53204400	-2.40801800	-2.41652400
C	-4.83651900	-2.43657900	-2.94981800
C	-5.94857700	-2.12449200	-2.15004500
C	-5.77957400	-1.76469900	-0.80424800
C	-4.49690200	-1.70685300	-0.21353700
C	3.87133000	-2.49438300	-1.68042200
C	2.65278900	-3.01322100	-0.87953100
C	2.24905800	-4.42764300	-1.38106900
C	-5.13839500	-0.03078400	1.60679900
C	-4.32910200	-1.30359600	1.25629800
C	-4.74489300	-2.47315600	2.19013300
H	0.07813700	4.33798300	-0.18674300
H	2.32917100	3.76237400	-0.82042900
H	-0.07033100	-4.17055900	1.19231700
H	-2.32623300	-3.82901600	0.41965000
H	-4.92845600	3.71606700	-0.68122100
H	-5.29064100	4.54527500	1.63035100
H	-3.48911500	4.33834100	3.32649500
H	-1.82874200	1.86916800	-1.75664700
H	1.43512700	1.84733900	-3.43244200
H	-4.75654500	2.46580000	-2.47849300
H	-4.18091100	0.97856400	-1.69413000
H	-3.63404000	1.39546000	-3.32966900

H	-3.10562300	4.49516500	-2.73470900
H	-2.11611400	3.39832000	-3.72454300
H	-1.38860600	4.27425600	-2.35904100
H	2.88968000	-0.24440300	-5.14437500
H	1.15618800	0.14510800	-5.21155000
H	1.84749500	-0.57341500	-3.73782400
H	2.70445500	3.57902500	-4.76511300
H	1.58831100	2.61642000	-5.75944300
H	3.32764400	2.29500500	-5.81829900
H	4.98186300	1.30005900	-4.64674400
H	6.94348900	1.20443900	-3.13002600
H	6.64183400	1.34064300	-0.67212200
H	-0.10235000	2.80074800	2.65046500
H	3.27139300	1.45173800	1.05550400
H	-2.35769000	2.81245600	4.72846800
H	-0.67523500	2.29316300	4.97971300
H	-1.70560800	1.39642100	3.83829700
H	-1.36839200	5.23145200	4.06439600
H	-0.15900100	5.32793200	2.76959900
H	0.26149800	4.58023400	4.32722800
H	4.85006900	-0.48195100	1.15777400
H	4.89118800	0.56119300	2.58123000
H	6.21408200	0.64066700	1.39831600
H	5.80596700	3.22169900	1.09731800
H	4.57452400	3.07776600	2.37496200
H	4.15893600	3.82470600	0.82281900
H	3.51986400	-3.04648800	4.50332700
H	5.29710700	-3.81423500	2.94938500
H	4.91370200	-3.77207600	0.49741300
H	0.13901400	-1.76513900	3.39782200
H	-1.42966200	-2.79547600	-2.67665700
H	2.41421500	-1.15335400	5.36188500
H	0.74089800	-0.55750100	5.44304900
H	1.76995000	-0.08224400	4.07135000
H	0.16581600	-4.12664200	4.30753200
H	-0.23083700	-2.92018600	5.55199500
H	1.38903700	-3.64436700	5.49901600
H	-2.93247100	-1.41709700	-4.97029600
H	-1.19112600	-1.77298900	-4.92182300
H	-1.89403100	-0.62115000	-3.76209600
H	-2.66064600	-4.89686400	-3.35455900
H	-1.56846200	-4.29239600	-4.62070600
H	-3.31500700	-4.04402900	-4.76556700
H	-4.98326300	-2.70487500	-3.99263100
H	-6.94734000	-2.15608100	-2.57922700
H	-6.64808900	-1.51211500	-0.20330400
H	1.82059000	-2.32989800	-1.08951000
H	-3.27853900	-1.05309200	1.46841400
H	4.73126700	-3.17265200	-1.60375400
H	4.18369800	-1.50392000	-1.33193800
H	3.61177700	-2.41335000	-2.74436800
H	2.06216900	-4.41457900	-2.46367600



H	1.34161200	-4.79264000	-0.88261200
H	3.04993700	-5.15220900	-1.18229900
H	-4.86783300	0.80542400	0.95231300
H	-4.89935000	0.26923400	2.63379600
H	-6.22467700	-0.18925700	1.54333100
H	-4.15733500	-3.38200500	2.00013100
H	-5.80694100	-2.72951900	2.06673000
H	-4.57926200	-2.18353600	3.23506300
O	1.43369500	0.83000100	1.92108700
O	-1.43926500	-0.18607100	2.08224500
O	-1.29967600	-0.96300800	-0.80479800
O	1.29544400	0.65816600	-1.06999400
N	-2.04992600	-2.01724500	-0.47941200
N	2.04735800	1.75986900	-1.09712700

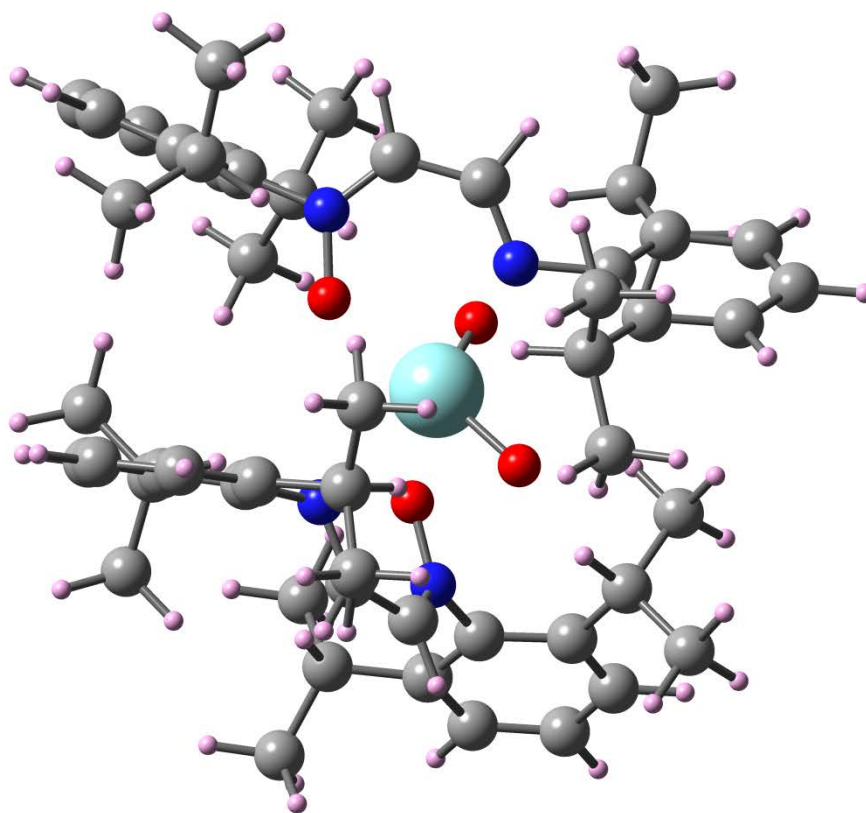
**Dioxo Complex (higher energy conformation)**

Fig. S49: NCCNO Dioxo Complex (higher energy conformation)

	SCF	E <sub>ZP</sub>	H	G
	-2591.0754021	-2589.927498	-2589.857937	-2590.035817
Zr		-0.38641300	-0.39588700	-0.08974600
O		1.90112300	-0.10786800	-0.11633800
O		-1.94430300	1.26483300	-0.64217600
O		-0.66125900	-1.03285900	-1.84468800
N		-0.09450400	1.70216800	1.41749400
N		-2.85920800	1.62552900	0.26853100
N		0.58789700	-2.69428600	-0.09382800
N		2.75303500	-0.76826400	-0.93546900
C		-1.20228600	2.01744800	2.03781700
C		-2.55001200	1.83482800	1.54076300
C		1.71362600	-3.00720900	-0.69361700
C		2.71539500	-2.07477400	-1.14646400
C		1.13782800	2.21232300	1.99981100
C		1.64780100	1.67298800	3.21030200
C		2.79616900	2.27846800	3.76644800
C		3.42467700	3.36381100	3.14065300
C		2.92658500	3.85111800	1.92055200
C		1.78393800	3.28424900	1.32320200
C		2.07817400	-0.66588900	4.10047000

C	1.02533100	0.45647400	3.90775400
C	0.39195600	0.83993100	5.27161500
C	-4.69334400	-1.73732700	-0.69701100
C	-4.69708000	-0.67617200	0.43546600
C	-5.60459300	-1.11789000	1.61098100
C	-4.23521900	1.78528900	-0.22597900
C	-5.11798300	0.68510500	-0.12410900
C	-6.42938900	0.88452400	-0.61155200
C	-6.81662200	2.10593700	-1.18197400
C	-5.89780800	3.16364300	-1.29183600
C	-4.57789100	3.02613800	-0.81769200
C	2.30965300	4.22396300	-1.00780700
C	1.21499400	3.85635800	0.02138500
C	0.31354700	5.08759100	0.31553700
C	-3.08154700	4.18273700	-2.49088100
C	-3.55914400	4.15327100	-1.01267100
C	-4.10406800	5.53428500	-0.57291900
C	-0.34803500	-3.79234000	0.10952500
C	-0.90091500	-4.47258300	-1.01819400
C	-1.79380500	-5.53554100	-0.76203300
C	-2.12826900	-5.91730000	0.54438600
C	-1.57847900	-5.22500600	1.63396400
C	-0.69125300	-4.14878400	1.44212400
C	-1.93540400	-3.75294000	-3.23138700
C	-0.62329400	-4.08720300	-2.47828500
C	0.16792800	-5.20160700	-3.21438300
C	5.84889600	0.79804000	1.38519100
C	5.31927800	-0.27906200	0.40681200
C	6.33378600	-1.44760800	0.27251200
C	3.75218600	0.06604100	-1.61808300
C	4.98511400	0.30776700	-0.96830400
C	5.92711200	1.09357300	-1.66435300
C	5.63272000	1.61454300	-2.93537700
C	4.38999400	1.36389900	-3.53896600
C	3.40862600	0.58257000	-2.89132700
C	-1.13189000	-2.98523800	3.66457800
C	-0.06034300	-3.46901200	2.65794600
C	0.97482500	-4.41575000	3.32592700
C	1.36165200	1.60134700	-4.03116600
C	2.06278500	0.29944600	-3.56858400
C	2.24844700	-0.67259200	-4.76471200
H	-1.15962300	2.54460300	2.99765600
H	-3.37864100	2.04918500	2.20392500
H	1.92065400	-4.04556000	-0.95942200
H	3.50682300	-2.45792900	-1.77993100
H	3.20185600	1.89317300	4.69870300
H	4.30058700	3.82217300	3.59386000
H	3.42954900	4.68178700	1.43299700
H	0.22967700	0.04515900	3.27574100
H	-3.66541800	-0.63909700	0.80906200
H	2.89068300	-0.34884000	4.76704700
H	2.51984200	-0.95732300	3.13928600

H	1.60817100	-1.55142200	4.54402700
H	1.14711600	1.23802100	5.96275100
H	-0.06627900	-0.04090800	5.73966300
H	-0.38798900	1.60436700	5.15651600
H	-5.69398900	-1.87957700	-1.13070800
H	-4.34791600	-2.69746500	-0.29516100
H	-4.00110000	-1.44507300	-1.49473100
H	-5.60351500	-0.37735800	2.42291200
H	-5.23289500	-2.06565600	2.01978300
H	-6.64644300	-1.27215200	1.29637700
H	-7.14450500	0.06889700	-0.55071500
H	-7.83123000	2.23232900	-1.55276500
H	-6.20718600	4.09743600	-1.75303200
H	0.58049500	3.08596400	-0.43227200
H	-2.67521500	3.94103800	-0.39919400
H	2.93148900	5.06171800	-0.66548900
H	1.84494300	4.53020900	-1.95443000
H	2.96704700	3.37052200	-1.21121700
H	0.89925000	5.90041000	0.76580000
H	-0.49799800	4.83593500	1.01091400
H	-0.13661800	5.46401600	-0.61301500
H	-2.64322800	3.21917800	-2.77366200
H	-2.32379300	4.96555000	-2.63169200
H	-3.91903700	4.39416000	-3.16886300
H	-4.93996000	5.86125200	-1.20424400
H	-3.31465200	6.29290000	-0.65495100
H	-4.45492700	5.51609300	0.46711300
H	-2.23882600	-6.06276800	-1.60205600
H	-2.81403300	-6.74478100	0.71226800
H	-1.84036900	-5.52358800	2.64559900
H	-0.05381600	-3.15292600	-2.49766700
H	4.39905100	-0.68137800	0.84683500
H	-2.63287800	-4.60149900	-3.25619100
H	-1.70598100	-3.47225600	-4.26849700
H	-2.41641900	-2.89480300	-2.75360600
H	1.12045200	-5.43129700	-2.71504700
H	0.38890400	-4.89148600	-4.24489700
H	-0.40783700	-6.13610800	-3.26326200
H	6.80217000	1.22287400	1.04435100
H	6.01982100	0.35250200	2.37394500
H	5.12730100	1.61366600	1.50097600
H	5.95021800	-2.24495600	-0.37754600
H	6.54418200	-1.88405800	1.25754500
H	7.28344900	-1.09752900	-0.15292600
H	6.89126500	1.30223900	-1.20915800
H	6.37282500	2.21873300	-3.45480100
H	4.17518600	1.77948600	-4.51951000
H	0.46932300	-2.57743300	2.30683800
H	1.37335700	-0.18340600	-2.86580900
H	-1.72800800	-3.81728200	4.06335000
H	-1.78516100	-2.26882200	3.15461800
H	-0.65327900	-2.48658200	4.52023300

H	1.46325100	-3.91910300	4.17535100
H	1.75515800	-4.72376000	2.61598200
H	0.48907700	-5.32605200	3.70239800
H	1.24340200	2.30383300	-3.19762200
H	0.36169900	1.35634800	-4.40795200
H	1.91570000	2.10903200	-4.83302500
H	2.70306000	-1.62098200	-4.44769600
H	2.88919000	-0.23586000	-5.54320300
H	1.27180900	-0.90057100	-5.20824400
O	-1.60798600	-0.97572800	1.21522400

## Peroxo Complex

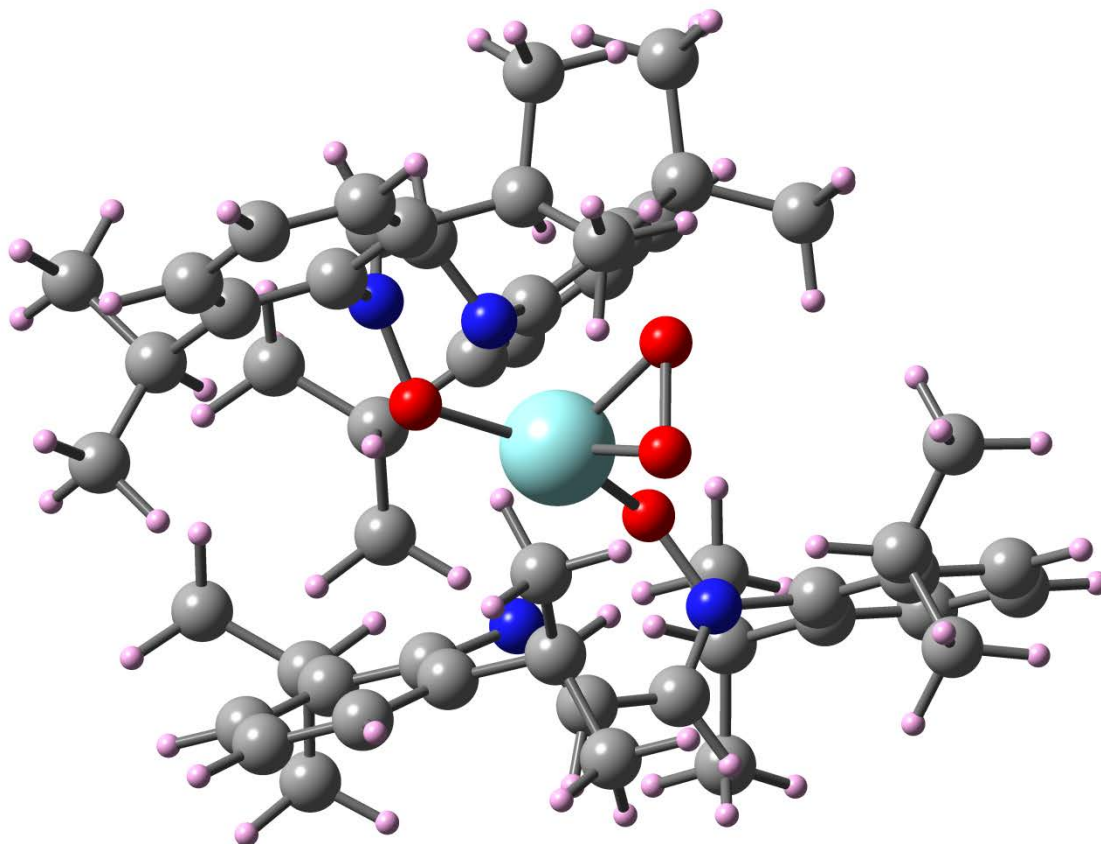


Fig. S50: NCCNO Peroxo Complex

SCF	E <sub>ZP</sub>	H	G
-2591.0542294	-2589.908017	-2589.838352	-2590.017931

Zr	-0.00083300	0.00092800	-0.37559200
O	2.05643600	0.29148400	0.06151400
O	-2.05856200	-0.29302500	0.07385500
O	-0.13561400	0.77220600	-2.25539900
O	0.11626300	-0.76930100	-2.25726300
N	0.06850000	-2.08412200	0.56652000
N	-2.81850100	-1.43570800	-0.16232400
N	-0.06768900	2.07973600	0.57708200
N	2.82078200	1.43532200	-0.15375200
C	-0.98370300	-2.94891200	0.49570900
C	-2.30774800	-2.65832400	0.12986100
C	0.98677700	2.94357400	0.51819100
C	2.31096900	2.65525900	0.15286500
C	1.32397600	-2.71964100	0.96614600
C	2.08729400	-3.45329500	0.01508800
C	3.25773800	-4.10549400	0.45992300
C	3.66713700	-4.03736800	1.79893900
C	2.90949200	-3.29781400	2.72011500

C	1.73559200	-2.62459700	2.32509600
C	2.82439500	-3.06355000	-2.39077400
C	1.69080800	-3.56701400	-1.46169200
C	1.28805800	-5.02079300	-1.82637100
C	-3.03907600	-0.68316200	-4.24681400
C	-3.14663400	-1.69908400	-3.08209000
C	-3.28219500	-3.14644200	-3.62760300
C	-4.13676300	-1.23244500	-0.73275200
C	-4.30517500	-1.36865900	-2.13558400
C	-5.61050200	-1.20389500	-2.64759800
C	-6.68914500	-0.90542600	-1.80125100
C	-6.48766700	-0.75969900	-0.41871000
C	-5.20506100	-0.91311300	0.14523600
C	1.78123700	-0.92451900	4.23829900
C	0.91107600	-1.86447700	3.36784200
C	0.10857500	-2.85169600	4.25822200
C	-5.63720700	0.50171900	2.22911500
C	-5.00029700	-0.78868800	1.65748900
C	-5.54929900	-2.04545600	2.38691800
C	-1.32315200	2.71466500	0.97774500
C	-1.73683600	2.61464100	2.33574800
C	-2.91090300	3.28703900	2.73170100
C	-3.66675200	4.03066000	1.81234000
C	-3.25512000	4.10413000	0.47428500
C	-2.08430000	3.45314500	0.02868600
C	-1.78666400	0.90520500	4.24040900
C	-0.91462000	1.84972900	3.37683100
C	-0.11462200	2.83278200	4.27405000
C	3.03038500	0.70418200	-4.23971700
C	3.14230200	1.71550300	-3.07144000
C	3.27680900	3.16499000	-3.61144500
C	4.13816100	1.23675800	-0.72734600
C	4.30350800	1.38066100	-2.12978500
C	5.60777200	1.21992700	-2.64561000
C	6.68857700	0.91825500	-1.80307400
C	6.49024100	0.76483900	-0.42092800
C	5.20856000	0.91353000	0.14653600
C	-2.81627800	3.07707700	-2.38108200
C	-1.68436200	3.57406300	-1.44655400
C	-1.27879100	5.02928500	-1.80233000
C	5.64379000	-0.51630300	2.21938800
C	5.00666200	0.77863300	1.65825700
C	5.55767800	2.02972100	2.39582000
H	-0.79077100	-3.99977400	0.71256200
H	-3.00929800	-3.47790500	0.03042300
H	0.79469900	3.99233400	0.74565100
H	3.01435000	3.47468700	0.06582100
H	3.85161800	-4.67213000	-0.25313700
H	4.56779200	-4.55422700	2.12237600
H	3.23149600	-3.24645800	3.75736700
H	0.82549300	-2.92523500	-1.64953200
H	-2.20090700	-1.63421500	-2.53639300

H	3.71853500	-3.69816100	-2.32291300
H	3.10974900	-2.03855800	-2.13032100
H	2.48277500	-3.06793800	-3.43376400
H	2.12500300	-5.71627500	-1.67661100
H	0.98609500	-5.07746600	-2.88066800
H	0.44817300	-5.37226500	-1.21234500
H	-3.91996200	-0.71191800	-4.90301500
H	-2.15418900	-0.91534500	-4.85151800
H	-2.91766700	0.33618600	-3.86617400
H	-3.30446900	-3.88410900	-2.81429500
H	-2.42993600	-3.38265600	-4.27758400
H	-4.20221900	-3.26660500	-4.21590900
H	-5.77896600	-1.30382500	-3.71645200
H	-7.68623300	-0.78289500	-2.21821400
H	-7.33128700	-0.52432300	0.22452100
H	0.18277300	-1.24426200	2.83268300
H	-3.92383400	-0.73006600	1.85202200
H	2.48221200	-1.48669900	4.86926300
H	1.14634700	-0.32808200	4.90634000
H	2.36383800	-0.23656200	3.61316800
H	0.78457000	-3.51546800	4.81379800
H	-0.55604500	-3.48005700	3.65185300
H	-0.50794700	-2.30578000	4.98531400
H	-5.23576600	1.39124500	1.73145500
H	-5.41663700	0.58427600	3.30166000
H	-6.72934800	0.50277300	2.11522300
H	-6.63119800	-2.15084800	2.23072500
H	-5.36820100	-1.97014400	3.46743900
H	-5.06645200	-2.96222300	2.02442200
H	-3.23452500	3.23172300	3.76825800
H	-4.56765400	4.54667200	2.13645300
H	-3.84741200	4.67426500	-0.23730700
H	-0.18486700	1.23229300	2.84044100
H	2.19847700	1.64923400	-2.52263200
H	-2.49058100	1.46394300	4.87114200
H	-1.15341600	0.30680900	4.90830100
H	-2.36611200	0.21921200	3.61025400
H	0.55115900	3.46449500	3.67245900
H	0.50047100	2.28349600	4.99982400
H	-0.79216100	3.49344800	4.83144200
H	3.90947600	0.73484900	-4.89822900
H	2.14395900	0.93925800	-4.84104200
H	2.90940600	-0.31656600	-3.86272300
H	3.30245300	3.89911600	-2.79505800
H	2.42242900	3.40444500	-4.25744100
H	4.19479900	3.28699100	-4.20253100
H	5.77393600	1.32586400	-3.71425900
H	7.68492000	0.79914200	-2.22280200
H	7.33549500	0.52670400	0.21915100
H	-0.81927900	2.93229700	-1.63553100
H	3.93044400	0.71946100	1.85432900
H	-3.70956000	3.71283500	-2.31245400



H	-3.10382600	2.05124400	-2.12648100
H	-2.47189000	3.08589400	-3.42312600
H	-0.97409100	5.09131300	-2.85555200
H	-0.44000900	5.37625900	-1.18425800
H	-2.11524600	5.72500600	-1.65092800
H	5.24128900	-1.40196600	1.71573100
H	5.42472000	-0.60677600	3.29160400
H	6.73575700	-0.51696800	2.10385300
H	5.07442500	2.94932100	2.04114400
H	6.63927700	2.13592200	2.23813300
H	5.37885900	1.94648100	3.47613400

## 5.4 Structures with five oxygen atoms

## Oxo Peroxo Complex (conformation 1 higher energy)

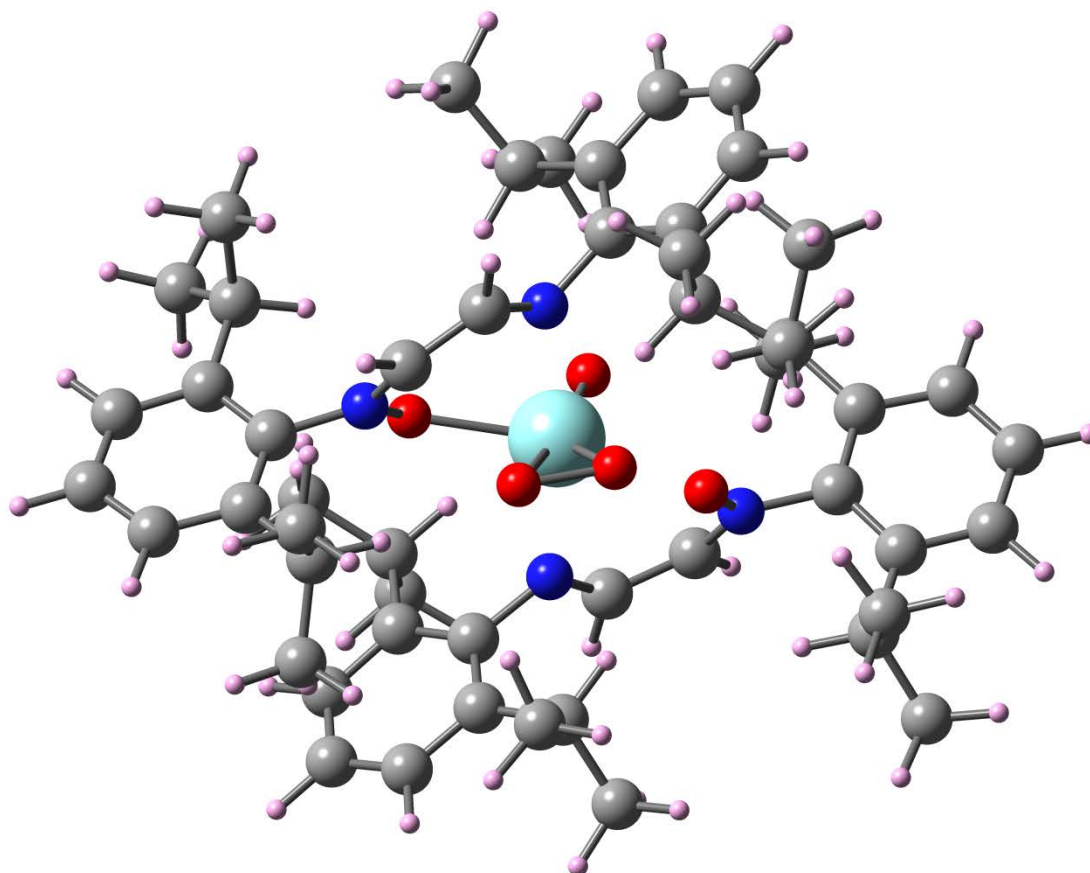


Fig. S51: NCCNO Oxo Peroxo Complex (conformation 1 higher energy)

SCF	$E_{ZP}$	H	G
-2666.24044048	-2665.088468	-2665.018221	-2665.196447

Zr	0.12067700	0.10585800	0.00833400
O	2.27350800	-0.85548500	0.28536200
O	-1.98746600	0.56210800	-0.48272200
O	0.95909600	0.70515500	-1.52975600
N	-0.10461000	2.28171600	0.85760800
N	-2.84758200	0.98037100	0.53404200
N	0.07130800	-2.14342800	-0.92347700
N	2.97464800	-1.39916900	-0.70145700
C	-1.16202400	2.47444000	1.61306800
C	-2.39226600	1.72573100	1.54285100
C	1.06124600	-2.62252000	-1.63335600
C	2.42536100	-2.14878000	-1.65128000
C	0.95273700	3.28161000	0.84981200
C	1.80806800	3.46059800	1.97476800
C	2.82150400	4.44037200	1.87728000

C	2.98275500	5.21845800	0.72277100
C	2.11820600	5.03235700	-0.36719200
C	1.09173400	4.06805300	-0.32942600
C	2.99374200	1.84761000	3.54445600
C	1.69392900	2.64648700	3.26904000
C	1.33719200	3.55385100	4.47580400
C	-4.46845100	-2.35731300	2.64750800
C	-4.17633500	-0.84237300	2.51213900
C	-4.58771000	-0.11543600	3.82389800
C	-4.26169300	0.64988000	0.38032800
C	-4.89146900	-0.22230500	1.30578200
C	-6.26743100	-0.48184800	1.11155400
C	-6.97448800	0.08565600	0.04420200
C	-6.32535400	0.95439200	-0.84913300
C	-4.96098300	1.26667900	-0.69611800
C	0.84357900	3.70615500	-2.85219700
C	0.11813700	3.95717400	-1.50828400
C	-0.78139400	5.22163800	-1.57854500
C	-4.82539200	2.32210000	-3.04457600
C	-4.29778300	2.32216900	-1.59029800
C	-4.48912500	3.73120900	-0.95864700
C	-1.14620400	-2.95258600	-0.88691700
C	-2.06087500	-2.90608800	-1.96986200
C	-3.19950700	-3.73611700	-1.89175000
C	-3.41605900	-4.57164300	-0.78556700
C	-2.49510000	-4.58980900	0.27450900
C	-1.34216600	-3.77884000	0.25208900
C	-3.06794300	-1.10635500	-3.46937900
C	-1.84389600	-2.01482100	-3.19909900
C	-1.50352500	-2.86707600	-4.45150400
C	4.39681700	-2.50135300	2.60374300
C	4.50073800	-3.06202500	1.15829000
C	5.22612600	-4.43027300	1.13973300
C	4.43434000	-1.20329900	-0.64280000
C	5.16787000	-2.03139500	0.24148800
C	6.56189600	-1.82682500	0.28719000
C	7.17403700	-0.84591800	-0.51069000
C	6.40498400	-0.03445900	-1.35873400
C	5.00241900	-0.18141100	-1.43783900
C	-0.94292300	-3.62106700	2.78364000
C	-0.31463000	-3.85813600	1.38894400
C	0.43916200	-5.21569400	1.33814000
C	4.53630300	2.21456500	-2.17308100
C	4.16545100	0.72113400	-2.35078800
C	4.32890800	0.29491300	-3.83555400
H	-1.17169900	3.28907600	2.34246100
H	-3.13425800	1.96215800	2.29694200
H	0.89679400	-3.51709900	-2.24169000
H	3.10489900	-2.54844500	-2.39265900
H	3.49134000	4.59015800	2.72062800
H	3.77078100	5.96674400	0.67403600
H	2.23592500	5.64676100	-1.25643400

H	0.91097900	1.89316100	3.15340400
H	-3.09404000	-0.72782100	2.39019900
H	3.86115100	2.50730300	3.68591500
H	3.20468000	1.16690900	2.71177300
H	2.87392500	1.24139600	4.45209400
H	2.12579900	4.29194400	4.67661200
H	1.20901700	2.94437400	5.38043400
H	0.40353900	4.10732200	4.30321200
H	-5.52587000	-2.55236300	2.87086800
H	-3.87574600	-2.77368600	3.47124100
H	-4.20353200	-2.89522200	1.73134100
H	-4.38065200	0.96182700	3.78593800
H	-4.03193000	-0.53172300	4.67348400
H	-5.66125600	-0.23884100	4.02131100
H	-6.78406800	-1.14309100	1.80113000
H	-8.03054200	-0.13846700	-0.08778300
H	-6.88844600	1.40217800	-1.66216900
H	-0.52448900	3.08855800	-1.34199300
H	-3.22536700	2.10911000	-1.63144000
H	1.57233600	4.49555000	-3.08408400
H	0.11203100	3.67612700	-3.67212700
H	1.34481300	2.73437000	-2.80694400
H	-0.18487200	6.12393700	-1.77020200
H	-1.32978100	5.37755600	-0.63930400
H	-1.51390400	5.12338700	-2.39180700
H	-4.75965600	1.32604700	-3.49702700
H	-4.22552600	3.01152200	-3.65269100
H	-5.86878300	2.65940300	-3.10525000
H	-5.55447900	3.99447800	-0.90996900
H	-3.97445000	4.49089000	-1.56065400
H	-4.08235500	3.77665500	0.05951200
H	-3.92207300	-3.72508900	-2.70366100
H	-4.29900100	-5.20534100	-0.74846300
H	-2.66967900	-5.24282600	1.12584600
H	-0.99776500	-1.34505600	-3.00831200
H	3.47380200	-3.23459500	0.81254800
H	-3.96498000	-1.69034100	-3.71532200
H	-2.85718700	-0.44081600	-4.31713300
H	-3.27915100	-0.49067700	-2.59038100
H	-0.60459600	-3.47975900	-4.29712000
H	-1.32651200	-2.21602000	-5.31758700
H	-2.32817000	-3.54761100	-4.70197800
H	5.39271300	-2.28307300	3.01179100
H	3.91238500	-3.23552000	3.26091300
H	3.80211000	-1.58199500	2.62257800
H	5.32166500	-4.82402200	0.11941300
H	4.66271300	-5.15867900	1.73700200
H	6.23278400	-4.36311600	1.57129700
H	7.16980300	-2.43490900	0.95082300
H	8.25162900	-0.70795400	-0.46286800
H	6.89185400	0.73181200	-1.95454200
H	0.42506200	-3.06242500	1.25048300

H	3.10218800	0.63196600	-2.08863600
H	-1.73932800	-4.34425200	3.00398200
H	-1.34549100	-2.60505700	2.84942800
H	-0.17185500	-3.72267400	3.55868300
H	1.21521600	-5.24835300	2.11445600
H	0.92039500	-5.37650300	0.36326400
H	-0.24662300	-6.05575200	1.51124100
H	4.41982600	2.53052300	-1.12992300
H	3.86398400	2.83046500	-2.78134600
H	5.56646400	2.42845000	-2.48995500
H	4.01992600	-0.74695300	-3.99729400
H	5.37186200	0.39118400	-4.16829600
H	3.70436700	0.93099900	-4.47509700
O	-0.91362200	-0.11623900	2.13375000
O	0.55608700	-0.00775500	2.09874000

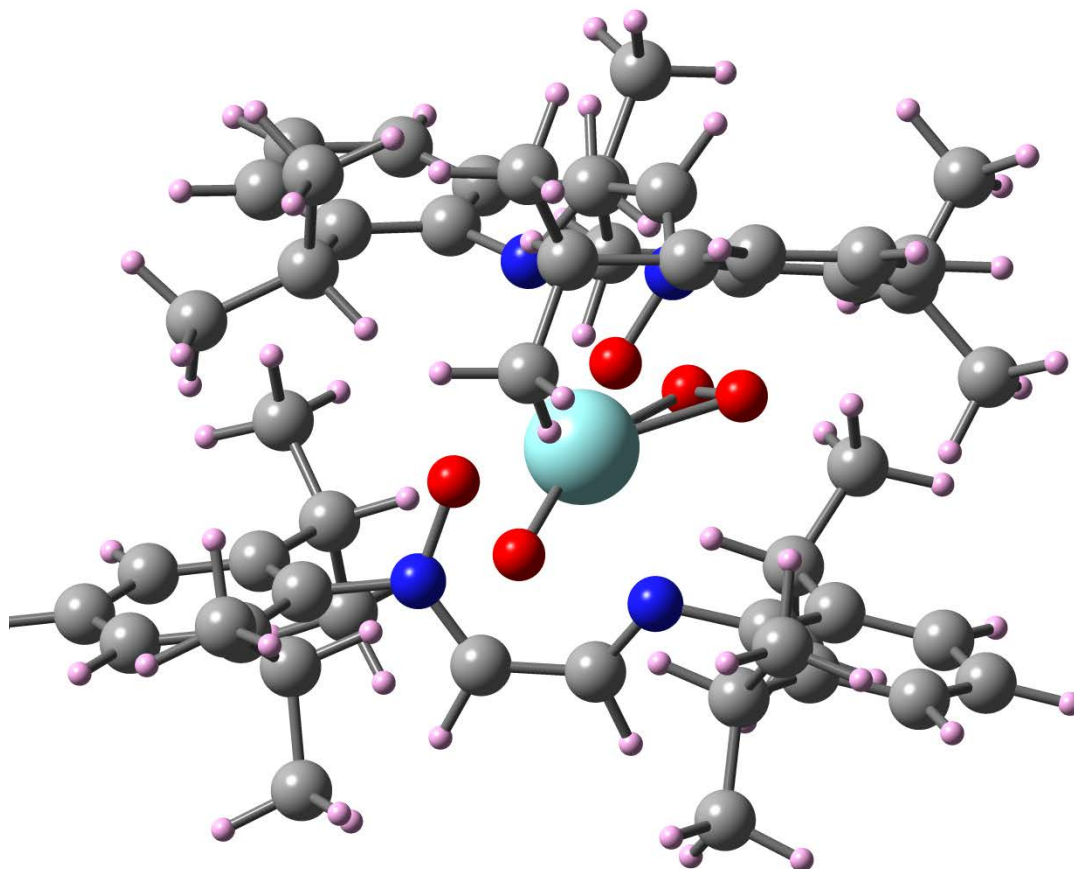
**Oxo Peroxo Complex (conformation 2 lowest energy)**

Fig. S52: NCCNO Oxo Peroxo Complex (conformation 2 lowest energy)

	<b>SCF</b>	<b>E<sub>ZP</sub></b>	<b>H</b>	<b>G</b>
	-2666.24191265	-2665.090548	-2665.020213	-2665.197779
Zr		-0.21880700	-0.08677600	-0.24052100
O		2.04472500	-0.10032400	-0.11827000
O		-2.03584900	1.24061500	-0.55349000
O		0.00750000	-0.02486100	-2.08586800
N		-0.05066000	1.68430100	1.43345800
N		-2.91210000	1.62016300	0.40257700
N		0.27622500	-2.44008800	-0.68069700
N		2.82605400	-0.76915800	-0.99273300
C		-1.14988500	2.01977500	2.08345300
C		-2.51157200	1.90888400	1.63554200
C		1.43599400	-2.83439300	-1.13714200
C		2.58127200	-1.99613700	-1.42078400
C		1.19889800	2.11584600	2.04754200
C		1.60844100	1.61540000	3.31584500
C		2.79140400	2.14737800	3.87575600
C		3.54259200	3.12542900	3.21131800
C		3.13114800	3.58443200	1.94881100

C	1.96018000	3.09172100	1.34185800
C	1.77982900	-0.71775400	4.30276400
C	0.86279500	0.51201400	4.07681400
C	0.30014100	1.02722900	5.42760700
C	-5.28496100	-1.79189500	0.91840300
C	-4.81715100	-0.41170000	1.44592900
C	-5.37104900	-0.16356900	2.87542100
C	-4.31654000	1.68924800	-0.00479300
C	-5.22542700	0.72487500	0.49967100
C	-6.56973200	0.84401400	0.08258700
C	-6.96926700	1.85091200	-0.80797000
C	-6.03228800	2.77044700	-1.30819600
C	-4.67979800	2.71412500	-0.91682100
C	2.62141500	4.09596700	-0.93316800
C	1.47312400	3.66108100	0.00513200
C	0.50433000	4.85365900	0.24353300
C	-3.23706600	3.26514200	-2.92053600
C	-3.66181100	3.70423300	-1.49196400
C	-4.18315800	5.16258500	-1.48654000
C	-0.73265300	-3.48221600	-0.49958900
C	-1.76429400	-3.58936900	-1.47279500
C	-2.71778700	-4.61438100	-1.30556300
C	-2.65883200	-5.49622000	-0.21619600
C	-1.63001000	-5.36801000	0.72763500
C	-0.64370100	-4.36560000	0.61083400
C	-3.20612800	-2.02414600	-2.89199800
C	-1.82294900	-2.69938600	-2.72044900
C	-1.45415400	-3.51968100	-3.98666400
C	5.72304700	0.06354700	1.93892600
C	5.14319100	-0.79763700	0.79077100
C	5.90856500	-2.14549200	0.67737200
C	4.04299000	-0.06583100	-1.42983600
C	5.15560400	-0.06366800	-0.55459100
C	6.31575700	0.59985600	-1.00378900
C	6.34548700	1.23025500	-2.25903200
C	5.21722100	1.21003900	-3.09398800
C	4.02564800	0.56175100	-2.70007800
C	-0.14788200	-4.14310100	3.09945300
C	0.45385100	-4.27670200	1.67797900
C	1.41687100	-5.49170900	1.59351400
C	2.50465900	1.89250100	-4.27620100
C	2.80840100	0.51731600	-3.63296100
C	3.02109300	-0.54703300	-4.74525500
H	-1.05717600	2.48873000	3.06597500
H	-3.29284400	2.19485000	2.32863300
H	1.59161000	-3.88692300	-1.38642700
H	3.35849400	-2.42045100	-2.04520600
H	3.12556000	1.78358700	4.84435700
H	4.44423800	3.52590400	3.66920600
H	3.72453300	4.33560000	1.43671200
H	0.03673700	0.14351400	3.46077000
H	-3.72530200	-0.46893400	1.50797200

H	2.64819000	-0.47652900	4.93174700
H	2.13810500	-1.10437800	3.34182300
H	1.21305100	-1.51829100	4.79477200
H	1.10383500	1.35025600	6.10361800
H	-0.26103900	0.22898300	5.93111900
H	-0.37634600	1.88234800	5.29024200
H	-6.37991800	-1.87991900	0.89938700
H	-4.89222500	-2.58292300	1.56858200
H	-4.90376000	-1.97691800	-0.09200600
H	-5.01784200	0.78939000	3.29325100
H	-5.04429100	-0.96717100	3.54749000
H	-6.46940800	-0.14039000	2.88043600
H	-7.30232000	0.12932500	0.44677000
H	-8.00910200	1.91571800	-1.11978900
H	-6.35558200	3.53923000	-2.00389100
H	0.90589100	2.87833700	-0.51333700
H	-2.75766400	3.67740500	-0.87241000
H	3.16203100	4.96776200	-0.54148700
H	2.21069500	4.38285600	-1.90957200
H	3.34128600	3.28386500	-1.08892000
H	1.02444300	5.67880500	0.74878500
H	-0.35153300	4.56318800	0.86500100
H	0.11729600	5.22750600	-0.71383200
H	-2.77260100	2.27434900	-2.89382700
H	-2.50830000	3.97572600	-3.33327800
H	-4.10339000	3.23457900	-3.59555800
H	-5.02656600	5.29859400	-2.17561400
H	-3.38480200	5.84248400	-1.81113000
H	-4.51031200	5.47205700	-0.48525900
H	-3.50977700	-4.72556300	-2.04208100
H	-3.40618300	-6.27884100	-0.10581600
H	-1.59190100	-6.05233400	1.57156700
H	-1.09148600	-1.88989700	-2.62776700
H	4.10375600	-1.01887600	1.05753600
H	-4.01049200	-2.75704400	-3.04702500
H	-3.18572000	-1.35571300	-3.76247700
H	-3.45603200	-1.41792400	-2.01339300
H	-0.45507700	-3.96798800	-3.89573200
H	-1.45378200	-2.86801400	-4.87051000
H	-2.17112200	-4.33386200	-4.16228100
H	6.78785100	0.28429300	1.78712000
H	5.63065100	-0.47648800	2.89017300
H	5.18125200	1.01052800	2.03285200
H	5.48097400	-2.79106600	-0.10108200
H	5.86412600	-2.68873900	1.63023700
H	6.96525000	-1.97760800	0.43050100
H	7.19729000	0.62464500	-0.36963100
H	7.25017200	1.73736100	-2.58637200
H	5.25520000	1.70686600	-4.05900900
H	1.02759500	-3.36108100	1.50973200
H	1.90809700	0.24068200	-3.06607900
H	-0.75566600	-5.01599800	3.37321600



H	-0.76515200	-3.24104200	3.14821000
H	0.65882200	-4.05247000	3.84053600
H	2.21164500	-5.40143400	2.34668000
H	1.88997700	-5.56900600	0.60442500
H	0.88496700	-6.43461900	1.77835200
H	2.38901200	2.66944800	-3.51301300
H	1.56110900	1.82589500	-4.83117500
H	3.28736600	2.21032600	-4.97951600
H	3.18259400	-1.55061200	-4.32953900
H	3.88860400	-0.30075300	-5.37374500
H	2.13209600	-0.59233200	-5.38649900
O	-1.63100700	-1.02251900	1.04048100
O	-0.29401500	-1.18697800	1.69260800

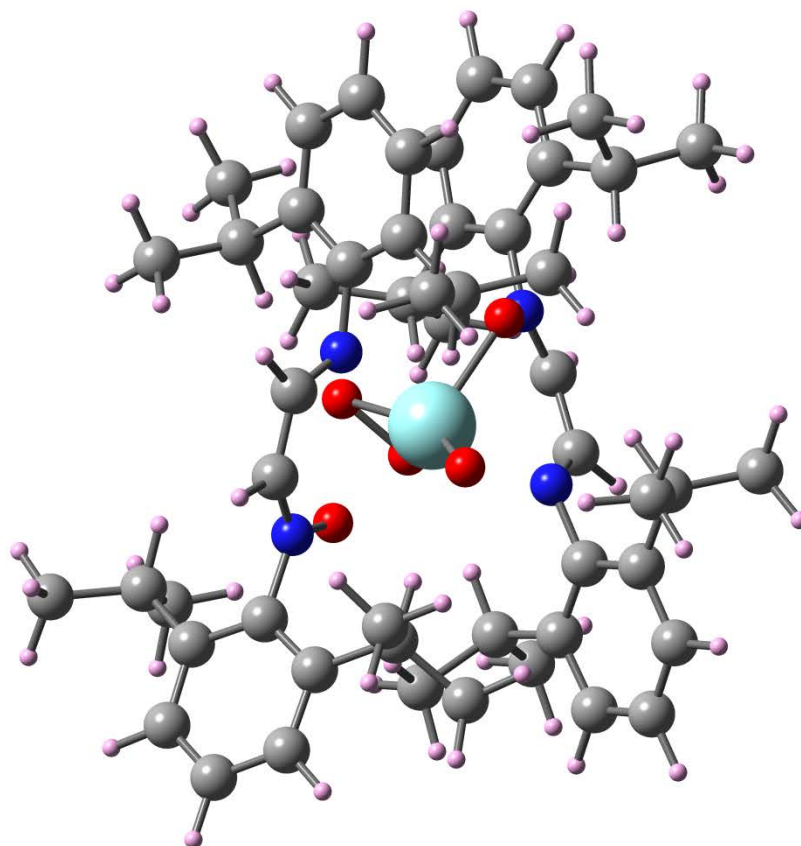
**Oxo Peroxo Complex (conformation 3 higher energy)**

Fig. S53: NCCNO Oxo Peroxo Complex (conformation 3 higher energy)

SCF	E <sub>ZP</sub>	H	G
-2666.23672257	-2665.084989	-2665.014674	-2665.192064

Zr	-0.04315700	-0.10825000	0.01958000
O	2.06866300	-0.74852700	0.25704300
O	-2.01585400	0.90148800	-0.61117600
O	0.07114800	-0.48124800	-2.10105700
O	0.49990000	0.93463500	-1.87187400
N	0.22085100	2.04226400	1.06963600
N	-2.72046000	1.74547500	0.13184800
N	-0.11776400	-2.47627700	-0.40407900
N	2.67903700	-1.34315600	-0.82683800
C	-0.82333000	2.75284800	1.41512900
C	-2.20646600	2.56690800	1.04207100
C	0.82381300	-2.96765200	-1.16824400
C	2.08684900	-2.33006900	-1.48416700
C	1.49721200	2.47547000	1.64090300
C	1.81505700	2.09609100	2.97311300
C	3.03585200	2.56417200	3.50815400
C	3.90491500	3.36212300	2.75181300

C	3.57015100	3.70896200	1.43222800
C	2.36303000	3.27660600	0.84708000
C	1.64883700	-0.06028800	4.31591100
C	0.90322200	1.21069100	3.83286500
C	0.33267900	2.00085500	5.04018200
C	-4.92772700	-1.37188500	1.77803100
C	-4.40374300	0.08447600	1.83435700
C	-4.72164400	0.72313900	3.21358100
C	-4.16960500	1.74643500	-0.13043400
C	-4.98049700	0.93835100	0.69898900
C	-6.36724400	0.96076400	0.43317700
C	-6.88938900	1.72846300	-0.61972800
C	-6.03997100	2.48930200	-1.44146900
C	-4.64788100	2.51600200	-1.21804200
C	3.18348200	3.88629500	-1.50867600
C	1.96844300	3.71314000	-0.56861600
C	1.15358900	5.03698600	-0.52403100
C	-3.36560400	2.40581600	-3.39389600
C	-3.70654000	3.28079500	-2.15435600
C	-4.26829000	4.65753300	-2.58273400
C	-1.28618300	-3.30621100	-0.14838300
C	-2.23669900	-3.52186400	-1.18679500
C	-3.34173300	-4.35114500	-0.89481600
C	-3.50244500	-4.93969700	0.36761700
C	-2.55913500	-4.69393000	1.37746700
C	-1.43931800	-3.87022400	1.14617900
C	-3.35722900	-1.95731900	-2.84970400
C	-2.13690500	-2.87531200	-2.57562300
C	-1.99283300	-3.94460500	-3.69032600
C	5.15267700	-0.65194800	2.30824300
C	4.84578800	-1.62701900	1.14366900
C	5.71913900	-2.90653300	1.24710700
C	4.00740100	-0.85015500	-1.19157400
C	5.03675000	-0.95049200	-0.21855100
C	6.30632800	-0.44900000	-0.56832700
C	6.54153300	0.10863300	-1.83440400
C	5.50954700	0.16534400	-2.78214800
C	4.21101200	-0.30719700	-2.49144900
C	-1.07781700	-3.02482600	3.51778700
C	-0.41641100	-3.64752500	2.26352600
C	0.33011300	-4.96548800	2.60373000
C	2.99399200	1.16521200	-4.20361600
C	3.13325900	-0.24645900	-3.58487800
C	3.43974300	-1.29022100	-4.69584200
H	-0.68006700	3.60117200	2.09026000
H	-2.93295900	3.20545400	1.52936900
H	0.69790000	-3.95322100	-1.62531400
H	2.67403300	-2.77545800	-2.27760600
H	3.30561100	2.29407900	4.52623300
H	4.84019500	3.71013500	3.18433900
H	4.25440200	4.32149400	0.85328200
H	0.06276800	0.85506600	3.22648100

H	-3.31138100	0.02269700	1.73729200
H	2.49482600	0.18241700	4.97368500
H	2.02966200	-0.63281400	3.46187800
H	0.95833900	-0.70497700	4.87444600
H	1.13217200	2.34593400	5.71014200
H	-0.34435500	1.36244400	5.62302200
H	-0.23163600	2.88528700	4.71385500
H	-6.01020300	-1.43177700	1.95872700
H	-4.42394600	-1.96955400	2.54717000
H	-4.71136600	-1.83468200	0.80832000
H	-4.30639200	1.73670800	3.29739500
H	-4.28299500	0.11477400	4.01451000
H	-5.80503200	0.78812900	3.38605700
H	-7.03580100	0.36303100	1.04610100
H	-7.96047400	1.72734500	-0.80847900
H	-6.46137900	3.06382200	-2.26084000
H	1.32800000	2.93423700	-1.00123800
H	-2.76009800	3.46383700	-1.62959900
H	3.81132400	4.73929200	-1.21642700
H	2.83416100	4.07549400	-2.53130500
H	3.80934400	2.98639400	-1.52368400
H	1.75420700	5.84978000	-0.09294600
H	0.24215500	4.93718600	0.07829500
H	0.85533100	5.33129500	-1.53895800
H	-2.86559900	1.48077200	-3.09036400
H	-2.68880400	2.95127900	-4.06419400
H	-4.27653300	2.15258600	-3.95345300
H	-5.15229400	4.55478600	-3.22506500
H	-3.51005400	5.20223900	-3.15955700
H	-4.54677300	5.27173400	-1.71635500
H	-4.08433100	-4.53355400	-1.66788700
H	-4.35920100	-5.58000800	0.56495300
H	-2.69143400	-5.14782100	2.35657400
H	-1.25939000	-2.22389500	-2.61699500
H	3.79917300	-1.92443500	1.24775800
H	-4.30065100	-2.52026500	-2.84718500
H	-3.24962700	-1.47785800	-3.83168900
H	-3.42280600	-1.16514900	-2.09532400
H	-1.11117800	-4.58058100	-3.52975800
H	-1.88734800	-3.45729500	-4.66863500
H	-2.87124100	-4.60229400	-3.73505100
H	6.20214500	-0.32767600	2.29624600
H	4.96660000	-1.14588700	3.27118600
H	4.51787200	0.23824000	2.25171300
H	5.49357600	-3.61391500	0.43813400
H	5.53391700	-3.41245700	2.20391800
H	6.78958200	-2.66815600	1.19559500
H	7.11762900	-0.50694800	0.15223600
H	7.52848400	0.49057900	-2.08462200
H	5.70734700	0.59170400	-3.76125500
H	0.32254000	-2.92131800	1.91118100
H	2.15365800	-0.46891900	-3.15505100

H	-1.87778200	-3.66284700	3.91814700
H	-1.48262600	-2.04261400	3.25079400
H	-0.32872700	-2.89085400	4.31095800
H	1.09292600	-4.78276700	3.37272200
H	0.82897600	-5.38624800	1.71950800
H	-0.36044900	-5.72718200	2.99022800
H	2.67622800	1.87963600	-3.44126100
H	2.21534700	1.14461600	-4.97639800
H	3.92490100	1.51736300	-4.66905900
H	3.53598700	-2.31080100	-4.29842300
H	4.37780600	-1.05430800	-5.21649900
H	2.63097700	-1.29143500	-5.43746100
O	-1.06375300	-0.37851200	1.57026100

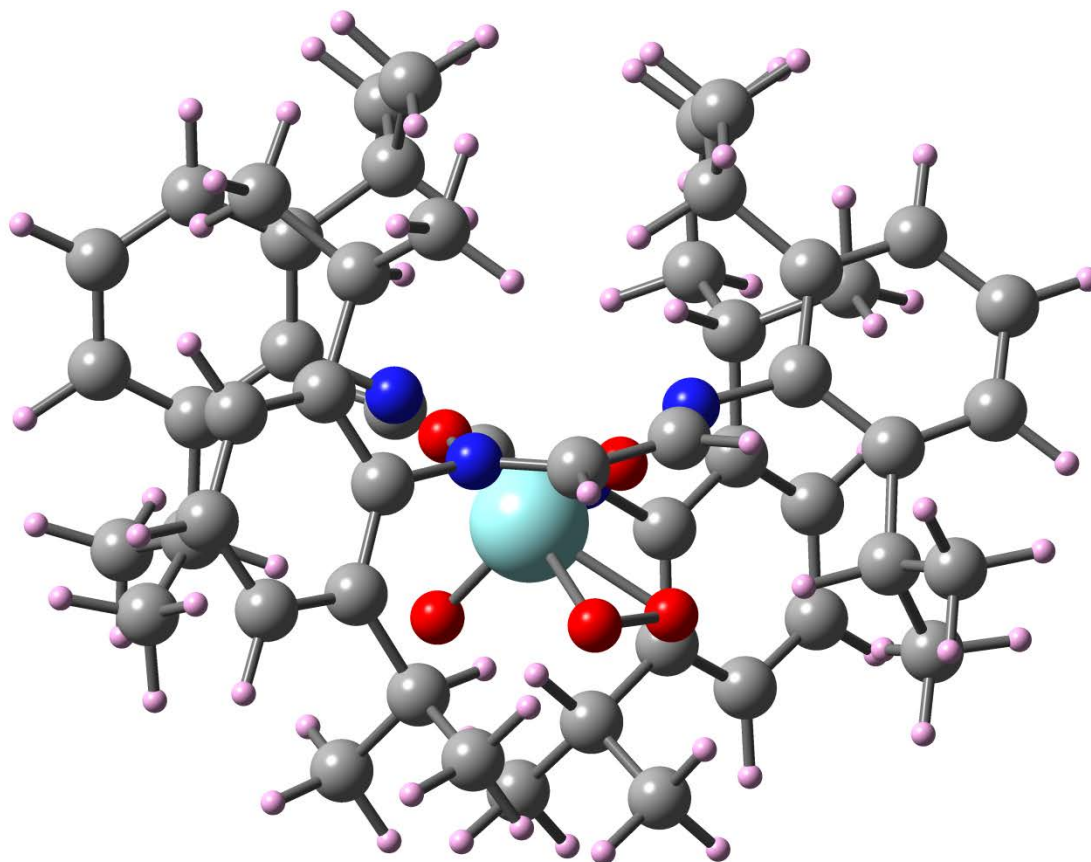
**Oxo Peroxo Complex (butterfly conformation)**

Fig. S54: NCCNO Oxo Peroxo Complex (butterfly conformation)

SCF	E <sub>ZP</sub>	H	G
-2666.248035	-2665.096245	-2665.025988	-2665.204376

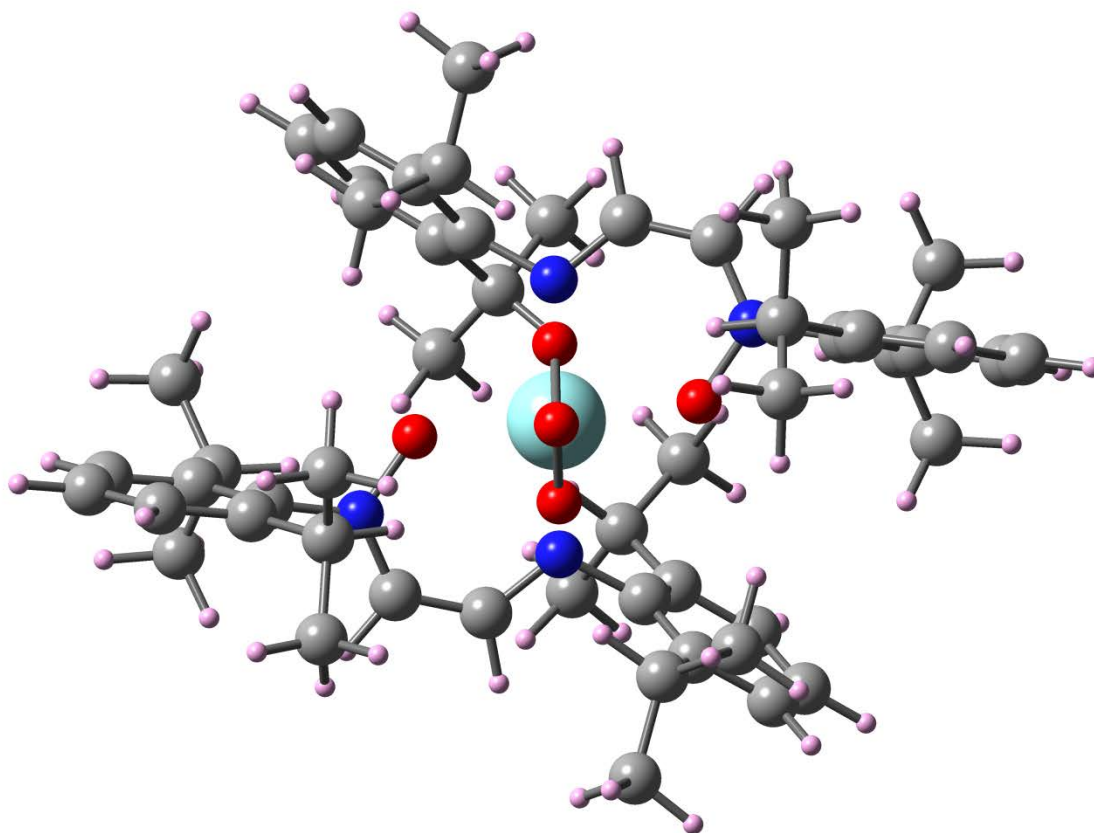
O	2.08359824	0.46550763	-0.04029076
O	0.91981243	-1.46117489	-1.96430182
N	-0.10570440	2.23985426	0.66766910
N	2.74419222	1.62759924	-0.20038365
N	-2.71281106	-1.37560391	-0.31422038
N	0.14127737	-2.34178147	0.52301479
C	0.88668319	3.08331981	0.57599237
C	2.22364200	2.80653039	0.07844697
C	-2.16589266	-2.58051194	-0.36787900
C	-0.86449496	-3.05058202	0.07040747
C	-1.36884073	2.80934413	1.13877073
C	-2.12949158	3.65362435	0.28077246
C	-3.33119779	4.18821471	0.79691426
C	-3.76224264	3.90855295	2.09978139
C	-2.98937090	3.07711718	2.92602720
C	-1.78560200	2.51103842	2.46432752

C	-2.85781029	3.68117797	-2.15978871
C	-1.72100957	4.00170108	-1.15633602
C	-1.30421069	5.49279984	-1.27140005
C	3.08701184	0.51999566	-4.04541320
C	3.19429769	1.75409882	-3.11026779
C	3.37768874	3.05857909	-3.92954567
C	4.12670181	1.50588006	-0.69934647
C	4.33022890	1.57568251	-2.09825372
C	5.66586837	1.46156924	-2.54283809
C	6.72151041	1.27712435	-1.63750430
C	6.46980116	1.18974002	-0.25832031
C	5.15753630	1.29141125	0.24600459
C	-1.69173125	0.77908382	4.35894211
C	-0.89444378	1.70062641	3.40852060
C	0.01821454	2.65871720	4.22546135
C	5.44173603	-0.16359630	2.31442420
C	4.89913768	1.17520128	1.75131541
C	5.50019853	2.38444850	2.51661965
C	-4.11551914	-1.13976848	-0.67254645
C	-4.49235256	-1.10378267	-2.03863048
C	-5.85811296	-0.86589823	-2.31675977
C	-6.78974691	-0.67029225	-1.28939799
C	-6.38029829	-0.71138772	0.05444495
C	-5.03366537	-0.94391783	0.39318093
C	-3.45164330	-0.06473048	-4.11720772
C	-3.52135072	-1.31617482	-3.20449363
C	-3.90748755	-2.57549372	-4.02528132
C	1.87270906	-0.92601424	4.07840065
C	0.98699260	-1.85566776	3.21691210
C	0.07253320	-2.73394945	4.11729481
C	1.32844173	-3.04197614	0.95909124
C	1.79394070	-2.75328375	2.27720468
C	2.95014292	-3.40098113	2.75082785
C	3.64772532	-4.31496430	1.94667593
C	3.18358778	-4.58862840	0.65375240
C	2.02697546	-3.97351260	0.12573208
C	-5.32559634	-0.04147283	2.77878386
C	-4.59966069	-1.05129471	1.85896022
C	-4.81192592	-2.50269256	2.37486012
C	2.78272413	-4.05985837	-2.30783684
C	1.62617588	-4.33169757	-1.31255286
C	1.15942331	-5.80953406	-1.41133813
H	0.74007346	4.13095287	0.85449418
H	2.88334721	3.65191018	-0.07732671
H	-2.84069151	-3.35392106	-0.72154273
H	-0.78734454	-4.14015846	0.00875655
H	-3.93543173	4.82988763	0.16102560
H	-4.68953740	4.33782492	2.47202337
H	-3.32362838	2.87558628	3.93955939
H	-0.88002157	3.36990325	-1.46105243
H	2.22903378	1.82527453	-2.59690756
H	-3.73807439	4.32264167	-2.01318986

H	-3.17193043	2.63614633	-2.06300109
H	-2.49643323	3.83022532	-3.18515635
H	-2.13494555	6.16474239	-1.01412687
H	-0.99475946	5.71756115	-2.30071130
H	-0.46486000	5.73661286	-0.60464147
H	4.01320507	0.35628104	-4.61444116
H	2.26700755	0.67571801	-4.75692722
H	2.85063402	-0.38521062	-3.47556555
H	3.43919204	3.94221299	-3.27896175
H	2.51980598	3.19158275	-4.59982361
H	4.28730061	3.03019220	-4.54501876
H	5.87244054	1.51164029	-3.60807137
H	7.74097048	1.19221384	-2.00611120
H	7.29583230	1.03252079	0.42980660
H	-0.24420917	1.06354037	2.79537696
H	3.81634847	1.17426051	1.92477584
H	-2.31718052	1.35107026	5.05620923
H	-1.00454415	0.17539676	4.96351182
H	-2.34017057	0.09853278	3.79543164
H	-0.58732220	3.32567124	4.85349289
H	0.63241861	3.28737271	3.56775932
H	0.69260022	2.09092428	4.88002294
H	4.98209265	-1.01937814	1.80759351
H	5.21595919	-0.23983259	3.38606108
H	6.53052240	-0.23755417	2.19697480
H	6.59147367	2.42082685	2.40464068
H	5.27421487	2.30784656	3.58822749
H	5.09556022	3.33689778	2.14913001
H	-6.18617772	-0.83113380	-3.35197919
H	-7.83387903	-0.48632046	-1.53173042
H	-7.11289091	-0.55894667	0.84099241
H	-2.50858866	-1.47669848	-2.82811456
H	0.33407235	-1.22875342	2.59872063
H	-4.42644184	0.17176618	-4.56604170
H	-2.73465173	-0.24249019	-4.92827194
H	-3.10361115	0.81021316	-3.55732141
H	-3.94565295	-3.47388627	-3.39412312
H	-3.16030802	-2.74614371	-4.81018521
H	-4.88773415	-2.46290040	-4.50823824
H	2.50772213	-1.49081273	4.77345068
H	1.24757147	-0.25767484	4.68353000
H	2.52424495	-0.30993238	3.44666318
H	-0.58819443	-3.36585793	3.51005282
H	-0.55520758	-2.11019660	4.76684024
H	0.67474223	-3.39478569	4.75538287
H	3.30262596	-3.19945059	3.75859661
H	4.53912967	-4.81029927	2.32475424
H	3.73107980	-5.29240121	0.03203826
H	-3.52918112	-0.82380628	1.91097364
H	0.81337815	-3.67924844	-1.63427801
H	-6.39872790	-0.25840047	2.85991739
H	-5.20388507	0.98395184	2.41204120



H	-4.90640008	-0.09378407	3.79206877
H	-4.46481220	-2.59568048	3.41261739
H	-4.26132852	-3.23214193	1.76726214
H	-5.87563079	-2.77440297	2.34533297
H	3.07989419	-3.00780537	-2.25768899
H	2.44350940	-4.26212923	-3.33241169
H	3.66058635	-4.69078021	-2.11122224
H	0.31526484	-6.02053725	-0.73932023
H	1.96843175	-6.50432823	-1.14719498
H	0.84255877	-6.03677150	-2.43803818
O	0.01889181	1.52165029	-2.03356152
O	-0.56601870	-1.53495176	-2.18191903
O	-1.98708062	-0.25586935	0.03897818
Zr	0.00474137	0.08398484	-0.89116603

$\eta^2$ -Ozone ComplexFig. S55: NCCNO  $\eta^2$ -Ozone Complex

SCF	$E_{ZP}$	H	G
-2666.202370	-2665.052570	-2664.982028	-2665.162667

Zr	0.00247200	0.05856200	-0.44484000
O	-2.07480700	0.22496000	-0.10330500
O	2.09075500	-0.20156400	-0.10195100
O	0.03434200	1.37679400	-2.08767100
N	0.00207100	-2.06991600	0.36331400
N	2.89012200	-1.30708100	-0.34577900
N	-0.00625400	1.92311800	0.83558300
N	-2.89857400	1.33795100	-0.01330100
C	1.07344200	-2.89769400	0.17927000
C	2.39282700	-2.55015000	-0.16125400
C	-1.09568000	2.75275800	0.90891800
C	-2.41413300	2.48995500	0.51081700
C	-1.22767600	-2.79996800	0.70831400
C	-1.64466100	-2.82557400	2.06911500
C	-2.79199400	-3.57129800	2.40907100
C	-3.51802300	-4.27355300	1.43654300

C	-3.09148000	-4.24346900	0.10293100
C	-1.94430100	-3.52031800	-0.29134100
C	-1.73870200	-1.30222300	4.12379900
C	-0.84392500	-2.14728600	3.18345300
C	-0.04545400	-3.20641200	3.99212900
C	5.52564700	0.24069900	2.41952200
C	5.00242900	-1.00293700	1.65822800
C	5.61250700	-2.30565000	2.24273600
C	4.24215500	-1.04472600	-0.81173700
C	5.27041800	-0.90133100	0.15439600
C	6.58096000	-0.68330600	-0.31865100
C	6.84546000	-0.59850700	-1.69478800
C	5.80371400	-0.72783800	-2.62654600
C	4.47442900	-0.94943400	-2.20822400
C	-2.65981800	-2.99405700	-2.67434300
C	-1.53757000	-3.56285600	-1.76875100
C	-1.15472200	-5.00183400	-2.20620300
C	3.35008000	0.03621100	-4.28093900
C	3.35568800	-1.11136800	-3.24039300
C	3.46287600	-2.48971400	-3.94829200
C	1.22384600	2.56428500	1.32451500
C	1.92219000	3.49830200	0.50520300
C	3.07326000	4.12064300	1.03602000
C	3.52082700	3.84917500	2.33544900
C	2.81170800	2.94042300	3.13368700
C	1.66112300	2.28443200	2.64946200
C	2.58975100	3.57720700	-1.95119700
C	1.48027300	3.87782700	-0.91213100
C	1.04956300	5.36732700	-0.98438000
C	-5.58809100	-0.86367300	2.25045100
C	-5.01781400	0.51314800	1.82715600
C	-5.58766500	1.64410100	2.72579200
C	-4.24469700	1.19974000	-0.54005400
C	-5.27932500	0.80900400	0.34810700
C	-6.58746100	0.72750800	-0.17221000
C	-6.84385800	1.00676700	-1.52411000
C	-5.79620000	1.37168100	-2.38403700
C	-4.46944900	1.47354700	-1.91418300
C	1.80483500	0.29908300	4.25246500
C	0.88747500	1.35591600	3.58862300
C	0.13238300	2.18197900	4.66565500
C	-3.31598900	1.03316200	-4.14939400
C	-3.34503400	1.89686600	-2.86347700
C	-3.46969600	3.40344500	-3.21926100
H	0.90201000	-3.96941400	0.27499900
H	3.10638000	-3.34964600	-0.32163100
H	-0.93177800	3.75861800	1.29362900
H	-3.14276100	3.28766500	0.59287800
H	-3.11448400	-3.61169200	3.44634000
H	-4.40072400	-4.84345100	1.71729600
H	-3.65210000	-4.79174700	-0.64989800
H	-0.11631700	-1.47458400	2.71730500

H	3.91830200	-1.04279700	1.81204300
H	-2.46364800	-1.92525800	4.66259900
H	-2.29696600	-0.54358000	3.56121800
H	-1.12583200	-0.79006200	4.87591600
H	-0.72334300	-3.91969000	4.47976700
H	0.56058200	-2.72554000	4.77147200
H	0.62785700	-3.77628700	3.33929000
H	6.61687200	0.33258600	2.34203900
H	5.27331100	0.16231300	3.48537000
H	5.07265100	1.15878300	2.02992400
H	5.21478700	-3.19710900	1.74037300
H	5.38387600	-2.38733100	3.31360200
H	6.70453300	-2.31649700	2.12876200
H	7.39595500	-0.57392200	0.39205800
H	7.86246500	-0.42809200	-2.04060800
H	6.02096000	-0.65123700	-3.68822400
H	-0.66818300	-2.92255700	-1.92915000
H	2.38715000	-1.07981100	-2.73350400
H	-3.56830600	-3.61098300	-2.63567000
H	-2.31552800	-2.95661300	-3.71575300
H	-2.92086600	-1.97550400	-2.36721800
H	-2.00289000	-5.69341800	-2.11193000
H	-0.33033000	-5.40211900	-1.60035500
H	-0.83544800	-5.00222700	-3.25681600
H	3.28851400	1.01378100	-3.78963600
H	2.47110800	-0.06289300	-4.92826800
H	4.24687300	0.02124500	-4.91588700
H	4.40641600	-2.58141900	-4.50377100
H	2.63430700	-2.60913400	-4.65756500
H	3.41318600	-3.31716000	-3.22794600
H	3.61952500	4.83083600	0.42023100
H	4.40629800	4.34600000	2.72518200
H	3.15025700	2.74406600	4.14792800
H	0.62200000	3.26808100	-1.20088300
H	-3.93353400	0.47456700	1.98213200
H	3.48057100	4.20064400	-1.79179200
H	2.21353700	3.77089800	-2.96374900
H	2.88959800	2.52506500	-1.89860200
H	0.22980300	5.58468500	-0.28631800
H	0.70577100	5.61015100	-1.99861600
H	1.88259800	6.04059000	-0.74072500
H	-6.68293700	-0.89069300	2.17209000
H	-5.32481800	-1.07267400	3.29582700
H	-5.17670000	-1.66712700	1.62982100
H	-5.15654600	2.61994700	2.46735000
H	-5.36534900	1.44221700	3.78203500
H	-6.67772800	1.72069100	2.61808400
H	-7.40682000	0.43917800	0.48092100
H	-7.85918800	0.93655500	-1.90773100
H	-6.00707600	1.57711800	-3.42986400
H	0.13540500	0.82411700	2.99593800
H	-2.38015800	1.75660500	-2.36814200

H	2.55487800	0.76510200	4.90408000
H	2.33524500	-0.29176700	3.49559100
H	1.21380000	-0.38642400	4.87258900
H	-0.45034300	1.52346500	5.32351700
H	-0.55728700	2.89869700	4.20206100
H	0.83641600	2.74888400	5.28936100
H	-3.23819200	-0.03249400	-3.90660500
H	-2.43837000	1.29933700	-4.74985000
H	-4.21281600	1.18593700	-4.76553800
H	-3.43916100	4.03303300	-2.32000500
H	-4.41048100	3.61270800	-3.74673500
H	-2.63853000	3.70234000	-3.87032200
O	0.02951800	0.32573400	-3.17041900
O	0.01926700	-0.91525300	-2.31453300

## 5.5 Structures with six oxygen atoms

## Bisperoxo Complex (spiro conformation)

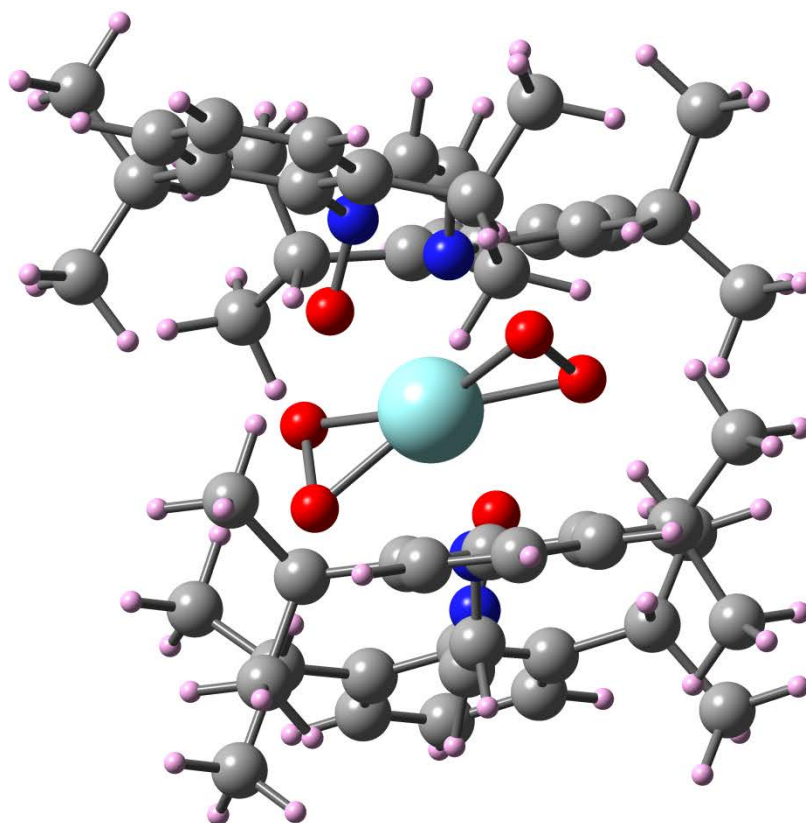


Fig. S56: NCCNO Bisperoxo Complex (spiro conformation)

SCF	$E_{ZP}$	H	G
-2741.41393279	-2740.259005	-2740.187597	-2740.367839

Zr	-0.00036100	-0.00889700	0.06173200
O	-2.24720300	-0.53267700	-0.13891900
O	2.00302000	0.79170900	0.76165200
O	-0.38764000	-0.54957500	2.02992100
O	-0.67871000	0.93813600	1.81735600
N	-0.01214900	2.22204200	-0.86526000
N	2.85821100	1.49082000	-0.01447600
N	-0.02081100	-2.44646000	0.14715000
N	-2.87788900	-1.43749600	0.61263600
C	1.11596600	2.68739200	-1.34322800
C	2.46296200	2.29235900	-0.99260000
C	-1.04605500	-3.12003100	0.58900400
C	-2.35829600	-2.60822300	0.94248300
C	-1.23162100	2.92450300	-1.25536300
C	-1.70031700	2.87463100	-2.59943200

C	-2.89695100	3.56551300	-2.89613900
C	-3.59313000	4.28461300	-1.91614300
C	-3.09171000	4.34378500	-0.60576500
C	-1.90432700	3.67555200	-0.24837900
C	-1.90857200	1.08854800	-4.40910700
C	-0.98305800	2.13140100	-3.73438800
C	-0.42870800	3.13129900	-4.78540900
C	5.02630200	-1.55518400	-1.87079600
C	4.62732700	-0.05935600	-1.82009900
C	5.16858300	0.68795100	-3.06946900
C	4.27629800	1.35239400	0.33220700
C	5.11935000	0.61099500	-0.53123700
C	6.47678200	0.51018600	-0.15500800
C	6.94852900	1.09753900	1.02842700
C	6.07483500	1.80895200	1.86743000
C	4.71262800	1.95915200	1.53719000
C	-2.36050900	4.00808500	2.26106800
C	-1.30066400	3.84918900	1.14866600
C	-0.33133000	5.06541300	1.15775200
C	3.43054800	1.88172200	3.72224700
C	3.76851200	2.72995700	2.46640500
C	4.34281500	4.11302800	2.86425300
C	1.17654300	-3.23965200	-0.15396100
C	2.09458200	-3.51088200	0.89489900
C	3.19831000	-4.33849100	0.59400900
C	3.38272600	-4.86745900	-0.69169700
C	2.47001700	-4.56014900	-1.71300300
C	1.35206600	-3.73478300	-1.47303100
C	3.17591500	-2.20300000	2.79938800
C	1.91702200	-2.96811800	2.31866900
C	1.55932200	-4.11099100	3.30640900
C	-5.15109300	-0.09319100	-2.31702300
C	-4.97148500	-1.36607400	-1.44865500
C	-5.86365000	-2.52552100	-1.96314700
C	-4.24746600	-1.08564500	1.02714200
C	-5.24784000	-1.05275000	0.02523000
C	-6.54989100	-0.70741600	0.44091700
C	-6.82512000	-0.41161900	1.78572200
C	-5.80201500	-0.44706500	2.74504900
C	-4.47525300	-0.77694800	2.39159100
C	1.07184300	-2.93577400	-3.88276900
C	0.36060300	-3.43076700	-2.60026000
C	-0.52936700	-4.66797000	-2.89741500
C	-3.33305100	0.53535200	4.25865900
C	-3.37625100	-0.79214400	3.46237000
C	-3.57051200	-1.99715400	4.42307400
H	1.08958700	3.51830800	-2.05327500
H	3.26585000	2.78919200	-1.52411200
H	-0.95262100	-4.20010400	0.73463500
H	-3.01489600	-3.26658100	1.49710400
H	-3.28376700	3.53473200	-3.91176200
H	-4.51377800	4.80440000	-2.17184700

H	-3.62524000	4.91894900	0.14482400
H	-0.15396200	1.55446100	-3.31846000
H	3.53291100	-0.02808200	-1.85771200
H	-2.79166800	1.55372800	-4.86919400
H	-2.23716600	0.34883100	-3.67262700
H	-1.35728800	0.55596800	-5.19547800
H	-1.23779900	3.68966800	-5.27580500
H	0.12723300	2.59152000	-5.56372100
H	0.24956300	3.86773600	-4.33161800
H	6.11528900	-1.68900900	-1.92581900
H	4.58466100	-2.02399100	-2.75868800
H	4.65491400	-2.09446800	-0.99291200
H	4.86545400	1.74371400	-3.07968800
H	4.78269200	0.21858500	-3.98316600
H	6.26591900	0.65709100	-3.10751700
H	7.16307300	-0.04500400	-0.78810800
H	7.99689300	0.99848800	1.30000800
H	6.45458500	2.25519500	2.78208500
H	-0.72110300	2.95276200	1.39128200
H	2.82049200	2.90359000	1.94536200
H	-2.88729500	4.97096500	2.20093600
H	-1.87211100	3.95765600	3.24231600
H	-3.10159200	3.20246500	2.21181400
H	-0.86766300	5.99668500	0.92824200
H	0.47212500	4.95066100	0.41807300
H	0.13279100	5.17249100	2.14760300
H	2.92978900	0.95298500	3.43264000
H	2.75356100	2.43998600	4.38168200
H	4.33834800	1.63560600	4.29021000
H	5.24698900	4.01787800	3.47921300
H	3.60118800	4.66608400	3.45485400
H	4.59564600	4.71540600	1.98185600
H	3.91435100	-4.57219300	1.37793300
H	4.23558900	-5.50993400	-0.89862900
H	2.62636700	-4.96368300	-2.70994000
H	1.09574800	-2.24459400	2.33245200
H	-3.92728200	-1.67670400	-1.56045200
H	4.05711600	-2.85590700	2.86044500
H	2.99676600	-1.78566600	3.79889300
H	3.40505000	-1.37182700	2.12312800
H	0.63862400	-4.63073500	3.00710000
H	1.40680600	-3.70535800	4.31515200
H	2.36153800	-4.85975200	3.35787900
H	-6.18260700	0.28039000	-2.26578100
H	-4.92311100	-0.31755700	-3.36696900
H	-4.47767200	0.70370500	-1.98393300
H	-5.72805000	-3.43493500	-1.36302200
H	-5.60684300	-2.76146500	-3.00396700
H	-6.92855800	-2.26094400	-1.93573200
H	-7.35113500	-0.67036900	-0.29202500
H	-7.83685500	-0.14791700	2.08467900
H	-6.02796100	-0.20293000	3.77907400



H	-0.27909700	-2.60102100	-2.28438400
H	-2.39388200	-0.88085300	2.98675500
H	1.73963400	-3.69543900	-4.31273000
H	1.64617700	-2.03119400	-3.65840000
H	0.32286000	-2.67986400	-4.64391700
H	-1.25915100	-4.43053100	-3.68306300
H	-1.08333100	-4.99441500	-2.00570300
H	0.07400700	-5.51928600	-3.24186600
H	-3.13965800	1.37699400	3.58755900
H	-2.50845200	0.49692900	4.98115200
H	-4.26300300	0.72260800	4.81329500
H	-3.56784900	-2.95726100	3.88777900
H	-4.52157900	-1.92553100	4.96847300
H	-2.75746300	-2.02028100	5.15959300
O	1.25165300	-0.26173500	-1.64533000
O	-0.21470100	-0.30666200	-2.01519400

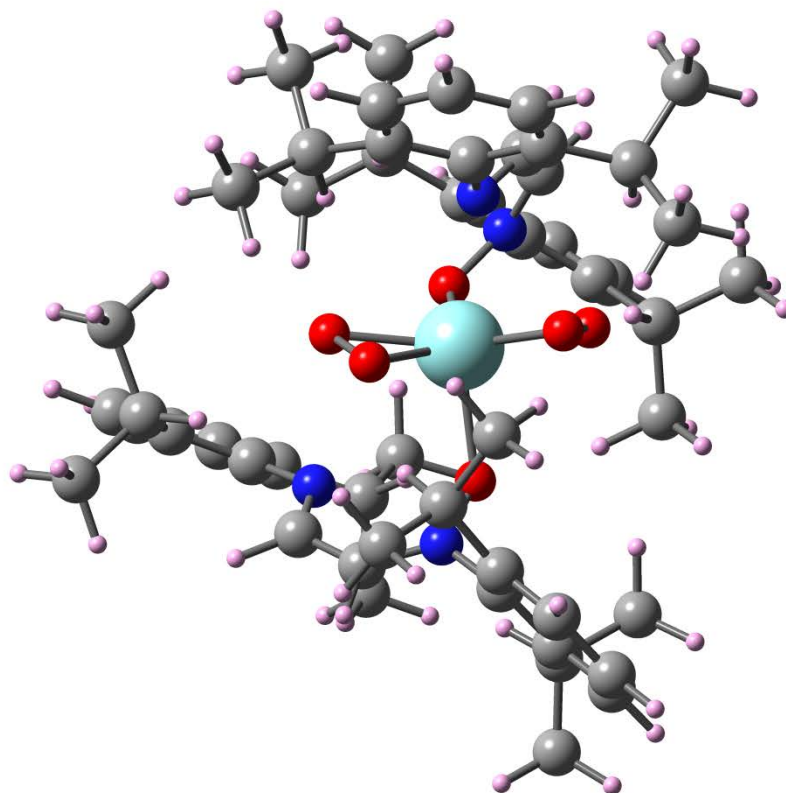
**Bisperoxo Complex (planar conformation 1 lower energy)**

Fig. S57: NCCNO Bisperoxo Complex (planar conformation 1 lower energy)

SCF	$E_{ZP}$	H	G
-2741.4044128	-2740.250742	-2740.178758	-2740.362962

Zr	-0.60405200	-0.34960400	-0.07366100
O	1.55470500	-0.81136600	-0.39888200
O	-1.06402900	1.71692200	-0.60810300
O	-2.09488900	-1.12327700	-1.27761600
N	0.74448000	2.51501300	1.47593000
N	-1.86859000	2.62316000	0.01102900
N	-0.54768600	-2.82754500	0.05651400
N	2.00231400	-1.73728900	-1.28691200
C	-0.33979900	3.08239300	1.92635900
C	-1.56265600	3.19809200	1.16005800
C	0.22626600	-3.42842500	-0.81468300
C	1.38644600	-2.88764800	-1.49392700
C	1.96834100	2.50556000	2.18991200
C	2.08221300	2.20488000	3.58598400
C	3.36539900	2.27888200	4.16686600
C	4.49884500	2.62022300	3.41455700
C	4.37924200	2.85829500	2.03420500
C	3.12923000	2.78816600	1.39544000

C	1.23050400	0.39373400	5.16127000
C	0.90744200	1.73360400	4.45323100
C	0.50160700	2.81156700	5.49447300
C	-5.00716900	0.05615600	0.41197300
C	-4.44120400	1.41588600	0.90083900
C	-5.30186000	1.99556000	2.05374900
C	-3.10592500	2.95761500	-0.70929200
C	-4.33022200	2.40328500	-0.26554100
C	-5.48986900	2.77824000	-0.97953700
C	-5.41736400	3.63607700	-2.08621000
C	-4.17760800	4.13767300	-2.51638900
C	-2.98807100	3.80760900	-1.83726400
C	4.20606300	2.66144100	-0.94006900
C	2.98289700	3.08897500	-0.09816700
C	2.67937600	4.59767900	-0.32025700
C	-1.23975300	3.53278900	-3.63356100
C	-1.63679300	4.31293200	-2.35082200
C	-1.63048100	5.84209700	-2.59782900
C	-1.62783200	-3.62200300	0.62605400
C	-2.60343800	-4.23740000	-0.21962900
C	-3.61175300	-5.00363100	0.40324100
C	-3.66178900	-5.16676700	1.79417000
C	-2.69256200	-4.55381700	2.60127600
C	-1.66339400	-3.77106400	2.04174300
C	-4.01322000	-3.53318300	-2.22838900
C	-2.65154500	-4.09804200	-1.74963600
C	-2.35778500	-5.45651400	-2.44392800
C	5.21859600	-1.22117200	1.11357600
C	4.51509700	-2.19586700	0.13410200
C	5.20073000	-3.58805200	0.14585200
C	3.24932200	-1.39736100	-1.97913000
C	4.46373200	-1.62112200	-1.28528300
C	5.65545800	-1.30138000	-1.96756900
C	5.62305800	-0.77710300	-3.27026600
C	4.39785800	-0.55293900	-3.91656700
C	3.17195100	-0.85117200	-3.28278800
C	-1.11062600	-2.61219000	4.25749200
C	-0.56256700	-3.20379100	2.93923500
C	0.50587100	-4.29713300	3.22089000
C	1.70922800	0.92758300	-4.35347300
C	1.84717600	-0.57614600	-4.00140800
C	1.70655400	-1.45391100	-5.27300000
H	-0.38437600	3.59200600	2.89401000
H	-2.32569100	3.86933600	1.54070600
H	0.03759700	-4.47258100	-1.07122400
H	1.86152900	-3.53039700	-2.22637400
H	3.47997900	2.05523700	5.22432300
H	5.47219500	2.68278500	3.89599100
H	5.26679900	3.09465600	1.45493300
H	0.05334900	1.51760900	3.80517200
H	-3.44627700	1.20488800	1.30556600
H	2.07244300	0.48271700	5.86057800

H	1.46372700	-0.37588600	4.41809100
H	0.35472300	0.05798800	5.73143400
H	1.32119200	3.00900900	6.19892500
H	-0.36676700	2.47206600	6.07470300
H	0.24297300	3.76898000	5.02108800
H	-6.03517400	0.15565600	0.03679100
H	-5.01371700	-0.65980700	1.24301700
H	-4.38194700	-0.35951500	-0.38626900
H	-4.89267500	2.94272300	2.43243400
H	-5.33278800	1.28290600	2.88751600
H	-6.33534200	2.18344300	1.73274600
H	-6.45227100	2.37882800	-0.67224200
H	-6.32445200	3.90445400	-2.62262200
H	-4.13401300	4.78712800	-3.38611100
H	2.11024200	2.52656200	-0.44947700
H	-0.86826200	4.09734200	-1.59973600
H	5.09602700	3.26480800	-0.71414900
H	3.98534100	2.79626900	-2.00726800
H	4.45568400	1.60578500	-0.78003000
H	3.51375300	5.21978000	0.03199600
H	1.77521000	4.90626600	0.21869200
H	2.52695200	4.80481900	-1.38845100
H	-1.20009700	2.45724600	-3.43053500
H	-0.25184800	3.85854400	-3.98615100
H	-1.96449000	3.70846700	-4.44003100
H	-2.32278000	6.12875000	-3.39976600
H	-0.62618300	6.16801300	-2.89848800
H	-1.91358300	6.39714600	-1.69392200
H	-4.37429800	-5.47053000	-0.21475300
H	-4.44968300	-5.76602700	2.24493700
H	-2.73172400	-4.68662000	3.67816900
H	-1.90668200	-3.36595300	-2.07117100
H	3.49172700	-2.32321500	0.50326200
H	-4.85089900	-4.19704600	-1.97537100
H	-3.99941900	-3.40893000	-3.31971100
H	-4.18515400	-2.54964500	-1.78211500
H	-1.38359800	-5.87183700	-2.14838900
H	-2.35836200	-5.33141200	-3.53510900
H	-3.12002300	-6.20580400	-2.19132900
H	6.26363500	-1.04409300	0.82644600
H	5.21618700	-1.64268500	2.12697100
H	4.70199600	-0.25562700	1.14895500
H	4.68772000	-4.29561900	-0.51890100
H	5.19112100	-4.00548200	1.16092500
H	6.24687200	-3.52089300	-0.18006500
H	6.61174000	-1.46274000	-1.47737200
H	6.55381100	-0.53884200	-3.77958900
H	4.38889900	-0.13754900	-4.92063900
H	-0.07655200	-2.37557600	2.41549900
H	1.00645600	-0.82202600	-3.34510100
H	-1.58924500	-3.36970700	4.89376400
H	-1.83192800	-1.81744700	4.03825100

H	-0.28708400	-2.17157400	4.83184400
H	1.32613400	-3.88067400	3.82125100
H	0.93309100	-4.69283900	2.28880700
H	0.07214600	-5.14139500	3.77490000
H	1.78605100	1.55029900	-3.45377300
H	0.72811000	1.11130300	-4.80723900
H	2.48127300	1.25194600	-5.06446900
H	1.77025800	-2.52372300	-5.03311600
H	2.48853600	-1.22766200	-6.01057300
H	0.73218700	-1.27267700	-5.74321600
O	-1.65923100	-0.14332300	1.68841300
O	-0.13000500	-0.18188100	1.95555800
O	-0.81919400	-0.94031200	-2.10423400

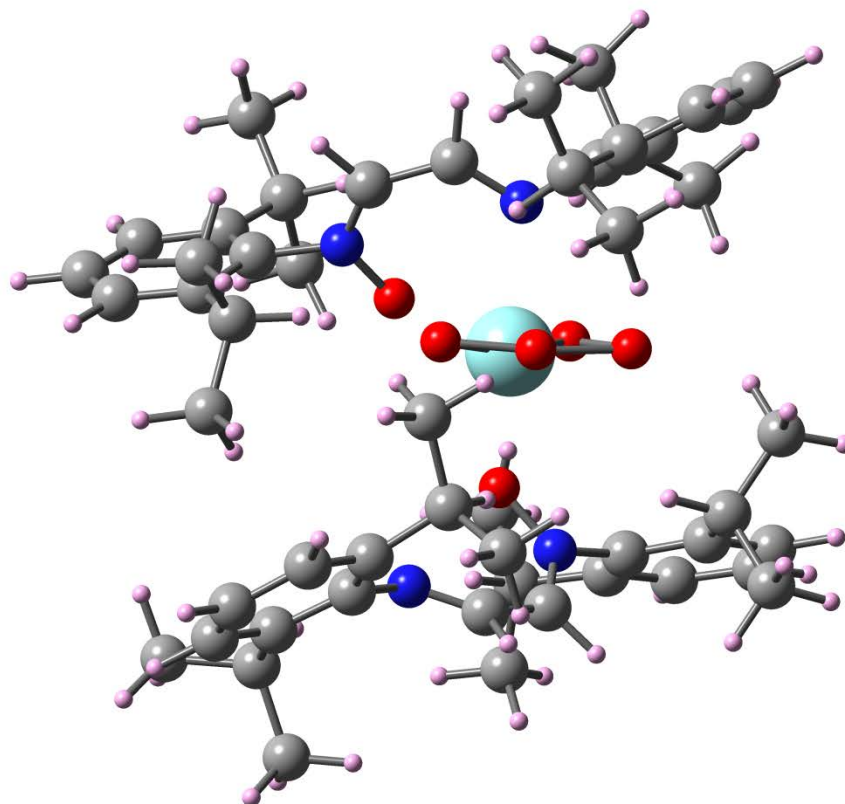
**Bisperoxo Complex (planar conformation 2 higher energy)**

Fig. S58: NCCNO Bisperoxo Complex (planar conformation 2 higher energy)

SCF	E <sub>ZP</sub>	H	G
-2741.399655	-2740.246131	-2740.174198	-2740.357543

Zr	0.94355271	-0.14377247	-0.19758879
O	0.64156836	1.87728907	-1.13102052
O	-0.63437586	-1.43867209	-1.01327849
O	2.26655164	-0.61823478	-1.72912551
N	-3.32077666	-1.54082038	0.21861622
N	-0.80650181	-2.78040818	-1.02979620
N	2.58868298	1.26097210	0.93592569
N	0.50167335	3.02454068	-0.42938319
C	-2.85555815	-2.73814383	0.39678477
C	-1.82343058	-3.36051458	-0.42496332
C	2.24407260	2.47854202	1.26285332
C	1.19094391	3.28109971	0.66946475
C	-4.31840889	-0.99339757	1.07204701
C	-4.16496441	-0.93548863	2.49260302
C	-5.21747791	-0.35743382	3.23522500
C	-6.37169048	0.14231574	2.61486859

C	-6.48391078	0.11352744	1.21308270
C	-5.46066592	-0.43168641	0.41937348
C	-2.25832050	-0.20742029	4.02222184
C	-2.89801705	-1.38213779	3.23692470
C	-3.19001169	-2.58498406	4.17365748
C	2.50503347	-4.33666824	1.04210421
C	1.06599650	-4.53483867	0.49904976
C	0.46861691	-5.87517723	1.00830478
C	0.18093787	-3.59332372	-1.76661639
C	1.03202829	-4.45756601	-1.03275603
C	1.90742740	-5.26689530	-1.78558798
C	1.94790581	-5.18958045	-3.18511323
C	1.11836546	-4.28922891	-3.87046672
C	0.21391925	-3.46134247	-3.17613819
C	-6.30913390	0.71567812	-1.72115985
C	-5.57700554	-0.49853945	-1.10489160
C	-6.26387353	-1.82241550	-1.54450393
C	0.24070770	-1.36388593	-4.57826451
C	-0.65592339	-2.46657133	-3.95068137
C	-1.52302278	-3.16864442	-5.02660483
C	3.74463517	0.69358122	1.62016867
C	4.88864659	0.37896945	0.83496865
C	6.01498702	-0.14855989	1.49572766
C	6.00974902	-0.36734924	2.88189732
C	4.86771568	-0.05660970	3.63252985
C	3.70949229	0.48091822	3.02987370
C	5.59014189	-0.44583486	-1.48680270
C	4.95425531	0.69524665	-0.66056947
C	5.70211658	2.03874970	-0.88596253
C	-3.47915616	2.70425763	0.65604909
C	-2.12082782	3.40854076	0.89604969
C	-2.19324974	4.33049770	2.14259284
C	-0.43642713	4.00330309	-0.99132437
C	-1.68110303	4.19476985	-0.34457002
C	-2.54215766	5.16131107	-0.90949800
C	-2.18204911	5.86791083	-2.06641932
C	-0.94816907	5.62655711	-2.69322158
C	-0.03941610	4.68575887	-2.16853273
C	2.04361083	-0.49937283	4.69187059
C	2.48939351	0.76751733	3.91818411
C	2.77757960	1.93299841	4.90353871
C	1.05286819	3.59835117	-4.17459617
C	1.29224458	4.41570311	-2.87616449
C	2.07304097	5.72075373	-3.17307868
H	-3.26430472	-3.41715035	1.15795485
H	-1.84343348	-4.44125045	-0.51320114
H	2.80832153	3.01155816	2.03195315
H	0.99460959	4.24723040	1.11876050
H	-5.12533801	-0.29438064	4.31655424
H	-7.17216807	0.56623088	3.21678258
H	-7.37020752	0.52539002	0.73925856
H	-2.13639849	-1.69060417	2.51496886

H	0.46794028	-3.71466298	0.91357686
H	-2.95357471	0.22848811	4.75250905
H	-1.91665023	0.56566794	3.32615173
H	-1.37312284	-0.56700884	4.56202346
H	-3.91034336	-2.31441822	4.95729698
H	-2.26529510	-2.91288858	4.66622152
H	-3.60850517	-3.43997810	3.62404672
H	3.15957854	-5.17601591	0.77071385
H	2.48107322	-4.27445678	2.13820033
H	2.93371458	-3.41112435	0.64549659
H	-0.57061252	-6.02179431	0.68135291
H	0.48677370	-5.90392246	2.10552798
H	1.05223164	-6.72889778	0.63964175
H	2.58259075	-5.94205693	-1.26780442
H	2.63923656	-5.81874418	-3.74067350
H	1.17641691	-4.22318506	-4.95329833
H	-4.55242893	-0.51706545	-1.49887270
H	-1.33438926	-1.96512750	-3.25290348
H	-7.37539124	0.73104139	-1.45814340
H	-6.24526152	0.67215612	-2.81647414
H	-5.86204215	1.66173598	-1.39173250
H	-7.29478595	-1.86976051	-1.16804198
H	-5.72505901	-2.69897991	-1.16324137
H	-6.29684805	-1.89342259	-2.64016544
H	0.88887216	-0.91480101	-3.81749018
H	-0.38398908	-0.58066406	-5.02896644
H	0.88267256	-1.78067245	-5.36644951
H	-0.90365836	-3.65060006	-5.79398017
H	-2.16170487	-2.43180899	-5.53145174
H	-2.17097065	-3.93745044	-4.58480746
H	6.90274917	-0.38965254	0.91828484
H	6.88885911	-0.77865608	3.37291309
H	4.86750935	-0.24030729	4.70389829
H	3.93379747	0.79835923	-1.03917944
H	-1.39807247	2.61409092	1.11077594
H	6.64600073	-0.61446593	-1.23094150
H	5.54085670	-0.19735631	-2.55492856
H	5.02502201	-1.37042603	-1.33396130
H	5.22268212	2.86547386	-0.34194418
H	5.71095226	2.29322759	-1.95455004
H	6.74414231	1.97445368	-0.54285053
H	-4.29033968	3.42401265	0.48133308
H	-3.74558997	2.10252875	1.53213413
H	-3.42134070	2.02914750	-0.20530036
H	-1.22680916	4.80807265	2.35487186
H	-2.47982945	3.74344980	3.02391305
H	-2.93656368	5.12794899	2.00882501
H	-3.50596661	5.34897396	-0.44497894
H	-2.86546422	6.60275017	-2.48520755
H	-0.68774838	6.17545574	-3.59376045
H	1.63685911	1.03789901	3.28921832
H	1.92165597	3.79551999	-2.22824022



H	2.82606074	-0.86972604	5.36778055
H	1.77426738	-1.28888521	3.98393459
H	1.15561463	-0.27064256	5.29698298
H	1.88638822	2.14829114	5.50835251
H	3.06442466	2.85540662	4.37852564
H	3.59708186	1.68026389	5.58949195
H	0.56290644	2.64613557	-3.94467000
H	2.00989820	3.38063909	-4.66596315
H	0.42372289	4.15517795	-4.88214781
H	2.24259437	6.30607965	-2.25996035
H	1.54197249	6.36004155	-3.88983546
H	3.05019707	5.47809199	-3.60977449
O	0.57510624	-0.58123916	1.78659858
O	-0.24816215	0.65801811	1.38064929
O	2.42000429	-1.52548082	-0.46250982

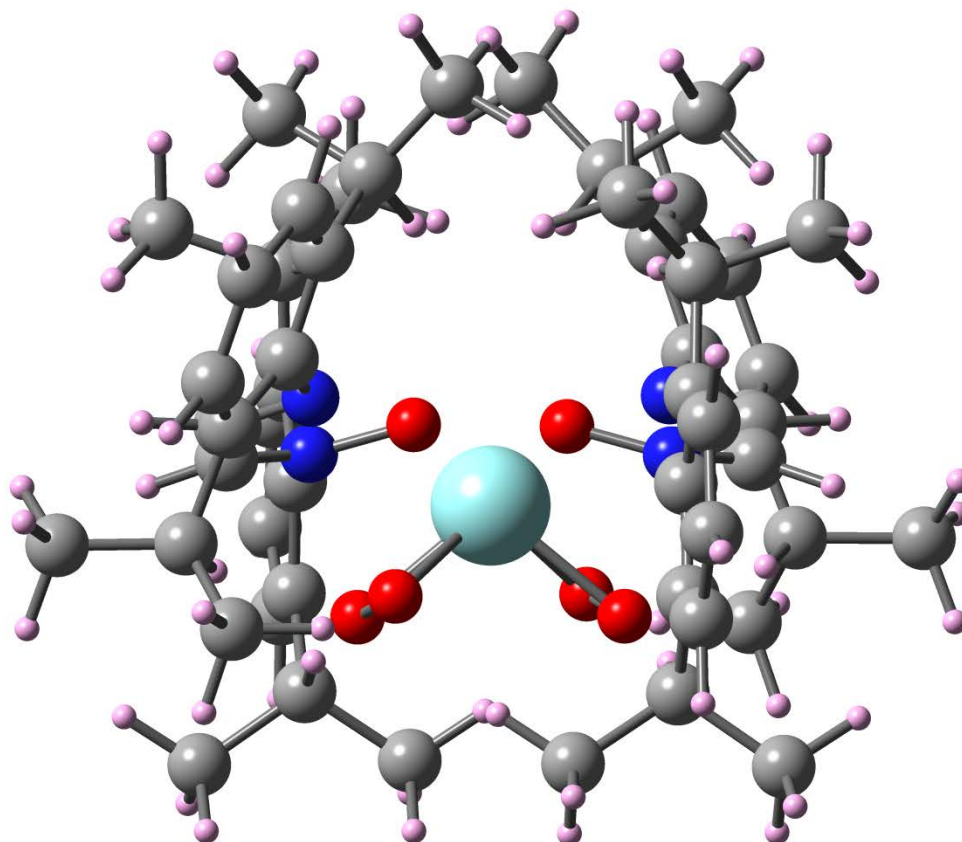
**Bisperoxo Complex (butterfly conformation)**

Fig. S59: NCCNO Bisperoxo Complex (butterfly conformation)

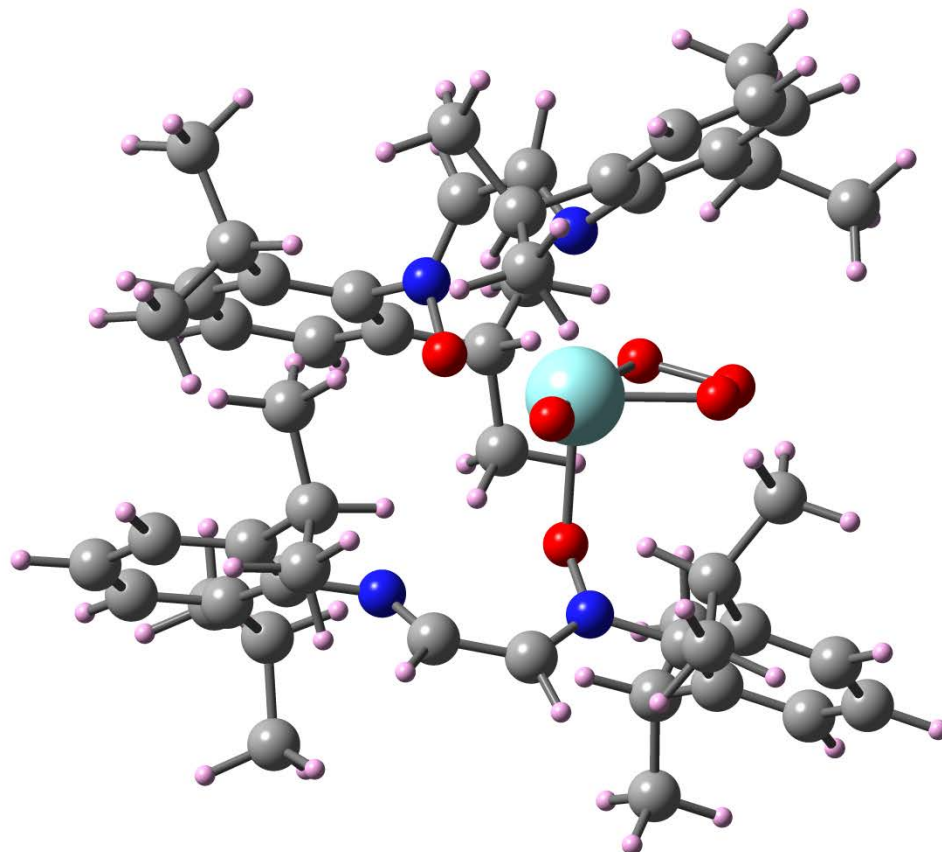
SCF	E <sub>ZP</sub>	H	G
-2741.404045	-2740.249500	-2740.178212	-2740.357924

O	-1.96324127	-0.45319935	0.12108889
O	-1.01694445	1.45821502	-1.92233704
N	0.24171321	-2.30289943	0.46746102
N	-2.65794864	-1.57947692	-0.23208882
N	2.65805606	1.57980672	-0.22451194
N	-0.24161505	2.30196585	0.47776866
C	-0.72934051	-3.11707317	0.12788763
C	-2.07016970	-2.76153211	-0.29377459
C	2.07117396	2.76260996	-0.27999232
C	0.73016085	3.11691368	0.14201359
C	1.47440575	-2.91006629	0.94358518
C	2.22885369	-3.81584729	0.13719788
C	3.42714887	-4.33146240	0.68042008
C	3.86619533	-3.98879537	1.96447644
C	3.09470100	-3.11989017	2.75211818
C	1.89358035	-2.57295303	2.26401872

C	2.96159757	-3.98196619	-2.30111310
C	1.83488423	-4.26616891	-1.27657471
C	1.45455144	-5.77216499	-1.29335670
C	-3.46632912	-0.11744039	-3.93980506
C	-3.49460612	-1.42350040	-3.10392565
C	-3.85016010	-2.64501724	-3.99295303
C	-4.07641629	-1.38849931	-0.56229912
C	-4.46376722	-1.30757550	-1.92313125
C	-5.84079108	-1.11725968	-2.17956854
C	-6.77075300	-1.01358698	-1.13714451
C	-6.34813178	-1.09742068	0.20015731
C	-4.98873659	-1.28014065	0.51912661
C	1.75982229	-0.92142001	4.23309917
C	0.98854552	-1.74686849	3.18027333
C	-0.03806523	-2.68320010	3.88073274
C	-5.23836927	-0.40168531	2.91307112
C	-4.54419814	-1.42203551	1.97871320
C	-4.79212060	-2.87318750	2.47791822
C	4.07630989	1.38972927	-0.55617027
C	4.46290245	1.31708928	-1.91773201
C	5.83971188	1.12843263	-2.17619834
C	6.77029404	1.01840473	-1.13492567
C	6.34838086	1.09351156	0.20307655
C	4.98910341	1.27402544	0.52403304
C	3.46618508	0.14032931	-3.94260252
C	3.49260291	1.43999782	-3.09686634
C	3.84503618	2.66891802	-3.97688537
C	-1.76585776	0.90264642	4.23420348
C	-0.99213449	1.73222977	3.18644168
C	0.03564329	2.66287927	3.89271882
C	-1.47404446	2.90818128	0.95559175
C	-1.89495246	2.56482782	2.27392503
C	-3.09565051	3.11105208	2.76380072
C	-3.86501281	3.98539381	1.98005479
C	-3.42440574	4.33390610	0.69812040
C	-2.22655266	3.81906553	0.15317755
C	5.23497173	0.37118053	2.90866759
C	4.54581816	1.40471329	1.98502497
C	4.80215068	2.84951592	2.49802909
C	-2.95782506	3.99729481	-2.28467422
C	-1.83120206	4.27530485	-1.25831716
C	-1.44882166	5.78084646	-1.26814002
H	-0.57416288	-4.19801854	0.16930291
H	-2.70919848	-3.57429709	-0.62065647
H	2.71105912	3.57663232	-0.60205081
H	0.57567056	4.19776540	0.18803868
H	4.02568356	-5.01016253	0.07846423
H	4.79426387	-4.40139912	2.35338908
H	3.42734578	-2.87803029	3.75700357
H	0.97885970	-3.68070809	-1.61663860
H	-2.47498876	-1.57635701	-2.74285308
H	3.87037475	-4.56292874	-2.09230001

H	3.21225357	-2.91711307	-2.29781238
H	2.61901750	-4.24325449	-3.31104795
H	2.30605447	-6.40409106	-1.00680793
H	1.13968032	-6.06976020	-2.30250548
H	0.63238691	-5.99828026	-0.59932986
H	-4.45974329	0.13807015	-4.33406773
H	-2.78208781	-0.24257999	-4.78829391
H	-3.09045375	0.71898731	-3.34142904
H	-3.86050118	-3.57927206	-3.41461235
H	-3.10300449	-2.74890038	-4.78941220
H	-4.83508665	-2.53228316	-4.46591179
H	-6.17907573	-1.04742199	-3.20951787
H	-7.82427161	-0.86686353	-1.36325688
H	-7.08009377	-1.01631931	0.99808028
H	0.42210901	-1.04968639	2.55070457
H	-3.46732818	-1.22499769	2.03072244
H	2.26404754	-1.56324525	4.96724672
H	1.06711969	-0.28047069	4.79081378
H	2.51343059	-0.28242369	3.76033562
H	0.47979586	-3.41395186	4.51633837
H	-0.63733431	-3.23897868	3.14905045
H	-0.72457111	-2.10478793	4.51280621
H	-5.07522631	0.62513063	2.56615244
H	-4.83352912	-0.48992709	3.92968179
H	-6.31966199	-0.57745536	2.97847067
H	-5.86267203	-3.11608974	2.45355023
H	-4.43958431	-2.98875531	3.51141483
H	-4.26740023	-3.61006624	1.85591310
H	6.17743200	1.06497534	-3.20674904
H	7.82371454	0.87331416	-1.36254204
H	7.08077689	1.00718655	1.00009274
H	2.47304607	1.58800192	-2.73364078
H	-0.42658408	1.03736254	2.55353060
H	4.45952800	-0.10975732	-4.34048908
H	2.78020619	0.27022757	-4.78896239
H	3.09344255	-0.70159740	-3.34998027
H	3.85436947	3.59872225	-3.39139574
H	3.09683655	2.77758185	-4.77171111
H	4.82969956	2.56148859	-4.45166003
H	-2.26756805	1.54153193	4.97263888
H	-1.07526456	0.25561243	4.78748308
H	-2.52187475	0.26934714	3.75765265
H	0.63707505	3.22087480	3.16452378
H	0.72005595	2.07994478	4.52288572
H	-0.48149120	3.39164980	4.53118551
H	-3.42969945	2.86439144	3.76706626
H	-4.79273792	4.39747486	2.37034064
H	-4.02138925	5.01659555	0.09914622
H	3.46792190	1.21317685	2.03590017
H	-0.97579106	3.69022440	-1.60061405
H	6.31741457	0.53970197	2.97400775
H	5.06493540	-0.65118274	2.55210205

H	4.83212028	0.45204322	3.92668095
H	4.45116007	2.95699848	3.53293025
H	4.28096930	3.59525283	1.88363298
H	5.87398235	3.08684431	2.47510743
H	-3.20959587	2.93270896	-2.28660132
H	-2.61455107	4.26313980	-3.29319025
H	-3.86602163	4.57825242	-2.07337809
H	-0.62661547	6.00275350	-0.57280081
H	-2.29959307	6.41260409	-0.97905323
H	-1.13319481	6.08258566	-2.27582105
O	-0.47896790	-1.53699332	-2.18891832
O	1.01531341	-1.44823435	-1.93052608
O	0.47698682	1.54739521	-2.18262186
O	1.96251078	0.45219465	0.12242911
Zr	-0.00041228	0.00220026	-0.84384401

Oxo  $\eta^2$ -Ozone Complex (conformation 1 lowest energy)Fig. S60: NCCNO Oxo  $\eta^2$ -Ozone Complex (conformation 1 lowest energy)

SCF	$E_{ZP}$	H	G
-2741.39635270	-2740.243536	-2740.171925	-2740.354967

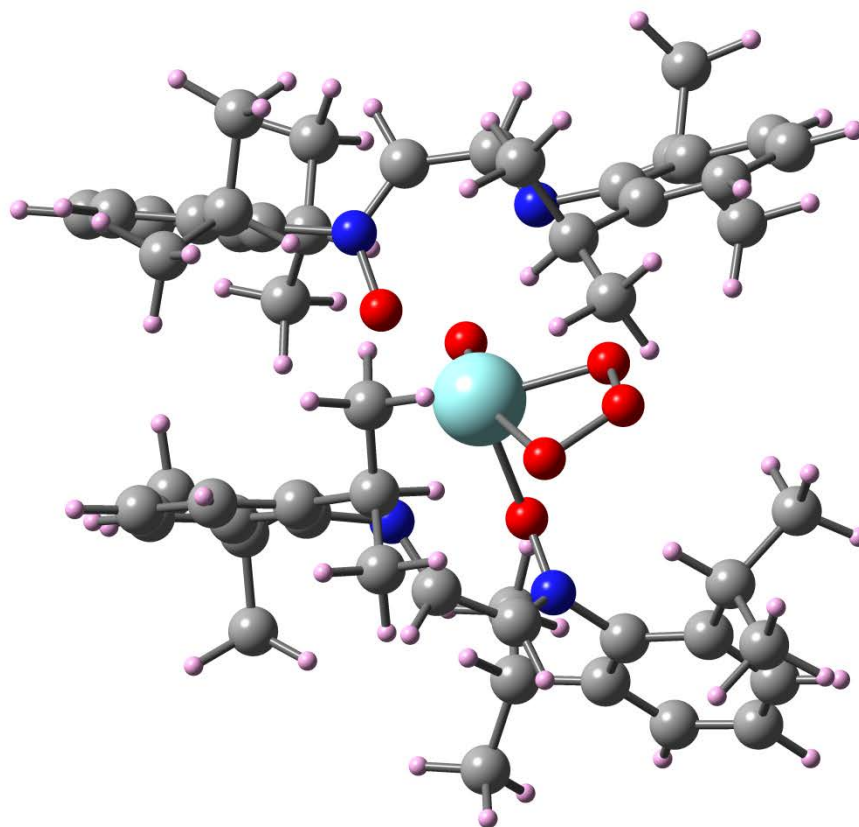
Zr	-1.03551600	-0.12960200	-0.04626400
O	0.90323700	-1.18409000	-0.46090900
O	-0.28420100	1.89456500	-0.59536000
O	-2.96921700	0.30522200	-0.70533900
N	2.08223300	2.14743900	1.10823900
N	-0.63292800	3.02908400	0.05989100
N	-1.58055700	-2.46331500	0.16805900
N	1.14921600	-2.33843500	-1.10817200
C	1.28328300	3.00763500	1.66283700
C	0.06917900	3.53169300	1.05408100
C	-0.93566900	-3.46041900	-0.39616000
C	0.33514800	-3.38568300	-1.06983300
C	3.27027500	1.71122000	1.75547000
C	3.28703000	1.21148300	3.09565800
C	4.53811300	0.85262400	3.64124600
C	5.72448100	0.96259000	2.90063600
C	5.67874200	1.39304700	1.56273200

C	4.46016300	1.75361900	0.96120500
C	1.92986500	-0.53016300	4.35903500
C	2.01731500	0.95568300	3.92186600
C	1.94041800	1.88654000	5.16103500
C	-4.34079600	2.14585500	1.79830500
C	-3.10369300	3.08038700	1.75573000
C	-3.15434900	4.11724400	2.90981200
C	-1.83828400	3.72191400	-0.43342200
C	-2.98853300	3.77549700	0.39316000
C	-4.09189900	4.49708200	-0.11181000
C	-4.05371700	5.09781000	-1.37780200
C	-2.90869400	4.98484500	-2.18219200
C	-1.76934700	4.29010000	-1.73081800
C	5.37493400	1.52413000	-1.42988600
C	4.39862500	2.25816400	-0.48208400
C	4.64169000	3.79281100	-0.53395300
C	-0.86175900	3.17021000	-3.80334700
C	-0.54675500	4.15417100	-2.64354800
C	-0.06406200	5.52394400	-3.18444000
C	-2.86829800	-2.81113600	0.78198800
C	-3.98967600	-3.08611800	-0.05062900
C	-5.19235300	-3.45904100	0.58647800
C	-5.28490100	-3.55016500	1.98240300
C	-4.16612700	-3.25971500	2.77714900
C	-2.93725800	-2.88034300	2.19947600
C	-5.12469400	-2.11708700	-2.12062700
C	-3.95597100	-2.98066800	-1.58142800
C	-3.98080200	-4.38823100	-2.23921700
C	4.46390100	-2.51731600	1.26017000
C	3.48007300	-3.32873700	0.37925400
C	3.73357900	-4.85333700	0.52124300
C	2.43958900	-2.40783400	-1.80936100
C	3.55703600	-2.89234500	-1.08770900
C	4.78026400	-2.96425900	-1.78568300
C	4.87031400	-2.55967500	-3.12763000
C	3.74157500	-2.06567100	-3.80000300
C	2.49046700	-1.96867400	-3.15323800
C	-2.03146600	-1.71935700	4.29084000
C	-1.71479900	-2.64485900	3.09264200
C	-1.12731700	-4.00198600	3.56837100
C	1.53708100	0.00963100	-4.43402800
C	1.27125200	-1.42050300	-3.89941000
C	0.85132100	-2.37112800	-5.05177300
H	1.51023800	3.47390900	2.63036700
H	-0.33329700	4.44757400	1.47278400
H	-1.38137100	-4.45668700	-0.39162600
H	0.68726700	-4.26373100	-1.59698900
H	4.58104600	0.47223000	4.65889100
H	6.67561000	0.69479100	3.35490700
H	6.59723600	1.44281700	0.98497100
H	1.13173200	1.13514800	3.30340400
H	-2.23955400	2.42630400	1.91339700

H	2.74447200	-0.80655900	5.04159800
H	1.96848200	-1.19441000	3.48709200
H	0.97891000	-0.70674900	4.87576800
H	2.78646100	1.71431600	5.83989300
H	1.01429600	1.69861200	5.71968900
H	1.95816700	2.94753700	4.87710800
H	-5.28298800	2.70773200	1.73300400
H	-4.34395600	1.58799400	2.74335700
H	-4.30117600	1.42433900	0.97552400
H	-2.26588100	4.76520500	2.92581900
H	-3.21202500	3.59869600	3.87553200
H	-4.03477600	4.76849400	2.82377800
H	-4.99675600	4.56355700	0.48517700
H	-4.92181700	5.63980000	-1.74547500
H	-2.89960100	5.43763800	-3.16955600
H	3.37661900	2.07635200	-0.83631300
H	0.27790200	3.71423900	-2.07328000
H	6.42506000	1.73956700	-1.18965500
H	5.20392800	1.85184100	-2.46387400
H	5.22902200	0.43734400	-1.39169700
H	5.64998000	4.04131800	-0.17525500
H	3.91837100	4.33317100	0.08969800
H	4.54522300	4.16192000	-1.56392300
H	-1.16073900	2.19095700	-3.41508300
H	0.02696600	3.04014200	-4.43557900
H	-1.67485500	3.55366000	-4.43482800
H	-0.81563000	5.99600000	-3.83005800
H	0.84544600	5.38742600	-3.78439800
H	0.16609400	6.22236100	-2.36883800
H	-6.06827500	-3.66708100	-0.02172200
H	-6.22393200	-3.84033000	2.44809000
H	-4.24478200	-3.33061700	3.85835700
H	-3.03778000	-2.47043100	-1.88821300
H	2.47324700	-3.12171500	0.76026900
H	-6.10170500	-2.58759300	-1.94170800
H	-5.01012700	-1.97833100	-3.20309900
H	-5.11097800	-1.12751200	-1.65505300
H	-3.13195600	-5.01046100	-1.92154700
H	-3.94067300	-4.29295600	-3.33245200
H	-4.90075900	-4.93035600	-1.98090400
H	5.50714500	-2.69726900	0.96972500
H	4.35523300	-2.80920000	2.31261600
H	4.27050400	-1.44192500	1.18420100
H	3.01634700	-5.43970900	-0.06831900
H	3.64111700	-5.15781000	1.57174600
H	4.74222300	-5.12075100	0.18085200
H	5.66558500	-3.33236000	-1.27430800
H	5.82322700	-2.62414300	-3.64745400
H	3.82944500	-1.74639000	-4.83476100
H	-0.95424800	-2.12211500	2.50472800
H	0.41622900	-1.33569200	-3.22134000
H	-2.81660900	-2.12770300	4.94117300



H	-2.33579300	-0.73496700	3.92172700
H	-1.13090900	-1.58685000	4.90499800
H	-0.22136900	-3.83704400	4.16760200
H	-0.86305500	-4.64847100	2.71952900
H	-1.84990900	-4.54885200	4.18932000
H	1.80927500	0.68804700	-3.61675900
H	0.62432900	0.39714000	-4.90070500
H	2.34045100	0.02473600	-5.18351200
H	0.62663900	-3.38034100	-4.68092900
H	1.63925700	-2.45914200	-5.81234700
H	-0.05175100	-1.98238400	-5.53744500
O	-1.16461000	0.27931200	1.74669600
O	-2.76234000	0.06316100	-2.19063500
O	-1.43934500	-0.61273100	-2.25945300

Oxo  $\eta^2$ -Ozone Complex (conformation 2 higher energy)Fig. S61: NCCNO Oxo  $\eta^2$ -Ozone Complex (conformation 2 higher energy)

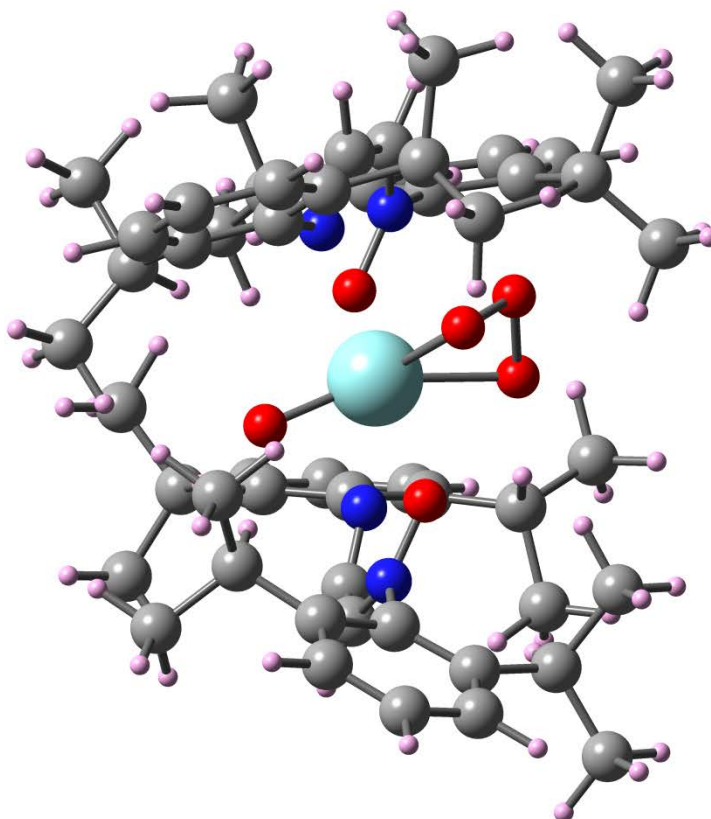
SCF	$E_{ZP}$	H	G
-2741.3926268	-2740.238296	-2740.167490	-2740.346525

Zr	0.38331700	-0.06888200	-0.43467900
O	-1.82610200	0.05223700	-0.08024900
O	2.36682900	-1.06616900	-0.64161500
O	1.34197800	1.80552200	-0.44512400
N	0.41473700	-1.87269600	1.27585400
N	3.25335000	-1.29069100	0.35286600
N	-1.31522400	2.93659100	-0.43043200
N	-2.76813300	0.33328600	-1.02758200
C	1.52223600	-1.95101500	1.98407500
C	2.85961400	-1.58875400	1.58421100
C	-2.11360300	2.71642800	-1.43859900
C	-2.88298100	1.50470500	-1.62667900
C	-0.75536100	-2.50921600	1.86620400
C	-1.30452500	-2.03057900	3.08900600
C	-2.38502600	-2.75148600	3.64366500
C	-2.90969400	-3.88749900	3.01330300
C	-2.36983300	-4.32161500	1.79108900

C	-1.28838000	-3.64609900	1.19376500
C	-1.95879700	0.27965000	3.91746500
C	-0.81630300	-0.76315300	3.80450400
C	-0.23647200	-1.08604500	5.20721400
C	4.88300500	2.41865100	0.36958700
C	4.81136000	1.10223600	1.18679500
C	5.51104600	1.26157700	2.56192700
C	4.66549600	-1.19383900	-0.02441700
C	5.40837300	-0.06181700	0.38939800
C	6.76590800	-0.01953900	0.00048800
C	7.33230500	-1.03945300	-0.77677700
C	6.55340500	-2.13319900	-1.19093100
C	5.19726100	-2.23774400	-0.82431600
C	-1.64399300	-4.87447400	-1.04124300
C	-0.64342700	-4.17691300	-0.09145500
C	0.52526200	-5.14493000	0.24847200
C	3.92666600	-3.17023500	-2.79977700
C	4.34509700	-3.40939800	-1.32256900
C	5.05537300	-4.77562900	-1.15679400
C	-0.63477100	4.17195500	-0.28293500
C	0.03974900	4.83039300	-1.36237200
C	0.61072000	6.09151800	-1.10125600
C	0.54353700	6.68064900	0.17091400
C	-0.04926800	5.98328700	1.23692100
C	-0.62023800	4.71338400	1.04147000
C	1.81807200	4.02907400	-2.98541900
C	0.29482400	4.18177000	-2.73099500
C	-0.38614300	4.96573600	-3.88337700
C	-5.41603300	-0.86878900	2.11704300
C	-4.91060100	-0.09003100	0.88071900
C	-5.86212100	1.10269300	0.57667600
C	-3.73611200	-0.73995300	-1.32522700
C	-4.75764900	-0.96939100	-0.36612400
C	-5.68983400	-1.98540500	-0.65267500
C	-5.60837400	-2.72511400	-1.84481400
C	-4.59901900	-2.45397700	-2.77863300
C	-3.62934400	-1.45105300	-2.54687000
C	-0.53080000	4.14978400	3.54014000
C	-1.26700000	3.94741800	2.19638000
C	-2.76983100	4.31883100	2.33249000
C	-1.83840300	-2.42219400	-4.09926200
C	-2.57817800	-1.14876700	-3.62169400
C	-3.23873700	-0.42729400	-4.82875700
H	1.48271500	-2.40329900	2.97861900
H	3.65021400	-1.70094200	2.31590200
H	-2.32815700	3.48166500	-2.19302400
H	-3.67537400	1.54595600	-2.36621800
H	-2.82169200	-2.41069400	4.57922500
H	-3.73701900	-4.42931900	3.46581600
H	-2.78998200	-5.19575000	1.30339900
H	-0.03001400	-0.28162400	3.21503500
H	3.74984800	0.92138400	1.37360800

H	-2.79980800	-0.09723100	4.51524800
H	-2.33112300	0.54925200	2.92243700
H	-1.58247500	1.19137800	4.39837300
H	-0.99952300	-1.51551900	5.87044000
H	0.14189200	-0.16940200	5.67785100
H	0.59292800	-1.80456200	5.15081700
H	5.91998300	2.70275300	0.14303600
H	4.41678900	3.23035000	0.94016500
H	4.32948100	2.31941300	-0.57042400
H	5.44650700	0.34215700	3.16037500
H	5.03209000	2.06921900	3.12925400
H	6.57427400	1.51291200	2.44930300
H	7.37438800	0.82978100	0.29834200
H	8.37801500	-0.97958300	-1.06909100
H	7.00312200	-2.91042800	-1.80187100
H	-0.21282300	-3.32397400	-0.63220600
H	3.42022500	-3.44815300	-0.73414100
H	-2.01247000	-5.82013000	-0.62183000
H	-1.14828600	-5.11300900	-1.99095800
H	-2.50706500	-4.23464100	-1.25832500
H	0.15104900	-6.02545700	0.78781800
H	1.28407500	-4.66213100	0.87655300
H	1.01566600	-5.48969900	-0.67171500
H	3.34714100	-2.24581100	-2.88995500
H	3.30701500	-4.00321200	-3.15817800
H	4.80913400	-3.09776300	-3.44981600
H	5.94326700	-4.85455600	-1.79698400
H	4.37296900	-5.58603400	-1.44446600
H	5.37043900	-4.94533600	-0.11893100
H	1.13466800	6.61128300	-1.89962800
H	0.97874700	7.66348200	0.33794700
H	-0.05055500	6.42588400	2.22843200
H	-0.10246400	3.16276800	-2.72836300
H	-3.92640000	0.31689600	1.13506500
H	2.32484200	5.00186600	-3.03864300
H	1.98629500	3.50624800	-3.93673700
H	2.26572300	3.43490100	-2.18229700
H	-1.47348600	5.04423900	-3.74183400
H	-0.20101800	4.46615100	-4.84354600
H	0.00894300	5.98776200	-3.95521200
H	-6.45369000	-1.20639300	1.99279500
H	-5.38960400	-0.21614700	2.99911800
H	-4.78707100	-1.74174700	2.31983600
H	-5.50239400	1.71013700	-0.26335600
H	-5.94101700	1.75698000	1.45458300
H	-6.86906700	0.74270900	0.32640600
H	-6.48519700	-2.19615300	0.05528900
H	-6.33803700	-3.50564500	-2.04777100
H	-4.55579100	-3.02462100	-3.70194700
H	-1.20832900	2.88460300	1.93968900
H	-1.79494500	-0.50537000	-3.20692600
H	-0.61756700	5.17956100	3.91325200

H	0.53228400	3.90108500	3.44197100
H	-0.96570700	3.49081800	4.30343600
H	-3.23900900	3.73044200	3.13330900
H	-3.31428400	4.12072200	1.40022800
H	-2.89115600	5.38349900	2.57656700
H	-1.33505900	-2.91368100	-3.26055200
H	-1.06509100	-2.13760500	-4.82270400
H	-2.50947100	-3.14591100	-4.58307800
H	-3.74345800	0.50194700	-4.52961400
H	-3.98667400	-1.06645700	-5.31825800
H	-2.47275200	-0.16947600	-5.57114200
O	1.58785000	2.01182500	1.02193500
O	1.20524200	0.72371000	1.62993000
O	0.07343100	-0.21509400	-2.22954100

Oxo  $\eta^3$ -Ozone ComplexFig. S62: NCCNO Oxo  $\eta^3$ -Ozone Complex

SCF	$E_{ZP}$	H	G
-2741.39251827	-2740.237776	-2740.166229	-2740.346537

Zr	0.26999600	0.13555000	-0.18296400
O	-1.95618200	0.40887000	0.23738200
O	2.22929700	-1.00317900	-0.73809000
O	1.00620600	1.03161100	-1.97992200
N	0.02943800	-2.13695500	0.83352400
N	2.96429500	-1.76998500	0.06030300
N	-0.23592600	2.60738100	-0.16821000
N	-2.82040800	1.12283800	-0.52057500
C	1.06584900	-2.80761400	1.26517800
C	2.46400200	-2.57320100	0.98628700
C	-1.33026700	3.08587700	-0.70010800
C	-2.54081700	2.33759600	-0.95845500
C	-1.25622100	-2.63617300	1.32484000
C	-1.62990600	-2.35405800	2.66689800
C	-2.84121800	-2.90895500	3.13486000
C	-3.64958500	-3.69825400	2.30488800
C	-3.26236600	-3.94525400	0.97731900

C	-2.06036000	-3.42415100	0.45733600
C	-1.60083200	-0.32620000	4.21759500
C	-0.77802400	-1.48982100	3.60850300
C	-0.14898200	-2.34829300	4.73915900
C	4.90735400	1.55685200	1.44879500
C	4.54363700	0.07050400	1.69968300
C	4.97181000	-0.36826500	3.12490800
C	4.41710500	-1.70855100	-0.17410200
C	5.17493600	-0.83181900	0.63370000
C	6.56726300	-0.80552900	0.39774300
C	7.14461300	-1.59181000	-0.61078100
C	6.34492900	-2.41682100	-1.42070700
C	4.95078800	-2.49287100	-1.22550600
C	-2.77376100	-3.97291800	-1.94979100
C	-1.60109500	-3.75856100	-0.96585500
C	-0.68933000	-5.01846200	-0.96500800
C	3.71441200	-2.48238200	-3.42669700
C	4.06106300	-3.31750100	-2.16079600
C	4.68525300	-4.67997800	-2.54561800
C	0.84031900	3.55312200	0.09756600
C	1.49157900	4.24175100	-0.96879200
C	2.53152300	5.13391700	-0.62520100
C	2.90045100	5.35659200	0.70761100
C	2.22582800	4.68504800	1.73910800
C	1.19079500	3.77202400	1.46180900
C	2.37448600	3.61655300	-3.27958900
C	1.14488800	4.07418500	-2.45517600
C	0.54795600	5.38516300	-3.03592500
C	-5.37121300	-0.01166500	2.79662700
C	-4.71797100	0.82442100	1.67305900
C	-5.16933000	2.30972500	1.78496100
C	-4.11732900	0.49277100	-0.81835500
C	-5.01500400	0.29314400	0.26531400
C	-6.24210700	-0.32978700	-0.02929100
C	-6.55839300	-0.72388100	-1.34103900
C	-5.65830400	-0.48676300	-2.38722000
C	-4.40754600	0.13195500	-2.15899800
C	1.27847600	2.65130900	3.76919400
C	0.38891500	3.14980400	2.60869600
C	-0.68001500	4.15917000	3.11328100
C	-3.16957300	-0.86956700	-4.16824700
C	-3.48769600	0.40988700	-3.35602800
C	-4.11728000	1.49964600	-4.26831700
H	0.90424300	-3.65939200	1.93205000
H	3.19128600	-3.15426300	1.53968700
H	-1.39700600	4.14358900	-0.96554500
H	-3.33066100	2.82845600	-1.51318000
H	-3.15064900	-2.71886600	4.15981600
H	-4.57584400	-4.12084900	2.68811600
H	-3.89904700	-4.55238900	0.34112300
H	0.03206300	-1.02284500	3.03725200
H	3.44962600	0.00897000	1.64227000

H	-2.42526000	-0.68800900	4.84697400
H	-2.02042400	0.30548400	3.42614000
H	-0.95082800	0.30014200	4.84234900
H	-0.92226500	-2.82199500	5.35932700
H	0.47139900	-1.71990700	5.39187300
H	0.48665300	-3.14853200	4.33644800
H	5.98603300	1.73968300	1.55057800
H	4.38433500	2.19234000	2.17328900
H	4.59601900	1.87323300	0.44654500
H	4.68471100	-1.40846700	3.33106200
H	4.48536300	0.26979300	3.87366800
H	6.05886600	-0.28612000	3.26264200
H	7.19577100	-0.15388500	0.99833200
H	8.21864000	-1.55298800	-0.77731100
H	6.80700400	-3.00104100	-2.21068800
H	-1.01360100	-2.91185600	-1.34221600
H	3.11146300	-3.52609300	-1.65095500
H	-3.32420200	-4.90039300	-1.73798300
H	-2.38435900	-4.04877500	-2.97271100
H	-3.48108900	-3.13655700	-1.91773300
H	-1.23838200	-5.89660700	-0.59753900
H	0.19525600	-4.88480800	-0.33029000
H	-0.34193200	-5.23252000	-1.98436400
H	3.18535400	-1.56344000	-3.15441000
H	3.06592800	-3.06373100	-4.09509500
H	4.62692000	-2.21672900	-3.97774100
H	5.57796900	-4.55601000	-3.17199600
H	3.96173800	-5.26694000	-3.12554500
H	4.96916900	-5.26348900	-1.65990400
H	3.05673300	5.65835900	-1.41922700
H	3.70212200	6.05318500	0.94219400
H	2.50155000	4.87715200	2.77198200
H	0.40998500	3.27344100	-2.56470800
H	-3.63541100	0.78470900	1.82831100
H	3.20009200	4.33913800	-3.22787400
H	2.09279400	3.50045900	-4.33485400
H	2.72094000	2.64354200	-2.91860600
H	-0.34350800	5.71227400	-2.48150500
H	0.26216900	5.23733900	-4.08597800
H	1.27551900	6.20689900	-2.99905400
H	-6.46530300	0.08375800	2.79723700
H	-5.01372800	0.34267300	3.77184200
H	-5.11048300	-1.07136800	2.70375500
H	-4.68196100	2.94474400	1.03431500
H	-4.91697100	2.70777400	2.77634700
H	-6.25548200	2.39712600	1.64794200
H	-6.95665300	-0.50646500	0.76779100
H	-7.51079700	-1.20739900	-1.54515300
H	-5.92016200	-0.78636400	-3.39789000
H	-0.11997700	2.26446500	2.22021000
H	-2.52087900	0.77750700	-3.00573100
H	1.85874000	3.45823900	4.23745900



H	1.95522400	1.87601200	3.39660500
H	0.64951800	2.20405200	4.55121600
H	-1.29773900	3.69932000	3.89681300
H	-1.34550400	4.48347500	2.30088800
H	-0.20809800	5.05703000	3.53554200
H	-2.58002800	-1.55971800	-3.56002300
H	-2.56049600	-0.60272200	-5.04108400
H	-4.07606800	-1.37493000	-4.52826800
H	-4.33714000	2.42581300	-3.71790700
H	-5.05800900	1.15206500	-4.71555400
H	-3.42591300	1.74549900	-5.08402200
O	1.15655200	0.33820100	1.43550700
O	-0.35029300	0.54623500	-2.50850400
O	-0.48798200	-0.90145100	-2.03637300

## Reactant for Ligand Cyclization

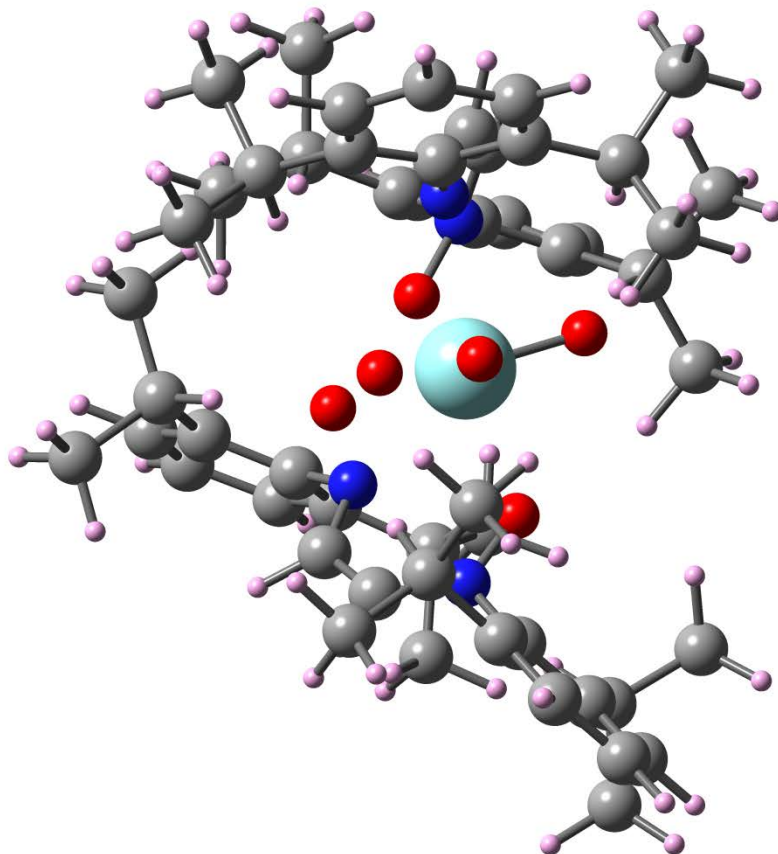


Fig. S63: NCCNO Reactant for Ligand Cyclization

	SCF	E <sub>ZP</sub>	H	G
	-2741.39852398	-2740.243660	-2740.172289	-2740.351026
Zr	0.42060000	0.28724200	-0.35392400	
O	-1.86666600	0.04103200	-0.12577100	
O	2.02067500	-1.27382200	-0.56745300	
O	2.07817100	1.62383600	-0.34058400	
N	0.06661000	-1.55134600	1.43056500	
N	2.90878100	-1.58274800	0.40740900	
N	-0.61126500	2.60587100	-0.54130400	
N	-2.76527800	0.52636200	-1.00103500	
C	1.15834000	-1.79677300	2.12199800	
C	2.52602900	-1.69886800	1.67270700	
C	-1.72810000	2.76625300	-1.19936600	
C	-2.71060300	1.74700400	-1.49926200	
C	-1.16691800	-2.03703200	2.04116800	
C	-1.69719000	-1.42538700	3.20934500	
C	-2.83795600	-2.01387400	3.79964000	
C	-3.43996900	-3.15423200	3.25205300	
C	-2.91283800	-3.72685200	2.08271100	

C	-1.77271900	-3.18573500	1.45742800
C	-2.15990700	0.97049500	3.91283500
C	-1.10255500	-0.16150800	3.84313400
C	-0.52734600	-0.44721300	5.25608900
C	5.49019400	1.61429500	0.47974200
C	5.07869800	0.32323900	1.23310200
C	5.83094000	0.20274800	2.58541400
C	4.28560900	-1.81261100	-0.03683800
C	5.30851500	-0.91607800	0.36213500
C	6.61306900	-1.19438800	-0.10396300
C	6.87396600	-2.29048600	-0.93672500
C	5.83054200	-3.14661700	-1.32512600
C	4.51109000	-2.93157300	-0.88204100
C	-2.19320600	-4.51510300	-0.70484000
C	-1.14988400	-3.87441700	0.23882300
C	-0.12060000	-4.94810800	0.69326600
C	2.99654800	-3.56968900	-2.80525000
C	3.39026500	-3.87386300	-1.33425300
C	3.76641300	-5.36601700	-1.15248900
C	0.19861200	3.82323200	-0.42625700
C	0.83756700	4.33939500	-1.58620700
C	1.54136300	5.55444800	-1.45159200
C	1.61900100	6.22242900	-0.22098900
C	1.00795800	5.66806400	0.91429400
C	0.29700700	4.45385700	0.83900400
C	2.33085900	3.24119800	-3.31307000
C	0.87058800	3.60366800	-2.93288000
C	0.19098300	4.42757300	-4.05732100
C	-5.77303300	-0.29353100	1.91095700
C	-5.13272500	0.44989100	0.71501400
C	-5.94438900	1.73409700	0.38332800
C	-3.86933400	-0.37639500	-1.38198000
C	-5.00136400	-0.43121300	-0.53246000
C	-6.04824600	-1.28937200	-0.92575700
C	-5.95594800	-2.04704000	-2.10527200
C	-4.81928400	-1.95682700	-2.92275200
C	-3.73682100	-1.11527400	-2.58287000
C	0.48429200	3.95991300	3.34214600
C	-0.40055100	3.88300600	2.07601400
C	-1.76441100	4.59095100	2.30603500
C	-1.98639800	-2.35261200	-3.99018000
C	-2.52851500	-0.98209700	-3.51713300
C	-2.89968700	-0.10508800	-4.74548500
H	1.07116400	-2.21097000	3.13140300
H	3.31056900	-1.90249800	2.39065200
H	-1.98460100	3.75109100	-1.59840100
H	-3.51614000	2.00881000	-2.17382600
H	-3.25665400	-1.57033800	4.69993600
H	-4.31155000	-3.59516000	3.73047400
H	-3.38899700	-4.60719500	1.66098700
H	-0.28116600	0.20958000	3.22180000
H	4.01464000	0.43754800	1.44951800

H	-3.00970100	0.69652800	4.55240300
H	-2.54606000	1.20472100	2.91284300
H	-1.70864600	1.88054100	4.32695500
H	-1.30863800	-0.79171500	5.94720400
H	-0.08159800	0.46456000	5.67443900
H	0.25285800	-1.21932700	5.22647800
H	6.55549500	1.61352900	0.21069600
H	5.29618400	2.48661300	1.11566600
H	4.89000500	1.73052500	-0.42862400
H	5.52978300	-0.69494400	3.14413000
H	5.61364500	1.07864400	3.20957300
H	6.91847700	0.15311900	2.44020800
H	7.42549300	-0.53123300	0.17946800
H	7.88621500	-2.47566900	-1.28824900
H	6.04380200	-3.99107400	-1.97421000
H	-0.60236700	-3.11498700	-0.33254900
H	2.50091300	-3.68323200	-0.72443200
H	-2.69774400	-5.37061800	-0.23646500
H	-1.69582300	-4.89005100	-1.60889600
H	-2.95780900	-3.79083100	-1.00893100
H	-0.61628800	-5.73816300	1.27340300
H	0.66761300	-4.51534100	1.32180300
H	0.35892500	-5.41370900	-0.17833900
H	2.65105700	-2.53545000	-2.90147500
H	2.18562500	-4.23733300	-3.12709900
H	3.84996100	-3.72201800	-3.48003800
H	4.59123900	-5.66421200	-1.81213800
H	2.90465400	-5.99964700	-1.40072900
H	4.06453700	-5.58450000	-0.11867300
H	2.04872000	5.96869400	-2.31935100
H	2.16456600	7.16012200	-0.14324800
H	1.08864400	6.17990300	1.86904100
H	0.34665900	2.64692600	-2.84340100
H	-4.12800700	0.75515900	1.03070200
H	2.94275700	4.13831500	-3.48244300
H	2.33877600	2.64298900	-4.23398400
H	2.78604300	2.65006700	-2.51190900
H	-0.85929200	4.65325600	-3.82205100
H	0.21556900	3.86848600	-5.00216700
H	0.70425900	5.38471400	-4.22116800
H	-6.82552200	-0.54162300	1.72065800
H	-5.74416800	0.34640200	2.80229100
H	-5.23145400	-1.21719700	2.13819400
H	-5.48106000	2.31330000	-0.42563700
H	-6.01051400	2.38070300	1.26782200
H	-6.96524300	1.47860400	0.07038700
H	-6.93684900	-1.36805900	-0.30689600
H	-6.77420900	-2.70484500	-2.38871500
H	-4.76558300	-2.54470700	-3.83436000
H	-0.59367000	2.82011800	1.89084300
H	-1.69734500	-0.49026800	-2.99646100
H	0.68905200	4.99677000	3.64071300

H	1.43538900	3.44709600	3.16849700
H	-0.02156600	3.47100400	4.18544600
H	-2.28694700	4.15370700	3.16742900
H	-2.41931600	4.50091500	1.42811400
H	-1.61869700	5.66159200	2.50349700
H	-1.72866300	-2.99088800	-3.13843300
H	-1.07328800	-2.19201900	-4.57574000
H	-2.70340400	-2.89277400	-4.62418700
H	-3.23793300	0.89668200	-4.44741400
H	-3.70074400	-0.56630600	-5.33985400
H	-2.01954900	0.01837200	-5.38820300
O	2.20998900	1.86853200	1.13335100
O	1.37005300	0.81773400	1.74821300
O	0.12276200	0.22184100	-2.16195600

## Product for Ligand Cyclization

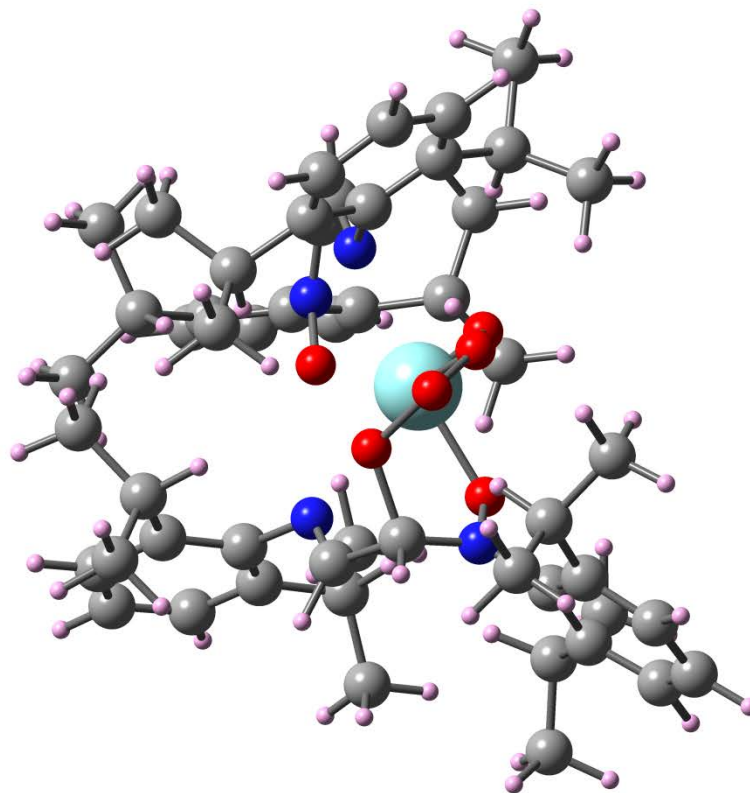


Fig. S64: NCCNO Product for Ligand Cyclization

SCF	E <sub>ZP</sub>	H	G
-2741.39361929	-2740.238217	-2740.167323	-2740.346083

Zr	0.41770300	0.37402900	-0.62301100
O	-1.85555200	-0.00022400	-0.24554900
O	1.84125800	-1.17911400	-0.83064100
O	2.08487800	1.71937000	-0.58054400
N	0.14024500	-1.44661300	1.44633600
N	2.90607200	-1.28045200	0.11702000
N	-0.65689000	2.63764000	-0.24927800
N	-2.82862000	0.62448000	-0.92980300
C	1.32327000	-1.63232800	1.94746400
C	2.54086800	-0.90189400	1.41632000
C	-1.82940100	2.88876600	-0.76631700
C	-2.82394300	1.92042300	-1.18176600
C	-0.96189500	-2.19585000	2.03783000
C	-1.47019000	-1.78526000	3.30410800
C	-2.49632200	-2.55613600	3.88942200
C	-3.02448700	-3.68168400	3.24072700
C	-2.53466300	-4.04514900	1.97814400
C	-1.50079100	-3.31658200	1.35286700
C	-2.11032600	0.39752500	4.45647800

C	-0.95146800	-0.54904500	4.05081800
C	-0.12310600	-0.95024400	5.30105100
C	6.04549400	1.41739600	-0.32625400
C	5.46929200	0.30493600	0.58766600
C	6.29165400	0.18490200	1.89915100
C	4.18123900	-1.77106600	-0.35481000
C	5.38770900	-1.03576700	-0.14669800
C	6.59275600	-1.56934200	-0.65365300
C	6.62108200	-2.76141800	-1.38570100
C	5.42771300	-3.46857300	-1.58770500
C	4.20334400	-3.01436400	-1.05910300
C	-2.10513600	-3.77875900	-1.07388600
C	-0.98075500	-3.78370600	-0.00821200
C	-0.34601500	-5.19473800	0.09782800
C	2.43996100	-3.76522400	-2.72249200
C	2.95893100	-3.88345400	-1.26467100
C	3.22807000	-5.36466300	-0.88958200
C	0.15257400	3.82457200	0.04460800
C	0.69543800	4.57707500	-1.03281100
C	1.42172500	5.74130700	-0.70684100
C	1.61183800	6.13785400	0.62473700
C	1.08867300	5.35831400	1.66711400
C	0.35850800	4.18290800	1.40003700
C	2.00545400	3.92355200	-3.10659200
C	0.59352400	4.14983300	-2.50360700
C	-0.21044200	5.17717700	-3.34345600
C	-5.46803000	-0.86981300	2.04323600
C	-4.99632200	0.14320300	0.97305100
C	-5.86374400	1.43249000	1.02744500
C	-3.97004400	-0.20246700	-1.37470900
C	-5.00761500	-0.44565600	-0.44196000
C	-6.10024600	-1.21223500	-0.89537900
C	-6.14051000	-1.70470700	-2.21048300
C	-5.09039300	-1.44045000	-3.10231000
C	-3.96651300	-0.68137400	-2.70758400
C	0.76473400	3.12374500	3.69226400
C	-0.24989400	3.37815000	2.55170000
C	-1.52624800	4.08569000	3.08592600
C	-2.38342900	-1.63065600	-4.48302100
C	-2.84430300	-0.37347400	-3.70484000
C	-3.29481200	0.73293500	-4.69842000
H	1.50401500	-2.35678300	2.74872500
H	3.38781000	-0.96903300	2.09912000
H	-2.13466500	3.92511300	-0.93446600
H	-3.68756800	2.29106500	-1.71957400
H	-2.88625600	-2.27070300	4.86323300
H	-3.80969500	-4.26695300	3.71327400
H	-2.94874400	-4.91444800	1.47355300
H	-0.29181500	0.01605000	3.38406100
H	4.46738800	0.63881300	0.84413100
H	-2.79521000	-0.07938400	5.16889800
H	-2.69331800	0.70499900	3.57879100

H	-1.71122000	1.29972600	4.93692000
H	-0.73595100	-1.51793000	6.01378500
H	0.25654000	-0.05700300	5.81468100
H	0.73648800	-1.57682500	5.03084800
H	7.07991100	1.20835800	-0.63030900
H	6.03512200	2.37894600	0.20416800
H	5.43398000	1.52419000	-1.22957700
H	5.87628200	-0.57926700	2.57182100
H	6.29494800	1.14415900	2.43399500
H	7.33512700	-0.09048900	1.69585600
H	7.51702700	-1.02011800	-0.49276300
H	7.55800500	-3.13634200	-1.79093000
H	5.45016900	-4.40008100	-2.14637000
H	-0.20276300	-3.09099200	-0.34669700
H	2.16653000	-3.50620300	-0.61219800
H	-2.89911800	-4.49589100	-0.82539500
H	-1.69573300	-4.06050600	-2.05285300
H	-2.55816100	-2.78620500	-1.16064700
H	-1.08336800	-5.93714600	0.43091200
H	0.48941900	-5.20847000	0.80898000
H	0.03284200	-5.51299900	-0.88112400
H	2.18980000	-2.72395300	-2.94762400
H	1.53854900	-4.37930900	-2.86151900
H	3.19745000	-4.11069200	-3.43981100
H	3.96201500	-5.83059600	-1.55910100
H	2.30234200	-5.94759800	-0.96678500
H	3.60681400	-5.45571800	0.13729100
H	1.85852900	6.33213700	-1.50781900
H	2.17458200	7.04092300	0.84904300
H	1.25024500	5.66481600	2.69698600
H	0.08550700	3.18275800	-2.57119200
H	-3.96508100	0.41571900	1.22755300
H	2.58617100	4.85566100	-3.14459200
H	1.91521200	3.53748800	-4.13054200
H	2.55458700	3.19032000	-2.50737900
H	-1.23072900	5.31496400	-2.95699800
H	-0.28362200	4.83768600	-4.38505100
H	0.27606800	6.16174000	-3.34555300
H	-6.52844900	-1.12652900	1.92191100
H	-5.34849500	-0.43471200	3.04365400
H	-4.87893600	-1.79181200	2.00438700
H	-5.51631100	2.18981100	0.31250800
H	-5.82836900	1.87316600	2.03220300
H	-6.91199000	1.20691100	0.79188200
H	-6.92077100	-1.42651900	-0.21733800
H	-6.99273700	-2.29459700	-2.53930400
H	-5.13460100	-1.83091700	-4.11465900
H	-0.55141700	2.39758800	2.16184700
H	-1.96013200	-0.00145200	-3.17322700
H	1.07208400	4.05741600	4.18054500
H	1.65716800	2.62155900	3.30527800
H	0.31539400	2.48420600	4.46364300



H	-1.99107000	3.49788700	3.88790300
H	-2.27053100	4.22698900	2.29016800
H	-1.27971600	5.07698400	3.48870400
H	-2.08742000	-2.43384700	-3.79938300
H	-1.51004400	-1.37313000	-5.09386500
H	-3.16232100	-2.01707300	-5.15501500
H	-3.57309500	1.66109100	-4.18081000
H	-4.15951400	0.40980600	-5.29460300
H	-2.47197500	0.96849500	-5.38438000
O	2.66988200	1.67661600	0.77484200
O	1.92435800	0.56842800	1.50498900
O	-0.07780000	0.57343700	-2.36110400

## Oxo Peroxo Complex with Adsorbed Propylene Oxide (conformation 1)

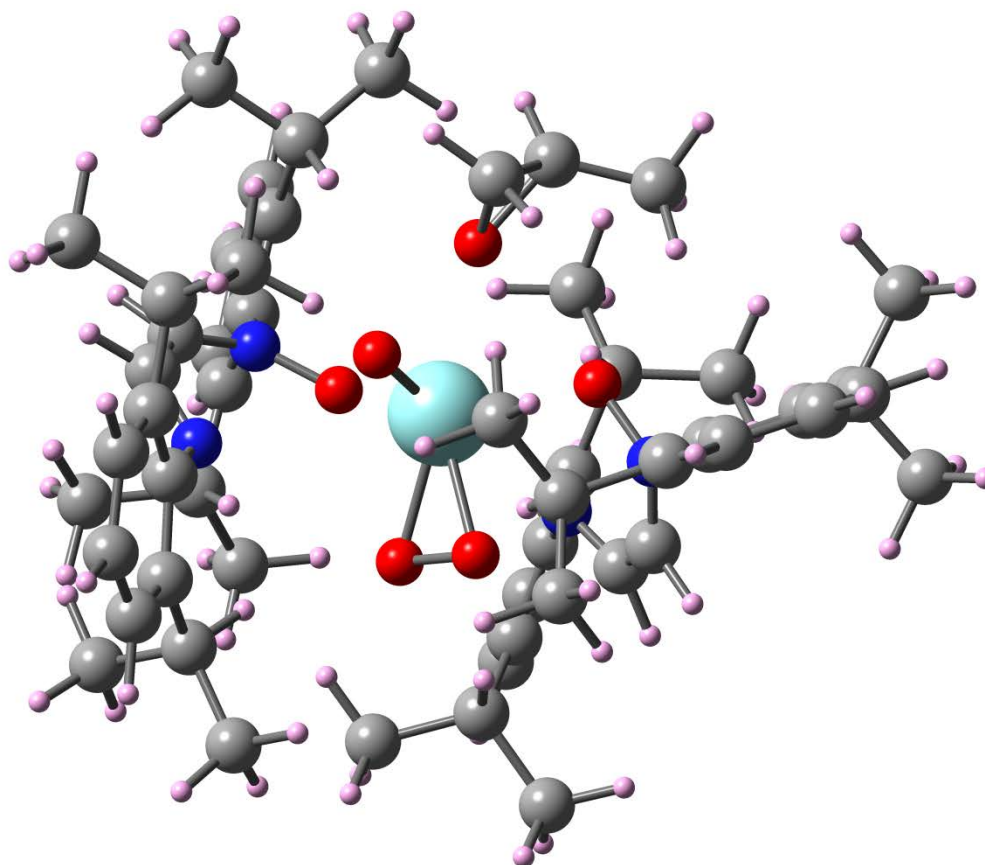


Fig. S65: NCCNO Oxo Peroxo Complex with Adsorbed Propylene Oxide (conformation 1)

SCF	E <sub>ZP</sub>	H	G
-2859.32437701	-2858.086119	-2858.009634	-2858.201418

Zr	0.42889000	0.27993700	-0.27383800
O	-1.79907400	-0.21058500	-0.40084600
O	2.44188900	-0.68690300	-0.71728600
O	0.60462100	1.81480000	-1.25280500
N	0.74857300	-1.98836100	1.28909700
N	3.37853400	-0.71289400	0.29635400
N	-1.77673300	2.85676900	0.01869500
N	-2.95375800	0.19152400	-0.96787500
C	1.86421400	-1.81727600	1.95449600
C	3.04493100	-1.09571400	1.52185900
C	-2.67820300	2.69777200	-0.90631600
C	-3.32907600	1.44003200	-1.21165300
C	-0.26260600	-2.83645800	1.87065300
C	-0.76409600	-2.63682900	3.19470800
C	-1.70900000	-3.56437200	3.68590100
C	-2.16268200	-4.64021000	2.91058400
C	-1.68887700	-4.79752700	1.59804000

C	-0.74453200	-3.90533100	1.05663000
C	-1.62620400	-0.61670400	4.47943900
C	-0.37812500	-1.45007400	4.09003500
C	0.38018900	-1.91546100	5.36134600
C	3.93998500	3.17859900	-0.71462200
C	4.17871800	2.16695900	0.43541700
C	4.72251800	2.88313100	1.69973900
C	4.73886200	-0.32071400	-0.06608800
C	5.11815700	1.04401300	-0.00819600
C	6.44711300	1.35447200	-0.37507500
C	7.34603100	0.35778100	-0.78031500
C	6.93623700	-0.98451800	-0.83374400
C	5.62114500	-1.35218400	-0.48572500
C	-1.22396600	-4.62821600	-1.36275200
C	-0.16983000	-4.13986900	-0.34230900
C	1.02045100	-5.13636100	-0.26513700
C	5.56201100	-3.49071100	-1.88934000
C	5.19821800	-2.82487100	-0.53785000
C	5.82046600	-3.61736300	0.64391500
C	-1.20156600	4.12222600	0.29476900
C	-0.75402900	5.02345500	-0.72717400
C	-0.24703100	6.27361500	-0.31857700
C	-0.16479700	6.62940900	1.03617000
C	-0.54776600	5.70933400	2.02686800
C	-1.04841100	4.44096000	1.68350400
C	0.74034200	4.79200000	-2.77551600
C	-0.70172100	4.66906400	-2.22036400
C	-1.69101600	5.53156300	-3.04870800
C	-4.82069300	-1.63688200	2.36633000
C	-4.70506400	-0.61827000	1.20761900
C	-5.81413800	0.46480500	1.32830400
C	-3.92182600	-0.89262200	-1.23974600
C	-4.76351600	-1.28644800	-0.17053600
C	-5.71341200	-2.29337300	-0.44134900
C	-5.80883500	-2.87327900	-1.71581100
C	-4.95308700	-2.46052800	-2.74880300
C	-3.98012200	-1.46026000	-2.53461000
C	-0.63705600	3.52274000	4.04467400
C	-1.48227700	3.43934200	2.75448000
C	-2.99268000	3.60628300	3.07988500
C	-2.58482800	-2.16868600	-4.55910500
C	-3.07789300	-0.99150300	-3.68200900
C	-3.81525700	0.04845900	-4.57175200
H	1.98839200	-2.25897300	2.94850500
H	3.83219300	-0.98673000	2.26078000
H	-3.09106400	3.53911200	-1.47580000
H	-4.28601600	1.50966500	-1.71891000
H	-2.10015000	-3.43375200	4.69213700
H	-2.88375800	-5.34384200	3.32047600
H	-2.05306700	-5.62467100	0.99492500
H	0.25657200	-0.76403300	3.52449100
H	3.20421600	1.75142000	0.70147600

H	-2.35749000	-1.20568600	5.04997500
H	-2.11062000	-0.22336900	3.57916500
H	-1.32281100	0.23859000	5.09732800
H	-0.24926900	-2.55839300	5.99185900
H	0.68093900	-1.04659100	5.96187300
H	1.28585400	-2.48678400	5.11384300
H	4.87668100	3.65047000	-1.04461300
H	3.25781900	3.96622900	-0.37369300
H	3.46636700	2.68658100	-1.57103100
H	4.86681400	2.17765600	2.52862800
H	4.00235800	3.64282800	2.02740700
H	5.68179100	3.38382600	1.50783000
H	6.77533400	2.38958300	-0.33855300
H	8.36410700	0.62454600	-1.05475600
H	7.64092400	-1.74853400	-1.15117900
H	0.22594400	-3.18241800	-0.69744300
H	4.10825000	-2.87897100	-0.43708000
H	-1.58747200	-5.63778700	-1.12932500
H	-0.78223600	-4.67033000	-2.36866600
H	-2.08758200	-3.95289600	-1.39385700
H	0.68742400	-6.11140400	0.11554200
H	1.80457800	-4.76212800	0.40520900
H	1.46585800	-5.29390700	-1.25752700
H	5.13962700	-2.93133900	-2.73268700
H	5.16641400	-4.51456400	-1.92216500
H	6.64813100	-3.55154700	-2.03431600
H	6.91704700	-3.60508600	0.59060000
H	5.49047400	-4.66452400	0.62104400
H	5.52870500	-3.18873500	1.61128400
H	0.10272900	6.97402700	-1.07312400
H	0.21723600	7.60804200	1.31890700
H	-0.44381900	5.97758300	3.07380100
H	-0.95683000	3.61275900	-2.33882700
H	-3.73346700	-0.12338300	1.31321100
H	1.14090400	5.81002800	-2.68020800
H	0.75176100	4.52684700	-3.84279600
H	1.38751800	4.09005400	-2.24205700
H	-2.72567500	5.43290700	-2.69057800
H	-1.66472000	5.23470500	-4.10641500
H	-1.42851000	6.59670100	-2.99379000
H	-5.80948100	-2.11405900	2.39489900
H	-4.67745400	-1.12163300	3.32411700
H	-4.05814100	-2.41867800	2.28731100
H	-5.72839800	1.22627300	0.54281600
H	-5.74081100	0.97298100	2.29818400
H	-6.81232300	0.01260700	1.25309400
H	-6.37857600	-2.62550500	0.34983900
H	-6.54967300	-3.64660900	-1.90448800
H	-5.03965200	-2.92240500	-3.72769300
H	-1.32635700	2.44085000	2.33279800
H	-2.19051600	-0.51403500	-3.25007800
H	-0.79461900	4.46131300	4.59555600

H	0.43047100	3.42176000	3.81642000
H	-0.91392400	2.69799400	4.71428300
H	-3.30772400	2.85494200	3.81761100
H	-3.61103200	3.48042600	2.18154500
H	-3.20037100	4.60168300	3.49821300
H	-2.08640700	-2.93510900	-3.95426300
H	-1.87642800	-1.79968000	-5.31257200
H	-3.40891000	-2.64634600	-5.10403900
H	-4.12128100	0.93311500	-4.00080700
H	-4.71671200	-0.39049600	-5.01982100
H	-3.16050500	0.38682700	-5.38574200
O	1.46608200	0.80490700	1.55744200
O	-0.00902000	0.67094300	1.76200000
C	1.17346700	-0.10847000	-3.52248100
H	0.65091500	0.58532900	-4.17430100
C	0.93647900	-1.57669500	-3.61659500
H	0.18601000	-1.90862700	-4.33113000
O	0.26951300	-0.76623200	-2.50675900
H	2.09989200	0.25160300	-3.08827800
C	1.97617700	-2.59762000	-3.22768300
H	1.50636400	-3.52666100	-2.88589800
H	2.59477700	-2.83338100	-4.10582200
H	2.60946200	-2.20411600	-2.42953700

## Oxo Peroxo Complex with Adsorbed Propylene Oxide (conformation 2)

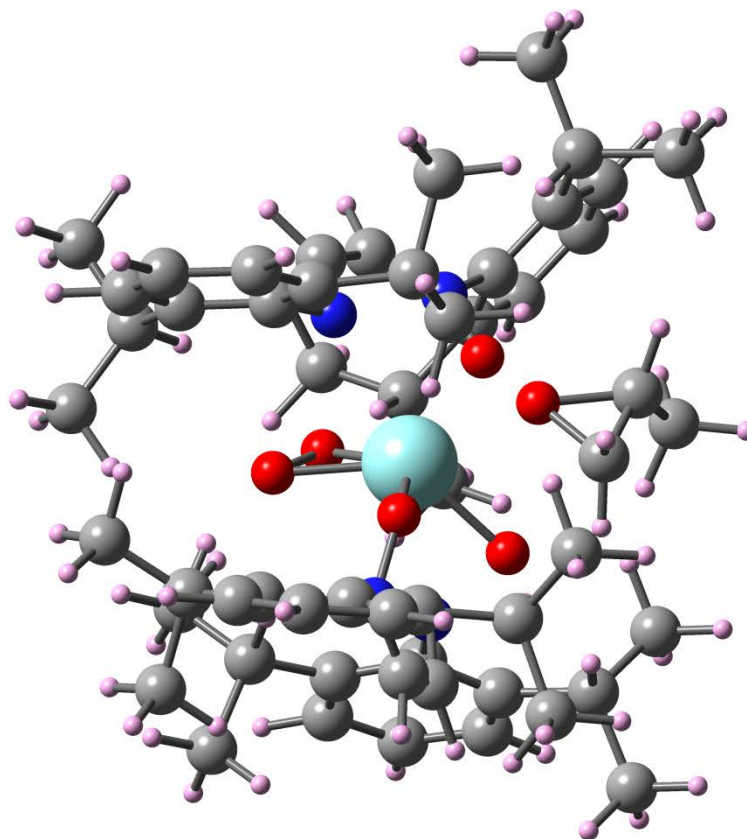


Fig. S66: NCCNO Oxo Peroxo Complex with Adsorbed Propylene Oxide (conformation 2)

SCF	E <sub>ZP</sub>	H	G
-2859.3224482	-2858.082065	-2858.007122	-2858.192347

Zr	0.12590200	0.06677700	-0.13748000
O	-1.87588100	0.18462000	-0.70067600
O	2.16449400	-0.88151800	-0.70898000
O	0.67324800	1.73517800	-1.25105000
N	0.05290500	-2.35305800	0.67091700
N	2.97466300	-1.59630100	0.09563200
N	-0.06598300	2.48347000	-0.14792000
N	-2.88931700	1.17914500	-0.51881500
C	1.14353000	-2.85329600	1.20548600
C	2.51438100	-2.45101400	0.99161400
C	-1.30589400	3.09983900	-0.55886000
C	-2.53237600	2.49940900	-0.64082900
C	-1.18810600	-3.00809600	1.06394600
C	-1.54779400	-3.12634800	2.44316500
C	-2.74528200	-3.80930500	2.74566000
C	-3.55896600	-4.35558200	1.74409700
C	-3.18736100	-4.22342700	0.39819300
C	-2.00426300	-3.55289600	0.03260000

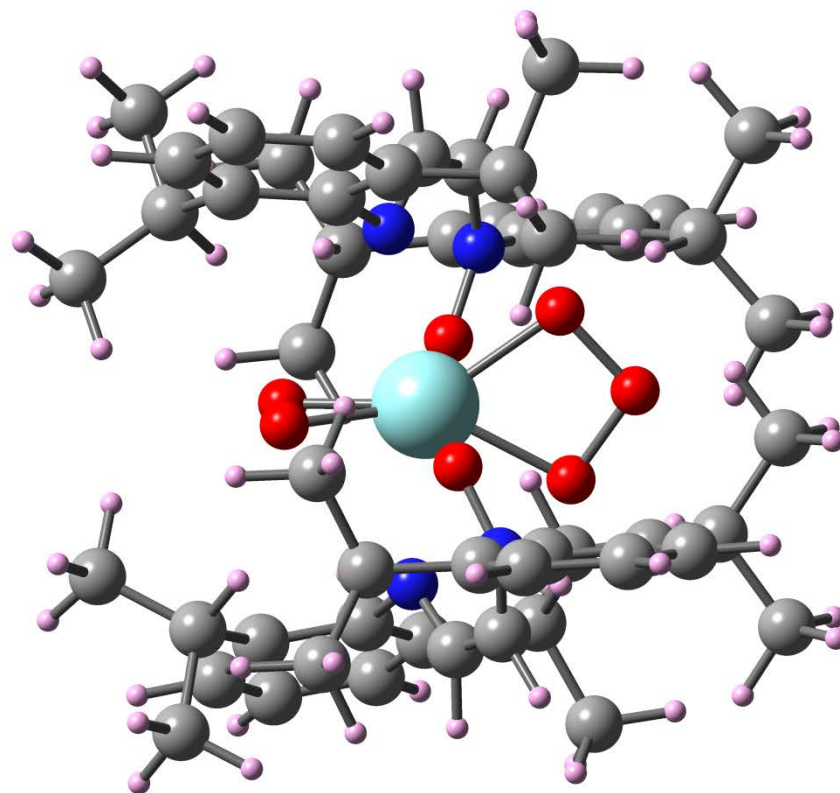
C	-1.58103700	-1.55393800	4.45588900
C	-0.73791000	-2.54354900	3.61291000
C	-0.16629600	-3.67071700	4.51585000
C	4.61966000	1.98294800	1.31577600
C	4.38515600	0.48668100	1.64079100
C	4.84108000	0.15860100	3.08786700
C	4.41779700	-1.41687400	-0.11460500
C	5.09073900	-0.41974700	0.62929900
C	6.48057100	-0.29661000	0.40996800
C	7.14673200	-1.11768700	-0.51205600
C	6.43845400	-2.08400400	-1.24586100
C	5.05020200	-2.25277100	-1.06833000
C	-2.72463000	-3.23127400	-2.40622500
C	-1.56202900	-3.52737000	-1.43115200
C	-0.86180100	-4.86587700	-1.79769500
C	4.54325600	-3.19273200	-3.38964500
C	4.29216900	-3.32075000	-1.86545400
C	4.66174700	-4.74497200	-1.36903200
C	0.83106500	3.47147000	0.49036000
C	1.67360100	4.30228200	-0.30773500
C	2.53659800	5.20436300	0.35111700
C	2.53605600	5.33320000	1.74646700
C	1.63275700	4.57654600	2.50435500
C	0.75872800	3.64550300	1.90148800
C	3.03365400	3.87435400	-2.41812700
C	1.66713200	4.32790300	-1.84469400
C	1.28548700	5.73410300	-2.37996600
C	-4.96301700	-0.63257900	2.79020100
C	-4.42482500	0.44228100	1.81858200
C	-4.69893900	1.86170000	2.39056900
C	-4.24461100	0.71955600	-0.72840900
C	-5.00646300	0.32988100	0.40727400
C	-6.33652600	-0.09260000	0.20346400
C	-6.89629400	-0.12497500	-1.08399300
C	-6.13276200	0.26716400	-2.19301600
C	-4.79408800	0.68802100	-2.03990500
C	0.30940000	2.32396100	4.05253600
C	-0.29407000	2.96524800	2.77998500
C	-1.40028700	3.99207700	3.15113900
C	-4.05422800	0.10116500	-4.41802700
C	-4.00168400	1.14140800	-3.27003300
C	-4.50991800	2.51787100	-3.78000700
H	1.06041200	-3.70201100	1.88734800
H	3.27166800	-2.95534300	1.58036100
H	-1.26525500	4.17237200	-0.72664800
H	-3.38182900	3.15511200	-0.81982200
H	-3.04622800	-3.90622300	3.78557300
H	-4.47425100	-4.87917100	2.01007600
H	-3.81867900	-4.65134900	-0.37505500
H	0.08921100	-1.94829400	3.21836500
H	3.30484100	0.31868300	1.59814400
H	-2.46995500	-2.03002000	4.89110900

H	-1.88975800	-0.71014500	3.83253100
H	-0.97181500	-1.15902600	5.28006400
H	-0.97105100	-4.25114700	4.98642900
H	0.44668900	-3.23743500	5.31745000
H	0.45857900	-4.37867100	3.95284400
H	5.67593700	2.26527300	1.42721100
H	4.02759800	2.60711100	1.99428200
H	4.30433400	2.21999800	0.29343400
H	4.63660400	-0.88855400	3.34881300
H	4.29821800	0.79413300	3.79808300
H	5.91683000	0.33678600	3.22212700
H	7.03895000	0.45288400	0.96356800
H	8.21750600	-1.00338200	-0.66300900
H	6.96707400	-2.70709400	-1.96223100
H	-0.82722900	-2.72855800	-1.55671700
H	3.21627400	-3.18058000	-1.70854400
H	-3.47110100	-4.03643600	-2.42050200
H	-2.33630000	-3.13344700	-3.43005000
H	-3.22776800	-2.29729100	-2.13278400
H	-1.55338200	-5.71319100	-1.69577700
H	0.00071400	-5.05680800	-1.14499900
H	-0.50495500	-4.84082300	-2.83681800
H	4.28352000	-2.19068100	-3.75166300
H	3.93278600	-3.92527000	-3.93388000
H	5.59325300	-3.38171100	-3.64637100
H	5.72918100	-4.95045000	-1.52214900
H	4.08830700	-5.50318300	-1.91815700
H	4.44888500	-4.86590900	-0.29899700
H	3.20157000	5.82765600	-0.24226500
H	3.20900900	6.03573000	2.23335000
H	1.59332000	4.71282800	3.58167500
H	0.92000100	3.61950800	-2.20198300
H	-3.33852300	0.32010900	1.74204900
H	3.84317200	4.55182000	-2.11387000
H	3.00576600	3.85942400	-3.51709100
H	3.27874700	2.86687200	-2.06302700
H	0.30940300	6.05597900	-1.99319400
H	1.22768400	5.71639200	-3.47745800
H	2.02290400	6.49680400	-2.09752200
H	-6.03170600	-0.49342600	3.00400700
H	-4.42899100	-0.56527600	3.74584500
H	-4.81549300	-1.64266600	2.39111700
H	-4.25309500	2.63943300	1.76044300
H	-4.26848200	1.95578000	3.39631900
H	-5.77927500	2.05086200	2.46109600
H	-6.94056800	-0.39530400	1.05339000
H	-7.92548100	-0.45022900	-1.22054800
H	-6.57929100	0.24458400	-3.18432400
H	-0.75394000	2.15417400	2.21424400
H	-2.95553900	1.25899700	-2.97179900
H	0.76474100	3.06873000	4.72085400
H	1.06003600	1.57911200	3.77087200



H	-0.48073900	1.81006100	4.61595200
H	-2.18425400	3.50445400	3.74630600
H	-1.86752200	4.41376000	2.25203000
H	-0.99125000	4.82239500	3.74370300
H	-3.73713900	-0.88977800	-4.07275300
H	-3.39869500	0.41295300	-5.24324500
H	-5.06784000	0.00308500	-4.82758600
H	-4.43452500	3.28749700	-3.00248100
H	-5.56139100	2.45684800	-4.09057400
H	-3.91887800	2.85014000	-4.64436600
O	1.13428100	0.18850300	1.67691600
O	-0.36922000	-0.01518400	1.88639900
C	-0.48641400	-0.15616600	-3.56461200
H	-1.31235700	-0.71129000	-3.99602700
C	0.91427700	-0.66746400	-3.66444400
H	1.05270600	-1.63818500	-4.14076000
O	0.12464200	-0.83312900	-2.37351300
H	-0.63677900	0.90778000	-3.40649800
C	2.10906800	0.25389800	-3.65751700
H	2.96437600	-0.22323700	-3.17002200
H	2.37996800	0.49445300	-4.69603000
H	1.88348300	1.17655700	-3.11824400

## 5.6 Structures with seven oxygen atoms

Peroxo  $\eta^2$ -Ozone ComplexFig. S67: NCCNO Peroxo  $\eta^2$ -Ozone Complex

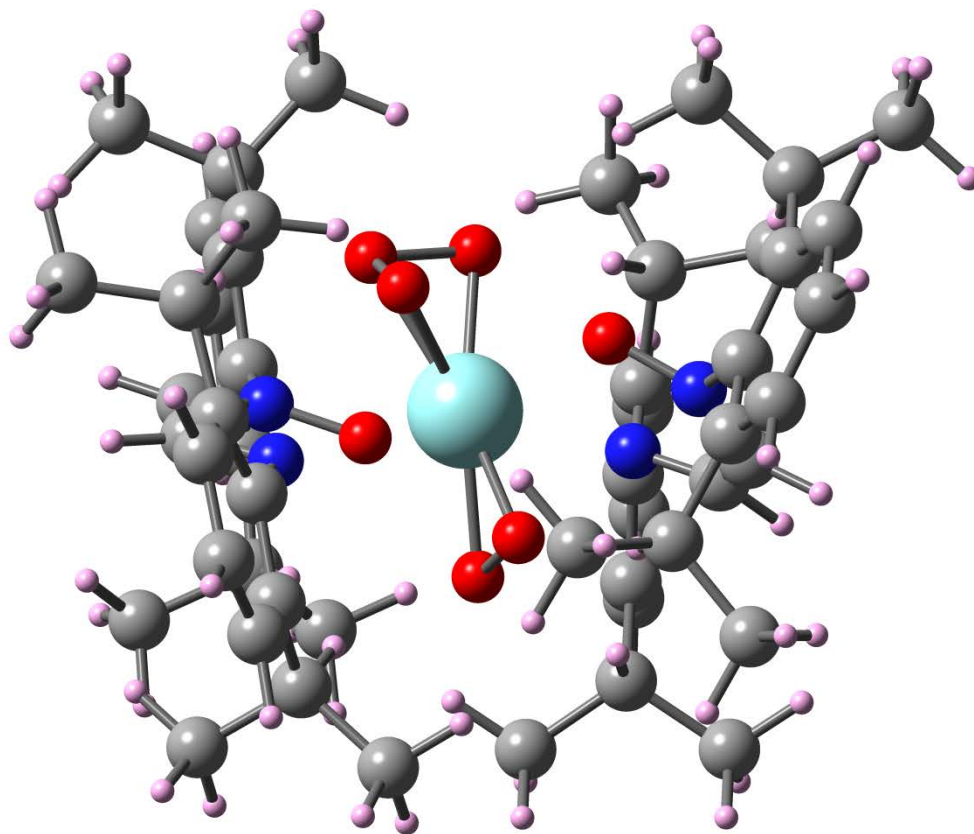
SCF	$E_{ZP}$	H	G
-2816.565471	-2815.407322	-2815.334599	-2815.519456

Zr	-0.00032300	0.00080700	0.24429300
O	-2.21780200	0.30451400	-0.12929600
O	2.21790100	-0.30629500	-0.12959800
O	-0.00986400	1.16549300	-1.63786400
N	0.17269000	-2.41526900	0.58455500
N	2.84133000	-1.38147000	-0.61518600
N	-0.17517200	2.41906600	0.57788500
N	-2.84161900	1.37747500	-0.62078100
C	1.15375900	-3.10586200	0.07212100
C	2.36266000	-2.61683800	-0.56637500
C	-1.15481100	3.10623800	0.05795000
C	-2.36287600	2.61296200	-0.57876500
C	-0.89041600	-3.17859500	1.25039500
C	-0.82683700	-3.33695600	2.66187600
C	-1.85345600	-4.07650200	3.28325000

C	-2.90572800	-4.63349600	2.54007200
C	-2.93924100	-4.46776600	1.14902500
C	-1.93624000	-3.74182300	0.46898200
C	-0.12636400	-2.09220000	4.78715500
C	0.34112000	-2.79939600	3.49353500
C	1.34089400	-3.94406600	3.81679600
C	5.28416300	0.53996600	1.77013800
C	5.08189800	-0.89060200	1.20306300
C	6.04163600	-1.90122700	1.88226500
C	4.16221200	-1.11735100	-1.20881700
C	5.24196000	-0.89215800	-0.32084100
C	6.50082800	-0.64389600	-0.90551600
C	6.65778000	-0.62114000	-2.30111200
C	5.55686400	-0.83337500	-3.14512400
C	4.26933500	-1.07684800	-2.61932300
C	-3.36691900	-3.07042500	-1.53756200
C	-2.00346800	-3.62910300	-1.05924700
C	-1.71421400	-5.00343900	-1.72223200
C	2.89577700	-0.04772000	-4.49632400
C	3.07505200	-1.27029900	-3.56044900
C	3.22286500	-2.57814600	-4.38279600
C	0.88741700	3.18725600	1.23873400
C	1.92830000	3.75455600	0.45360700
C	2.93009000	4.48578900	1.12992400
C	2.90015200	4.65309100	2.52075500
C	1.85259700	4.09220300	3.26773500
C	0.82750300	3.34736700	2.65030500
C	3.35409300	3.06447600	-1.54828300
C	1.99507900	3.63835400	-1.07443600
C	1.71978600	5.01310100	-1.74192500
C	-5.27926400	-0.53324700	1.77035800
C	-5.08388400	0.89641400	1.19809800
C	-6.04888200	1.90473600	1.87285900
C	-4.16166700	1.10943900	-1.21390200
C	-5.24253100	0.89009200	-0.32593600
C	-6.50059800	0.63736400	-0.91065000
C	-6.65548700	0.60445700	-2.30622100
C	-5.55330900	0.81065000	-3.15022900
C	-4.26679400	1.05854200	-2.62433500
C	0.13437600	2.10819800	4.78163300
C	-0.33696200	2.80760700	3.48523500
C	-1.34204400	3.94888800	3.80425100
C	-2.89307700	0.02502600	-4.50015500
C	-3.07112300	1.24776600	-3.56451700
C	-3.21546100	2.55567500	-4.38757600
H	1.11844400	-4.19780500	0.12492100
H	3.01296000	-3.36506500	-1.00363400
H	-1.11878400	4.19858700	0.10168400
H	-3.01271200	3.35861400	-1.02111600
H	-1.82754300	-4.21503400	4.36056500
H	-3.68930100	-5.19717500	3.04148600
H	-3.75116600	-4.90915100	0.57654800

H	0.85871400	-2.03328800	2.90986300
H	4.05787600	-1.18450600	1.45738600
H	-0.62274000	-2.77850500	5.48743700
H	-0.80989500	-1.27603500	4.53354100
H	0.74049600	-1.65997500	5.30470700
H	0.86587100	-4.72758000	4.42365100
H	2.19827700	-3.55155100	4.38023900
H	1.72395600	-4.42060600	2.90291300
H	6.29601900	0.91175400	1.55930400
H	5.14073700	0.53656200	2.85799700
H	4.55948900	1.23786500	1.33736200
H	5.89722400	-2.91826600	1.49466100
H	5.85919000	-1.91933500	2.96430900
H	7.09352600	-1.62822500	1.72753500
H	7.36048600	-0.46782400	-0.26475100
H	7.63833300	-0.43052800	-2.73086200
H	5.69189700	-0.79775300	-4.22259200
H	-1.24502400	-2.92022700	-1.40361000
H	2.15339800	-1.34223200	-2.97529700
H	-4.20241700	-3.73270200	-1.27331300
H	-3.36196300	-2.96168400	-2.63045600
H	-3.55444500	-2.08382600	-1.09945000
H	-2.46508200	-5.75258900	-1.43576000
H	-0.72943000	-5.39361500	-1.43008900
H	-1.72995400	-4.90775700	-2.81624300
H	2.74496100	0.86663200	-3.91270800
H	2.00603200	-0.19183500	-5.12088800
H	3.76107400	0.09440200	-5.15823100
H	4.11058600	-2.54878900	-5.02885600
H	2.34269100	-2.71836900	-5.02277700
H	3.31186300	-3.45946500	-3.73298100
H	3.73825500	4.93010500	0.55435200
H	3.68268100	5.22095700	3.01906100
H	1.82896100	4.23225700	4.34488700
H	1.23110200	2.93528200	-1.41810300
H	-4.06146400	1.19636500	1.45197500
H	4.19574400	3.71741400	-1.28022100
H	3.35217800	2.95585600	-2.64124900
H	3.52872500	2.07575700	-1.10966900
H	0.73948500	5.41452500	-1.44992100
H	1.73337800	4.91289100	-2.83553900
H	2.47871100	5.75565300	-1.45975000
H	-6.28901200	-0.91081200	1.55972100
H	-5.13684600	-0.52528300	2.85833300
H	-4.55056600	-1.22891900	1.34075200
H	-5.90873600	2.92111700	1.48193200
H	-5.86745900	1.92735600	2.95497900
H	-7.09942500	1.62656400	1.71829700
H	-7.36105600	0.46547700	-0.26982300
H	-7.63534700	0.41040500	-2.73601300
H	-5.68670100	0.76670500	-4.22760200
H	-0.85135300	2.03682700	2.90488500

H	-2.14998000	1.31786700	-2.97839700
H	0.62741400	2.79979600	5.47905700
H	0.82188300	1.29425400	4.53151000
H	-0.73030700	1.67402800	5.30118400
H	-2.19688100	3.55461700	4.37034200
H	-1.72841000	4.41921900	2.88855300
H	-0.87027100	4.73754600	4.40699700
H	-2.74580700	-0.89000100	-3.91661500
H	-2.00165100	0.16737100	-5.12273800
H	-3.75703600	-0.11499500	-5.16424500
H	-3.30322100	3.43758800	-3.73841100
H	-4.10290600	2.52757800	-5.03408100
H	-2.33449600	2.69392600	-5.02690200
O	0.77215000	0.05212100	2.15161600
O	-0.77033100	-0.04664700	2.15312400
O	0.00700300	-0.00056800	-2.57386300
O	0.01342000	-1.16683200	-1.63685400

Peroxo  $\eta^3$ -Ozone ComplexFig. S68: NCCNO Peroxo  $\eta^3$ -Ozone Complex

SCF	$E_{ZP}$	H	G
-2816.5525653	-2815.394732	-2815.322332	-2815.504574

Zr	0.19934600	0.09377000	-0.12801100
O	-2.07463400	0.30494600	0.12604800
O	2.15678600	-1.02440500	-0.78727500
O	1.01840800	1.11189300	-1.86914100
N	0.13650200	-2.20142600	0.82179900
N	3.00378600	-1.69733800	0.00102000
N	-0.28165800	2.61174300	0.01669700
N	-2.91190300	1.15353700	-0.48610600
C	1.21819400	-2.74959100	1.32505400
C	2.59273500	-2.44457300	1.01346700
C	-1.40179300	3.12802500	-0.41056400
C	-2.62805300	2.42231400	-0.72576600
C	-1.12067200	-2.84373900	1.20834700
C	-1.57624800	-2.79585600	2.55703100
C	-2.78457100	-3.46256000	2.86099300
C	-3.50806200	-4.15524000	1.88217800
C	-3.02573600	-4.20608600	0.56447500

C	-1.82638600	-3.56320800	0.20036100
C	-1.72254200	-0.97913600	4.33625400
C	-0.83648100	-2.07447700	3.69175400
C	-0.34071400	-3.08006900	4.76552900
C	5.05452100	1.54359300	1.44203200
C	4.76817800	0.03258700	1.64332300
C	5.39610500	-0.47641900	2.96757200
C	4.42483600	-1.58951500	-0.35498900
C	5.26744400	-0.78110300	0.44421200
C	6.62786300	-0.72175700	0.06846200
C	7.10050300	-1.41025000	-1.05818800
C	6.22203700	-2.17191700	-1.84726500
C	4.85644900	-2.27968900	-1.51600100
C	-2.32708500	-3.90776900	-2.30048200
C	-1.24835700	-3.73744000	-1.20784000
C	-0.27197500	-4.94779000	-1.23776200
C	3.49433100	-2.19482200	-3.64116300
C	3.89291700	-3.06193800	-2.41410400
C	4.46608600	-4.43025900	-2.85696700
C	0.80278400	3.56401000	0.27460600
C	1.42156800	4.26078100	-0.80586900
C	2.47967000	5.14205300	-0.48941700
C	2.89404000	5.35162900	0.83176400
C	2.23550800	4.69004300	1.87900600
C	1.18147500	3.78993000	1.62904800
C	2.19210300	3.74097300	-3.18812100
C	1.00380700	4.14247800	-2.27909700
C	0.36011600	5.46783200	-2.77318500
C	-5.27964900	-0.43800600	2.63315900
C	-4.84514000	0.68216700	1.65810600
C	-5.52146800	2.03004500	2.03664900
C	-4.22971600	0.60376800	-0.85458900
C	-5.14487300	0.33765600	0.19501600
C	-6.39775700	-0.19085300	-0.17345400
C	-6.70979700	-0.44245600	-1.51978900
C	-5.77800500	-0.16100700	-2.52864100
C	-4.50523400	0.37156500	-2.22534900
C	1.30248200	2.67432900	3.93804600
C	0.39542000	3.19666000	2.80055500
C	-0.61687900	4.24742600	3.33702200
C	-3.26099900	-0.53826900	-4.26643400
C	-3.53055900	0.69237700	-3.36578200
C	-4.05846100	1.88646600	-4.20818000
H	1.11078300	-3.57355400	2.03523000
H	3.36732800	-2.94695700	1.57934400
H	-1.47810600	4.20807500	-0.55942400
H	-3.42744800	2.99473400	-1.17979100
H	-3.15695600	-3.43642700	3.88233000
H	-4.43449700	-4.66162800	2.14382800
H	-3.58229400	-4.75902700	-0.18567600
H	0.02320300	-1.54232400	3.27827000
H	3.68100200	-0.06178400	1.72839100

H	-2.62586000	-1.39896300	4.80040400
H	-2.01861600	-0.24433300	3.58018800
H	-1.15582200	-0.45031900	5.11402300
H	-1.17812300	-3.59647400	5.25400200
H	0.22749600	-2.55241400	5.54319600
H	0.31181300	-3.85134700	4.33260200
H	6.13196600	1.75494700	1.40327500
H	4.62408800	2.11540600	2.27314400
H	4.59581100	1.90966500	0.51646100
H	5.16572600	-1.53593100	3.14536500
H	5.00355900	0.10110000	3.81419500
H	6.48928200	-0.36935100	2.96300900
H	7.31408100	-0.11762900	0.65556700
H	8.15134000	-1.34474000	-1.33044600
H	6.60012900	-2.68496700	-2.72656500
H	-0.67541900	-2.83981000	-1.46113600
H	2.96923900	-3.25797300	-1.85646400
H	-2.83729100	-4.87856600	-2.23032000
H	-1.85718300	-3.85286400	-3.29042400
H	-3.08160200	-3.11548600	-2.23845400
H	-0.79998900	-5.88117100	-0.99834000
H	0.54600800	-4.82915500	-0.51602500
H	0.17147800	-5.05097100	-2.23713800
H	3.00557100	-1.27105600	-3.31593300
H	2.79171400	-2.74633900	-4.27969000
H	4.37748500	-1.93959300	-4.24301900
H	5.33463100	-4.31465700	-3.51808300
H	3.70328200	-4.98678900	-3.41658900
H	4.77308500	-5.03998100	-1.99693300
H	2.97987900	5.67167200	-1.29590300
H	3.71165600	6.03643900	1.04508100
H	2.53581200	4.87958600	2.90558800
H	0.27165500	3.33888600	-2.38260800
H	-3.76315800	0.79986200	1.77569900
H	3.00090400	4.48348700	-3.16407600
H	1.85124500	3.64917900	-4.22833300
H	2.58479200	2.76838300	-2.87767400
H	-0.50706600	5.75786000	-2.16254300
H	0.02488900	5.36119600	-3.81378500
H	1.07810600	6.29779000	-2.73537300
H	-6.36966600	-0.56977900	2.64638900
H	-4.96680400	-0.18103100	3.65311500
H	-4.81541600	-1.39339400	2.36623400
H	-5.19068600	2.84841000	1.38340700
H	-5.27316000	2.30089600	3.07096400
H	-6.61426700	1.95701000	1.95644800
H	-7.13258300	-0.40717800	0.59610600
H	-7.68160300	-0.85432600	-1.78116400
H	-6.03389200	-0.35991000	-3.56534800
H	-0.16002600	2.32718200	2.44006700
H	-2.55908500	0.97454800	-2.95240500
H	1.88715900	3.47413700	4.41446700



H	1.98159400	1.91036600	3.54643600
H	0.68339200	2.20851700	4.71648800
H	-1.21975800	3.81410700	4.14666600
H	-1.30195200	4.59037800	2.54850400
H	-0.09825800	5.13119900	3.73423700
H	-2.79175100	-1.33830000	-3.68785800
H	-2.56403400	-0.25928300	-5.06645600
H	-4.17832700	-0.92077400	-4.73389300
H	-4.22523100	2.78222600	-3.59355700
H	-5.00969700	1.64030300	-4.69838800
H	-3.33161900	2.14204800	-4.98936400
O	1.52587700	0.39428900	1.45671200
O	0.08246600	0.26123800	1.94562700
O	-0.41729400	0.69540800	-2.20230500
O	-0.47768300	-0.81923300	-2.00005900

**Peroxo  $\eta^3$ -Ozone Complex (higher energy conformation with one octahedral-like coordination)**

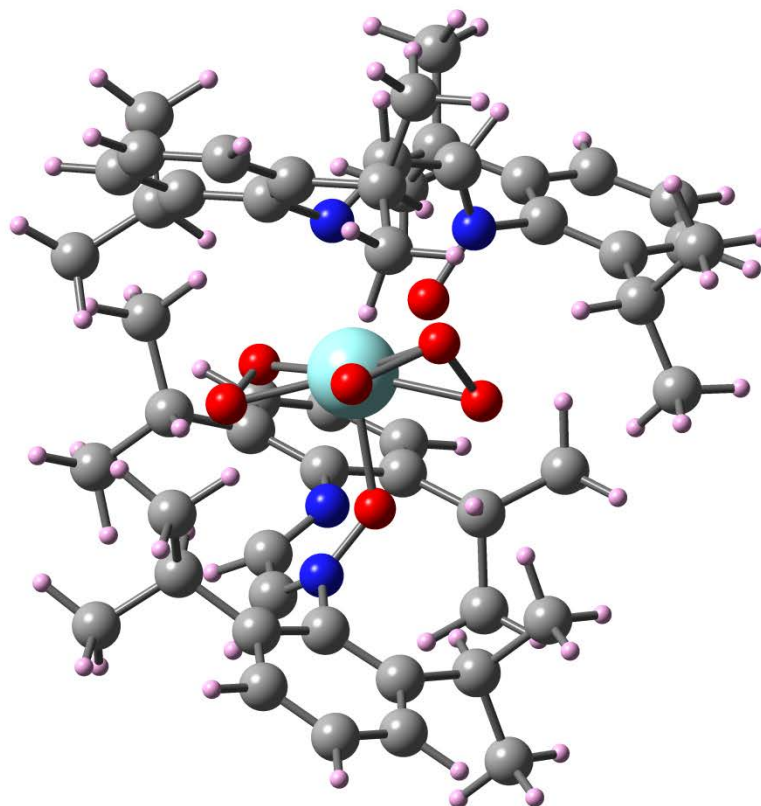


Fig. S69: NCCNO Peroxo  $\eta^3$ -Ozone Complex (higher energy conformation with one octahedral-like coordination)

SCF	E <sub>ZP</sub>	H	G
-2816.5490885	-2815.392746	-2815.319483	-2815.506813

Zr	0.91591300	0.25208000	-0.20969200
O	-1.15060700	1.11001300	-0.52329400
O	0.70700400	-1.91956300	-0.62415800
O	2.82888800	0.54831100	-1.05134300
N	-1.50772100	-2.53961600	1.18920400
N	1.22797300	-2.99686300	0.00467500
N	1.16878900	2.71081100	0.17721300
N	-1.58139400	2.25692300	-1.05192700
C	-0.55277900	-3.22621600	1.73927900
C	0.68972800	-3.56660100	1.06370400
C	0.38648800	3.60715700	-0.37110700
C	-0.89241000	3.38864500	-1.01147100
C	-2.74407700	-2.27595800	1.82667000
C	-2.86660300	-1.84390200	3.18763800
C	-4.16871700	-1.67196100	3.70284200

C	-5.30992900	-1.89366800	2.91744700
C	-5.17102100	-2.24758500	1.56396700
C	-3.89965900	-2.42281200	0.99034900
C	-1.79772700	-0.03274300	4.62312100
C	-1.66785600	-1.47715800	4.07433500
C	-1.49028100	-2.48596100	5.24007400
C	4.89711000	-1.46548000	1.00245000
C	3.92540900	-2.64700100	1.26716900
C	4.45333900	-3.55799000	2.40560100
C	2.42151600	-3.57467400	-0.64307200
C	3.68604300	-3.44028600	-0.02171600
C	4.78044000	-4.04637200	-0.67782700
C	4.61719100	-4.71855100	-1.89682300
C	3.35141300	-4.79413500	-2.50088200
C	2.21876400	-4.22082300	-1.88967200
C	-4.79100800	-2.20268500	-1.41116500
C	-3.73930700	-2.83916200	-0.47349200
C	-3.76168500	-4.38791700	-0.60444200
C	0.83457400	-3.25491100	-3.76717300
C	0.85768300	-4.27102200	-2.59144100
C	0.49453600	-5.69807700	-3.07303600
C	2.41233200	3.22173900	0.75901800
C	3.40592300	3.81021400	-0.07846800
C	4.57879000	4.28910300	0.54356100
C	4.76321500	4.20277000	1.92941800
C	3.76407100	3.63049600	2.73085100
C	2.57383000	3.12689900	2.17040000
C	4.48017200	3.19507900	-2.30661100
C	3.30429800	3.92521200	-1.60639400
C	3.23448800	5.41092400	-2.05278300
C	-4.69425100	1.95627700	1.58104400
C	-3.86038600	2.90542200	0.68217300
C	-4.23223700	4.38885400	0.94747200
C	-2.93235400	2.21922500	-1.63959200
C	-4.02206500	2.55224400	-0.79999800
C	-5.30233700	2.53757700	-1.39185900
C	-5.46954200	2.19281200	-2.74289800
C	-4.36276200	1.84075000	-3.53132400
C	-3.05726000	1.83463100	-2.99506100
C	1.97790100	1.70787800	4.22015300
C	1.45670900	2.61839200	3.08483500
C	0.65705800	3.82242700	3.65788200
C	-2.05866200	0.03689100	-4.49393300
C	-1.86004800	1.43829100	-3.86236900
C	-1.59159500	2.50529500	-4.95684000
H	-0.64715200	-3.68836300	2.72909500
H	1.24951100	-4.41136100	1.45254500
H	0.68724300	4.65724100	-0.35857400
H	-1.37657600	4.23982800	-1.47338900
H	-4.28973600	-1.34993200	4.73412300
H	-6.30021000	-1.77046700	3.35017000
H	-6.05849700	-2.38170100	0.95232600

H	-0.75989700	-1.47007500	3.46443200
H	2.98715500	-2.19341200	1.60019000
H	-2.68013400	0.09266300	5.26466200
H	-1.85621900	0.68306300	3.79544900
H	-0.91027500	0.21566300	5.21913900
H	-2.36253200	-2.47822200	5.90789700
H	-0.60603500	-2.22596600	5.83703600
H	-1.36657000	-3.51590300	4.87797700
H	5.89853800	-1.81851200	0.71921300
H	4.99323900	-0.85661800	1.91019200
H	4.51886000	-0.81853400	0.20259600
H	3.75546600	-4.37705900	2.63033500
H	4.59086200	-2.96875900	3.32131600
H	5.42138800	-4.00817900	2.14756900
H	5.76976800	-3.96929300	-0.23556100
H	5.47743200	-5.17024100	-2.38529800
H	3.24249100	-5.29979700	-3.45605700
H	-2.74611300	-2.50001600	-0.79029200
H	0.08091200	-3.95306500	-1.88722300
H	-5.80462100	-2.57721800	-1.21250100
H	-4.55282800	-2.44802100	-2.45482400
H	-4.80415800	-1.10968100	-1.31502300
H	-4.73006900	-4.79481100	-0.28189600
H	-2.97854600	-4.85014300	0.00941500
H	-3.59676900	-4.68721000	-1.64853800
H	1.02247400	-2.23703800	-3.40810200
H	-0.14782200	-3.27468000	-4.25944800
H	1.59540400	-3.50868800	-4.51845800
H	1.17692200	-6.05129600	-3.85677700
H	-0.51853100	-5.70014100	-3.49638600
H	0.52197000	-6.42339300	-2.24893400
H	5.35992200	4.72570400	-0.07318300
H	5.67693200	4.58047100	2.38240800
H	3.90603900	3.57859700	3.80618600
H	2.39647600	3.42326200	-1.95093000
H	-2.81197500	2.76660900	0.97080300
H	5.44786100	3.65298700	-2.06120300
H	4.35184300	3.24229500	-3.39631300
H	4.49679300	2.14240000	-2.00929500
H	2.38155200	5.93820100	-1.60137000
H	3.13661900	5.47389200	-3.14480700
H	4.14364100	5.95558200	-1.76626100
H	-5.77061800	2.06823900	1.39578100
H	-4.51146700	2.18634500	2.63845900
H	-4.42513500	0.90807600	1.41150000
H	-3.61698900	5.07497500	0.35015200
H	-4.08387300	4.63305700	2.00716200
H	-5.28402700	4.58344200	0.70106700
H	-6.17126900	2.78864500	-0.78993800
H	-6.46566100	2.18939100	-3.17880800
H	-4.51067400	1.56005900	-4.57028500
H	0.76966400	2.00210900	2.49821900

H	-0.96139900	1.35563400	-3.24319300
H	2.65371100	2.23421400	4.90823600
H	2.49340500	0.84186400	3.79277600
H	1.12944400	1.33648300	4.80879200
H	-0.17597700	3.46290300	4.27708100
H	0.24037400	4.45008000	2.85704800
H	1.29559000	4.46174100	4.28332000
H	-2.25745400	-0.71446000	-3.72048400
H	-1.14124500	-0.25788000	-5.01631100
H	-2.88675900	0.02322700	-5.21610600
H	-1.40292200	3.49548300	-4.51983600
H	-2.44301400	2.59848300	-5.64465000
H	-0.70890500	2.22157400	-5.54309800
O	1.73524500	-0.35096200	1.57787600
O	0.22600300	-0.00961600	1.71886500
O	1.86119100	1.17907100	-2.09689600
O	0.85531600	0.10579300	-2.43202500

## Planar Bisperoxo Complex with Adsorbed Propylene Oxide

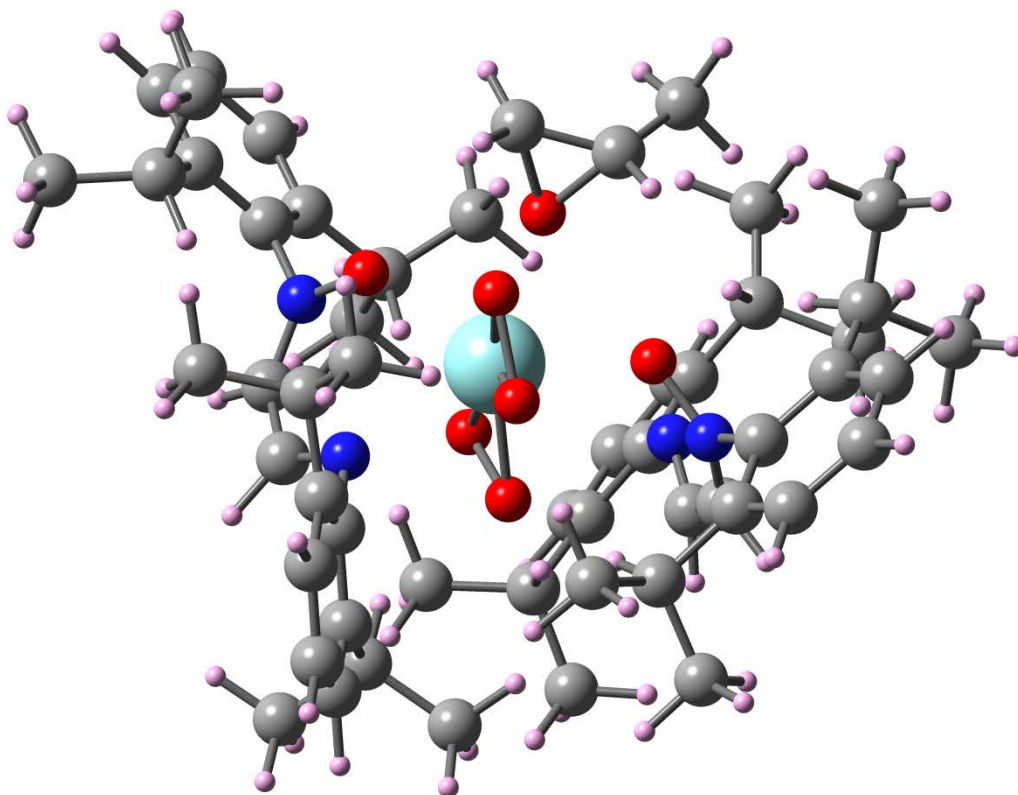


Fig. S70: NCCNO Planar Bisperoxo Complex with Adsorbed Propylene Oxide

SCF	E <sub>ZP</sub>	H	G
-2934.4941137	-2933.252394	-2933.175107	-2933.367590

Zr	-0.33545000	0.61000200	-0.64962400
O	-2.34393400	-0.40260400	-1.15210500
O	1.88264100	0.34344300	-1.08765800
O	-0.66678100	1.87217900	-2.26519000
N	2.58386500	-1.79051100	0.95606800
N	2.87320600	0.96226100	-0.38920500
N	-2.15586700	1.54715000	0.84094100
N	-3.08770900	-1.08046100	-0.24613300
C	3.01528400	-0.69324800	1.49929100
C	3.33017900	0.52420900	0.76675900
C	-2.94079300	0.69555300	1.44933700
C	-3.28390200	-0.62856300	0.98123400
C	2.41102600	-2.99621200	1.68479200
C	1.80733000	-3.07780600	2.98205000
C	1.72706600	-4.35081700	3.58703100
C	2.20575300	-5.50583100	2.95152400
C	2.75489100	-5.41693500	1.66046500
C	2.85384800	-4.17846600	1.00312900

C	-0.26762200	-2.13080900	4.13426000
C	1.20527200	-1.87577500	3.72526400
C	2.05724300	-1.50997000	4.97143200
C	1.42165200	4.86610100	0.49545700
C	2.43115500	3.71827300	0.74370300
C	3.34004200	4.04967600	1.96088900
C	3.49720800	2.13695600	-1.03280700
C	3.28425400	3.43014300	-0.49646500
C	3.93957600	4.50140000	-1.14339400
C	4.75225100	4.29233200	-2.26512000
C	4.94145300	2.99507400	-2.76724900
C	4.31869400	1.88583400	-2.16230000
C	3.25860000	-5.30458500	-1.27912900
C	3.48705100	-4.06372400	-0.38606500
C	5.00724100	-3.76122300	-0.26581100
C	4.47842700	0.37466000	-4.22069500
C	4.60713200	0.47150700	-2.68016600
C	6.01826100	0.00758800	-2.22368800
C	-2.12096200	2.90372000	1.36060000
C	-2.55271600	3.94180700	0.48545100
C	-2.57154300	5.25963600	0.98109600
C	-2.16898200	5.55065700	2.29390100
C	-1.73909200	4.51537400	3.13493800
C	-1.70487400	3.17269200	2.69778100
C	-2.62021800	4.65082000	-1.97977700
C	-3.09463000	3.63873000	-0.91329000
C	-4.64639600	3.55659600	-0.87068300
C	-0.69205900	-4.20684500	-0.72058600
C	-1.79780700	-3.70605500	0.24575400
C	-1.93735600	-4.65263500	1.46576400
C	-3.73508800	-2.29784700	-0.74567600
C	-3.12484700	-3.54984100	-0.50101600
C	-3.78429300	-4.68856400	-1.01496900
C	-4.97633800	-4.57056600	-1.74481800
C	-5.54004500	-3.30639000	-1.98541000
C	-4.92939800	-2.13566900	-1.49219700
C	0.22590500	2.41726100	4.18085000
C	-1.20478300	2.10030000	3.67709600
C	-2.17647100	1.93519800	4.87641900
C	-5.33413500	-0.41939700	-3.30784000
C	-5.52883900	-0.76099700	-1.80602800
C	-7.02168300	-0.66727600	-1.40145500
H	3.30897100	-0.63071700	2.55326900
H	4.08175500	1.16654400	1.21606200
H	-3.47082500	0.98889300	2.35915100
H	-3.88171000	-1.26140000	1.62655600
H	1.27782300	-4.43795400	4.57314500
H	2.14025700	-6.46938500	3.45185200
H	3.10142600	-6.31885800	1.16455100
H	1.16960500	-1.01551900	3.05299600
H	1.83911100	2.82942400	0.98494700
H	-0.37571100	-2.98730400	4.81318500

H	-0.87518300	-2.30058300	3.24003900
H	-0.66510000	-1.24448500	4.64775100
H	2.06338200	-2.32996300	5.70232800
H	1.64539400	-0.61983300	5.46576000
H	3.10321700	-1.29997400	4.70827300
H	1.92682900	5.82654900	0.32328700
H	0.77292200	4.98318300	1.37208000
H	0.78830900	4.62363300	-0.36222900
H	4.04417900	3.23831000	2.19388800
H	2.72421900	4.22819800	2.85133800
H	3.93163700	4.95544100	1.77172000
H	3.79662900	5.51000500	-0.76767900
H	5.23909000	5.13692600	-2.74693000
H	5.58187400	2.84376600	-3.63162600
H	3.02093200	-3.19627400	-0.86937700
H	3.87192500	-0.21487800	-2.24903300
H	3.79935200	-6.18612000	-0.90908400
H	3.62556000	-5.10383800	-2.29483100
H	2.19383900	-5.56043500	-1.34726300
H	5.53083500	-4.58611700	0.23670700
H	5.18396500	-2.84502200	0.31028800
H	5.45466200	-3.63029300	-1.26115100
H	3.49992100	0.73474100	-4.56078000
H	4.59618900	-0.66821200	-4.54331100
H	5.24969800	0.96440800	-4.73211600
H	6.80004600	0.65580700	-2.64119300
H	6.21060500	-1.01972500	-2.56071200
H	6.11276400	0.02791500	-1.13033600
H	-2.90504400	6.06485500	0.33295800
H	-2.19082700	6.57554100	2.65765900
H	-1.42285100	4.74892900	4.14872800
H	-2.70864600	2.66707700	-1.22970500
H	-1.46519500	-2.73187000	0.61953600
H	-2.99119600	5.66849100	-1.79228900
H	-2.98478500	4.34135100	-2.96812400
H	-1.52678700	4.66075700	-2.01703600
H	-4.99138100	2.80582300	-0.14527400
H	-5.03907300	3.28276000	-1.85984500
H	-5.08647200	4.52243300	-0.58545800
H	-0.94884100	-5.18489600	-1.15141800
H	0.25179200	-4.30681800	-0.17373900
H	-0.53599700	-3.48858500	-1.53339400
H	-2.70572000	-4.29854200	2.16644500
H	-0.98352600	-4.70639000	2.00339200
H	-2.20728800	-5.67212700	1.15914300
H	-3.35384300	-5.67162000	-0.84547400
H	-5.46405500	-5.46216700	-2.13184500
H	-6.45867500	-3.22873000	-2.56059200
H	-1.12188800	1.14687600	3.14936900
H	-4.98531100	0.00276400	-1.23912900
H	0.27294300	3.37083600	4.72374700
H	0.91898000	2.45509600	3.33455800



H	0.56730200	1.62609500	4.86272300
H	-1.82715400	1.13591600	5.54458900
H	-3.19469600	1.68299900	4.54868300
H	-2.24424400	2.85935400	5.46596600
H	-4.26970200	-0.42600500	-3.56794300
H	-5.73330300	0.58004700	-3.52389900
H	-5.85485200	-1.14130000	-3.95109300
H	-7.16496600	-0.89627300	-0.33749000
H	-7.64430000	-1.36060400	-1.98129500
H	-7.39625700	0.34773000	-1.58596100
O	0.32663300	0.64173800	1.35120400
O	-0.33721900	-0.69933800	1.05091600
O	-0.06816900	2.60951000	-1.02560200
O	-0.05802300	-0.96787900	-2.39977500
C	-0.73076000	-0.73744300	-3.73574500
H	-1.26623800	-1.61503200	-4.08855700
H	-1.24136400	0.21890500	-3.79452400
C	0.75907000	-0.75698000	-3.66044800
H	1.25485100	0.20973300	-3.64081900
C	1.57540600	-1.95179400	-4.08632600
H	1.92025400	-1.82215000	-5.12107600
H	2.45383300	-2.05984100	-3.44052400
H	0.98465700	-2.87280800	-4.02626100

## Catalyst Deformation Product with Oxygen Added to Ligand

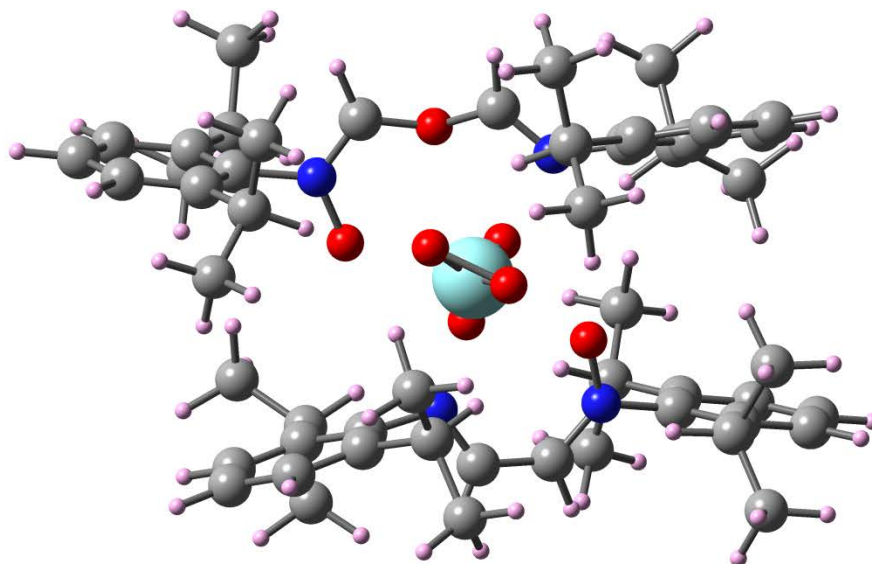


Fig. S71: NCCNO Catalyst Deformation Product with Oxygen Added to Ligand

SCF	E <sub>ZP</sub>	H	G
-2816.5979503	-2815.440310	-2815.367332	-2815.552206

Zr	-0.01827800	-0.01882000	-0.23852600
O	2.17223900	-0.55365500	0.28389400
O	-2.27668200	-0.20837300	-0.94822100
O	0.23269300	-1.72744100	-1.42993200
O	0.61056500	-0.43582400	-2.17360100
N	0.91309400	2.42105300	-0.87569600
N	-3.02832100	0.90939500	-1.16133800
N	-0.26554700	-1.90935300	1.23140700
N	2.66045500	-1.79396900	0.32101800
C	-0.18520200	2.96219500	-1.20670200
C	-2.48196900	2.05462200	-1.48947100
C	0.65342600	-2.82878400	1.35274000
C	1.99294300	-2.83146300	0.79627700
C	2.08184500	3.16077200	-0.47356600
C	2.05364800	4.04160900	0.64254400
C	3.24566000	4.73466500	0.94918300
C	4.41385200	4.55265600	0.19631600
C	4.42029100	3.65356700	-0.88395700
C	3.26165900	2.93674000	-1.23904000
C	1.13717600	3.97770200	3.01897600
C	0.81844100	4.25166600	1.52774000
C	0.23573400	5.67896800	1.34179700
C	-4.92915800	0.95555300	2.62406400
C	-4.41736400	1.62413900	1.32510100
C	-4.54342600	3.16915000	1.43281300
C	-4.48675700	0.77110800	-1.11395200

C	-5.15643100	1.11149100	0.08462600
C	-6.56329500	0.99113000	0.07524600
C	-7.24474700	0.53960000	-1.06587700
C	-6.53863200	0.19147400	-2.22990500
C	-5.13374300	0.29372500	-2.28043900
C	4.60328000	1.33987900	-2.74158900
C	3.23702900	2.00002300	-2.45048000
C	2.73741600	2.76099800	-3.71142500
C	-4.83218200	-1.38456700	-4.19237500
C	-4.35919800	-0.05375600	-3.55726100
C	-4.46318200	1.10561000	-4.58671400
C	-1.52078100	-2.18564100	1.94262200
C	-2.48782300	-3.01547900	1.31421600
C	-3.65080500	-3.32563900	2.05130700
C	-3.84180800	-2.83414800	3.35178300
C	-2.87266900	-2.00540100	3.93778500
C	-1.69419600	-1.65370800	3.24664100
C	-3.54373500	-3.44795500	-0.97637000
C	-2.28528700	-3.60145000	-0.08907500
C	-1.86810700	-5.09599700	-0.00711400
C	5.20718900	0.68803400	2.00999900
C	4.82129900	-0.81429000	2.04653500
C	5.56239100	-1.55402200	3.19038100
C	4.04689300	-1.94818100	-0.15227700
C	5.08225000	-1.47242000	0.68789600
C	6.40135000	-1.62242400	0.21306200
C	6.65703300	-2.21450900	-1.03478800
C	5.59896400	-2.66245400	-1.84053800
C	4.25558100	-2.53304600	-1.42504900
C	-1.24197100	0.52490600	4.50390800
C	-0.63606600	-0.77588800	3.92327000
C	0.11928800	-1.57906200	5.01647700
C	3.19609400	-2.41114200	-3.74524900
C	3.11364800	-3.02217000	-2.32423900
C	3.10774400	-4.57353900	-2.39580400
H	-0.47320100	4.01162100	-1.23721000
H	-3.07927300	2.94416600	-1.63926300
H	0.42846600	-3.72630100	1.93477000
H	2.53981000	-3.76570500	0.81848000
H	3.25711300	5.41657200	1.79567000
H	5.31788000	5.10035900	0.45318000
H	5.33404200	3.50801500	-1.45172800
H	0.05539400	3.51537900	1.26056000
H	-3.35095200	1.38283500	1.24142500
H	1.90403500	4.65774100	3.41450500
H	1.47372800	2.94288100	3.13582200
H	0.22850500	4.10705200	3.62247000
H	0.95603300	6.44776300	1.65299300
H	-0.67089300	5.80167800	1.94961500
H	-0.02461300	5.88435700	0.29285500
H	-5.96589700	1.23812100	2.85347500
H	-4.30360700	1.27135000	3.46771000

H	-4.87159700	-0.13601000	2.55649500
H	-4.14152500	3.67602700	0.54492100
H	-3.98275900	3.52871400	2.30439900
H	-5.59252000	3.47500300	1.54646400
H	-7.12487700	1.24365500	0.96964900
H	-8.32881700	0.45447600	-1.04773900
H	-7.08115300	-0.16630000	-3.10016700
H	2.51539000	1.19898200	-2.24559300
H	-3.30249800	-0.18597700	-3.29915900
H	5.35508200	2.07181700	-3.06828600
H	4.49293300	0.60539100	-3.54896000
H	4.99198100	0.81532200	-1.86027000
H	3.42863700	3.57287200	-3.97820500
H	1.74380300	3.19804800	-3.55190900
H	2.66524400	2.07332700	-4.56400800
H	-4.78457100	-2.20612400	-3.46924000
H	-4.18373200	-1.64005100	-5.04000700
H	-5.86052400	-1.31672900	-4.57143500
H	-5.50561400	1.26915600	-4.89140000
H	-3.87705100	0.86954100	-5.48399800
H	-4.08168300	2.04903800	-4.17410400
H	-4.41085600	-3.95921400	1.60212700
H	-4.74119700	-3.09532700	3.90504800
H	-3.03040400	-1.62577200	4.94397300
H	-1.48462900	-3.05052900	-0.59450700
H	3.74866500	-0.85537500	2.26503900
H	-4.39148200	-4.03899000	-0.60325800
H	-3.31703300	-3.79515600	-1.99327700
H	-3.84057800	-2.39632200	-1.03112200
H	-0.94012000	-5.23256600	0.56438900
H	-1.70458100	-5.49787500	-1.01568600
H	-2.64851500	-5.69764700	0.47901800
H	6.27878700	0.81895900	1.80690500
H	4.98524500	1.15764200	2.97695500
H	4.64107400	1.21898100	1.23768900
H	5.28195100	-2.61476300	3.23324000
H	5.31346200	-1.09537000	4.15605100
H	6.65186200	-1.49941400	3.06783300
H	7.23018700	-1.27434400	0.82341100
H	7.68226400	-2.32124200	-1.38138500
H	5.81244800	-3.10690500	-2.80850400
H	0.08075400	-0.44538700	3.16554600
H	2.15085600	-2.69186800	-1.91874200
H	-2.00394800	0.32665800	5.27066100
H	-1.68086400	1.11705800	3.69434400
H	-0.44853100	1.12668200	4.96643600
H	0.90085400	-0.95654200	5.47237500
H	0.59908800	-2.47712900	4.60164700
H	-0.56122400	-1.90668300	5.81473600
H	3.11918700	-1.32050600	-3.69678700
H	2.34868600	-2.76999000	-4.34197500
H	4.12324700	-2.68511100	-4.26815900

H	3.01648300	-5.03051300	-1.40027900
H	4.02900100	-4.95859500	-2.85455900
H	2.25816900	-4.91391200	-3.00103200
O	-1.07874100	1.29347100	1.04152200
O	0.37203400	1.09488400	1.49729000
O	-1.14176300	2.03354600	-1.68819200

## 5.7 Structures with eight oxygen atoms

## Bisozone Complex

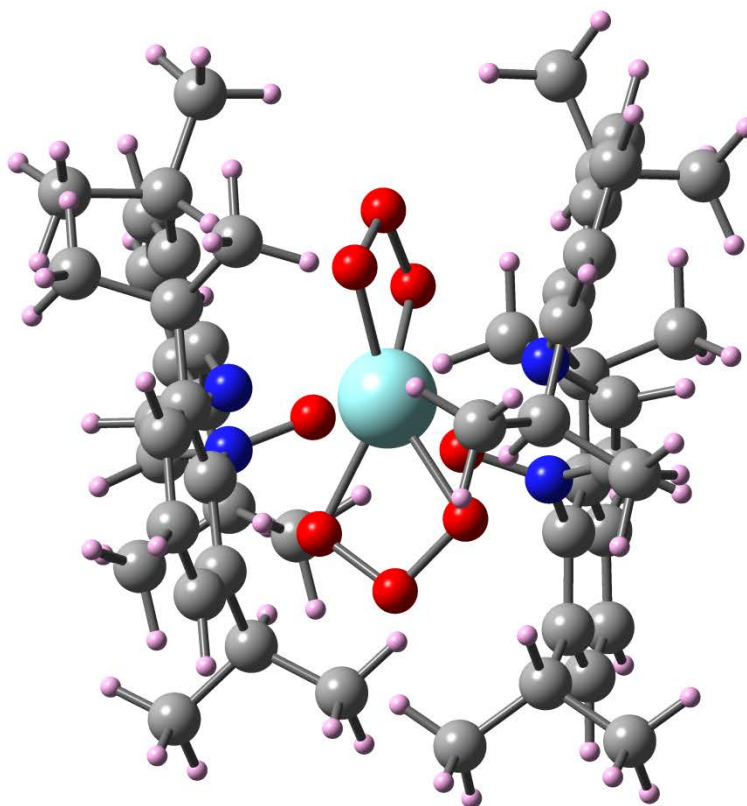


Fig. S72: NCCNO Bisozone Complex

	SCF	E <sub>ZP</sub>	H	G
	-2891.7057419	-2890.544318	-2890.470627	-2890.658358
Zr	-0.01563900	0.04372200	-0.17441500	
O	2.19697400	0.00263500	0.35283200	
O	-2.23589800	-0.10171900	0.31052700	
O	0.06027500	0.91534100	1.84224400	
N	-0.43136500	-2.25568900	-0.86109700	
N	-2.95707400	-1.18180600	0.61066100	
N	0.43799700	2.44017100	-0.17661100	
N	2.92825800	0.94240000	0.95184800	
C	-1.46004800	-2.91908900	-0.40694600	
C	-2.59163900	-2.43131000	0.35894400	
C	1.47942400	2.92691500	0.44224800	
C	2.58871900	2.21986900	1.05442500	
C	0.47274500	-3.00016800	-1.74931000	
C	0.17319700	-3.04595400	-3.13864800	
C	1.05151100	-3.77126600	-3.97011400	
C	2.17589800	-4.42836700	-3.44878100	
C	2.43648700	-4.37917900	-2.07221000	

C	1.59605800	-3.66659900	-1.19033500
C	-0.80815900	-1.70253300	-5.09379800
C	-1.08007500	-2.39256100	-3.73558000
C	-2.21519500	-3.44399800	-3.89350000
C	-5.66809100	0.84916700	-1.72386700
C	-5.18005100	-0.51137400	-1.16379800
C	-5.92346400	-1.68901000	-1.84990200
C	-4.26523400	-0.90455300	1.22820000
C	-5.33654500	-0.58479800	0.35937400
C	-6.58941100	-0.34902200	0.96214900
C	-6.74514000	-0.41665200	2.35661400
C	-5.64937100	-0.71187300	3.18228000
C	-4.37026500	-0.95719800	2.63699200
C	3.35674800	-3.42689000	0.65796600
C	1.87332600	-3.70549900	0.31714800
C	1.42937700	-5.07236900	0.90925900
C	-2.92257600	-0.06917300	4.52515000
C	-3.18059500	-1.25139400	3.55598700
C	-3.39229900	-2.57425100	4.33846900
C	-0.41983100	3.41866600	-0.85710200
C	-1.59902700	3.86956400	-0.20497400
C	-2.39237800	4.82321100	-0.87605300
C	-2.03394100	5.30864900	-2.14215400
C	-0.86124400	4.85023400	-2.75933800
C	-0.02694900	3.89726400	-2.13780700
C	-3.47915500	3.14028400	1.38334600
C	-1.96945800	3.43080200	1.21575300
C	-1.50704600	4.50234700	2.24266100
C	5.51991600	-0.53167900	-1.81557100
C	5.14607000	0.68731600	-0.93295500
C	5.99595700	1.92865500	-1.31488500
C	4.22194900	0.47609500	1.47914700
C	5.29101900	0.36202200	0.55807400
C	6.52975900	-0.06568900	1.07859900
C	6.67435200	-0.37079400	2.44219800
C	5.58028000	-0.26748800	3.31535800
C	4.31433500	0.15258500	2.85239600
C	1.05324600	3.15817300	-4.34366500
C	1.26294700	3.44639400	-2.83699100
C	2.38619000	4.50506400	-2.65093400
C	2.82372500	-1.15974600	4.43536600
C	3.12320100	0.22814100	3.81263600
C	3.36025400	1.29201300	4.91646700
H	-1.54476500	-3.98310600	-0.64293100
H	-3.30007600	-3.17828900	0.69665900
H	1.59785800	4.01218200	0.49807200
H	3.30754200	2.82830600	1.59029700
H	0.85294900	-3.81748800	-5.03690500
H	2.84023500	-4.97977100	-4.11035000
H	3.30038500	-4.90330800	-1.67218300
H	-1.42163900	-1.60771400	-3.05398000
H	-4.11815400	-0.58538700	-1.42140500

H	-0.56122100	-2.42360800	-5.88554200
H	0.00802100	-0.98080300	-4.99663500
H	-1.70478200	-1.15520200	-5.41362300
H	-1.91197400	-4.24877000	-4.57716900
H	-3.11662200	-2.96989200	-4.30529700
H	-2.48461100	-3.90891700	-2.93510400
H	-6.74269100	0.99891900	-1.55447200
H	-5.48818400	0.89091700	-2.80529400
H	-5.12569300	1.68171700	-1.26205200
H	-5.55688200	-2.66060400	-1.49284200
H	-5.77400400	-1.64775300	-2.93641400
H	-7.00310000	-1.64541000	-1.65431900
H	-7.44464300	-0.10737500	0.33709300
H	-7.72076400	-0.23183500	2.79990100
H	-5.78242800	-0.74598900	4.26015800
H	1.28348400	-2.92795500	0.81112000
H	-2.27116100	-1.35819500	2.95775800
H	4.02878200	-4.19952100	0.26055300
H	3.48886200	-3.40466900	1.74802200
H	3.66839500	-2.45483900	0.26165200
H	1.99906700	-5.90125500	0.46675700
H	0.36350400	-5.26450900	0.72552900
H	1.59123500	-5.08644900	1.99529100
H	-2.71693100	0.85131100	3.96752100
H	-2.04234600	-0.28582000	5.14219400
H	-3.77698900	0.10717700	5.19296200
H	-4.26806300	-2.51783400	4.99891400
H	-2.51300400	-2.78409700	4.96032800
H	-3.53798000	-3.42634700	3.66081500
H	-3.29661600	5.19004300	-0.39858500
H	-2.66206800	6.04197900	-2.64290200
H	-0.59113100	5.23007300	-3.74056600
H	-1.43542000	2.50659700	1.45488100
H	4.09766600	0.91484500	-1.15312100
H	-4.09424700	4.04256700	1.26314100
H	-3.67062400	2.74366100	2.38924500
H	-3.81312600	2.39074200	0.65789700
H	-0.42506800	4.67948700	2.17925800
H	-1.73289500	4.17102200	3.26485000
H	-2.01550700	5.46120200	2.07035300
H	6.57091700	-0.82192100	-1.68375500
H	5.36610200	-0.28539800	-2.87351900
H	4.88908400	-1.39549300	-1.57881800
H	5.71536100	2.80896100	-0.72141300
H	5.85000400	2.17242000	-2.37498200
H	7.06659400	1.74421400	-1.15560000
H	7.38220700	-0.16413200	0.41209700
H	7.63931300	-0.69768400	2.82233300
H	5.70392100	-0.52345900	4.36403400
H	1.58821500	2.50217300	-2.38983700
H	2.22369600	0.51237000	3.25871800
H	0.81924000	4.06779100	-4.91368800



H	0.24811300	2.43057000	-4.48025100
H	1.97176000	2.73035200	-4.76735300
H	3.31108300	4.16776800	-3.13853200
H	2.60954500	4.68993200	-1.59119200
H	2.09753100	5.46562800	-3.09926800
H	2.59327100	-1.89238800	3.65407100
H	1.94691700	-1.08707900	5.09011300
H	3.66804700	-1.53286500	5.03121900
H	3.54067000	2.28714200	4.48799200
H	4.22370600	1.03643900	5.54521200
H	2.47784400	1.35834500	5.56513200
O	-1.16700300	0.45131700	-1.91413600
O	1.15381200	0.18629900	-1.94833500
O	-0.02208000	-0.36357600	2.61140800
O	-0.10720900	-1.37176800	1.51205300
O	-0.00160400	0.49074000	-2.88248300

## 6. NCCNO Triplet Ground States

### 6.1 Structures with two oxygen atoms

#### Bare Complex

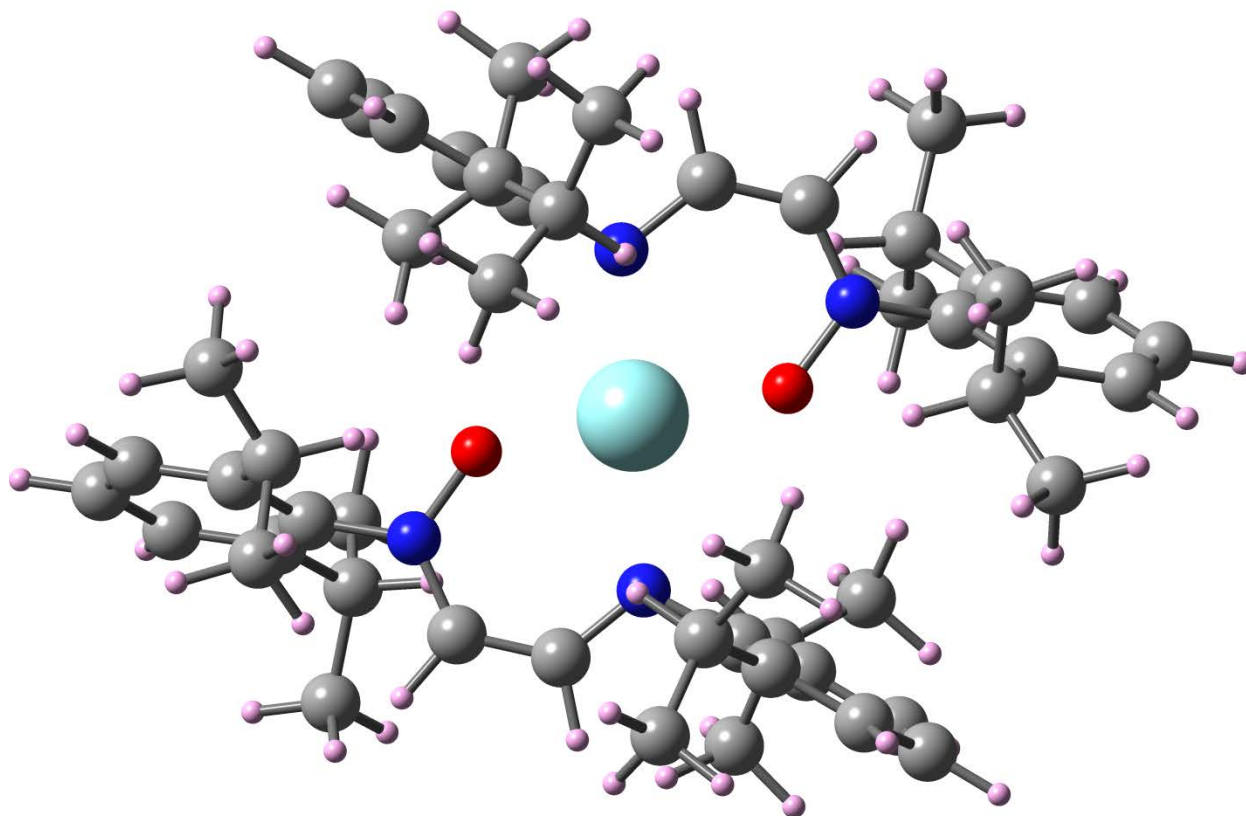


Fig. S73: NCCNO Bare Complex

SCF	$E_{ZP}$	H	G
-2440.617606	-2439.477753	-2439.410641	-2439.585321

Zr	0.00272452	0.05046653	0.15103464
O	2.00247379	0.39996794	0.01781330
O	-2.01306779	-0.41269896	-0.03187695
N	0.14431423	-2.20441646	0.25553395
N	-2.81980686	-1.53229314	-0.21303215
N	-0.14305096	2.19377960	0.34066687
N	2.83956714	1.52124792	-0.11022828
C	-0.92500833	-3.07166136	0.18685650
C	-2.26555845	-2.77416179	-0.04090259
C	0.95777818	3.07297429	0.32584932
C	2.28210708	2.76997607	0.10557005
C	1.41394582	-2.88353449	0.50690480

C	2.24166038	-3.24825412	-0.59209729
C	3.43528604	-3.95235617	-0.32879328
C	3.80855164	-4.28776702	0.98173246
C	2.98835303	-3.91157845	2.05551148
C	1.78497622	-3.20619232	1.84317552
C	3.01306373	-2.30962344	-2.84440663
C	1.84951847	-2.93761245	-2.03970577
C	1.31213775	-4.20921929	-2.75082526
C	-3.62487472	-1.31709435	-4.28632403
C	-3.60415666	-2.16129666	-2.98611335
C	-3.89515393	-3.65264888	-3.30646636
C	-4.19326803	-1.30650455	-0.60805930
C	-4.58382281	-1.62298353	-1.93658514
C	-5.93985820	-1.43414357	-2.28229307
C	-6.85778567	-0.92471990	-1.35333995
C	-6.44080622	-0.59800562	-0.05128057
C	-5.10440155	-0.78611794	0.35187878
C	1.69787303	-1.92813494	4.04780942
C	0.92011967	-2.82481213	3.05013551
C	0.35567123	-4.08130866	3.76401991
C	-5.41184381	0.67290044	2.44787537
C	-4.66521122	-0.51233042	1.79392563
C	-4.83183264	-1.79792450	2.65312492
C	-1.40391391	2.87957424	0.60640407
C	-1.80228045	3.12857955	1.95278278
C	-3.00983411	3.82055224	2.18397108
C	-3.81002034	4.26205424	1.11931455
C	-3.40373997	4.01806820	-0.20111220
C	-2.20166090	3.33441880	-0.48239291
C	-1.73466867	1.75560931	4.10533704
C	-0.95128540	2.69328344	3.15126953
C	-0.39546176	3.91991845	3.92211917
C	3.55150372	1.53601236	-4.19387105
C	3.59144815	2.31086106	-2.85147202
C	3.92577705	3.80647044	-3.09990739
C	4.19149267	1.28871675	-0.54603913
C	4.57470883	1.68245924	-1.85727832
C	5.91970231	1.48371101	-2.24038559
C	6.83781611	0.88366408	-1.36762044
C	6.43229922	0.47996505	-0.08283629
C	5.11029065	0.68218187	0.35762771
C	-2.84867706	2.33128730	-2.73317681
C	-1.78276101	3.12817307	-1.94053570
C	-1.47217349	4.48074008	-2.63425227
C	5.46770218	-0.85074521	2.39644973
C	4.68478377	0.33462891	1.78779898
C	4.81315646	1.58860679	2.69888520
H	-0.71175808	-4.13320074	0.31786150
H	-2.97499613	-3.59088050	-0.10052492
H	0.74015911	4.12455668	0.50726426
H	3.00620063	3.57682449	0.10315780
H	4.07815306	-4.24178301	-1.15653295

H	4.72982820	-4.83655495	1.16364704
H	3.28427953	-4.16847789	3.07030721
H	1.03368242	-2.20520015	-2.01726818
H	-2.58951826	-2.10084409	-2.57734315
H	3.83776665	-3.01932901	-2.99223046
H	3.41201051	-1.42739675	-2.33085099
H	2.66078990	-2.00561348	-3.83980115
H	2.08144452	-4.99242624	-2.78767378
H	1.01416387	-3.97660992	-3.78252198
H	0.43942979	-4.61896898	-2.22658686
H	-4.59451561	-1.38077850	-4.79682193
H	-2.85918768	-1.68359946	-4.98304149
H	-3.42051716	-0.26138754	-4.07690696
H	-3.83649589	-4.27783399	-2.40662785
H	-3.16828334	-4.03586220	-4.03471997
H	-4.89903408	-3.77482312	-3.73412262
H	-6.27399092	-1.67402500	-3.28849672
H	-7.89621490	-0.77822537	-1.64166630
H	-7.16304008	-0.19921521	0.65429670
H	0.06650133	-2.24162185	2.68808133
H	-3.60089076	-0.25573809	1.77486468
H	2.56401736	-2.45335263	4.47153508
H	1.04684406	-1.62877449	4.88039656
H	2.06200838	-1.01900640	3.55283809
H	1.16283049	-4.70925273	4.16409743
H	-0.23647126	-4.69682217	3.07472216
H	-0.29112879	-3.78897169	4.60237159
H	-5.32951627	1.58008103	1.83837311
H	-4.97222911	0.88700998	3.43035821
H	-6.47581399	0.45189564	2.60780924
H	-5.88604489	-2.10365348	2.69791758
H	-4.48585943	-1.61653294	3.67952171
H	-4.25110411	-2.63329324	2.24347195
H	-3.32472755	4.01776794	3.20658237
H	-4.73675783	4.79643291	1.31670267
H	-4.02391955	4.36791965	-1.02372548
H	-0.09318096	2.12993515	2.76945217
H	2.58648663	2.26317576	-2.41862510
H	-2.60504487	2.26119734	4.54459143
H	-1.08922599	1.42329039	4.92991603
H	-2.09414313	0.86628779	3.57184551
H	0.20131489	4.56253572	3.26278557
H	0.24592945	3.59355012	4.75216237
H	-1.20704971	4.52944076	4.34170983
H	4.51246835	1.58798140	-4.72218821
H	2.78633997	1.96686285	-4.85364879
H	3.31089769	0.47901764	-4.03291351
H	3.91032369	4.38090385	-2.16534802
H	3.19404716	4.25346989	-3.78601360
H	4.92229596	3.91967318	-3.54723107
H	6.24362319	1.78498862	-3.23362953
H	7.86663812	0.72783891	-1.68471307

H	7.15461071	0.01435556	0.58049605
H	-0.85947807	2.53847819	-1.94331898
H	3.62741828	0.05088047	1.75753963
H	-3.79722266	2.88077581	-2.80022220
H	-3.05025364	1.36903401	-2.24815485
H	-2.49918906	2.14285973	-3.75808009
H	-1.12992987	4.31283893	-3.66484777
H	-0.68691237	5.02856138	-2.09799546
H	-2.36227278	5.12306077	-2.67630423
H	5.41849864	-1.73546812	1.75105223
H	5.03252177	-1.11822091	3.36799877
H	6.52341380	-0.60104091	2.57004419
H	4.20169708	2.41798492	2.32529182
H	5.85732089	1.92643770	2.75205893
H	4.47858476	1.35390926	3.71857542

## 6.2 Structures with three oxygen atoms

### Oxo Complex

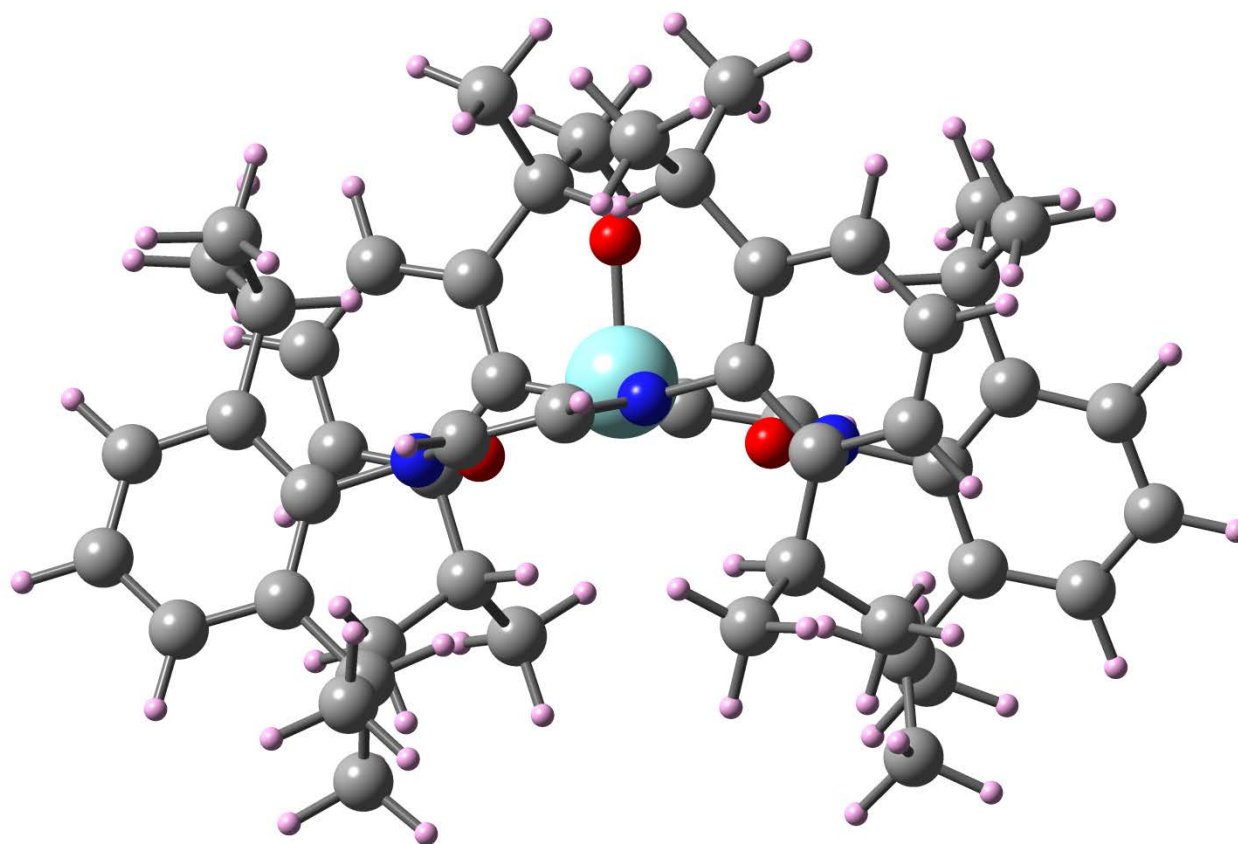


Fig. S74: NCCNO Oxo Complex

SCF	E <sub>ZP</sub>	H	G
-2515.928361	-2514.784299	-2514.715938	-2514.893339

Zr	-0.01113530	-0.00481867	-0.52226708
N	-0.21389481	-2.30651007	-0.29573169
N	0.21949895	2.29650343	-0.29665256
C	0.84464869	-3.14435662	-0.15048824
C	2.17983278	-2.81906625	0.12695306
C	-0.83143247	3.14434714	-0.15368474
C	-2.16912576	2.83296558	0.12810163
C	-1.48053876	-2.97169555	-0.58574608
C	-2.38248750	-3.22403769	0.48719132
C	-3.58386826	-3.90594638	0.20604831
C	-3.88779393	-4.33131811	-1.09735176
C	-2.99125156	-4.06872890	-2.14264719
C	-1.77660786	-3.38470593	-1.91595345
C	-3.23924280	-2.29122194	2.72303758

C	-2.03175739	-2.83808139	1.92749648
C	-1.39556108	-4.04450301	2.67241160
C	3.54916492	-1.38984254	4.42880352
C	3.51792374	-2.21502356	3.11730997
C	3.81806917	-3.71002769	3.41218426
C	4.07921434	-1.35397746	0.73914448
C	4.48430669	-1.66187835	2.06373372
C	5.84266400	-1.46098160	2.39138162
C	6.74600745	-0.95569215	1.44446960
C	6.31294445	-0.64476424	0.14422199
C	4.97037260	-0.83817975	-0.23872324
C	-1.51682052	-2.38488770	-4.25222553
C	-0.82298907	-3.14370310	-3.09303041
C	-0.21492935	-4.48148824	-3.59459459
C	5.15968810	0.68381681	-2.29980864
C	4.51058196	-0.57325986	-1.67598812
C	4.78211549	-1.82307560	-2.56005824
C	1.49164393	2.95085352	-0.58732417
C	1.79222038	3.35766537	-1.91828675
C	3.01163554	4.03308494	-2.14558616
C	3.90812714	4.29403370	-1.09991093
C	3.59955729	3.87483517	0.20444274
C	2.39375625	3.20104821	0.48596524
C	1.52909231	2.34817296	-4.24921702
C	0.83887439	3.11958110	-3.09618699
C	0.24509429	4.46026868	-3.60693827
C	-3.56342709	1.36036845	4.44224628
C	-3.50502255	2.19139653	3.13566433
C	-3.76494785	3.69244913	3.43870537
C	-4.08259188	1.38741649	0.74290182
C	-4.48230935	1.67312275	2.07462790
C	-5.84330695	1.48849853	2.39846761
C	-6.75641970	1.02164366	1.44024122
C	-6.32933127	0.73342125	0.13361070
C	-4.98245866	0.90982276	-0.24480970
C	3.24498030	2.27652218	2.72725364
C	2.03930841	2.82020742	1.92672942
C	1.40149739	4.02877301	2.66687259
C	-5.07174087	-0.68175943	-2.24985683
C	-4.53581852	0.65644467	-1.68755405
C	-4.95916488	1.84467495	-2.59506153
H	0.66002174	-4.21253928	-0.27429785
H	2.90419322	-3.62278706	0.17812367
H	-0.63733153	4.21031431	-0.28227569
H	-2.88592797	3.64359590	0.17673369
H	-4.28454004	-4.11142561	1.01078483
H	-4.81594377	-4.86306163	-1.29470399
H	-3.23331728	-4.39881645	-3.14998792
H	-1.27992472	-2.04100659	1.88535901
H	2.49875268	-2.15151082	2.72026820
H	-4.00815267	-3.05836995	2.88428122
H	-3.70161092	-1.44405252	2.20445473

H	-2.90775467	-1.95304958	3.71430817
H	-2.10457048	-4.88146337	2.73151787
H	-1.11639990	-3.76101076	3.69669995
H	-0.49424939	-4.40139063	2.15916298
H	4.52464410	-1.45551460	4.92793840
H	2.79333871	-1.76999977	5.12885009
H	3.33788626	-0.33258984	4.23531318
H	3.75057831	-4.32176634	2.50378016
H	3.10147439	-4.10686206	4.14333456
H	4.82765130	-3.83472968	3.82532379
H	6.19184684	-1.69198520	3.39452184
H	7.78738594	-0.80247692	1.71838733
H	7.02447486	-0.25189848	-0.57586901
H	-0.00724555	-2.49917218	-2.75672491
H	3.42892156	-0.40438836	-1.66299694
H	-2.37358982	-2.94147446	-4.65648185
H	-0.80261007	-2.22182668	-5.07009921
H	-1.85457402	-1.40116923	-3.90980591
H	-0.99363798	-5.15885025	-3.97121450
H	0.32353763	-5.00526413	-2.79324759
H	0.49245078	-4.29279600	-4.41336654
H	4.99901597	1.56814713	-1.67337153
H	4.70882413	0.88153747	-3.28048802
H	6.23959535	0.55528993	-2.45457588
H	5.85785774	-2.03995538	-2.61216856
H	4.41735713	-1.64962357	-3.58064403
H	4.27316682	-2.71173415	-2.16640991
H	3.25687592	4.35855335	-3.15369211
H	4.83936532	4.82032838	-1.29750271
H	4.30023123	4.07854817	1.00960979
H	0.01587736	2.48472831	-2.75887563
H	-2.48678932	2.10195548	2.74087386
H	2.39022734	2.89637326	-4.65580626
H	0.81507522	2.18404218	-5.06699938
H	1.86001317	1.36457870	-3.89968906
H	-0.28850941	4.99480678	-2.80944162
H	-0.46354256	4.27353625	-4.42508264
H	1.03095171	5.12719782	-3.98739140
H	-4.53670822	1.45373076	4.94136106
H	-2.79693966	1.71316070	5.14499808
H	-3.38467475	0.29814830	4.24343553
H	-3.67405203	4.30784116	2.53492157
H	-3.04213577	4.06426091	4.17686811
H	-4.77344564	3.84230937	3.84623684
H	-6.18847800	1.70324937	3.40655019
H	-7.80042879	0.88197261	1.71131318
H	-7.04776559	0.37193123	-0.59675048
H	1.28797869	2.02271489	1.88476041
H	-3.44288782	0.59828433	-1.70584801
H	4.01042692	3.04629489	2.89275210
H	3.71292427	1.43158840	2.21014863
H	2.91035139	1.93644697	3.71685121



H	1.12185554	3.74846799	3.69193192
H	0.50022301	4.38334784	2.15206067
H	2.11003073	4.86631227	2.72372452
H	-4.78053105	-1.52549960	-1.61477019
H	-4.65625341	-0.85538181	-3.25062539
H	-6.16627711	-0.67790843	-2.34239009
H	-4.53395883	2.79192312	-2.23918844
H	-6.05218115	1.95137669	-2.62056135
H	-4.60757652	1.67975349	-3.62168043
O	-0.01683960	-0.00164910	-2.33778286
O	-1.88340021	0.47127424	0.34675702
O	1.87190914	-0.45950069	0.33957132
N	-2.69939646	1.60057366	0.36626975
N	2.69906857	-1.58070101	0.35821315

### 6.3 Structures with four oxygen atoms

#### Dioxo Complex

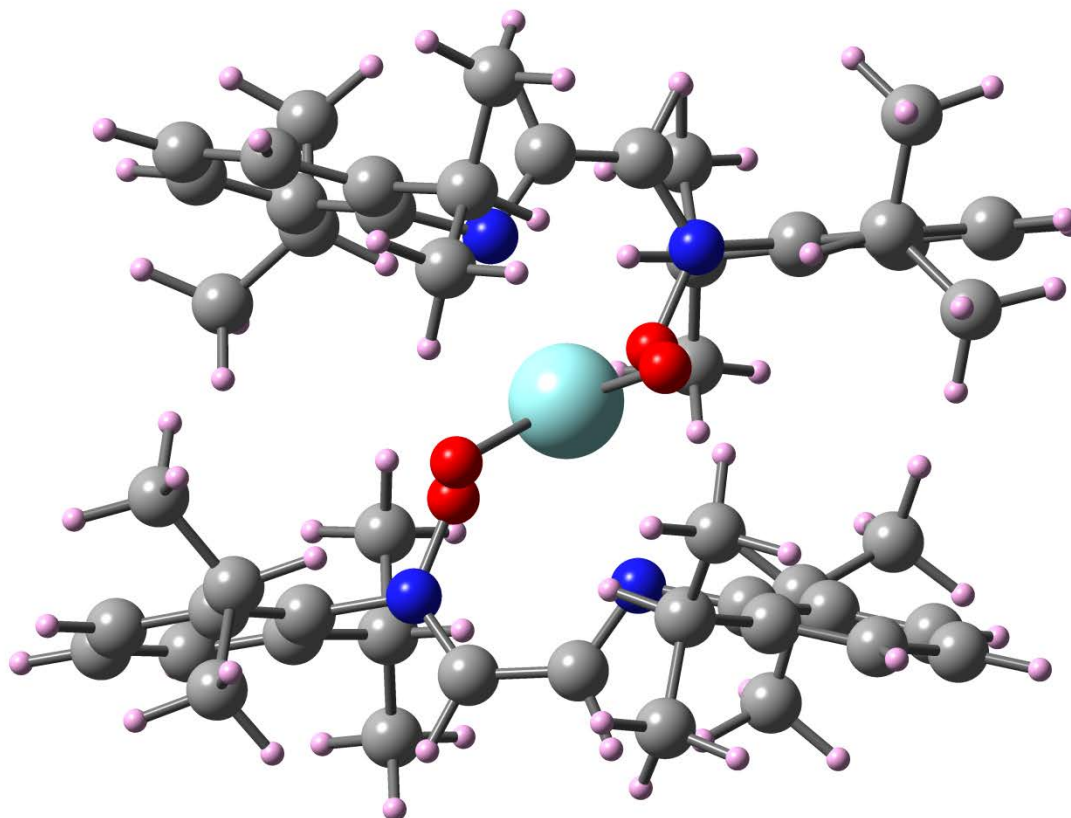


Fig. S75: NCCNO Dioxo Complex

SCF	E <sub>ZP</sub>	H	G
-2591.082361	-2589.936351	-2589.866325	-2590.046064

Zr	0.03396670	-0.13787538	-0.89128777
N	-0.51902601	-2.34564393	-0.62827893
N	0.54367205	2.28594380	-0.66178263
C	0.38335637	-3.26496941	-0.19821341
C	1.63704287	-3.03195259	0.38657224
C	-0.35951360	3.19503024	-0.39756267
C	-1.66980029	2.99189367	0.18215383
C	-1.80181156	-2.88885759	-1.05798029
C	-2.79119708	-3.18265505	-0.07524687
C	-4.01757242	-3.73410007	-0.50275436
C	-4.26674798	-3.98260873	-1.86158355
C	-3.28415715	-3.67905940	-2.81562954
C	-2.03941348	-3.13043764	-2.43944278
C	-3.71848352	-2.19879071	2.10304061

C	-2.54631191	-2.94592679	1.42017534
C	-2.26177121	-4.28479427	2.15434933
C	2.21543322	-0.55163679	4.53263318
C	2.41159936	-1.84303973	3.69611884
C	2.53044094	-3.08650038	4.61474898
C	3.47873594	-1.70556264	1.35043580
C	3.61757363	-1.71591838	2.76116464
C	4.92033727	-1.60460233	3.28957770
C	6.03364417	-1.49020025	2.44084514
C	5.86433010	-1.47340068	1.04692774
C	4.58073519	-1.56862588	0.46709453
C	-1.53337163	-1.87404299	-4.59790506
C	-0.98864906	-2.84144659	-3.51636240
C	-0.47079574	-4.15777352	-4.15530288
C	5.16662638	-0.37335064	-1.71975577
C	4.40998357	-1.55043182	-1.05597241
C	4.86346736	-2.90230701	-1.67161832
C	1.81240756	2.80149824	-1.19053894
C	1.91478993	3.11614858	-2.56978415
C	3.14158034	3.64696069	-3.02443144
C	4.21871344	3.84776249	-2.15050750
C	4.09263954	3.51107241	-0.79262207
C	2.89131380	2.97899343	-0.28232600
C	1.21001773	1.97655669	-4.73274353
C	0.77061163	2.89997008	-3.56758204
C	0.22899490	4.25446705	-4.09897053
C	-1.97149892	0.87176194	4.47046002
C	-2.23710365	2.16365751	3.65180326
C	-2.32120089	3.40428256	4.57639371
C	-3.44562339	1.84572571	1.38340861
C	-3.49325248	2.00098565	2.78982313
C	-4.76975868	1.96740540	3.38715624
C	-5.92594253	1.78640026	2.61029351
C	-5.83197102	1.62352139	1.21965961
C	-4.58115568	1.63804767	0.56427546
C	4.05016453	2.17501814	1.87093291
C	2.73900029	2.66032700	1.21053249
C	2.19511665	3.89585575	1.98254063
C	-5.27805451	0.19898108	-1.42860961
C	-4.49753633	1.45027607	-0.95447944
C	-5.00348122	2.72076131	-1.69064388
H	0.13070849	-4.31890617	-0.32629845
H	2.28531527	-3.88033698	0.57111858
H	-0.14201034	4.24420948	-0.61765807
H	-2.34274220	3.83895750	0.22488091
H	-4.78269010	-3.97153309	0.23287647
H	-5.21757050	-4.40980935	-2.17293549
H	-3.48199180	-3.87247585	-3.86736413
H	-1.65714615	-2.31434850	1.52109686
H	1.51226074	-1.96479192	3.08369626
H	-4.64069380	-2.79467482	2.10196135
H	-3.92588300	-1.24743296	1.60038643

H	-3.46758351	-1.98271734	3.15057642
H	-3.12253666	-4.96327656	2.08035368
H	-2.06100445	-4.10559661	3.21984464
H	-1.39240945	-4.79834895	1.72556628
H	3.08086868	-0.35549086	5.18015235
H	1.32872659	-0.64715627	5.17405220
H	2.07203658	0.31400917	3.87538861
H	2.63601591	-4.00691577	4.02635041
H	1.63342977	-3.18322255	5.24083743
H	3.39857369	-3.01421080	5.28314457
H	5.06484917	-1.61245932	4.36723545
H	7.03213909	-1.41140796	2.86514613
H	6.73424162	-1.37687926	0.40299188
H	-0.13300023	-2.34422893	-3.05049174
H	3.35019048	-1.41248653	-1.29509904
H	-2.37180658	-2.31587782	-5.15468266
H	-0.73937360	-1.63272345	-5.31714664
H	-1.87168697	-0.94061904	-4.13387708
H	-1.27845353	-4.70413824	-4.66186127
H	-0.03733100	-4.82558890	-3.39858956
H	0.30616651	-3.93574743	-4.89903550
H	4.84180407	0.58952723	-1.30990565
H	4.95302738	-0.36372989	-2.79562277
H	6.25500981	-0.45693515	-1.59263874
H	5.93201171	-3.08330141	-1.48983247
H	4.69770632	-2.89390005	-2.75646992
H	4.30127370	-3.74570099	-1.25067556
H	3.25161602	3.89533489	-4.07679901
H	5.15463757	4.25660675	-2.52413576
H	4.93646288	3.66010913	-0.12572089
H	-0.05135072	2.38198490	-3.06336391
H	-1.36983892	2.30310897	2.99570143
H	2.02817446	2.41896870	-5.31759634
H	0.36382514	1.80696584	-5.41239754
H	1.53082354	1.00978463	-4.33106442
H	-0.12368127	4.90284542	-3.28399339
H	-0.61128616	4.08222436	-4.78435120
H	1.00380987	4.80594232	-4.64839935
H	-2.79732109	0.66537151	5.16411185
H	-1.05100713	0.98029562	5.05875791
H	-1.85407551	0.01015167	3.80426683
H	-2.50226073	4.32256232	4.00280197
H	-1.37963638	3.52556548	5.12725670
H	-3.12565797	3.30627130	5.31637987
H	-4.85961325	2.08229584	4.46381583
H	-6.90085202	1.76569856	3.09130317
H	-6.73447245	1.47024297	0.63527384
H	2.01119519	1.84467041	1.30663369
H	-3.45567467	1.28537519	-1.25439599
H	4.80247259	2.97354608	1.92449225
H	4.48353523	1.32707806	1.33033758
H	3.84812048	1.84793768	2.89850872

H	2.06546135	3.65555375	3.04665999
H	1.22700084	4.23470155	1.59193937
H	2.89699398	4.73729529	1.90681953
H	-4.92671279	-0.70593584	-0.92064232
H	-5.11503324	0.05641730	-2.50340494
H	-6.35938923	0.29690247	-1.26061007
H	-4.42863515	3.61349531	-1.40819383
H	-6.06063523	2.91845318	-1.46636122
H	-4.90384990	2.58566369	-2.77469887
O	1.19346208	-0.27739794	-2.32350046
O	-1.57115743	0.43664574	-2.00108424
O	-1.40913862	0.74806838	0.80321826
O	1.37940640	-0.67656045	0.76751744
N	-2.11928562	1.87678699	0.74104546
N	2.15067968	-1.83372462	0.78453199

## Peroxo Complex

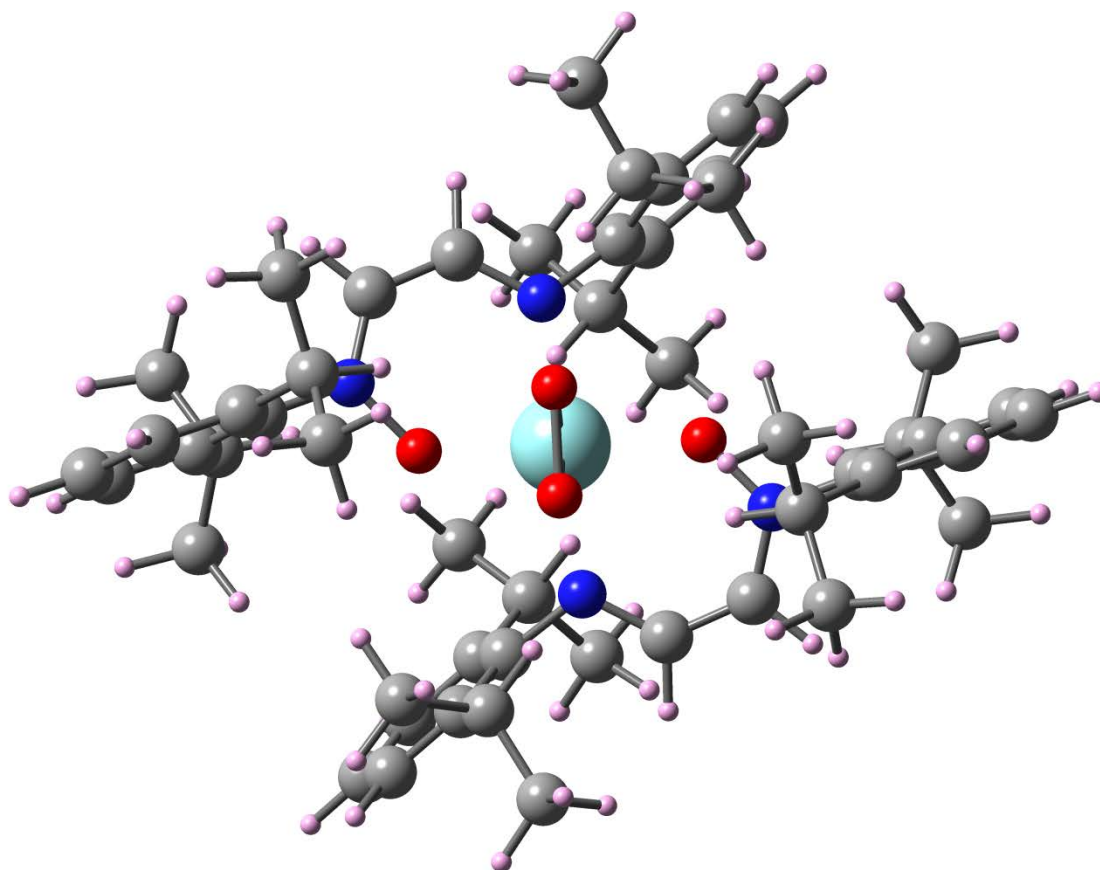


Fig. S76: NCCNO Peroxo Complex

SCF	E <sub>ZP</sub>	H	G
-2591.081598	-2589.935344	-2589.865585	-2590.048101

Zr	-0.00146300	0.01280800	-0.41422603
O	2.02630615	0.31464102	0.06748400
O	-2.02614316	-0.33404103	0.05673500
O	-0.12775201	0.87029506	-2.25239617
O	0.10070701	-0.67143305	-2.32477218
N	0.12648201	-2.17075617	0.32391502
N	-2.80009122	-1.46879211	-0.20429902
N	-0.12831101	2.11917216	0.52065404
N	2.80254621	1.46980011	-0.05742000
C	-0.93997307	-3.01678223	0.28859202
C	-2.27419217	-2.70866221	-0.00982000
C	0.94092807	2.95935323	0.58801104
C	2.27701317	2.68129020	0.27023502
C	1.37841011	-2.81001521	0.72459806
C	2.17855716	-3.46982627	-0.24850402
C	3.34411926	-4.13582031	0.18799501

C	3.71282528	-4.14935032	1.54109312
C	2.91898723	-3.48002527	2.48511319
C	1.74729213	-2.79736121	2.09846016
C	2.97846423	-3.03020123	-2.63104720
C	1.80660614	-3.50224127	-1.73478613
C	1.33091810	-4.91792037	-2.15922717
C	-3.24196625	-0.42725803	-4.22857832
C	-3.26414725	-1.48539211	-3.09797424
C	-3.38774126	-2.91523022	-3.69239728
C	-4.14973832	-1.22977510	-0.67929505
C	-4.38092333	-1.23262310	-2.08021116
C	-5.70768046	-1.02808208	-2.51511519
C	-6.74784550	-0.81961207	-1.59574612
C	-6.48521848	-0.81047206	-0.21634702
C	-5.17759940	-1.01032008	0.27194302
C	1.72682713	-1.16062009	4.06402431
C	0.89084107	-2.10299816	3.16259724
C	0.11952801	-3.14181524	4.02053931
C	-5.45425044	0.24088102	2.47922919
C	-4.90716037	-1.02725308	1.77835614
C	-5.49044341	-2.31193618	2.42735619
C	-1.38589111	2.72371121	0.95752107
C	-1.77893914	2.58683120	2.31765518
C	-2.95668523	3.23451124	2.74431621
C	-3.73258129	3.98909931	1.85105514
C	-3.33908026	4.09931631	0.50926904
C	-2.16653717	3.47326127	0.03441500
C	-1.78977214	0.80203106	4.15274032
C	-0.93856407	1.79915214	3.32830726
C	-0.15664101	2.75927221	4.26513833
C	3.24034425	0.83884607	-4.15307732
C	3.26595625	1.79624614	-2.93551122
C	3.39473626	3.27107825	-3.40486126
C	4.15259832	1.28842710	-0.55545204
C	4.38426034	1.44882111	-1.94688115
C	5.71342944	1.30652710	-2.39968519
C	6.75477052	1.00697708	-1.50739711
C	6.49086051	0.83905806	-0.13817301
C	5.18103539	0.96939607	0.36674103
C	-2.92403122	3.32424725	-2.40158718
C	-1.75958814	3.64661728	-1.43280111
C	-1.21875109	5.07901339	-1.69250913
C	5.49519542	-0.50725704	2.42550518
C	4.90619737	0.81034806	1.86406314
C	5.44121543	2.03616015	2.65337520
H	-0.75206806	-4.07087931	0.49594004
H	-2.98577523	-3.51983727	-0.10699601
H	0.75406206	3.98578730	0.90570407
H	2.99096123	3.49606627	0.26862502
H	3.96616230	-4.64926336	-0.54098804
H	4.61060635	-4.67553036	1.85753914
H	3.21151524	-3.49061427	3.53245527

H	0.97956608	-2.80712221	-1.90544114
H	-2.29460917	-1.41695411	-2.59596320
H	3.82832929	-3.72543429	-2.59474920
H	3.33279326	-2.04154516	-2.31819618
H	2.64509620	-2.96046623	-3.67449928
H	2.12533316	-5.66312744	-2.01630615
H	1.04873208	-4.92171837	-3.22051725
H	0.45938304	-5.24128540	-1.57495312
H	-4.14592432	-0.46799104	-4.85193537
H	-2.37464618	-0.60534705	-4.87559637
H	-3.14519924	0.58352404	-3.81880229
H	-3.35350825	-3.68226428	-2.90757922
H	-2.56018220	-3.10432824	-4.38804934
H	-4.33116533	-3.03683423	-4.24221633
H	-5.92455243	-1.02599208	-3.57971927
H	-7.76273560	-0.66266305	-1.95411715
H	-7.29989754	-0.64496705	0.48372104
H	0.14213701	-1.48896811	2.64799520
H	-3.82202929	-1.03900308	1.92899615
H	2.45904319	-1.71644813	4.66416736
H	1.07221908	-0.62122605	4.76121036
H	2.27180718	-0.42381803	3.46162227
H	0.81447506	-3.79955929	4.55945335
H	-0.52283004	-3.77364429	3.39429026
H	-0.51527804	-2.63688420	4.76147436
H	-5.02197539	1.14806409	2.04323016
H	-5.19842440	0.21967702	3.54702227
H	-6.54750449	0.30635602	2.40207918
H	-6.58166151	-2.35262118	2.31131918
H	-5.26343840	-2.33374118	3.50155927
H	-5.07035539	-3.21806125	1.97184715
H	-3.26868125	3.14925024	3.78250229
H	-4.63610935	4.48560634	2.19765617
H	-3.94764730	4.67953936	-0.17982301
H	-0.19640101	1.21593009	2.77011121
H	2.29673117	1.68797013	-2.43962719
H	-2.51099519	1.32032210	4.79788437
H	-1.14384309	0.19706501	4.80269137
H	-2.34792218	0.12573401	3.49428627
H	0.49862804	3.42660626	3.69121028
H	0.46699004	2.19197617	4.96956538
H	-0.84596407	3.38513126	4.84745937
H	4.14863532	0.92569707	-4.76503236
H	2.37832118	1.07903108	-4.78704737
H	3.13323624	-0.20227902	-3.83167429
H	3.36187926	3.96880830	-2.55768419
H	2.56905620	3.52134127	-4.08324131
H	4.33911833	3.43601026	-3.94149030
H	5.93100744	1.42640611	-3.45745727
H	7.77163361	0.90183207	-1.87886914
H	7.30617057	0.60299005	0.54043804
H	-0.95601307	2.93977722	-1.65850013



H	3.82088829	0.76660106	2.00740415
H	-3.73943829	4.05598231	-2.32105418
H	-3.33570525	2.32914818	-2.19864517
H	-2.56117120	3.33921926	-3.43738826
H	-0.91250807	5.18507940	-2.74180821
H	-0.34898703	5.30136938	-1.06068308
H	-1.98721615	5.83603145	-1.48405512
H	5.10516239	-1.37453410	1.88154114
H	5.22380140	-0.61851205	3.48376527
H	6.59126750	-0.52215204	2.36169118
H	4.99034838	2.97098423	2.29583118
H	6.53058850	2.12739916	2.54955519
H	5.21001640	1.93357115	3.72201228

**Oxo Complex with Propylene Oxide Molecule (reaction products of dioxo complex)**

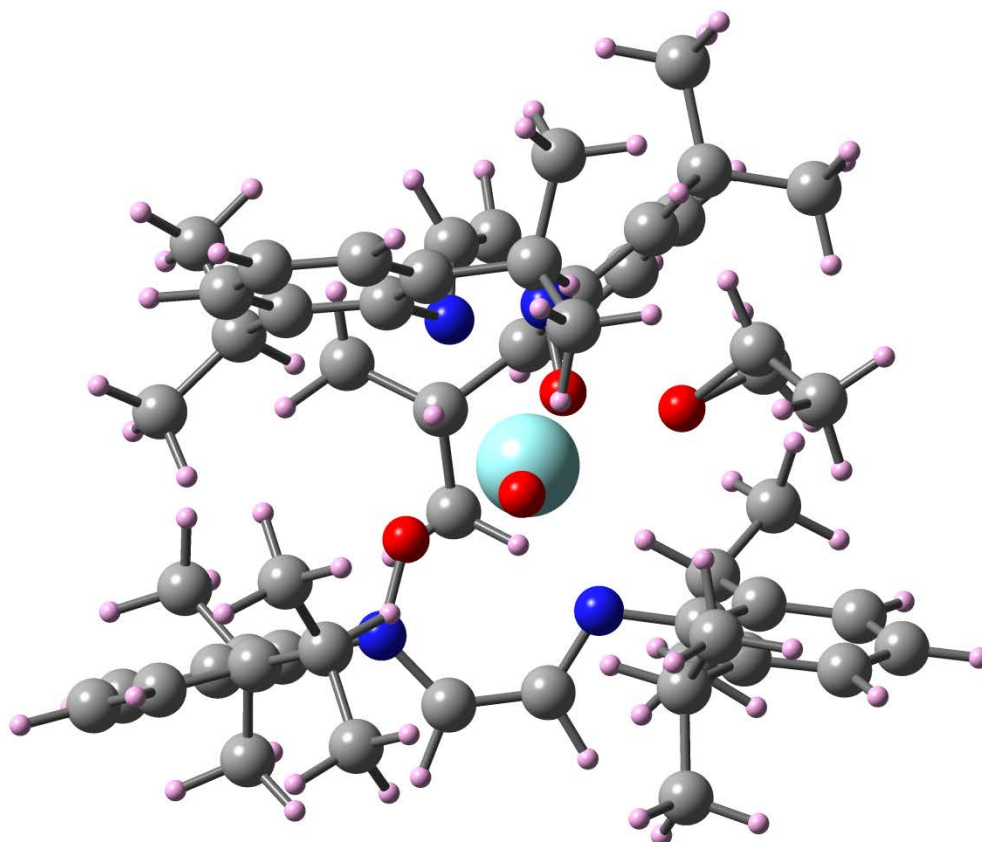


Fig. S77: Oxo Complex with Propylene Oxide Molecule (reaction products of dioxo complex)

SCF	E <sub>ZP</sub>	H	G
-2709.009799	-2707.777864	-2707.704041	-2707.889924

Zr	0.10023700	0.67548900	0.34402300
N	-0.16418200	1.62264100	-1.80389900
N	0.20909700	-0.64695500	2.24998700
C	0.76628400	1.48215400	-2.78235400
C	1.93452400	0.70813100	-2.76297500
C	-0.68108600	-1.60069900	2.65156100
C	-1.81238000	-2.10550500	2.00369500
C	-1.15229400	2.66040700	-2.05499800
C	-2.45300900	2.29939100	-2.51251300
C	-3.39964000	3.32477200	-2.72382700
C	-3.07267900	4.67318700	-2.50119900
C	-1.77943400	5.01393100	-2.07612300
C	-0.79610400	4.02565300	-1.84891800
C	-4.26218000	0.46049400	-2.57295200
C	-2.79042500	0.84402000	-2.85365400
C	-2.44868600	0.56141000	-4.34391500

C	2.65351600	-4.16967200	-2.63042700
C	2.77592500	-2.71107000	-3.14008400
C	2.98529500	-2.68268500	-4.67776900
C	3.66500300	-0.72745100	-1.74937900
C	3.89498900	-1.95532300	-2.41859400
C	5.21117600	-2.46288900	-2.41982500
C	6.24762300	-1.77625400	-1.76767700
C	5.98654800	-0.57187900	-1.09430400
C	4.68765900	-0.02138900	-1.06239400
C	0.64034200	5.34883700	-0.17871200
C	0.62104000	4.45490900	-1.44284700
C	1.32738000	5.16974300	-2.62731900
C	5.02159500	1.32497600	1.09006200
C	4.42112100	1.30133800	-0.33736500
C	4.95904500	2.49366400	-1.17486800
C	1.35885400	-0.52759900	3.14972300
C	1.41217600	0.53475400	4.09382600
C	2.52011700	0.61451500	4.96222400
C	3.55300400	-0.33275100	4.91268000
C	3.48340400	-1.38303700	3.98603800
C	2.39697100	-1.50471900	3.09285700
C	0.80485500	3.01196500	4.07057900
C	0.28608000	1.56139600	4.23130200
C	-0.47265100	1.37341900	5.57319900
C	-1.46665200	-3.24198200	-2.95257900
C	-1.63049700	-3.51715900	-1.43734900
C	-1.16813400	-4.95662300	-1.08223400
C	-3.38828400	-2.45281400	0.13381500
C	-3.07084900	-3.29229600	-0.96725600
C	-4.12915800	-3.98214500	-1.59355100
C	-5.45081300	-3.85357200	-1.13746800
C	-5.73706300	-3.02897800	-0.03972400
C	-4.71643500	-2.30602400	0.61446100
C	3.70038100	-2.92783500	1.40021600
C	2.35445200	-2.69950600	2.13010000
C	1.94326700	-3.99898800	2.87822700
C	-6.16825400	-0.37619000	1.44548600
C	-5.07809900	-1.41772100	1.80990700
C	-5.53162500	-2.26937000	3.02583600
H	0.64368600	2.08157800	-3.68627200
H	2.63097500	0.80644200	-3.58739800
H	-0.48914600	-2.07433300	3.61597800
H	-2.36176200	-2.90425100	2.48795500
H	-4.39477000	3.06988700	-3.07852000
H	-3.81379900	5.45049900	-2.67472300
H	-1.52396200	6.06088800	-1.92899700
H	-2.16070900	0.19828900	-2.23215500
H	1.82787000	-2.20756500	-2.92128100
H	-4.95941400	0.96664600	-3.25465500
H	-4.55370200	0.70384400	-1.54357800
H	-4.39581300	-0.62020400	-2.70695300
H	-3.02872600	1.21804600	-5.00693900

H	-2.68608200	-0.47936700	-4.60340900
H	-1.38417000	0.72675300	-4.54707700
H	3.56263400	-4.74897300	-2.83781500
H	1.81658600	-4.67696700	-3.12883900
H	2.47582100	-4.19219200	-1.54849700
H	3.02999400	-1.65301300	-5.05481600
H	2.15868700	-3.19591600	-5.18719100
H	3.92025500	-3.18462400	-4.96039800
H	5.42579400	-3.39849900	-2.93023000
H	7.25701200	-2.18150400	-1.78013000
H	6.79570200	-0.05703400	-0.58359000
H	1.19541800	3.56137400	-1.18640000
H	3.34201400	1.43648600	-0.21628600
H	0.02076800	6.24928300	-0.29314700
H	1.66823000	5.67328500	0.03035500
H	0.29451100	4.77906600	0.68840900
H	0.81539600	6.10557300	-2.89069600
H	1.34814500	4.53787000	-3.52481300
H	2.36368400	5.41548100	-2.35911200
H	4.65122100	0.48730000	1.69185900
H	4.71841400	2.25038700	1.59433100
H	6.12011300	1.28863600	1.07861100
H	6.04822000	2.42867500	-1.30682000
H	4.73179300	3.43943700	-0.66620100
H	4.49827800	2.52458900	-2.17087700
H	2.57036800	1.42373000	5.68728100
H	4.40006700	-0.25629400	5.59080800
H	4.28248100	-2.11941400	3.95432800
H	-0.42285800	1.37708500	3.41836000
H	-0.97793600	-2.81319300	-0.91449700
H	1.54861100	3.26380900	4.83849300
H	-0.02403500	3.72913600	4.17209700
H	1.25659400	3.12460400	3.07913500
H	-0.87865600	0.35690500	5.66457800
H	-1.30716600	2.08597900	5.65112400
H	0.19108600	1.54552200	6.43080500
H	-2.07096900	-3.92699900	-3.56241800
H	-0.41712000	-3.37338700	-3.24502800
H	-1.75941700	-2.21477000	-3.19600800
H	-1.25066000	-5.14542700	-0.00421500
H	-0.11957600	-5.09929900	-1.37269800
H	-1.77129100	-5.71144900	-1.60483600
H	-3.91576800	-4.63442500	-2.43643800
H	-6.25224900	-4.39745300	-1.63191600
H	-6.76330400	-2.93882900	0.30754900
H	1.60118100	-2.49287400	1.36291200
H	-4.17937100	-0.87066500	2.11705600
H	4.49691300	-3.22588600	2.09500800
H	4.02556200	-2.02707900	0.87177100
H	3.59387400	-3.73319100	0.66106000
H	1.88951900	-4.84378500	2.17744000
H	0.96553900	-3.89820500	3.36458800

H	2.67944300	-4.24899000	3.65447400
H	-5.88094100	0.21688900	0.56814000
H	-6.33956000	0.30797700	2.28769500
H	-7.12526900	-0.86112200	1.21557400
H	-4.75413200	-2.98179800	3.32851900
H	-6.43683600	-2.84368500	2.78992300
H	-5.75538400	-1.62370300	3.88547700
O	1.22526100	1.96441700	0.98472700
O	-1.70897600	1.97006900	0.98758100
O	-1.69841400	-0.72941700	0.05595200
O	1.45122300	-0.52692000	-0.77437200
N	-2.30560600	-1.73366800	0.78374200
N	2.33645800	-0.14797000	-1.78335100
C	-2.49655900	2.81087800	1.97071800
H	-2.41946900	2.39870800	2.97542700
C	-3.20452000	1.97810800	0.94910800
H	-3.65188800	1.03137800	1.22679300
H	-3.59831800	2.46065600	0.05946300
C	-2.37068400	4.30739300	1.84771900
H	-2.38740800	4.61863300	0.79911100
H	-3.21086100	4.78310500	2.37324500
H	-1.43913700	4.65691900	2.30365700

## Dioxo Complex with Coordinated Propene Molecule

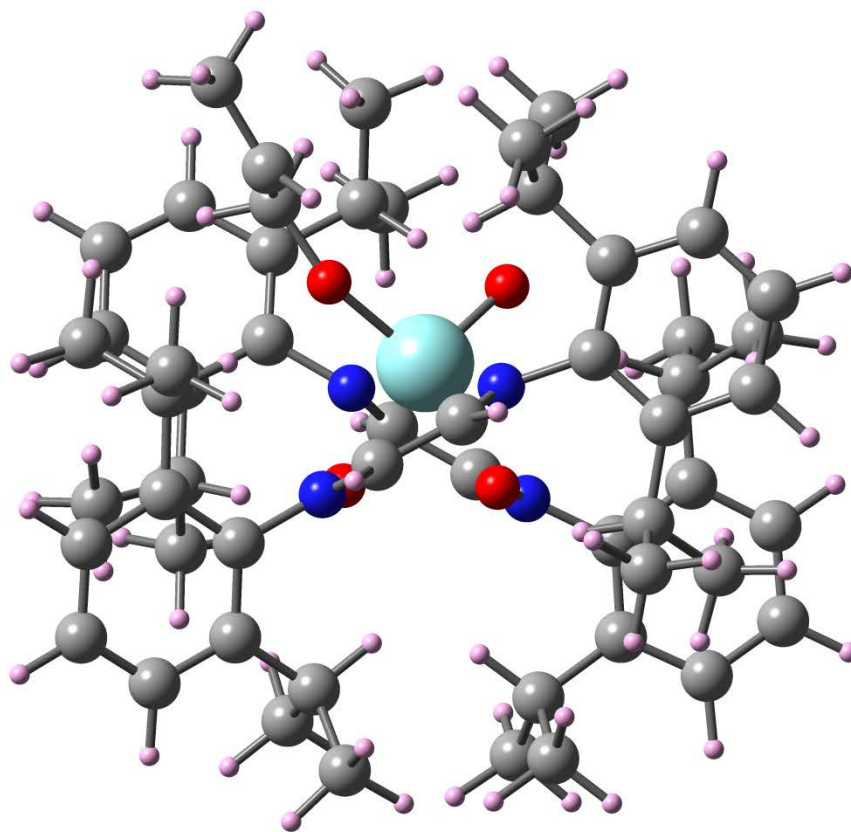


Fig. S78: NCCNO Dioxo Complex with Coordinated Propene Molecule

SCF	E <sub>ZP</sub>	H	G
-2708.999321	-2707.771762	-2707.698350	-2707.884547

Zr	-0.03951200	0.87773900	0.05214200
N	-0.37950700	0.84921600	-2.29704600
N	0.45938200	0.21983700	2.27164300
C	0.58721800	0.56292700	-3.16728900
C	1.87054100	0.01697500	-2.89144900
C	-0.33918700	-0.54238300	3.02365700
C	-1.44544700	-1.34346500	2.63066100
C	-1.56760200	1.48457800	-2.86099500
C	-2.70519500	0.68009100	-3.15147400
C	-3.84417200	1.31243900	-3.69079000
C	-3.85566600	2.69367800	-3.94520300
C	-2.71862200	3.46487000	-3.66474000
C	-1.55307200	2.88527700	-3.11625900
C	-4.03750100	-1.44815100	-2.57576800
C	-2.66919300	-0.84064400	-2.95958000
C	-2.13342700	-1.53325900	-4.24474400

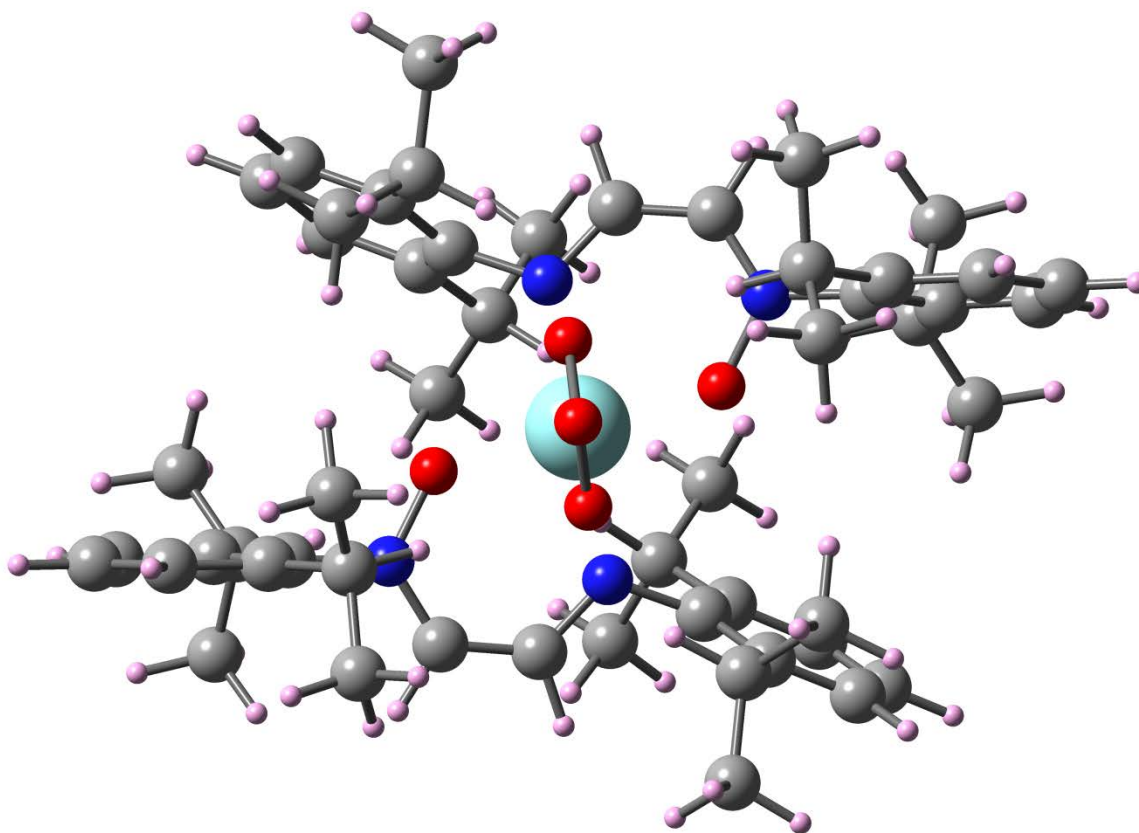
C	2.89538900	-4.44941800	-1.01496700
C	2.91864400	-3.33480200	-2.09319900
C	3.11555600	-3.93706300	-3.50918600
C	3.69393100	-0.92318300	-1.57562000
C	3.99451100	-2.29133400	-1.77862800
C	5.34874400	-2.67518700	-1.68467000
C	6.34608700	-1.73166700	-1.39066600
C	6.00840700	-0.38648800	-1.17163400
C	4.66942000	0.05364800	-1.25006700
C	-0.65694300	5.09386100	-2.15362000
C	-0.31562700	3.75883500	-2.86070900
C	0.42964800	4.04903600	-4.19368100
C	4.96816900	2.08421600	0.27655900
C	4.31627200	1.52615300	-1.01290400
C	4.72600700	2.38598600	-2.23972800
C	1.61835600	0.76674300	2.98071000
C	1.60025200	2.11713600	3.42280300
C	2.72214000	2.60134000	4.12773800
C	3.82680400	1.78009900	4.39385500
C	3.82661200	0.44952400	3.94880300
C	2.73361100	-0.08449100	3.23405300
C	0.79315100	4.33672400	2.45928300
C	0.39750600	3.04108200	3.21099500
C	-0.29579200	3.36117800	4.56281800
C	-1.18794200	-4.51048000	-1.23682400
C	-1.32223900	-4.32194800	0.29788200
C	-0.96386900	-5.62564700	1.05580200
C	-2.98515500	-2.52633200	1.15055900
C	-2.72985000	-3.82693500	0.64557500
C	-3.83939000	-4.67605300	0.45572800
C	-5.14084900	-4.24694600	0.76140800
C	-5.35995700	-2.94914400	1.24683400
C	-4.28941300	-2.05010200	1.44238700
C	4.14087600	-1.94227100	2.16177600
C	2.77475300	-1.54923200	2.77569200
C	2.44037300	-2.51173000	3.94969900
C	-5.64423500	0.08478500	1.07608500
C	-4.57518300	-0.62829800	1.94241200
C	-5.01485100	-0.64100300	3.43133900
H	0.42614500	0.80145300	-4.22040500
H	2.59416400	-0.00894900	-3.69664400
H	-0.13921400	-0.58516400	4.09689600
H	-2.02145600	-1.82020300	3.41364800
H	-4.72671400	0.72137800	-3.91799900
H	-4.74292800	3.16301700	-4.36445000
H	-2.73342600	4.53182100	-3.87144100
H	-1.97345100	-1.05972200	-2.14131800
H	1.93897300	-2.84509800	-2.06947100
H	-4.75699000	-1.40114300	-3.40473200
H	-4.47267000	-0.93305500	-1.71269800
H	-3.91542100	-2.50580200	-2.30914800
H	-2.78981700	-1.32470600	-5.10063100

H	-2.09331100	-2.62207300	-4.10305900
H	-1.12504000	-1.18784300	-4.50127700
H	3.85435900	-4.98127900	-0.96355600
H	2.11751200	-5.18873800	-1.24706900
H	2.68544200	-4.02649500	-0.02544500
H	3.10335400	-3.15597000	-4.28018600
H	2.31250200	-4.65102700	-3.73527000
H	4.07202300	-4.47037500	-3.58768600
H	5.62304300	-3.71529400	-1.84201400
H	7.38537500	-2.04571600	-1.32591500
H	6.78863200	0.32936600	-0.92931200
H	0.36526700	3.22193800	-2.19162300
H	3.23388700	1.63188300	-0.87414900
H	-1.26973800	5.75451900	-2.78243100
H	0.27066100	5.62859200	-1.91233500
H	-1.19352800	4.91686900	-1.21460200
H	-0.21190500	4.60728700	-4.88981900
H	0.74091100	3.12452000	-4.69679900
H	1.32890200	4.64977300	-4.00208400
H	4.69454300	1.48531300	1.15255200
H	4.60500500	3.10442100	0.44925100
H	6.06470000	2.12234800	0.20818000
H	5.81162100	2.35112100	-2.40856500
H	4.43794400	3.43132000	-2.07157500
H	4.23012700	2.04436600	-3.15796600
H	2.72521800	3.63184700	4.47418600
H	4.68054200	2.17196700	4.94208900
H	4.68812100	-0.18059700	4.15327500
H	-0.33406700	2.52306400	2.58356000
H	-0.59673800	-3.55540300	0.58631100
H	1.53406300	4.92322500	3.02014700
H	-0.09329000	4.97038800	2.31497400
H	1.20216800	4.07892000	1.47630400
H	-0.61271300	2.44509700	5.08056200
H	-1.18435900	3.98419100	4.39318000
H	0.37687500	3.90914600	5.23640000
H	-1.89441900	-5.26391200	-1.61051100
H	-0.17357800	-4.84055000	-1.49444000
H	-1.38200200	-3.56489500	-1.75458300
H	-1.04834600	-5.49222400	2.14203400
H	0.06934700	-5.91943400	0.82824100
H	-1.61728700	-6.45930600	0.76715000
H	-3.68208600	-5.68126000	0.07364900
H	-5.98227700	-4.92008400	0.61526400
H	-6.37337800	-2.62322100	1.46428800
H	2.02044600	-1.68100600	1.99204900
H	-3.66207200	-0.03012300	1.86168100
H	4.94299900	-1.93566600	2.91183500
H	4.42439300	-1.26416500	1.35113600
H	4.08737700	-2.95896900	1.75073400
H	2.46718500	-3.55623800	3.60941300
H	1.44592400	-2.31773500	4.36984900



H	3.17279200	-2.40046800	4.76079300
H	-5.34727500	0.10217900	0.02175600
H	-5.75389300	1.12287000	1.41330900
H	-6.62579900	-0.40181700	1.14990700
H	-4.25475700	-1.09878700	4.07773900
H	-5.94773900	-1.20525400	3.56329700
H	-5.18580500	0.38461500	3.78293300
O	1.15573100	2.26520500	-0.11071700
O	-1.78925700	1.73891700	0.49969800
O	-1.18210700	-1.20882500	0.28085700
O	1.49613400	-0.63525000	-0.63898700
N	-1.84237600	-1.64111400	1.37630500
N	2.30818000	-0.48207500	-1.72177600
C	-3.36738700	2.96280400	1.91950300
H	-2.91934000	2.42806800	2.75593300
C	-2.76385400	2.77792800	0.55187400
H	-3.56299100	2.56145000	-0.18471300
H	-2.30499200	3.73410600	0.22094100
C	-4.37140000	4.06026300	2.15615500
H	-5.10523000	4.11870200	1.33619500
H	-4.92229700	3.91444600	3.09408300
H	-3.89321600	5.05607900	2.21431400

## 6.4 Structures with five oxygen atoms

 $\eta^2$ -ozone ComplexFig. S79: NCCNO  $\eta^2$ -ozone Complex

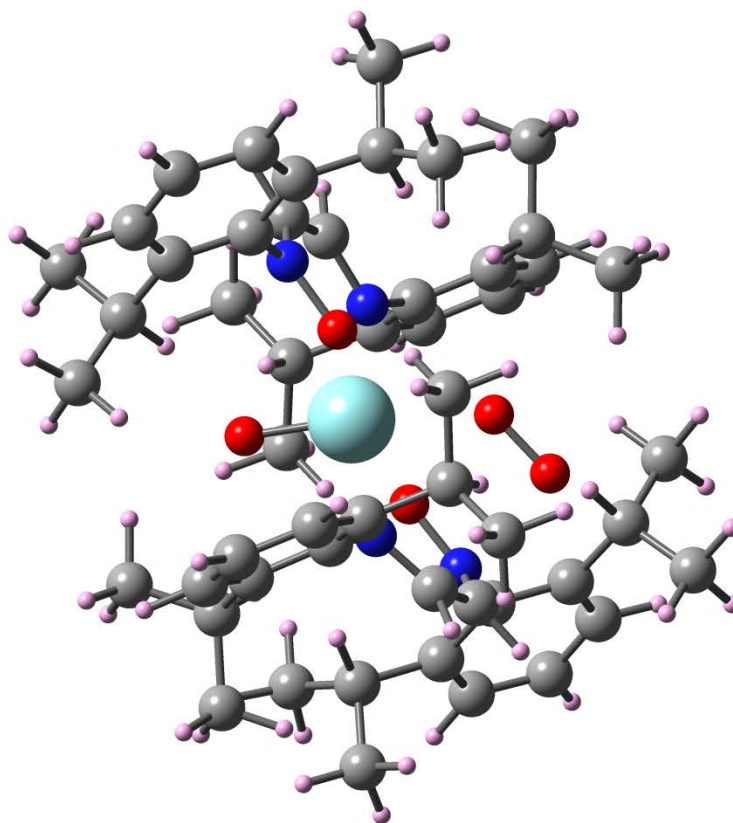
SCF	E <sub>ZP</sub>	H	G
-2666.226166	-2665.075984	-2665.005465	-2665.186472

Zr	0.00242412	-0.04414539	-0.45288925
O	-2.03872843	0.26930668	-0.04388547
O	2.03934589	-0.27252712	0.00772849
O	-0.03811094	0.91994149	-2.32103919
N	-0.09205857	-2.03288781	0.67910993
N	2.84053992	-1.41263683	0.00535389
N	0.09214835	2.13190166	0.24666671
N	-2.83555373	1.38256151	-0.30626252
C	0.98916921	-2.86279695	0.76487305
C	2.31993019	-2.59971051	0.41743319
C	-0.98708974	2.96205058	0.13637743
C	-2.31439122	2.63063919	-0.16167855
C	-1.33500210	-2.63779496	1.16798199
C	-1.74888832	-2.36719374	2.50281419

C	-2.91653385	-2.99313543	2.98515988
C	-3.66231573	-3.86176046	2.17402732
C	-3.23926668	-4.11960708	0.86336425
C	-2.07422221	-3.52271589	0.33345948
C	-1.79325476	-0.47890916	4.23899913
C	-0.92446541	-1.48394189	3.44462804
C	-0.08461881	-2.36266667	4.41274526
C	5.45799352	0.69157456	2.49984823
C	4.86724794	-0.63930146	1.97286070
C	5.34840303	-1.83613619	2.83831338
C	4.21034434	-1.24808569	-0.44771567
C	5.19933762	-0.87400037	0.49726521
C	6.52803109	-0.76365033	0.03907756
C	6.84838515	-1.00440740	-1.30683491
C	5.84579038	-1.35974904	-2.22226306
C	4.49968425	-1.48505734	-1.81705498
C	-2.77248553	-3.53608564	-2.11566000
C	-1.65372409	-3.87218979	-1.09768708
C	-1.24045810	-5.36409790	-1.21045761
C	3.45836021	-1.02382703	-4.10617025
C	3.42560691	-1.89833825	-2.82782971
C	3.57221336	-3.40104027	-3.19227482
C	1.32547911	2.82601834	0.62992602
C	2.09137507	3.51709842	-0.35080678
C	3.23748635	4.22369588	0.07516908
C	3.61693595	4.25786420	1.42362427
C	2.84792387	3.57409802	2.37719947
C	1.69852458	2.84803619	2.00348739
C	2.87163979	2.97891563	-2.71155038
C	1.72282898	3.54359054	-1.83774528
C	1.33759732	4.97574562	-2.29506610
C	-5.44787771	-0.07016614	2.60270290
C	-4.87092037	1.11155919	1.78484055
C	-5.37160687	2.46844426	2.35104828
C	-4.20692429	1.12501342	-0.70975866
C	-5.19925355	0.99396118	0.29441299
C	-6.52880787	0.78823500	-0.12799903
C	-6.84630723	0.70572883	-1.49322713
C	-5.84016596	0.82612366	-2.46446028
C	-4.49370734	1.03408001	-2.09698053
C	1.71132121	1.31938794	4.05830496
C	0.85520275	2.17106045	3.08861963
C	0.02727209	3.22557918	3.87275991
C	-3.47661206	0.07903086	-4.24248057
C	-3.41390309	1.19528493	-3.17072841
C	-3.51745816	2.59446648	-3.83795266
H	0.81128851	-3.87342986	1.13288150
H	3.03752562	-3.40935990	0.46946111
H	-0.81018574	4.02816340	0.28019209
H	-3.02932739	3.43318695	-0.29620150
H	-3.24294092	-2.80495713	4.00468366
H	-4.56032803	-4.33659184	2.56269178

H	-3.81731812	-4.79615183	0.23856408
H	-0.21798815	-0.90565469	2.83741855
H	3.77799244	-0.57105353	2.06996904
H	-2.47741177	-0.98938046	4.92878704
H	-2.39299099	0.14361415	3.56456688
H	-1.15623053	0.18087492	4.84183832
H	-0.73765533	-2.97977521	5.04415737
H	0.53338806	-1.73597870	5.06969551
H	0.58170931	-3.03657777	3.85981572
H	6.55579151	0.68161537	2.48890233
H	5.13971724	0.85739915	3.53757967
H	5.11312458	1.54030358	1.89912436
H	4.89383131	-2.77915154	2.50824235
H	5.08006982	-1.67918503	3.89149749
H	6.43892965	-1.95029051	2.77928985
H	7.31422512	-0.48557464	0.73564661
H	7.87909114	-0.91312104	-1.64195536
H	6.10701867	-1.53728561	-3.26184309
H	-0.79269827	-3.26173935	-1.37795796
H	2.43615687	-1.76551946	-2.38067557
H	-3.66713057	-4.15564815	-1.96316478
H	-2.41097814	-3.70719554	-3.13785161
H	-3.06588863	-2.48365113	-2.03165677
H	-2.07740746	-6.03338980	-0.96856850
H	-0.41282223	-5.60526958	-0.52979590
H	-0.91397514	-5.58839512	-2.23466982
H	3.37425297	0.04033577	-3.85955740
H	2.60784054	-1.28285653	-4.74760978
H	4.38044144	-1.17528066	-4.68414461
H	4.54211921	-3.60327638	-3.66705827
H	2.78015573	-3.69386819	-3.89300803
H	3.49087813	-4.04051374	-2.30337615
H	3.83370475	4.75537179	-0.66232437
H	4.49921710	4.81499642	1.73045498
H	3.14043848	3.61162237	3.42357074
H	0.86213018	2.89342667	-2.00753982
H	-3.78118858	1.08302238	1.89662053
H	3.77188053	3.60690847	-2.66142165
H	2.55196806	2.92523383	-3.76026660
H	3.14145909	1.96792152	-2.38583032
H	0.48987232	5.36767212	-1.71689677
H	1.05100410	4.96865204	-3.35506872
H	2.17505317	5.67677910	-2.17601136
H	-6.54524221	-0.08354080	2.57623235
H	-5.14402739	0.01769219	3.65425983
H	-5.08088144	-1.02910605	2.22093838
H	-4.93365589	3.31630764	1.80875141
H	-5.09984546	2.56455689	3.41065852
H	-6.46401440	2.54847611	2.27300968
H	-7.31786316	0.68888986	0.61259718
H	-7.87749335	0.54552997	-1.79980510
H	-6.09935465	0.75308983	-3.51690861

H	0.14236922	1.49902316	2.59677179
H	-2.42710107	1.12958659	-2.70344701
H	2.41574669	1.93792861	4.62886356
H	2.28942788	0.56403153	3.51268089
H	1.06782910	0.80405363	4.78260610
H	-0.60691823	2.73924202	4.62626067
H	-0.62131910	3.79981385	3.19940006
H	0.68750414	3.93515261	4.38914474
H	-3.42985472	-0.91463628	-3.78308227
H	-2.61738577	0.17243854	-4.91704536
H	-4.39212045	0.13875961	-4.84719029
H	-3.41763249	3.40097777	-3.09974046
H	-4.48140201	2.72106143	-4.34992661
H	-2.71694919	2.71415368	-4.57876873
O	-0.00326156	-0.31676620	-3.18364389
O	0.03912234	-1.36029426	-2.09511134

Oxo Complex with weakly adsorbed O<sub>2</sub> moleculeFig. S80: NCCNO Oxo Complex with weakly adsorbed O<sub>2</sub> molecule

SCF	E <sub>ZP</sub>	H	G
-2666.255567	-2665.105301	-2665.034245	-2665.214683

Zr	-0.12302900	-0.07182000	-0.32584400
O	-2.10288200	0.53492900	0.17482800
O	2.06764900	-0.38916100	-0.18690200
O	-0.48387500	-0.79069300	-1.95444200
N	0.03282900	-2.08002800	0.92278700
N	2.87350900	-1.05112300	0.69236500
N	-0.02606400	2.11683700	-0.97964900
N	-2.95118600	1.25271400	-0.67278600
C	1.05147800	-2.40211700	1.69876300
C	2.39211800	-1.89222800	1.60480600
C	-1.13252400	2.72626400	-1.48581700
C	-2.46370900	2.29854900	-1.40013900
C	-1.15981700	-2.92856400	0.99627800
C	-2.05259600	-2.84761900	2.10050300
C	-3.20064200	-3.66924700	2.07779200
C	-3.44834600	-4.55047900	1.01706500

C	-2.53489500	-4.63724900	-0.04500600
C	-1.37668100	-3.83552100	-0.08135200
C	-2.94311600	-0.83705800	3.37543300
C	-1.83492200	-1.91799500	3.29918900
C	-1.74393200	-2.71584900	4.62705000
C	4.80403700	2.38992000	2.27310800
C	4.37015100	0.90641200	2.36131400
C	4.67352100	0.33388000	3.77339700
C	4.31890800	-0.88504000	0.49090700
C	5.03182100	0.04837600	1.28014700
C	6.42454600	0.13562700	1.06304300
C	7.06074300	-0.65656400	0.09694600
C	6.31881100	-1.56304000	-0.67763200
C	4.92735200	-1.69867100	-0.50070500
C	-0.97697400	-4.02191000	-2.61396900
C	-0.34887800	-4.04163200	-1.20080800
C	0.43553800	-5.36050600	-0.95384100
C	4.51725300	-2.73091900	-2.81370800
C	4.13978900	-2.73437900	-1.31187700
C	4.34143100	-4.15259100	-0.70828900
C	1.19620700	2.90475500	-1.03851700
C	2.06534000	2.77054300	-2.15600200
C	3.23105100	3.56539900	-2.19244400
C	3.52554800	4.47145200	-1.16227900
C	2.65144000	4.59592700	-0.07031200
C	1.47730300	3.81940200	0.01665500
C	2.89442100	0.81425300	-3.56783800
C	1.74997200	1.82828500	-3.32284600
C	1.43586600	2.63017200	-4.61406700
C	-4.88645000	2.48705200	2.84380300
C	-4.47826700	2.70309500	1.36477400
C	-4.82821700	4.14770300	0.91329200
C	-4.37113000	0.97555400	-0.55381400
C	-5.12068700	1.67492900	0.42763200
C	-6.50654400	1.42082900	0.49061300
C	-7.11054200	0.50141200	-0.38196100
C	-6.34039700	-0.18648400	-1.33308400
C	-4.94956100	0.02920900	-1.43721900
C	1.22908200	3.94344700	2.57005300
C	0.51727700	4.01205900	1.19702700
C	-0.26010200	5.34908300	1.05234000
C	-4.46786400	-2.20214700	-2.59150100
C	-4.12088800	-0.69647200	-2.50129000
C	-4.30393600	-0.01445000	-3.88550900
H	0.93173200	-3.19726100	2.43761100
H	3.13191200	-2.31103700	2.27589000
H	-0.98935500	3.66382700	-2.02525400
H	-3.22058300	2.86093700	-1.93349000
H	-3.90626800	-3.61442600	2.90298100
H	-4.34059500	-5.17221200	1.02147000
H	-2.71956500	-5.33975300	-0.85325600
H	-0.88911600	-1.38839600	3.17522900

H	3.28499100	0.87389700	2.22444500
H	-3.93360000	-1.28890700	3.52410600
H	-2.96426200	-0.24800300	2.45267400
H	-2.74858200	-0.15876800	4.21726800
H	-2.68351600	-3.23709100	4.85233500
H	-1.53176700	-2.03320600	5.46043000
H	-0.94564000	-3.46985000	4.59173300
H	5.87387700	2.51640700	2.48531400
H	4.24992300	2.98093000	3.01251600
H	4.59416500	2.80562800	1.28148200
H	4.32074800	-0.70035300	3.87707400
H	4.16907600	0.93591400	4.53922200
H	5.75202000	0.34548300	3.98103100
H	7.01066000	0.83553400	1.65109300
H	8.13396000	-0.56825500	-0.05408700
H	6.82395800	-2.16815900	-1.42468700
H	0.36244800	-3.21160500	-1.17550600
H	3.07395000	-2.48833200	-1.25404800
H	-1.74986700	-4.79230400	-2.73927400
H	-0.19948700	-4.20545400	-3.36806100
H	-1.40574500	-3.03510700	-2.81040900
H	-0.23264100	-6.23109300	-0.99608700
H	0.92368100	-5.36328300	0.03068900
H	1.21038800	-5.49223200	-1.72147800
H	4.41158500	-1.73121000	-3.24828100
H	3.85450200	-3.41176000	-3.36287300
H	5.54784800	-3.07164700	-2.97793200
H	5.39636300	-4.45252200	-0.75980900
H	3.74862800	-4.89031300	-1.26369900
H	4.03182200	-4.19294500	0.34418100
H	3.90862200	3.47867200	-3.03879300
H	4.42541400	5.08071000	-1.21239100
H	2.88172100	5.30603500	0.72057800
H	0.85729300	1.24599100	-3.07327100
H	-3.39049500	2.58630100	1.30887500
H	3.82485400	1.31330500	-3.87226200
H	2.60884900	0.11395500	-4.36413600
H	3.09155700	0.23897800	-2.65670100
H	0.59045100	3.31433700	-4.46318800
H	1.17699700	1.94473000	-5.43214300
H	2.29976600	3.22931900	-4.93314200
H	-5.95754800	2.66905900	3.00170600
H	-4.33483600	3.18331900	3.48924200
H	-4.66125100	1.46660100	3.17150000
H	-4.49930700	4.33696800	-0.11606400
H	-4.33813500	4.88159400	1.56682800
H	-5.91176400	4.32123600	0.95870000
H	-7.11493400	1.94149900	1.22532200
H	-8.18121900	0.31962500	-0.31926500
H	-6.82201100	-0.89947800	-1.99608700
H	-0.21195200	3.19627100	1.17762900
H	-3.06013900	-0.62242000	-2.23727000



H	1.98065200	4.73617000	2.68504100
H	1.71949100	2.97339700	2.70546200
H	0.49433800	4.06139000	3.37774600
H	-0.97243800	5.47032900	1.87997900
H	-0.82187200	5.38367300	0.11024500
H	0.42558100	6.20724200	1.06619300
H	-4.35037000	-2.69496400	-1.61921700
H	-3.79253600	-2.69271500	-3.30291100
H	-5.49542600	-2.36835000	-2.94287900
H	-4.00603900	1.04118800	-3.85372500
H	-5.35064600	-0.06423800	-4.21668000
H	-3.68031000	-0.51644200	-4.63621900
O	0.23938100	0.50410000	2.07153200
O	1.12862900	-0.00436500	2.93309600

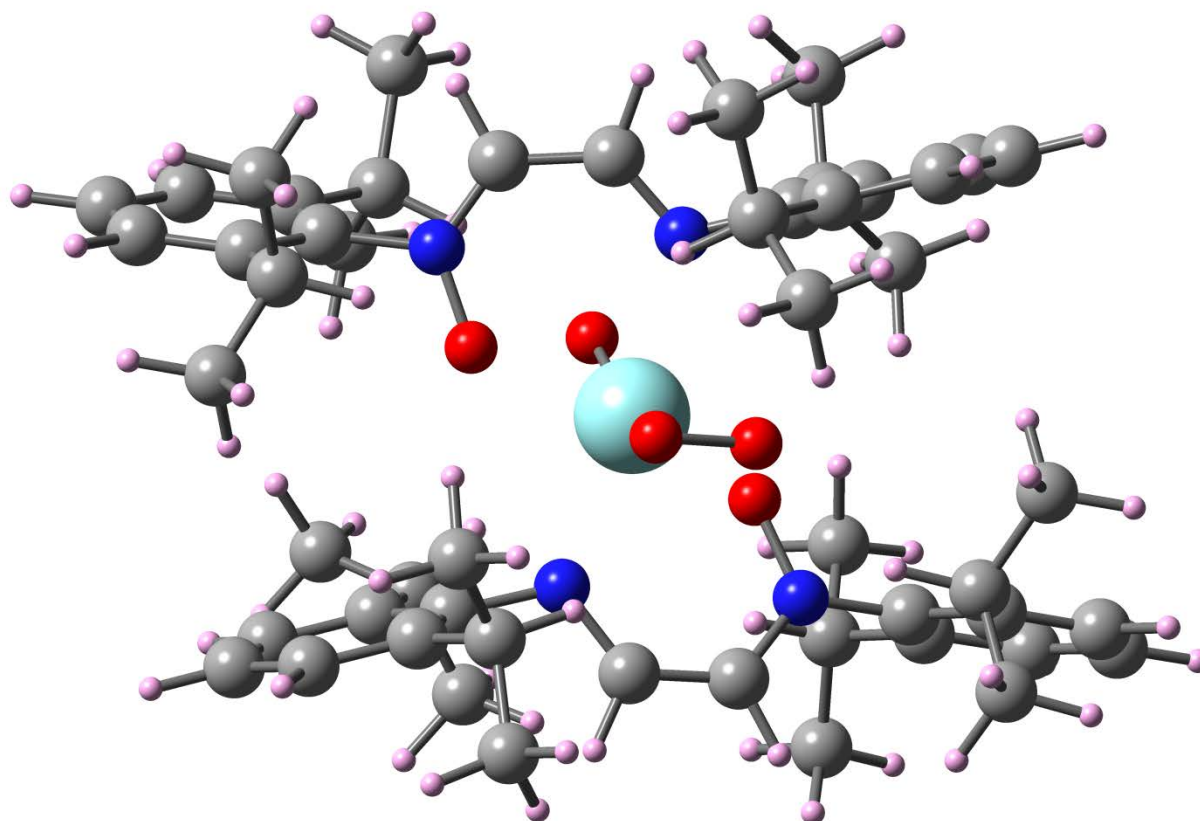
**Oxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation 1 lower energy)**

Fig. S81: NCCNO Oxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G
-2666.253675	-2665.102355	-2665.031790	-2665.211288

Zr	0.12817901	-0.00958600	-0.11615801
O	-2.13617716	0.42261103	0.19699002
O	2.03228016	-0.86191507	-0.57318304
O	-0.37834903	0.02124900	-1.88229214
N	-0.12027901	-2.05278516	0.91080407
N	2.86339822	-1.57302412	0.28815502
N	-0.02861900	2.44049219	-0.41808003
N	-2.84870722	1.24345810	-0.57952305
C	0.97003607	-2.69325221	1.42408911
C	2.32805418	-2.45910719	1.17694609
C	-1.12673808	3.03905523	-0.78322506
C	-2.42753419	2.43148419	-0.98455207
C	-1.39716711	-2.64885420	1.28624910
C	-1.90101315	-2.48722019	2.60802920
C	-3.12360124	-3.11260824	2.93986823

C	-3.83204429	-3.87134330	1.99919515
C	-3.32063526	-4.02151731	0.69951406
C	-2.10103016	-3.42599026	0.31890602
C	-2.05043415	-0.50414004	4.20612132
C	-1.17447609	-1.67125513	3.68480628
C	-0.71027205	-2.57172520	4.86054037
C	5.02636938	1.53900612	1.88433314
C	4.64475835	0.04085100	1.99182015
C	5.17694240	-0.56843105	3.31652525
C	4.27810733	-1.52796712	-0.03198600
C	5.14356639	-0.75636506	0.78386606
C	6.51551351	-0.74933206	0.45018303
C	6.99513055	-1.46324711	-0.65843405
C	6.11107746	-2.20662117	-1.45767011
C	4.73374336	-2.25817617	-1.16121809
C	-2.59218920	-3.99319031	-2.14427316
C	-1.51975612	-3.66424328	-1.08028508
C	-0.46417804	-4.80595137	-1.04984208
C	3.74225429	-2.53543319	-3.48580326
C	3.79090229	-3.08816023	-2.03784215
C	4.18689332	-4.58799135	-2.02733616
C	1.16902909	3.27870025	-0.31272102
C	2.09644316	3.25886025	-1.39035111
C	3.23935425	4.07813131	-1.28012510
C	3.45603127	4.88083937	-0.15026601
C	2.52281819	4.88095937	0.89656007
C	1.36092411	4.08265731	0.84449306
C	3.08795324	1.61783812	-3.08831123
C	1.85524414	2.45885519	-2.67684720
C	1.43096111	3.41434226	-3.82627429
C	-5.44317243	0.15688501	2.49171319
C	-4.96759338	1.21573409	1.46595011
C	-5.66097041	2.58271620	1.71819513
C	-4.19543932	0.78243306	-0.97135207
C	-5.20218140	0.75480006	0.02366100
C	-6.48505650	0.33416603	-0.38308903
C	-6.73464051	-0.04400900	-1.71140713
C	-5.70665444	-0.00821600	-2.66600920
C	-4.40036833	0.40448903	-2.32480518
C	1.06440108	3.88003929	3.37447226
C	0.36738203	4.12361332	2.01242415
C	-0.41545803	5.46500343	2.02746815
C	-3.28698225	-0.81358206	-4.28773133
C	-3.30094925	0.45265803	-3.39689026
C	-3.47052027	1.71005513	-4.29598633
H	0.78121506	-3.51668427	2.11424316
H	3.05738423	-3.05469223	1.71270313
H	-1.10643408	4.10746931	-1.01520708
H	-3.16265124	3.01652223	-1.52162312
H	-3.51992227	-3.00181723	3.94689530
H	-4.77154236	-4.34609733	2.27384517
H	-3.87395430	-4.61482535	-0.02171500

H	-0.28640002	-1.21453909	3.24187625
H	3.55245427	-0.00415700	2.01727815
H	-2.96330623	-0.86809207	4.69713336
H	-2.33813518	0.15693401	3.38104126
H	-1.48581411	0.09201601	4.93476938
H	-1.56412512	-3.03709023	5.37141843
H	-0.15936401	-1.97561415	5.60048741
H	-0.05119700	-3.37856326	4.51369235
H	6.11525944	1.68489413	1.89844815
H	4.59971035	2.09226116	2.73065321
H	4.63099135	1.98172615	0.96290407
H	4.87395437	-1.61812212	3.42642526
H	4.78157037	-0.00938300	4.17473632
H	6.27386149	-0.52912604	3.36265326
H	7.20860256	-0.17289901	1.05755408
H	8.05522260	-1.43965911	-0.90105507
H	6.49421851	-2.75469721	-2.31487618
H	-1.00782308	-2.74706621	-1.39702911
H	2.77681721	-3.00604223	-1.63553712
H	-3.01872723	-4.99500238	-1.99678015
H	-2.13776116	-3.97594430	-3.14319324
H	-3.41449926	-3.26788825	-2.12688216
H	-0.92700307	-5.75004343	-0.72987506
H	0.35905903	-4.57840235	-0.36471603
H	-0.03875100	-4.95580238	-2.05177016
H	3.40499426	-1.49351112	-3.48852427
H	3.03887823	-3.12301624	-4.09067631
H	4.72739536	-2.58482920	-3.96962030
H	5.18463240	-4.74599536	-2.45815619
H	3.47013326	-5.17179540	-2.61997820
H	4.19393432	-4.99181138	-1.00657408
H	3.96184730	4.08953431	-2.09166416
H	4.34510233	5.50384842	-0.08705801
H	2.69921520	5.50332544	1.76983013
H	1.03433008	1.75147713	-2.51892219
H	-3.89274729	1.34840110	1.62566112
H	3.96002630	2.24364817	-3.32170126
H	2.84849622	1.03164108	-3.98522731
H	3.36201625	0.91687807	-2.29230417
H	0.52548004	3.98062130	-3.56678927
H	1.22139209	2.83825122	-4.73704936
H	2.22368917	4.13984732	-4.05530931
H	-6.52703152	-0.00760400	2.43181519
H	-5.21409840	0.49570104	3.51003127
H	-4.93754238	-0.80092806	2.32918618
H	-5.30490741	3.35163326	1.01949308
H	-5.45410142	2.92871922	2.73917921
H	-6.74980954	2.50269619	1.60215012
H	-7.29108055	0.30343602	0.34438603
H	-7.73090061	-0.36781203	-2.00295215
H	-5.91453447	-0.31293002	-3.68719428
H	-0.35263503	3.30840525	1.89093315

H	-2.31649118	0.48935604	-2.91316922
H	1.77545413	4.68018936	3.61991327
H	1.59737312	2.92430622	3.36017926
H	0.31452702	3.84313729	4.17573232
H	-1.14071409	5.47411242	2.85216622
H	-0.96317507	5.62918744	1.08897509
H	0.26361302	6.31680247	2.16572617
H	-3.19554924	-1.72054613	-3.68438528
H	-2.41964719	-0.77050906	-4.95797338
H	-4.18740832	-0.89771707	-4.91174138
H	-3.44305026	2.64608720	-3.72257729
H	-4.42634734	1.68276913	-4.83717337
H	-2.66100220	1.74847713	-5.03584339
O	1.41340011	0.93149207	1.60905312
O	0.11292001	0.86355707	2.10290216

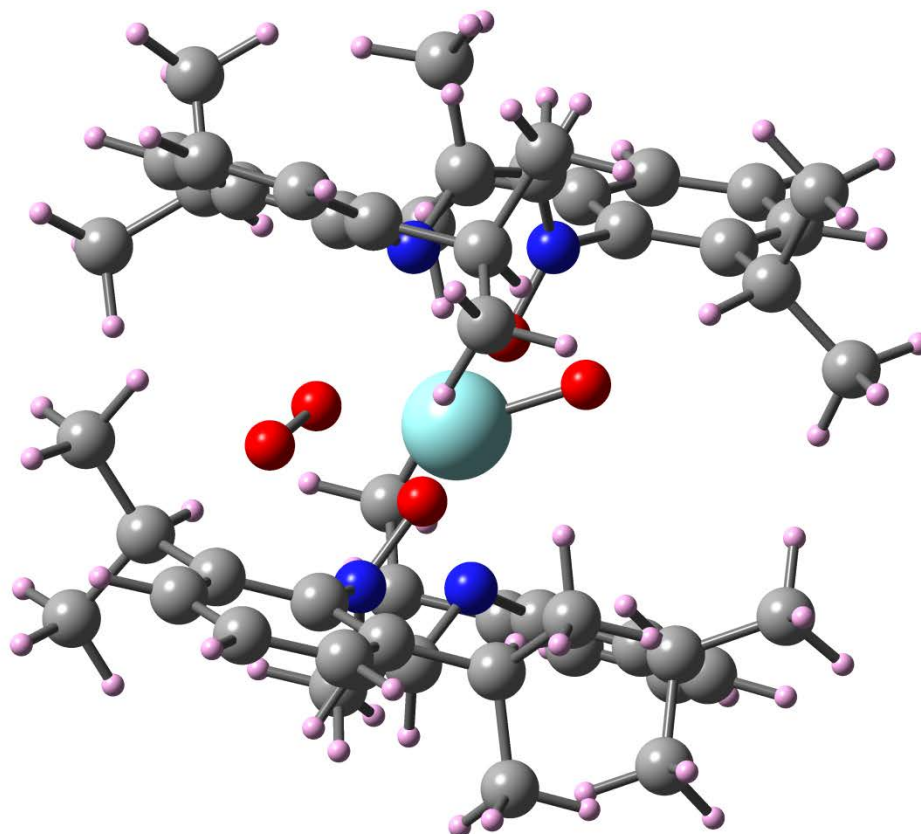
**Oxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation 2 higher energy)**

Fig. S82: NCCNO Oxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation 2 higher energy)

SCF	E <sub>ZP</sub>	H	G
-2666.252034	-2665.101731	-2665.031389	-2665.212183

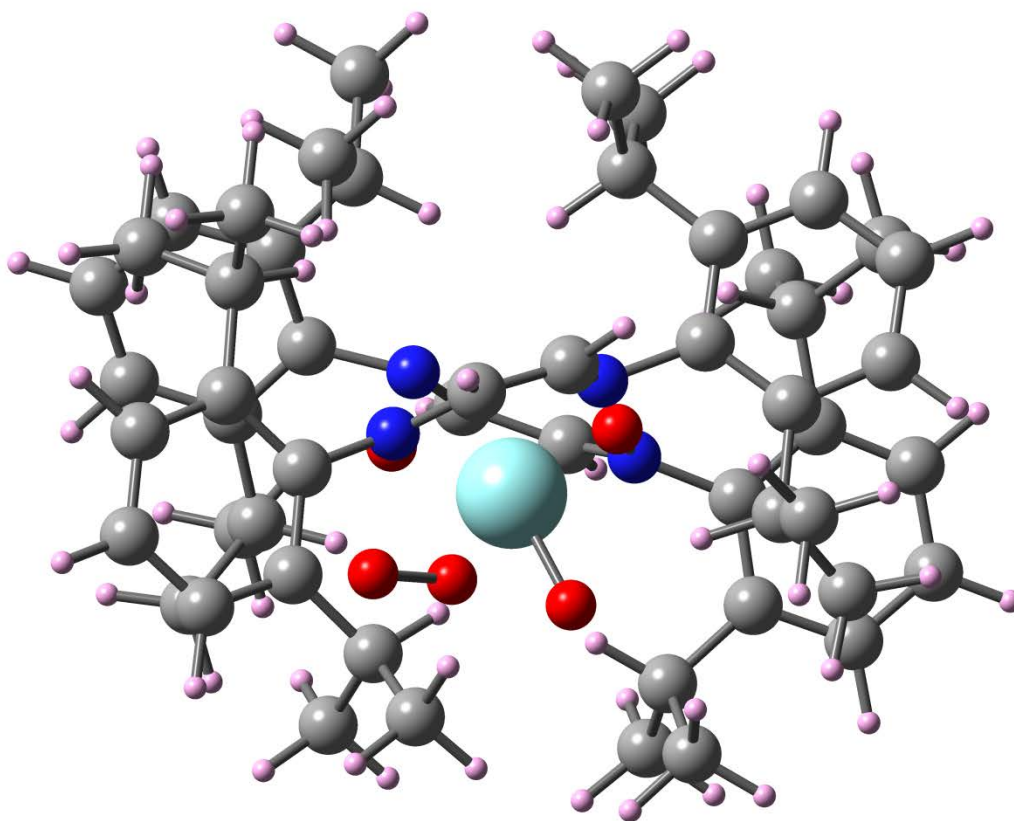
Zr	-0.02547100	-0.09727000	-0.00349500
O	2.27616800	0.41697600	-0.20090200
O	-2.08002500	-0.58861700	0.32359600
O	0.54179400	-0.47911600	1.70347100
N	-0.09781000	-2.07882500	-1.09438400
N	-2.96595000	-1.11312000	-0.61741100
N	0.12127900	2.22240100	0.76418200
N	2.98664600	1.09931300	0.68853700
C	-1.23067600	-2.49557300	-1.72537500
C	-2.53442200	-2.01920800	-1.54657700
C	1.19077100	2.69846600	1.34224300
C	2.50923700	2.10525800	1.40972700
C	1.06045400	-2.95480700	-1.20706900
C	1.95227300	-2.82760000	-2.30629400
C	3.07168400	-3.68735400	-2.35979100

C	3.30122100	-4.64482100	-1.36203100
C	2.39879400	-4.76941000	-0.29215100
C	1.26504900	-3.93785800	-0.19412000
C	2.91684700	-0.85462600	-3.60373300
C	1.71931100	-1.82262000	-3.43883900
C	1.40914900	-2.54943100	-4.77448900
C	-4.76401500	2.45014300	-1.91452400
C	-4.43628800	0.94797300	-2.09874700
C	-4.85265300	0.46770400	-3.51536400
C	-4.37418200	-0.91703700	-0.31626900
C	-5.09237700	0.07680800	-1.02546700
C	-6.46669700	0.21846800	-0.73489300
C	-7.08826800	-0.58345600	0.23414500
C	-6.34750100	-1.55061600	0.93261400
C	-4.97453100	-1.74012800	0.67317800
C	0.88354700	-4.43790600	2.30494300
C	0.24311600	-4.14514800	0.92937800
C	-0.74322600	-5.28311700	0.54436500
C	-4.31611800	-2.68125100	2.95522900
C	-4.19789000	-2.83134100	1.41738100
C	-4.67149600	-4.23964800	0.96576400
C	-1.05536300	3.09821100	0.79872000
C	-1.97121000	2.96049900	1.87613500
C	-3.06603600	3.84972700	1.91339500
C	-3.24382300	4.82924800	0.92453200
C	-2.32711100	4.93360100	-0.13220100
C	-1.21466100	4.07105400	-0.22395700
C	-3.05868500	1.15569700	3.32991600
C	-1.76686900	1.94346500	3.00600100
C	-1.22403300	2.65117900	4.27819700
C	5.47710600	1.91581300	-2.59937100
C	4.87412800	2.28038800	-1.21956600
C	5.23864200	3.74141800	-0.83648800
C	4.41386000	0.73784000	0.80877900
C	5.31717000	1.31014000	-0.11862400
C	6.67876600	0.98020000	0.04082800
C	7.09709900	0.11890300	1.06822000
C	6.16403400	-0.43768400	1.95656300
C	4.78652000	-0.14703900	1.84673300
C	-0.90781100	4.23990700	-2.75921400
C	-0.21396600	4.23708100	-1.37437400
C	0.63305300	5.52464700	-1.17935000
C	4.00564400	-2.24951700	3.06308800
C	3.77471000	-0.73606300	2.83676700
C	3.84051200	0.02249800	4.19169800
H	-1.13868700	-3.31707400	-2.43794200
H	-3.32443200	-2.43813900	-2.15818700
H	1.13362200	3.66865200	1.84445400
H	3.22991000	2.57744100	2.06517200
H	3.76622000	-3.60560500	-3.19290400
H	4.17097200	-5.29577000	-1.41979800
H	2.57648000	-5.52445100	0.46935200

H	0.85146100	-1.20728100	-3.18601800
H	-3.35007600	0.83875600	-2.01960500
H	3.83276200	-1.38813500	-3.89435900
H	3.10443000	-0.32278400	-2.66486200
H	2.69499600	-0.11039300	-4.37988800
H	2.25824800	-3.16496400	-5.10168000
H	1.19744500	-1.81697800	-5.56507800
H	0.53645400	-3.20907000	-4.67870800
H	-5.83186300	2.65797300	-2.06654800
H	-4.20186000	3.04416200	-2.64638000
H	-4.48475900	2.79715300	-0.91357000
H	-4.58630500	-0.58482900	-3.67680200
H	-4.34298500	1.06549600	-4.28195800
H	-5.93652800	0.56944900	-3.66547200
H	-7.05008700	0.96532900	-1.26656600
H	-8.14774000	-0.45614100	0.44510200
H	-6.83992200	-2.16505300	1.68196700
H	-0.32926600	-3.21849200	1.03770000
H	-3.13668300	-2.73452400	1.16916800
H	1.41983600	-5.39677200	2.31898700
H	0.10105100	-4.48679100	3.07385900
H	1.58017600	-3.64239800	2.58363200
H	-0.20857500	-6.23482400	0.41842800
H	-1.26556700	-5.06197600	-0.39446900
H	-1.49885400	-5.41812600	1.33062900
H	-3.96343000	-1.69655600	3.28051000
H	-3.70491400	-3.44479300	3.45427300
H	-5.35166500	-2.80720600	3.29850300
H	-5.73205400	-4.39665300	1.20357200
H	-4.09051600	-5.01903000	1.47604700
H	-4.54450300	-4.37553500	-0.11579700
H	-3.78261000	3.77568200	2.72682600
H	-4.09339300	5.50608700	0.97623200
H	-2.47627800	5.69134400	-0.89696200
H	-1.01961000	1.20445300	2.69735300
H	3.78494600	2.21971800	-1.32640600
H	-3.85536600	1.80425100	3.71866500
H	-2.84314200	0.39916200	4.09588200
H	-3.42767800	0.64128000	2.43649500
H	-0.27342300	3.16630600	4.08238600
H	-1.05072100	1.91546800	5.07429500
H	-1.93732400	3.39880900	4.65150700
H	6.56886300	2.02827400	-2.60965100
H	5.06856500	2.58135600	-3.37054900
H	5.23496900	0.88471500	-2.87781500
H	4.78425200	4.03598500	0.11858600
H	4.88606200	4.43647700	-1.60943200
H	6.32575900	3.86213000	-0.74125600
H	7.41309100	1.39564900	-0.64321200
H	8.15222100	-0.12185500	1.17366500
H	6.50503900	-1.10958900	2.73828000
H	0.46610900	3.37943500	-1.37606800



H	2.75581100	-0.62420100	2.44176500
H	-1.60984200	5.07781100	-2.86660200
H	-1.44605700	3.29930500	-2.91536500
H	-0.15395900	4.33148100	-3.55233300
H	1.36701600	5.62427900	-1.99018600
H	1.17723500	5.51338300	-0.22467500
H	-0.00246200	6.42021200	-1.18658000
H	3.93305800	-2.80621300	2.12142300
H	3.23982100	-2.63513500	3.74637700
H	4.98467800	-2.45760500	3.51521400
H	3.63749400	1.09495700	4.07123800
H	4.82901100	-0.08191800	4.66029100
H	3.08846400	-0.38257500	4.88002600
O	0.36451200	0.95542200	-2.03847700
O	-1.02875700	0.91170700	-2.03129100

**Oxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)**Fig. S83: NCCNO Oxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)

SCF	E <sub>ZP</sub>	H	G
-2666.250739	-2665.100113	-2665.029174	-2665.211025

O	-2.20063567	-0.51455241	-0.27804372
O	-1.04167802	1.26125279	-2.10362012
N	-0.06256477	-2.04500591	0.85484287
N	-2.98343497	-1.63449301	-0.01848543
N	2.80781247	1.13260099	-0.37397297
N	0.34841929	2.81268633	0.42786722
C	-1.14370030	-2.83496671	1.10789257
C	-2.46796436	-2.68518691	0.67417365
C	2.64978537	2.44400154	-0.37201155
C	1.49225627	3.24908376	-0.01850593
C	1.15807535	-2.55831791	1.47834738
C	1.93092436	-3.55134985	0.81076680
C	3.04670141	-4.09513631	1.48457871
C	3.39003939	-3.68604990	2.78068024
C	2.61858728	-2.70648605	3.42428667
C	1.50084767	-2.12532507	2.79022992

C	2.77020623	-4.05394446	-1.54958656
C	1.56527028	-4.09118613	-0.57650434
C	0.99753523	-5.53300794	-0.47379059
C	-3.18984827	-1.14457998	-3.90888604
C	-3.37910976	-2.26276574	-2.84944232
C	-3.57450805	-3.64192437	-3.52939754
C	-4.33556687	-1.59626415	-0.54068531
C	-4.53638954	-1.92129823	-1.90775164
C	-5.86087140	-1.89681178	-2.39288055
C	-6.93476355	-1.56300262	-1.55243832
C	-6.70433522	-1.22963119	-0.20857078
C	-5.39750618	-1.22690099	0.32332852
C	1.50351839	0.01145068	4.20008604
C	0.64940091	-1.10480367	3.55129120
C	-0.22325501	-1.81237825	4.62377804
C	-5.67743851	0.61675364	2.05052780
C	-5.16758401	-0.82293007	1.78222330
C	-5.82370437	-1.83283583	2.76029239
C	4.10422730	0.54847580	-0.78681906
C	4.31259686	0.25180733	-2.15509174
C	5.56046684	-0.31708448	-2.49504229
C	6.53615110	-0.56769425	-1.52111113
C	6.29332251	-0.25021950	-0.17427450
C	5.06651393	0.31262423	0.22849988
C	2.90535692	-0.72009756	-4.05625681
C	3.29639412	0.55244673	-3.26132507
C	3.84343576	1.65354167	-4.21093516
C	-2.17593462	1.64068912	3.26253651
C	-1.03455358	2.63901129	2.94365244
C	-0.57627210	3.39440123	4.22021594
C	-0.73893906	3.72382045	0.61574131
C	-1.45358689	3.62172010	1.84852288
C	-2.53888949	4.48622231	2.07513049
C	-2.93510837	5.41999420	1.10533065
C	-2.25324363	5.48253475	-0.11788721
C	-1.15199982	4.64861620	-0.40276359
C	5.40593936	-0.32445186	2.69126859
C	4.82769368	0.70416010	1.69107889
C	5.41786511	2.11402355	1.97935329
C	-1.60440720	4.53327731	-2.91347585
C	-0.53460727	4.73714141	-1.80805102
C	0.21059673	6.08421140	-2.01289427
H	-0.97309395	-3.73505265	1.70074208
H	-3.17491099	-3.47754987	0.88987586
H	3.52043815	2.99071642	-0.71712429
H	1.67356794	4.31956221	-0.16592530
H	3.64193960	-4.85893658	0.99018200
H	4.24323930	-4.13135947	3.28800195
H	2.88235448	-2.39887331	4.43358069
H	0.79402465	-3.45272754	-1.01353647
H	-2.44837388	-2.31158536	-2.27709035
H	3.57403744	-4.73694152	-1.24079001

H	3.18692874	-3.04206015	-1.61556493
H	2.44377517	-4.35108758	-2.55464642
H	1.73843767	-6.22667327	-0.05190294
H	0.71656874	-5.90025155	-1.47004543
H	0.10401195	-5.56755178	0.16321742
H	-4.07403449	-1.05256264	-4.55534060
H	-2.32069437	-1.37496359	-4.53709346
H	-3.00696436	-0.17743955	-3.42753835
H	-3.69865717	-4.44145674	-2.78704482
H	-2.69457008	-3.87850933	-4.14100121
H	-4.45346138	-3.65233619	-4.18830276
H	-6.05097277	-2.14142953	-3.43460162
H	-7.94879247	-1.55519102	-1.94599647
H	-7.54309423	-0.95984785	0.42853396
H	-0.02865502	-0.63121287	2.83283672
H	-4.08922835	-0.82639730	1.97493191
H	2.19400511	-0.38821803	4.95400521
H	0.85727052	0.74167790	4.70283969
H	2.09460456	0.54150744	3.44316551
H	0.40582248	-2.32003963	5.36740017
H	-0.87787613	-2.56450414	4.16685288
H	-0.85521695	-1.08578119	5.15316613
H	-5.18876969	1.33615815	1.38266991
H	-5.46206464	0.90819488	3.08718843
H	-6.76202702	0.69377386	1.89906949
H	-6.91331472	-1.86438998	2.62853714
H	-5.61841715	-1.54667963	3.80050415
H	-5.43841110	-2.84865083	2.60347717
H	5.76172263	-0.56442843	-3.53331248
H	7.48722131	-1.00920440	-1.80878969
H	7.05896679	-0.45029707	0.56875665
H	2.37406778	0.93608584	-2.81854115
H	-0.18202259	2.06149032	2.57173871
H	3.78104148	-1.20391724	-4.51007578
H	2.21305594	-0.44782314	-4.86301084
H	2.38478457	-1.43890450	-3.41593600
H	4.10011056	2.57252420	-3.66584718
H	3.08433294	1.90421101	-4.96216050
H	4.74430231	1.31547975	-4.74000698
H	-3.06570016	2.15679598	3.64655733
H	-1.85103884	0.92129726	4.02556187
H	-2.46648037	1.08391032	2.36386419
H	0.26109243	4.07065042	4.00376613
H	-0.25202420	2.68458742	4.99196589
H	-1.39198470	3.99597816	4.64223551
H	-3.07723808	4.43030429	3.01765973
H	-3.77515700	6.08373826	1.29491252
H	-2.58999387	6.18433972	-0.87600181
H	3.74571129	0.74326091	1.86317645
H	0.18359112	3.92387879	-1.94384092
H	6.50366221	-0.33785389	2.67261972
H	5.03810258	-1.33302677	2.47946340

H	5.09972930	-0.05896609	3.71126308
H	5.21947099	2.40350257	3.01956877
H	4.98668885	2.88401897	1.32688935
H	6.50516264	2.11656025	1.82678913
H	-2.09523782	3.56207007	-2.79458241
H	-1.12329465	4.54971609	-3.90056647
H	-2.36736298	5.32221024	-2.90033250
H	1.00443080	6.23527388	-1.26785796
H	-0.47985692	6.93378690	-1.92989518
H	0.66634254	6.11847795	-3.01137386
O	0.14213561	-1.58787614	-2.12980096
O	0.33554300	1.43684277	-2.13393886
O	1.87409802	0.25058376	0.04625223
Zr	-0.13551694	-0.38229613	-0.81337624

## 6.5 Structures with six oxygen atoms

### Oxo Complex with adsorbed ozone group (conformation 1 lower energy)

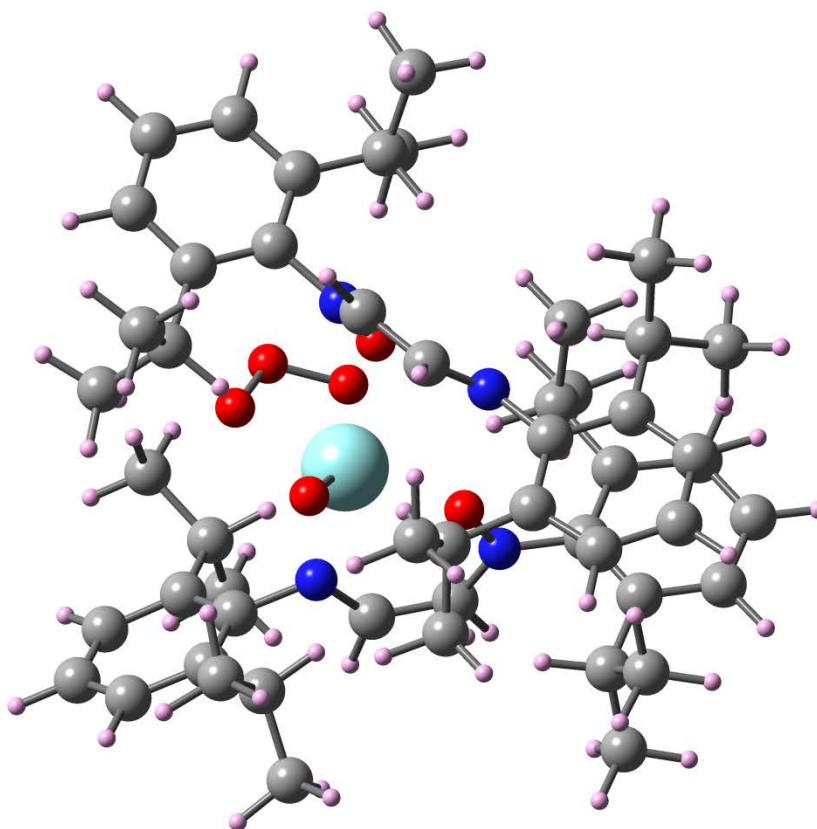


Fig. S84: NCCNO Oxo Complex with adsorbed ozone group (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G
-2741.401498	-2740.248894	-2740.176349	-2740.363029

Zr	-0.92430599	-0.27379342	-0.00216095
O	0.96576072	-1.07123326	-0.49614491
O	-0.47604832	1.87885245	-0.42209627
O	-2.98618888	0.25844665	-0.71480433
N	1.92505319	2.07667089	1.30014126
N	-0.85230553	2.91897201	0.36979493
N	-1.50439609	-2.48463861	-0.20393193
N	1.32659009	-2.12843041	-1.32802989
C	1.05945958	2.76859907	1.97645475
C	-0.17217790	3.31536999	1.42506056
C	-0.75815745	-3.39137370	-0.88904294
C	0.51762096	-3.21975788	-1.44544071
C	3.12688207	1.60223748	1.88911303
C	3.15734672	0.89742559	3.13482148

C	4.42033044	0.51914798	3.63674093
C	5.60541590	0.80219062	2.94118600
C	5.54963755	1.43611629	1.68732820
C	4.31965147	1.82801453	1.13078110
C	1.89021212	-1.09940900	4.06686653
C	1.89660089	0.44096502	3.88433717
C	1.75496047	1.14853899	5.25814441
C	-4.55195070	1.64680892	1.91441078
C	-3.34719368	2.61966626	1.99359118
C	-3.43749520	3.49413908	3.27361930
C	-2.07577340	3.63067641	-0.04447166
C	-3.24987307	3.49652337	0.73860521
C	-4.37990910	4.22482513	0.30776248
C	-4.34055006	5.01739332	-0.84839105
C	-3.16367614	5.10432141	-1.60877355
C	-1.99844417	4.41090562	-1.22493897
C	5.28010750	2.04216862	-1.24334453
C	4.24649385	2.55372322	-0.21410592
C	4.39065804	4.08851016	-0.01353540
C	-0.94220893	3.89146179	-3.47090079
C	-0.72716052	4.52873993	-2.07245436
C	-0.26167641	6.00313869	-2.19660420
C	-2.77162038	-2.98990250	0.32309695
C	-3.88334406	-3.17810611	-0.54956836
C	-5.08154825	-3.68718530	-0.00508496
C	-5.19007333	-3.99923040	1.35734743
C	-4.08621445	-3.81056383	2.20099873
C	-2.86281589	-3.30945261	1.70789190
C	-5.00705901	-1.98456106	-2.51482004
C	-3.82699324	-2.87752908	-2.05254315
C	-3.79854874	-4.19181404	-2.88133911
C	4.50685895	-2.86002368	1.18733591
C	3.55104640	-3.41058080	0.09839505
C	3.74255937	-4.94095785	-0.07742447
C	2.65277117	-2.04846636	-1.90810523
C	3.73151296	-2.67685160	-1.23377409
C	5.00397592	-2.61234628	-1.83917267
C	5.19302361	-1.92954968	-3.05131705
C	4.11233736	-1.29254189	-3.68123351
C	2.81719499	-1.33666104	-3.12338395
C	-2.00984706	-2.40241417	3.94223161
C	-1.66670352	-3.19843951	2.65960857
C	-1.12050472	-4.61109147	3.00507315
C	1.86983403	0.92200617	-3.77190227
C	1.65945312	-0.61469128	-3.81647256
C	1.45921154	-1.10763754	-5.27233226
H	1.23377681	3.06999298	3.01688658
H	-0.61480640	4.15329023	1.95343022
H	-1.18480491	-4.38386829	-1.03727924
H	0.94006265	-4.02928838	-2.02837625
H	4.47427246	-0.01836069	4.58021864
H	6.56496020	0.51038850	3.36172431

H	6.46930940	1.61952695	1.13962109
H	1.00595080	0.66670613	3.28903373
H	-2.45538250	1.98901222	2.07127636
H	2.71497649	-1.44334838	4.70508768
H	1.96870140	-1.60358543	3.09638524
H	0.94655509	-1.40919954	4.53128881
H	2.60124767	0.91206620	5.91715088
H	0.83469453	0.82030337	5.75849338
H	1.71583968	2.24177799	5.15456562
H	-5.51234092	2.17988925	1.93590042
H	-4.52818765	0.96431508	2.77333229
H	-4.50398198	1.04687015	1.00006179
H	-2.57147303	4.16232452	3.38230978
H	-3.48194701	2.85222230	4.16261037
H	-4.33899144	4.12130068	3.26313895
H	-5.30290061	4.15200653	0.87552957
H	-5.22871243	5.56076953	-1.16180749
H	-3.14814464	5.71596828	-2.50669914
H	3.24293361	2.36927256	-0.61681758
H	0.07802537	3.96464285	-1.59080776
H	6.31055363	2.28424387	-0.94966286
H	5.09950171	2.51737110	-2.21672701
H	5.20580762	0.95630226	-1.37808395
H	5.37510066	4.33664766	0.40628148
H	3.62433581	4.47611869	0.66973895
H	4.28767519	4.61243855	-0.97350693
H	-1.21613754	2.83492261	-3.37890626
H	-0.01850893	3.95938363	-4.06070614
H	-1.73646438	4.40742545	-4.02662975
H	-1.00094733	6.61812537	-2.72574231
H	0.67821874	6.05328109	-2.76180241
H	-0.09202089	6.45584184	-1.21080474
H	-5.93921752	-3.83581362	-0.65648047
H	-6.12385619	-4.38896571	1.75645919
H	-4.17020726	-4.06453018	3.25466686
H	-2.90295412	-2.33124290	-2.26498235
H	2.52820010	-3.23985636	0.45125001
H	-5.96762338	-2.51125675	-2.43654061
H	-4.87078737	-1.69744757	-3.56595613
H	-5.06402482	-1.07061828	-1.91514201
H	-2.93849659	-4.82087177	-2.61755175
H	-3.73905999	-3.96571332	-3.95460592
H	-4.70831884	-4.78228961	-2.70861056
H	5.55894937	-3.04064581	0.92995243
H	4.30905245	-3.35780776	2.14594005
H	4.37196642	-1.78175099	1.32850567
H	3.03766000	-5.35300168	-0.81101885
H	3.58032571	-5.45763987	0.87766352
H	4.75892088	-5.17623727	-0.42027778
H	5.85189692	-3.09084035	-1.35581616
H	6.18243929	-1.88955984	-3.50123874
H	4.27403253	-0.75893568	-4.61422996



H	-0.87139912	-2.64679646	2.15131292
H	0.73261932	-0.82266096	-3.27362428
H	-2.83707051	-2.85746162	4.50286740
H	-2.27324395	-1.37194197	3.68213575
H	-1.13672736	-2.37129815	4.60800870
H	-0.23268678	-4.53072333	3.64738687
H	-0.83857829	-5.16204663	2.09784347
H	-1.87204168	-5.20838945	3.53923231
H	1.95489502	1.27177834	-2.73617000
H	1.01378445	1.42967674	-4.23263229
H	2.77855369	1.21669992	-4.31482825
H	1.29275554	-2.19209878	-5.30706868
H	2.32902374	-0.87910893	-5.90252262
H	0.58479371	-0.61464441	-5.71585868
O	-1.04220717	0.02342589	1.78802864
O	-2.81359471	0.41293120	-2.14804971
O	-1.54828408	-0.00044631	-2.52057164

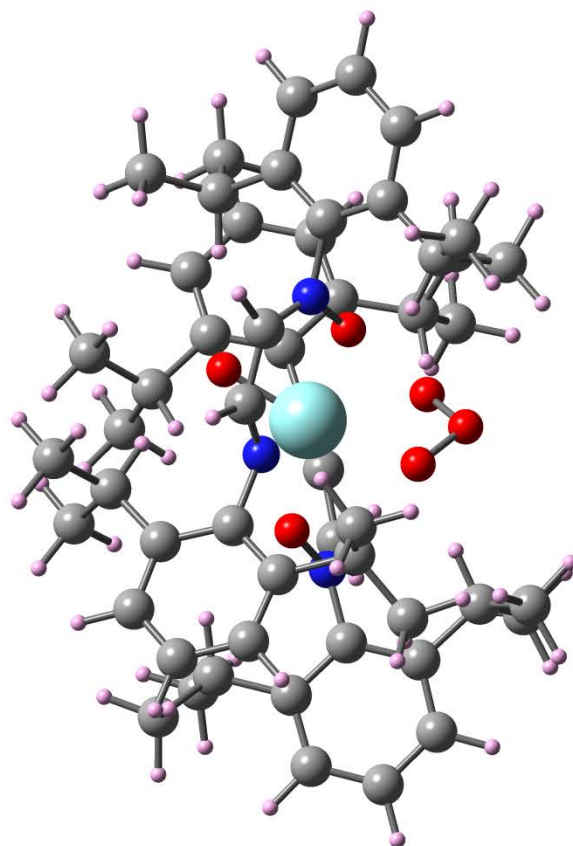
**Oxo Complex with adsorbed ozone group (conformation 2 higher energy)**

Fig. S85: NCCNO Oxo Complex with adsorbed ozone group (conformation 2 higher energy)

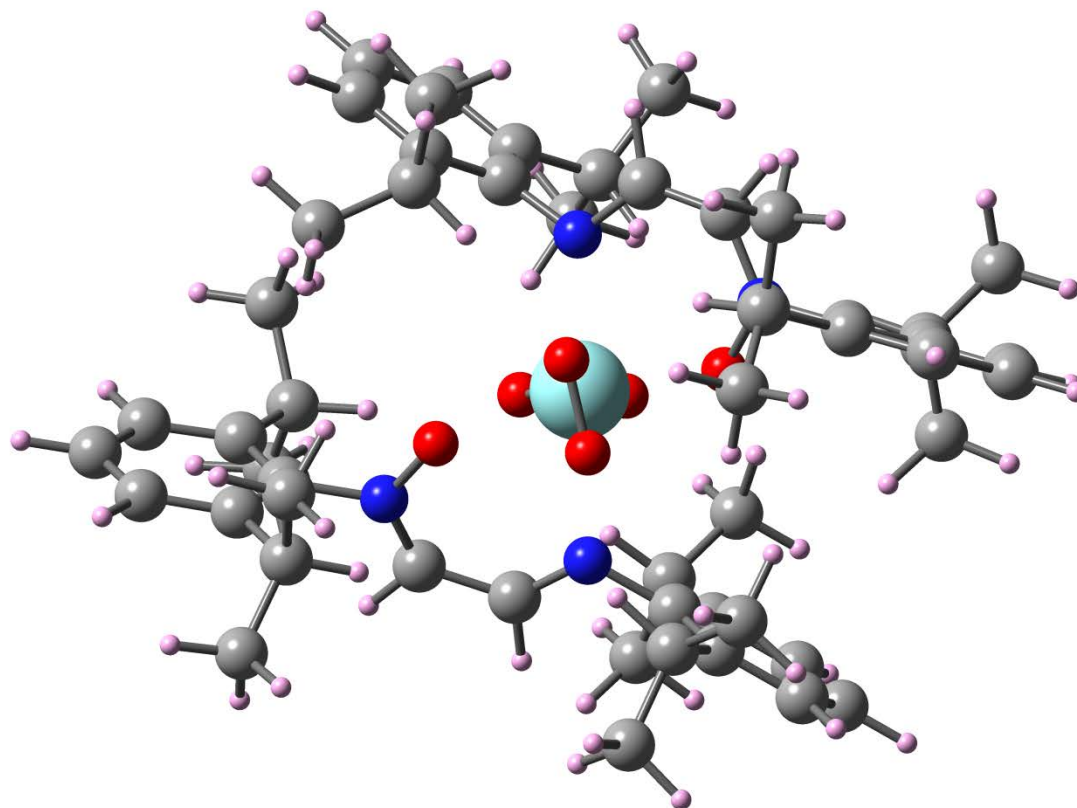
SCF	$E_{ZP}$	H	G
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Zr	0.19522683	0.20019623	-0.10870643
O	-1.92270800	0.43160638	0.06023605
O	2.07967897	-1.00769042	-0.60514023
O	0.69111321	0.52791908	-2.38867339
N	-0.17885257	-1.99192029	1.08939925
N	2.78309394	-1.75071581	0.25019946
N	0.00740111	2.47885832	-0.41247182
N	-2.73746791	1.21864390	-0.76648002
C	0.84918470	-2.65867074	1.54000635
C	2.25300392	-2.47486374	1.22107534
C	-1.10781893	3.07528547	-0.89899682
C	-2.35725301	2.48012063	-1.11904862
C	-1.47294119	-2.42961134	1.63217083
C	-1.87200710	-1.95457654	2.91050936
C	-3.08889264	-2.44218629	3.43414201
C	-3.87972632	-3.35311096	2.71991794

C	-3.46242860	-3.79943389	1.45672637
C	-2.25300563	-3.35236360	0.88656950
C	-1.86674846	0.24242830	4.21065886
C	-1.03155981	-0.97498737	3.74036118
C	-0.39294524	-1.69385491	4.96007854
C	4.87468973	1.57259396	1.48569427
C	4.43499370	0.11828335	1.79392965
C	4.82645250	-0.27814704	3.24241252
C	4.23947742	-1.75847388	0.02065933
C	5.02910296	-0.86418186	0.77900329
C	6.42148919	-0.90781562	0.54779732
C	6.97035278	-1.77796647	-0.40649262
C	6.14183055	-2.62221381	-1.16520603
C	4.74516725	-2.63108335	-0.97299707
C	-2.91919976	-4.06896736	-1.48545019
C	-1.77619255	-3.91921853	-0.45367964
C	-1.06396637	-5.28471653	-0.24202897
C	3.65182386	-2.81519142	-3.24131179
C	3.83626226	-3.49277568	-1.85475187
C	4.35210900	-4.94455089	-2.00675626
C	1.11777417	3.38122729	-0.11006551
C	2.00501321	3.80092650	-1.14227738
C	3.05991148	4.67772886	-0.80283793
C	3.22988019	5.14298009	0.50739136
C	2.33207222	4.73821905	1.50719019
C	1.26766594	3.85787483	1.22496166
C	3.11165527	2.65083723	-3.13446806
C	1.84826760	3.37733386	-2.60686965
C	1.50317485	4.59614243	-3.50432957
C	-5.48424801	0.43694155	2.42490743
C	-4.79890787	1.23677210	1.29235314
C	-5.26012876	2.72147339	1.32730423
C	-4.03820837	0.67061910	-1.10165889
C	-5.04386583	0.64300852	-0.09827342
C	-6.30423668	0.12219324	-0.45157596
C	-6.55458944	-0.34443365	-1.75314455
C	-5.54705744	-0.29645540	-2.72733659
C	-4.26240694	0.20620368	-2.42426487
C	0.98172964	3.01791442	3.62408068
C	0.27478212	3.50461736	2.33655008
C	-0.65808563	4.71112748	2.63166810
C	-3.01530119	-1.07690036	-4.25831456
C	-3.19316928	0.27286205	-3.52045094
C	-3.52107910	1.40471636	-4.53294563
H	0.68589568	-3.46117583	2.26491617
H	2.96694063	-3.04071794	1.80757271
H	-1.05413798	4.13670315	-1.14516639
H	-3.13003234	3.06093837	-1.60803538
H	-3.41749274	-2.10234243	4.41293763
H	-4.81288851	-3.71527199	3.14510424
H	-4.07925151	-4.50581758	0.90877444
H	-0.22232531	-0.57447799	3.12081926

H	3.34035692	0.10825154	1.72692291
H	-2.68176627	-0.05143331	4.88577106
H	-2.30206666	0.76814092	3.35310692
H	-1.22260017	0.94764379	4.75031614
H	-1.16183890	-2.09157773	5.63634260
H	0.23109555	-0.99256085	5.52953590
H	0.24141888	-2.53536409	4.64901946
H	5.95895472	1.70817266	1.60056641
H	4.37084105	2.26332227	2.17164001
H	4.59623922	1.86385472	0.46639423
H	4.48284650	-1.29109476	3.49382803
H	4.36900503	0.41942392	3.95509587
H	5.91505158	-0.24768064	3.38763654
H	7.07355960	-0.24522627	1.10968911
H	8.04535096	-1.79062775	-0.56984541
H	6.58252105	-3.27417352	-1.91372556
H	-1.04853021	-3.22651947	-0.88577003
H	2.84119017	-3.54617986	-1.39601477
H	-3.62674956	-4.86047762	-1.20402017
H	-2.50043136	-4.33463766	-2.46459743
H	-3.47760650	-3.13244727	-1.59511831
H	-1.75148243	-6.02113294	0.19573069
H	-0.20096715	-5.19372232	0.43136246
H	-0.70497892	-5.67990511	-1.20174076
H	3.21953105	-1.81507507	-3.13113533
H	2.97575360	-3.41228011	-3.86672070
H	4.61358873	-2.72549535	-3.76400452
H	5.30305598	-4.98333233	-2.55308262
H	3.62532124	-5.53949370	-2.57429283
H	4.50238403	-5.42610847	-1.03167679
H	3.74761839	5.00344006	-1.57979173
H	4.04615666	5.82121009	0.74644019
H	2.45495107	5.11664336	2.51904643
H	1.02517029	2.66422831	-2.68314178
H	-3.72077032	1.21325518	1.48073115
H	3.99606018	3.30275101	-3.11520230
H	2.95220374	2.32524795	-4.17086471
H	3.32449257	1.75859399	-2.53469855
H	0.58617336	5.09658811	-3.16519467
H	1.35072578	4.27116612	-4.54249028
H	2.31043467	5.34088845	-3.49923555
H	-6.57924587	0.49928343	2.36668189
H	-5.18635572	0.84661289	3.39900285
H	-5.19287181	-0.61877919	2.39632065
H	-4.73976288	3.32235480	0.57164512
H	-5.05063012	3.16141978	2.31148092
H	-6.33996911	2.80039308	1.14112068
H	-7.09603751	0.08483860	0.29069451
H	-7.53518245	-0.74103016	-2.00678871
H	-5.75494721	-0.65826939	-3.73063671
H	-0.34335824	2.67429758	1.98674148
H	-2.23135563	0.51158077	-3.05707864

H	1.64442543	3.78303272	4.05088693
H	1.56242977	2.11667315	3.40138451
H	0.23443091	2.76785468	4.38983618
H	-1.39556396	4.44456439	3.40135869
H	-1.20265057	5.02392283	1.73090954
H	-0.08620625	5.57594443	2.99513981
H	-2.74722369	-1.87349168	-3.55752428
H	-2.20420043	-0.99170675	-4.99257420
H	-3.92520405	-1.37359360	-4.79695385
H	-3.60759457	2.37920696	-4.03555507
H	-4.46829945	1.20763287	-5.05292548
H	-2.72726956	1.47840774	-5.28750678
O	1.07225094	0.48064323	1.47594108
O	0.26731466	-0.71863861	-2.94558124
O	-0.35840013	-1.48249658	-1.95942999

Peroxo Complex with adsorbed O<sub>2</sub> molecule (spiro conformation)Fig. S86: NCCNO Peroxo Complex with adsorbed O<sub>2</sub> molecule (spiro conformation)

SCF	E <sub>ZP</sub>	H	G
-2741.415563	-2740.261585	-2740.189919	-2740.370951

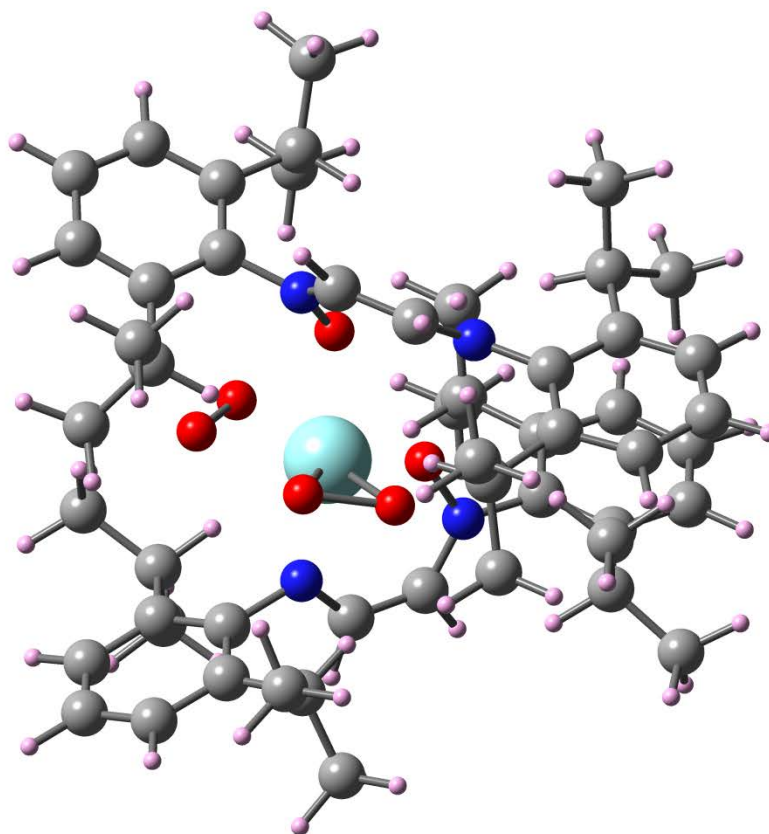
Zr	0.00345304	-0.10956504	0.07215292
O	2.10935021	-0.51629803	0.17886493
O	-1.88289911	0.64354198	-0.92767916
O	0.28417808	-0.85251609	-2.09759325
O	0.62524008	0.48976402	-2.05721724
N	0.11796401	2.40515915	0.37787895
N	-2.73789719	1.56102904	-0.43022312
N	-0.14702093	-2.34634921	0.33673394
N	2.76414428	-1.61242410	-0.37536011
C	-1.00420509	3.03243818	0.61072796
C	-2.35221519	2.60806413	0.27380394
C	0.88787817	-3.18138326	0.04875192
C	2.19834326	-2.85479821	-0.32088011
C	1.33996209	3.10631123	0.76669398
C	1.60110710	3.39554326	2.14027108
C	2.80078918	4.07625033	2.44177610

C	3.70109024	4.46522938	1.44103403
C	3.41100023	4.18541335	0.09780292
C	2.23184015	3.50670128	-0.26734410
C	1.40895411	2.15187716	4.35980425
C	0.67292504	3.01390621	3.30273117
C	0.06141397	4.28016030	3.96263022
C	-5.05088333	-0.83979619	2.09912008
C	-4.59952132	0.57340293	1.65448904
C	-5.14439638	1.64950400	2.63340112
C	-4.15078230	1.35809500	-0.78136114
C	-5.03540936	0.88242594	0.21708093
C	-6.38210644	0.70724991	-0.16997810
C	-6.80232652	0.97439192	-1.48172320
C	-5.88711843	1.42916697	-2.44519927
C	-4.53174033	1.63538201	-2.11777125
C	3.07427523	2.74999124	-2.56372428
C	1.89296712	3.32579526	-1.74875722
C	1.40871807	4.67240335	-2.35522826
C	-3.29559123	1.03198399	-4.25012141
C	-3.54620526	2.12964107	-3.18206433
C	-4.02645833	3.44884616	-3.83996138
C	-1.35815701	-3.01963828	0.80004498
C	-2.31734007	-3.46647934	-0.15279610
C	-3.44281914	-4.17925341	0.31530794
C	-3.61872015	-4.44306343	1.68172504
C	-2.66696209	-3.98705338	2.60674712
C	-1.52595402	-3.26892131	2.19139408
C	-3.39525517	-2.62723129	-2.31792026
C	-2.13861007	-3.24857132	-1.65958821
C	-1.75455901	-4.57669441	-2.36723626
C	4.90566741	0.53906510	2.17289908
C	4.74430242	-0.92262402	1.68173304
C	5.59383348	-1.89627007	2.53995211
C	4.13384038	-1.38783706	-0.79322614
C	5.09324545	-1.03913202	0.19503193
C	6.41773155	-0.81468397	-0.23259010
C	6.77611256	-0.94940898	-1.58338520
C	5.81080652	-1.30844303	-2.53598328
C	4.46534541	-1.52579407	-2.16843725
C	-1.14162201	-2.01568121	4.38284225
C	-0.49340394	-2.82123925	3.23007816
C	0.29874114	-4.03955933	3.77618421
C	3.42043532	-0.89779704	-4.41550842
C	3.44221634	-1.91166211	-3.24372633
C	3.71408339	-3.34628222	-3.77213737
H	-0.98020110	4.01917926	1.08053900
H	-3.15563726	3.26803916	0.57941096
H	0.69297917	-4.25261734	0.11014692
H	2.86976033	-3.66284326	-0.58516713
H	3.03115520	4.29884935	3.48018718
H	4.61760430	4.98747743	1.70502105
H	4.10161527	4.50427339	-0.67789813

H	-0.13706301	2.38357015	2.92843614
H	-3.50605224	0.58308095	1.71933805
H	2.25150816	2.68743522	4.81806428
H	1.77565615	1.22973310	3.89940021
H	0.71143706	1.87245412	5.16060131
H	0.83959702	4.91627536	4.40497125
H	-0.63115408	3.99065726	4.76419928
H	-0.49239108	4.89617833	3.23962416
H	-6.14494444	-0.92592621	2.14686108
H	-4.65330430	-1.05336519	3.09858515
H	-4.67129829	-1.61136124	1.42128603
H	-4.80106737	2.65917709	2.36899910
H	-4.80230235	1.43388299	3.65329119
H	-6.24263447	1.66224399	2.63785812
H	-7.10078952	0.34585387	0.55983496
H	-7.84376359	0.82401889	-1.75572622
H	-6.22811845	1.62809598	-3.45748535
H	1.06941908	2.61374919	-1.83440023
H	-2.57875119	2.32963310	-2.70870229
H	3.92177128	3.44716430	-2.60913128
H	2.75196421	2.55020321	-3.59354636
H	3.42531127	1.80842117	-2.12741225
H	2.19990111	5.43301143	-2.31200626
H	0.53694299	5.06722137	-1.81532522
H	1.12572205	4.53484034	-3.40744734
H	-2.88275218	0.12980993	-3.78778037
H	-2.57670818	1.39186203	-4.99730947
H	-4.22457629	0.76454695	-4.77143145
H	-4.95845640	3.30629513	-4.40179642
H	-3.26777827	3.81188220	-4.54511943
H	-4.20145036	4.23342922	-3.09211432
H	-4.18023920	-4.53840545	-0.39846611
H	-4.48818821	-5.00119049	2.02240507
H	-2.80706909	-4.19458540	3.66484320
H	-1.31331101	-2.54798025	-1.81397822
H	3.69197835	-1.18664706	1.81599005
H	-4.26376622	-3.29648936	-2.25654326
H	-3.20228716	-2.43190928	-3.38140934
H	-3.66009421	-1.67756222	-1.83857522
H	-0.83334993	-5.00039343	-1.94734823
H	-1.59085700	-4.40445540	-3.43964434
H	-2.54916306	-5.32771246	-2.25990026
H	5.94537646	0.88150514	2.07625807
H	4.62021338	0.61693510	3.23041816
H	4.26414135	1.21410214	1.59692204
H	5.47166450	-2.93496516	2.20602508
H	5.28246048	-1.83739807	3.59133719
H	6.66349559	-1.65160304	2.49489611
H	7.17493260	-0.54414094	0.49894995
H	7.80478365	-0.77743995	-1.89213823
H	6.10055356	-1.40902603	-3.57871636
H	0.21137310	-2.14287819	2.74297913



H	2.44155326	-1.89961613	-2.80324130
H	-1.86580405	-2.61481826	4.95293330
H	-1.64474506	-1.13088315	3.97911522
H	-0.36511996	-1.67536516	5.08089930
H	1.05930719	-3.70688630	4.49571426
H	0.80874919	-4.57994536	2.96759315
H	-0.36437690	-4.75037340	4.28881325
H	3.19868828	0.11168004	-4.05382339
H	2.63812526	-1.17843607	-5.13264648
H	4.37679739	-0.87113802	-4.95503746
H	3.68784440	-4.08728228	-2.96247431
H	4.69932146	-3.41240921	-4.25305141
H	2.95488333	-3.62702125	-4.51392443
O	-1.24332606	0.22812997	1.69022005
O	0.23257506	0.21729699	2.09892807

**Peroxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation)**Fig. S87: NCCNO Peroxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation)

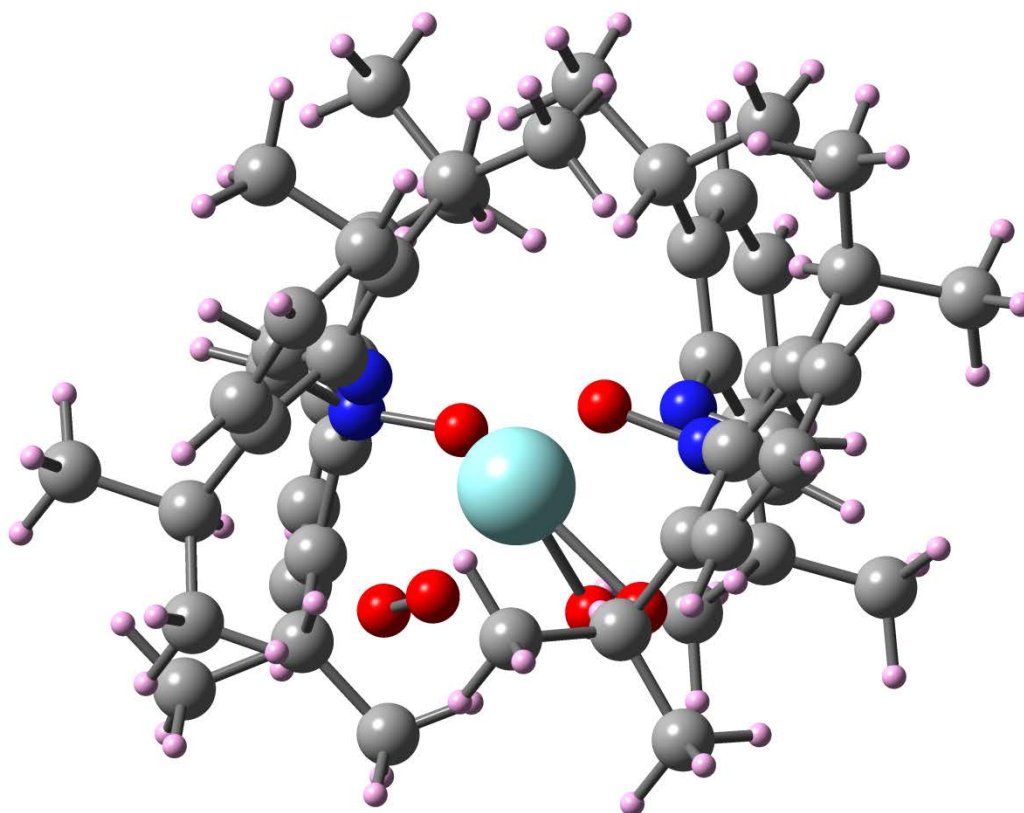
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O	0.76171006	-1.36640611	-0.94115507
O	-0.45548904	1.68092113	-0.86686207
O	-2.89589222	-0.02668100	-0.73600205
N	1.83349314	2.54621320	0.77660906
N	-0.91160407	2.90201222	-0.48489404
N	-1.45709111	-2.44562318	0.45717003
N	1.27843210	-2.65113720	-0.91623807
C	0.91975307	3.39307326	1.14864809
C	-0.30311802	3.65514028	0.40971903
C	-0.72706405	-3.56478627	0.20110202
C	0.52684004	-3.67111828	-0.41521403
C	3.03381723	2.35024018	1.50134911
C	3.08618923	2.20103217	2.92644622
C	4.35805133	2.05456616	3.51757227
C	5.53275843	2.04249416	2.75032721

C	5.45816540	2.12538216	1.34893810
C	4.21868932	2.25573817	0.69969005
C	1.84328714	0.76987806	4.62785935
C	1.84306814	2.09449816	3.82193129
C	1.72214813	3.31503025	4.77350736
C	-4.65028436	2.04229715	1.25632109
C	-3.47197527	3.02880723	1.04899808
C	-3.63561628	4.26829832	1.97049415
C	-2.13434516	3.37084326	-1.16043109
C	-3.34098325	3.44949827	-0.42073603
C	-4.47113034	3.94013030	-1.10981709
C	-4.39960633	4.30190933	-2.46279719
C	-3.19169524	4.17869932	-3.16786424
C	-2.02527715	3.70832728	-2.53252020
C	5.16412440	1.50413212	-1.56980112
C	4.12699731	2.37411118	-0.82309606
C	4.24847732	3.86094329	-1.26093510
C	-0.84309206	2.36751418	-4.31936733
C	-0.72464505	3.55681027	-3.32798525
C	-0.33599003	4.86363337	-4.06485731
C	-2.74815921	-2.69201820	1.10477208
C	-3.87861130	-3.03686123	0.30884302
C	-5.10782139	-3.26609225	0.96353807
C	-5.22022740	-3.16547824	2.35751818
C	-4.09054531	-2.84715422	3.12590324
C	-2.83717422	-2.60837820	2.52371019
C	-4.91783838	-2.46934519	-1.96730715
C	-3.79759329	-3.22603624	-1.21102009
C	-3.82611929	-4.73721036	-1.57305412
C	3.67052428	-1.53624512	1.37736311
C	3.57762327	-2.99951923	0.86249407
C	4.60845935	-3.89964530	1.58278312
C	2.58657720	-2.82033721	-1.51536111
C	3.70779228	-3.02241123	-0.66528105
C	4.96586438	-3.17351424	-1.28436210
C	5.09955939	-3.11016024	-2.68171221
C	3.97479630	-2.89857022	-3.49326927
C	2.69063220	-2.75290821	-2.92726622
C	-1.87003214	-1.30698010	4.51452134
C	-1.61071512	-2.35838318	3.40912326
C	-1.12214809	-3.69801128	4.02783231
C	1.53695012	-1.09712808	-4.45834034
C	1.47465311	-2.51311519	-3.82612429
C	1.33501010	-3.60478428	-4.91738938
H	1.04231808	4.05016431	2.01747515
H	-0.80793406	4.59334935	0.61559305
H	-1.15657709	-4.51765934	0.51106204
H	0.97169707	-4.65316836	-0.52109104
H	4.42831934	1.93720615	4.59598735
H	6.49944451	1.94623815	3.23951024
H	6.37053947	2.08002716	0.76156406
H	0.94907407	2.04541116	3.19465524

H	-2.56723520	2.49361419	1.35762910
H	2.70730021	0.69220205	5.30109739
H	1.84028914	-0.08349601	3.94221330
H	0.93233207	0.71005806	5.23765940
H	2.57480320	3.36504525	5.46389543
H	0.80656806	3.23816024	5.37467541
H	1.69180113	4.26601533	4.22326132
H	-5.62177541	2.52153819	1.07473708
H	-4.64542235	1.67731313	2.29098118
H	-4.55771135	1.17863409	0.59037405
H	-2.79199321	4.96726238	1.88259914
H	-3.70160128	3.94975130	3.01859223
H	-4.55084035	4.82440437	1.72742113
H	-5.41863739	4.01747731	-0.58473704
H	-5.28773640	4.66908536	-2.97142722
H	-3.15361924	4.45038234	-4.21902232
H	3.12505624	2.03085516	-1.10642409
H	0.08968101	3.31148125	-2.63786520
H	6.19214546	1.85821314	-1.41284711
H	4.96873238	1.54063312	-2.64967620
H	5.10862439	0.45520503	-1.25354809
H	5.22993440	4.27073233	-0.98534808
H	3.47740526	4.48055534	-0.78583706
H	4.13514032	3.95107730	-2.34989718
H	-1.09245608	1.44299211	-3.78763529
H	0.10818101	2.22012817	-4.84773237
H	-1.62349813	2.55404119	-5.06959139
H	-1.07612608	5.13718339	-4.82764437
H	0.62826405	4.73276736	-4.57308435
H	-0.24289502	5.70681044	-3.36788426
H	-5.98359845	-3.52691627	0.37480203
H	-6.17769649	-3.34378126	2.84216222
H	-4.17977532	-2.78934321	4.20749132
H	-2.84503322	-2.81736522	-1.56172512
H	2.58164020	-3.36901626	1.13372409
H	-5.91355248	-2.86470022	-1.72505313
H	-4.77368836	-2.57500820	-3.05091823
H	-4.89579137	-1.40241211	-1.72348213
H	-3.00249523	-5.28310840	-1.09459409
H	-3.73886829	-4.87118237	-2.65991821
H	-4.76738536	-5.20074540	-1.24814709
H	4.64509635	-1.09666508	1.12712909
H	3.55574027	-1.51022912	2.46847319
H	2.88677222	-0.90714407	0.94292107
H	4.59524335	-4.92696138	1.19560609
H	4.37775534	-3.93601630	2.65506120
H	5.63054642	-3.51075727	1.48541711
H	5.84768742	-3.33508425	-0.67237005
H	6.08144544	-3.22465124	-3.13538524
H	4.09230431	-2.85189422	-4.57277735
H	-0.80358206	-1.96124915	2.78815522
H	0.57224704	-2.54602020	-3.20691124

H	-2.65019520	-1.62543613	5.21965540
H	-2.15844816	-0.35280503	4.06203531
H	-0.94918007	-1.14340709	5.09018339
H	-0.22135402	-3.53123327	4.63425735
H	-0.87741506	-4.43411234	3.25035925
H	-1.89220615	-4.13878131	4.67590936
H	1.57925312	-0.32940403	-3.67767928
H	0.64382805	-0.91597407	-5.07062039
H	2.42031419	-0.98835907	-5.10253639
H	1.28044510	-4.60805635	-4.47545934
H	2.17955117	-3.59046127	-5.61877143
H	0.41865203	-3.43746526	-5.49828545
O	-1.24076809	0.51588204	1.80214414
O	0.23355802	0.00292300	1.72682013
O	-2.20188617	-0.41466703	-1.88349414

Peroxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)Fig. S88: NCCNO Peroxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)

SCF	E <sub>ZP</sub>	H	G
-2741.399877	-2740.246009	-2740.174721	-2740.354124

O	1.97152515	0.20581994	-0.02365896
O	0.68835904	-0.29002104	-2.54900016
N	-0.04028093	1.87203916	1.13419713
N	2.86699626	1.12437497	0.51992708
N	-2.74433127	-1.18633096	-0.78418402
N	0.14901792	-2.06683415	-0.51298600
C	1.09434418	2.39014015	1.68021117
C	2.42623127	2.08762207	1.37290514
C	-2.13270226	-2.16197306	-1.43955707
C	-0.80965818	-2.68188116	-1.16116305
C	-1.26824100	2.53250626	1.57923216
C	-1.59358396	3.84825537	1.12652813
C	-2.82649703	4.40552747	1.53342416
C	-3.70441013	3.71313746	2.37741622
C	-3.33692616	2.45221534	2.87071426
C	-2.11962609	1.85143125	2.49544923

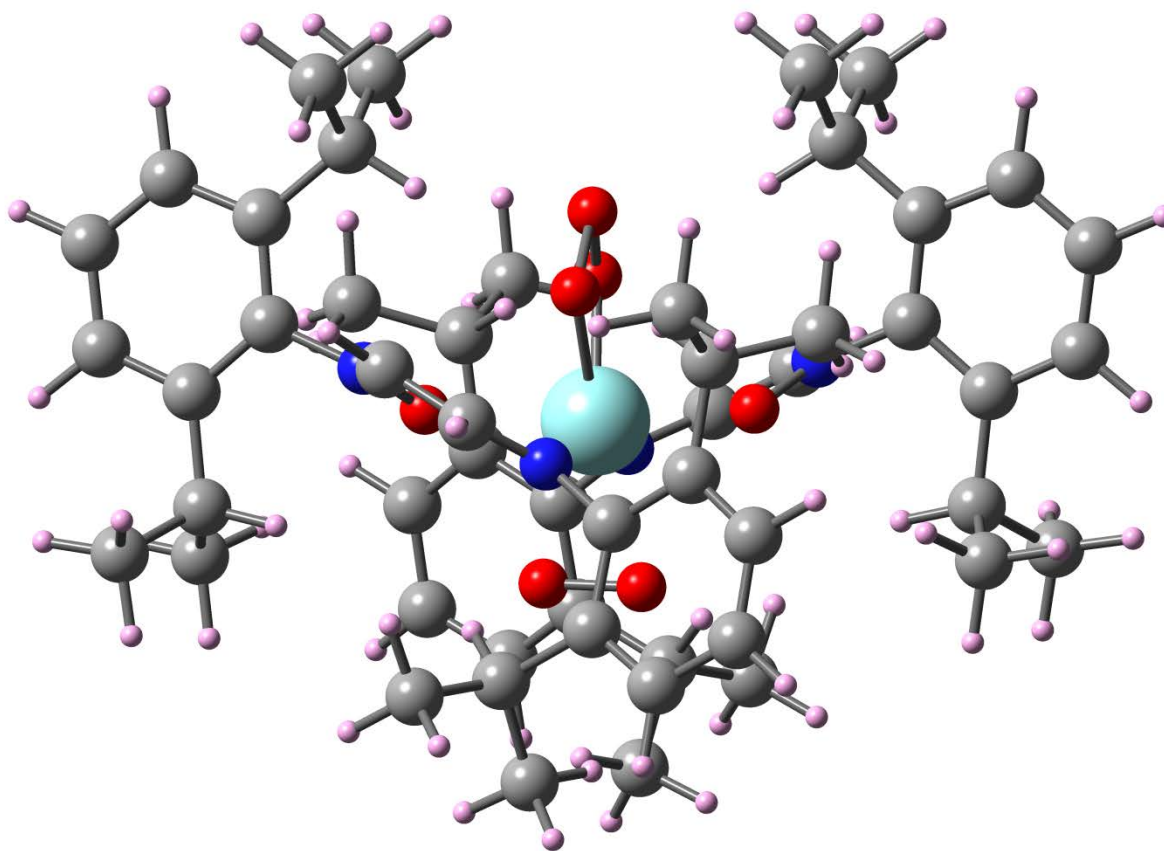
C	-1.33033388	5.34053549	-0.95293203
C	-0.64678886	4.72573840	0.29397206
C	-0.04471276	5.85460647	1.17834913
C	3.49824634	1.74961600	-3.39686822
C	3.68938538	2.39369704	-1.99959611
C	4.16953548	3.86388613	-2.12883512
C	4.25230236	0.98925790	0.10382505
C	4.64780242	1.58288894	-1.12351605
C	5.99518849	1.43227786	-1.51521508
C	6.90909353	0.73422377	-0.71197602
C	6.49414951	0.17045775	0.50515108
C	5.15552640	0.27693781	0.93578711
C	-2.81257724	-0.45345190	3.39479430
C	-1.66872811	0.55970212	3.17921128
C	-0.98114904	0.90644813	4.53040139
C	5.26710732	-1.75538635	2.48952923
C	4.72853434	-0.31961721	2.28012122
C	5.17703142	0.59583084	3.45336830
C	-4.19958037	-1.01684889	-0.83011602
C	-4.75154337	0.01041522	-1.63594008
C	-6.15945448	0.11366928	-1.66625009
C	-6.97114559	-0.75974775	-0.93010903
C	-6.39254457	-1.76575085	-0.14012297
C	-4.99342347	-1.91725992	-0.06503596
C	-4.20501122	2.43932538	-2.15402513
C	-3.91236127	0.95656925	-2.49461315
C	-4.14373929	0.67777824	-4.00417226
C	1.12509498	-2.32076521	3.59564932
C	0.45330191	-2.76320622	2.27480921
C	-0.59359122	-3.87950526	2.54682024
C	1.30059797	-2.89749326	-0.15670897
C	1.45623997	-3.23219129	1.21706913
C	2.50135201	-4.10339541	1.57923116
C	3.37667306	-4.62507748	0.61424308
C	3.21058606	-4.27640545	-0.73162002
C	2.17323002	-3.41506134	-1.15464805
C	-5.07895753	-3.16182601	2.17929321
C	-4.39914747	-3.04400903	0.79166310
C	-4.48935354	-4.40771914	0.05034404
C	3.35926715	-2.39998631	-3.15440820
C	2.06487602	-3.08773631	-2.64826216
C	1.75410994	-4.35407039	-3.48885523
H	0.97811920	3.17865721	2.42402323
H	3.20866235	2.68436308	1.82578418
H	-2.75661434	-2.73078708	-2.11816812
H	-0.65781722	-3.70794824	-1.50715307
H	-3.09535701	5.39971354	1.18599213
H	-4.65213618	4.16079253	2.66793725
H	-3.99725323	1.93716833	3.56280531
H	0.17964418	4.11076732	-0.07026597
H	2.70637731	2.41613608	-1.52369707
H	-2.13427691	6.03702355	-0.67838701

H	-1.74728595	4.55494543	-1.58948808
H	-0.59281780	5.90265651	-1.54149208
H	-0.83071079	6.52635857	1.54844016
H	0.66660232	6.45519550	0.59517009
H	0.48455326	5.45163641	2.05188520
H	4.45138940	1.67017595	-3.93812326
H	2.81390331	2.36282707	-3.99627427
H	3.05461726	0.75239694	-3.31394821
H	4.29236351	4.33420116	-1.14416505
H	3.43318845	4.44637320	-2.69690217
H	5.13055656	3.92927809	-2.65628916
H	6.32899255	1.87164588	-2.45159815
H	7.94397161	0.63213272	-1.03078504
H	7.21370854	-0.36389332	1.11905412
H	-0.91857507	0.08460806	2.53817623
H	3.63388226	-0.37476417	2.29317421
H	-3.54651428	-0.09548384	4.12917736
H	-2.41196825	-1.40343299	3.77427433
H	-3.32995129	-0.64445189	2.44993623
H	-1.67890307	1.43260220	5.19563844
H	-0.10850795	1.55360614	4.37732637
H	-0.64379006	-0.00443896	5.04275642
H	4.98418427	-2.40878038	1.65799517
H	4.85069127	-2.17925436	3.41308830
H	6.36065740	-1.76893040	2.58674524
H	6.27150252	0.68134980	3.48314331
H	4.84254837	0.17939482	4.41300338
H	4.76420443	1.60791793	3.36055230
H	-6.61789745	0.88493436	-2.27836613
H	-8.05314664	-0.65960669	-0.97096303
H	-7.03378764	-2.43259387	0.42857507
H	-2.85267019	0.78196319	-2.30363314
H	-0.08753709	-1.89925013	1.87330718
H	-5.24338029	2.71424644	-2.38605214
H	-3.54241914	3.08481340	-2.74172617
H	-4.01990320	2.64650839	-1.09394804
H	-3.89671732	-0.36017985	-4.26121729
H	-3.49577822	1.33126327	-4.60059131
H	-5.18589037	0.86625130	-4.29725329
H	1.62208498	-3.15717030	4.10356036
H	0.37109394	-1.92269215	4.28574437
H	1.87085807	-1.53721619	3.41675530
H	-1.11970327	-4.16727626	1.62669117
H	-1.34027426	-3.53997020	3.27693729
H	-0.10741422	-4.77907135	2.94696527
H	2.62805101	-4.38321343	2.62140024
H	4.17780109	-5.29826158	0.91011111
H	3.89415909	-4.67797751	-1.47505807
H	-3.33996638	-2.82533006	0.97231411
H	1.26444899	-2.36078722	-2.80329617
H	-6.11670764	-3.50848299	2.09542820
H	-5.08091449	-2.20341394	2.70875025



H	-4.53905052	-3.89261709	2.79543425
H	-4.04841254	-5.20551321	0.66249809
H	-3.96533450	-4.39023016	-0.91346803
H	-5.53621761	-4.67147011	-0.14806297
H	3.57548820	-1.50504425	-2.56131515
H	3.23470015	-2.09354329	-4.20107928
H	4.22867619	-3.06949341	-3.09742620
H	0.82150585	-4.83942140	-3.16806920
H	2.55722297	-5.09945749	-3.41189422
H	1.64770795	-4.08381137	-4.54759231
O	0.34228712	2.38288618	-1.69174909
O	-1.03926399	2.18596722	-1.60748008
O	-0.80250009	-0.40417198	-2.57821216
O	-2.02414817	-0.31940793	0.01109504
Zr	-0.02891299	0.40410104	-0.72898102

## 6.6 Structures with seven oxygen atoms

 $\eta^2$ -ozone Complex with adsorbed O<sub>2</sub> moleculeFig. S89: NCCNO  $\eta^2$ -ozone Complex with adsorbed O<sub>2</sub> molecule

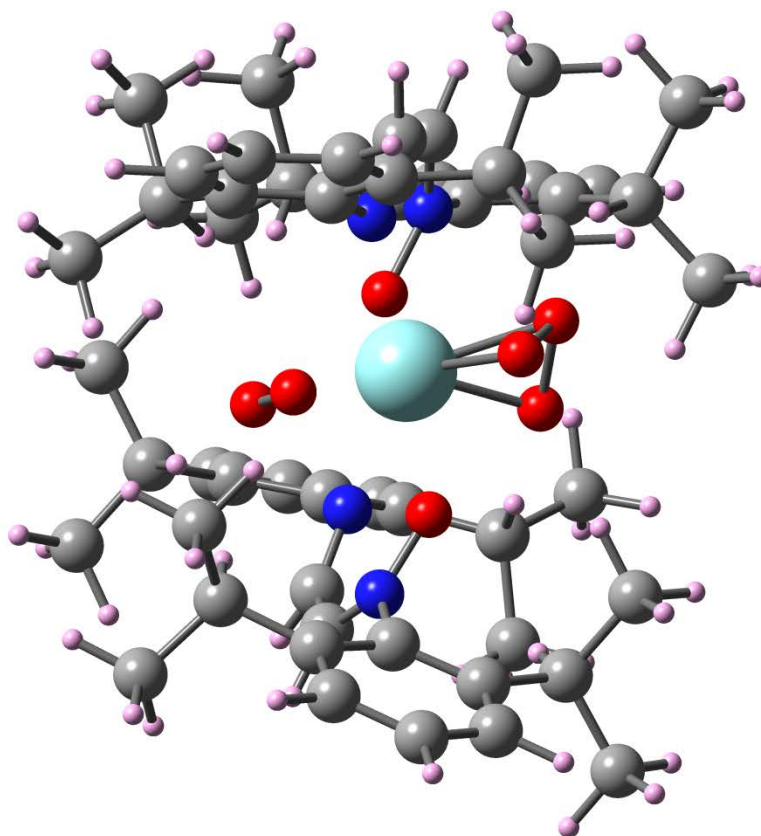
SCF	E <sub>ZP</sub>	H	G
-2816.559460	-2815.402518	-2815.329690	-2815.514488

Zr	0.07674202	-0.02530106	0.07463297
O	-2.15500933	0.21735600	-0.18947007
O	2.16422533	-0.31370312	0.02983496
O	0.00551001	0.57539603	-2.00638536
N	0.18382301	-1.98174036	1.25614215
N	2.86478943	-1.49850131	-0.16835807
N	-0.24225701	2.41777632	-0.29160609
N	-2.81867841	0.96323913	-1.08275021
C	1.20963417	-2.85715450	1.07595212
C	2.41517735	-2.65552048	0.39104601
C	-1.19769715	2.85164840	-1.07108421
C	-2.36261133	2.12322129	-1.53331628
C	-0.84518814	-2.41918642	2.19924529
C	-0.65836511	-2.17193038	3.59136351

C	-1.66513127	-2.59152844	4.48631764
C	-2.81874245	-3.24559252	4.03085857
C	-2.97108648	-3.51124857	2.66214136
C	-1.99470332	-3.11486151	1.72292121
C	0.32476905	-0.40739512	5.17231275
C	0.61844108	-1.53582130	4.15339359
C	1.52699621	-2.62275247	4.79238169
C	5.32516283	1.12346808	1.63199720
C	5.03941878	-0.39036016	1.45413917
C	5.92080893	-1.23674529	2.41031432
C	4.17189564	-1.36326530	-0.78140117
C	5.22948580	-0.82512322	-0.00231405
C	6.49449496	-0.71159222	-0.61438914
C	6.69322906	-1.12173729	-1.94297534
C	5.62699585	-1.64685935	-2.68905646
C	4.33676865	-1.77055137	-2.12955837
C	-3.58496057	-3.33342653	-0.28573609
C	-2.14926935	-3.53169957	0.25578099
C	-1.71294630	-5.01326280	0.07574797
C	2.98124545	-1.51392331	-4.26949270
C	3.18518047	-2.33116644	-2.96866850
C	3.41450249	-3.83192267	-3.29156155
C	0.73776215	3.41369046	0.16032398
C	1.88438832	3.68375749	-0.63596615
C	2.80711847	4.63393164	-0.14696607
C	2.60175445	5.29541773	1.07150312
C	1.44802027	5.02892771	1.82353724
C	0.49159812	4.08913856	1.38869617
C	3.53004657	2.41038029	-2.12462637
C	2.12427136	3.04963439	-2.01166735
C	1.91137734	4.10339155	-3.13371552
C	-5.28526780	0.13407101	1.91059925
C	-5.05426375	1.18714717	0.79477707
C	-6.00648193	2.39977936	0.96576211
C	-4.12541561	0.44162105	-1.50999627
C	-5.20000279	0.55515508	-0.59367613
C	-6.44808495	0.05287101	-1.01481920
C	-6.60236806	-0.52877608	-2.28378139
C	-5.50973785	-0.62847310	-3.15809553
C	-4.23226364	-0.15285104	-2.79064047
C	-0.52049704	3.71731852	3.71594853
C	-0.79277608	3.88658155	2.20175529
C	-1.78063122	5.05964074	1.95010625
C	-2.83020943	-1.77262930	-4.16872468
C	-3.05306546	-0.29483007	-3.75883562
C	-3.25629948	0.60045706	-5.01063381
H	1.11019415	-3.84276265	1.53136419
H	3.10030245	-3.48967062	0.29880200
H	-1.17834014	3.89092855	-1.41082626
H	-3.00330643	2.61806637	-2.25291239
H	-1.54025925	-2.40745840	5.55025880
H	-3.58407858	-3.55980156	4.73727168

H	-3.85295462	-4.04478164	2.31761631
H	1.17296818	-1.08377723	3.32659746
H	3.99357262	-0.55001317	1.73348422
H	-0.15653702	-0.79091617	6.08225090
H	-0.32665604	0.35170201	4.72706068
H	1.26287521	0.07760895	5.47382682
H	1.02311514	-3.11176954	5.63722781
H	2.45678737	-2.17218940	5.16605174
H	1.79324925	-3.40049759	4.06515857
H	6.36524796	1.36940511	1.37809817
H	5.15269780	1.41977912	2.67501136
H	4.66390874	1.72323917	0.99676211
H	5.70546284	-2.30832446	2.30845131
H	5.73183687	-0.94830824	3.45280549
H	6.99016407	-1.08777128	2.20977129
H	7.32847512	-0.30517516	-0.04761705
H	7.67781217	-1.03011828	-2.39622641
H	5.79306686	-1.95364140	-3.71848461
H	-1.48166124	-2.92103549	-0.35795510
H	2.25659033	-2.24842142	-2.39694441
H	-4.31127968	-3.99414963	0.20701699
H	-3.61149858	-3.56452556	-1.35894425
H	-3.91742361	-2.29779837	-0.15431707
H	-2.34445340	-5.68684591	0.67185206
H	-0.67129514	-5.16445584	0.38536201
H	-1.79594231	-5.30776089	-0.97912520
H	2.77664243	-0.46256215	-4.03816566
H	2.11766032	-1.90628337	-4.82058978
H	3.85888759	-1.56427133	-4.92889380
H	4.32100663	-3.97911269	-3.89469965
H	2.56207536	-4.22892472	-3.85789563
H	3.51963051	-4.42862876	-2.37578641
H	3.69291561	4.85896366	-0.73502216
H	3.32935956	6.02086883	1.42771017
H	1.28641025	5.55635879	2.75946938
H	1.40161525	2.24502528	-2.17142837
H	-4.02840359	1.55157022	0.91691809
H	4.33270770	3.15400039	-2.02748136
H	3.64185058	1.92780621	-3.10456652
H	3.66958358	1.64356017	-1.35595025
H	0.90196319	4.53636363	-3.09703451
H	2.04466135	3.63741249	-4.11890468
H	2.63057445	4.92925668	-3.04781951
H	-6.29864693	-0.28615504	1.85967324
H	-5.16012077	0.59844408	2.89709640
H	-4.56557670	-0.68762112	1.83112123
H	-5.83495584	3.16010348	0.19235798
H	-5.84670490	2.86697544	1.94608326
H	-7.05977903	2.09631833	0.90981310
H	-7.30221306	0.11866003	-0.34648410
H	-7.57431214	-0.90909512	-2.58865444
H	-5.64271385	-1.09067817	-4.13218968

H	-1.27414716	2.96225442	1.86885524
H	-2.13066432	0.02344897	-3.26588555
H	-0.11646597	4.63344265	4.16685759
H	0.18740406	2.90021939	3.88848654
H	-1.45579318	3.47692150	4.23837460
H	-2.71259536	4.90168271	2.50972633
H	-2.03377725	5.15750375	0.88527009
H	-1.34729414	6.01470688	2.27564030
H	-2.64017142	-2.39530139	-3.28795655
H	-1.94930031	-1.84243432	-4.81772678
H	-3.69114357	-2.18404136	-4.71307677
H	-3.37624450	1.65875423	-4.74025976
H	-4.14557562	0.29967903	-5.58075492
H	-2.38555435	0.51846605	-5.67308391
O	0.71099113	0.99454908	2.03717226
O	-0.64215709	0.67243405	2.10831828
O	0.08910202	-0.79707518	-2.59360044
O	-0.02812701	-1.62522830	-1.34768826

$\eta^3$ -ozone Complex with adsorbed O<sub>2</sub> molecule (conformation 1 lower energy)Fig. S90: NCCNO  $\eta^3$ -ozone Complex with adsorbed O<sub>2</sub> molecule (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G
-2816.543155	-2815.385880	-2815.313527	-2815.495178

Zr	0.21413962	0.24595682	-0.36207268
O	-1.85297878	0.32092826	0.12458030
O	2.17746923	-0.98809261	-0.68684543
O	1.10888223	0.88360476	-2.18910757
N	-0.00260423	-2.06469861	0.84423294
N	2.92496384	-1.78456644	0.07015296
N	-0.21427834	2.54416232	-0.17404203
N	-2.83552675	1.08421690	-0.52407750
C	1.01723619	-2.75515322	1.29100261
C	2.42198463	-2.58566539	0.99546158
C	-1.40209676	3.08173802	-0.54610878
C	-2.60247851	2.40080207	-0.77487429
C	-1.29350352	-2.57717818	1.32902103
C	-1.65808383	-2.37361143	2.68798354
C	-2.85260535	-2.97337173	3.14113674
C	-3.65394605	-3.73989412	2.28482519

C	-3.27463239	-3.91656189	0.94508239
C	-2.08955308	-3.34704723	0.43779509
C	-1.64434042	-0.37445558	4.27519822
C	-0.82431332	-1.54647051	3.67755083
C	-0.24969783	-2.43707224	4.81238277
C	5.28151902	0.94082335	2.03453037
C	4.84744533	-0.54710556	1.98992413
C	5.40994417	-1.32952871	3.20644736
C	4.36184142	-1.78311934	-0.25233133
C	5.26759147	-1.20380326	0.66899155
C	6.63196827	-1.22419126	0.30607397
C	7.05020875	-1.77023884	-0.91596253
C	6.11373457	-2.30995042	-1.81287741
C	4.73839312	-2.33057457	-1.50554658
C	-2.81108558	-3.77607409	-1.99019917
C	-1.63595892	-3.64155247	-0.99506474
C	-0.76307290	-4.92770267	-1.03427231
C	3.46372259	-1.85833499	-3.64092842
C	3.72721708	-2.89230789	-2.51086909
C	4.17321434	-4.25711387	-3.09322535
C	0.81359755	3.53020024	0.16218427
C	1.55739328	4.18703307	-0.85926414
C	2.54035398	5.12363420	-0.46904914
C	2.77455112	5.42304750	0.87978220
C	2.00141466	4.80099971	1.87164303
C	1.00900005	3.85768121	1.53791645
C	2.59077256	3.54806053	-3.10677666
C	1.30516810	3.97579011	-2.35673785
C	0.69847020	5.25457456	-2.99618458
C	-5.39307019	-0.28193811	2.73954705
C	-4.68435435	0.56865482	1.66181281
C	-5.07700235	2.06353727	1.84547384
C	-4.08996460	0.42663577	-0.83970889
C	-4.98161881	0.11818256	0.22687844
C	-6.18511545	-0.53641890	-0.09665791
C	-6.50337847	-0.84978695	-1.42995830
C	-5.62727245	-0.49809535	-2.46453789
C	-4.39866609	0.14819447	-2.19761382
C	0.88087552	2.91121243	3.92619746
C	0.10946784	3.28401150	2.63794786
C	-1.03733845	4.28211274	2.96253153
C	-3.13206369	-0.63439483	-4.28400081
C	-3.50394285	0.56102033	-3.37229402
C	-4.18643660	1.68832389	-4.19540362
H	0.83003583	-3.59752106	1.96274345
H	3.13256772	-3.21754583	1.51261678
H	-1.45069334	4.16171689	-0.68658671
H	-3.44949614	2.94625458	-1.17201766
H	-3.15503152	-2.83515318	4.17616425
H	-4.56743901	-4.19792049	2.65693951
H	-3.90244363	-4.50935868	0.28725720
H	0.01977574	-1.09324470	3.15195629

H	3.75605572	-0.54611933	2.06685820
H	-2.50637632	-0.73398207	4.85223209
H	-2.01182680	0.28616503	3.48199403
H	-1.01232853	0.21923840	4.94843625
H	-1.05176847	-2.90356181	5.39907916
H	0.36116322	-1.83368620	5.49676126
H	0.38022833	-3.24548588	4.41630294
H	6.37246430	1.04896195	1.97681088
H	4.94461101	1.39797540	2.97338837
H	4.82882238	1.50219000	1.21052803
H	5.07760292	-2.37691653	3.20751741
H	5.07336171	-0.86468468	4.14182154
H	6.50756447	-1.33082250	3.20787177
H	7.36672316	-0.79258622	0.97991075
H	8.10608601	-1.76714465	-1.17531150
H	6.45301804	-2.71908467	-2.75957992
H	-1.02201662	-2.80305571	-1.34080814
H	2.76791261	-3.05161037	-2.00475303
H	-3.39829825	-4.68789742	-1.81336004
H	-2.41966502	-3.83181542	-3.01363462
H	-3.48369790	-2.91343623	-1.93087352
H	-1.34004514	-5.80146723	-0.70130072
H	0.12143021	-4.84433224	-0.38931168
H	-0.41596817	-5.11655889	-2.05860918
H	3.03077122	-0.93911947	-3.23431436
H	2.75144150	-2.27236076	-4.36621257
H	4.39374955	-1.61507565	-4.17319142
H	5.06853001	-4.16118319	-3.72077613
H	3.37459061	-4.66412467	-3.72620074
H	4.38966816	-4.98753914	-2.30228401
H	3.12283206	5.62763483	-1.23662837
H	3.53896110	6.14642529	1.15507028
H	2.16548628	5.05701715	2.91486198
H	0.59155879	3.15946752	-2.47889902
H	-3.60362857	0.48006960	1.81798452
H	3.37077539	4.32071004	-3.05914271
H	2.36294131	3.36227048	-4.16484191
H	2.98740000	2.61901919	-2.68458264
H	-0.23701613	5.54847383	-2.50103983
H	0.48127630	5.07950229	-4.05863219
H	1.39100024	6.10473575	-2.92910233
H	-6.47980113	-0.12056326	2.73517872
H	-5.02676987	0.00526360	3.73371999
H	-5.19719440	-1.34999410	2.60054358
H	-4.53489068	2.71545488	1.15242380
H	-4.84525445	2.39298752	2.86730912
H	-6.15391325	2.20214056	1.67858733
H	-6.88378759	-0.79736443	0.69168078
H	-7.43901316	-1.35533446	-1.65869168
H	-5.89268982	-0.72809240	-3.49302459
H	-0.35123248	2.36715302	2.25722452
H	-2.56272406	0.95596863	-2.98475955



H	1.28912084	3.79614745	4.43247808
H	1.70570096	2.22620610	3.70121978
H	0.20479881	2.41319263	4.63417651
H	-1.70811593	3.86287080	3.72547267
H	-1.63475389	4.50558001	2.06985970
H	-0.63415674	5.22950686	3.34554283
H	-2.54767616	-1.37154465	-3.72636266
H	-2.51151040	-0.28101686	-5.11746199
H	-4.01973596	-1.12419441	-4.70737380
H	-4.42884782	2.55812862	-3.56996222
H	-5.12013641	1.33781868	-4.65554092
H	-3.51834393	2.02361186	-4.99936270
O	1.96175245	1.06265365	0.97212429
O	1.02304906	0.36932712	1.73771070
O	-0.34223277	0.53286968	-2.50569285
O	-0.43396181	-0.92563737	-2.05604379

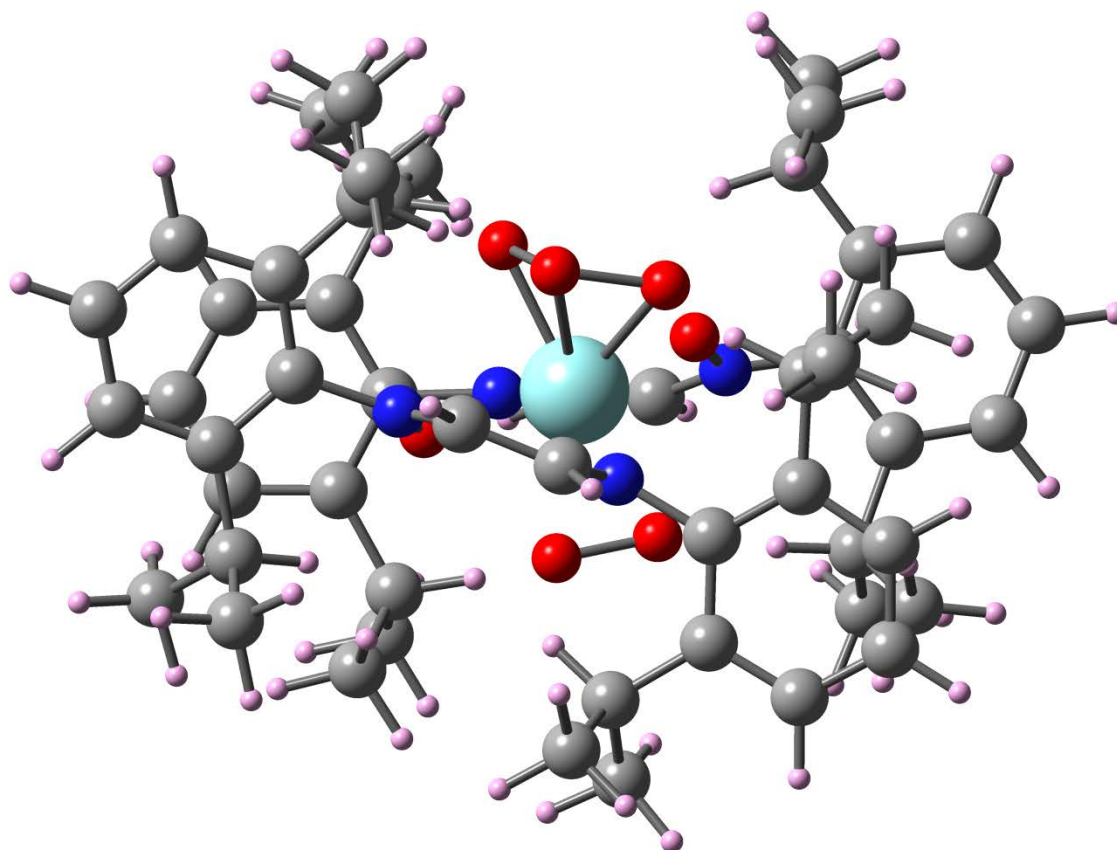
$\eta^3$ -ozone Complex with adsorbed O<sub>2</sub> molecule (conformation 2 higher energy)

Fig. S91: NCCNO  $\eta^3$ -ozone Complex with adsorbed O<sub>2</sub> molecule (conformation 2 higher energy)

SCF	E <sub>ZP</sub>	H	G
-2816.540097	-2815.383427	-2815.311620	-2815.492692

Zr	0.19414982	-0.12322767	-0.26584468
O	-2.06522548	0.41185284	0.10976006
O	2.12770810	-0.96888457	-0.60953892
O	0.84653306	0.49808768	-2.24970580
N	0.04764028	-2.08997299	0.93495346
N	2.98217744	-1.62546726	0.26655738
N	-0.11657560	2.46174762	-0.41216515
N	-2.85229737	1.17363697	-0.66228779
C	1.13425389	-2.72786664	1.45403588
C	2.48704822	-2.49296119	1.19201208
C	-1.19321483	2.99584138	-0.91925634
C	-2.46516840	2.33877405	-1.15686934
C	-1.23320005	-2.67295901	1.34034178
C	-1.76537650	-2.40446158	2.63435663
C	-3.01011743	-2.97639709	2.97997324

C	-3.70489649	-3.80386409	2.08835786
C	-3.14078662	-4.10261251	0.83818259
C	-1.89859729	-3.56325024	0.44582098
C	-1.86126128	-0.37456062	4.19100557
C	-1.02448816	-1.57881159	3.69372497
C	-0.59596857	-2.47184628	4.88987805
C	5.00502120	1.45515547	2.04736716
C	4.71564205	-0.06748370	2.08384115
C	5.31374298	-0.71133456	3.36292798
C	4.39122864	-1.50189460	-0.05124229
C	5.23175486	-0.76382090	0.82043316
C	6.59936064	-0.67310890	0.48143067
C	7.09627432	-1.26737425	-0.68779872
C	6.23476121	-1.97363766	-1.54364640
C	4.86466917	-2.11408957	-1.24316419
C	-2.25905688	-4.29031696	-1.99815784
C	-1.24617008	-4.02566716	-0.86130749
C	-0.39331644	-5.30081544	-0.60527999
C	3.60853097	-2.01669489	-3.44116594
C	3.93897883	-2.88014028	-2.19316711
C	4.52656080	-4.25377470	-2.60367874
C	0.97907787	3.39573788	-0.10294323
C	1.91792223	3.77117501	-1.10330437
C	2.96956510	4.63344514	-0.72008815
C	3.07814615	5.12701526	0.58577903
C	2.10731152	4.78573147	1.53851336
C	1.03881229	3.92399306	1.22010172
C	3.10108706	2.59757155	-3.03472439
C	1.82587169	3.34678463	-2.57325561
C	1.54548667	4.57426301	-3.48153912
C	-5.30567070	0.32027604	2.74368505
C	-4.73018825	1.16969584	1.58635059
C	-5.19088151	2.64973292	1.71514454
C	-4.22152749	0.67570704	-0.90613276
C	-5.10671739	0.62641403	0.20283744
C	-6.40585041	0.14104038	-0.04105579
C	-6.79670771	-0.27456259	-1.32445923
C	-5.89793773	-0.19866866	-2.39588018
C	-4.58063409	0.28130406	-2.22055725
C	0.51532459	3.34537664	3.66623167
C	-0.05473489	3.66984320	2.26463258
C	-1.01921754	4.88689468	2.33476407
C	-3.51692117	-0.98796740	-4.16879060
C	-3.65781823	0.37299238	-3.44308996
C	-4.16503238	1.46882862	-4.42078276
H	0.94436917	-3.53244428	2.16475405
H	3.23276708	-3.06128552	1.73401969
H	-1.19966585	4.05831284	-1.17990994
H	-3.21369745	2.87956513	-1.72182345
H	-3.42908490	-2.77748561	3.96392474
H	-4.66462078	-4.23107741	2.37119143
H	-3.66627732	-4.77171142	0.16312715

H	-0.11803136	-1.16640417	3.24716280
H	3.62850260	-0.17708614	2.12874044
H	-2.78135181	-0.69891512	4.69557430
H	-2.13444422	0.27530416	3.35247275
H	-1.27591204	0.22070586	4.90448587
H	-1.46751758	-2.89666248	5.40586633
H	-0.02643556	-1.88121042	5.62036960
H	0.03503083	-3.30803847	4.56105185
H	6.08318474	1.66440892	2.03039217
H	4.58077993	1.93778427	2.93737594
H	4.55018885	1.92085797	1.16555894
H	5.08527124	-1.78395871	3.41833061
H	4.90135075	-0.22867707	4.25884588
H	6.40606108	-0.60051376	3.39288396
H	7.27394553	-0.12083073	1.13071408
H	8.15165034	-1.17754108	-0.93534454
H	6.63183423	-2.42561325	-2.44838838
H	-0.57000578	-3.23916032	-1.20796088
H	2.98947593	-3.06474721	-1.67975140
H	-2.86552932	-5.18775328	-1.81162162
H	-1.72158330	-4.44568509	-2.94237901
H	-2.93325443	-3.43711758	-2.12818892
H	-1.02205286	-6.12452063	-0.23919626
H	0.39287697	-5.11781687	0.13696831
H	0.09006633	-5.62698876	-1.53636698
H	3.07958769	-1.10548927	-3.14502003
H	2.95774041	-2.57770955	-4.12535438
H	4.52344529	-1.74321657	-3.98553189
H	5.43353474	-4.14541311	-3.21294863
H	3.79237649	-4.80565885	-3.20517893
H	4.77848262	-4.86416755	-1.72638459
H	3.70593160	4.92414323	-1.46468804
H	3.90069882	5.78522027	0.85508807
H	2.17634889	5.19527337	2.54231006
H	1.00687188	2.63579038	-2.69110014
H	-3.64103961	1.14232513	1.68541185
H	3.99639520	3.23132818	-2.97094757
H	2.98696656	2.27438064	-4.07732493
H	3.26408529	1.70205433	-2.42557779
H	0.62328613	5.09513569	-3.18713901
H	1.43599700	4.25114542	-4.52533185
H	2.36476338	5.30435791	-3.44065820
H	-6.40122942	0.37300816	2.78820741
H	-4.92153964	0.69425685	3.70082684
H	-5.00882008	-0.72961924	2.64497004
H	-4.75212232	3.28237872	0.93203927
H	-4.88803606	3.05698629	2.68849144
H	-6.28346669	2.72788115	1.63781944
H	-7.11717412	0.08795568	0.77684646
H	-7.80323094	-0.65192970	-1.48755710
H	-6.21406303	-0.52001201	-3.38405660
H	-0.63562790	2.79584922	1.95748633

H	-2.64849071	0.64346207	-3.12647958
H	1.03695129	4.20444085	4.10875044
H	1.21126816	2.50214950	3.61094026
H	-0.30186549	3.06989716	4.34577579
H	-1.82516118	4.69574842	3.05645821
H	-1.47775456	5.10002036	1.35917144
H	-0.48579744	5.79232871	2.65336132
H	-3.07036710	-1.73139891	-3.50269462
H	-2.84964993	-0.87460044	-5.03243084
H	-4.48078237	-1.36636203	-4.53403080
H	-4.24676756	2.45111890	-3.93396984
H	-5.15513001	1.21808681	-4.82349799
H	-3.47175542	1.56606298	-5.26578449
O	1.46294938	0.72948742	1.47179696
O	0.13160352	0.63969512	1.86467909
O	-0.64201294	0.22523424	-2.29052088
O	-0.78470600	-1.23138657	-1.82661008

## Peroxo Complex with adsorbed ozone group

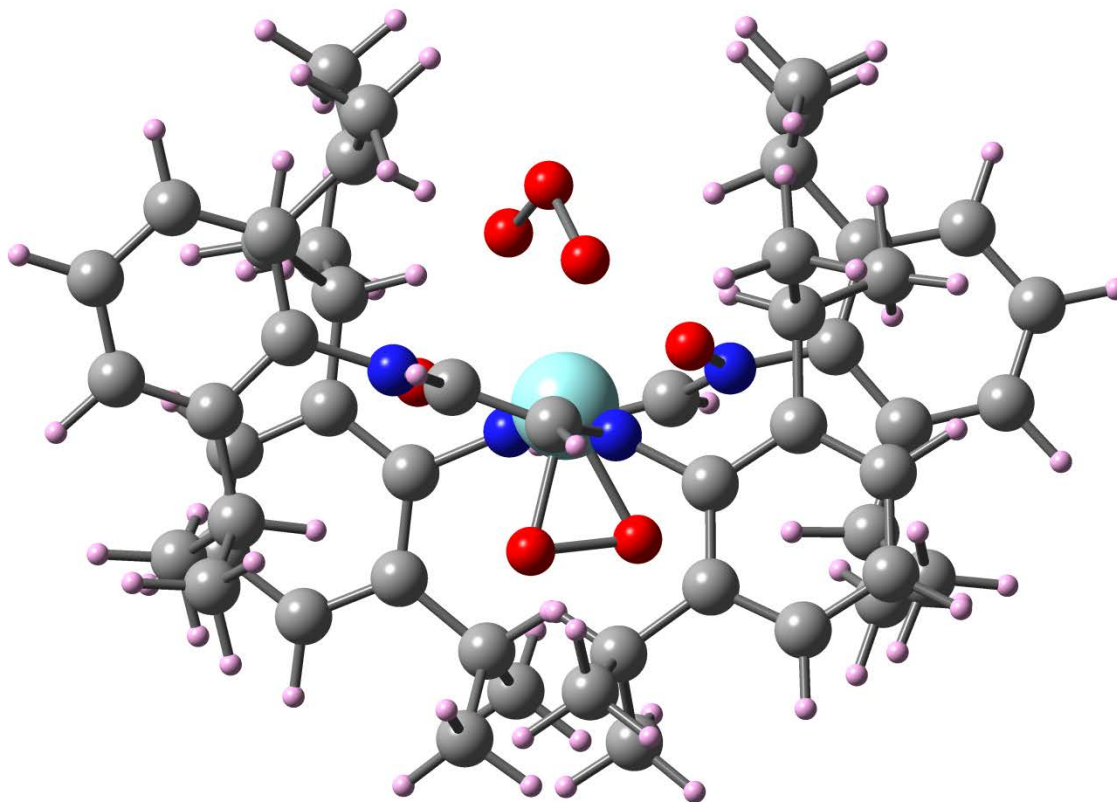


Fig. S92: NCCNO Peroxo Complex with adsorbed ozone group

SCF	$E_{ZP}$	H	G
-2816.555122	-2815.398443	-2815.325323	-2815.513318

Zr	0.08441568	-0.09566736	0.00477697
O	-2.12990585	0.19748422	-0.36612528
O	1.98648116	-0.67384896	-0.70424286
O	-0.07042493	0.72983498	-2.18054229
N	0.05503583	-2.23377856	0.81716300
N	2.89695416	-1.59673036	-0.20819967
N	-0.03494176	2.43883097	-0.13768389
N	-2.85142134	1.25115482	-0.75462157
C	1.17283454	-3.00442489	0.88486846
C	2.47303268	-2.71028533	0.44957187
C	-1.14526644	3.06589349	-0.41233930
C	-2.42928341	2.50527617	-0.79454533
C	-1.10662298	-2.79164084	1.51646394
C	-1.21553078	-2.62315398	2.93022397
C	-2.34190329	-3.17001404	3.58119769
C	-3.33031662	-3.87060446	2.87403373

C	-3.18983653	-4.05692382	1.49228149
C	-2.07951474	-3.53665635	0.79175647
C	-0.70634981	-0.89889038	4.75855327
C	-0.12919073	-1.94569642	3.77474484
C	0.69224701	-3.01507201	4.54883749
C	4.94957916	1.21136369	2.05056775
C	4.61023313	-0.26999887	1.75096724
C	5.17148503	-1.19684463	2.86318261
C	4.27901087	-1.35608684	-0.56863616
C	5.11852903	-0.71051435	0.37450481
C	6.46411912	-0.50067944	0.00444965
C	6.93704218	-0.89858513	-1.25659513
C	6.07415661	-1.51441239	-2.17807551
C	4.72251902	-1.75525081	-1.85479974
C	-3.15608912	-3.36149656	-1.51752779
C	-1.93732510	-3.85417507	-0.69885383
C	-1.70510514	-5.37372860	-0.91818195
C	3.58582120	-1.49870864	-4.11025717
C	3.78639591	-2.41234594	-2.87274816
C	4.29562670	-3.81543172	-3.29255569
C	1.06635269	3.27509171	0.33912346
C	2.18495772	3.48408290	-0.51683930
C	3.21707823	4.32549892	-0.05692606
C	3.15544769	4.93262950	1.20673453
C	2.05031017	4.70124019	2.03572062
C	0.98161701	3.87297711	1.63005511
C	3.63687791	2.42264088	-2.35158256
C	2.23321222	2.92260244	-1.93948088
C	1.71428262	3.98488509	-2.94887678
C	-5.13576724	-0.36650943	2.19525402
C	-4.80451698	0.92666173	1.40685742
C	-5.50191719	2.15988098	2.04100046
C	-4.24536137	0.93745077	-1.12426509
C	-5.17895830	0.78539953	-0.07195847
C	-6.50915698	0.50277006	-0.44578747
C	-6.86906450	0.37145510	-1.79680328
C	-5.90537320	0.51035427	-2.80781907
C	-4.55758079	0.79015405	-2.49623803
C	0.34564118	3.05153330	3.95028112
C	-0.17323911	3.63926227	2.61237902
C	-0.98078359	4.94228303	2.85438101
C	-3.47389894	-0.35904577	-4.49318462
C	-3.51734568	0.91782802	-3.61472965
C	-3.78808741	2.17522570	-4.48382296
H	1.07628863	-3.97486751	1.37242479
H	3.25702939	-3.42754399	0.66178108
H	-1.17099971	4.15728010	-0.35184914
H	-3.18532228	3.21414769	-1.11143137
H	-2.43970686	-3.05065917	4.65716648
H	-4.19072937	-4.28137982	3.39802587
H	-3.93920906	-4.62707047	0.94825788
H	0.54850904	-1.40685869	3.10928312

H	3.51837476	-0.35194700	1.76638914
H	-1.36761919	-1.35378621	5.50962931
H	-1.25779995	-0.13170626	4.20671561
H	0.11444587	-0.40431690	5.29552526
H	0.05678670	-3.56968568	5.25308770
H	1.49534511	-2.53325144	5.12309031
H	1.15234785	-3.74410526	3.86889433
H	6.03349743	1.37995834	2.11260251
H	4.50839191	1.50376709	3.01173261
H	4.53894692	1.87469816	1.28110463
H	4.88944554	-2.24400932	2.69332079
H	4.77723951	-0.89397050	3.84186816
H	6.26805107	-1.14548692	2.90663979
H	7.14163470	-0.01602614	0.70246680
H	7.97710022	-0.72410850	-1.52330852
H	6.45264079	-1.80910313	-3.15381002
H	-1.05939185	-3.33346414	-1.08360370
H	2.80223380	-2.53883520	-2.41015078
H	-4.07989761	-3.87854928	-1.22301072
H	-2.99083091	-3.55057424	-2.58670141
H	-3.30524596	-2.28480525	-1.37733880
H	-2.56116739	-5.96610549	-0.56769838
H	-0.81441120	-5.72175017	-0.37854034
H	-1.56104745	-5.58511306	-1.98646813
H	3.16885612	-0.53075638	-3.81111721
H	2.88724536	-1.96710563	-4.81584482
H	4.53363934	-1.32135418	-4.63663071
H	5.26632441	-3.75768740	-3.80261365
H	3.58226992	-4.28443226	-3.98291337
H	4.41177478	-4.47478664	-2.42254373
H	4.07308162	4.51168893	-0.69866297
H	3.96338440	5.57901212	1.54155536
H	2.01416643	5.16184579	3.01947599
H	1.55588120	2.06724698	-2.00456064
H	-3.72245335	1.07413219	1.49292213
H	4.36840855	3.23945570	-2.41836228
H	3.58251915	1.95162465	-3.34167485
H	4.01378967	1.67504398	-1.64459663
H	0.69370057	4.30810128	-2.70325318
H	1.69898594	3.56599188	-3.96347507
H	2.35842041	4.87520033	-2.95258948
H	-6.21423718	-0.57447752	2.19419061
H	-4.81397130	-0.25968137	3.23868077
H	-4.61542781	-1.23259064	1.77293130
H	-5.24773122	3.08703124	1.50990224
H	-5.18986293	2.27048529	3.08724455
H	-6.59446538	2.05311686	2.02542782
H	-7.26438059	0.38138957	0.32559935
H	-7.90075741	0.15306421	-2.06147576
H	-6.19678073	0.39078694	-3.84748935
H	-0.84182706	2.87780357	2.20194639
H	-2.52151643	1.02884358	-3.17363952



H	1.01228915	3.75032796	4.47400095
H	0.88237361	2.11729847	3.76014578
H	-0.50049744	2.83166890	4.61504287
H	-1.81900096	4.74844681	3.53737378
H	-1.38945178	5.35147353	1.91944039
H	-0.35462189	5.72241196	3.30763785
H	-3.26994474	-1.24756484	-3.88609670
H	-2.67368460	-0.26903108	-5.23800563
H	-4.41932855	-0.51535562	-5.02932367
H	-3.77712437	3.09468976	-3.88305172
H	-4.76448925	2.11349200	-4.98210895
H	-3.01784463	2.26871154	-5.25969843
O	1.06120484	0.46728812	1.71022337
O	-0.47235514	0.55735523	1.86670413
O	-0.25375668	-0.47854227	-2.94238907
O	-0.40984323	-1.53326671	-2.05924560

## 7. NCCNO Singlet Transition States

## Spiro Bisperoxo Complex to Oxo Peroxo Complex (conformation 1 lower energy)

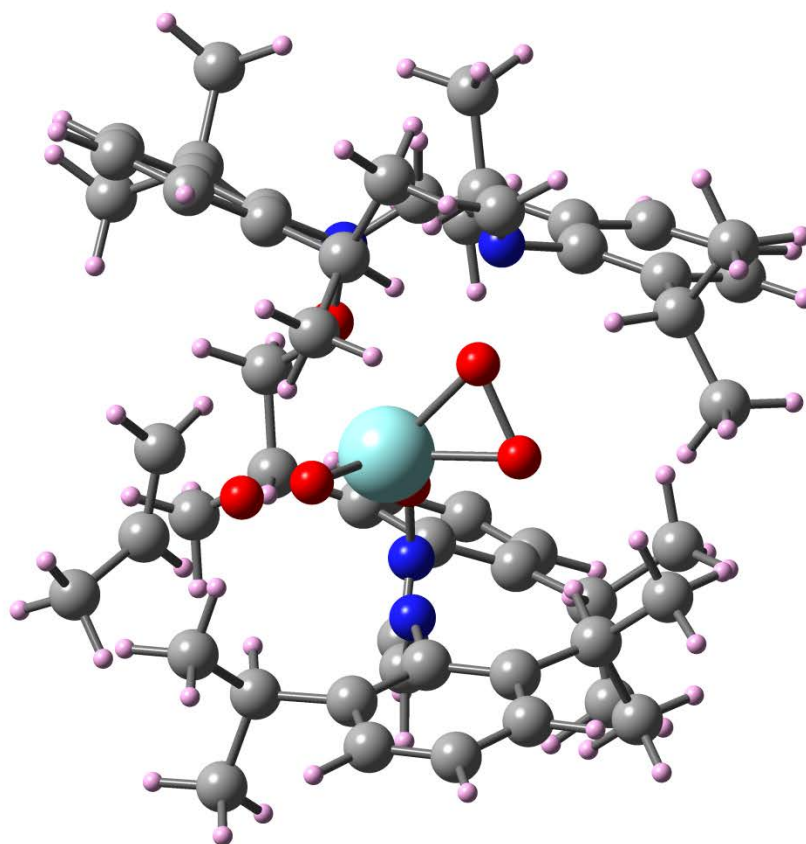


Fig. S93: NCCNO Spiro Bisperoxo Complex to Oxo Peroxo Complex (conformation 1 lower energy)

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2859.256339	-2858.021043	-2857.944435	-2858.135973	-474

Zr	1.21804309	0.18865001	-0.27325802
O	-0.37918303	-0.97328107	0.92472907
O	-0.14053201	1.97503715	0.14966101
O	2.99095123	0.89394207	-0.15792301
N	-2.67043721	1.10842709	-1.38814210
N	-0.27644102	2.97101623	-0.77273606
N	2.28903618	-1.96830215	0.29906502
N	-0.41045603	-2.06247816	1.69917913
C	-2.00445015	1.85286514	-2.21608617
C	-1.06109308	2.89569422	-1.82495514
C	1.92457515	-2.79166422	1.24449309
C	0.64641005	-2.82944322	1.93147515
C	-3.65364528	0.17786401	-1.82797414

C	-3.46808826	-0.71619206	-2.93260823
C	-4.53983635	-1.57310412	-3.26603925
C	-5.74296446	-1.57193912	-2.54573020
C	-5.89226643	-0.72086806	-1.43699911
C	-4.85861837	0.15071501	-1.05263108
C	-1.66026313	-2.29811117	-3.80779529
C	-2.16168117	-0.83402106	-3.73329428
C	-2.32798618	-0.26285402	-5.16850040
C	3.63706228	3.29429325	-2.31016718
C	2.13733217	3.65872528	-2.45489019
C	1.87721714	4.40119534	-3.79536629
C	0.49643004	4.19806932	-0.49712104
C	1.63838913	4.50486834	-1.27736610
C	2.32303418	5.69719645	-0.94758007
C	1.89364014	6.52451851	0.09790501
C	0.75315006	6.18684845	0.84576806
C	0.02819500	5.01235238	0.56746204
C	-5.87687346	0.53818404	1.27909210
C	-5.03599439	1.11864108	0.11912701
C	-5.64579244	2.46076219	-0.37407003
C	-1.09054908	4.86833937	2.87062022
C	-1.25821010	4.69595436	1.34077510
C	-2.42643819	5.57902842	0.82036906
C	3.56972827	-2.28506917	-0.35722003
C	4.79191336	-1.89411914	0.25004202
C	5.98787045	-2.24515217	-0.41252603
C	5.97644043	-2.95170622	-1.62209112
C	4.75348436	-3.33244225	-2.19344617
C	3.52618127	-3.01065823	-1.57893112
C	5.73688543	0.13979301	1.46175511
C	4.87520237	-1.14203709	1.58180112
C	5.41907343	-2.08013416	2.69490920
C	-2.85602322	-4.48153234	-0.65789605
C	-1.82262514	-4.37349033	0.49355104
C	-1.36361810	-5.78542544	0.94742807
C	-1.73350913	-2.43606519	2.23584617
C	-2.38198118	-3.56550627	1.67150113
C	-3.62814628	-3.92547430	2.22644217
C	-4.20430132	-3.17874724	3.26474325
C	-3.55244727	-2.04130915	3.76466129
C	-2.29994518	-1.63761412	3.25865725
C	2.16440116	-3.34853526	-3.72401828
C	2.21438417	-3.51838927	-2.18809717
C	1.97686315	-5.00242338	-1.79140213
C	-2.40881019	0.88519307	3.35807625
C	-1.62702412	-0.37912303	3.80478829
C	-1.46590511	-0.42561303	5.34518838
H	-2.19553917	1.85239514	-3.29457125
H	-0.98820807	3.74811329	-2.49470119
H	2.59355520	-3.60528828	1.53711712
H	0.48387804	-3.63623428	2.63531820
H	-4.42479534	-2.25663617	-4.10328831

H	-6.55338249	-2.23592617	-2.83814721
H	-6.81859252	-0.73926406	-0.87010507
H	-1.36254610	-0.27798202	-3.23457725
H	1.59778012	2.70669221	-2.48828119
H	-2.35085718	-2.94885922	-4.36197833
H	-1.51904411	-2.71032621	-2.80247921
H	-0.68803405	-2.31794018	-4.31144633
H	-3.07352623	-0.83455806	-5.73834141
H	-1.37227811	-0.31594502	-5.70543643
H	-2.65638620	0.78548406	-5.16117239
H	4.28001732	4.18531032	-2.28766717
H	3.94444430	2.68040720	-3.16700724
H	3.79800929	2.70244621	-1.40294911
H	0.81475406	4.64932735	-3.93239730
H	2.18691717	3.76718829	-4.63566535
H	2.44629419	5.33927843	-3.84931129
H	3.20783425	5.96977745	-1.51535311
H	2.44382819	7.43344357	0.32993003
H	0.42527603	6.84258151	1.64758813
H	-4.03120231	1.33975110	0.49772104
H	-1.52278612	3.64864428	1.16515309
H	-6.92759955	0.39119103	0.99463407
H	-5.86614444	1.23343709	2.12961316
H	-5.47568444	-0.42487103	1.61937713
H	-6.65248850	2.30465518	-0.78538006
H	-5.02585638	2.91231022	-1.15834809
H	-5.72307243	3.17782824	0.45505403
H	-0.25745402	4.26496833	3.24873725
H	-2.00750115	4.54965935	3.38411326
H	-0.90729607	5.91442345	3.14759924
H	-2.21876917	6.64426752	0.98791307
H	-3.35842626	5.32646440	1.34356610
H	-2.59170620	5.43374641	-0.25506802
H	6.93722951	-1.95079215	0.02643100
H	6.91179651	-3.20537724	-2.11559916
H	4.75011136	-3.88600630	-3.12775624
H	3.87651330	-0.79222806	1.85758914
H	-0.95070407	-3.85260329	0.08159701
H	6.77715154	-0.07998101	1.18382909
H	5.75220644	0.66852405	2.42432919
H	5.28673340	0.80189706	0.71659206
H	4.78149137	-2.96585923	2.83349122
H	5.47413242	-1.54687112	3.65379028
H	6.42959348	-2.43754019	2.45442219
H	-3.73013629	-5.07587839	-0.36288503
H	-2.39640218	-4.97557938	-1.52323312
H	-3.20709124	-3.49372226	-0.97591107
H	-0.59518705	-5.73608146	1.73036013
H	-0.94641207	-6.33978951	0.09744601
H	-2.20709917	-6.36285947	1.34715110
H	-4.15822032	-4.78537536	1.82771814
H	-5.16694939	-3.47503426	3.67384628

H	-4.01699731	-1.45977211	4.55581335
H	1.39161711	-2.91539222	-1.79117814
H	-0.62838205	-0.30112802	3.36876126
H	2.93709123	-3.93802730	-4.23540232
H	2.28252317	-2.29210518	-3.98429030
H	1.19061909	-3.68495428	-4.10265631
H	1.02037308	-5.35893043	-2.19872517
H	1.95636615	-5.13631339	-0.70016105
H	2.77451621	-5.64595442	-2.18670617
H	-2.41629419	0.96748007	2.26563517
H	-1.93269215	1.78399013	3.76957329
H	-3.44669126	0.85651407	3.71556228
H	-0.92528207	-1.32503310	5.66830443
H	-2.43733718	-0.41527303	5.85620146
H	-0.90142107	0.45145003	5.68482942
O	0.64926105	0.70988106	-2.22296917
O	1.00953108	-0.78036906	-2.11099016
C	1.89888515	0.78805406	3.81767529
H	1.32194210	-0.12056001	3.98423430
C	1.38412510	1.78417814	3.00489223
H	0.36207903	1.76189014	2.64208120
O	2.28971217	0.87232207	1.60112112
H	1.89287514	2.74024921	2.92066523
C	3.23993525	0.87246507	4.49619934
H	3.84254929	-0.02375200	4.30175533
H	3.80294029	1.74192813	4.14028331
H	3.12554624	0.95577607	5.58950740

## Spiro Bisperoxo Complex to Oxo Peroxo Complex (conformation 2 higher energy)

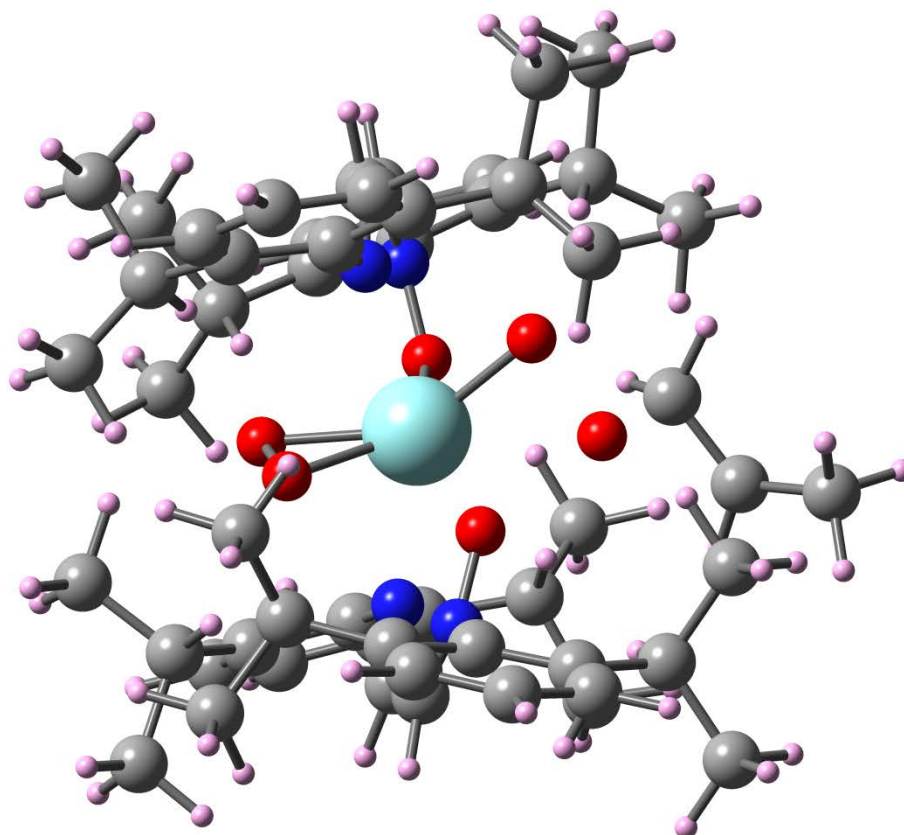


Fig. S94: NCCNO Spiro Bisperoxo Complex to Oxo Peroxo Complex (conformation 2 higher energy)

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2859.24779765	-2858.012526	-2857.937259	-2858.125106	-370

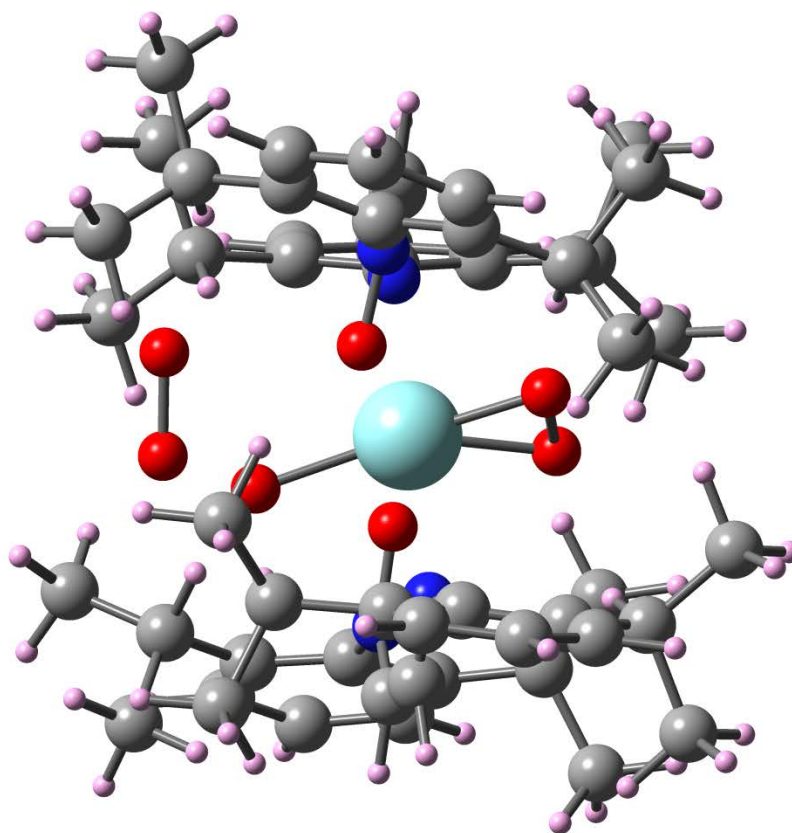
Zr	-0.12095300	0.10226300	0.11251900
O	2.07040200	0.16527700	0.43096200
O	-2.18504800	-0.65418200	0.64374200
O	-0.29809700	1.07011100	1.87949400
N	-0.04912800	-2.27536100	-0.68623100
N	-2.97647300	-1.55329100	0.05752500
N	0.08947700	2.46815900	-0.02716400
N	2.91505500	1.23922400	0.42071200
C	-1.16203000	-2.91567600	-0.97455400
C	-2.52582700	-2.58921300	-0.64133100
C	1.23810100	3.09733600	0.19785000
C	2.53187300	2.52466800	0.36080500
C	1.14559800	-2.85226100	-1.30219900
C	1.25903500	-2.90418100	-2.72556900
C	2.40042100	-3.53505500	-3.26524900

C	3.39610500	-4.08564200	-2.44661000
C	3.26976600	-4.00863200	-1.05194200
C	2.14838900	-3.39758300	-0.45630100
C	0.88548600	-1.28877700	-4.66614700
C	0.23055400	-2.30814600	-3.69919200
C	-0.49275900	-3.42414700	-4.50278200
C	-4.85862500	1.21795400	-2.39254500
C	-4.50346100	-0.26215700	-2.10060600
C	-4.91399000	-1.16917000	-3.29194700
C	-4.41827900	-1.34805200	0.25257100
C	-5.15115200	-0.74466400	-0.79774300
C	-6.53855300	-0.58870800	-0.58968600
C	-7.14135900	-0.99028100	0.61259000
C	-6.36939700	-1.54682100	1.64525300
C	-4.98023400	-1.73548400	1.49190900
C	3.28020900	-3.16235900	1.83062700
C	1.96853000	-3.44228000	1.06086100
C	1.37077200	-4.81725600	1.47402800
C	-4.03853900	-1.23617900	3.78062500
C	-4.14063000	-2.29073200	2.64584200
C	-4.69701200	-3.63616600	3.17662200
C	-1.05742300	3.33539600	-0.32748900
C	-1.84699500	3.89255000	0.71857900
C	-2.95619400	4.68988300	0.35506700
C	-3.26016800	4.95824300	-0.98523100
C	-2.43325400	4.44720800	-1.99688200
C	-1.32078000	3.63464500	-1.69803300
C	-2.71380000	3.06377200	2.96945400
C	-1.53556500	3.72199900	2.20929600
C	-1.15098200	5.08259800	2.85027100
C	4.72082800	-0.46481300	-3.05257900
C	4.27411800	0.65676300	-2.08611300
C	4.47846400	2.04844000	-2.74903800
C	4.33877600	0.90420100	0.48062200
C	4.99990400	0.60189200	-0.73712700
C	6.37736500	0.30914700	-0.66231700
C	7.05434700	0.31797300	0.56871400
C	6.36782400	0.61893900	1.75473400
C	4.98728800	0.91331700	1.73925500
C	-1.14772400	2.61201600	-4.04672500
C	-0.38852300	3.19550600	-2.83185700
C	0.50919600	4.38707100	-3.26799400
C	4.51848300	0.21514400	4.15321200
C	4.25886100	1.26281100	3.04140300
C	4.65988200	2.68083800	3.53239400
H	-1.09432700	-3.83084700	-1.56718700
H	-3.29394400	-3.25690100	-1.01126400
H	1.23702500	4.18808000	0.23473700
H	3.36020400	3.22125000	0.42431500
H	2.51189600	-3.58624500	-4.34524500
H	4.26223900	-4.57023900	-2.89126200
H	4.04135100	-4.43975600	-0.42055900

H	-0.51062500	-1.73764400	-3.13358900
H	-3.41273500	-0.30245400	-2.00570700
H	1.66633800	-1.74813300	-5.28736500
H	1.30865400	-0.46146100	-4.08968900
H	0.12201200	-0.87449900	-5.33855500
H	0.21312800	-3.98544100	-5.12969700
H	-1.25019600	-2.98275700	-5.16413600
H	-0.99541900	-4.14943400	-3.84745800
H	-5.93319000	1.35374400	-2.57554500
H	-4.31857400	1.55598100	-3.28511200
H	-4.56233200	1.86760900	-1.56161700
H	-4.62764600	-2.21639100	-3.12432700
H	-4.42084500	-0.82688600	-4.21054900
H	-5.99942500	-1.14151500	-3.45833700
H	-7.14476800	-0.13478600	-1.36846500
H	-8.21173800	-0.85697800	0.75058700
H	-6.84683000	-1.83259100	2.57843100
H	1.24238600	-2.67024000	1.34003900
H	-3.11806000	-2.46712200	2.29406000
H	4.01838300	-3.96185800	1.68560400
H	3.08003500	-3.09897500	2.90823300
H	3.72744000	-2.21705200	1.50342400
H	2.04709000	-5.63450400	1.18986700
H	0.40328600	-4.99558400	0.98673600
H	1.21691800	-4.86822900	2.56034600
H	-3.54967300	-0.32662000	3.41595200
H	-3.44010500	-1.63354000	4.60973900
H	-5.03137200	-0.97295100	4.16960400
H	-5.69422400	-3.51720300	3.61972500
H	-4.03464700	-4.03228000	3.95728800
H	-4.77055500	-4.38628400	2.37819300
H	-3.57893200	5.11254400	1.13976200
H	-4.11938300	5.57521400	-1.23943000
H	-2.64981300	4.68509800	-3.03502000
H	-0.69352300	3.03498300	2.31701800
H	3.20094400	0.52185400	-1.91164300
H	-3.62998900	3.66868300	2.91708000
H	-2.45281900	2.93663600	4.02913300
H	-2.91994700	2.07226400	2.55232300
H	-0.29764300	5.54359600	2.33375300
H	-0.87402100	4.93822300	3.90378600
H	-1.98402100	5.79830800	2.81784800
H	5.76258500	-0.33729200	-3.37708700
H	4.09151000	-0.44582000	-3.95082200
H	4.61592700	-1.45270600	-2.59168800
H	4.10978700	2.86078500	-2.11077600
H	3.93175100	2.09477600	-3.69938900
H	5.54194500	2.23196200	-2.95481600
H	6.92343200	0.07285200	-1.57058600
H	8.11744400	0.09100600	0.60208100
H	6.90466300	0.62097300	2.69946000
H	0.25105200	2.39005900	-2.46435200



H	3.18109200	1.27273400	2.84568600
H	-1.80013000	3.35132100	-4.53278800
H	-1.74467800	1.75287700	-3.72577000
H	-0.42656900	2.26215700	-4.79796800
H	1.21255400	4.06736700	-4.04954500
H	1.09332100	4.78193000	-2.42543000
H	-0.09363300	5.21306100	-3.67086700
H	4.26944500	-0.79734100	3.81513900
H	3.90317900	0.44239800	5.03334400
H	5.56803300	0.21627800	4.47454300
H	4.42882300	3.44840500	2.78291300
H	5.73546500	2.73405900	3.74660100
H	4.11662700	2.93273200	4.45245000
O	-1.13043000	0.32128300	-1.67958900
O	0.39071300	0.26262800	-1.91828400
C	0.96908300	-0.72561800	3.47669100
H	1.91847300	-0.76134200	2.93556500
C	0.52183000	-1.97999500	4.07275400
H	0.80259400	-2.91460000	3.59697500
O	-0.15742900	-0.57851800	2.47026000
H	0.91547200	0.14767600	4.13595300
C	-0.42545500	-2.01969700	5.23603600
H	-1.14697300	-2.84440500	5.15289000
H	0.11275500	-2.16737000	6.19191000
H	-0.98349000	-1.07901200	5.31951600

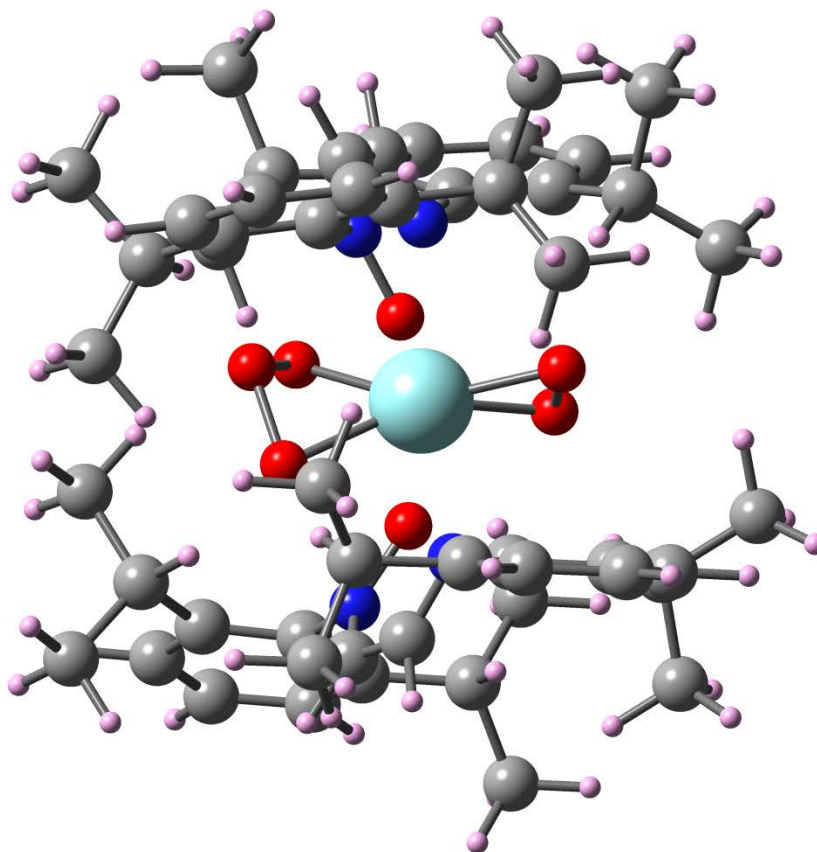
Oxo Peroxo Complex to Peroxo  $\eta^2$ -Ozone ComplexFig. S95: NCCNO Oxo Peroxo Complex to Peroxo  $\eta^2$ -Ozone Complex

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2816.533200	-2815.376073	-2815.303839	-2815.486802	-10
Zr	0.00400000	0.07795300	0.17920500	
O	-2.23449000	0.23998800	-0.05243200	
O	2.09214900	-0.48590200	-0.28197500	
O	-0.43668000	-0.30697000	-1.87058500	
N	0.03411200	-2.05522200	1.07259400	
N	2.92389900	-1.27405500	0.41990900	
N	-0.10623500	2.28652400	-0.63622600	
N	-2.97995300	1.14227500	-0.70201100	
C	1.14787700	-2.68981100	1.41701700	
C	2.49565000	-2.29561800	1.17520000	
C	-1.20501100	2.86206500	-1.08112600	
C	-2.53090800	2.31632300	-1.15125800	
C	-1.21419600	-2.74459700	1.42158400	
C	-1.79606200	-2.51660000	2.69879000	
C	-3.00157000	-3.18861300	2.99565700	
C	-3.59881600	-4.05807400	2.07139200	
C	-2.98485800	-4.29093100	0.83127600	
C	-1.77943500	-3.64811600	0.47911700	

C	-2.09980400	-0.64222700	4.42371100
C	-1.12481500	-1.65362200	3.77551000
C	-0.47887900	-2.55971000	4.86032400
C	4.67441200	2.11597700	2.23894300
C	4.29825700	0.61503500	2.19798300
C	4.59117500	-0.05685600	3.56830400
C	4.36125500	-1.05206200	0.22125400
C	5.02127400	-0.13451400	1.07465500
C	6.41059500	0.02084000	0.88316200
C	7.09140700	-0.70081300	-0.11068800
C	6.39889200	-1.59618800	-0.94069300
C	5.00873800	-1.79127000	-0.79800100
C	-2.06239600	-4.09326100	-2.03172600
C	-1.08276400	-3.98793900	-0.84232900
C	-0.26965900	-5.30573300	-0.70572900
C	4.51551100	-2.47042100	-3.19946800
C	4.26365800	-2.77662900	-1.70394500
C	4.64965700	-4.24020200	-1.36184900
C	1.08873100	3.14234000	-0.62667300
C	1.97970700	3.09232100	-1.73145500
C	3.10038100	3.94960200	-1.70797400
C	3.32516700	4.82370700	-0.63458300
C	2.42647400	4.85391400	0.44262700
C	1.29225300	4.01559500	0.47772300
C	2.97490700	1.35935200	-3.32792700
C	1.73088000	2.20003800	-2.95179100
C	1.25965400	3.05538000	-4.16001900
C	-5.29858800	1.09020800	2.68815300
C	-4.84533800	1.88420500	1.43561800
C	-5.35863700	3.34754600	1.49184700
C	-4.40108700	0.79642300	-0.87104000
C	-5.29832200	1.18791500	0.14828900
C	-6.66468800	0.90227000	-0.06323300
C	-7.09107300	0.24288600	-1.22549300
C	-6.16087700	-0.16450500	-2.19755000
C	-4.78379400	0.09579000	-2.04239600
C	1.05348500	3.93639400	3.02230500
C	0.32541400	4.09965400	1.66508300
C	-0.47824900	5.42793000	1.62304900
C	-4.18172100	-1.64072200	-3.83109200
C	-3.75384000	-0.35391100	-3.08603100
C	-3.48140000	0.76134700	-4.13585900
H	1.05516100	-3.63221300	1.95883600
H	3.28397300	-2.89384100	1.61326900
H	-1.14023500	3.88475200	-1.45845900
H	-3.29080700	2.93437300	-1.61212300
H	-3.46990200	-3.03390900	3.96424400
H	-4.52963800	-4.56250400	2.32117600
H	-3.44309200	-4.98197400	0.12922200
H	-0.33479600	-1.05721200	3.31341700
H	3.21692500	0.56354900	2.03395600
H	-2.93063700	-1.13784500	4.94509900

H	-2.50559900	0.03205200	3.66340500
H	-1.56058700	-0.02911300	5.15744700
H	-1.23810500	-3.15774100	5.38283500
H	0.04146400	-1.94373400	5.60581700
H	0.25100000	-3.25627500	4.42562100
H	5.73081700	2.26853000	2.49884200
H	4.06856000	2.62461200	2.99859900
H	4.48007200	2.60171900	1.27616600
H	4.27895900	-1.10943200	3.57630800
H	4.04229400	0.46240900	4.36394700
H	5.66268300	-0.01954700	3.80772100
H	6.96084200	0.71144400	1.51547700
H	8.16283100	-0.56427800	-0.23825400
H	6.93697500	-2.14366800	-1.70953700
H	-0.37645900	-3.19086100	-1.09262400
H	3.18651300	-2.65661000	-1.55621800
H	-2.73014400	-4.96200100	-1.94835500
H	-1.49695000	-4.19496300	-2.96638500
H	-2.67562000	-3.19083200	-2.10520500
H	-0.92921100	-6.15368100	-0.47375200
H	0.48398800	-5.24085400	0.08999900
H	0.25135800	-5.52193900	-1.64766100
H	4.22985300	-1.43709300	-3.41717300
H	3.89696400	-3.12705300	-3.82149300
H	5.56668100	-2.61747900	-3.48287400
H	5.72181400	-4.41752500	-1.52154100
H	4.09156200	-4.93479500	-2.00267600
H	4.42257900	-4.48724700	-0.31572700
H	3.79693500	3.93366000	-2.54207900
H	4.19285300	5.47948200	-0.63828000
H	2.60741600	5.53427000	1.27077100
H	0.92969300	1.49386400	-2.71975700
H	-3.75026900	1.91215500	1.46037800
H	3.81417800	1.98951200	-3.65309100
H	2.72266400	0.67771800	-4.14930500
H	3.29993600	0.75276600	-2.47615600
H	0.34257400	3.61387200	-3.92636300
H	1.05368800	2.40818400	-5.02239100
H	2.02808400	3.78339000	-4.45397200
H	-6.39280300	1.05841300	2.77209200
H	-4.90573100	1.56605300	3.59564400
H	-4.92648800	0.05988500	2.65521600
H	-5.00716500	3.93155700	0.63101600
H	-5.00029600	3.83927600	2.40523000
H	-6.45591200	3.38454400	1.49618400
H	-7.39268000	1.18939400	0.69059000
H	-8.14812700	0.03256200	-1.37023800
H	-6.50643700	-0.69912500	-3.07645000
H	-0.37782200	3.26418900	1.60789300
H	-2.81047700	-0.56049200	-2.56246700
H	1.79750600	4.72650700	3.19405700
H	1.54439700	2.95911700	3.06102300

H	0.32302800	3.97991100	3.84119300
H	-1.19673600	5.46281600	2.45301600
H	-1.03725200	5.53573500	0.68290800
H	0.18537300	6.29859000	1.71438500
H	-4.51536300	-2.42483300	-3.14184500
H	-3.32828500	-2.02999900	-4.39869700
H	-4.99324400	-1.44418200	-4.54514000
H	-3.08743000	1.67573100	-3.67987900
H	-4.40095500	1.01628300	-4.68072400
H	-2.73623300	0.40965400	-4.85979900
O	0.97141700	0.73770700	1.86621100
O	-0.55268900	0.92193300	1.97535700
O	0.33998200	-0.95301100	-2.94503800
O	1.18841200	-1.94188900	-2.44231600

Peroxo  $\eta^2$ -Ozone Complex to Peroxo  $\eta^3$ -Ozone ComplexFig. S96: NCCNO Peroxo  $\eta^2$ -Ozone Complex to Peroxo  $\eta^3$ -Ozone Complex

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2816.550425	-2815.392853	-2815.320942	-2815.502102	-14

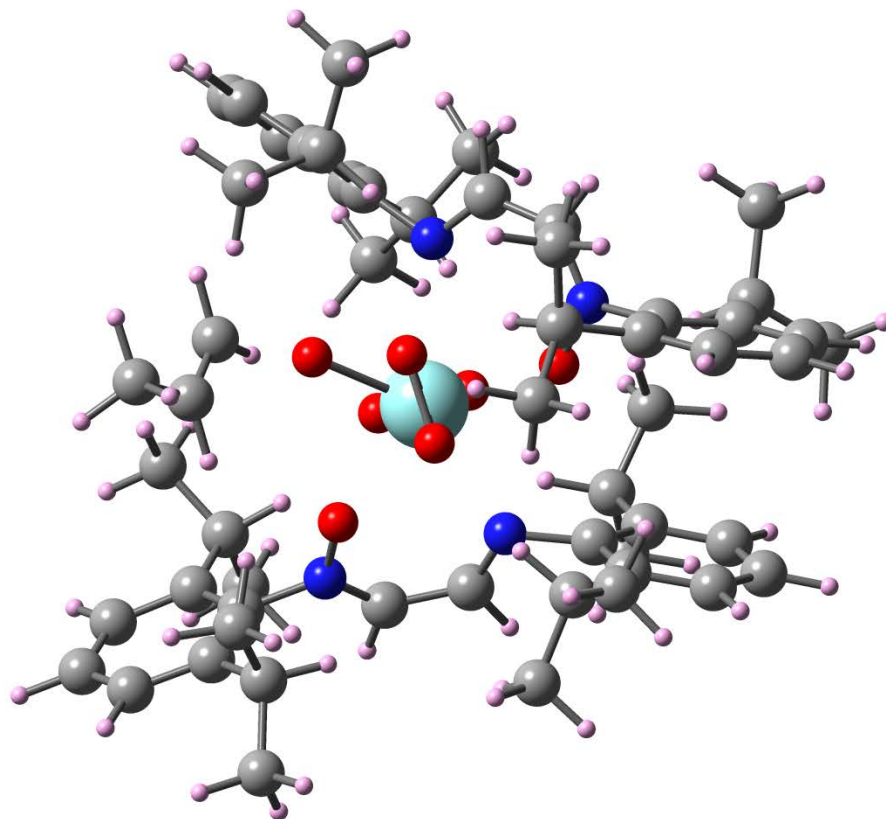
Zr	-0.19942402	0.09575101	-0.34651903
O	2.06395116	0.22909402	0.05513200
O	-2.41957119	-0.64846305	-0.20011902
O	-1.19818309	1.35038111	1.18170509
N	-0.19278401	-2.39272218	-0.47350804
N	-2.88514822	-1.57593912	0.63297405
N	0.36637503	2.56056120	-0.64055505
N	2.81473622	1.19509309	0.58870704
C	-1.02673108	-3.13338724	0.20768802
C	-2.24249817	-2.70900120	0.87025207
C	1.38586111	3.13253324	-0.05697600
C	2.52452819	2.48631119	0.55808404
C	0.90149607	-3.10786124	-1.13687909
C	0.82424506	-3.27536725	-2.54691219
C	1.86887314	-3.97815031	-3.17963024
C	2.94766022	-4.49733935	-2.44662619

C	2.99408623	-4.32629133	-1.05620708
C	1.97662615	-3.63070428	-0.36596403
C	-0.03116000	-2.21543617	-4.72203436
C	-0.39696603	-2.81375022	-3.34523626
C	-1.39885911	-3.99216431	-3.50323827
C	-5.36497638	-0.37667803	-1.96033015
C	-5.21675240	-1.67867913	-1.12672709
C	-6.23628445	-2.75322021	-1.58065512
C	-4.20306732	-1.30348110	1.22759709
C	-5.32867138	-1.36445310	0.36871903
C	-6.58287248	-1.08660109	0.94829107
C	-6.69533952	-0.76799406	2.31197618
C	-5.55340042	-0.70736306	3.12401824
C	-4.26708932	-0.96281808	2.59962020
C	3.47422426	-3.04150923	1.62392312
C	2.06687116	-3.49167726	1.16095109
C	1.69369013	-4.82717137	1.86423714
C	-2.92643023	0.57394804	4.11730931
C	-3.03476523	-0.84611407	3.50487627
C	-3.05874623	-1.93205415	4.61354435
C	-0.62339605	3.47067427	-1.22790910
C	-1.42058811	4.31249833	-0.39574503
C	-2.37032018	5.14449739	-1.02984908
C	-2.51523219	5.16788440	-2.42223819
C	-1.68359713	4.36778834	-3.22002425
C	-0.72168206	3.51168027	-2.64971620
C	-2.67218221	4.12907031	1.82217914
C	-1.30951010	4.39099533	1.13377109
C	-0.73092205	5.76348845	1.57509812
C	5.23921640	-0.84744506	-1.87845514
C	5.03480438	0.53250904	-1.20035809
C	6.03803444	1.57919312	-1.75354913
C	4.07579031	0.74120806	1.19904709
C	5.14150639	0.42032203	0.32428002
C	6.34367050	-0.01030900	0.92251207
C	6.45949448	-0.11488601	2.31824618
C	5.37373644	0.20373802	3.14846024
C	4.14347732	0.63750205	2.60897620
C	-0.37839503	2.17665017	-4.81763737
C	0.27269102	2.77688521	-3.55136027
C	1.43312511	3.74047429	-3.93164830
C	2.56613220	-0.25188402	4.40492234
C	2.97104723	0.96934207	3.54003527
C	3.30699025	2.19293017	4.43448434
H	-0.84688407	-4.20889932	0.28165102
H	-2.73639421	-3.40532826	1.53556512
H	1.44512911	4.22304632	-0.02302800
H	3.26530225	3.12782824	1.01973908
H	1.83446914	-4.12228931	-4.25552832
H	3.74365229	-5.03642839	-2.95551923
H	3.83087929	-4.73549936	-0.49650404
H	-0.89113407	-2.01066815	-2.79192721

H	-4.21417232	-2.06976416	-1.33509010
H	0.40925303	-2.95759122	-5.40311641
H	0.66687205	-1.38254311	-4.59080835
H	-0.93683307	-1.82203914	-5.20162840
H	-0.95295107	-4.81850237	-4.07436131
H	-2.29743818	-3.65478928	-4.03733931
H	-1.71344613	-4.39287034	-2.52887619
H	-6.34870451	0.08530901	-1.79999314
H	-5.26153340	-0.60002304	-3.03006723
H	-4.58844535	0.34470803	-1.68679213
H	-6.14264945	-3.67465628	-0.99105307
H	-6.06580847	-3.00327023	-2.63566620
H	-7.27100256	-2.39840319	-1.49136311
H	-7.47537055	-1.12087109	0.33024003
H	-7.67359759	-0.55938504	2.73861521
H	-5.65395241	-0.44387203	4.17313332
H	1.36456910	-2.71813121	1.49065811
H	-2.12509616	-0.98576407	2.91274722
H	4.23587232	-3.80629829	1.42290711
H	3.47093327	-2.85887622	2.70605721
H	3.77346229	-2.11605616	1.12319708
H	2.38576718	-5.62810945	1.57122812
H	0.67910405	-5.16170139	1.61130312
H	1.74929714	-4.71199036	2.95514422
H	-2.81396022	1.31832910	3.32302625
H	-2.03460516	0.63059305	4.75459936
H	-3.80132629	0.82723506	4.73172536
H	-3.92421630	-1.81101614	5.27912040
H	-2.15022117	-1.86115614	5.22512040
H	-3.10373824	-2.94582722	4.19122032
H	-3.00279923	5.78095145	-0.41657103
H	-3.25771125	5.81536147	-2.88321222
H	-1.77442213	4.41194033	-4.30113733
H	-0.64616505	3.59792928	1.48474812
H	4.02571631	0.86331607	-1.46766711
H	-3.41875426	4.89195138	1.56386312
H	-2.54755820	4.13827331	2.91363722
H	-3.05543223	3.14569824	1.53292712
H	0.25485602	5.95695946	1.12866109
H	-0.62295105	5.79671247	2.66793020
H	-1.39104211	6.58907851	1.27765010
H	6.23887345	-1.25293109	-1.67145613
H	5.13307839	-0.74772406	-2.96607623
H	4.49258434	-1.57099912	-1.53391112
H	5.88620544	2.56549620	-1.29542010
H	5.90993544	1.68406013	-2.83840521
H	7.07710455	1.27814910	-1.56620412
H	7.19073854	-0.26494502	0.29150202
H	7.39588754	-0.44869403	2.75876921
H	5.47678640	0.10865301	4.22589833
H	0.69247705	1.93305415	-2.99814123
H	2.08911816	1.22071710	2.94371222



H	-0.76141606	2.94586622	-5.50366342
H	-1.19309909	1.50320711	-4.53311235
H	0.36748503	1.58702912	-5.36687438
H	2.17489417	3.21332025	-4.54702235
H	1.94643615	4.12932431	-3.04034623
H	1.06319808	4.60174535	-4.50549534
H	2.21473517	-1.07312208	3.77192129
H	1.74180313	0.02851000	5.07259739
H	3.39919326	-0.60992805	5.02448638
H	3.57593827	3.07349823	3.83528629
H	4.14762732	1.97890615	5.10773939
H	2.43870619	2.45495219	5.05215038
O	-0.94658507	0.15534801	-2.24882917
O	0.59879405	-0.01020200	-2.24135017
O	-0.02212100	0.74649506	1.93872615
O	-0.10666701	-0.75637106	1.67438513

Peroxo  $\eta^3$ -Ozone Complex to Spiro Bisperoxo ComplexFig. S97: NCCNO Peroxo  $\eta^3$ -Ozone Complex to Spiro Bisperoxo Complex

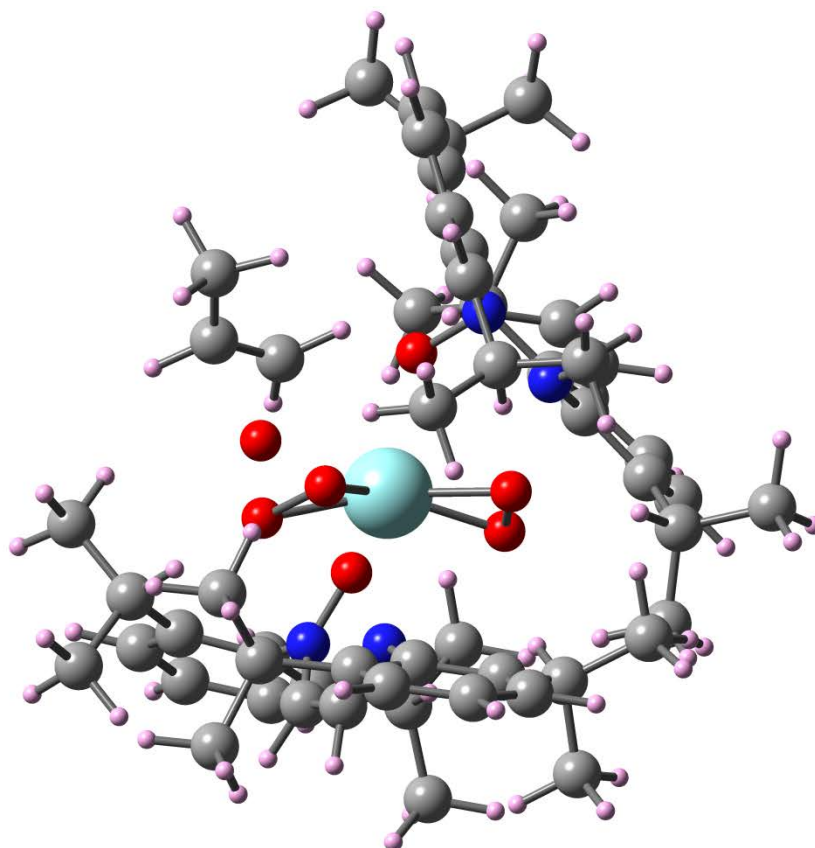
SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2934.421423	-2933.182058	-2933.104869	-2933.295695	-335

Zr	0.26242000	0.20053300	-0.09512900
O	-2.05048600	0.04046400	0.15919800
O	2.14003900	-1.10028900	-0.73441600
O	1.35621800	1.55141900	-1.40505600
N	0.01773200	-2.21402100	0.78167200
N	2.92724100	-1.86242200	0.04305100
N	-0.70195100	2.68480400	0.37201700
N	-3.02767400	0.80935000	-0.33283000
C	1.05492200	-2.82547500	1.30867400
C	2.44563400	-2.60602900	1.02605700
C	-1.93178500	3.00584600	0.07534500
C	-3.00300600	2.12952300	-0.34216800
C	-1.25643100	-2.84885700	1.11704400
C	-1.71955600	-2.88947000	2.46303000
C	-2.89585000	-3.62536200	2.72770400
C	-3.58677700	-4.29485900	1.70983000

C	-3.11514700	-4.23129900	0.38866200
C	-1.94536800	-3.51690000	0.06357600
C	-1.96067500	-1.10397800	4.25597200
C	-1.02697600	-2.17129400	3.62971000
C	-0.54225100	-3.17312700	4.71098300
C	5.50550300	0.79266900	2.10438400
C	4.85978000	-0.60570000	1.92896400
C	5.22851100	-1.50860000	3.13903800
C	4.35704000	-1.86817200	-0.28996800
C	5.27649800	-1.27018800	0.60921300
C	6.63910500	-1.31238500	0.24094800
C	7.04892500	-1.89683100	-0.96680700
C	6.10505600	-2.46334200	-1.83890700
C	4.73189200	-2.46964400	-1.51917900
C	-2.46021100	-3.72865500	-2.44864100
C	-1.37779500	-3.55299600	-1.35985300
C	-0.32461300	-4.69009100	-1.49521300
C	3.45062200	-2.13476000	-3.68126900
C	3.71485400	-3.08885100	-2.48453800
C	4.15272900	-4.49178600	-2.97559200
C	0.17948700	3.82276500	0.60584400
C	0.43213100	4.74301600	-0.45758000
C	1.31156900	5.81566600	-0.19477900
C	1.90480800	5.98790900	1.06390700
C	1.61410100	5.08728300	2.10057300
C	0.74919500	3.99306400	1.89893000
C	0.89722900	4.56319400	-2.97173900
C	-0.18149700	4.63755900	-1.86378600
C	-1.15691200	5.81723700	-2.12981400
C	-5.69657500	-1.17011100	2.47293300
C	-5.04448700	-0.08360000	1.58778600
C	-5.66366000	1.30211300	1.93515400
C	-4.22271800	0.11097500	-0.85312800
C	-5.17499500	-0.36337600	0.08521400
C	-6.29905300	-1.03299000	-0.43667700
C	-6.45958500	-1.20742000	-1.82213200
C	-5.50877100	-0.69793000	-2.71692400
C	-4.35896100	-0.01709000	-2.25690200
C	1.50970800	2.74060700	4.01105500
C	0.33602800	3.10684600	3.07510600
C	-0.80784100	3.79839800	3.86962100
C	-2.90011300	-0.41886200	-4.33043200
C	-3.38200700	0.59750000	-3.26750100
C	-4.03717700	1.83131600	-3.94978500
H	0.88691600	-3.65075700	2.00575700
H	3.17178600	-3.18711700	1.57963100
H	-2.23343800	4.05692200	0.08989800
H	-3.90145500	2.60070800	-0.72045600
H	-3.26852300	-3.67297800	3.74831000
H	-4.48355900	-4.86558100	1.94143400
H	-3.65686100	-4.75255000	-0.39424900
H	-0.16807900	-1.61373800	3.24798400

H	3.77399200	-0.45523600	1.93375700
H	-2.88133200	-1.54844000	4.65981100
H	-2.22873600	-0.35253700	3.50512600
H	-1.44379800	-0.58756200	5.07573500
H	-1.38134500	-3.71076200	5.17326400
H	-0.00795700	-2.63853600	5.50776500
H	0.13947800	-3.92688000	4.29271300
H	6.59417700	0.72969300	2.23443600
H	5.09170100	1.27582400	2.99869200
H	5.29844200	1.43893800	1.24455800
H	4.75222600	-2.49616700	3.08067300
H	4.90350700	-1.03406400	4.07364700
H	6.31398800	-1.66683800	3.19582100
H	7.38074700	-0.86873000	0.89895100
H	8.10381600	-1.90823400	-1.23076500
H	6.43760800	-2.91114400	-2.77088300
H	-0.87245100	-2.59959800	-1.54942200
H	2.75858000	-3.20642700	-1.96348500
H	-2.91164200	-4.73019100	-2.42080400
H	-2.00612200	-3.60370400	-3.43970600
H	-3.25962600	-2.98627600	-2.34482800
H	-0.78883200	-5.67169900	-1.32566000
H	0.49604600	-4.57548800	-0.77731600
H	0.10723200	-4.68492300	-2.50510100
H	3.01557600	-1.19341300	-3.33175300
H	2.73883400	-2.59467500	-4.37902300
H	4.37895100	-1.92245700	-4.22952000
H	5.04942000	-4.44402800	-3.60687900
H	3.35169300	-4.93775200	-3.57905200
H	4.36452600	-5.16696400	-2.13618600
H	1.53407700	6.52348500	-0.98947400
H	2.57819000	6.82392600	1.23880300
H	2.05478100	5.24050800	3.08141800
H	-0.74247200	3.70276100	-1.94627100
H	-3.97765500	-0.05564500	1.83802200
H	1.56245400	5.43710100	-2.96327800
H	0.41532100	4.51916300	-3.95806700
H	1.48608900	3.65332200	-2.84076500
H	-1.95470800	5.87315200	-1.37592700
H	-1.62530200	5.70719500	-3.11717000
H	-0.62800200	6.77928100	-2.11552000
H	-6.79187600	-1.15862500	2.39118800
H	-5.44623800	-0.98297900	3.52477600
H	-5.33372200	-2.16810600	2.21062900
H	-5.18683800	2.12073300	1.38319700
H	-5.54611000	1.50819000	3.00684500
H	-6.73646000	1.31533000	1.70058800
H	-7.05200800	-1.42088200	0.24146900
H	-7.33297400	-1.73238700	-2.20192900
H	-5.65389600	-0.82664800	-3.78558000
H	-0.04539300	2.16061000	2.68000200
H	-2.47849900	0.93335700	-2.75167400

H	1.93738600	3.61638100	4.51959800
H	2.29700500	2.22930300	3.44676500
H	1.15493600	2.04771200	4.78510700
H	-1.14865200	3.14724800	4.68595600
H	-1.67228900	4.01421200	3.22607100
H	-0.47079600	4.74855700	4.30791100
H	-2.32690100	-1.21878100	-3.85624500
H	-2.23058400	0.08699300	-5.03708300
H	-3.73055400	-0.85474700	-4.90273900
H	-4.36154700	2.58363000	-3.21726200
H	-4.91753300	1.54134200	-4.53902000
H	-3.31687600	2.30694500	-4.62728000
O	1.57093600	0.35405800	1.54826300
O	0.12862600	0.18258700	2.00563800
O	-0.35596700	1.03164200	-1.98702600
O	-0.29813600	-0.46542100	-2.07233800
C	3.11343600	2.38883300	-0.41664100
H	2.93947600	1.94997100	0.56016500
H	2.98004200	3.46253700	-0.50899500
C	3.51914300	1.63135600	-1.49034400
H	3.64945300	0.56348400	-1.35576900
C	3.85848400	2.17219400	-2.85282300
H	3.78617400	3.26415500	-2.89324600
H	4.87863800	1.87766900	-3.14072300
H	3.17072800	1.74792400	-3.59645100

Peroxo  $\eta^3$ -Ozone Complex to Planar Bisperoxo ComplexFig. S98: NCCNO Peroxo  $\eta^3$ -Ozone Complex to Planar Bisperoxo Complex

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2934.41547840	-2933.176962	-2933.099532	2933.293042	-368

Zr	0.09307800	0.69870700	-0.34570900
O	-1.99277100	-0.23044700	-0.48817000
O	2.00676600	-0.42241600	-0.85743500
O	0.74207500	2.52981100	-1.13228600
N	1.33997600	-2.64631700	1.07517200
N	3.14264800	-0.49954200	-0.10667600
N	-1.47189400	2.44753000	0.68945600
N	-3.20216200	0.30248200	-0.65291900
C	2.28973700	-2.01834400	1.70233200
C	3.22029100	-1.10442000	1.06331200
C	-2.75092400	2.49854000	0.44193100
C	-3.56136200	1.50778600	-0.23973300
C	0.53866400	-3.65186900	1.68125200
C	-0.01360000	-3.56689100	3.00207400
C	-0.73942600	-4.67749400	3.48258700
C	-0.94233400	-5.82568500	2.70339900

C	-0.45020100	-5.87050200	1.38852900
C	0.27571000	-4.79252100	0.85175200
C	-1.33172500	-1.84774000	4.33930200
C	0.07620400	-2.31828500	3.89079000
C	0.98332600	-2.56316500	5.12616400
C	3.47378100	3.65558700	0.09444900
C	3.89995900	2.28136300	0.66862700
C	4.73557400	2.46012700	1.96589700
C	4.33803300	0.12284400	-0.70374000
C	4.67864500	1.45081100	-0.35534400
C	5.83232800	1.99287500	-0.96557900
C	6.59400200	1.24640800	-1.87472000
C	6.22934400	-0.07345700	-2.19070400
C	5.09116400	-0.66776600	-1.61142400
C	-0.10898700	-5.55102600	-1.57497500
C	0.84334200	-4.86587700	-0.56724600
C	2.22969300	-5.56773000	-0.56397500
C	4.95215800	-2.52832100	-3.38249400
C	4.73924600	-2.13266800	-1.90131100
C	5.56337900	-3.07389600	-0.97766800
C	-0.90538800	3.62688500	1.35037600
C	-0.78232700	4.84855000	0.62625500
C	-0.21456500	5.95053600	1.30227800
C	0.19997000	5.85970900	2.63736500
C	0.03650500	4.65355400	3.33543300
C	-0.51747300	3.51608700	2.71457800
C	-0.11349700	5.61271800	-1.72293500
C	-1.24118400	5.04363900	-0.82590300
C	-2.49670700	5.95778100	-0.88558000
C	-3.95653300	-3.11246300	1.26256200
C	-4.55868800	-1.70598400	1.00388000
C	-5.81603800	-1.46626300	1.87933500
C	-4.19538100	-0.57719100	-1.29876700
C	-4.86451800	-1.52009000	-0.48535300
C	-5.83495600	-2.32622300	-1.11784700
C	-6.10093400	-2.19274200	-2.48933500
C	-5.38942200	-1.26374800	-3.26679400
C	-4.40317600	-0.43454200	-2.69226200
C	0.34470200	1.89495300	4.50477600
C	-0.80479500	2.25813200	3.53764100
C	-2.14283700	2.43437300	4.31016600
C	-3.19942800	-0.03048800	-4.91168200
C	-3.61827900	0.56870800	-3.54642000
C	-4.43875900	1.86910800	-3.77007600
H	2.54196400	-2.21817700	2.74910900
H	4.16789400	-0.95605900	1.57370700
H	-3.32636600	3.37442500	0.75324800
H	-4.59851000	1.75922300	-0.42268800
H	-1.15935100	-4.63807100	4.48461500
H	-1.49302900	-6.67070300	3.11052400
H	-0.63466500	-6.74961100	0.77761000
H	0.47990800	-1.49067500	3.30304100

H	2.98497800	1.75025200	0.94528900
H	-1.84817500	-2.59721400	4.95390500
H	-1.95102000	-1.62077300	3.46397500
H	-1.24299600	-0.93025900	4.93490700
H	0.57145500	-3.34970700	5.77337000
H	1.07001200	-1.64535400	5.72316900
H	1.99574200	-2.87677100	4.83660700
H	4.34191900	4.27781400	-0.16397700
H	2.88019900	4.19773800	0.84120500
H	2.84803100	3.52672300	-0.79470200
H	5.01403600	1.49350400	2.40820200
H	4.15026900	3.01585700	2.70919600
H	5.66084200	3.01988800	1.77263000
H	6.12810200	3.01037900	-0.72643800
H	7.47403300	1.68885900	-2.33573000
H	6.83371300	-0.64124200	-2.89193900
H	1.00304300	-3.83381300	-0.89457200
H	3.67757200	-2.28397800	-1.67418900
H	-0.21998400	-6.62562600	-1.37640100
H	0.28949100	-5.44627500	-2.59277900
H	-1.10732700	-5.09578000	-1.55325100
H	2.14273200	-6.60538300	-0.21360000
H	2.93534400	-5.04601100	0.09462100
H	2.65411800	-5.58515200	-1.57754400
H	4.41986300	-1.85108100	-4.05893400
H	4.57632300	-3.54579000	-3.55192100
H	6.01478100	-2.52330500	-3.65741300
H	6.63874000	-2.96042900	-1.16884800
H	5.29131800	-4.12157500	-1.16028200
H	5.38609600	-2.85813400	0.08339800
H	-0.09510000	6.88959600	0.76845700
H	0.63531400	6.72413600	3.13368200
H	0.33474000	4.59507600	4.37813900
H	-1.49720200	4.07206200	-1.25655100
H	-3.79751000	-0.97840900	1.30790200
H	0.20713700	6.61301000	-1.40144500
H	-0.46915000	5.69299100	-2.75919300
H	0.74433700	4.93472200	-1.70901500
H	-3.32933500	5.55534300	-0.29093700
H	-2.83887400	6.06497100	-1.92390300
H	-2.27514500	6.96171900	-0.49932900
H	-4.66309400	-3.90698800	0.98825400
H	-3.71066800	-3.22967100	2.32487300
H	-3.03484400	-3.25673500	0.68804300
H	-6.23444500	-0.46369700	1.71972200
H	-5.55797400	-1.56263300	2.94160800
H	-6.60451000	-2.19767800	1.65978700
H	-6.37846800	-3.06300300	-0.53292200
H	-6.85531100	-2.82090800	-2.95689400
H	-5.59200100	-1.19047700	-4.33091300
H	-0.90888600	1.41101000	2.85400400
H	-2.68907500	0.83021500	-3.02734700



H	0.51075800	2.66172300	5.27439900
H	1.26856400	1.74215300	3.93778500
H	0.10758200	0.95738500	5.02508300
H	-2.38616300	1.51800700	4.86521800
H	-2.97784500	2.64857600	3.62794000
H	-2.08069900	3.26296100	5.02950100
H	-2.67535300	-0.98480800	-4.78312000
H	-2.52202300	0.66607300	-5.42025500
H	-4.06117500	-0.19724500	-5.57160500
H	-4.70156400	2.35827000	-2.82353500
H	-5.37170200	1.65759000	-4.31015700
H	-3.85266800	2.58292000	-4.36215700
O	1.11546700	0.80746200	1.48675100
O	-0.10088100	-0.13627500	1.53967000
O	-0.49305700	2.10476900	-1.91513900
O	-0.13848100	0.44432700	-2.55819000
C	0.17013900	-1.73520100	-2.96977900
H	0.92929900	-2.04422600	-2.25910500
H	-0.83319700	-2.13269100	-2.84529800
C	0.46481100	-0.83353200	-3.97227400
H	-0.31840700	-0.58592200	-4.68643800
C	1.84536300	-0.33166700	-4.31202200
H	2.24752600	-0.86619000	-5.18736500
H	1.80229600	0.73587600	-4.55529100
H	2.52191400	-0.45773600	-3.46382400

## Oxo Peroxo Complex to Dioxo Complex

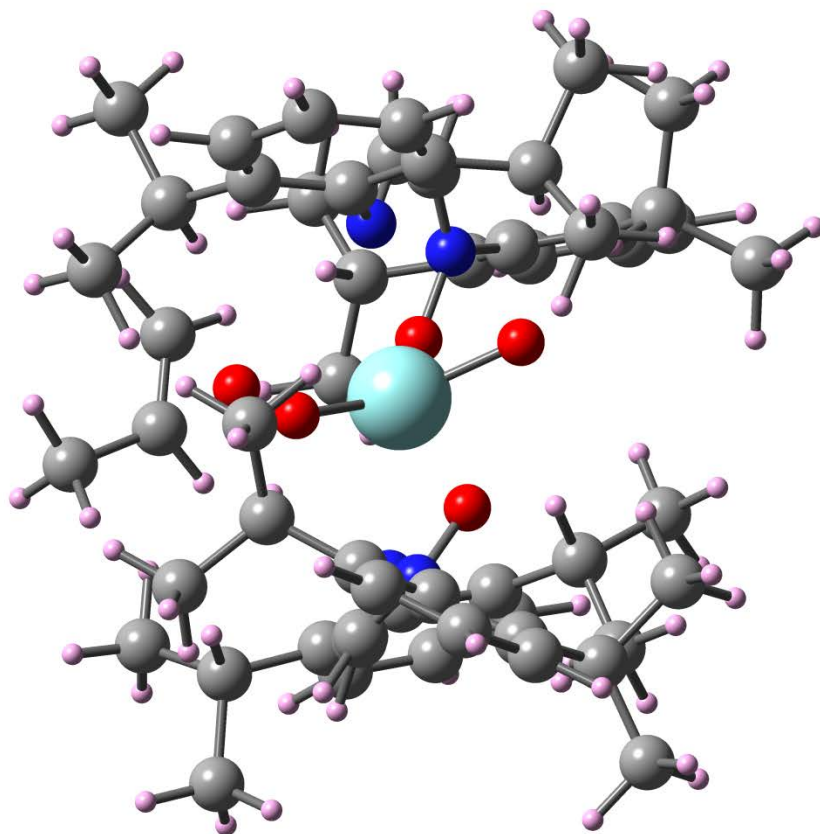


Fig. S99: NCCNO Oxo Peroxo Complex to Dioxo Complex

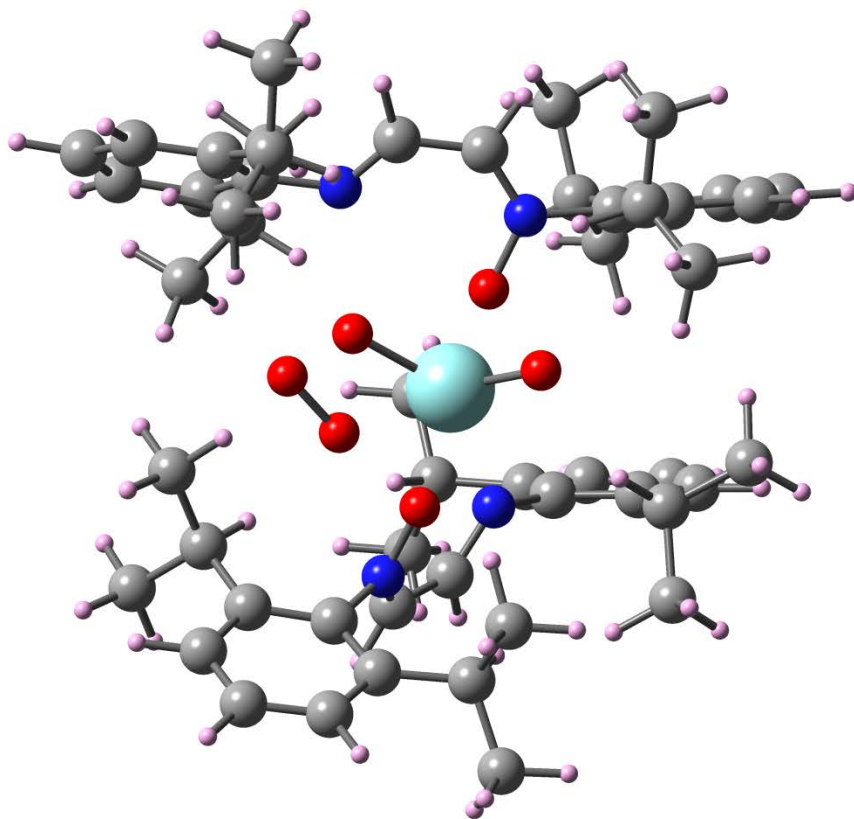
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Zr	0.12985800	0.16853300	0.13111800
O	-2.16541300	0.37800600	0.17670700
O	1.96513700	-0.84710100	-1.08796800
O	0.01352600	1.02544500	-1.54543300
N	0.00441400	-2.41948300	0.24813500
N	2.84539700	-1.66593100	-0.52027400
N	-0.08593100	2.59739100	0.59062400
N	-2.87426500	1.47183800	-0.15737900
C	1.11597700	-3.06965400	0.50969500
C	2.47740800	-2.63271800	0.31389000
C	-1.20011500	3.25875800	0.42268800
C	-2.49470900	2.72463700	0.06140400
C	-1.23563300	-3.18969800	0.24999500
C	-1.66792000	-3.98707500	1.35769000
C	-2.90489400	-4.65990000	1.23812200
C	-3.68456600	-4.57582400	0.07969300

C	-3.22308400	-3.82647100	-1.01265300
C	-1.99870100	-3.13481900	-0.95926800
C	-1.75863600	-4.11175300	3.93144100
C	-0.87436600	-4.21073700	2.65835300
C	-0.18911700	-5.60882500	2.65305600
C	5.21558700	1.10937600	1.54692100
C	4.74454200	-0.35368600	1.35028400
C	5.29073300	-1.25953900	2.48640400
C	4.25319900	-1.50332700	-0.92374200
C	5.15773200	-0.89325900	-0.02274900
C	6.49906000	-0.78664100	-0.45480300
C	6.89495500	-1.23608500	-1.72255800
C	5.95620300	-1.80302700	-2.60073700
C	4.60698100	-1.95135900	-2.22216000
C	-2.51822700	-2.05395100	-3.24119100
C	-1.43919500	-2.46879600	-2.22050300
C	-0.42310800	-3.42487400	-2.90942100
C	3.14494100	-1.42474900	-4.21467500
C	3.58153900	-2.52328600	-3.20591000
C	4.09571600	-3.78482700	-3.94199800
C	1.11712800	3.42880000	0.73016200
C	1.68135700	4.03425200	-0.43065700
C	2.82376800	4.84636500	-0.25363700
C	3.38284200	5.06463600	1.01209000
C	2.80038000	4.46426200	2.13781500
C	1.66710000	3.63407100	2.02377800
C	2.19907500	3.26226900	-2.80050800
C	1.12791700	3.85489000	-1.84983700
C	0.57682300	5.19549600	-2.40441400
C	-5.23950900	-1.11421200	1.67960900
C	-5.14121800	0.40711500	1.39742500
C	-6.21265400	1.19325400	2.19685800
C	-4.15242900	1.22354500	-0.84879000
C	-5.23257500	0.69588300	-0.10190200
C	-6.43798800	0.45612900	-0.79402300
C	-6.55114400	0.74041200	-2.16334600
C	-5.46039300	1.27055500	-2.87070700
C	-4.22410000	1.52309300	-2.23759900
C	2.05804400	2.32607700	4.17544400
C	1.02512500	3.05599200	3.28451900
C	0.28409700	4.16885100	4.07454900
C	-2.93658100	1.50867500	-4.46345500
C	-3.05380300	2.11397500	-3.04189700
C	-3.20367000	3.65691500	-3.17930800
H	1.06283800	-4.11548200	0.81743700
H	3.27452400	-3.24251200	0.71913400
H	-1.19035000	4.35128300	0.46147700
H	-3.26094100	3.45707500	-0.16008300
H	-3.26043300	-5.25906000	2.07114600
H	-4.63515800	-5.10040000	0.02171900
H	-3.81752700	-3.78696900	-1.91866900
H	-0.09305300	-3.44702900	2.74377200

H	3.64952200	-0.32246400	1.42391100
H	-2.43276600	-4.97261900	4.01969300
H	-2.36921400	-3.20323400	3.94058000
H	-1.12116800	-4.10407300	4.82448600
H	-0.94534500	-6.40358100	2.61676900
H	0.40345400	-5.74613200	3.56732300
H	0.47397200	-5.75772200	1.79139800
H	6.31103400	1.19953800	1.56429200
H	4.82939500	1.48961700	2.50006500
H	4.82319600	1.75654900	0.75442000
H	4.93090900	-2.29406400	2.39448800
H	4.95992600	-0.87476500	3.45950700
H	6.38957800	-1.28805300	2.48684100
H	7.23089800	-0.33006800	0.20519600
H	7.93254500	-1.13584500	-2.03258100
H	6.27438500	-2.13291100	-3.58536500
H	-0.89585800	-1.55814800	-1.94493000
H	2.68300200	-2.81441700	-2.64937600
H	-3.01898500	-2.92209400	-3.69112500
H	-2.04001600	-1.49728500	-4.05493100
H	-3.27928400	-1.41007600	-2.78521500
H	-0.92854500	-4.33567600	-3.25924400
H	0.38358700	-3.72447000	-2.23041000
H	0.03257900	-2.92697100	-3.77477200
H	2.69216600	-0.57809100	-3.68855500
H	2.40595800	-1.82967100	-4.91947700
H	4.00501500	-1.06257900	-4.79405100
H	4.92982500	-3.55285700	-4.61637400
H	3.29048400	-4.21047200	-4.55496500
H	4.43439800	-4.55575700	-3.23748300
H	3.27500500	5.31288400	-1.12591300
H	4.25984100	5.69900000	1.12109800
H	3.22713100	4.64242200	3.12149000
H	0.33097800	3.10527600	-1.83076600
H	-4.16100800	0.73680600	1.75312800
H	3.08371800	3.90842300	-2.89063900
H	1.77171700	3.12909900	-3.80377700
H	2.50958300	2.27649100	-2.43920900
H	-0.21822300	5.60392600	-1.76425700
H	0.16126700	5.04701100	-3.41097600
H	1.36478100	5.95800000	-2.47758800
H	-6.21505400	-1.51328300	1.37028700
H	-5.12158300	-1.30609800	2.75410400
H	-4.45905100	-1.66451800	1.14341200
H	-6.13754000	2.27331300	2.01554700
H	-6.08063200	1.01757300	3.27226700
H	-7.22935700	0.87725800	1.93002800
H	-7.29131200	0.05305700	-0.25519000
H	-7.48900200	0.55125400	-2.68029100
H	-5.56407500	1.48041800	-3.93085700
H	0.30594900	2.29149100	2.98176500
H	-2.10936100	1.89068300	-2.52747400

H	2.87358200	2.98564700	4.50446500
H	2.47045900	1.47999100	3.61664700
H	1.56626600	1.93686700	5.07787000
H	-0.21649300	3.74433000	4.95629500
H	-0.47858800	4.66346200	3.45635900
H	0.98124500	4.94343900	4.42393400
H	-2.93443500	0.41622100	-4.43787000
H	-1.99297300	1.83769900	-4.91531300
H	-3.75231100	1.83836200	-5.12151200
H	-3.22705400	4.17093100	-2.21132300
H	-4.12916700	3.91132400	-3.71396300
H	-2.35732300	4.06222800	-3.74777600
O	1.65611300	0.27020200	1.37373900
O	0.06789900	0.17620800	2.42325100
C	-0.90355600	-0.73117700	3.62394600
H	-1.24382300	-1.58196100	3.04101300
C	-1.73927300	0.38962000	3.63873100
H	-2.56156800	0.48012600	2.93971000
H	-1.54153800	1.22542000	4.30372500
C	0.07451000	-1.04340500	4.73634000
H	0.40789700	-0.12040600	5.22136600
H	-0.38276100	-1.69296200	5.49734800
H	0.96107000	-1.54519000	4.33124000

Dioxo Complex to Oxo  $\eta^2$ -Ozone ComplexFig. S100: NCCNO Dioxo Complex to Oxo  $\eta^2$ -Ozone Complex

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
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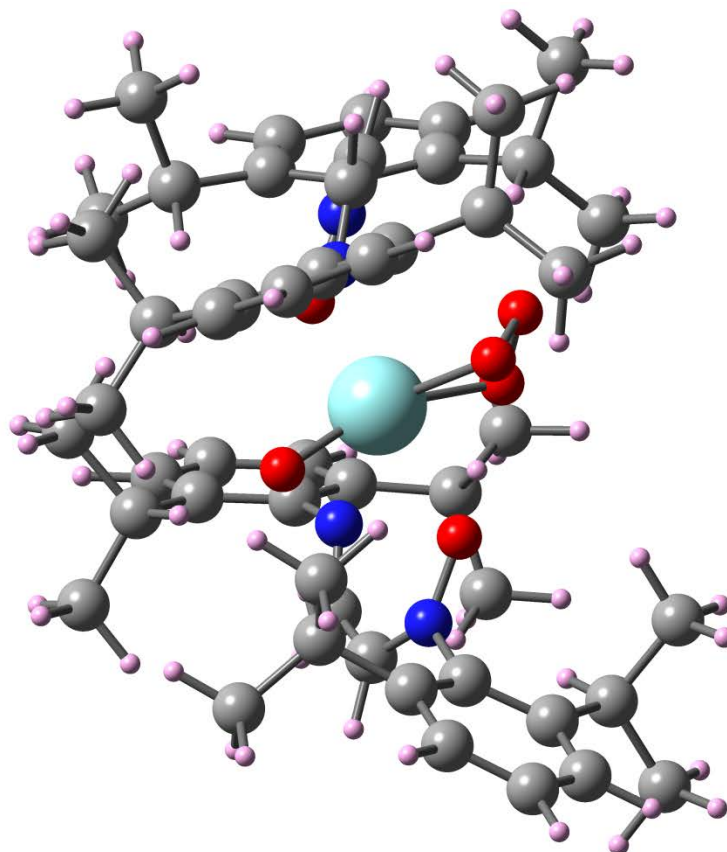
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O	-1.82963714	0.03157100	-0.06619401
O	2.55909220	-0.82247806	-0.66580405
O	0.84990207	1.62943412	-1.09614308
N	0.74361006	-2.00990415	1.19223609
N	3.45685126	-0.99697308	0.30688402
N	-1.71488713	2.97331423	-0.27505302
N	-2.83973022	0.23680602	-0.96193507
C	1.86408014	-2.05060616	1.87061614
C	3.14263224	-1.48903311	1.49583011
C	-2.46831019	2.69366320	-1.29824110
C	-3.11915124	1.41278611	-1.49587211
C	-0.36267603	-2.78123621	1.74158613
C	-0.91434207	-2.44339219	3.01052623
C	-1.93144515	-3.27960525	3.52018327
C	-2.39118718	-4.39205634	2.80186421

C	-1.85441814	-4.68103636	1.53612812
C	-0.83574607	-3.88571430	0.97599408
C	-1.70726213	-0.23110102	3.97766931
C	-0.50555304	-1.19742709	3.80970229
C	0.09459001	-1.57039312	5.19079340
C	4.22200132	2.85457422	0.00699000
C	4.49304534	1.68318013	0.98857407
C	5.15024339	2.18974417	2.29784018
C	4.84585437	-0.66601205	-0.04681100
C	5.34336240	0.60990805	0.30369402
C	6.68037450	0.88567707	-0.05894100
C	7.45468856	-0.05851400	-0.74904506
C	6.90986851	-1.30348310	-1.10627609
C	5.58383743	-1.63863812	-0.76579106
C	-1.18119409	-4.92951238	-1.34925810
C	-0.19826601	-4.24917532	-0.36947903
C	1.04694408	-5.15416040	-0.15098001
C	4.59557935	-2.88181322	-2.72990221
C	4.97181238	-2.96596023	-1.22461910
C	5.89476647	-4.17708432	-0.94340707
C	-1.09290708	4.22167932	-0.07761701
C	-0.47451204	4.98682938	-1.12266909
C	0.05109900	6.24901148	-0.78198906
C	-0.00390400	6.74164052	0.53093804
C	-0.53632404	5.94437546	1.55927412
C	-1.05980908	4.67002635	1.28478610
C	1.25736210	4.47150634	-2.91299922
C	-0.24986402	4.46338334	-2.54802019
C	-1.07859408	5.25976340	-3.59086727
C	-5.08990739	-1.38370911	2.29411518
C	-4.76976336	-0.50536404	1.06269508
C	-5.87246747	0.57690205	0.87866207
C	-3.70738828	-0.92141107	-1.25473110
C	-4.61273435	-1.31232610	-0.23249702
C	-5.44591140	-2.41550418	-0.49937404
C	-5.38371640	-3.08495723	-1.73305313
C	-4.49873634	-2.65117720	-2.72899821
C	-3.63275528	-1.55297512	-2.52164819
C	-0.90346207	3.94873930	3.74249128
C	-1.63680512	3.78716629	2.39182118
C	-3.15947024	4.04418131	2.56563420
C	-1.94066815	-2.22402917	-4.32789633
C	-2.74233721	-1.07235308	-3.67489928
C	-3.60376728	-0.33508403	-4.73891736
H	1.90009615	-2.61145620	2.80925722
H	3.96049830	-1.57092412	2.20076017
H	-2.74096721	3.43462826	-2.05876316
H	-3.94566130	1.39201811	-2.19843817
H	-2.37121318	-3.04807723	4.48729734
H	-3.17029324	-5.02555838	3.21969925
H	-2.22884717	-5.53430644	0.97944407
H	0.24859202	-0.63566805	3.25119425

H	3.51426027	1.26958310	1.24849510
H	-2.52254519	-0.69069605	4.55236235
H	-2.09643616	0.06995401	2.99852623
H	-1.38525510	0.67437105	4.50835234
H	-0.63963205	-2.08834716	5.82200042
H	0.41265103	-0.66381905	5.72202646
H	0.96703007	-2.23103117	5.09160839
H	5.15796939	3.32905925	-0.32006002
H	3.59799828	3.60969127	0.49842504
H	3.67162828	2.50080719	-0.87116607
H	5.34145043	1.36819111	3.00182823
H	4.48387434	2.91011422	2.78829221
H	6.10529446	2.69676920	2.10546116
H	7.10784356	1.85234514	0.19165001
H	8.48033667	0.17906401	-1.02133708
H	7.51664357	-2.01631315	-1.65717612
H	0.13546901	-3.32387225	-0.85363607
H	4.03689131	-3.13631124	-0.67663605
H	-1.46800611	-5.93753945	-1.01815408
H	-0.70375605	-5.02969638	-2.33208818
H	-2.09128516	-4.33221133	-1.47772111
H	0.75998706	-6.10979447	0.30955702
H	1.79037014	-4.67615036	0.50023604
H	1.52992511	-5.36923039	-1.11344109
H	3.88052730	-2.07093416	-2.90506322
H	4.13424432	-3.82244529	-3.05814224
H	5.48621841	-2.70368221	-3.34739126
H	6.81791052	-4.13294431	-1.53511112
H	5.37914839	-5.10812339	-1.21172609
H	6.17558047	-4.23409132	0.11643201
H	0.52740204	6.84846453	-1.55367412
H	0.39346003	7.72866759	0.75727506
H	-0.52650104	6.31425046	2.58012420
H	-0.54602604	3.41174926	-2.58975020
H	-3.82369729	0.00708200	1.26567009
H	1.68129713	5.48456044	-2.91024522
H	1.39780411	4.05132031	-3.91849530
H	1.80786514	3.84516730	-2.20433217
H	-2.15468716	5.23816740	-3.36742025
H	-0.92847207	4.84264637	-4.59571535
H	-0.77228406	6.31415246	-3.61595628
H	-6.08676748	-1.83934714	2.22429117
H	-5.07799439	-0.76503706	3.20077224
H	-4.35037833	-2.18200417	2.41553019
H	-5.64895142	1.24814309	0.03997900
H	-5.95758648	1.18918509	1.78587214
H	-6.84799954	0.11020101	0.68705905
H	-6.15032246	-2.74827721	0.25644602
H	-6.03351548	-3.93672830	-1.92018414
H	-4.47157434	-3.16917024	-3.68284528
H	-1.50972612	2.75221221	2.05610216
H	-1.98688215	-0.38568103	-3.28239925



H	-1.06835008	4.93795138	4.19163832
H	0.17620701	3.79631329	3.62504128
H	-1.27661110	3.20197125	4.45624634
H	-3.57597827	3.37551226	3.33189425
H	-3.70075728	3.86674330	1.62793412
H	-3.35019325	5.08048439	2.87809722
H	-1.24848109	-2.64664720	-3.59550628
H	-1.33771510	-1.82270414	-5.15277639
H	-2.58954320	-3.01023723	-4.73838336
H	-4.16696232	0.50745604	-4.31306333
H	-4.33154033	-1.01662008	-5.19968040
H	-2.95839422	0.05843400	-5.53479344
O	1.09172808	1.98599915	0.85690106
O	1.06816208	0.73214006	1.47386311
O	-0.01705000	-1.20016209	-2.06330916

Oxo  $\eta^2$ -Ozone Complex to Oxo  $\eta^3$ -Ozone ComplexFig. S101: NCCNO Oxo  $\eta^2$ -Ozone Complex to Oxo  $\eta^3$ -Ozone Complex

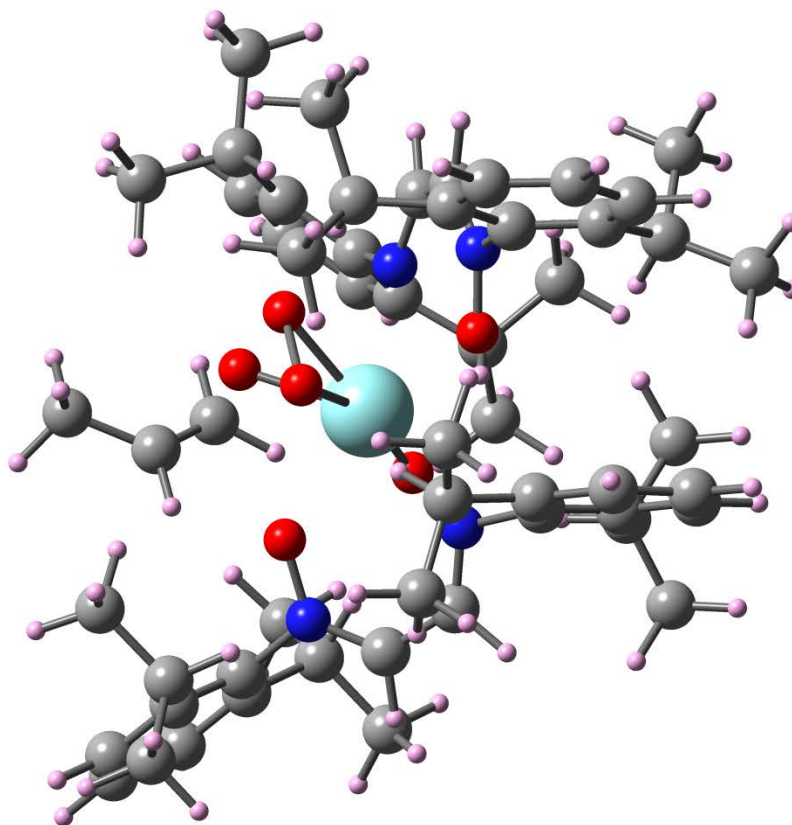
SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2741.392519	-2740.237910	-2740.167190	-2740.345135	-58

Zr	0.26806502	0.14673701	-0.16554701
O	-1.94770915	0.43859803	0.26332402
O	2.21516617	-1.01680508	-0.73057406
O	1.01183908	1.04431808	-1.95847915
N	0.00819300	-2.12850016	0.84435607
N	2.94555723	-1.78601214	0.06960701
N	-0.21651202	2.60989620	-0.17847601
N	-2.80364421	1.13206009	-0.52942104
C	1.03964308	-2.80607822	1.27693410
C	2.43976619	-2.58172320	0.99905207
C	-1.30235410	3.08309323	-0.73533905
C	-2.51187619	2.33475118	-0.99307708
C	-1.28143910	-2.62186420	1.33118610
C	-1.65875513	-2.33853618	2.67179320
C	-2.87459922	-2.88756622	3.13480324
C	-3.68348728	-3.67260828	2.30131917

C	-3.29219325	-3.92128530	0.97524407
C	-2.08564616	-3.40582226	0.46019504
C	-1.62440012	-0.31205502	4.22447732
C	-0.80573506	-1.47943611	3.61703627
C	-0.18464301	-2.34231818	4.74876136
C	4.91632137	1.52592512	1.45239011
C	4.54302834	0.04242800	1.70635613
C	4.97177838	-0.39715303	3.13112324
C	4.39874334	-1.73674013	-0.16629401
C	5.16500739	-0.86580406	0.63997105
C	6.55714451	-0.85112506	0.40188303
C	7.12656352	-1.64273313	-0.60697205
C	6.31896549	-2.46180319	-1.41505211
C	4.92456737	-2.52633619	-1.21771009
C	-2.79158521	-3.95714230	-1.94848615
C	-1.62187112	-3.74169028	-0.96133507
C	-0.71122005	-5.00251238	-0.95680407
C	3.68846428	-2.51074419	-3.41901026
C	4.02710431	-3.34526425	-2.15062017
C	4.63847535	-4.71477436	-2.53118819
C	0.85950707	3.55442227	0.09037801
C	1.52213812	4.23788332	-0.97278508
C	2.56284520	5.12688739	-0.62355305
C	2.92238522	5.35225840	0.71138805
C	2.23660717	4.68705536	1.73947013
C	1.19999409	3.77748829	1.45671211
C	2.42214818	3.59790027	-3.27265825
C	1.18812209	4.06783631	-2.46178519
C	0.60638705	5.38090943	-3.05293423
C	-5.38168743	0.03192600	2.78590821
C	-4.71077236	0.84840306	1.65847613
C	-5.15051139	2.33875618	1.74906613
C	-4.09739931	0.49820004	-0.82772506
C	-4.99966438	0.30430102	0.25387502
C	-6.22447750	-0.32296402	-0.04075700
C	-6.53662752	-0.72503506	-1.35101410
C	-5.63428543	-0.49125304	-2.39586818
C	-4.38490133	0.13013701	-2.16751117
C	1.26858910	2.65113220	3.76157629
C	0.38731503	3.16458924	2.60109020
C	-0.66702705	4.18901532	3.10616624
C	-3.15057524	-0.87528207	-4.17834932
C	-3.46441226	0.40443503	-3.36515926
C	-4.09149931	1.49556911	-4.27778233
H	0.87146306	-3.65724728	1.94300915
H	3.16265624	-3.16598924	1.55480512
H	-1.36017110	4.13510832	-1.02340108
H	-3.29174825	2.81702722	-1.56899012
H	-3.18721324	-2.69622120	4.15855332
H	-4.61344435	-4.09056131	2.68063820
H	-3.92942630	-4.52502534	0.33643403
H	0.00901600	-1.01677308	3.04903223

H	3.44855027	-0.01150100	1.65178913
H	-2.45313519	-0.67029605	4.85017437
H	-2.03762515	0.32276402	3.43226626
H	-0.97346807	0.30987602	4.85267737
H	-0.96239707	-2.81229821	5.36611740
H	0.43719203	-1.71793913	5.40391340
H	0.44777803	-3.14568124	4.34719733
H	5.99653345	1.70139613	1.55085312
H	4.39976034	2.16590116	2.17763317
H	4.60432735	1.84313614	0.45060003
H	4.67794635	-1.43499711	3.33970226
H	4.49171734	0.24550702	3.88005730
H	6.05970546	-0.32246702	3.26614325
H	7.19185257	-0.20429002	1.00115508
H	8.20061564	-1.61277412	-0.77513806
H	6.77510850	-3.05052923	-2.20514317
H	-1.03192808	-2.89606922	-1.33703310
H	3.07557223	-3.54329927	-1.64020212
H	-3.34313426	-4.88384438	-1.73625713
H	-2.39912718	-4.03576631	-2.97001023
H	-3.49847127	-3.12033924	-1.92038915
H	-1.26233110	-5.87968243	-0.59013104
H	0.17185201	-4.86955137	-0.31992802
H	-0.36136803	-5.21781140	-1.97506115
H	3.16963924	-1.58527112	-3.14917624
H	3.03323223	-3.08721923	-4.08503931
H	4.60325935	-2.25659017	-3.97164530
H	5.53313140	-4.60108735	-3.15669824
H	3.91001430	-5.29623642	-3.11047624
H	4.91561737	-5.29866942	-1.64359312
H	3.09653124	5.64671046	-1.41496511
H	3.72515128	6.04619647	0.95004507
H	2.50443219	4.88162937	2.77400221
H	0.44818103	3.27245425	-2.57522120
H	-3.63011828	0.80160506	1.82308014
H	3.25260225	4.31449333	-3.21547725
H	2.14997316	3.48009927	-4.33026133
H	2.75793521	2.62380520	-2.90451822
H	-0.28733202	5.71686645	-2.50755119
H	0.32860103	5.23073940	-4.10479231
H	1.33960910	6.19744946	-3.01329423
H	-6.47480348	0.13806501	2.77623821
H	-5.02893538	0.39437103	3.75989329
H	-5.13071939	-1.03139108	2.70797021
H	-4.65154036	2.96084422	0.99527708
H	-4.90294937	2.74631621	2.73781421
H	-6.23476148	2.43355219	1.60200712
H	-6.94120554	-0.49578004	0.75514406
H	-7.48760058	-1.21139909	-1.55509812
H	-5.89318847	-0.79596906	-3.40575726
H	-0.13635601	2.28881918	2.21081517
H	-2.49630119	0.76851506	-3.01510023

H	1.86066614	3.44905727	4.23048432
H	1.93361015	1.86615914	3.38825826
H	0.63263205	2.21277217	4.54301435
H	-1.29249710	3.73711829	3.88814430
H	-1.32635210	4.52456935	2.29339617
H	-0.18209201	5.07883239	3.53063127
H	-2.56480120	-1.56818812	-3.56986527
H	-2.53939519	-0.60985005	-5.05018539
H	-4.05833931	-1.37693010	-4.54028934
H	-4.31029933	2.42242519	-3.72807328
H	-5.03282938	1.14952009	-4.72495936
H	-3.39952626	1.73994714	-5.09344339
O	1.16731409	0.33339603	1.44520411
O	-0.30090302	0.54295104	-2.56252820
O	-0.49759504	-0.87441107	-2.02363715

Oxo  $\eta^3$ -Ozone Complex to Oxo Peroxo ComplexFig. S102: NCCNO Oxo  $\eta^3$ -Ozone Complex to Oxo Peroxo Complex

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2859.250587	-2858.014156	-2857.937999	-2858.127412	-393

Zr	0.30624300	0.21489500	-0.19580500
O	-1.98741100	0.06206300	0.19701200
O	2.19562900	-1.12523600	-0.75787400
O	1.41462200	1.52588100	-1.52994300
N	-0.03671000	-2.18070600	0.76019700
N	2.91294700	-1.89504000	0.05797400
N	-0.67853200	2.65329800	0.28429100
N	-2.97640900	0.78251500	-0.35709000
C	0.97372300	-2.86914200	1.22479300
C	2.38011400	-2.67244700	0.98314800
C	-1.89340500	2.98690600	-0.06190800
C	-2.95480400	2.09808600	-0.46306100
C	-1.32152800	-2.72406700	1.20272900
C	-1.70670700	-2.55076100	2.55904500
C	-2.87318000	-3.21616000	2.99410900
C	-3.62799100	-4.00850200	2.11695600

C	-3.24139700	-4.13161400	0.77167100
C	-2.08246300	-3.49476900	0.28423900
C	-1.79031600	-0.55418600	4.14358300
C	-0.91073500	-1.68145600	3.54508400
C	-0.29127000	-2.53710600	4.68242000
C	5.27563500	0.91318000	2.20497800
C	4.62282700	-0.47843200	2.00673300
C	4.82015200	-1.33143100	3.29098200
C	4.36907100	-1.88669500	-0.15928800
C	5.18601000	-1.20738300	0.77794800
C	6.57618100	-1.23346900	0.53245700
C	7.10368800	-1.88128300	-0.59556500
C	6.25452000	-2.52408200	-1.51123500
C	4.85832200	-2.54610300	-1.31355200
C	-2.77467000	-3.91535200	-2.15474100
C	-1.61152000	-3.68999100	-1.16175600
C	-0.61631600	-4.88133400	-1.26253400
C	3.77279900	-2.34126400	-3.59426000
C	3.93690600	-3.22899100	-2.33039300
C	4.42709700	-4.65014900	-2.70443300
C	0.21414400	3.76980000	0.54130500
C	0.47326800	4.72522900	-0.48904600
C	1.36575600	5.77747900	-0.18912200
C	1.96680700	5.89429800	1.07192400
C	1.67871200	4.95328000	2.07428200
C	0.80056400	3.87856900	1.83547500
C	0.95082500	4.60778500	-3.00436300
C	-0.13365600	4.67037800	-1.90131000
C	-1.08806000	5.87268300	-2.14007200
C	-5.71937100	-0.92215600	2.58751900
C	-5.00562400	0.05625000	1.62676300
C	-5.56184200	1.49143500	1.86253000
C	-4.17478300	0.05003300	-0.82201500
C	-5.13646500	-0.33507600	0.14887400
C	-6.27196300	-1.02399000	-0.31982000
C	-6.44001500	-1.29704500	-1.68836800
C	-5.48489300	-0.86752800	-2.61873800
C	-4.32194900	-0.17317000	-2.21310500
C	1.49676500	2.69994600	4.01371200
C	0.39316600	2.92209700	2.95758000
C	-0.91012000	3.42794000	3.63727700
C	-2.88805100	-0.73206200	-4.26698000
C	-3.34973400	0.35988800	-3.27244400
C	-4.00426600	1.54715600	-4.03383100
H	0.77692600	-3.72415200	1.87891800
H	3.07856200	-3.27568800	1.54824100
H	-2.18493300	4.04000600	-0.08393700
H	-3.84459800	2.54304500	-0.88951200
H	-3.18907800	-3.11281500	4.02972400
H	-4.51452500	-4.52646300	2.47661800
H	-3.84226000	-4.73466500	0.09785700
H	-0.09594100	-1.18055600	3.01000500

H	3.54531500	-0.31091600	1.87172700
H	-2.64514100	-0.95393300	4.70622500
H	-2.17000000	0.10064800	3.35082900
H	-1.19296500	0.06012200	4.83046700
H	-1.06706400	-3.04156400	5.27446300
H	0.29104800	-1.90027300	5.36148400
H	0.37909500	-3.31278000	4.28822500
H	6.33061200	0.83588700	2.50126900
H	4.74735100	1.45201000	3.00171300
H	5.21691300	1.51693300	1.29277900
H	4.32070300	-2.30641100	3.22289900
H	4.40162500	-0.80282600	4.15673600
H	5.88611800	-1.51507500	3.48351100
H	7.24652800	-0.72849700	1.22155000
H	8.17783500	-1.87983400	-0.76520000
H	6.67812200	-3.01430200	-2.38300600
H	-1.08420300	-2.77728400	-1.46876200
H	2.93779400	-3.33208400	-1.89132900
H	-3.26713200	-4.88473000	-1.99432100
H	-2.38797300	-3.91251600	-3.18157800
H	-3.53062500	-3.12669400	-2.07538500
H	-1.10478700	-5.82097900	-0.96901400
H	0.26054600	-4.74129600	-0.61936500
H	-0.26098400	-4.98789700	-2.29607100
H	3.31345300	-1.38208300	-3.33466300
H	3.11911800	-2.83943500	-4.32171100
H	4.74286800	-2.15552500	-4.07555200
H	5.38280400	-4.62543000	-3.24355100
H	3.69303400	-5.13351800	-3.36178300
H	4.55694000	-5.28038300	-1.81485100
H	1.59423500	6.51168700	-0.95776000
H	2.64940600	6.71633900	1.27536900
H	2.13595800	5.05996200	3.05310900
H	-0.70739800	3.74659100	-2.01525200
H	-3.94044700	0.05253500	1.88477500
H	1.63858300	5.46326500	-2.96231000
H	0.47397800	4.60941900	-3.99406700
H	1.51317800	3.67776200	-2.90199500
H	-1.88910900	5.92280600	-1.38899700
H	-1.55265300	5.79635900	-3.13223000
H	-0.54335900	6.82508300	-2.09779100
H	-6.81203300	-0.85065500	2.50089600
H	-5.45825200	-0.67374400	3.62410700
H	-5.41812700	-1.95645000	2.40003300
H	-5.04130600	2.24546000	1.26143100
H	-5.44817500	1.76984300	2.91832700
H	-6.62996700	1.53622900	1.61128900
H	-7.02982400	-1.34651200	0.38624000
H	-7.32310500	-1.83380300	-2.02721200
H	-5.63602700	-1.06774700	-3.67539700
H	0.21336100	1.94216800	2.50011000
H	-2.43591400	0.72278000	-2.79461200



H	1.70934400	3.60349100	4.60297800
H	2.42181900	2.35831600	3.53577700
H	1.17761400	1.91715000	4.71420900
H	-1.23598200	2.71857900	4.40998000
H	-1.72999100	3.53722200	2.91487500
H	-0.75147700	4.40480600	4.11607100
H	-2.30701300	-1.49494500	-3.74357100
H	-2.22435400	-0.27935600	-5.01367500
H	-3.72733900	-1.20398300	-4.79727400
H	-4.32061600	2.35111300	-3.35407700
H	-4.88950200	1.22259300	-4.59793200
H	-3.28369000	1.97042300	-4.74477100
O	1.21301100	0.31357100	1.44936400
O	-0.35737800	0.97757800	-2.17058100
O	-0.28802300	-0.52407500	-2.19295800
C	3.10403500	2.29206500	-0.50879100
H	2.92636400	1.82781900	0.45507400
H	3.00634000	3.37173300	-0.57313800
C	3.45413100	1.54521300	-1.62020100
H	3.58200500	0.47479300	-1.50763500
C	3.81953500	2.11713100	-2.96395900
H	3.74588800	3.20941400	-2.98134600
H	4.84811900	1.83319300	-3.23292900
H	3.15002800	1.70789500	-3.73125200

## TS for Ligand Cyclization

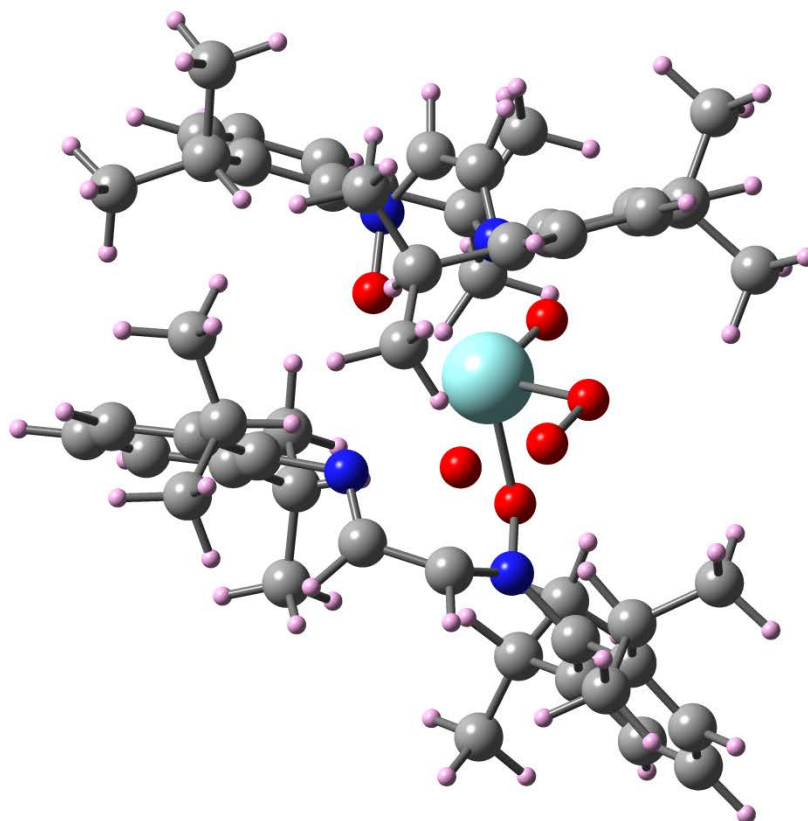


Fig. S103: NCCNO TS for Ligand Cyclization

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2741.391709	-2740.237205	-2740.166673	-2740.344046	-164

Zr	0.44577500	0.30202800	-0.52207300
O	-1.84978200	0.02181400	-0.19708700
O	1.87480100	-1.31471500	-0.70571500
O	2.11912100	1.61737300	-0.52167000
N	0.05516700	-1.45719500	1.44635000
N	2.87346500	-1.43323300	0.27873600
N	-0.59342300	2.62006600	-0.39831100
N	-2.77761300	0.59442400	-0.98392500
C	1.18847700	-1.65376400	2.05062000
C	2.49302800	-1.15257100	1.54959500
C	-1.73314700	2.84291800	-0.99561200
C	-2.72995000	1.85791900	-1.36276100
C	-1.12229000	-2.06642700	2.05305500
C	-1.64638100	-1.53527900	3.26409500
C	-2.73328400	-2.20833500	3.86246200
C	-3.29490000	-3.35261900	3.27890200

C	-2.78278800	-3.83617300	2.06504700
C	-1.69453800	-3.20609400	1.42792400
C	-2.21425500	0.77381600	4.17350500
C	-1.09356800	-0.27106400	3.93639800
C	-0.38059400	-0.60474700	5.27468800
C	5.85954200	1.45867000	-0.08119500
C	5.32206900	0.30663100	0.80597500
C	6.11281100	0.21688600	2.13904800
C	4.19452200	-1.83441500	-0.18040700
C	5.34237900	-1.02848200	0.05890700
C	6.58399500	-1.49382100	-0.42876800
C	6.68954900	-2.68692100	-1.15268900
C	5.54251600	-3.46105500	-1.38243800
C	4.28268800	-3.06858500	-0.88975900
C	-2.20142600	-4.14310300	-0.89909200
C	-1.11155200	-3.80373900	0.14556700
C	-0.27039200	-5.06611800	0.47794100
C	2.61681800	-3.87290400	-2.62189500
C	3.07689300	-3.97959300	-1.14340800
C	3.37152600	-5.45176400	-0.75591800
C	0.22599500	3.81766000	-0.18271100
C	0.83487500	4.44937000	-1.30193900
C	1.55965400	5.63473200	-1.06082700
C	1.68515400	6.16765800	0.23042600
C	1.09909800	5.50447100	1.31848600
C	0.36927100	4.31235500	1.13692000
C	2.23391900	3.58496800	-3.23680700
C	0.79826200	3.87410000	-2.72455400
C	0.03935700	4.81184100	-3.70045300
C	-5.64705800	-0.51040500	1.97537800
C	-5.05006300	0.35154600	0.83800800
C	-5.84807800	1.67865200	0.69448900
C	-3.91256700	-0.25481500	-1.40189800
C	-5.00090200	-0.38670700	-0.50438000
C	-6.08282500	-1.18241600	-0.93216300
C	-6.06608700	-1.80790700	-2.19024400
C	-4.96994000	-1.64742300	-3.05061700
C	-3.85411900	-0.86462700	-2.67899600
C	0.69673700	3.43961800	3.51385700
C	-0.29239500	3.63205400	2.33824600
C	-1.54964100	4.42701600	2.78669300
C	-2.20948800	-1.98638800	-4.29348500
C	-2.68695700	-0.66100600	-3.65112800
C	-3.08319600	0.35520300	-4.75827800
H	1.23671200	-2.22808900	2.98224300
H	3.29888500	-1.16920000	2.27710700
H	-2.00352300	3.86303000	-1.28129700
H	-3.55576800	2.18810300	-1.98017600
H	-3.14354200	-1.83150200	4.79614000
H	-4.12429300	-3.86193300	3.76393200
H	-3.22573700	-4.71964100	1.61302100
H	-0.35357400	0.19353500	3.27569600

H	4.29535900	0.58139300	1.03885600
H	-2.98269100	0.39685100	4.86041600
H	-2.70482900	1.04517300	3.23022200
H	-1.79285600	1.68517500	4.61516400
H	-1.07587000	-1.06214000	5.99105000
H	0.02582600	0.30785400	5.72994900
H	0.45067500	-1.30614700	5.12629800
H	6.90900600	1.30672700	-0.36780100
H	5.78866400	2.40908700	0.46337300
H	5.25720600	1.54997100	-0.99193300
H	5.72459900	-0.57825100	2.79186700
H	6.04163100	1.16794500	2.68287900
H	7.17657800	0.00726200	1.96363200
H	7.47354400	-0.89483700	-0.25252600
H	7.65454700	-3.01209900	-1.53436000
H	5.62834900	-4.38967900	-1.93984200
H	-0.43854000	-3.06668700	-0.30671500
H	2.24291300	-3.63107900	-0.52842600
H	-2.86236100	-4.94952100	-0.55446700
H	-1.73123900	-4.48220300	-1.83142100
H	-2.82082900	-3.26778400	-1.12428400
H	-0.89503800	-5.83910600	0.94566300
H	0.54989100	-4.83403800	1.16960800
H	0.16556500	-5.48655600	-0.43692100
H	2.33564800	-2.84090900	-2.85350800
H	1.74617800	-4.51997500	-2.79967300
H	3.41603400	-4.18509100	-3.30825100
H	4.14177100	-5.89958400	-1.39666800
H	2.46257100	-6.05724800	-0.86748500
H	3.71150000	-5.53330000	0.28508100
H	2.04432900	6.13519900	-1.89521100
H	2.24655800	7.08546400	0.38887000
H	1.21105600	5.91368300	2.31894100
H	0.28955100	2.90506300	-2.71600600
H	-4.02359600	0.60073100	1.13283700
H	2.82400100	4.50602400	-3.34265000
H	2.18652800	3.09732100	-4.21957600
H	2.74785900	2.91362500	-2.54157400
H	-0.99584200	4.99126900	-3.37541300
H	0.00900100	4.36726000	-4.70402300
H	0.53253500	5.78983400	-3.78157800
H	-6.71180200	-0.72164100	1.81138600
H	-5.56356700	0.02688200	2.92875500
H	-5.11323600	-1.46092300	2.07442600
H	-5.41667700	2.33601600	-0.07133800
H	-5.85184000	2.22521900	1.64647100
H	-6.89007600	1.47662500	0.41389700
H	-6.94007900	-1.31537300	-0.27940600
H	-6.91092200	-2.41863700	-2.49966900
H	-4.97217200	-2.13627600	-4.02028800
H	-0.62097600	2.63283700	2.02687900
H	-1.82011800	-0.24968400	-3.11975100

H	1.04276700	4.40047900	3.91641200
H	1.56691000	2.86257900	3.18606700
H	0.20981300	2.89653300	4.33518300
H	-2.05043600	3.92460200	3.62473400
H	-2.27412200	4.52899300	1.96690200
H	-1.27401300	5.43855400	3.11340600
H	-1.94654200	-2.72568700	-3.52908300
H	-1.31086700	-1.79099200	-4.89063800
H	-2.96557800	-2.42829700	-4.95736700
H	-3.37422600	1.32740900	-4.33742100
H	-3.92443700	-0.01433700	-5.36115900
H	-2.22880900	0.52408200	-5.42502500
O	2.53204100	1.71446200	0.91047400
O	1.77482600	0.63923700	1.60832800
O	0.02041600	0.37652800	-2.29237000

## 8. NCCNO Triplet Transition States

## Oxo Peroxo Complex to Dioxo Complex

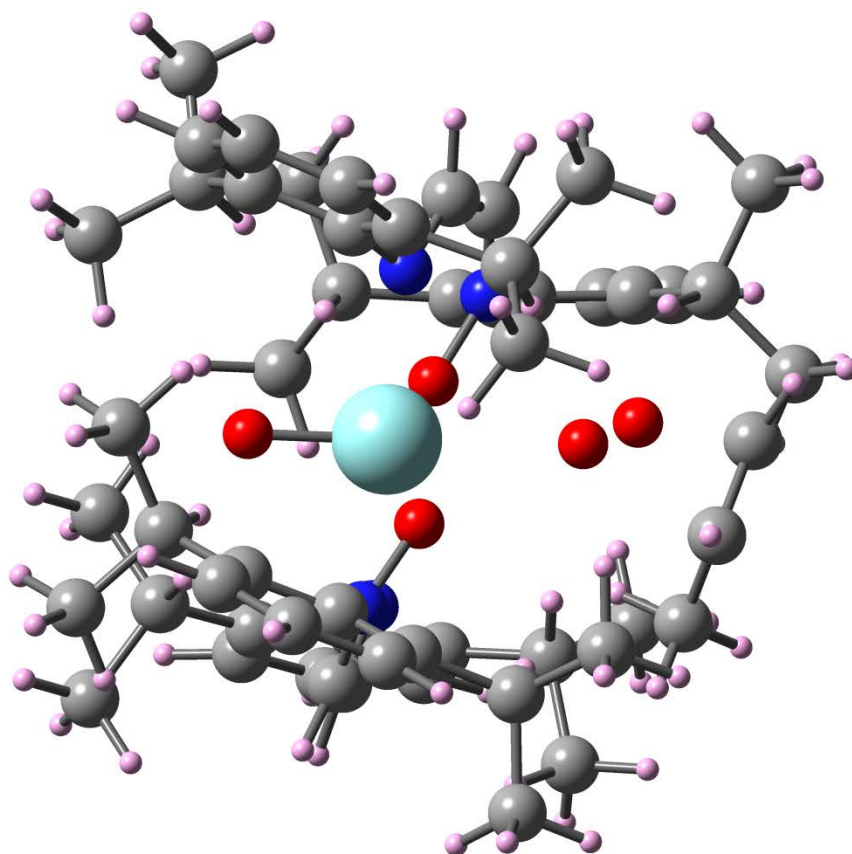


Fig. S104: NCCNO Oxo Peroxo Complex to Dioxo Complex

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2784.099789	-2782.867471	-2782.792810	-2782.981144	-125

Zr	-0.11492831	0.13193385	-0.25975422
O	2.01694570	0.40342491	-0.08293213
O	-1.95643358	-0.70370910	0.46209474
O	-0.41660228	-0.10385159	3.22039451
O	0.52065185	-0.44965732	2.16504029
N	0.18060951	-2.09819472	-1.00177004
N	-2.79395738	-1.53424390	-0.29638932
N	-0.07965418	2.33346988	0.45235199
N	2.80786177	1.28039768	0.64099432
C	-0.91905384	-2.84256551	-1.28798954
C	-2.26883009	-2.57556171	-1.00379093
C	1.01480750	2.97238430	0.93890025
C	2.32242101	2.48524265	1.06206596

C	1.40770894	-2.58149766	-1.62585409
C	1.59718618	-2.41430292	-3.02917555
C	2.77667384	-2.93194579	-3.60981124
C	3.74909237	-3.58149086	-2.83852327
C	3.55440640	-3.72518706	-1.45527128
C	2.39021112	-3.23695874	-0.82980727
C	1.22778460	-0.49794126	-4.66856424
C	0.58329306	-1.70073646	-3.93352177
C	-0.05295828	-2.68594726	-4.94950632
C	-4.34726630	1.62403935	-2.57318667
C	-4.03393806	0.12075551	-2.37523247
C	-4.30228233	-0.66955589	-3.68526364
C	-4.21913960	-1.28000980	-0.21015276
C	-4.82863846	-0.48499599	-1.21561363
C	-6.22507870	-0.29167134	-1.13166911
C	-6.97563302	-0.85230882	-0.08728072
C	-6.34421460	-1.62160301	0.90393154
C	-4.95319150	-1.84587973	0.86448697
C	3.44828917	-3.49380814	1.50251044
C	2.15159949	-3.47736360	0.66209824
C	1.36378810	-4.80154464	0.87064312
C	-4.64343976	-2.25284440	3.36665483
C	-4.27957582	-2.71204973	1.93192709
C	-4.63445418	-4.21061335	1.73233437
C	-1.22150601	3.20205366	0.18122567
C	-2.27948508	3.29896356	1.12759210
C	-3.36149609	4.16015498	0.84673327
C	-3.40074326	4.91318951	-0.33573228
C	-2.34830618	4.81092894	-1.25775062
C	-1.24640560	3.96107744	-1.02578535
C	-3.54253215	1.77291092	2.74995983
C	-2.23636735	2.55131040	2.46187494
C	-1.90649066	3.52876130	3.62299963
C	4.91064961	0.33906556	-2.88764879
C	4.48155597	1.30876296	-1.76054539
C	4.93118381	2.76130277	-2.08309133
C	4.20553358	0.91676490	0.77921545
C	5.01683531	0.89015656	-0.38737540
C	6.37442167	0.54474103	-0.23029898
C	6.90776101	0.25047720	1.03486816
C	6.08850721	0.29828280	2.17238562
C	4.71831178	0.62255463	2.07098374
C	-0.63551534	3.51729993	-3.46657321
C	-0.11639571	3.91076768	-2.06093238
C	0.65237277	5.25931519	-2.10351271
C	3.98149990	-0.60343093	4.19309768
C	3.85902778	0.68443186	3.34009523
C	4.23191965	1.92664457	4.19516591
H	-0.76786800	-3.75838015	-1.86314971
H	-3.01178067	-3.24900203	-1.41628941
H	0.89669041	4.01470427	1.24223793
H	3.06949982	3.13623661	1.49969398

H	2.93292567	-2.81705723	-4.67996037
H	4.65012941	-3.97118692	-3.30717387
H	4.31388615	-4.22567865	-0.86145410
H	-0.21089743	-1.27713358	-3.31446983
H	-2.96331662	0.05096009	-2.15797136
H	2.04340699	-0.80894248	-5.33691454
H	1.61907684	0.22347189	-3.94293603
H	0.46989509	0.01768013	-5.27278377
H	0.70178789	-3.11223959	-5.62493561
H	-0.79955992	-2.16546004	-5.56471555
H	-0.55372198	-3.52076177	-4.44094543
H	-5.38461272	1.79279151	-2.89550649
H	-3.68460722	2.03528187	-3.34414366
H	-4.17420973	2.19094069	-1.65157830
H	-4.03071493	-1.72790637	-3.57857441
H	-3.70369879	-0.24877594	-4.50327699
H	-5.36168591	-0.61783462	-3.97399780
H	-6.72469209	0.30739958	-1.88786400
H	-8.05023283	-0.68926676	-0.04374377
H	-6.93690349	-2.04907748	1.70894642
H	1.53087365	-2.65085149	1.02574340
H	-3.19689997	-2.60227755	1.81142047
H	4.07588202	-4.36495742	1.27187234
H	3.20004996	-3.55271913	2.57172581
H	4.04285140	-2.58806621	1.33473897
H	1.93217993	-5.65364077	0.47395300
H	0.39453182	-4.77328335	0.35934975
H	1.18317257	-4.98613557	1.93964204
H	-4.40329165	-1.19223421	3.51251735
H	-4.09544413	-2.85067490	4.10986182
H	-5.71269404	-2.38455001	3.57499889
H	-5.71601199	-4.37448647	1.82554306
H	-4.13214234	-4.83338282	2.48585192
H	-4.32557271	-4.56232833	0.74031315
H	-4.17519343	4.24706079	1.56302796
H	-4.24093948	5.57447697	-0.53587061
H	-2.38195777	5.39777505	-2.17272414
H	-1.42675858	1.81932456	2.41337064
H	3.38926616	1.29281417	-1.72288359
H	-4.40918837	2.44110949	2.84094529
H	-3.45133256	1.22342817	3.69901005
H	-3.74398752	1.05027471	1.95188481
H	-0.94968758	4.03882914	3.45143659
H	-1.83937317	2.98718447	4.57799063
H	-2.68259185	4.29921958	3.72675162
H	5.99785877	0.34743043	-3.04597236
H	4.43825881	0.63764702	-3.83244550
H	4.59923883	-0.68729832	-2.66560139
H	4.58587146	3.46692906	-1.31638901
H	4.51600994	3.07964660	-3.04851867
H	6.02589675	2.83339999	-2.14294413
H	7.02119465	0.51521738	-1.10265196



H	7.95917090	-0.00970720	1.13372457
H	6.51539661	0.07387072	3.14655938
H	0.58653403	3.12847031	-1.76409630
H	2.81004141	0.77566010	3.03978695
H	-1.39009800	4.22320489	-3.84039413
H	-1.06093895	2.50970662	-3.42529655
H	0.19763713	3.50830317	-4.18368344
H	1.48548908	5.19899785	-2.81713092
H	1.06342986	5.51894897	-1.11861959
H	-0.00278964	6.08243781	-2.41986189
H	3.67515416	-1.48490986	3.61981763
H	3.34597074	-0.52444205	5.08776552
H	5.00783307	-0.76793142	4.54488547
H	4.12427212	2.85701870	3.62436940
H	5.27192961	1.86766586	4.54273446
H	3.58307411	1.99569068	5.07923271
O	-0.64315793	0.58604414	-1.94700116
C	-0.98101241	-1.64812418	4.12152512
H	-2.02660206	-1.44568735	4.33165487
C	0.01717581	-0.66008094	4.58028979
H	-0.25531774	0.05212222	5.35661914
H	1.06870474	-0.93527189	4.55380736
C	-0.56809265	-2.80867877	3.31461280
H	-0.10601731	-2.37071445	2.39377781
H	0.22799091	-3.39299767	3.79321090
H	-1.39969310	-3.45329478	3.02748456

### Oxo Complex with weakly adsorbed O<sub>2</sub> molecule to Oxo Peroxo Complex

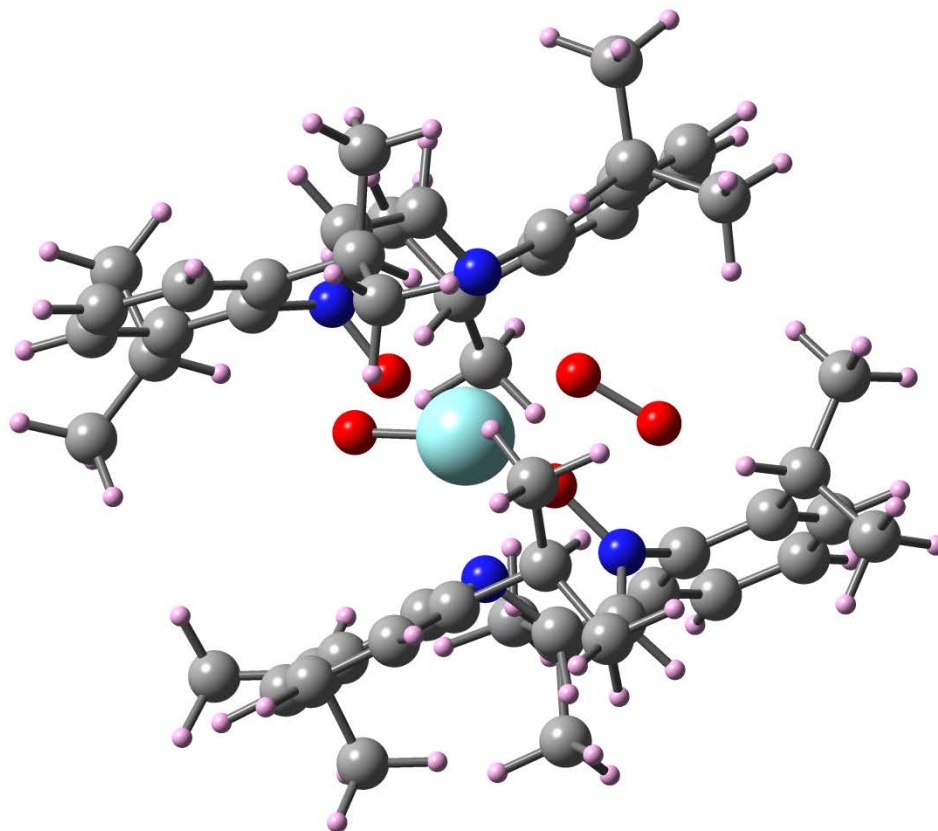


Fig. S105: NCCNO Oxo Complex with weakly adsorbed O<sub>2</sub> molecule to Oxo Peroxo Complex

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2666.243621	-2665.093622	-2665.024225	-2665.199364	-223

Zr	-0.02223145	-0.17050223	-0.24501654
O	-2.17886191	0.39389488	0.14836515
O	2.05150507	-0.55051681	-0.34722818
O	-0.58212790	-0.47054595	-1.96617285
N	-0.00207595	-2.16073699	0.83889145
N	2.91975236	-1.27615647	0.46192945
N	-0.02628899	2.21827835	-0.78280277
N	-2.93066346	1.23243956	-0.57829741
C	1.11390850	-2.67404652	1.42472119
C	2.44283318	-2.26470138	1.26970482
C	-1.12246281	2.86697391	-1.09013667
C	-2.47004818	2.35124687	-1.12478120
C	-1.23906386	-2.88792362	1.10054270
C	-1.90975116	-2.71468252	2.34281835
C	-3.11624751	-3.41931383	2.55033343

C	-3.63930800	-4.27065472	1.56755576
C	-2.94895889	-4.44882513	0.35667055
C	-1.73784683	-3.77442757	0.10069187
C	-2.35937531	-0.71123818	3.86102592
C	-1.35944707	-1.82516182	3.46447986
C	-0.97121562	-2.67493168	4.70460738
C	4.65010087	1.97869746	2.39533500
C	4.35412907	0.45954940	2.34149582
C	4.76859718	-0.22473753	3.67265321
C	4.33868444	-1.05189548	0.24741001
C	5.03938496	-0.21652142	1.15158207
C	6.42588120	-0.04953380	0.93922362
C	7.07291236	-0.67682271	-0.13517452
C	6.34935301	-1.49236015	-1.02252899
C	4.96599139	-1.69906452	-0.85188464
C	-1.81704736	-4.43064307	-2.39276645
C	-0.93913481	-4.05157439	-1.17882891
C	0.10936129	-5.17162791	-0.92445964
C	4.62475411	-2.53212010	-3.26066251
C	4.19016372	-2.64206469	-1.77924341
C	4.33361395	-4.11213234	-1.29242851
C	1.20351625	3.00800911	-0.76652995
C	2.13549847	2.80409342	-1.82238049
C	3.31696931	3.57138506	-1.81183959
C	3.56654323	4.50815195	-0.79693019
C	2.62580928	4.69934412	0.22453828
C	1.42202300	3.96279814	0.26768614
C	3.05080354	1.03146872	-3.43426621
C	1.83135109	1.87719542	-3.00411216
C	1.28740864	2.70809170	-4.20018048
C	-5.33228498	1.35651207	2.92751941
C	-4.71865710	1.95027097	1.63577151
C	-5.01017234	3.47482325	1.54988741
C	-4.36113089	0.89872152	-0.70055002
C	-5.21823473	1.23891319	0.37363754
C	-6.58717120	0.94401452	0.20976183
C	-7.05939267	0.33545765	-0.96430774
C	-6.17357943	0.00526259	-2.00110789
C	-4.79120283	0.27409193	-1.89652689
C	1.08580247	4.07162823	2.80124603
C	0.42963102	4.23660019	1.40665593
C	-0.19687682	5.65069040	1.26004206
C	-4.13960379	-1.46499685	-3.65255769
C	-3.84096481	-0.07057769	-3.04962095
C	-3.92675662	1.00885383	-4.16585919
H	0.98077866	-3.52684303	2.09128508
H	3.20905601	-2.78966053	1.82681575
H	-1.05522371	3.92006689	-1.37400290
H	-3.22207746	2.96334723	-1.60636465
H	-3.64650566	-3.29870237	3.49240456
H	-4.57258259	-4.80095735	1.74466580
H	-3.35430920	-5.12385022	-0.39147625

H	-0.45368005	-1.32217345	3.11518108
H	3.27056976	0.34554901	2.23927342
H	-3.29671977	-1.12735233	4.25614869
H	-2.59341162	-0.08296043	2.99502736
H	-1.91816107	-0.07111017	4.63625155
H	-1.84688627	-3.17803933	5.13711038
H	-0.53171784	-2.03345690	5.48006450
H	-0.23626557	-3.44925131	4.44717661
H	5.71384532	2.18207267	2.58064348
H	4.07458490	2.43715701	3.20925545
H	4.36291811	2.47135202	1.45949224
H	4.51579936	-1.29301464	3.67068398
H	4.24407527	0.24427981	4.51481020
H	5.84940222	-0.13403250	3.84821198
H	6.99717318	0.57999868	1.61614814
H	8.14092117	-0.53271719	-0.28321051
H	6.86549837	-1.97042661	-1.85002075
H	-0.39945422	-3.13630541	-1.44607645
H	3.12961216	-2.37155918	-1.72963100
H	-2.28080592	-5.41988662	-2.27481879
H	-1.19773801	-4.46380061	-3.29854292
H	-2.61035688	-3.69365308	-2.55318592
H	-0.38743450	-6.11075149	-0.64378091
H	0.80333367	-4.90035188	-0.12114733
H	0.69837310	-5.35492508	-1.83383899
H	4.58027791	-1.49683761	-3.61608116
H	3.95604696	-3.13634678	-3.88732984
H	5.64545895	-2.90603716	-3.41676468
H	5.38417726	-4.43152805	-1.32115161
H	3.75340109	-4.78436779	-1.93832682
H	3.96873339	-4.23368958	-0.26573585
H	4.04385897	3.43771366	-2.60770023
H	4.48604717	5.08868708	-0.80565638
H	2.82669828	5.42833986	1.00518829
H	1.04040510	1.17490378	-2.72139814
H	-3.63318852	1.81775107	1.70672798
H	3.85768143	1.64730061	-3.85484112
H	2.74445558	0.31349801	-4.20615339
H	3.44558824	0.47103642	-2.58081214
H	0.38735788	3.27304218	-3.92148400
H	1.02462673	2.04267005	-5.03277686
H	2.03812629	3.42667069	-4.55683001
H	-6.40980051	1.55484814	2.99497073
H	-4.85724125	1.80967735	3.80665193
H	-5.17654178	0.27359604	2.97835617
H	-4.53593634	3.93082319	0.67093485
H	-4.62784868	3.98507003	2.44331520
H	-6.08978035	3.66374107	1.48461953
H	-7.28508349	1.18810855	1.00504440
H	-8.11913949	0.11561748	-1.06927366
H	-6.55427685	-0.47484944	-2.89735800
H	-0.37069132	3.49241816	1.36675971

H	-2.80445938	-0.09987532	-2.68914247
H	1.93042760	4.75978760	2.94077945
H	1.43163524	3.04276142	2.94160465
H	0.34730303	4.28797886	3.58546449
H	-0.93395725	5.82369157	2.05574417
H	-0.70228908	5.77808585	0.29239618
H	0.56857534	6.43438862	1.33617419
H	-4.17624999	-2.23487826	-2.87409032
H	-3.34355999	-1.73440044	-4.35706955
H	-5.09165279	-1.48404472	-4.20038051
H	-3.65739919	2.00705926	-3.79653350
H	-4.94156856	1.06751762	-4.58286449
H	-3.23481665	0.75734988	-4.97941534
O	0.05324618	1.04609773	1.72981201
O	0.96894348	0.62687039	2.66833702

## 9. ONCCNO Singlet Ground States

### 9.1 Structures with four oxygen atoms

#### Bare Complex (conformation 1 higher energy with distorted N-O bonds)

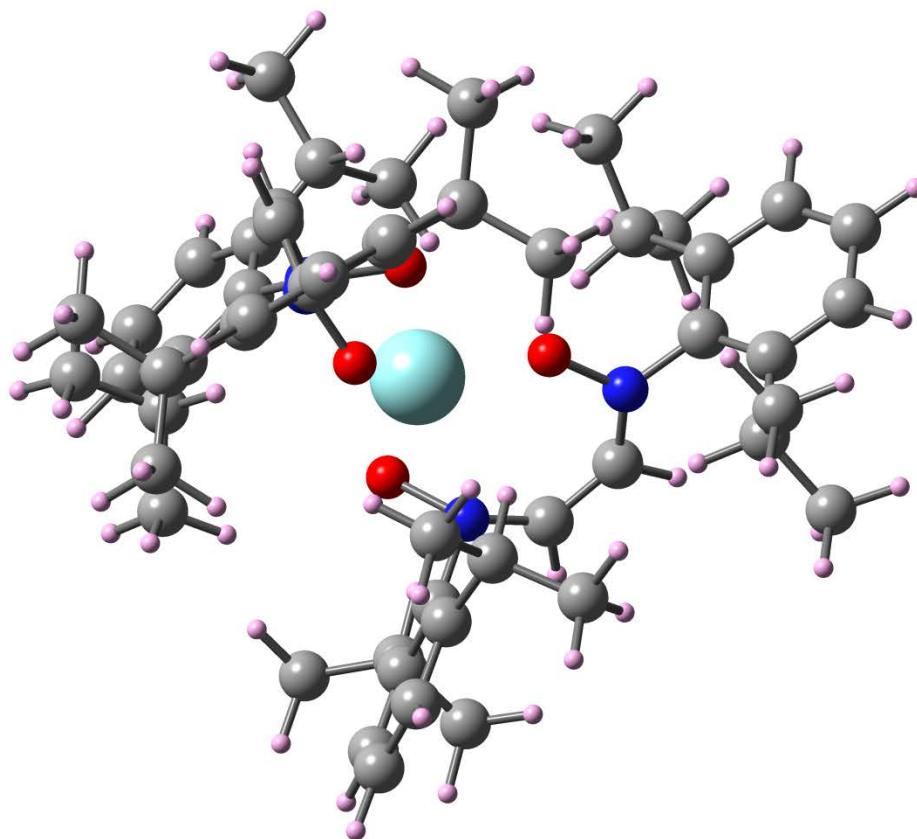


Fig. S106: ONCCNO Bare Complex (conformation 1 higher energy with distorted N-O bonds)

SCF	$E_{ZP}$	H	G
-2591.055276	-2589.906171	-2589.838037	-2590.011783

Zr	-0.09258087	-0.40947889	-0.05958153
O	-1.12222367	1.33101839	-0.30657235
O	1.89036933	0.05629461	-0.32246230
O	-0.16381149	-1.56931331	-1.74008283
O	-0.52125487	-1.74171565	1.43789793
N	0.60066204	-0.87897064	2.10139211
N	3.05570013	-0.54389395	0.23047524
N	-1.65588680	-1.20848877	-1.57626191
N	-1.85074021	1.87282926	-1.41358554
C	1.87532181	-1.54208556	2.18505424
C	2.94304626	-1.32164944	1.34727722
C	-2.12010654	-0.30613922	-2.59548250
C	-2.19246410	1.05619388	-2.46238241

C	0.08595009	-0.37542772	3.38710595
C	0.14418402	1.02166979	3.64141577
C	-0.37750552	1.49732001	4.86446261
C	-0.92376983	0.62315302	5.81208316
C	-0.92882671	-0.75698909	5.56073408
C	-0.42113656	-1.29017493	4.35851155
C	-0.09167712	3.21837193	2.33565201
C	0.82510957	2.02629111	2.70470346
C	2.14659613	2.53074842	3.34767325
C	5.16628255	2.96349651	0.60213854
C	5.03273846	1.47263886	1.00507446
C	6.01717406	1.12177533	2.15221794
C	4.25202271	-0.42083217	-0.56879592
C	5.22684261	0.54330400	-0.19484734
C	6.40888191	0.62207985	-0.96108960
C	6.60210532	-0.20800531	-2.07604195
C	5.61340335	-1.13340000	-2.44578442
C	4.42094222	-1.25984734	-1.70290468
C	-1.79246657	-3.45925339	4.39277873
C	-0.39436241	-2.81921848	4.20005668
C	0.61922770	-3.44661990	5.19779430
C	2.82596296	-1.95500296	-3.55054915
C	3.36525487	-2.28014644	-2.13335182
C	3.91763828	-3.72825265	-2.06678813
C	-2.49224337	-2.40666840	-1.38986415
C	-3.53665089	-2.32732830	-0.42592858
C	-4.31865978	-3.47804683	-0.19766396
C	-4.08801680	-4.66605943	-0.90517975
C	-3.09461681	-4.70154351	-1.89320892
C	-2.29198032	-3.57506016	-2.17666284
C	-3.96992884	-1.19332882	1.83683924
C	-3.91369785	-1.02924989	0.29908165
C	-5.26587605	-0.49493977	-0.24885659
C	1.78391739	3.52219748	-1.86543312
C	0.48874104	3.18937045	-2.65119337
C	0.67966459	3.45172605	-4.16780376
C	-1.82043747	3.31549096	-1.48715394
C	-0.70784910	3.96309097	-2.09044822
C	-0.72020152	5.37209652	-2.15528033
C	-1.79378809	6.11018776	-1.63219575
C	-2.87516651	5.45162826	-1.02640620
C	-2.90653980	4.04436602	-0.93377661
C	-0.16091207	-4.69743150	-2.98687696
C	-1.28112666	-3.68114282	-3.32751354
C	-1.98223526	-4.05587137	-4.66021833
C	-4.31384945	3.83991917	1.18340141
C	-4.09485928	3.34678097	-0.26998249
C	-5.38577596	3.52405910	-1.11304197
H	2.01563364	-2.24792846	2.99525567
H	3.86316056	-1.84838445	1.58672377
H	-2.44686217	-0.75106614	-3.53067778
H	-2.59563711	1.61175338	-3.30493646

H	-0.34880823	2.56307644	5.07479456
H	-1.32767922	1.01037693	6.74457910
H	-1.32916190	-1.43285027	6.31185456
H	1.10141078	1.51897947	1.77480900
H	4.01608160	1.32589148	1.38177798
H	-0.38081285	3.79700337	3.22276640
H	-0.99808723	2.87283475	1.82855806
H	0.43245572	3.89847565	1.65135374
H	1.94662488	3.08456389	4.27439111
H	2.67160642	3.20448599	2.65791931
H	2.81386799	1.69469962	3.59232835
H	6.17681747	3.19862469	0.24309331
H	4.96375568	3.60882501	1.46740711
H	4.45550532	3.22108069	-0.19231648
H	5.89821496	0.07957794	2.47538505
H	5.84044077	1.76998921	3.02082937
H	7.06005415	1.25736877	1.83613017
H	7.17724362	1.34146387	-0.68896020
H	7.51818850	-0.13111144	-2.65745394
H	5.77009623	-1.76644563	-3.31553081
H	-0.08285446	-3.06445850	3.18372520
H	2.51488672	-2.21776578	-1.44806042
H	-2.18994785	-3.28337801	5.40125413
H	-1.72831386	-4.54569765	4.24546090
H	-2.50845974	-3.06163325	3.66689914
H	0.30522072	-3.28585156	6.23773011
H	1.62283472	-3.01496270	5.08788270
H	0.69217432	-4.52992528	5.03212260
H	2.39539388	-0.94774482	-3.57858009
H	2.03618406	-2.66462733	-3.82289727
H	3.62043225	-2.01599965	-4.30689088
H	4.75623498	-3.87200476	-2.76115980
H	3.13053704	-4.44410594	-2.33638229
H	4.27125324	-3.97486224	-1.05703643
H	-5.11533923	-3.44079875	0.54080476
H	-4.68993895	-5.54892681	-0.70295438
H	-2.94467799	-5.61402090	-2.46485032
H	-3.15748878	-0.26943240	0.08380217
H	0.30480879	2.11759916	-2.52645142
H	-4.72900832	-1.92563125	2.14214166
H	-4.22593991	-0.23451340	2.30797879
H	-2.99796114	-1.51535325	2.22180129
H	-5.21581697	-0.32317039	-1.33139013
H	-5.52583399	0.45368418	0.23964604
H	-6.07899583	-1.20698931	-0.05545329
H	2.05039612	4.58302377	-1.96632581
H	2.61928419	2.91980429	-2.24367076
H	1.66120979	3.29549231	-0.80020768
H	-0.22267105	3.19136813	-4.73615495
H	1.51186717	2.84830008	-4.55293783
H	0.90990284	4.50655533	-4.36764110
H	0.11505382	5.89445458	-2.61514658



H	-1.78557792	7.19616261	-1.69335746
H	-3.69787158	6.03431501	-0.61947804
H	-0.79628471	-2.71319729	-3.46193848
H	-3.86911782	2.27681655	-0.22509127
H	-0.56832361	-5.70318113	-2.81639952
H	0.37204420	-4.38382044	-2.08230536
H	0.56110239	-4.76283141	-3.81260101
H	-1.25094289	-4.05944383	-5.48001655
H	-2.77358165	-3.33728729	-4.91237442
H	-2.43904097	-5.05318767	-4.61847914
H	-3.41129736	3.69498453	1.78938087
H	-5.13430550	3.28105754	1.65308120
H	-4.57671296	4.90554765	1.21538639
H	-5.25283979	3.13688913	-2.13142942
H	-5.66839513	4.58248875	-1.19015711
H	-6.22262025	2.98408056	-0.65057484

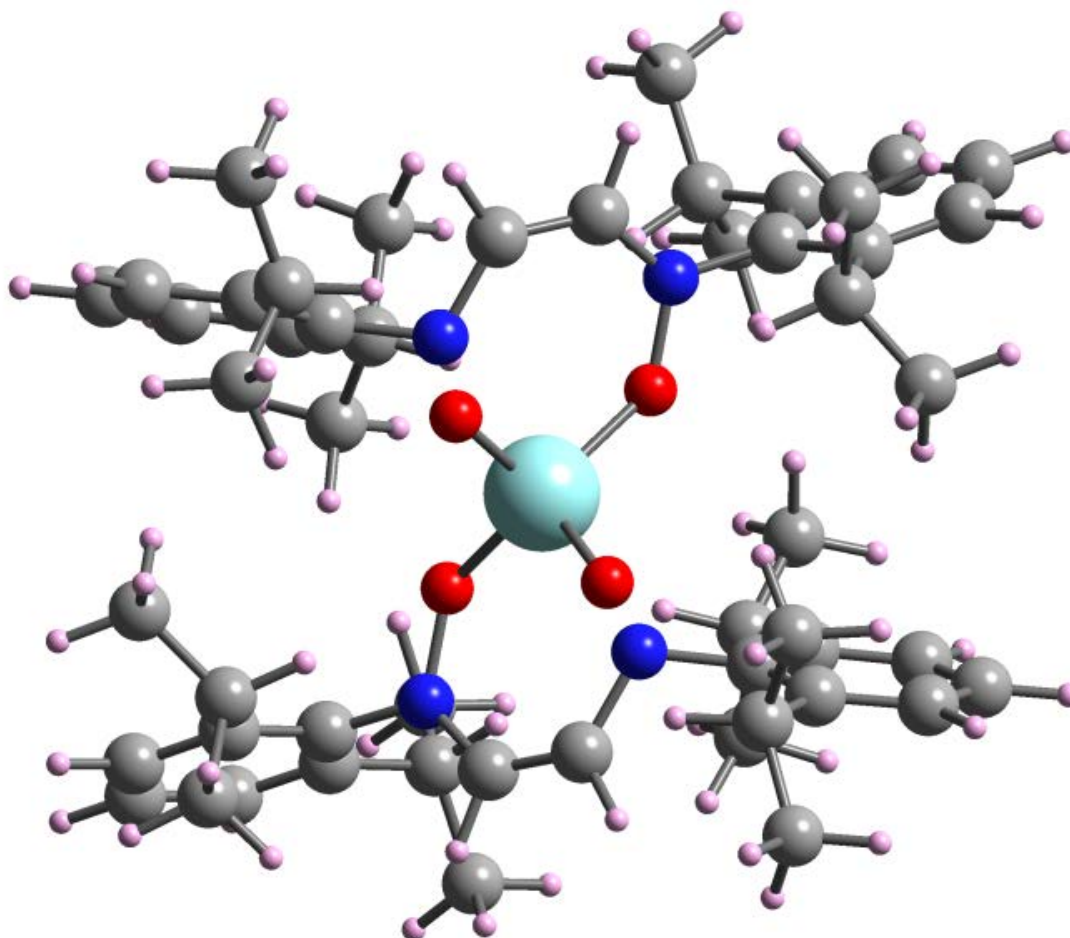
**Bare Complex (conformation 2 lower energy with distorted N-O bonds)**

Fig. S107: ONCCNO Bare Complex (conformation 2 lower energy with distorted N-O bonds)

SCF	E <sub>ZP</sub>	H	G
-2591.059596	-2589.910390	-2589.842214	-2590.015860

Zr	-0.00037700	-0.00444800	0.62726100
O	-0.47854500	1.29891800	2.12658900
O	-1.64584600	-0.65402700	-0.39219900
N	0.39276800	-2.28086600	0.89831700
N	-2.42528900	-1.84811300	-0.33815400
N	2.42803500	1.84862800	-0.30943800
N	-0.39321000	2.26949700	0.92236900
C	-0.74371800	-3.16292800	0.94595500
C	-1.96090900	-2.92843100	0.36153000
C	1.96254000	2.92115400	0.40106700
C	0.74374900	3.14995000	0.98451300
C	1.67180400	-2.98915400	0.72659800
C	2.21109300	-3.08112600	-0.58603300
C	3.44027300	-3.75348900	-0.75331900
C	4.10985300	-4.32477200	0.33770600

C	3.53603200	-4.26182000	1.61554700
C	2.30167100	-3.61575600	1.83995900
C	2.36789500	-1.72867800	-2.76383500
C	1.47178700	-2.57629100	-1.83047200
C	0.85723300	-3.77904900	-2.59904800
C	-2.89974700	-1.90091000	-4.48337100
C	-2.91678100	-2.61746300	-3.11007000
C	-3.04041000	-4.15426700	-3.29717400
C	-3.77145600	-1.72716800	-0.84578200
C	-4.02639300	-2.09663900	-2.19388900
C	-5.35413000	-2.01289800	-2.66267100
C	-6.38710400	-1.56414700	-1.82437000
C	-6.11118400	-1.18946200	-0.50013800
C	-4.79961500	-1.25735400	0.01489100
C	2.56404900	-2.78450800	4.23043400
C	1.71471400	-3.64447600	3.25972000
C	1.57356600	-5.09756500	3.78526400
C	-5.06291300	0.55021100	1.79627900
C	-4.52664300	-0.86562500	1.46912100
C	-5.12269300	-1.91691200	2.44432300
C	3.77163900	1.73682400	-0.82535900
C	4.02258700	2.13868200	-2.16481200
C	5.34827400	2.06197400	-2.64088300
C	6.38276900	1.58875200	-1.81831600
C	6.11080800	1.18297000	-0.50230300
C	4.80177100	1.24327500	0.01975300
C	2.87393600	1.98013600	-4.44500400
C	2.91193700	2.68389000	-3.06531500
C	3.05333000	4.22054400	-3.23899700
C	-2.57363300	2.74217800	4.25461900
C	-1.72151500	3.60953000	3.29308600
C	-1.57994900	5.05804600	3.83115600
C	-1.67136800	2.98004100	0.75366800
C	-2.30519900	3.59408000	1.87175900
C	-3.53984400	4.24075400	1.65074500
C	-4.11018000	4.31638200	0.37200200
C	-3.43632200	3.75824900	-0.72317700
C	-2.20655800	3.08603200	-0.55954900
C	5.08223400	-0.59458800	1.76880700
C	4.53292700	0.82145400	1.46645200
C	5.11942600	1.86117600	2.46000000
C	-2.35420800	1.75454800	-2.75086100
C	-1.46285700	2.59581700	-1.80724700
C	-0.85033100	3.80784600	-2.56276700
H	-0.60938500	-4.09928800	1.47819000
H	-2.70351500	-3.71709600	0.44875400
H	2.70579200	3.70783900	0.50017400
H	0.60908700	4.07941100	1.52861700
H	3.87345400	-3.83140600	-1.74672800
H	5.06254800	-4.82829200	0.19110100
H	4.04818100	-4.72954600	2.45257200
H	0.63709300	-1.94278100	-1.51260700

H	-1.95841500	-2.41688200	-2.61973300
H	3.19644700	-2.31675400	-3.17919100
H	2.78161600	-0.87014200	-2.22663500
H	1.77367400	-1.35437100	-3.60883500
H	1.64328800	-4.46131100	-2.94855300
H	0.29974100	-3.42567800	-3.47692000
H	0.17154400	-4.34886700	-1.96014000
H	-3.80851700	-2.10892900	-5.06336900
H	-2.04399800	-2.24765200	-5.07817900
H	-2.81568900	-0.81462100	-4.36237400
H	-2.99200100	-4.67827400	-2.33420500
H	-2.22597800	-4.53109700	-3.92978700
H	-3.99308400	-4.41726300	-3.77614300
H	-5.58129600	-2.29710500	-3.68685400
H	-7.40527900	-1.50618600	-2.20277900
H	-6.91957800	-0.84071000	0.13719900
H	0.72142000	-3.19429500	3.24288100
H	-3.44277600	-0.84657100	1.62456500
H	3.60116500	-3.14348900	4.28524200
H	2.13847400	-2.82105400	5.24238500
H	2.56925300	-1.74043500	3.89966700
H	2.54796500	-5.58784000	3.90823500
H	0.97287100	-5.71594200	3.10463400
H	1.07977100	-5.09202400	4.76631200
H	-4.64386400	1.30145900	1.11777200
H	-4.78599700	0.82851600	2.82076700
H	-6.15789100	0.59465600	1.72315600
H	-6.21511500	-1.97330300	2.34538600
H	-4.88934700	-1.64667500	3.48245200
H	-4.71507200	-2.91810400	2.25429200
H	5.57228900	2.37075100	-3.65869800
H	7.39920700	1.53632700	-2.20216600
H	6.92064600	0.81606200	0.12281200
H	1.95514900	2.49068000	-2.56914900
H	-0.72862500	3.15849700	3.27457500
H	3.78382000	2.17569100	-5.02756600
H	2.02183000	2.34833800	-5.03208100
H	2.76979900	0.89469400	-4.33251800
H	3.02193100	4.73591200	-2.27060800
H	2.23704000	4.61362800	-3.85922100
H	4.00391900	4.47670600	-3.72571600
H	-3.61050400	3.10166300	4.31069900
H	-2.14990300	2.76935200	5.26763500
H	-2.57936000	1.70111400	3.91456700
H	-0.97688300	5.68132000	3.15711000
H	-1.08861900	5.04387300	4.81335700
H	-2.55412600	5.54839400	3.95561400
H	-4.05501800	4.69883600	2.49123600
H	-5.06336300	4.81974600	0.22807300
H	-3.86673300	3.84612800	-1.71696800
H	3.44932800	0.78977200	1.62151800
H	-0.62679000	1.96192400	-1.49363900

H	6.17793500	-0.62681300	1.70027300
H	4.67373200	-1.33693700	1.07427200
H	4.80360100	-0.89522400	2.78650000
H	4.89201900	1.56883700	3.49344300
H	4.69950800	2.86087700	2.28993100
H	6.21084300	1.93198200	2.35902700
H	-2.76723200	0.89033600	-2.22240900
H	-1.75660500	1.38921600	-3.59744400
H	-3.18304700	2.34445200	-3.16306400
H	-0.16811500	4.37391400	-1.91678300
H	-1.63756600	4.49096600	-2.90792500
H	-0.28957500	3.46468800	-3.44260600
O	0.47268800	-1.32401400	2.11396200
O	1.64775200	0.65614700	-0.38168100

## 9.2 Structures with five oxygen atoms

## Oxo Complex

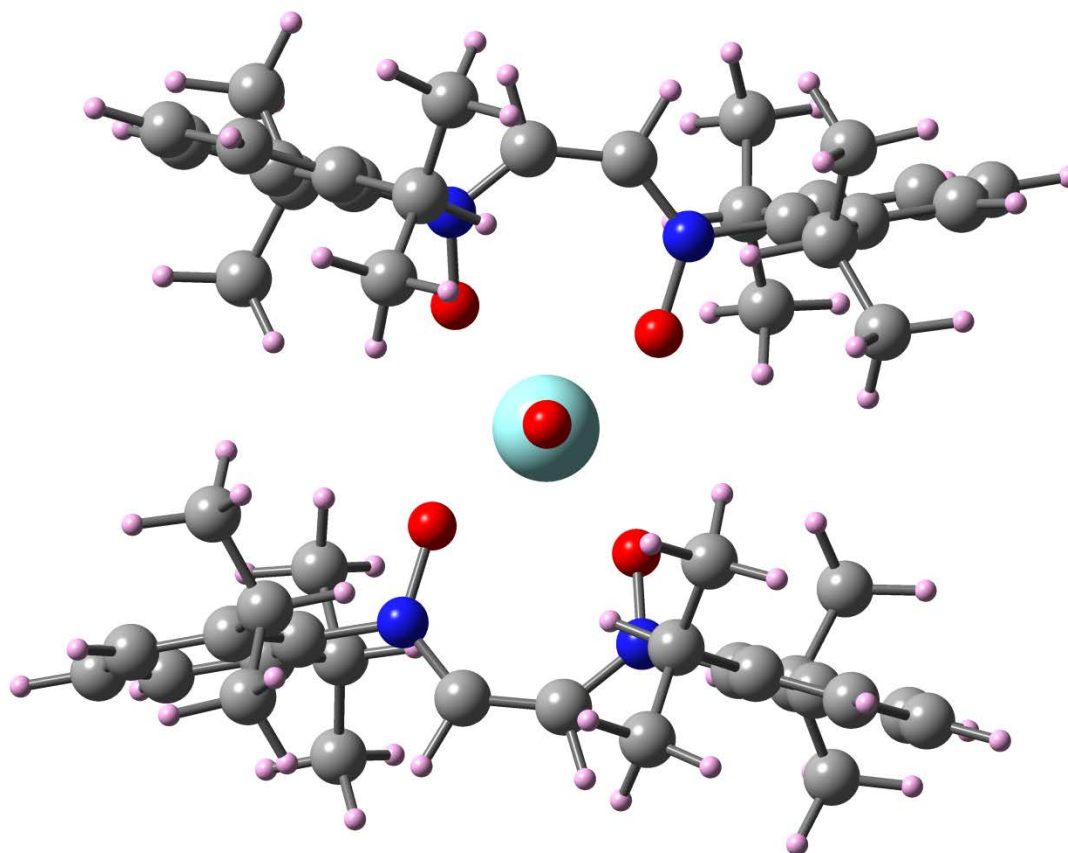


Fig. S108: ONCCNO Oxo Complex

SCF	E <sub>ZP</sub>	H	G
-2666.25984069	-2665.108325	-2665.037239	-2665.223969

N	-0.99166172	-3.03663397	-0.13623739
N	0.99234534	3.03610469	-0.13860398
C	0.15098281	-3.77988822	-0.19706550
C	1.49370331	-3.51290920	0.09781246
C	-0.15079133	3.77861123	-0.19931323
C	-1.49342202	3.51129322	0.09581789
C	-2.25715904	-3.54069412	-0.63315672
C	-3.25974780	-3.88133007	0.31451636
C	-4.48952841	-4.35899753	-0.18024126
C	-4.70766382	-4.50043884	-1.56095222
C	-3.70338382	-4.14713230	-2.47441433
C	-2.45946375	-3.64352614	-2.03520496
C	-3.83879866	-2.50027115	2.35259625
C	-3.04241988	-3.72231827	1.82162543
C	-3.40472803	-5.00876666	2.60586042

C	3.18749410	-1.44740371	4.15070512
C	3.04330313	-2.70113096	3.24704663
C	3.19133000	-4.00404656	4.07345531
C	3.61882073	-2.47390464	0.74259811
C	4.03874382	-2.64346833	2.08601198
C	5.42540821	-2.72608623	2.33010692
C	6.34954675	-2.63493603	1.27646027
C	5.90504447	-2.44156899	-0.04112869
C	4.52857872	-2.34407031	-0.33631177
C	-1.95966734	-2.12717746	-4.02189647
C	-1.40884335	-3.21802498	-3.06813066
C	-0.88669366	-4.44155020	-3.86714703
C	4.64247346	-0.76290956	-2.32362997
C	4.06446152	-2.09266639	-1.77377355
C	4.43212352	-3.28015191	-2.70197845
C	2.25756035	3.54167537	-0.63492830
C	2.46094824	3.64289989	-2.03689847
C	3.70417906	4.14856087	-2.47568372
C	4.70684992	4.50520863	-1.56172355
C	4.48783594	4.36495307	-0.18103174
C	3.25860408	3.88531375	0.31323323
C	1.96677089	2.12414949	-4.02309980
C	1.41200128	3.21339768	-3.06982054
C	0.88582586	4.43471694	-3.86955201
C	-3.19217355	1.45241025	4.15028437
C	-3.04740900	2.70489424	3.24497298
C	-3.19770929	4.00892303	4.06918648
C	-3.61871932	2.47257405	0.74004691
C	-4.04092629	2.64465886	2.08242119
C	-5.42801796	2.72739920	2.32403694
C	-6.35034697	2.63401410	1.26900450
C	-5.90359230	2.43814764	-0.04745626
C	-4.52662161	2.34029867	-0.34015987
C	3.83805521	2.50622317	2.35241626
C	3.04038498	3.72693987	1.82027091
C	3.40039488	5.01423966	2.60413778
C	-4.63978062	0.75752431	-2.32652325
C	-4.06001035	2.08636812	-1.77639542
C	-4.42314158	3.27390304	-2.70636898
H	-0.03417797	-4.78801094	-0.55220361
H	2.14523448	-4.37462486	-0.00417441
H	0.03377592	4.78663435	-0.55502233
H	-2.14529882	4.37254132	-0.00785980
H	-5.27822343	-4.62800389	0.51742109
H	-5.66152472	-4.87733081	-1.92317654
H	-3.89085087	-4.24403099	-3.54065095
H	-1.98235568	-3.51129693	1.99655701
H	2.02941121	-2.68138052	2.83346413
H	-4.91912302	-2.63727279	2.20608656
H	-3.52876877	-1.58838233	1.83118297
H	-3.65625069	-2.36511314	3.42750979
H	-4.47449416	-5.24478006	2.53276455

H	-3.16876403	-4.87705503	3.67026980
H	-2.84210426	-5.87593528	2.23600116
H	4.18101222	-1.40263626	4.61713087
H	2.43756763	-1.46980523	4.95272552
H	3.04026213	-0.53110876	3.56761637
H	3.06379430	-4.89345295	3.44290284
H	2.43338962	-4.03703917	4.86726843
H	4.17740599	-4.06960338	4.55199493
H	5.78307425	-2.85938625	3.34807548
H	7.41508107	-2.70465244	1.48332816
H	6.63159917	-2.35611283	-0.84521606
H	-0.56083573	-2.76173554	-2.54904687
H	2.97393655	-1.99146826	-1.77655208
H	-2.83920887	-2.47569716	-4.58036614
H	-1.18430287	-1.84329008	-4.74444073
H	-2.22545469	-1.22702239	-3.45844201
H	-1.69222557	-4.91496221	-4.44458917
H	-0.45820166	-5.20542068	-3.20434237
H	-0.10689537	-4.12688051	-4.57302890
H	4.36050897	0.08215350	-1.68505814
H	4.25215030	-0.57264026	-3.33171081
H	5.73854028	-0.79446520	-2.38660408
H	5.51992467	-3.41906694	-2.76142476
H	4.06019343	-3.09579709	-3.71822580
H	3.99304923	-4.22050347	-2.34371090
H	3.89246925	4.24437165	-3.54187488
H	5.66022871	4.88369544	-1.92355718
H	5.27540961	4.63633770	0.51697378
H	0.56549938	2.75437553	-2.55066683
H	-2.03283384	2.68522478	2.83305624
H	2.84307213	2.47668791	-4.58413262
H	1.19135719	1.83471387	-4.74333924
H	2.23933990	1.22641061	-3.45897577
H	0.45400359	5.19713725	-3.20725217
H	0.10765517	4.11698657	-4.57586193
H	1.69002017	4.91098300	-4.44652460
H	-4.18651081	1.40754991	4.61495816
H	-2.44372053	1.47665630	4.95362817
H	-3.04312737	0.53537307	3.56884347
H	-3.06986222	4.89748870	3.43750944
H	-2.44104345	4.04368095	4.86414328
H	-4.18456461	4.07447444	4.54611828
H	-5.78741863	2.86261640	3.34114228
H	-7.41624557	2.70391056	1.47393417
H	-6.62880485	2.35089100	-0.85255369
H	1.98046956	3.51458155	1.99456092
H	-2.96972035	1.98270287	-1.77682235
H	4.91830012	2.64472093	2.20673257
H	3.52978017	1.59366722	1.83111830
H	3.65480441	2.37124760	3.42723186
H	3.16387426	4.88272140	3.66844517
H	2.83686184	5.88047138	2.23347341



H	4.46989631	5.25165274	2.53167275
H	-4.36137786	-0.08771814	-1.68663387
H	-4.24731496	0.56552760	-3.33343000
H	-5.73560763	0.79152441	-2.39235238
H	-3.98279141	4.21360946	-2.34798648
H	-5.51052950	3.41506745	-2.76813397
H	-4.04947176	3.08788970	-3.72167329
O	-0.00398606	0.00050727	-1.91842051
O	-1.65913196	1.13847371	0.60978355
O	1.66072222	-1.13871824	0.60456520
N	-2.19202352	2.39882172	0.46815869
N	2.19261009	-2.39995508	0.46825444
O	-1.04985522	-1.79218128	0.46345512
O	1.05160612	1.79126147	0.45987358
Zr	-0.00026679	-0.00023197	-0.09542775

### 9.3 Structures with six oxygen atoms

#### Peroxo Complex

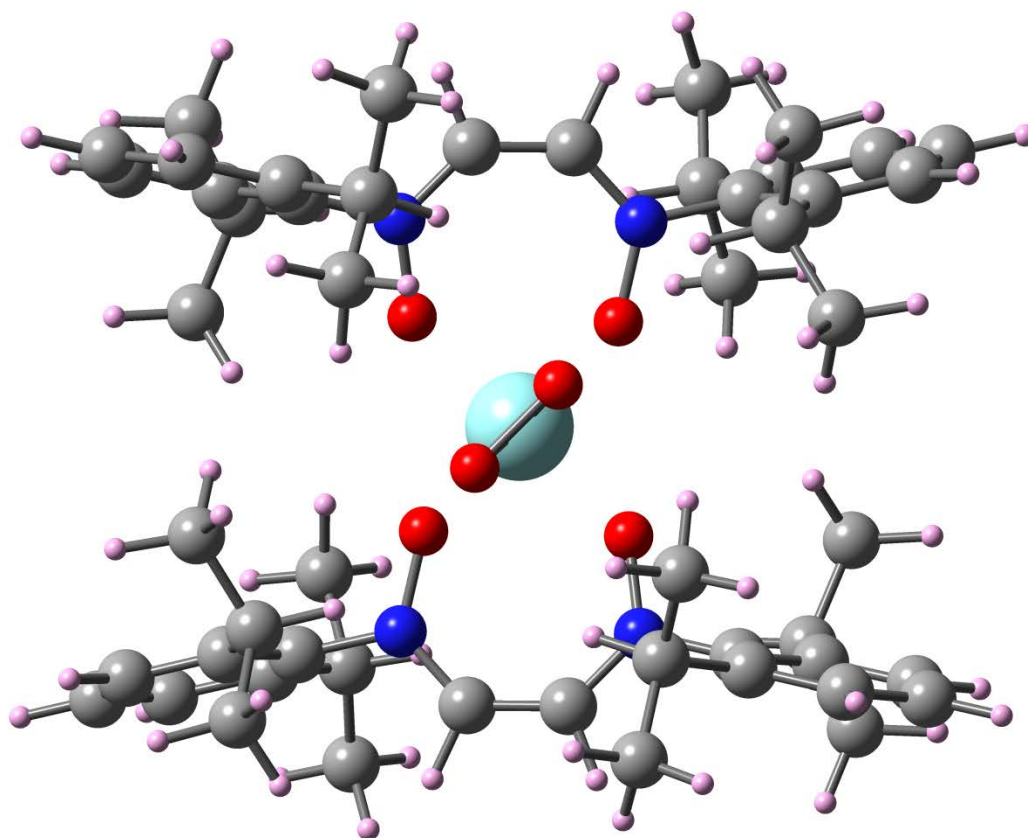


Fig. S109: ONCCNO Peroxo Complex

SCF	E <sub>ZP</sub>	H	G
-2741.418446	-2740.263703	-2740.191687	-2740.379485

O	-1.38450735	-1.51858911	0.28827603
O	1.38421986	1.51863166	0.28710657
O	0.58035595	-0.53257289	-2.15141397
O	-0.57909106	0.52793787	-2.15288970
N	-1.71971242	2.66211377	0.60018216
N	1.49094670	2.83115031	-0.13028591
N	1.71956795	-2.66185947	0.60049934
N	-1.49102968	-2.83081844	-0.13000284
C	-0.86540722	3.68507315	0.30963739
C	0.49131563	3.75246467	-0.02838126
C	0.86530429	-3.68478172	0.30987263
C	-0.49144310	-3.75214241	-0.02824185
C	-3.12432805	2.91374794	0.88219034
C	-4.04671155	2.87314635	-0.19360114
C	-5.40137018	3.13167306	0.10504649

C	-5.81380309	3.39855081	1.42032376
C	-4.88067705	3.40130555	2.46984716
C	-3.51412612	3.15253931	2.22407673
C	-4.33076667	1.27145068	-2.14545417
C	-3.62080606	2.54947737	-1.62831159
C	-3.87677979	3.74867201	-2.57829235
C	2.14740002	2.04987257	-4.07233502
C	1.82121586	3.17176843	-3.05242838
C	1.48683575	4.50279438	-3.77704079
C	2.79994056	3.18783571	-0.64799999
C	2.96192898	3.36404758	-2.04705034
C	4.24995081	3.71428874	-2.50785737
C	5.32590278	3.85437010	-1.61854538
C	5.13972969	3.64561343	-0.24152909
C	3.87258839	3.30871453	0.27476106
C	-2.78710786	1.85546660	4.27256698
C	-2.51652484	3.09964996	3.38430686
C	-2.53072124	4.40004015	4.22707532
C	4.31658255	1.69989846	2.17781819
C	3.68631221	3.05993997	1.77395885
C	4.25382535	4.21561411	2.63625182
C	3.12417190	-2.91370120	0.88246202
C	3.51385956	-3.15340661	2.22421682
C	4.88034063	-3.40269857	2.46983989
C	5.81347855	-3.39958609	1.42031987
C	5.40115200	-3.13172349	0.10521150
C	4.04656945	-2.87259871	-0.19328957
C	2.78642568	-1.85621792	4.27238086
C	2.51623951	-3.10075299	3.38444107
C	2.53080589	-4.40087612	4.22756080
C	-2.14635457	-2.05127587	-4.07319484
C	-1.82022737	-3.17226356	-3.05225978
C	-1.48514112	-4.50374588	-3.77569715
C	-2.79989680	-3.18744000	-0.64815635
C	-2.96131853	-3.36409442	-2.04721719
C	-4.24916577	-3.71452405	-2.50839462
C	-5.32547960	-3.85425960	-1.61947476
C	-5.13985256	-3.64500952	-0.24245633
C	-3.87291588	-3.30798169	0.27424220
C	4.33150423	-1.26969713	-2.14390413
C	3.62076649	-2.54769850	-1.62774884
C	3.87602571	-3.74627917	-2.57867353
C	-4.31684302	-1.69822493	2.17648202
C	-3.68722708	-3.05883701	1.77345491
C	-4.25588506	-4.21378429	2.63594677
H	-1.36985627	4.64519117	0.31844037
H	0.83472463	4.74921267	-0.28400956
H	1.36981279	-4.64487168	0.31827663
H	-0.83476031	-4.74883053	-0.28422986
H	-6.13668530	3.11557120	-0.69529050
H	-6.86312872	3.59439390	1.62918659
H	-5.21687835	3.59074939	3.48612315

H	-2.54700370	2.33794477	-1.64178754
H	0.92300042	2.84376178	-2.52058965
H	-5.41945947	1.40785231	-2.20135252
H	-4.12280419	0.41699903	-1.49147386
H	-3.96520389	1.02363256	-3.14955502
H	-4.94659174	3.98902909	-2.64261178
H	-3.52404943	3.50782921	-3.58935393
H	-3.34916153	4.64980359	-2.23878144
H	3.05312265	2.27550365	-4.65220565
H	1.31082906	1.93526235	-4.77300691
H	2.27470346	1.08949030	-3.56203544
H	1.22508659	5.29707956	-3.06473070
H	0.63546592	4.35816337	-4.45455703
H	2.33642704	4.85782551	-4.37582469
H	4.41189015	3.86209005	-3.57239261
H	6.31063317	4.11832697	-1.99765816
H	5.98359824	3.74995207	0.43533065
H	-1.50921780	2.98298681	2.96984837
H	2.61305263	2.98637338	1.98007951
H	-3.78437033	1.90310739	4.73031519
H	-2.04542115	1.79590778	5.08041483
H	-2.72532136	0.93553033	3.67968585
H	-3.50149796	4.55453234	4.71589524
H	-2.32301335	5.28136861	3.60652724
H	-1.76689653	4.34887026	5.01411264
H	3.84974364	0.88051972	1.62095573
H	4.16894939	1.51712589	3.25106154
H	5.39670384	1.68850117	1.97733836
H	5.34413929	4.29991103	2.53954076
H	4.03074498	4.03583989	3.69634088
H	3.81463419	5.18118588	2.35339759
H	5.21646694	-3.59290474	3.48599483
H	6.86273718	-3.59590674	1.62907153
H	6.13647691	-3.11531762	-0.69511057
H	1.50887584	-2.98449648	2.96998306
H	-0.92233445	-2.84345952	-2.52036896
H	3.78372326	-1.90342320	4.73010116
H	2.04473410	-1.79671752	5.08022963
H	2.72429753	-0.93647616	3.67924447
H	2.32347679	-5.28246805	3.60725964
H	1.76686033	-4.34971202	5.01448187
H	3.50154435	-4.55490287	4.71659531
H	-3.05175463	-2.27760690	-4.65329829
H	-1.30950778	-1.93696513	-4.77358511
H	-2.27412726	-1.09056311	-3.56364163
H	-1.22348529	-5.29743051	-3.06267657
H	-0.63349243	-4.35936989	-4.45291573
H	-2.33435290	-4.85948820	-4.37460820
H	-4.41065868	-3.86275488	-3.57293462
H	-6.31005636	-4.11836805	-1.99888141
H	-5.98399025	-3.74912460	0.43409739
H	2.54709657	-2.33549229	-1.64108161

H	-2.61402161	-2.98587233	1.98009228
H	5.42009861	-1.40679470	-2.20007411
H	4.12421632	-0.41567802	-1.48914293
H	3.96594813	-1.02078017	-3.14773074
H	3.52345027	-3.50437524	-3.58953500
H	3.34784096	-4.64737050	-2.23992718
H	4.94569504	-3.98724758	-2.64318628
H	-3.84913578	-0.87936353	1.61960031
H	-4.16972870	-1.51518408	3.24975434
H	-5.39683920	-1.68624583	1.97536513
H	-3.81742788	-5.17981203	2.35350768
H	-5.34624996	-4.29720947	2.53905813
H	-4.03289421	-4.03384481	3.69602808
O	-1.35825724	1.34142853	0.64403327
O	1.35794803	-1.34129767	0.64547503
Zr	0.00002677	-0.00014728	-0.27102941

## Dioxo Complex

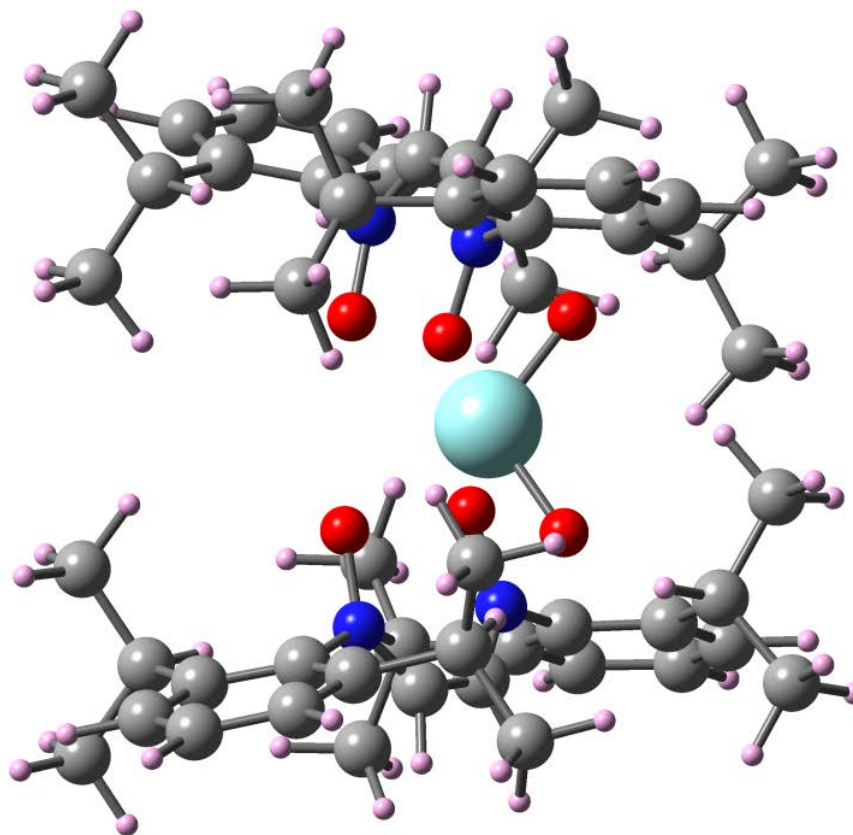


Fig. S110: ONCCNO Dioxo Complex

SCF	E <sub>ZP</sub>	H	G
-2741.430518	-2740.273171	-2740.201764	-2740.384290
O	-0.29931310	-1.48817895	1.22264616
O	2.24586953	0.00470378	-0.26814580
O	-0.25059029	-1.53919155	-1.73370880
N	0.73549769	2.73353394	1.00466443
N	3.01701150	1.03490245	-0.66951589
N	-3.01681699	-1.03506223	-0.66976165
N	-0.73564594	-2.73314195	1.00541556
C	1.77261699	3.07101416	0.24358583
C	2.76636542	2.32450434	-0.47868526
C	-2.76628220	-2.32460598	-0.47833928
C	-1.77250336	-3.07089539	0.24412227
C	-0.05302834	3.79306891	1.65727504
C	-0.98693904	4.51553063	0.87701649
C	-1.72828251	5.51433682	1.54770128
C	-1.55601681	5.75135632	2.91961871
C	-0.63826628	4.99022070	3.66372517
C	0.13643518	3.98693000	3.04754230
C	-2.69722202	3.79327487	-0.85184655

C	-1.23153386	4.24058276	-0.61126447
C	-0.88555023	5.48221899	-1.47354987
C	2.33630050	-0.28448703	-4.36118509
C	2.88938128	0.96418472	-3.62259965
C	3.16101568	2.12268836	-4.61724428
C	4.22057321	0.63416577	-1.41710322
C	4.15178083	0.60615182	-2.83106641
C	5.32447062	0.20332316	-3.50860963
C	6.48396390	-0.16072052	-2.80742146
C	6.50126779	-0.14142275	-1.40286642
C	5.36151075	0.25094533	-0.67177432
C	0.29658406	2.10233118	4.72464762
C	1.09652252	3.12575080	3.87413861
C	2.03898612	3.97591402	4.76199051
C	5.58908528	-1.20755271	1.39442782
C	5.38352262	0.23421808	0.85996735
C	6.46101216	1.19629954	1.42466307
C	-4.22077021	-0.63457893	-1.41689626
C	-4.15291083	-0.60751561	-2.83093705
C	-5.32595290	-0.20483014	-3.50795386
C	-6.48489018	0.15996854	-2.80623653
C	-6.50127716	0.14156507	-1.40166405
C	-5.36113318	-0.25062828	-0.67107741
C	-2.33812081	0.28121600	-4.36299874
C	-2.89126099	-0.96667809	-3.62315417
C	-3.16425162	-2.12569491	-4.61682914
C	-0.29858736	-2.10299283	4.72608934
C	-1.09759479	-3.12640950	3.87471308
C	-2.04006517	-3.97746850	4.76170448
C	0.05316860	-3.79242219	1.65804229
C	-0.13668644	-3.98675623	3.04819883
C	0.63826283	-4.98986484	3.66436394
C	1.55663237	-5.75036506	2.92036866
C	1.72927958	-5.51286962	1.54858335
C	0.98770562	-4.51421975	0.87792291
C	-5.58679346	1.20942227	1.39423121
C	-5.38207987	-0.23280571	0.86066468
C	-6.45947951	-1.19412128	1.42682279
C	2.69860478	-3.79077379	-0.84981692
C	1.23290643	-4.23853008	-0.61012275
C	0.88759271	-5.47982335	-1.47317399
H	1.91830202	4.14352696	0.17987581
H	3.50647710	2.96216940	-0.95105184
H	-3.50653912	-2.96240201	-0.95029954
H	-1.91800548	-4.14343687	0.18048085
H	-2.45320682	6.09959262	0.98827498
H	-2.14241468	6.52323208	3.41285233
H	-0.52496199	5.17716912	4.72814961
H	-0.60508630	3.40782897	-0.95703208
H	2.08880730	1.29051437	-2.94682989
H	-3.42039837	4.56649384	-0.55578790
H	-2.91756185	2.87292407	-0.29838883

H	-2.84227257	3.57788242	-1.91771043
H	-1.52664088	6.34158353	-1.23165903
H	-1.02458874	5.24279488	-2.53506417
H	0.15892183	5.79386793	-1.33365864
H	3.07636099	-0.71495157	-5.05141358
H	1.44898511	0.00077318	-4.94020850
H	2.02159474	-1.05343238	-3.64673423
H	3.54513438	3.01541035	-4.10415184
H	2.22512615	2.39952913	-5.11828851
H	3.88812712	1.84081092	-5.39157601
H	5.32072806	0.17062268	-4.59465883
H	7.37269778	-0.46737274	-3.35425898
H	7.40241293	-0.43780426	-0.87218084
H	1.72487521	2.54396233	3.18992193
H	4.40898033	0.57060603	1.23112732
H	-0.36572596	2.61500459	5.43529250
H	0.98283376	1.46389014	5.29694911
H	-0.31247720	1.46143905	4.07803016
H	1.48529704	4.53007696	5.53063913
H	2.60583652	4.70291810	4.16591975
H	2.75526429	3.32397736	5.27906397
H	4.80463292	-1.87582951	1.02167406
H	5.55261930	-1.21407175	2.49184150
H	6.56132819	-1.61403634	1.08625362
H	7.46984932	0.89395248	1.11523285
H	6.43360533	1.19538284	2.52233991
H	6.30009762	2.22594989	1.07900804
H	-5.32294394	-0.17289458	-4.59402864
H	-7.37391229	0.46648078	-3.35268448
H	-7.40199367	0.43852447	-0.87057408
H	-2.09034224	-1.29302801	-2.94780891
H	-1.72589238	-2.54460610	3.19046654
H	-3.07855014	0.71168399	-5.05283170
H	-1.45149066	-0.00491595	-4.94263870
H	-2.02231378	1.05040249	-3.64929787
H	-3.54842853	-3.01788245	-4.10285160
H	-2.22888105	-2.40334285	-5.11839300
H	-3.89181129	-1.84395343	-5.39079341
H	0.36364781	-2.61564822	5.43681897
H	-0.98543945	-1.46516898	5.29835567
H	0.31044788	-1.46148545	4.08005839
H	-2.60632213	-4.70441334	4.16499679
H	-2.75686724	-3.32612851	5.27880332
H	-1.48646439	-4.53179215	5.53030141
H	0.52465292	-5.17718099	4.72869143
H	2.14322628	-6.52209779	3.41359250
H	2.45471920	-6.09758440	0.98925870
H	-4.40738364	-0.56925303	1.23137764
H	0.60645576	-3.40571787	-0.95574524
H	-6.55910416	1.61600750	1.08640863
H	-4.80236718	1.87716924	1.02047375
H	-5.54959453	1.21671238	2.49161516



H	-6.43127934	-1.19242992	2.52447889
H	-6.29916680	-2.22407207	1.08178449
H	-7.46843923	-0.89165348	1.11791119
H	2.91851795	-2.87069568	-0.29573329
H	2.84407780	-3.57474414	-1.91549447
H	3.42181142	-4.56400904	-0.55387606
H	-0.15687640	-5.79177207	-1.33392578
H	1.52875275	-6.33916646	-1.23139961
H	1.02708360	-5.23986119	-2.53450822
O	0.25129238	1.53808841	-1.73437203
O	-2.24552914	-0.00472018	-0.26911838
O	0.29878317	1.48874853	1.22190180
Zr	0.00026548	-0.00030394	-0.66200721

## Octahedral Complex

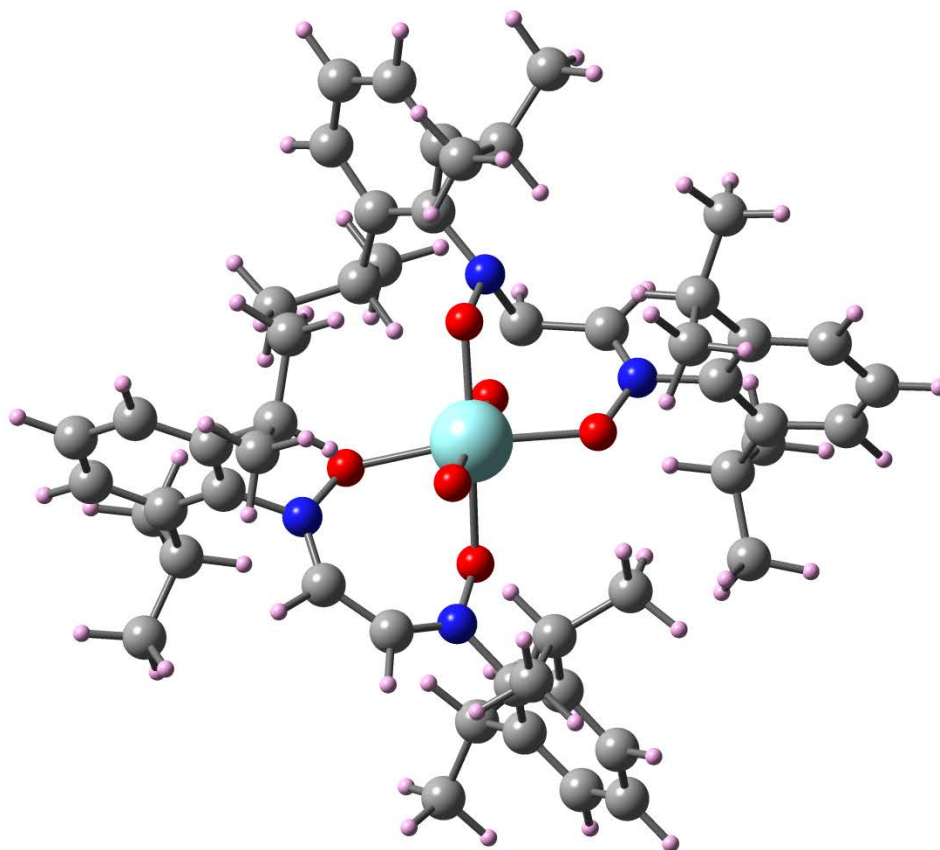


Fig. S111: ONCCNO Octahedral Complex

SCF	$E_{ZP}$	H	G
-2741.465835	-2740.308624	-2740.237817	-2740.420987

O	-0.15061444	2.06594553	0.44329706
O	0.29043565	0.74002039	-1.83295358
N	2.86713434	1.09417311	-0.52598524
N	0.21134859	2.89061532	-0.71528815
C	2.32966549	1.94396077	-1.36670377
C	0.84629800	2.02769856	-1.74752151
C	4.31051262	1.05125444	-0.27904461
C	5.10986451	0.27394230	-1.14969877
C	6.49777734	0.25417509	-0.89561560
C	7.04258923	0.95793446	0.19025555
C	6.21033360	1.68756062	1.05501756
C	4.81687596	1.74754827	0.84384796
C	4.80562386	-2.05658824	-2.10861038
C	4.52314950	-0.54383655	-2.30488569
C	5.05507172	-0.05265014	-3.67645225
C	-0.20749583	4.89717153	2.37632299
C	0.48866829	5.15005717	1.01188166

C	1.31948279	6.45683495	1.04628005
C	-0.69016148	3.98601695	-0.96808026
C	-0.53651174	5.13068987	-0.12370757
C	-1.36806674	6.24738881	-0.33242927
C	-2.31826253	6.25881989	-1.36638286
C	-2.46503722	5.13081941	-2.18404500
C	-1.68458242	3.96806411	-1.99285656
C	3.78371817	1.67773390	3.14789942
C	3.90874035	2.48862433	1.82912140
C	4.39553605	3.93231269	2.10706755
C	-3.44766930	2.30320049	-2.76728215
C	-1.96984570	2.75672830	-2.88981658
C	-1.61540756	3.05259172	-4.37233066
H	3.03103294	2.63137582	-1.83302465
H	0.80862836	2.58555456	-2.69718741
H	7.15165917	-0.32261369	-1.54451998
H	8.11481934	0.92887833	0.36965215
H	6.64483776	2.21120367	1.90194988
H	3.43433352	-0.42576353	-2.30874402
H	1.17194991	4.31271201	0.83848318
H	5.88211162	-2.27240102	-2.13007510
H	4.32939665	-2.63433869	-2.91157989
H	4.40383354	-2.40829800	-1.15119002
H	4.82532676	1.00839537	-3.83952465
H	4.59417305	-0.62846025	-4.48936598
H	6.14365176	-0.17524788	-3.75192234
H	-0.94070854	5.68558715	2.59859195
H	0.53280921	4.88313640	3.18925947
H	-0.72015337	3.93022043	2.35933819
H	1.79510840	6.65420382	0.07635229
H	2.10926418	6.38031443	1.80618550
H	0.70397851	7.32942907	1.30263038
H	-1.26330613	7.12049233	0.30692446
H	-2.94232529	7.13543301	-1.52695177
H	-3.21425692	5.14021419	-2.97253240
H	2.90072617	2.55584506	1.40531137
H	-1.36453981	1.90826996	-2.56429852
H	4.75974699	1.56824208	3.64049854
H	3.37712936	0.68020853	2.94978370
H	3.10447306	2.19029264	3.84105326
H	3.68275840	4.44313355	2.76676150
H	4.47933068	4.51519982	1.18077899
H	5.37390382	3.94412597	2.60522646
H	-3.68489774	2.03400410	-1.73086443
H	-3.61409305	1.41861915	-3.39748985
H	-4.14943342	3.08374023	-3.09032436
H	-0.56617611	3.35838593	-4.48289968
H	-2.23985089	3.85854808	-4.78228059
H	-1.77217696	2.15570680	-4.98662808
O	-0.35445713	-0.73326269	1.93155664
O	2.17679958	0.15058194	0.20760844
O	-2.21263740	-0.47190596	-0.20168183

N	-0.27569773	-3.18369812	0.22709482
N	-2.96976401	-1.32411945	0.50321304
C	-1.41736916	-3.31539872	0.89020778
C	-2.59998536	-2.50702911	0.98994482
C	0.74529760	-4.24086399	0.29645600
C	1.54236521	-4.34242358	1.46226601
C	2.51300294	-5.36949217	1.47227930
C	2.68348035	-6.22223776	0.37219241
C	1.88930201	-6.06856961	-0.77704865
C	0.89872278	-5.06889479	-0.84451923
C	2.74248280	-2.61253803	2.87767507
C	1.42008806	-3.39500541	2.66111038
C	1.01776654	-4.16746249	3.94472368
C	-5.56031021	-1.28617604	-2.71202834
C	-5.07611013	-2.01237703	-1.43118973
C	-5.72129508	-3.41995996	-1.31957526
C	-4.34252691	-0.84967873	0.76319319
C	-5.35051312	-1.18182803	-0.17280318
C	-6.65267244	-0.71689459	0.10424192
C	-6.91523659	0.05428255	1.24849626
C	-5.88132225	0.37932061	2.14012244
C	-4.55900266	-0.06362717	1.91934918
C	0.92293609	-4.16637572	-3.20617455
C	0.07123709	-4.87793129	-2.11956807
C	-0.51529415	-6.20902743	-2.65178884
C	-3.20366557	1.84585417	2.89212707
C	-3.44021999	0.31242610	2.89609757
C	-3.74977295	-0.19671238	4.32801335
H	-1.47802964	-4.23904066	1.45491413
H	-3.38185587	-2.97173068	1.58051502
H	3.14609555	-5.48769862	2.34720065
H	3.44076731	-7.00201589	0.40464980
H	2.04009579	-6.72944394	-1.62584847
H	0.65518193	-2.63298713	2.46975834
H	-3.99297967	-2.14579392	-1.53626242
H	3.58679753	-3.28098693	3.09678103
H	2.62241260	-1.92432588	3.72364810
H	2.98979368	-2.01263583	1.99395843
H	0.07101761	-4.71012687	3.81308217
H	0.88856870	-3.46189281	4.77485963
H	1.78310659	-4.89914019	4.23841862
H	-6.65119005	-1.16464358	-2.72161351
H	-5.28217096	-1.86696578	-3.60117068
H	-5.10556221	-0.29322648	-2.79413962
H	-5.35095779	-3.96657804	-0.44217850
H	-5.49501111	-4.01557202	-2.21368141
H	-6.81289979	-3.34653111	-1.23030342
H	-7.46119431	-0.95046767	-0.58307749
H	-7.92550279	0.40768696	1.44054481
H	-6.09665146	0.98590406	3.01535137
H	-0.77202109	-4.21317524	-1.89792741
H	-2.49515715	-0.14891369	2.58600487

H	1.79617179	-4.77359263	-3.48113723
H	1.26926841	-3.19309505	-2.84309405
H	0.32270190	-4.00192435	-4.11065471
H	-1.16174001	-6.01130564	-3.51671841
H	-1.11327852	-6.72184040	-1.88708004
H	0.27140787	-6.89891242	-2.98298465
H	-2.91286886	2.19759951	1.89602650
H	-2.38641816	2.09189925	3.58122817
H	-4.09978918	2.39667888	3.21066169
H	-3.90418141	-1.28431883	4.34558766
H	-4.64690889	0.27829842	4.74825517
H	-2.90494894	0.03406754	4.98852385
O	0.04305983	-2.13806932	-0.56123109
Zr	-0.02801207	-0.00623689	0.24645827

## 9.4 Structures with seven oxygen atoms

### Oxo Peroxo Complex (conformation 1)

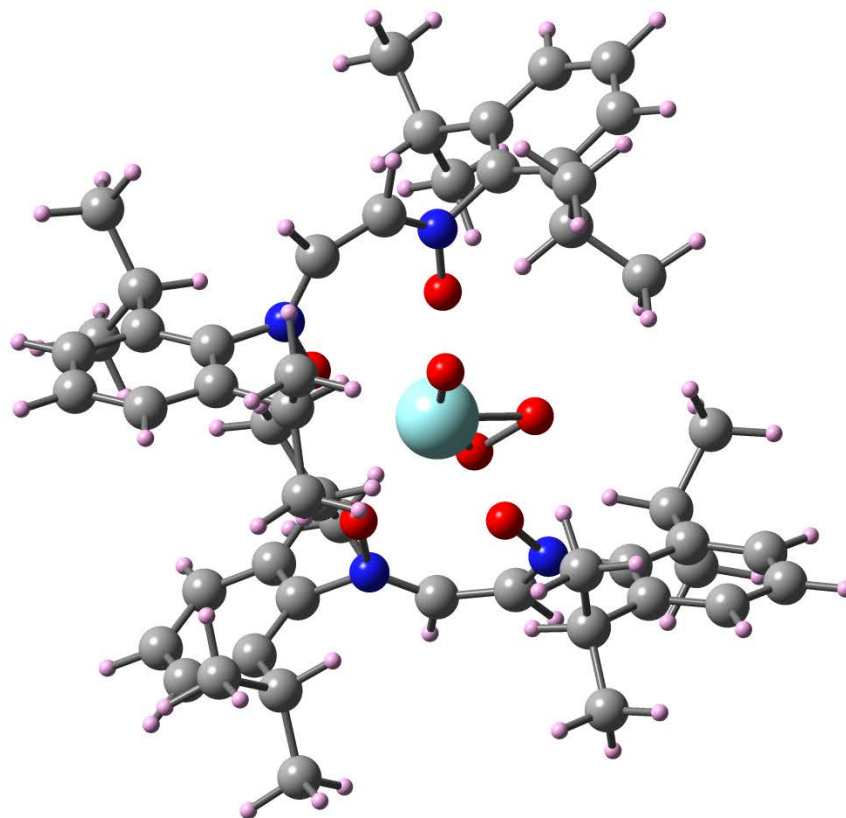


Fig. S112: ONCCNO Oxo Peroxo Complex (conformation 1)

SCF	E <sub>ZP</sub>	H	G
-2816.583435	-2815.423771	-2815.351243	-2815.536655

Zr	0.37014364	0.06807951	0.15375743
O	1.54548408	-1.72013343	0.86951966
O	-1.80850447	0.88488059	0.12069129
O	1.01459570	-0.51938233	-2.00591122
O	2.06557047	0.09251999	-1.15113169
N	0.37496681	3.33811814	0.08973059
N	-2.27928920	1.72432221	1.06166358
N	-0.80823693	-2.61659949	-1.08483342
N	2.30252432	-2.34483211	-0.09874037
C	-0.54920915	3.57714566	1.01920710
C	-1.71209074	2.86284322	1.44841488
C	0.36417823	-3.04670466	-1.55744822
C	1.73348595	-2.92277951	-1.15421137
C	1.43237881	4.33892468	-0.14199176
C	2.52839768	4.37230149	0.75151366

C	3.51682832	5.34957537	0.49832049
C	3.41728458	6.21662917	-0.59949239
C	2.32980615	6.12310561	-1.48475998
C	1.30821848	5.17427043	-1.27917666
C	3.96631011	2.52049867	1.70781342
C	2.69768142	3.38986126	1.91582881
C	2.74944830	4.12832667	3.27815031
C	-1.95007525	-1.29440351	3.59875604
C	-2.15173282	0.24464714	3.61840809
C	-2.07906896	0.79453824	5.06559283
C	-3.53940182	1.29946344	1.69775919
C	-3.47166794	0.61404482	2.93484781
C	-4.70272412	0.23543947	3.51479466
C	-5.92323293	0.51728361	2.88273532
C	-5.94493750	1.17780380	1.64336146
C	-4.74789565	1.57834772	1.01533323
C	0.64318683	4.17577024	-3.49925390
C	0.16384905	5.02022801	-2.28528447
C	-0.42188016	6.37713561	-2.74556374
C	-5.51506111	1.41902388	-1.40421977
C	-4.79096913	2.28645817	-0.34241577
C	-5.45305815	3.68509959	-0.22486015
C	-2.05412486	-3.06407840	-1.71533631
C	-2.46754895	-2.46775635	-2.93283680
C	-3.67698341	-2.93406334	-3.49371211
C	-4.43426075	-3.93354288	-2.86422832
C	-4.00334292	-4.48742232	-1.64765575
C	-2.80515497	-4.05851855	-1.04141773
C	-2.49707967	-0.02145015	-3.59256908
C	-1.68925949	-1.34576914	-3.62722962
C	-1.30879816	-1.72530818	-5.08140565
C	2.88120084	-2.58189496	3.67584314
C	3.00324705	-3.57058971	2.48597599
C	3.31442912	-5.00683490	2.98089602
C	3.72540927	-2.50755711	0.20940247
C	4.04837978	-3.07254968	1.47784611
C	5.41336615	-3.19158102	1.80671936
C	6.41783278	-2.79986626	0.90951712
C	6.06877181	-2.28106084	-0.34363829
C	4.72029856	-2.11104797	-0.72801856
C	-3.42086964	-4.43960376	1.39558271
C	-2.35602262	-4.66518040	0.29125936
C	-2.02579092	-6.17352900	0.13801919
C	5.12293565	-0.14309114	-2.29658114
C	4.43553400	-1.51968662	-2.11559378
C	4.87294496	-2.50490329	-3.23352736
H	-0.39360817	4.51508719	1.53981890
H	-2.25871869	3.36013778	2.24213813
H	0.24354951	-3.67440755	-2.43504018
H	2.42470922	-3.43401544	-1.81260014
H	4.37636374	5.41707642	1.15958859
H	4.19371103	6.95753293	-0.77544445

H	2.27771726	6.78912032	-2.34116837
H	1.85630827	2.68794373	1.94768121
H	-1.30472419	0.66438292	3.06342548
H	4.88356120	3.12591159	1.71026455
H	3.91349592	1.97527907	0.75814202
H	4.03993246	1.78041119	2.51403995
H	3.61343256	4.80379846	3.34487246
H	2.82951226	3.39651223	4.09174585
H	1.84330455	4.72598985	3.44976780
H	-2.73931880	-1.81512417	4.15993064
H	-0.98188716	-1.54114604	4.05190766
H	-1.94276968	-1.67390260	2.57033246
H	-2.20395702	1.88585569	5.09120084
H	-1.09864791	0.55771915	5.49713544
H	-2.84750832	0.35323558	5.71521965
H	-4.69924829	-0.29063855	4.46546826
H	-6.85738180	0.21546234	3.35062151
H	-6.89655748	1.37890072	1.15845688
H	-0.64912740	4.45764990	-1.80907437
H	-3.76474650	2.42979993	-0.69837999
H	1.46654936	4.68006670	-4.02315270
H	-0.18037650	4.03618087	-4.21249006
H	0.98949291	3.19019603	-3.17102509
H	0.30366583	6.95641150	-3.33066823
H	-0.73847242	6.99257801	-1.89328905
H	-1.29528587	6.20634688	-3.38841379
H	-5.04454030	0.43340794	-1.49182896
H	-5.47072510	1.90943757	-2.38552738
H	-6.57301131	1.27209004	-1.15066711
H	-6.49668485	3.60408915	0.10605985
H	-5.44709490	4.19255346	-1.19847269
H	-4.92267253	4.32184072	0.49540256
H	-4.02768324	-2.50448352	-4.42844087
H	-5.36140936	-4.27667442	-3.31761208
H	-4.60209596	-5.25519897	-1.16454593
H	-0.75749528	-1.15259736	-3.08920674
H	2.02444886	-3.59148848	2.00083195
H	-3.45163518	-0.11552208	-4.12923454
H	-1.91420409	0.77893810	-4.06624521
H	-2.70564813	0.27749578	-2.55858741
H	-0.72586457	-2.65541605	-5.11560273
H	-0.69793049	-0.92842942	-5.52368463
H	-2.19609103	-1.86149366	-5.71460665
H	3.83926004	-2.47460598	4.20389169
H	2.13609816	-2.94687003	4.39635627
H	2.56069665	-1.59911442	3.31625588
H	3.42229127	-5.70704873	2.14181026
H	2.49444351	-5.36197261	3.61948182
H	4.23521708	-5.05105436	3.57683594
H	5.69073890	-3.60834482	2.77081496
H	7.46500100	-2.90323163	1.18422086
H	6.85241690	-1.98414062	-1.03503258



H	-1.44652990	-4.15211446	0.61948064
H	3.36908918	-1.31969545	-2.21618636
H	-4.36133181	-4.95587474	1.16100931
H	-3.63636086	-3.37193913	1.51644847
H	-3.05567713	-4.82676526	2.35600716
H	-1.66995717	-6.58361237	1.09238326
H	-1.24471075	-6.33796544	-0.61582906
H	-2.91125471	-6.74768034	-0.16560667
H	4.76268888	0.55789053	-1.53681562
H	4.86260054	0.27067353	-3.27941507
H	6.21786813	-0.20850549	-2.23452354
H	4.37520088	-3.48142877	-3.14211142
H	5.95580887	-2.68746471	-3.20940291
H	4.62257648	-2.08839647	-4.21800244
O	0.51253523	0.85523978	1.82309853
O	0.46599085	2.24880331	-0.67683113
O	-0.99608180	-1.72540730	-0.06230729

## Oxo Peroxo Complex (conformation 2)

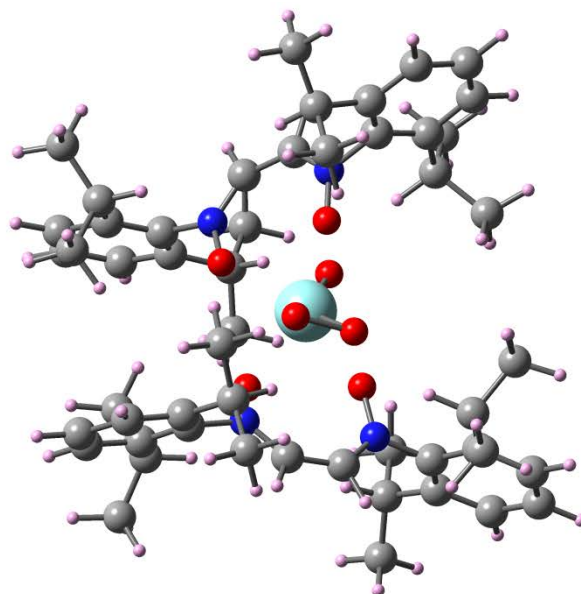


Fig. S113: ONCCNO Oxo Peroxo Complex (conformation 2)

SCF	E <sub>ZP</sub>	H	G
-2816.5798682	-2815.420531	-2815.347816	-2815.534821

Zr	-0.16660000	0.25876200	0.05097200
O	1.99207700	-0.43063000	0.17026300
O	-2.33299800	-0.02760900	0.72825900
O	0.12164400	1.11540100	1.68006100
N	-1.09963800	-2.43389700	-1.20389400
N	-3.40299200	-0.54975200	0.11272000
N	1.85458200	2.88217500	-0.02949800
N	2.83568200	-0.02048400	1.14614600
C	-2.38935200	-2.24117600	-1.49708600
C	-3.40167100	-1.46189300	-0.87229700
C	2.74488600	2.50482500	0.89431200
C	3.14216400	1.24178500	1.42832800
C	-0.29416300	-3.40451400	-1.95160200
C	-0.05700300	-3.22187900	-3.34285800
C	0.73089000	-4.19847900	-3.99130300
C	1.26241600	-5.29418000	-3.29905100
C	0.99319900	-5.45501600	-1.93160300
C	0.19880400	-4.52845500	-1.22757800
C	0.52242300	-1.31729400	-4.93582900
C	-0.60587600	-2.05631400	-4.17409000
C	-1.69879400	-2.55099100	-5.16021500
C	-4.35438900	3.15242800	-1.36770800
C	-4.57633400	1.62272000	-1.48920000
C	-5.39642500	1.28816800	-2.76330800
C	-4.68187800	0.02771000	0.54793500

C	-5.25134700	1.06165300	-0.23275200
C	-6.48681100	1.58386400	0.20932400
C	-7.09421000	1.11250300	1.38330400
C	-6.47639500	0.11204800	2.15279500
C	-5.24856700	-0.45426200	1.75287300
C	1.15380700	-4.60526600	1.12049800
C	-0.11436800	-4.80123800	0.24978500
C	-0.72081100	-6.21373700	0.45611100
C	-3.80841900	-0.77858700	3.80019400
C	-4.53793800	-1.49122400	2.62734500
C	-5.49109900	-2.59372800	3.14857600
C	1.73327600	4.31562500	-0.34813500
C	0.93890600	5.11316000	0.50686300
C	0.84582700	6.48478500	0.18286100
C	1.48897200	7.00583400	-0.95045000
C	2.23098900	6.16656900	-1.79958000
C	2.36818900	4.79135600	-1.52042300
C	-1.34629000	4.78593100	1.55788600
C	0.17758500	4.54011400	1.70819100
C	0.70218600	5.13253600	3.04188000
C	4.54250900	-2.68204000	-1.11936600
C	4.96616700	-1.52835100	-0.17162600
C	6.49121400	-1.26436800	-0.25821100
C	3.47677900	-1.10519100	1.90279600
C	4.51674400	-1.82348300	1.26280600
C	5.12585100	-2.85951300	1.99960400
C	4.70799300	-3.15758900	3.30720500
C	3.66182600	-2.43494200	3.90021500
C	3.00628300	-1.39257600	3.20798100
C	2.14407800	3.43197500	-3.63648600
C	3.10075700	3.85407200	-2.48540800
C	4.41143700	4.46196400	-3.03985700
C	0.70281900	-1.62904900	4.25365200
C	1.83862700	-0.64740700	3.86453700
C	2.31504200	0.15894900	5.10111300
H	-2.73489100	-2.80972400	-2.35216700
H	-4.39485100	-1.64239500	-1.26863700
H	3.27894000	3.34442200	1.32436000
H	3.87213100	1.32595300	2.22642400
H	0.93689900	-4.08598900	-5.05183500
H	1.87527700	-6.02389800	-3.82305100
H	1.38988100	-6.31886400	-1.40543900
H	-1.02872900	-1.30374400	-3.50427600
H	-3.58232700	1.17816900	-1.60487200
H	1.03045200	-1.96360500	-5.66503600
H	1.25882200	-0.92340800	-4.22826800
H	0.09780700	-0.46205000	-5.47636800
H	-1.28770600	-3.25572000	-5.89619300
H	-2.11961000	-1.69823000	-5.70850700
H	-2.52494200	-3.06218500	-4.64485100
H	-5.30379000	3.70406000	-1.32595000
H	-3.78868600	3.51144000	-2.23625000

H	-3.77651600	3.39222900	-0.46740700
H	-5.52676900	0.20452800	-2.88838500
H	-4.87765200	1.66996700	-3.65168400
H	-6.39558000	1.74372800	-2.73054100
H	-6.96514100	2.37389600	-0.36345700
H	-8.04388000	1.53268700	1.70657300
H	-6.94985900	-0.22828800	3.06933700
H	-0.84812100	-4.07068000	0.59872000
H	-3.76393500	-1.98307100	2.02610000
H	1.94705100	-5.31006800	0.83527400
H	0.91819200	-4.77347600	2.17997000
H	1.53842200	-3.58629900	1.01042300
H	-0.00851700	-7.01027600	0.20520400
H	-1.61831600	-6.35948500	-0.15941400
H	-1.00369600	-6.34479800	1.50918300
H	-3.07784600	-0.05768200	3.41786400
H	-3.27671100	-1.51480200	4.41807300
H	-4.52506000	-0.24756900	4.44175000
H	-6.24011400	-2.19184100	3.84294500
H	-4.91699300	-3.35456900	3.69313900
H	-6.02325600	-3.08971200	2.32633100
H	0.25323200	7.14105600	0.81464900
H	1.40072700	8.06469800	-1.18268500
H	2.70183100	6.58235500	-2.68548600
H	0.30524400	3.45146100	1.74961600
H	4.45205600	-0.62817400	-0.52523100
H	-1.59515700	5.85631100	1.57277600
H	-1.87956900	4.29821300	2.38326300
H	-1.71689500	4.35828400	0.61882000
H	1.77282100	4.92880100	3.18085600
H	0.16194500	4.68486400	3.88562400
H	0.55984500	6.22114700	3.08653200
H	5.01847900	-3.62889000	-0.83021100
H	4.84020100	-2.45314900	-2.15101900
H	3.45612800	-2.81969500	-1.10021400
H	6.79491900	-0.43951500	0.39976200
H	6.76838700	-1.00074900	-1.28727300
H	7.07368000	-2.15084900	0.02436700
H	5.93047500	-3.43411700	1.54861000
H	5.19381200	-3.95804200	3.86050700
H	3.33885500	-2.68684100	4.90678700
H	3.36845500	2.93627200	-1.94631600
H	1.39400400	0.05907300	3.15274000
H	1.81190100	4.31027300	-4.20709300
H	1.26563800	2.91199400	-3.24058300
H	2.66172800	2.75140600	-4.32565300
H	4.93918800	3.71399700	-3.64556300
H	5.08254500	4.78562100	-2.23324300
H	4.21873400	5.32659100	-3.68799200
H	0.36010500	-2.19543700	3.37934700
H	-0.15237400	-1.06112300	4.64049800
H	1.01919100	-2.34299100	5.02723900

H	3.09159400	0.88865300	4.83318800
H	2.72719000	-0.49574800	5.88158500
H	1.47004300	0.71092500	5.53165900
O	-1.31169100	0.88839300	-1.62809200
O	-0.14252700	0.17362500	-2.20556400
O	-0.54468100	-1.95164100	-0.03978000
O	1.02545300	2.10257500	-0.71062400

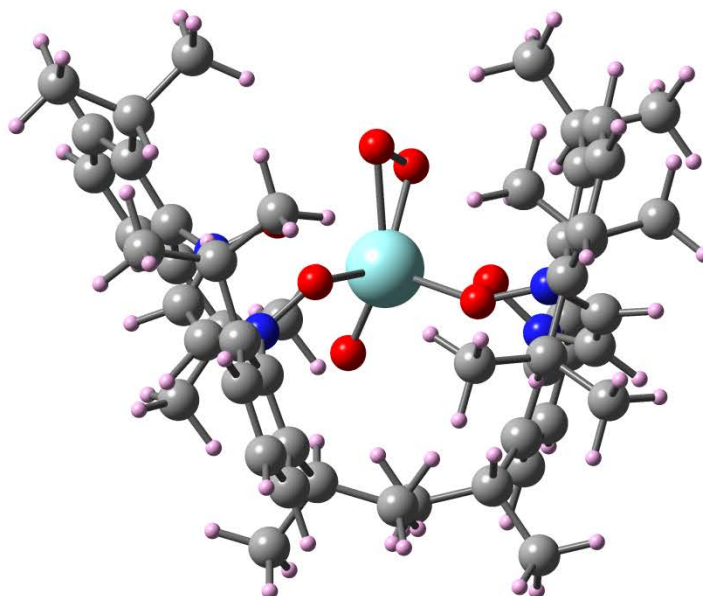
**Oxo Peroxo Complex (conformation 3)**

Fig. S114: ONCCNO Oxo Peroxo Complex (conformation 3)

SCF	E <sub>ZP</sub>	H	G
-2816.57276635	-2815.414170	-2815.341195	-2815.528580
O	0.29593600	-2.06069500	-0.11399900
O	-0.84503700	2.23558600	-0.39598500
O	0.94111200	0.47407500	1.20064100
N	-3.19250700	0.43529100	-0.57456900
N	-1.65424400	2.92380100	0.40849000
N	3.35385300	-0.75114300	-0.31113200
N	0.96623800	-2.66147900	0.91211900
C	-3.66897200	1.61428000	-0.15717900
C	-2.97082800	2.67253600	0.48976200
C	3.29044300	-1.65825500	0.68630800
C	2.25253000	-2.45736200	1.22441100
C	-3.98604900	-0.41625900	-1.46642500
C	-3.95955900	-0.13922800	-2.85623000
C	-4.75447600	-0.96361100	-3.68134500
C	-5.51156100	-2.01597900	-3.14405700
C	-5.48716100	-2.27802200	-1.76456500
C	-4.71677700	-1.48449400	-0.89041700
C	-2.22070400	0.47309800	-4.62498800
C	-3.12196700	0.98702900	-3.47326700
C	-4.03833800	2.14437000	-3.95605300
C	0.35367700	4.94092700	-2.05255300
C	-0.98848100	5.18518800	-1.30891400
C	-1.68413000	6.47276800	-1.81777000
C	-1.06881600	4.10800300	1.04788600

C	-0.75722900	5.20748200	0.20582900
C	-0.18004000	6.33636500	0.82095300
C	0.07463800	6.35794400	2.20229400
C	-0.22865900	5.24307500	2.99672700
C	-0.80122000	4.07983700	2.43671300
C	-4.00261000	-3.16911300	0.86000100
C	-4.68553200	-1.79930500	0.60762800
C	-6.10404200	-1.75788600	1.23307800
C	0.29253600	2.29883300	3.86846900
C	-1.05089700	2.85785100	3.32633700
C	-2.04037100	3.18927600	4.47427200
C	4.66014300	-0.18340500	-0.67140300
C	5.11954500	0.93022000	0.06844600
C	6.37906700	1.45655900	-0.29273800
C	7.11155500	0.90929000	-1.35779700
C	6.59836300	-0.17036800	-2.09722100
C	5.35141500	-0.74364500	-1.77276800
C	4.01731500	3.06318300	0.89536200
C	4.29719900	1.56751500	1.19406900
C	5.00236300	1.40211400	2.56594400
C	-0.62326500	-5.19654600	-1.41051500
C	0.53388900	-5.24113500	-0.37586300
C	1.28457800	-6.59482100	-0.43449700
C	0.18865400	-3.66365800	1.64071400
C	0.00085200	-4.92738600	1.02517600
C	-0.74146600	-5.88811500	1.74181100
C	-1.26590000	-5.59526400	3.01197200
C	-1.07704800	-4.32706800	3.58177600
C	-0.35489500	-3.32134400	2.90211600
C	4.02164500	-1.25609400	-3.86047500
C	4.74447400	-1.86283200	-2.62386100
C	5.78258000	-2.92876300	-3.04918900
C	-1.60358900	-1.29038500	3.76096700
C	-0.20930400	-1.92692300	3.52055100
C	0.60795300	-1.97849200	4.83767700
H	-4.72414400	1.77117000	-0.35558300
H	-3.55583900	3.42517500	1.00441500
H	4.25418300	-1.81964500	1.15540400
H	2.57365900	-3.07194900	2.05919300
H	-4.76499600	-0.78791800	-4.75301700
H	-6.11236600	-2.63944300	-3.80203000
H	-6.06756300	-3.10481700	-1.36367200
H	-2.44103300	1.38842000	-2.71507900
H	-1.64103300	4.34000200	-1.55756400
H	-2.80892400	0.04560800	-5.44866100
H	-1.50624900	-0.27087600	-4.25703800
H	-1.63145600	1.30742900	-5.02511200
H	-4.72108400	1.80608800	-4.74712900
H	-3.42734700	2.95957800	-4.36417800
H	-4.64963600	2.55125900	-3.13839300
H	1.07995500	5.73211900	-1.82114100
H	0.18758500	4.93380100	-3.13752100

H	0.77961500	3.97257500	-1.77262300
H	-2.62477500	6.66468000	-1.28444900
H	-1.91073800	6.37271000	-2.88710500
H	-1.04404500	7.35682500	-1.70212300
H	0.07285500	7.20240800	0.21626900
H	0.52054900	7.24003600	2.65577300
H	-0.00499800	5.26495800	4.05978300
H	-4.07623300	-1.04315100	1.11535700
H	-1.49260000	2.05822500	2.72181700
H	-4.56282600	-3.98602400	0.38591500
H	-3.94813400	-3.37601100	1.93634300
H	-2.98244000	-3.17364400	0.46112400
H	-6.75768100	-2.52637200	0.80069900
H	-6.58556700	-0.78322300	1.07768400
H	-6.04472200	-1.94116500	2.31389100
H	0.87751800	1.87325300	3.04403100
H	0.09624500	1.49431400	4.59071600
H	0.87344200	3.07597900	4.38333400
H	-1.62412500	3.93842200	5.16045900
H	-2.25351400	2.28558100	5.06008000
H	-2.99311000	3.58009400	4.09097500
H	6.77734800	2.30743900	0.25374100
H	8.07787100	1.33263600	-1.62275000
H	7.16807900	-0.56622700	-2.93286200
H	3.31781300	1.07894600	1.25610300
H	1.24126400	-4.45626000	-0.66541700
H	4.94241400	3.65508400	0.85955800
H	3.37425800	3.48269000	1.67950100
H	3.49694700	3.17735100	-0.06277200
H	5.17362100	0.34394000	2.80562000
H	4.37981000	1.83194700	3.36134100
H	5.97556400	1.91189700	2.58335400
H	-1.39253500	-5.94582700	-1.17791000
H	-0.23856500	-5.40231500	-2.41793900
H	-1.08792700	-4.20490600	-1.42019000
H	2.10106100	-6.63543700	0.29833600
H	1.71484000	-6.73881200	-1.43406300
H	0.61449900	-7.44255200	-0.24071600
H	-0.90705700	-6.86968000	1.30626500
H	-1.82782700	-6.35348400	3.55269800
H	-1.50049500	-4.10983800	4.55900100
H	3.97549600	-2.37290300	-2.02992300
H	0.31739400	-1.26568900	2.82280800
H	4.72640300	-0.68450000	-4.48035500
H	3.20283000	-0.59901500	-3.55041900
H	3.59558200	-2.05902200	-4.47690900
H	5.27425300	-3.75533900	-3.56254900
H	6.32159700	-3.34024500	-2.18541600
H	6.52345500	-2.52032800	-3.74887600
H	-2.15930200	-1.21210800	2.81889100
H	-1.48342500	-0.27882600	4.16772400
H	-2.20357400	-1.87386000	4.47284100



H	1.60809800	-2.40118200	4.67322700
H	0.10800300	-2.58863300	5.60247700
H	0.73465600	-0.96569200	5.24087900
O	0.45890100	1.06434400	-2.34133500
O	0.38308700	-0.36465600	-2.66660300
O	2.34586500	-0.29321600	-1.04674200
O	-2.03187900	-0.09012300	-0.12410900
Zr	0.16581700	0.11211400	-0.45321000

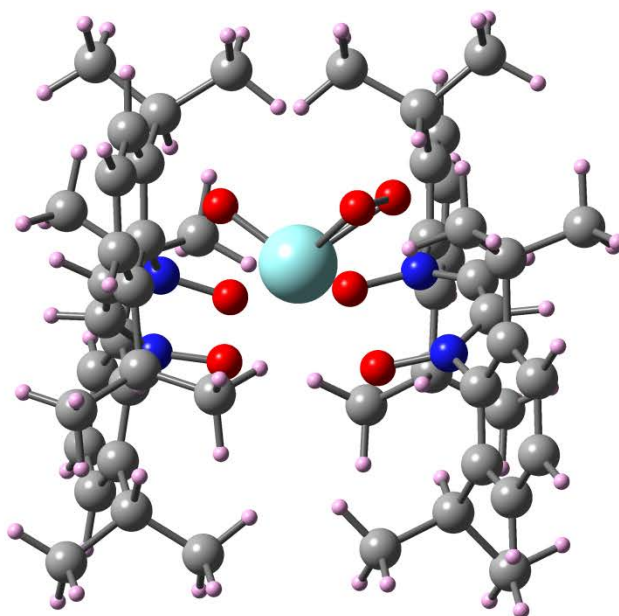
**Oxo Peroxo Complex (butterfly conformation)**

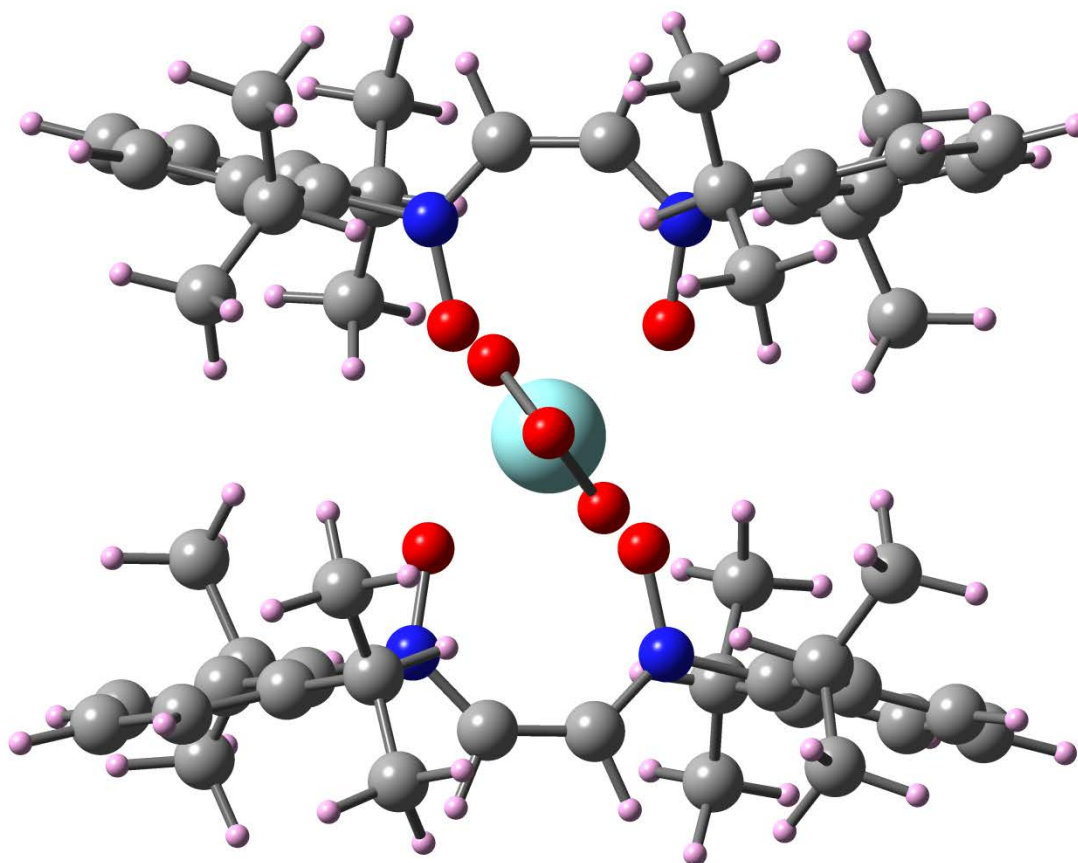
Fig. S115: ONCCNO Oxo Peroxo Complex (butterfly conformation)

SCF	E <sub>ZP</sub>	H	G
-2816.6033332	-2815.443249	-2815.370701	-2815.556085
O	0.10342200	1.55687700	1.12995500
O	-2.35724700	-0.38127600	-0.11024500
O	-1.12630800	1.59459000	-1.79200900
N	-0.29100800	-2.74081500	0.94011100
N	-2.97399500	-1.51306700	-0.48004800
N	2.83136200	1.21055800	-0.65444900
N	0.38609000	2.84243200	0.82965000
C	-1.33120100	-3.28135000	0.31251000
C	-2.50367300	-2.74414700	-0.31924400
C	2.51338500	2.49519900	-0.51324300
C	1.43334000	3.21804600	0.09868500
C	0.71956200	-3.63144200	1.54096600
C	1.68641400	-4.22049500	0.69220700
C	2.63581300	-5.06468500	1.31075400
C	2.62327600	-5.28271900	2.69644100
C	1.66102200	-4.65622600	3.50616200
C	0.68275200	-3.81037200	2.94530200
C	3.10588400	-3.32790400	-1.21034700
C	1.74905200	-3.96853600	-0.81829500
C	1.50550400	-5.27873200	-1.61227500
C	-2.85632200	-0.24733400	-4.26897000
C	-3.13407500	-1.52939300	-3.43802200
C	-3.31563300	-2.76525200	-4.35710100
C	-4.28632100	-1.31098700	-1.11991000

C	-4.35420800	-1.32755100	-2.53297900
C	-5.62939100	-1.11063600	-3.10195100
C	-6.75438200	-0.87162300	-2.29946200
C	-6.63557800	-0.83297400	-0.89972800
C	-5.39144300	-1.04748700	-0.27369300
C	0.36065600	-1.94376800	4.61841800
C	-0.33247700	-3.09577700	3.84231400
C	-1.05338700	-4.06803200	4.80908100
C	-5.25706000	0.56541600	1.66555700
C	-5.25307500	-0.93068600	1.24748300
C	-6.34194700	-1.72642400	2.00881300
C	4.13635700	0.84939900	-1.23008700
C	4.26732500	0.77509000	-2.63836000
C	5.53728900	0.40638000	-3.13531500
C	6.60480500	0.12007500	-2.27110000
C	6.42800200	0.18490900	-0.87931900
C	5.18252800	0.54421200	-0.32521700
C	2.68933000	-0.26753200	-4.32607900
C	3.11387600	1.04283200	-3.60968200
C	3.47671700	2.14566200	-4.63712100
C	-0.54748600	1.95488800	4.43990200
C	0.34237500	3.01887400	3.74435400
C	1.15891100	3.82949500	4.78315900
C	-0.49461600	3.85605800	1.43098600
C	-0.51208800	3.92448700	2.85025800
C	-1.36381200	4.87910000	3.43973600
C	-2.15125700	5.73315900	2.65082600
C	-2.10336700	5.64285900	1.25329500
C	-1.28054900	4.69708700	0.60070900
C	5.26043200	-0.80737600	1.82728700
C	4.99912700	0.58474900	1.19563500
C	5.90209800	1.66727000	1.84343500
C	-2.72745800	4.42101800	-1.47517400
C	-1.29238300	4.63340800	-0.93139600
C	-0.65834700	5.91317000	-1.54054800
H	-1.29667200	-4.36501000	0.29873100
H	-3.16204900	-3.50474500	-0.72385700
H	3.26484900	3.15155600	-0.94077500
H	1.51437200	4.29162300	-0.02339000
H	3.39428900	-5.54435300	0.69815600
H	3.36716900	-5.93493300	3.14811800
H	1.66994100	-4.82546200	4.57935800
H	0.97903400	-3.24631300	-1.11626800
H	-2.23408500	-1.69267100	-2.83430700
H	3.95758200	-3.97648000	-0.96136900
H	3.23539700	-2.36268400	-0.70832200
H	3.12463500	-3.14331700	-2.29171700
H	2.28503800	-6.02771100	-1.41465200
H	1.50743800	-5.06339800	-2.68802300
H	0.53580300	-5.73130700	-1.36176400
H	-3.71557800	0.02588000	-4.89814000
H	-1.99193600	-0.41930600	-4.92307900

H	-2.60488700	0.59368700	-3.61273500
H	-3.49570900	-3.68138500	-3.77684900
H	-2.40605700	-2.91595900	-4.95178400
H	-4.15605400	-2.63920000	-5.05364500
H	-5.73199100	-1.11683100	-4.18352700
H	-7.72339300	-0.70296300	-2.76353000
H	-7.51317400	-0.62979100	-0.29243600
H	-1.09857600	-2.63176600	3.21037200
H	-4.27997100	-1.33897200	1.54628100
H	1.15153000	-2.33116600	5.27491300
H	-0.37067500	-1.41189500	5.24102900
H	0.80505600	-1.22634200	3.92012800
H	-0.35856900	-4.51114700	5.53399300
H	-1.54135300	-4.88792400	4.26615300
H	-1.82185000	-3.52877400	5.37837800
H	-4.43804900	1.10310300	1.17617500
H	-5.13124100	0.65768900	2.75264700
H	-6.20472300	1.04658100	1.38892500
H	-7.34372900	-1.31328400	1.83529800
H	-6.15199300	-1.67999000	3.08918200
H	-6.35564600	-2.78204200	1.70761600
H	5.68462200	0.33900200	-4.20974900
H	7.57219100	-0.16078100	-2.68112000
H	7.25931000	-0.04987400	-0.21948200
H	2.23185200	1.38713000	-3.06105200
H	1.05310800	2.47042400	3.11869800
H	3.52049000	-0.70554400	-4.89711200
H	1.86713500	-0.05555100	-5.02079900
H	2.32474800	-1.00612400	-3.60358200
H	3.77814300	3.07790500	-4.14021600
H	2.60268500	2.36452800	-5.26311000
H	4.29626200	1.83791200	-5.30113700
H	-1.30439000	2.42850500	5.08002600
H	0.06810900	1.29766400	5.06846300
H	-1.05530100	1.33972800	3.68959300
H	1.78263400	4.59162400	4.29791400
H	1.81807900	3.15564200	5.34638200
H	0.51054500	4.33733400	5.50881700
H	-1.40437700	4.96023800	4.52244300
H	-2.80048100	6.46530600	3.12539500
H	-2.72233000	6.30338900	0.65270500
H	3.95745900	0.83891300	1.41876700
H	-0.72592800	3.76452200	-1.27309600
H	6.29629200	-1.13457300	1.66708000
H	4.59154300	-1.56174400	1.39798200
H	5.08286700	-0.76977400	2.91015600
H	5.72758000	1.70944000	2.92671300
H	5.69873700	2.66199400	1.42553600
H	6.96599500	1.44848900	1.68347400
H	-3.15317000	3.49549400	-1.07378500
H	-2.68946600	4.31475300	-2.56593800
H	-3.39567700	5.25954800	-1.23314300

H	0.37429200	6.06631300	-1.19530000
H	-1.23092600	6.81303700	-1.27655000
H	-0.63889200	5.83208300	-2.63472200
O	-0.22817400	-1.50284400	-1.76908300
O	0.38484700	1.66763300	-1.99488400
O	2.07411400	0.14467100	-0.30263000
O	-0.04261800	-1.43373400	1.08241600
Zr	-0.17562800	0.04246300	-0.74121200

$\eta^2$ -Ozone ComplexFig. S116: ONCCNO  $\eta^2$ -Ozone Complex

SCF	E <sub>ZP</sub>	H	G
-2816.572522	-2815.414334	-2815.341422	-2815.530360

O	-1.64639400	1.25230300	0.14826600
O	1.64650300	-1.25210700	0.14882900
O	0.59949200	0.99542700	-2.11220100
N	-1.20847900	-2.87432300	0.62642000
N	1.97245600	-2.54850500	-0.18515200
N	1.20849300	2.87439700	0.62623200
N	-1.97248400	2.54874900	-0.18527200
C	-0.21147100	-3.75338500	0.32181500
C	1.13093800	-3.61016200	-0.05150100
C	0.21151500	3.75349300	0.32161200
C	-1.13091700	3.61035800	-0.05163700
C	-2.54440000	-3.33866800	0.96973900
C	-2.84893800	-3.55699900	2.33739700
C	-4.14608500	-4.01433000	2.64890300
C	-5.09433600	-4.23499300	1.63658100
C	-4.76952700	-3.98728300	0.29358600

C	-3.48787500	-3.52236400	-0.07187600
C	-2.26878400	-2.00326700	4.24897100
C	-1.84161400	-3.26614600	3.45320400
C	-1.64313000	-4.47848300	4.39759700
C	4.53523100	-1.07814300	2.26155700
C	4.07654300	-2.49786700	1.83305500
C	4.71619700	-3.58631500	2.73141600
C	3.34490600	-2.72878300	-0.63199200
C	4.37155100	-2.72295700	0.34796400
C	5.69682100	-2.90031400	-0.09796700
C	5.98104700	-3.07630300	-1.46252000
C	4.94590900	-3.06111900	-2.40956600
C	3.60206300	-2.87287500	-2.01909700
C	-4.12802700	-2.17254600	-2.12989700
C	-3.16096300	-3.23040000	-1.53900900
C	-3.17975900	-4.53067500	-2.38556800
C	2.77471000	-1.70699300	-4.12555400
C	2.49766900	-2.81765600	-3.07964300
C	2.31999800	-4.19514100	-3.77213000
C	2.54444300	3.33875300	0.96944500
C	3.48788000	3.52228200	-0.07224100
C	4.76954500	3.98725100	0.29308800
C	5.09442800	4.23514100	1.63603700
C	4.14623600	4.01460800	2.64843600
C	2.84907400	3.55722500	2.33705900
C	4.12744200	2.17179100	-2.12999800
C	3.16084100	3.23017600	-1.53932300
C	3.18018800	4.53027100	-2.38614700
C	-4.53492700	1.07798300	2.26136200
C	-4.07627000	2.49777800	1.83307000
C	-4.71562100	3.58609200	2.73181500
C	-3.34497200	2.72897800	-0.63200400
C	-4.37149500	2.72314700	0.34805700
C	-5.69682900	2.90034100	-0.09776200
C	-5.98120100	3.07628900	-1.46228800
C	-4.94616400	3.06114000	-2.40944500
C	-3.60227500	2.87296900	-2.01910300
C	2.26922700	2.00404700	4.24918700
C	1.84183400	3.26658000	3.45299200
C	1.64324100	4.47922400	4.39696400
C	-2.77540000	1.70654100	-4.12541700
C	-2.49804900	2.81743800	-3.07982100
C	-2.32036900	4.19472500	-3.77268000
H	-0.55718800	-4.78065000	0.35777900
H	1.62386100	-4.54610600	-0.29153000
H	0.55728700	4.78073700	0.35755000
H	-1.62381900	4.54633000	-0.29159200
H	-4.41667400	-4.19462200	3.68612800
H	-6.08893100	-4.59093400	1.89577500
H	-5.51808200	-4.14729400	-0.47785200
H	-0.87204100	-3.04209300	2.99475800
H	2.99179600	-2.53998100	1.97998000

H	-3.23598700	-2.15678300	4.74630000
H	-2.35818000	-1.13792100	3.58243100
H	-1.52274700	-1.77004200	5.02047900
H	-2.56591800	-4.72841300	4.93724600
H	-0.87334500	-4.25074000	5.14674100
H	-1.32614100	-5.37086300	3.84256700
H	5.61882400	-0.95542200	2.12911400
H	4.30113300	-0.90606800	3.32092600
H	4.02387400	-0.31385300	1.66644100
H	4.39407800	-4.59282000	2.43413500
H	4.42342600	-3.42863600	3.77796100
H	5.81278700	-3.55730100	2.68849400
H	6.50943300	-2.90181200	0.62383900
H	7.00962600	-3.21612500	-1.78738900
H	5.18202400	-3.18065300	-3.46358000
H	-2.15698200	-2.80105900	-1.60846500
H	1.54879800	-2.56111400	-2.59809600
H	-5.16487200	-2.53539000	-2.15626800
H	-3.82530600	-1.92946100	-3.15589400
H	-4.09982100	-1.24713800	-1.54311600
H	-4.17618300	-4.99332000	-2.39057900
H	-2.46685100	-5.27157500	-1.99971700
H	-2.90584400	-4.30489800	-3.42409000
H	2.86549000	-0.72910300	-3.64049400
H	1.93622500	-1.64568700	-4.82914300
H	3.69163700	-1.90559900	-4.69766800
H	3.23252400	-4.49631500	-4.30429200
H	1.50317600	-4.14450800	-4.50344300
H	2.07875000	-4.98415900	-3.04709700
H	5.51805900	4.14717700	-0.47840700
H	6.08904200	4.59110000	1.89512800
H	4.41687300	4.19504600	3.68562500
H	2.15666600	2.80127400	-1.60866000
H	-2.99148200	2.53982000	1.97977100
H	5.16444700	2.53418200	-2.15639400
H	3.82464900	1.92866100	-3.15596200
H	4.09880300	1.24649700	-1.54306000
H	2.46761200	5.27156800	-2.00044300
H	2.90615900	4.30439700	-3.42461800
H	4.17681300	4.99247900	-2.39127800
H	-5.61857300	0.95539500	2.12923100
H	-4.30051100	0.90560700	3.32061400
H	-4.02383300	0.31379400	1.66588600
H	-4.39365800	4.59264300	2.43452000
H	-4.42241500	3.42829900	3.77822000
H	-5.81222300	3.55703800	2.68936800
H	-6.50938800	2.90170900	0.62409400
H	-7.00982900	3.21597900	-1.78706100
H	-5.18240900	3.18055000	-3.46344500
H	0.87227100	3.04224400	2.99467000
H	-1.54911400	2.56090000	-2.59840100
H	3.23642300	2.15788000	4.74643100



H	2.35873400	1.13847900	3.58295200
H	1.52325900	1.77098300	5.02080700
H	0.87367300	4.25156700	5.14635800
H	1.32590400	5.37131100	3.84165900
H	2.56608300	4.72960100	4.93631900
H	-2.86600400	0.72874900	-3.64012700
H	-1.93714800	1.64511600	-4.82927100
H	-3.69252400	1.90502600	-4.69725200
H	-2.07887300	4.98390000	-3.04789900
H	-3.23296300	4.49588700	-4.30472900
H	-1.50371400	4.14380800	-4.50416200
O	-0.00007700	-0.00020300	-3.08345700
O	-0.59941300	-0.99583300	-2.11203500
O	1.05714900	1.51682600	0.62917100
O	-1.05711700	-1.51675800	0.62930800
Zr	-0.00005400	0.00001300	-0.36044500

## 9.5 Structures with eight oxygen atoms

## Bisperoxo Complex (spiro conformation 1 lower energy)

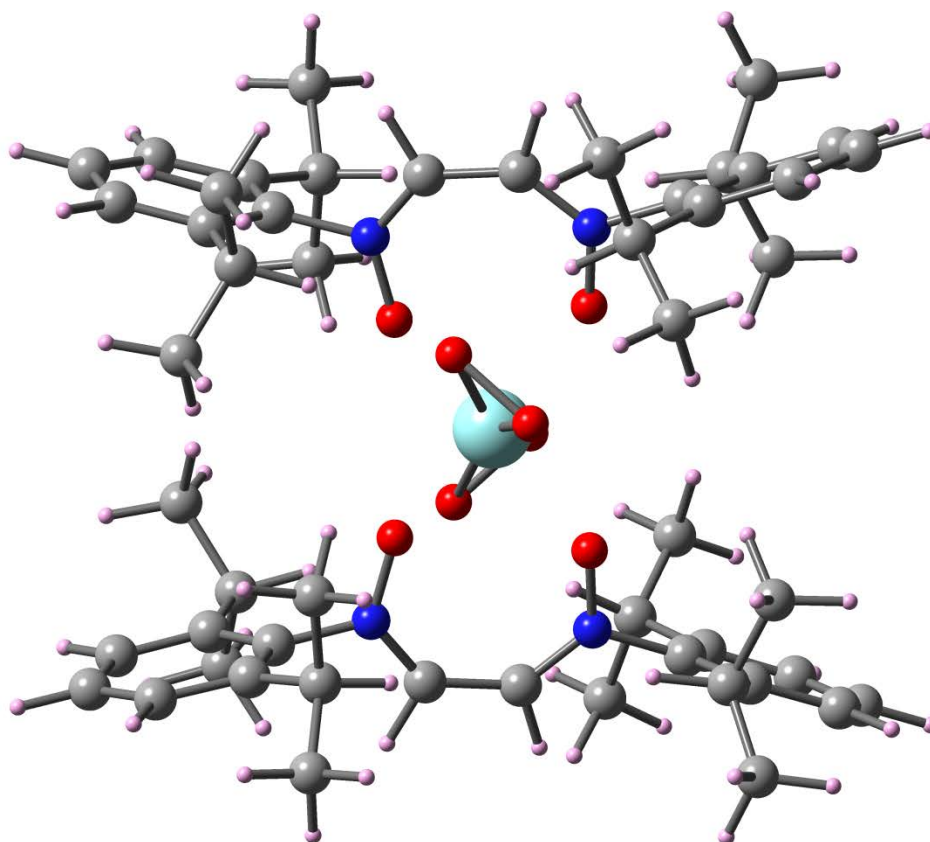


Fig. S117: ONCCNO Bisperoxo Complex (spiro conformation 1 lower energy)

SCF	$E_{ZP}$	H	G
-2891.748604	-2890.585775	-2890.512054	-2890.700079

Zr	0.16992393	0.00025500	0.00079131
O	1.56829367	-1.75966083	0.24401889
O	-1.25141065	1.57064065	-0.80326077
O	-0.39323615	-1.06186394	-1.73462631
O	0.70935252	-0.06631954	-2.04100788
N	1.59966246	2.89873723	0.46864678
N	-1.59637651	2.76395029	-0.30718657
N	-1.58758977	-2.76850635	0.30768113
N	1.60883571	-2.89350844	-0.46922517
C	0.56046668	3.70556830	0.68617001
C	-0.81776940	3.65241402	0.32227952
C	-0.80698308	-3.65373329	-0.32356332
C	0.57170904	-3.70305058	-0.68657683
C	2.93715939	3.28583760	0.94120702
C	3.22302044	3.20822815	2.32662271

C	4.52252576	3.59389119	2.72468694
C	5.48066390	4.00420324	1.78637821
C	5.16520009	4.03952681	0.41795493
C	3.88171752	3.68108040	-0.04058604
C	2.78749940	1.55823747	4.21647398
C	2.21397783	2.72764581	3.37684835
C	1.77591165	3.90033417	4.29522782
C	-4.33566331	1.04890911	2.17002853
C	-3.54279542	2.34597280	1.86527318
C	-3.74930182	3.39437042	2.99025039
C	-3.00547063	3.11415392	-0.55220325
C	-3.93307595	2.91916090	0.49768733
C	-5.27579876	3.26320454	0.22597041
C	-5.65914760	3.74591358	-1.03452853
C	-4.71081410	3.89000694	-2.06178243
C	-3.35391766	3.57328540	-1.84615562
C	4.22447923	2.47961562	-2.24012356
C	3.56413697	3.69797516	-1.53959990
C	3.98437095	5.02714704	-2.21598715
C	-2.42022293	2.40427272	-3.88612390
C	-2.33100224	3.66625843	-2.98273297
C	-2.47856129	4.96218184	-3.81686727
C	-2.99620704	-3.12167510	0.55130246
C	-3.92354015	-2.92961355	-0.49947170
C	-5.26562815	-3.27665783	-0.22844737
C	-5.64883235	-3.75952905	1.03201453
C	-4.70093570	-3.90078335	2.06005201
C	-3.34465815	-3.58091242	1.84528137
C	-4.33314121	-1.06544296	-2.17776196
C	-3.53370315	-2.35711139	-1.86745573
C	-3.73208322	-3.40941150	-2.99036673
C	4.22845811	-2.47230051	2.24208603
C	3.57208027	-3.69197901	1.54009334
C	3.99474466	-5.02042132	2.21636280
C	2.94746727	-3.27818120	-0.94080553
C	3.89145554	-3.67329081	0.04148777
C	5.17610721	-4.02880451	-0.41613587
C	5.49311486	-3.99040277	-1.78412939
C	4.53541080	-3.58006259	-2.72292151
C	3.23472070	-3.19760705	-2.32571789
C	-2.41668279	-2.40997715	3.88673135
C	-2.32243390	-3.67115722	2.98269224
C	-2.46648714	-4.96797233	3.81598578
C	2.79805558	-1.54629601	-4.21431741
C	2.22565292	-2.71704369	-3.37587804
C	1.78919477	-3.88937984	-4.29548874
H	0.82908851	4.60078539	1.23515210
H	-1.36986260	4.53831839	0.61595989
H	-1.35677918	-4.54027810	-0.61954854
H	0.84297953	-4.59765334	-1.23527595
H	4.78584391	3.55470950	3.77789760
H	6.47624966	4.28889214	2.11892564

H	5.92047761	4.34959720	-0.29873470
H	1.32721196	2.32547382	2.87916768
H	-2.48495132	2.06243014	1.86266189
H	3.67121755	1.85680846	4.79804916
H	3.05056239	0.71673362	3.56752702
H	2.02061950	1.20224421	4.91517403
H	2.62567001	4.30671463	4.86070681
H	1.02548871	3.55012993	5.01535825
H	1.33329959	4.72716732	3.72174736
H	-5.41633177	1.23469528	2.23668216
H	-4.00160764	0.63041137	3.12738649
H	-4.16076549	0.29194413	1.39683856
H	-3.16530030	4.30624441	2.80569332
H	-3.42778645	2.97679802	3.95264969
H	-4.80458162	3.68569486	3.08195603
H	-6.02365574	3.13953923	1.00458662
H	-6.69958326	4.00151858	-1.22156927
H	-5.02726855	4.25028092	-3.03629498
H	2.48301840	3.58589551	-1.67567435
H	-1.32330381	3.66877663	-2.54959289
H	5.31715866	2.50410692	-2.12793761
H	3.98893594	2.48708677	-3.31240497
H	3.84610928	1.54488564	-1.81410383
H	5.07327751	5.16507389	-2.20721006
H	3.53034989	5.89476790	-1.71924457
H	3.66283269	5.02619556	-3.26563561
H	-2.20010365	1.50092875	-3.30868519
H	-1.68597332	2.47280795	-4.69930013
H	-3.42050353	2.31295935	-4.33211799
H	-3.42213785	4.98238896	-4.37736083
H	-1.66390065	5.02460035	-4.54973145
H	-2.44032150	5.85911808	-3.18464903
H	-6.01321761	-3.15513406	-1.00764910
H	-6.68880037	-4.01751557	1.21838745
H	-5.01722387	-4.26138966	3.03450110
H	-2.47750264	-2.06754766	-1.86316836
H	2.49047362	-3.58278982	1.67483264
H	-5.41250185	-1.25750208	-2.24826702
H	-3.99783196	-0.64709306	-3.13473941
H	-4.16571952	-0.30579762	-1.40554237
H	-3.14385536	-4.31787769	-2.80246626
H	-3.41053901	-2.99254891	-3.95307319
H	-4.78568073	-3.70631342	-3.08357691
H	5.32134154	-2.49415779	2.13137287
H	3.99147105	-2.48080009	3.31403809
H	3.84848479	-1.53824360	1.81601154
H	3.54361378	-5.88893870	1.71855733
H	3.67177364	-5.02082220	3.26557043
H	5.08400745	-5.15555166	2.20902389
H	5.93115169	-4.33871622	0.30086701
H	6.48962568	-4.27264816	-2.11599279
H	4.80008784	-3.53835516	-3.77570135

H	-1.31433293	-3.66999626	2.55051317
H	1.33822944	-2.31639202	-2.87811992
H	-3.41747474	-2.32253895	4.33234797
H	-2.19956201	-1.50562954	3.30973854
H	-1.68251011	-2.47623935	4.70016585
H	-1.65254123	-5.02787003	4.54985709
H	-2.42424276	-5.86448875	3.18341022
H	-3.41070955	-4.99183777	4.37524806
H	3.06220313	-0.70570180	-3.56458048
H	2.03025922	-1.18935231	-4.91149201
H	3.68108023	-1.84388857	-4.79747890
H	1.34669527	-4.71689804	-3.72293635
H	2.63975189	-4.29471270	-4.86051828
H	1.03905929	-3.53923010	-5.01593782
O	-0.39320339	1.06062731	1.73706105
O	0.71461221	0.06991083	2.04080115
O	1.56132925	1.76572323	-0.24631170
O	-1.24399785	-1.57640442	0.80809571

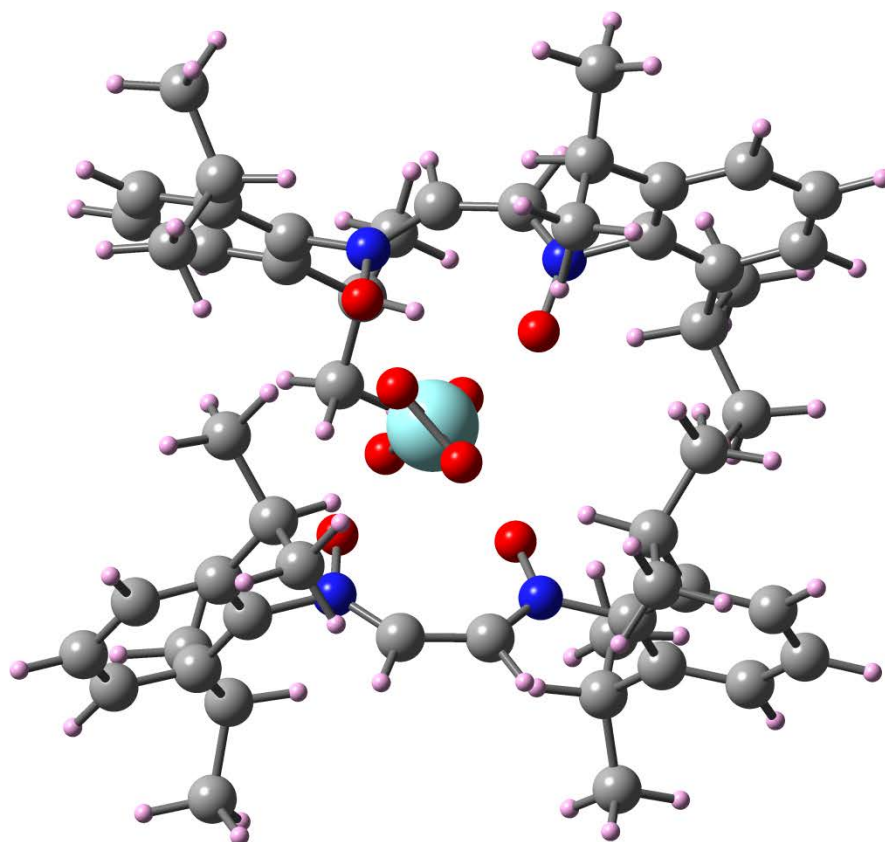
**Bisperoxo Complex (spiro conformation 2 higher energy)**

Fig. S118: ONCCNO Bisperoxo Complex (spiro conformation 2 higher energy)

SCF	$E_{ZP}$	H	G
-2891.746730	-2890.584397	-2890.512396	-2890.695242

O	2.23388100	-1.03105700	0.20168500
O	-1.76066700	0.85296300	-0.58922100
C	1.39346400	4.16171300	0.91836300
C	1.48953000	4.30288800	2.32947700
C	2.57334400	5.06785700	2.81493500
C	3.51121500	5.64371300	1.94792700
C	3.38616700	5.47625600	0.55935000
C	2.32344000	4.73554600	0.00725100
C	1.25644400	2.77990400	4.35824700
C	0.51486300	3.67935100	3.33706400
C	-0.30832100	4.78152900	4.05738000
C	-4.52649000	-0.64999200	1.94267700
C	-4.33778700	0.85790700	1.63505000
C	-5.07433200	1.73469000	2.68149700
C	-3.92587400	1.70299400	-0.77403200
C	-4.79882100	1.18846900	0.21099700

C	-6.13777600	0.97003800	-0.18014500
C	-6.55593400	1.23212200	-1.49410300
C	-5.64569600	1.70893700	-2.45299800
C	-4.29763000	1.95292100	-2.11780000
C	3.29024000	3.60211800	-2.04148200
C	2.21669300	4.59187600	-1.51598700
C	2.31863000	5.96031900	-2.23755600
C	-2.70583300	1.15033900	-3.91585300
C	-3.28042200	2.39238700	-3.17646000
C	-3.85998700	3.41552300	-4.18252800
C	-1.72857900	-3.72066000	0.65501900
C	-2.63108600	-3.90053400	-0.42220000
C	-3.82749500	-4.59544700	-0.13651200
C	-4.11041100	-5.05574900	1.15773400
C	-3.20116100	-4.83298700	2.20540900
C	-1.98352600	-4.16017500	1.97990200
C	-3.53901100	-2.48670400	-2.33575700
C	-2.37162400	-3.37679600	-1.83960200
C	-2.12620700	-4.55133500	-2.82499500
C	4.93915600	-1.28982300	2.45987900
C	4.63982100	-2.59114800	1.66590500
C	5.35622600	-3.80992200	2.29996000
C	4.02360300	-2.19094500	-0.81439900
C	5.00048800	-2.41009600	0.18808600
C	6.34715400	-2.41867600	-0.22829400
C	6.68819800	-2.21946400	-1.57675200
C	5.69048900	-1.99312500	-2.53652300
C	4.32439100	-1.96021300	-2.17780200
C	-1.51172100	-2.72187100	4.01335400
C	-1.01210400	-3.90334700	3.13714300
C	-0.76954400	-5.17032500	3.99527900
C	3.55109000	-0.36209200	-4.00103600
C	3.25470900	-1.67812700	-3.23904800
C	3.13356700	-2.87047000	-4.22532400
H	2.68700700	5.19582400	3.88759500
H	4.34030000	6.22021100	2.35163900
H	4.11739600	5.93100800	-0.10282100
H	-0.16922200	3.00458200	2.81450800
H	-3.26510800	1.06025300	1.72638900
H	2.00788000	3.33414800	4.93800400
H	1.73359200	1.94607100	3.83331800
H	0.53133900	2.35464900	5.06505900
H	0.33816800	5.44382000	4.64919400
H	-1.03232200	4.32019500	4.74154700
H	-0.86507300	5.41309500	3.34945600
H	-5.58363200	-0.94488900	1.89850300
H	-4.15339100	-0.87258800	2.94979600
H	-3.96506300	-1.26939400	1.23405500
H	-4.70406100	1.50760900	3.68926200
H	-6.15688000	1.54987200	2.66950300
H	-4.91458100	2.80511000	2.49493300
H	-6.85068300	0.58618600	0.54480000

H	-7.59142000	1.05638600	-1.77643400
H	-5.98542200	1.88852000	-3.46859800
H	1.24501400	4.15732000	-1.76837900
H	-2.43410100	2.87434100	-2.67105200
H	4.30417000	3.96118700	-1.81714000
H	3.19921000	3.48922900	-3.12981500
H	3.15515600	2.61732600	-1.58352200
H	3.30940300	6.41717500	-2.11712900
H	1.57123100	6.67176600	-1.86188500
H	2.14959200	5.82355600	-3.31380400
H	-2.17474300	0.48817100	-3.22502400
H	-1.99042100	1.47257900	-4.68343500
H	-3.51060900	0.58682900	-4.40860900
H	-4.62439300	2.96309600	-4.82737100
H	-3.05884800	3.78044300	-4.83754200
H	-4.30924600	4.27952700	-3.67526300
H	-4.54601800	-4.76275300	-0.93401700
H	-5.04143500	-5.58291900	1.35291300
H	-3.43669600	-5.18828400	3.20453900
H	-1.48237600	-2.73800100	-1.84401700
H	3.56042600	-2.76400400	1.74825500
H	-4.47881300	-3.04828200	-2.42656000
H	-3.29222300	-2.07796900	-3.32324100
H	-3.70223800	-1.64151500	-1.65738700
H	-1.27651000	-5.17542600	-2.51506000
H	-1.90715200	-4.15916700	-3.82620900
H	-3.00711500	-5.20374000	-2.89961900
H	6.00126600	-1.01884400	2.38864400
H	4.68996300	-1.42925000	3.52017500
H	4.33425800	-0.46101100	2.07829200
H	5.16279700	-4.73180500	1.73582900
H	5.00211100	-3.95637500	3.32857600
H	6.44317400	-3.66388100	2.34507400
H	7.13240100	-2.58204900	0.50450000
H	7.73364800	-2.23384500	-1.87641100
H	5.97018300	-1.82447400	-3.57283700
H	-0.04482800	-3.59541200	2.72443600
H	2.28297000	-1.53217600	-2.75819500
H	-2.50891800	-2.93200000	4.42530500
H	-1.55071900	-1.79990700	3.42514900
H	-0.82215500	-2.56032100	4.85214800
H	0.00105700	-4.96330200	4.74918600
H	-0.43125400	-6.01653600	3.38277900
H	-1.67514300	-5.48187600	4.53192000
H	3.61104100	0.48130200	-3.30474200
H	2.72920700	-0.15427400	-4.69624400
H	4.48668500	-0.41641000	-4.57564000
H	2.87681700	-3.80372000	-3.70466000
H	4.07208800	-3.03993900	-4.77103500
H	2.34414200	-2.66758300	-4.96000600
O	-0.39222200	1.04201300	1.81494100
O	1.03230100	0.58899300	1.89428400



O	0.10286100	-1.18264600	-1.65764300
O	0.68980400	0.17507900	-2.06003600
O	-0.40709700	-1.78697500	0.99236400
O	0.68149400	2.33189500	-0.42513600
N	0.30574600	3.36086400	0.34968700
N	-2.52234600	1.92911800	-0.39095300
N	2.61198000	-2.16438400	-0.39504900
N	-0.46705600	-3.00578000	0.41728600
Zr	0.27134800	0.12379700	-0.00716700
C	1.85944600	-3.25033200	-0.58683300
H	2.39806900	-4.04236000	-1.09472500
C	0.51810400	-3.60881500	-0.24828200
H	0.24572800	-4.60317600	-0.58409200
C	-0.96403400	3.73710700	0.50891700
H	-1.08155200	4.68346200	1.02276300
C	-2.18391500	3.13327000	0.09532300
H	-3.04904400	3.77824400	0.20553300

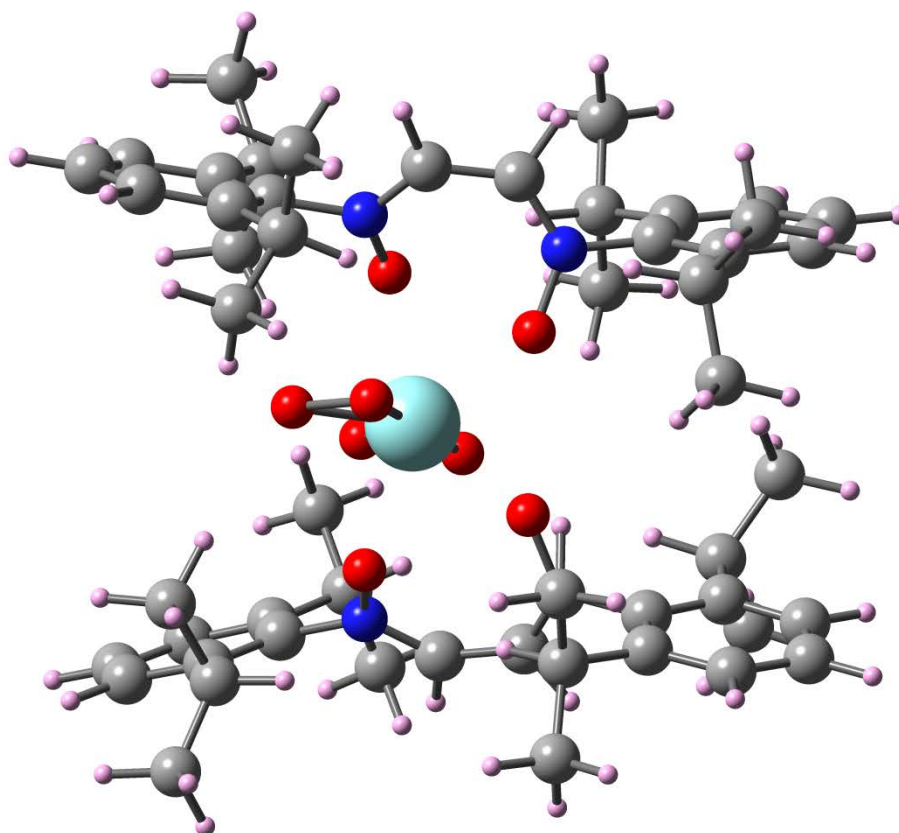
**Bisepoxo Complex (planar conformation)**

Fig. S119: ONCCNO Bisepoxo Complex (planar conformation)

SCF	$E_{ZP}$	H	G
-2891.73752862	-2890.575134	-2890.501691	-2890.687997

Zr	-0.58801700	0.01899400	-0.16971300
O	-1.64228500	0.50800000	1.55385600
O	-0.11716000	0.65742800	1.78887700
O	-0.91332300	-0.53064800	-2.15539100
O	-2.23744400	-0.24718800	-1.40146400
C	-2.58633400	3.49131600	0.75422700
C	-3.49221300	3.88273400	-0.27481600
C	-4.79330000	4.25037800	0.12361200
C	-5.17141200	4.25366100	1.47356500
C	-4.24986700	3.87939600	2.46143800
C	-2.93853800	3.47546300	2.13548200
C	-3.76032100	2.73751100	-2.52093600
C	-3.13651300	3.94346300	-1.76700300
C	-3.56076200	5.28892000	-2.41165100
C	2.42978800	1.96803600	-4.02961000
C	2.37202900	3.13213900	-3.00320200
C	2.43772400	4.50850800	-3.71427700
C	3.21961500	2.60941500	-0.61419900

C	3.48085600	2.97599300	-1.95698700
C	4.83286700	3.16651000	-2.31246300
C	5.85983000	2.99850100	-1.36854700
C	5.55925600	2.61990700	-0.05016600
C	4.22534800	2.40267200	0.35886000
C	-2.65868800	1.96718800	4.17881800
C	-2.00583700	3.04539700	3.27762000
C	-1.57679800	4.27525900	4.12577800
C	4.69068600	0.67256900	2.16764200
C	3.91959500	1.96349900	1.79602000
C	4.23789800	3.09898400	2.80697400
C	2.85989300	-2.93658000	0.66320700
C	2.86748100	-3.08127700	2.07160800
C	4.13036700	-3.23983400	2.68282000
C	5.30920300	-3.24295100	1.92118500
C	5.25894800	-3.07136400	0.52749600
C	4.02660400	-2.90718900	-0.13851700
C	1.57653500	-1.78021300	3.83556600
C	1.59578700	-3.03894800	2.92663500
C	1.43624100	-4.33605300	3.76249800
C	-2.71456900	-2.02547500	-4.28783400
C	-2.22516200	-3.12380100	-3.30961300
C	-1.98677300	-4.46179300	-4.06177700
C	-2.85218200	-3.29211800	-0.76993700
C	-3.20844100	-3.31541400	-2.14765800
C	-4.57406500	-3.50536800	-2.44547900
C	-5.53402200	-3.63724600	-1.43350200
C	-5.14778600	-3.59988600	-0.08512100
C	-3.79910100	-3.43639700	0.28605800
C	4.37594300	-1.19681700	-1.96796600
C	3.97823400	-2.66406400	-1.65012400
C	4.85655300	-3.66618800	-2.43955200
C	-3.84000700	-2.12338200	2.45961300
C	-3.43549600	-3.45846300	1.77741100
C	-4.06733900	-4.67301600	2.50756700
H	-5.51312000	4.54609000	-0.63373800
H	-6.18113300	4.54403500	1.75467200
H	-4.55778800	3.87464600	3.50286400
H	-2.05299900	3.85222300	-1.88013500
H	1.39869900	3.06061900	-2.50575000
H	-4.85516300	2.73465300	-2.41814100
H	-3.36298000	1.79148700	-2.13831100
H	-3.52052800	2.80262500	-3.59160000
H	-4.65163500	5.40368800	-2.45450100
H	-3.18959200	5.33076500	-3.44440300
H	-3.15110200	6.14952600	-1.86536500
H	3.38418900	1.96601600	-4.57446200
H	1.61703900	2.06921000	-4.76021900
H	2.30815900	1.00370000	-3.52440600
H	2.39663400	5.33674000	-2.99408100
H	1.58933700	4.61248600	-4.40309600
H	3.35784300	4.61877900	-4.30361900

H	5.08173100	3.44952700	-3.33212100
H	6.89507000	3.15714300	-1.66251100
H	6.36546500	2.48145000	0.66559500
H	-1.11799000	2.56368600	2.86165200
H	2.85212900	1.72885600	1.87910000
H	-3.57505500	2.32383600	4.66844000
H	-1.95077600	1.67327800	4.96570200
H	-2.87947100	1.08184900	3.57646700
H	-2.44194500	4.73556200	4.62185800
H	-1.09705900	5.05886300	3.52070300
H	-0.86691100	3.96607900	4.90435800
H	4.46717000	-0.13738800	1.46436200
H	4.39819800	0.33937000	3.17191600
H	5.77734200	0.83557200	2.17081800
H	5.30463600	3.36048900	2.78592000
H	3.98665000	2.77924000	3.82683600
H	3.66722100	4.01148500	2.58907600
H	4.18786800	-3.35628200	3.76165400
H	6.27013400	-3.36924600	2.41455400
H	6.18156700	-3.06352000	-0.04582400
H	0.72230600	-2.95623400	2.27174800
H	-1.27596400	-2.74969700	-2.91552800
H	2.46372900	-1.73776500	4.48271900
H	0.68671900	-1.80241700	4.47773400
H	1.51565700	-0.86544800	3.23602100
H	1.43191000	-5.23081200	3.12540900
H	0.48981600	-4.30726400	4.31734000
H	2.24700200	-4.44882900	4.49436000
H	-3.63825500	-2.31425600	-4.80892100
H	-1.94257500	-1.84382900	-5.04732400
H	-2.87387500	-1.09304100	-3.74002400
H	-1.59698800	-5.25242500	-3.40404100
H	-1.26470200	-4.31174200	-4.87549600
H	-2.91944600	-4.83683700	-4.50468400
H	-4.88918500	-3.51941000	-3.48448100
H	-6.58221400	-3.76501300	-1.69408600
H	-5.90091700	-3.70904600	0.68971200
H	2.94465300	-2.79087200	-1.99452800
H	-2.34938200	-3.54382700	1.88146000
H	5.39872500	-0.98213100	-1.62991300
H	3.69226300	-0.49491500	-1.47880100
H	4.33152200	-1.02089300	-3.05075400
H	4.72278500	-3.50900100	-3.51761700
H	4.59086500	-4.70666000	-2.20984700
H	5.92409600	-3.53500200	-2.21954100
H	-3.27199000	-1.28528400	2.04340000
H	-3.62914600	-2.17549600	3.53705800
H	-4.91379500	-1.92647300	2.33279100
H	-3.81321000	-5.62153500	2.01519000
H	-5.16135100	-4.60098900	2.55765300
H	-3.69642100	-4.71282200	3.54050100
O	-1.17406800	-2.15965500	0.52178500

N	-1.45564200	-3.11899000	-0.38199700
O	1.20520500	-1.51212500	-0.24382900
O	-1.11772200	2.23261900	-0.69127500
O	1.32778200	1.22222300	-0.62829000
N	1.55867200	-2.77293200	-0.00392400
N	1.81055300	2.40528800	-0.22959700
N	-1.24121500	3.09893000	0.33993700
C	1.20557400	3.38971300	0.45041500
H	1.90258100	4.16937400	0.74141300
C	-0.14050700	3.63936300	0.85079700
H	-0.28282600	4.43277100	1.57238700
C	-0.49487700	-3.96495100	-0.75875700
H	-0.80922000	-4.84379800	-1.30650000
C	0.86737900	-3.86575000	-0.35405800
H	1.43529100	-4.78829100	-0.30057700

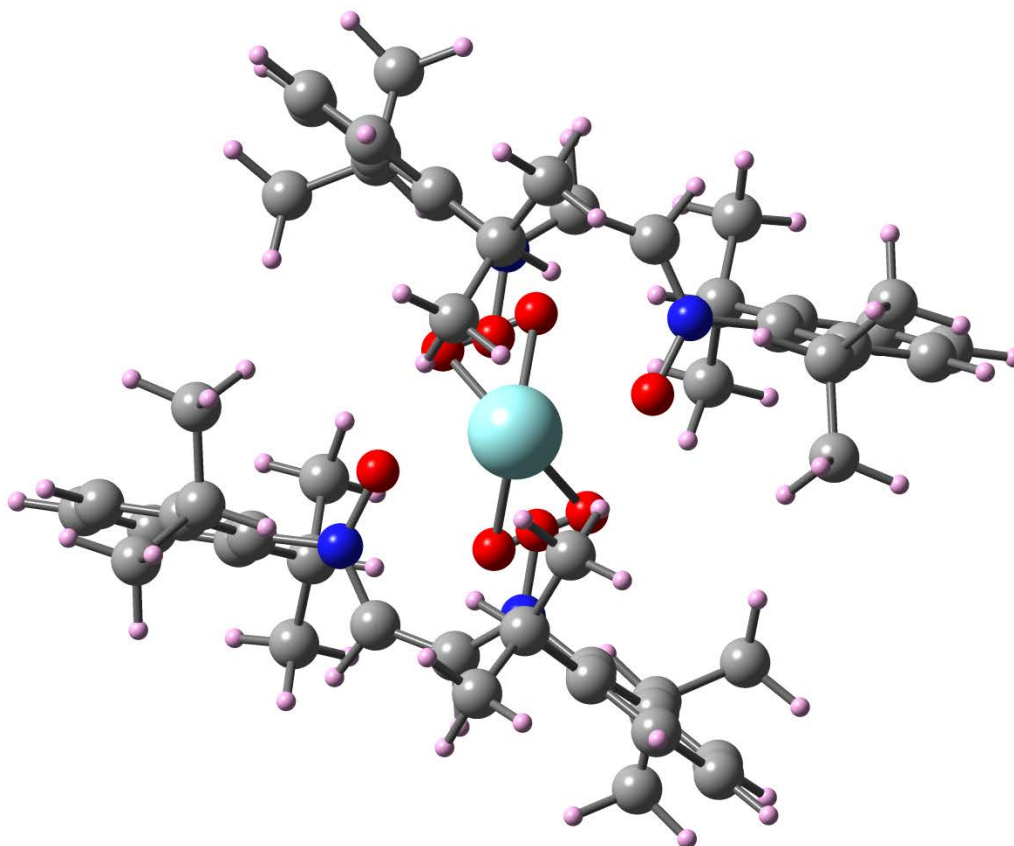
**Bisperoxo Complex (butterfly conformation)**

Fig. S120: ONCCNO Bisperoxo Complex (butterfly conformation)

SCF	$E_{ZP}$	H	G
-2891.759470	-2890.596997	-2890.523075	-2890.712818

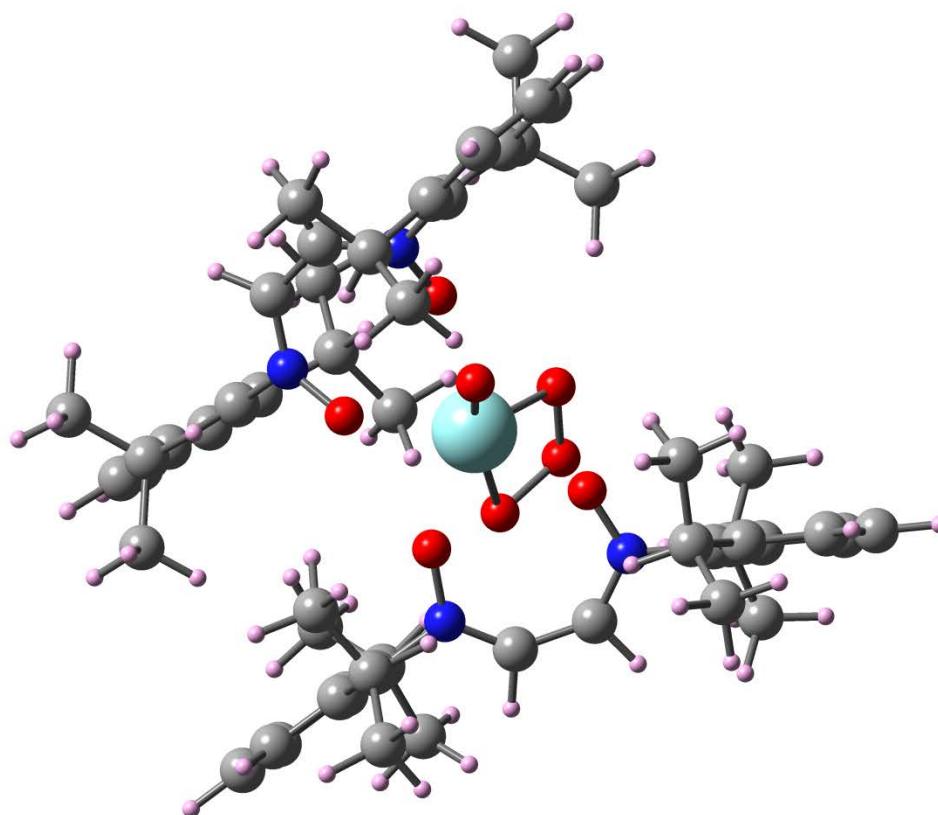
O	0.34006475	-1.49254076	0.89252217
O	2.10355225	0.58302413	-0.07733657
O	1.10193530	-1.22294366	-2.12909069
N	-0.12723569	2.79028429	0.86040473
N	2.67675706	1.74293972	-0.46147593
N	-2.67153045	-1.73522334	-0.50158753
N	0.12235991	-2.81562147	0.81136393
C	0.91366939	3.40022475	0.29965834
C	2.13576057	2.94516369	-0.30493171
C	-2.13582630	-2.94234399	-0.36931078
C	-0.92033182	-3.41157619	0.23814509
C	-1.18319513	3.60958565	1.48235141
C	-2.12461051	4.26059132	0.64865611
C	-3.10583772	5.04390102	1.29643581
C	-3.15069620	5.14796217	2.69440336
C	-2.21381557	4.46441585	3.48676338
C	-1.20504531	3.67590012	2.89728405

C	-3.48466370	3.61802080	-1.40184184
C	-2.12482605	4.14613872	-0.87925643
C	-1.77348947	5.50765786	-1.53671829
C	2.95667269	0.76256642	-4.37164848
C	3.12923194	1.98022258	-3.42376659
C	3.39363295	3.28141742	-4.22603962
C	4.03704744	1.60548699	-1.01007987
C	4.24447012	1.71995806	-2.40671712
C	5.57240640	1.55122426	-2.86093201
C	6.62017037	1.27129952	-1.97311880
C	6.36859935	1.14633251	-0.59654896
C	5.06754297	1.30694115	-0.08135331
C	-0.93200958	1.74304477	4.50278198
C	-0.21266350	2.91160345	3.77826289
C	0.50618522	3.84024294	4.78939083
C	4.87947473	-0.38371602	1.78993364
C	4.80632784	1.12161433	1.41737667
C	5.77214706	1.96196476	2.29040313
C	-4.02499758	-1.57562089	-1.06015283
C	-4.22405244	-1.67275781	-2.45955699
C	-5.54656038	-1.48295906	-2.92121209
C	-6.59738956	-1.19991351	-2.03815483
C	-6.35427992	-1.09299728	-0.65863881
C	-5.05913079	-1.27506011	-0.13577119
C	-2.91655770	-0.70980762	-4.40865085
C	-3.10579251	-1.93438195	-3.47291578
C	-3.37802334	-3.22579696	-4.28827906
C	0.85060959	-1.87459831	4.48964803
C	0.14967572	-3.02943835	3.72581207
C	-0.57906743	-3.98623555	4.70287056
C	1.16730631	-3.65258657	1.42951182
C	1.16044556	-3.76528519	2.84143363
C	2.16027099	-4.56962974	3.42492606
C	3.11621225	-5.22270693	2.62955945
C	3.10000847	-5.07175259	1.23519904
C	2.12842485	-4.27110322	0.59409273
C	-4.87182173	0.38875300	1.75977634
C	-4.80896608	-1.11193619	1.36750643
C	-5.79028037	-1.95504333	2.22052601
C	3.51777810	-3.51378783	-1.39407107
C	2.16121046	-4.10088589	-0.92796360
C	1.86657277	-5.44518410	-1.64497442
H	0.83115615	4.48109845	0.32905783
H	2.76098530	3.74893813	-0.67756784
H	-2.75881698	-3.73650252	-0.76547859
H	-0.84399435	-4.49326683	0.25517306
H	-3.84593967	5.56471984	0.69554217
H	-3.91888807	5.75524148	3.16749379
H	-2.26526095	4.54435777	4.56929610
H	-1.38067382	3.41235385	-1.19917632
H	2.16865995	2.09328909	-2.91217926
H	-4.31000379	4.31200751	-1.18837920

H	-3.71715635	2.64422754	-0.95694098
H	-3.42398937	3.47541736	-2.48697447
H	-2.51890286	6.27830552	-1.29584018
H	-1.74149376	5.39397773	-2.62741078
H	-0.79224284	5.87864916	-1.20872561
H	3.88166734	0.53601363	-4.92095150
H	2.16841435	0.98050788	-5.10367180
H	2.64363276	-0.12518908	-3.81057165
H	3.50411563	4.15276616	-3.56506811
H	2.55026473	3.47398418	-4.90094120
H	4.30326364	3.20826378	-4.83778295
H	5.77693643	1.63002088	-3.92496440
H	7.63128538	1.14242398	-2.35225275
H	7.18735482	0.92011026	0.08103468
H	0.55428474	2.45918886	3.14025916
H	3.78623718	1.45110349	1.64418189
H	-1.72740972	2.11520995	5.16255108
H	-0.21623631	1.17982799	5.11536232
H	-1.37593421	1.05814014	3.77167148
H	-0.19558704	4.27464744	5.51307151
H	1.01871966	4.66735983	4.28098856
H	1.25485968	3.27116853	5.35620511
H	4.13571612	-0.95322281	1.22317721
H	4.67671801	-0.52153742	2.86048299
H	5.87498175	-0.79501198	1.57534985
H	6.81248661	1.62960787	2.18247785
H	5.50315213	1.85963338	3.35004338
H	5.73046472	3.02704757	2.02722601
H	-5.74427185	-1.54733994	-3.98751018
H	-7.60401703	-1.05456855	-2.42323225
H	-7.17520449	-0.86468879	0.01558109
H	-2.14900913	-2.06000200	-2.95735637
H	-0.61057879	-2.56626518	3.08713676
H	-3.83500458	-0.47171803	-4.96401374
H	-2.12354246	-0.92712348	-5.13573444
H	-2.60250877	0.17075076	-3.83679168
H	-3.49859999	-4.10239010	-3.63598669
H	-2.53372961	-3.41936111	-4.96178131
H	-4.28464548	-3.13935246	-4.90273306
H	1.63922949	-2.25817102	5.15091749
H	0.12247588	-1.33165066	5.10603336
H	1.30022624	-1.16845075	3.78258747
H	-1.07722864	-4.80467529	4.16703787
H	-1.34052721	-3.43532744	5.27057451
H	0.11409944	-4.43231059	5.42766082
H	2.19008194	-4.68569376	4.50496311
H	3.87712057	-5.84264706	3.09798447
H	3.85444298	-5.56947873	0.63241892
H	-3.79396552	-1.45345367	1.59873486
H	1.40358389	-3.37767798	-1.24022033
H	-5.86106555	0.81254277	1.54047199
H	-4.11659827	0.95865151	1.20881749



H	-4.67924762	0.51003005	2.83424426
H	-5.52862778	-1.87108370	3.28363286
H	-5.75741122	-3.01656702	1.94207731
H	-6.82629586	-1.61039475	2.10951273
H	3.70828638	-2.54949505	-0.91018935
H	3.48205192	-3.33461440	-2.47488508
H	4.35776240	-4.19020209	-1.18085081
H	0.88981239	-5.85626518	-1.35414173
H	2.62932174	-6.20269969	-1.41716918
H	1.85581538	-5.28919181	-2.73076962
O	0.32398684	1.81399153	-1.91065716
O	-1.10226844	1.26155875	-2.09863974
O	-0.32150500	-1.78280281	-1.94145781
O	-2.09523101	-0.59022694	-0.07642511
O	-0.32838158	1.46266014	0.92707398
Zr	0.00169302	0.00592038	-0.87355651

Oxo  $\eta^2$ -Ozone ComplexFig. S121: ONCCNO Oxo  $\eta^2$ -Ozone Complex

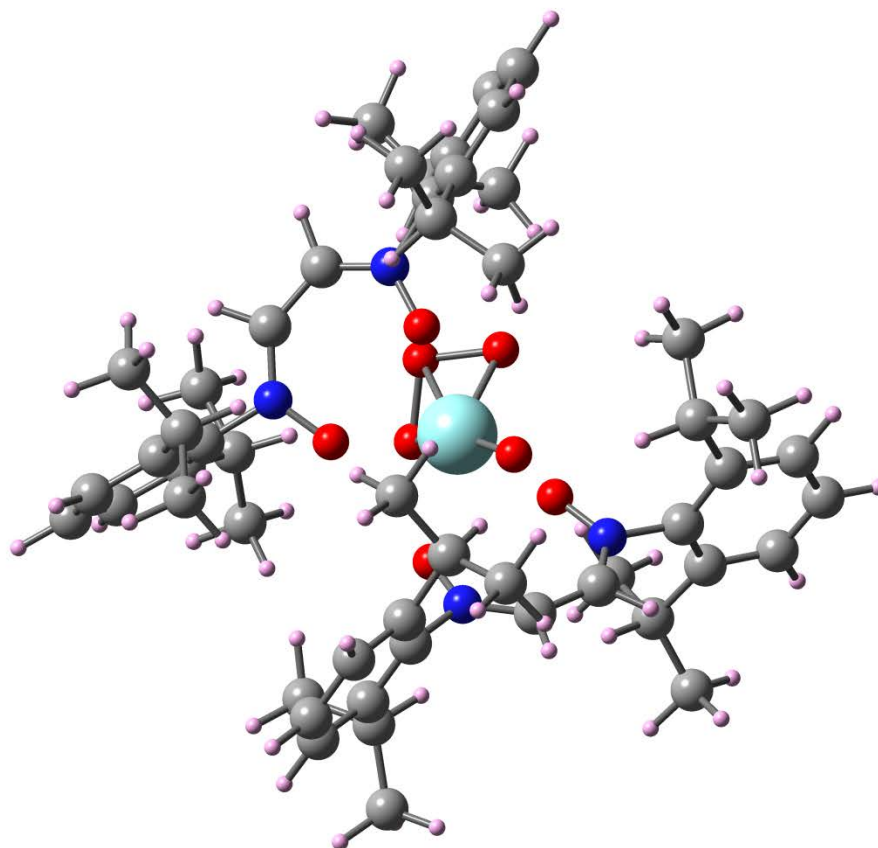
SCF	E <sub>ZP</sub>	H	G
-2891.736357	-2890.573469	-2890.499783	-2890.686288

O	2.46465654	-0.56444541	0.30389399
O	-1.86067275	0.57151686	0.00638743
O	0.39461468	-1.22143547	-1.70800310
N	-0.83275332	3.47306155	0.21007174
N	-2.92683231	1.31053890	-0.29537655
N	0.04876377	-2.80343640	0.65175602
N	3.02994130	-1.67381867	-0.17820233
C	-2.13582895	3.53895181	0.48793845
C	-3.10015443	2.59950544	0.01421303
C	1.11021242	-3.32152956	0.02496918
C	2.40929325	-2.85454587	-0.31720258
C	0.13456185	4.42038498	0.75684605
C	0.27117476	4.55304349	2.16682155
C	1.23042828	5.47977117	2.62451243
C	2.02279746	6.21507513	1.73201110
C	1.86483665	6.05251749	0.34773401
C	0.91381043	5.15708494	-0.17991924

C	0.40558617	3.02851681	4.20483033
C	-0.52843662	3.75447899	3.20440908
C	-1.54253989	4.67049449	3.94305924
C	-4.92593387	-1.52429384	1.84989963
C	-4.96877606	-0.07316473	1.30673723
C	-6.17418021	0.70566970	1.89760144
C	-4.00695297	0.59901420	-0.99931820
C	-4.99403877	-0.05404198	-0.22458654
C	-6.03339260	-0.69596869	-0.92979333
C	-6.06117986	-0.69231333	-2.33405760
C	-5.04490427	-0.05763760	-3.06551650
C	-3.98231306	0.60531210	-2.41449861
C	1.96201112	4.31896663	-2.33726697
C	0.75318754	5.05877253	-1.70293132
C	0.55150381	6.45647939	-2.34596466
C	-2.05917619	0.19669446	-4.02387435
C	-2.86318953	1.26164369	-3.22988534
C	-3.42288628	2.35802032	-4.17356022
C	-1.09860829	-3.65761101	0.96350015
C	-1.89653732	-4.16804449	-0.09311600
C	-2.97477015	-5.00624334	0.26857643
C	-3.25346930	-5.29877118	1.61137739
C	-2.45251117	-4.76164236	2.63234963
C	-1.35143548	-3.93415468	2.33349844
C	-2.91714665	-3.30029759	-2.25913318
C	-1.64525988	-3.86057538	-1.57501167
C	-1.14708812	-5.12578670	-2.32605516
C	4.70497230	0.27085388	2.56187881
C	4.76378017	-1.21672433	2.11943248
C	5.58069014	-2.06789817	3.12424622
C	4.47167735	-1.55485575	-0.43816460
C	5.30568705	-1.32782260	0.68971437
C	6.68615867	-1.18353829	0.44706567
C	7.20732978	-1.26861925	-0.85432961
C	6.35333999	-1.49218814	-1.94280992
C	4.95853646	-1.63164178	-1.76640157
C	-1.25247959	-2.23496609	4.20737103
C	-0.49045885	-3.36644014	3.46692050
C	-0.02472742	-4.46548956	4.45537019
C	4.17625878	-0.60387306	-3.94957821
C	4.06593305	-1.82252904	-2.99693818
C	4.40177206	-3.14397334	-3.73696125
H	-2.48152854	4.41623321	1.01924128
H	-4.11603842	2.95519855	-0.11839856
H	0.96280391	-4.36531012	-0.23013775
H	3.04762591	-3.61791777	-0.74701271
H	1.37499307	5.60531065	3.69344811
H	2.76535957	6.91129464	2.11477323
H	2.48117698	6.63240140	-0.33281290
H	-1.07849305	2.95938791	2.69372575
H	-4.05186016	0.41903945	1.65080520
H	1.01158810	3.73028710	4.79341121

H	1.05186162	2.34670458	3.64343036
H	-0.19740522	2.43783381	4.90880207
H	-1.02644699	5.46180121	4.50256901
H	-2.12985010	4.08180425	4.66027381
H	-2.24242723	5.16255644	3.25187935
H	-5.82956654	-2.08437540	1.57522338
H	-4.85779437	-1.51342737	2.94544890
H	-4.05739739	-2.06609047	1.46040468
H	-6.19664754	1.74558734	1.54517326
H	-6.11705187	0.71875042	2.99376080
H	-7.12648997	0.23772759	1.61624084
H	-6.81846801	-1.20528165	-0.37748115
H	-6.87097345	-1.19365700	-2.85882422
H	-5.07028261	-0.07999741	-4.15144594
H	-0.13283641	4.45989676	-1.93424991
H	-2.15211792	1.74292315	-2.55006177
H	2.90755254	4.81991343	-2.08689619
H	1.86122242	4.31065358	-3.43122103
H	2.00631284	3.27936266	-1.99859087
H	1.44636175	7.08490542	-2.25284247
H	-0.28913962	6.99646572	-1.88942114
H	0.34287812	6.34122554	-3.41775286
H	-1.57361108	-0.51637405	-3.34928863
H	-1.26603403	0.68787681	-4.60053715
H	-2.70571659	-0.35086166	-4.72394901
H	-4.09702711	1.93521528	-4.93036676
H	-2.59607417	2.84912662	-4.70200874
H	-3.97899842	3.12632152	-3.61919131
H	-3.60653107	-5.42208810	-0.51135727
H	-4.09327488	-5.94243449	1.86295818
H	-2.67721777	-4.99526227	3.66938724
H	-0.87728472	-3.08533069	-1.66867173
H	3.73322093	-1.58727006	2.13839108
H	-3.73190894	-4.03660956	-2.28162023
H	-2.68607079	-3.02298626	-3.29503650
H	-3.27783917	-2.40394995	-1.74357479
H	-0.22662287	-5.53236060	-1.88528804
H	-0.93635776	-4.88008587	-3.37472646
H	-1.90220865	-5.92358356	-2.30832564
H	5.70244584	0.73131752	2.52901217
H	4.32754615	0.34271534	3.59058563
H	4.02724973	0.83524194	1.91440635
H	5.64393365	-3.11781451	2.80847145
H	5.10046069	-2.03482558	4.11100107
H	6.60372047	-1.68930347	3.24667204
H	7.35754765	-1.00688498	1.28250582
H	8.27650421	-1.15538001	-1.01823635
H	6.76583895	-1.54304373	-2.94671630
H	0.40369720	-2.90680532	3.03470286
H	3.01958268	-1.85896611	-2.68593106
H	-2.17830986	-2.61272753	4.66376339
H	-1.50154414	-1.42911200	3.50930556

H	-0.62456379	-1.81537183	5.00410723
H	0.64808088	-4.02847768	5.20488934
H	0.51604734	-5.26898196	3.93828605
H	-0.86691855	-4.91845585	4.99449963
H	3.86437267	0.31119488	-3.43507853
H	3.50859589	-0.74522453	-4.80890136
H	5.19915985	-0.47002199	-4.32766605
H	4.29785601	-4.01798999	-3.07848825
H	5.42937609	-3.14146030	-4.12455635
H	3.72237058	-3.27766010	-4.58867049
O	0.86143507	1.37339376	1.57112130
O	1.24865071	-0.35594304	-2.53003857
O	1.37061040	0.93174139	-1.79376637
O	-0.05111567	-1.52230997	1.10581837
O	-0.39101104	2.56877906	-0.67288326
Zr	0.43913559	0.38970684	0.08699361

Oxo  $\eta^3$ -Ozone ComplexFig. S122: ONCCNO Oxo  $\eta^3$ -Ozone Complex

SCF	E <sub>ZP</sub>	H	G
-2891.730615	-2890.567393	-2890.493900	-2890.679936

O	-1.87336349	-0.05745758	-0.23512442
O	2.45879356	-0.79145552	-0.81325733
O	1.39362536	1.78550969	-1.27965279
N	0.48308242	-2.82061211	0.92233513
N	3.28936996	-1.45448948	-0.01315535
N	-1.06581102	3.15615618	0.09896784
N	-2.85169558	0.62659888	-0.83080683
C	1.72692019	-2.89712791	1.37685403
C	2.96627503	-2.32613642	0.94025346
C	-2.14537012	3.07232069	-0.67271692
C	-2.94908082	1.94570176	-1.03171562
C	-0.58371080	-3.57677364	1.59610476
C	-1.01754192	-3.16046144	2.87990737
C	-2.04225092	-3.92630403	3.47953476
C	-2.61098651	-5.02723418	2.82227270
C	-2.16726561	-5.39475086	1.54125755
C	-1.13958236	-4.67753936	0.89627750

C	-1.56273807	-0.94012577	3.99856049
C	-0.44457539	-1.94382471	3.61789272
C	0.34561627	-2.38338309	4.87882784
C	4.24024637	2.18958257	0.93974870
C	4.44853499	0.76095471	1.51365226
C	5.10099552	0.81359195	2.91762521
C	4.71215553	-1.13109123	-0.22970683
C	5.27035904	-0.07825539	0.53000263
C	6.63162584	0.21562484	0.29443209
C	7.37058393	-0.49413440	-0.66433532
C	6.76348708	-1.50599291	-1.42784550
C	5.40889079	-1.84537182	-1.23382400
C	-1.76899890	-4.70400200	-1.55095464
C	-0.68323629	-5.08152100	-0.50882136
C	-0.31821285	-6.58489325	-0.59639645
C	4.23982946	-2.16927328	-3.44502164
C	4.71041398	-2.86685741	-2.13673848
C	5.58466665	-4.10496704	-2.44683809
C	-0.40975596	4.44633780	0.34840515
C	0.13335449	5.18556303	-0.73687390
C	0.76744346	6.40579379	-0.41498777
C	0.87113165	6.85144131	0.90896026
C	0.33061765	6.08780446	1.95554905
C	-0.32822449	4.86839655	1.70544805
C	1.51910314	4.67782196	-2.81530388
C	0.09504471	4.74677046	-2.20717828
C	-0.82077626	5.68800602	-3.03674269
C	-5.04261564	-1.20785291	2.11427340
C	-4.94548347	-0.02097806	1.12134032
C	-6.05756383	1.02491986	1.40158958
C	-3.98809151	-0.21210336	-1.27917052
C	-4.99727282	-0.50476383	-0.33152539
C	-6.09086723	-1.27354116	-0.78197574
C	-6.15418472	-1.73077610	-2.10788577
C	-5.11873532	-1.43919429	-3.00952748
C	-3.99750832	-0.67594711	-2.61642898
C	0.20975294	3.33713610	3.65408209
C	-0.91616867	4.07675494	2.88125182
C	-1.74941064	4.97490606	3.83147133
C	-2.40776751	-1.61916171	-4.38049406
C	-2.87838246	-0.35999004	-3.61205383
C	-3.32433527	0.74508765	-4.60759578
H	1.83096558	-3.55122081	2.23546435
H	3.82871148	-2.68285077	1.49251130
H	-2.49138568	4.01899172	-1.06843526
H	-3.84400745	2.21062578	-1.58255670
H	-2.40301027	-3.64590702	4.46546793
H	-3.40228483	-5.59633977	3.30483061
H	-2.61982901	-6.24597559	1.04013655
H	0.23544498	-1.38988391	2.95907788
H	3.44733234	0.32950696	1.62976401
H	-2.28431298	-1.36677096	4.70972082

H	-2.10600913	-0.61189012	3.10491147
H	-1.11220034	-0.05230664	4.45977369
H	-0.29967507	-2.89866419	5.60400315
H	0.77759327	-1.50367552	5.37285721
H	1.17013018	-3.06471567	4.62631237
H	5.19896481	2.70523294	0.78620190
H	3.63780839	2.78357140	1.63881193
H	3.70523230	2.15479867	-0.01656448
H	5.24956729	-0.19260246	3.33296086
H	4.45052820	1.37041290	3.60399163
H	6.07673418	1.31831486	2.89946325
H	7.10730994	1.01330750	0.85831643
H	8.41716825	-0.24895322	-0.83009832
H	7.34340152	-2.02723448	-2.18374720
H	0.21196433	-4.50716298	-0.76931385
H	3.80650268	-3.22522723	-1.62768160
H	-2.70603944	-5.24584638	-1.36297090
H	-1.42635538	-4.95556415	-2.56340149
H	-1.97321229	-3.62903799	-1.51215725
H	-1.18947139	-7.22865240	-0.41911043
H	0.45432750	-6.85513608	0.13550660
H	0.06431439	-6.81752417	-1.59882276
H	3.55683465	-1.34278398	-3.22193096
H	3.71289318	-2.88700800	-4.08787541
H	5.09879342	-1.77426328	-4.00452798
H	6.45485169	-3.84561527	-3.06330698
H	4.99721952	-4.84174510	-3.00994139
H	5.94947128	-4.58571622	-1.52952973
H	1.20197273	6.99933333	-1.21403157
H	1.37591586	7.78956753	1.12715039
H	0.41603829	6.44561649	2.97720262
H	-0.29696453	3.73033022	-2.27982167
H	-3.97852156	0.46258760	1.30000616
H	2.03011286	5.64965416	-2.79019688
H	1.45302094	4.35601532	-3.86265581
H	2.11283076	3.93265621	-2.27752005
H	-1.84656895	5.72672782	-2.64111495
H	-0.87081195	5.33863796	-4.07593479
H	-0.43466083	6.71595484	-3.04570403
H	-6.00812354	-1.72357747	2.03117412
H	-4.94551679	-0.84383166	3.14532275
H	-4.24720188	-1.93970404	1.93422721
H	-5.97522914	1.89004382	0.73061306
H	-5.98740535	1.38722819	2.43556927
H	-7.05562149	0.58875354	1.26425987
H	-6.89213520	-1.51793265	-0.08974132
H	-7.00706630	-2.32024124	-2.43620769
H	-5.17240422	-1.81293922	-4.02795173
H	-1.58553376	3.30323147	2.49169858
H	-1.99407703	-0.00233381	-3.07353576
H	0.95398427	4.04786580	4.03991997
H	0.70745194	2.61117088	3.00359055



H	-0.21682338	2.79526444	4.50952300
H	-2.23193993	4.35169447	4.59586656
H	-2.53292184	5.52157030	3.28995630
H	-1.12634123	5.70963746	4.35687766
H	-2.11067441	-2.41249958	-3.68549260
H	-1.52922328	-1.36098058	-4.98316238
H	-3.18115954	-2.01465035	-5.05419757
H	-3.60954084	1.67159682	-4.09073085
H	-4.18382517	0.41920309	-5.21027154
H	-2.49772582	0.98390280	-5.28804746
O	1.11542899	-0.06951203	1.52072478
O	0.12887740	1.52041781	-2.14681443
O	0.13106415	0.03466819	-2.44468688
O	-0.56302338	2.11408335	0.77633423
O	0.09244817	-2.09651170	-0.14549181
Zr	0.43917169	0.22158312	-0.18974709

## Reactant for Ligand Cyclization Reaction

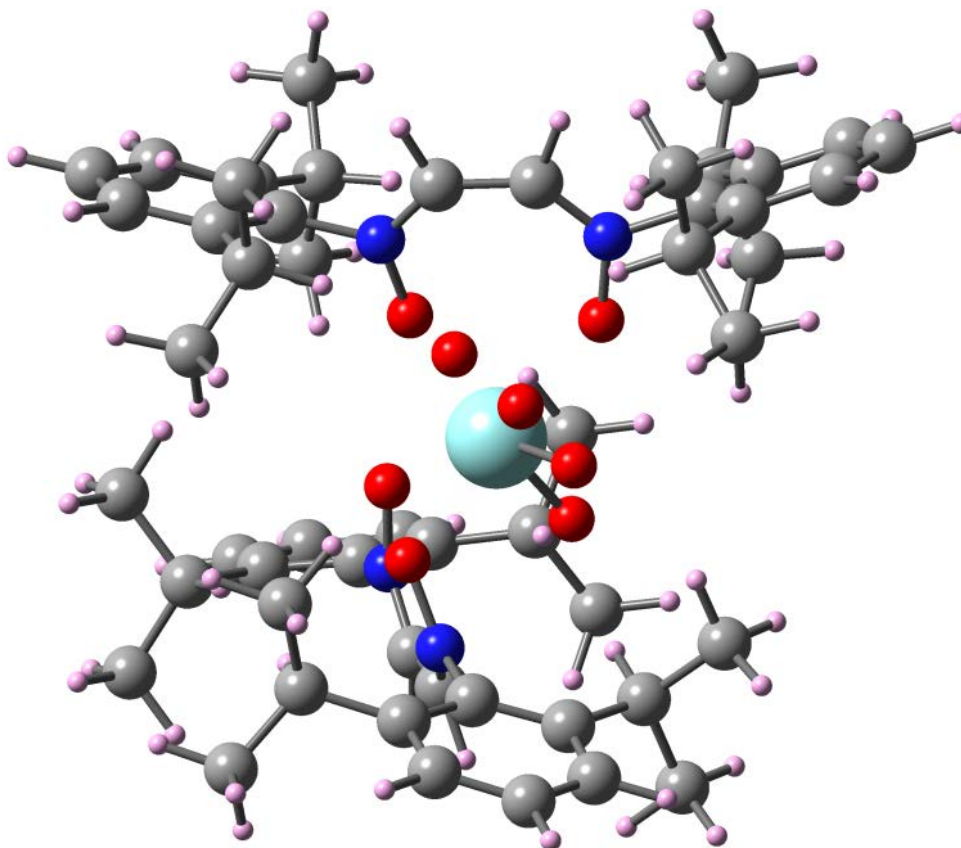


Fig. S123: ONCCNO Reactant for Ligand Cyclization Reaction

SCF	E <sub>ZP</sub>	H	G
-2891.7463375	-2890.582690	-2890.509270	-2890.695305

O	-2.31558100	-0.18441300	-0.80139100
O	1.77393200	-0.73950600	-0.56116300
O	-1.28015500	0.73415800	1.88943000
N	2.14201800	2.55310300	-0.17194100
N	2.76668600	-0.38932700	-1.37613500
N	-1.07697700	-2.06108600	1.66932700
N	-3.38684500	-0.52702500	-0.07192200
C	2.89218900	2.14940300	-1.18706000
C	3.20834700	0.83709300	-1.66519700
C	-2.36430600	-1.79771000	1.88559300
C	-3.37726100	-1.16126700	1.10775400
C	1.98530500	3.98398400	0.11977900
C	1.31139700	4.80910100	-0.81716300
C	1.21827200	6.18089400	-0.49366600
C	1.74141400	6.68817000	0.70328500
C	2.37295900	5.83145800	1.61962800

C	2.51060700	4.45582500	1.35134100
C	-0.84527200	4.65596700	-2.14827800
C	0.66411500	4.30065500	-2.11169700
C	1.39863300	4.86259800	-3.35820800
C	0.49618800	-2.22870400	-4.14345400
C	1.66835100	-1.23080300	-3.95551900
C	2.05528100	-0.57420500	-5.30621200
C	3.40494700	-1.53068400	-2.06155200
C	2.87252500	-1.92555100	-3.31074400
C	3.50173700	-3.01745500	-3.94721900
C	4.58573500	-3.67927300	-3.34865400
C	5.06387200	-3.27157300	-2.09247700
C	4.47793200	-2.18339100	-1.41227300
C	2.20443100	3.27584400	3.56075000
C	3.17961100	3.53999600	2.38152600
C	4.53058000	4.10525300	2.88741700
C	4.71283500	-2.90151400	1.00924400
C	4.98198400	-1.77578200	-0.02433500
C	6.48358900	-1.39021800	-0.05065700
C	-0.32114100	-2.91797400	2.58798200
C	0.02287300	-2.44021400	3.87779400
C	0.75542600	-3.31755200	4.70878900
C	1.14053700	-4.59089200	4.26738800
C	0.79597000	-5.02457700	2.97649400
C	0.05347700	-4.20116900	2.10713700
C	0.91371100	-0.25719500	4.83379000
C	-0.34678900	-1.04655800	4.39697700
C	-1.36361900	-1.14143500	5.56622800
C	-3.59543500	-1.55536500	-3.70776100
C	-4.28375600	-2.03090000	-2.39952600
C	-5.12664500	-3.30793000	-2.64102000
C	-4.67204700	-0.14203000	-0.67462300
C	-5.10894000	-0.88952000	-1.79768300
C	-6.33509800	-0.51468100	-2.38204700
C	-7.08389100	0.55558500	-1.86509500
C	-6.61248800	1.28102400	-0.76188600
C	-5.38479000	0.95926700	-0.14089000
C	0.94926000	-4.64008500	-0.21903000
C	-0.30039300	-4.69529100	0.70015600
C	-0.92234900	-6.11453600	0.71489400
C	-4.65724600	3.27880500	0.58458700
C	-4.88423500	1.81059500	1.02934300
C	-5.85743000	1.73726800	2.23537200
H	3.37621300	2.95276700	-1.72954100
H	3.97944800	0.82893200	-2.42766000
H	-2.73425900	-2.21434100	2.81605000
H	-4.36829700	-1.24502000	1.53991000
H	0.70898700	6.84959800	-1.18160800
H	1.64779500	7.74787900	0.92906000
H	2.76324800	6.23492200	2.54952400
H	0.70131700	3.20674200	-2.14905600
H	1.29345800	-0.43700800	-3.29826300

H	-1.01687300	5.74158700	-2.15622000
H	-1.35141800	4.21409300	-1.28377500
H	-1.29492500	4.23340600	-3.05611700
H	1.33182400	5.95821100	-3.40630900
H	0.94393000	4.45625400	-4.27062700
H	2.46608900	4.59684000	-3.36521500
H	0.75529300	-3.03960100	-4.83861500
H	-0.37589900	-1.69835700	-4.54436100
H	0.20738400	-2.67398300	-3.18367500
H	2.86799000	0.15422500	-5.18206400
H	1.18916000	-0.04335100	-5.72039400
H	2.38175100	-1.32038000	-6.04384200
H	3.13407500	-3.35337000	-4.91310800
H	5.05373900	-4.51889200	-3.85727900
H	5.89329100	-3.80478900	-1.63502000
H	3.38164100	2.56895900	1.91686300
H	4.42003800	-0.89751000	0.31347600
H	1.95550300	4.21140900	4.07990300
H	2.66490200	2.59374900	4.28820400
H	1.27729600	2.82242400	3.19575400
H	4.39836600	5.03403800	3.45694000
H	5.21840700	4.31350800	2.05714700
H	5.01040800	3.37800400	3.55576800
H	3.64314500	-3.13156100	1.06706500
H	5.04980300	-2.58817600	2.00602300
H	5.24960500	-3.82214500	0.74456100
H	7.11202400	-2.24215800	-0.34068800
H	6.80709300	-1.06126400	0.94546200
H	6.67728500	-0.57465600	-0.75965300
H	1.03435300	-2.98927900	5.70634700
H	1.70925400	-5.24421800	4.92506100
H	1.09902800	-6.01379700	2.64491100
H	-0.80768700	-0.45897200	3.59668500
H	-3.48318800	-2.29426900	-1.69914300
H	1.42543500	-0.73050000	5.68319800
H	0.62498700	0.75754800	5.13425600
H	1.62599100	-0.17055900	4.00463300
H	-2.28063100	-1.66774700	5.26682400
H	-1.64741300	-0.13425800	5.89689300
H	-0.94112400	-1.67591700	6.42823200
H	-4.34108400	-1.26733600	-4.46137300
H	-2.98057600	-2.36292500	-4.12741600
H	-2.94836700	-0.69470200	-3.50768800
H	-5.62103500	-3.64434200	-1.72025500
H	-4.47953100	-4.11972700	-2.99866500
H	-5.90220500	-3.14874000	-3.40106600
H	-6.70524800	-1.06196500	-3.24448600
H	-8.02920800	0.82833100	-2.32850100
H	-7.19224900	2.11772600	-0.38195200
H	-1.03959000	-4.01518000	0.26387600
H	-3.90844500	1.44787900	1.36129200
H	1.75152700	-5.28439500	0.16691900

H	1.32116800	-3.61311200	-0.29220100
H	0.69276100	-4.98847600	-1.22874700
H	-1.24146900	-6.39096100	-0.29869700
H	-1.79854200	-6.16494900	1.37464900
H	-0.20370900	-6.87367000	1.04981700
H	-3.90541100	3.32425500	-0.21015600
H	-4.27584600	3.86314700	1.43083300
H	-5.58566600	3.74768700	0.22989400
H	-6.00955700	0.70294000	2.57479000
H	-6.84265400	2.15449000	1.98678700
H	-5.45047400	2.31366200	3.07575900
O	0.15036700	1.02959800	-1.92025000
O	-1.65285100	2.13183400	1.63303800
O	-1.26880100	2.34707000	0.21272200
O	-0.38327600	-1.65740100	0.56871700
O	1.51873000	1.69502200	0.66490400
Zr	-0.24503200	0.49060700	-0.19973000

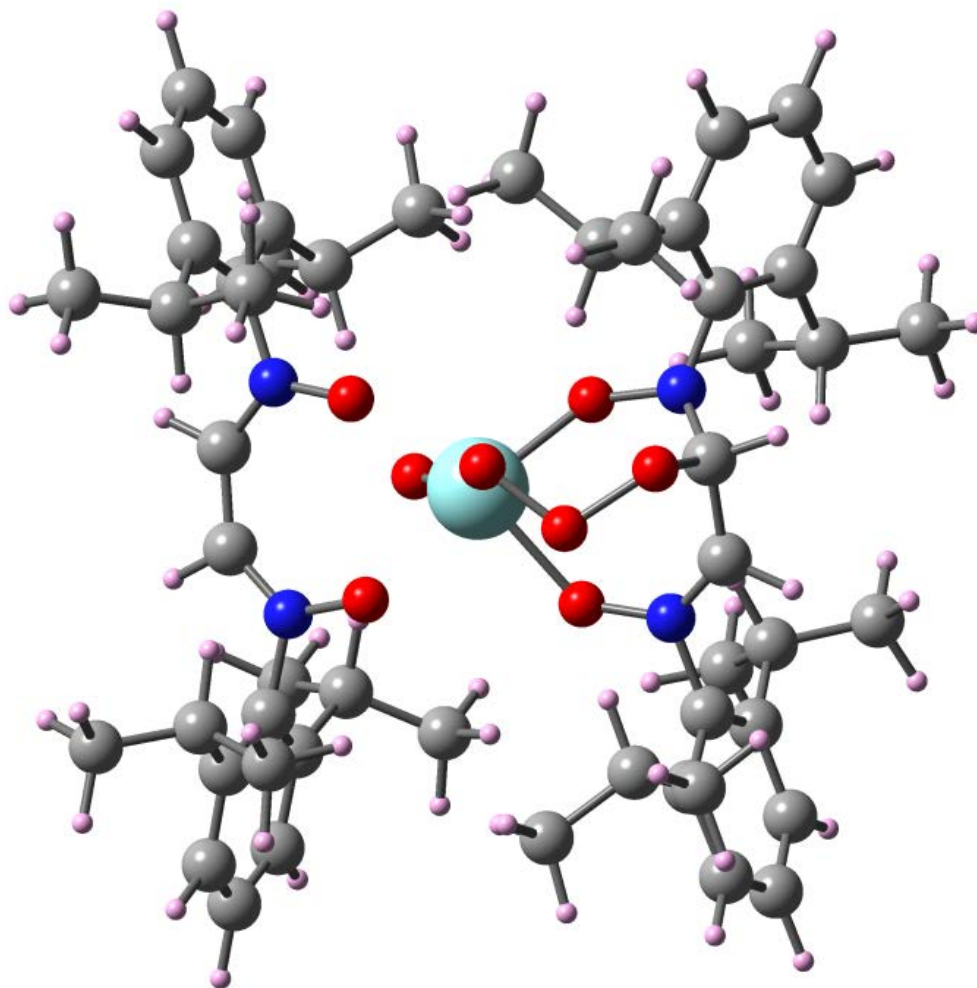
**Ligand Cyclization (conformation 1 lower energy)**

Fig. S124: ONCCNO Ligand Cyclization (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G
-2891.7437044	-2890.579968	-2890.506771	-2890.694187

O	2.02712700	0.03789800	0.04230500
O	-2.43531700	0.47296500	-0.40427300
O	0.91644000	-1.96287500	-2.83756000
N	-0.67538800	3.17639000	0.41901900
N	-3.23671400	1.10040100	0.46080600
N	0.66773000	-3.04914500	-0.56730300
N	2.95294800	-0.74081200	-0.57812400
C	-1.83462200	3.13445900	1.06599000
C	-2.94933300	2.22707100	1.10067300
C	1.51488600	-2.64561400	-1.62719100
C	2.76528200	-1.84976300	-1.25507100
C	0.20652100	4.34144000	0.60613600
C	1.03051200	4.37774200	1.75544800

C	1.87373500	5.50253300	1.89024300
C	1.89680700	6.51368100	0.91730900
C	1.07732600	6.42669700	-0.22072500
C	0.20897200	5.33143500	-0.40613500
C	2.45550600	2.63972600	2.93801100
C	1.04377200	3.26851500	2.81331200
C	0.55394800	3.80266500	4.18511800
C	-3.25462500	-2.11896000	2.92517100
C	-3.60086700	-0.60901200	2.84569800
C	-3.99623700	-0.05892600	4.24136500
C	-4.54350300	0.45303400	0.67477900
C	-4.71224000	-0.35977900	1.81977600
C	-5.97544900	-0.97325400	1.97438100
C	-6.99067200	-0.79504000	1.02304100
C	-6.76993800	-0.00119900	-0.11558200
C	-5.53368800	0.64374200	-0.32090900
C	0.22880900	4.89939100	-2.90217200
C	-0.65355500	5.22568300	-1.66767500
C	-1.49830100	6.50294400	-1.90583100
C	-4.90106300	0.51516500	-2.76809800
C	-5.27378500	1.45991700	-1.59170000
C	-6.46329200	2.37694700	-1.96741400
C	0.03529400	-4.35193400	-0.52039400
C	-1.14599500	-4.62559600	-1.26036900
C	-1.69277100	-5.92660300	-1.17748100
C	-1.10220800	-6.91348500	-0.37755000
C	0.04714000	-6.61625000	0.37523200
C	0.63005200	-5.33442700	0.32662900
C	-3.31146200	-3.35792400	-1.65061200
C	-1.84968100	-3.57367300	-2.12064000
C	-1.80437200	-3.95091700	-3.62393600
C	4.55030800	-0.92343900	3.16060800
C	4.53835800	-1.58002100	1.75590500
C	5.33279400	-2.91265500	1.76269200
C	4.32115000	-0.20910700	-0.42986300
C	5.07876900	-0.62055700	0.69106500
C	6.38752500	-0.10427200	0.79731500
C	6.89377200	0.78566700	-0.16359200
C	6.09877500	1.18802700	-1.24858600
C	4.78206700	0.70509000	-1.40536100
C	1.33344000	-4.24028100	2.48685700
C	1.82935200	-4.98296500	1.21347500
C	2.70979800	-6.19484100	1.59376500
C	3.75107700	2.70788000	-2.58040000
C	3.92306600	1.16702200	-2.58669600
C	4.51779800	0.68064900	-3.93488300
H	-1.98060600	4.00122500	1.70207900
H	-3.74291300	2.54982000	1.76549700
H	1.87684600	-3.56805200	-2.09666600
H	3.68880500	-2.25459200	-1.65855400
H	2.52224600	5.57777200	2.75880000
H	2.55847900	7.36768600	1.04153100

H	1.11261400	7.21310700	-0.96961200
H	0.37375600	2.45439100	2.51322300
H	-2.67945300	-0.10238500	2.53445200
H	3.20807200	3.37587400	3.25268400
H	2.77177100	2.20127000	1.98436800
H	2.43009700	1.83752400	3.68627300
H	1.21949900	4.58322000	4.57834300
H	0.52551300	2.98275000	4.91365900
H	-0.45668300	4.22828300	4.11694000
H	-4.10959400	-2.72048500	3.26388900
H	-2.42854700	-2.26916200	3.63119000
H	-2.92790800	-2.49856300	1.95012500
H	-4.21379000	1.01775800	4.20574600
H	-3.17012300	-0.21240000	4.94708400
H	-4.88388500	-0.56623900	4.64392000
H	-6.15388000	-1.60556000	2.83981600
H	-7.95281300	-1.28264700	1.16163500
H	-7.56209300	0.11514700	-0.84934900
H	-1.34954200	4.38689500	-1.55176700
H	-4.40416400	2.10744600	-1.42188800
H	0.96377100	5.69464100	-3.08659200
H	-0.39724700	4.79829200	-3.79811200
H	0.76430400	3.95616000	-2.75277600
H	-0.86540200	7.37759700	-2.10314400
H	-2.13214500	6.73525900	-1.03997500
H	-2.14871100	6.36341100	-2.77894300
H	-3.98858500	-0.04435900	-2.53924300
H	-4.72217100	1.10036700	-3.67968000
H	-5.71401700	-0.19541100	-2.97091700
H	-7.34382200	1.79781600	-2.27329000
H	-6.18486900	3.01599100	-2.81534800
H	-6.75740500	3.02483600	-1.13118700
H	-2.58998100	-6.16261200	-1.74439900
H	-1.53742300	-7.90970200	-0.33149400
H	0.48453700	-7.38667400	1.00290800
H	-1.33212000	-2.61940300	-2.01488600
H	3.49272900	-1.81475000	1.52837900
H	-3.92087400	-4.26369400	-1.77652600
H	-3.77377900	-2.55464200	-2.23798200
H	-3.34554800	-3.06582300	-0.59382000
H	-0.76910800	-4.02706300	-3.97735200
H	-2.30003200	-3.17195500	-4.21747100
H	-2.30994800	-4.90716400	-3.82051500
H	5.57161500	-0.69011900	3.48935400
H	4.10731100	-1.60626800	3.89695300
H	3.96804600	0.00422500	3.16230100
H	5.29906100	-3.40834800	0.78364200
H	4.91052300	-3.60036400	2.50636400
H	6.38758000	-2.74657700	2.01795600
H	7.01021800	-0.39706200	1.63844000
H	7.90621600	1.16964000	-0.06383700
H	6.50024200	1.88500100	-1.97912600



H	2.45726300	-4.27334700	0.65905700
H	2.92035900	0.73708600	-2.49760000
H	0.67893500	-4.89366400	3.08054500
H	0.77228800	-3.34005000	2.21532600
H	2.18468300	-3.94855600	3.11921200
H	3.61200300	-5.84934700	2.11583700
H	3.02494000	-6.76525300	0.70984600
H	2.18715100	-6.88122700	2.27294800
H	3.28881800	3.04707200	-1.64597000
H	3.10279700	3.01167200	-3.41199700
H	4.71286700	3.22495900	-2.69701400
H	4.61191100	-0.41261500	-3.96180300
H	5.51247800	1.11056200	-4.11429900
H	3.86279000	0.98060200	-4.76216900
O	-0.69733700	0.51144900	1.71992200
O	0.69494500	-0.45123600	-2.54910800
O	-0.69454700	-0.20365800	-2.16666000
O	0.00600600	-2.03018700	0.18775300
O	-0.19277800	2.25287600	-0.42846400
Zr	-0.19860000	0.00688300	0.00890300

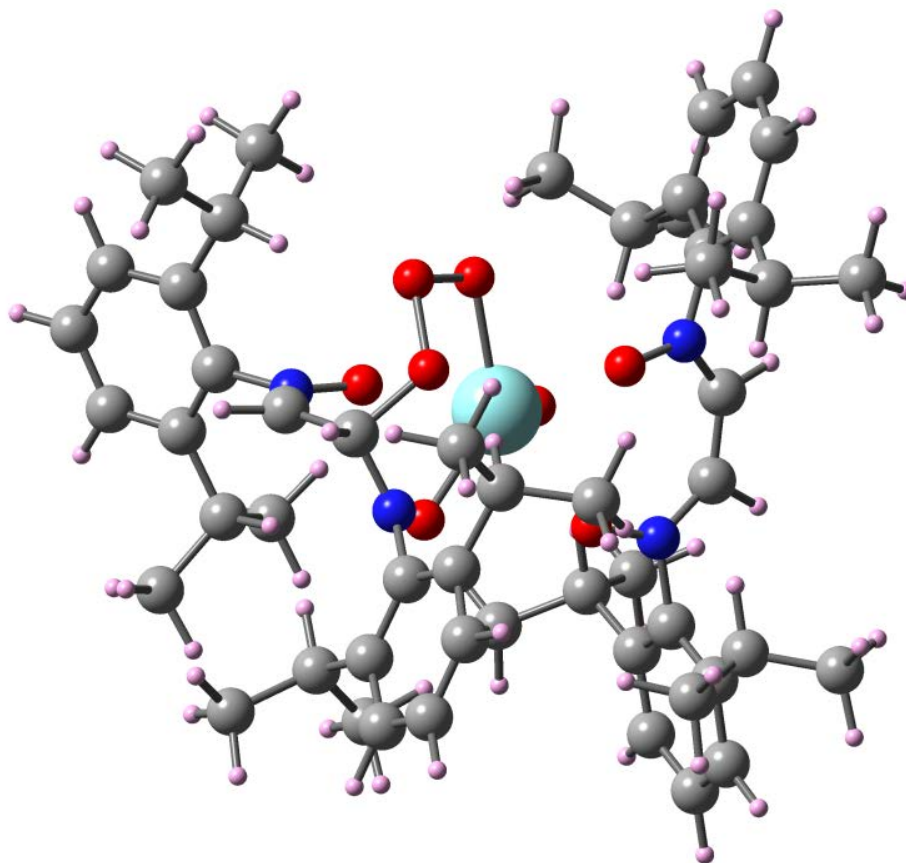
**Ligand Cyclization (conformation 2 higher energy)**

Fig. S125: ONCCNO Ligand Cyclization (conformation 2 higher energy)

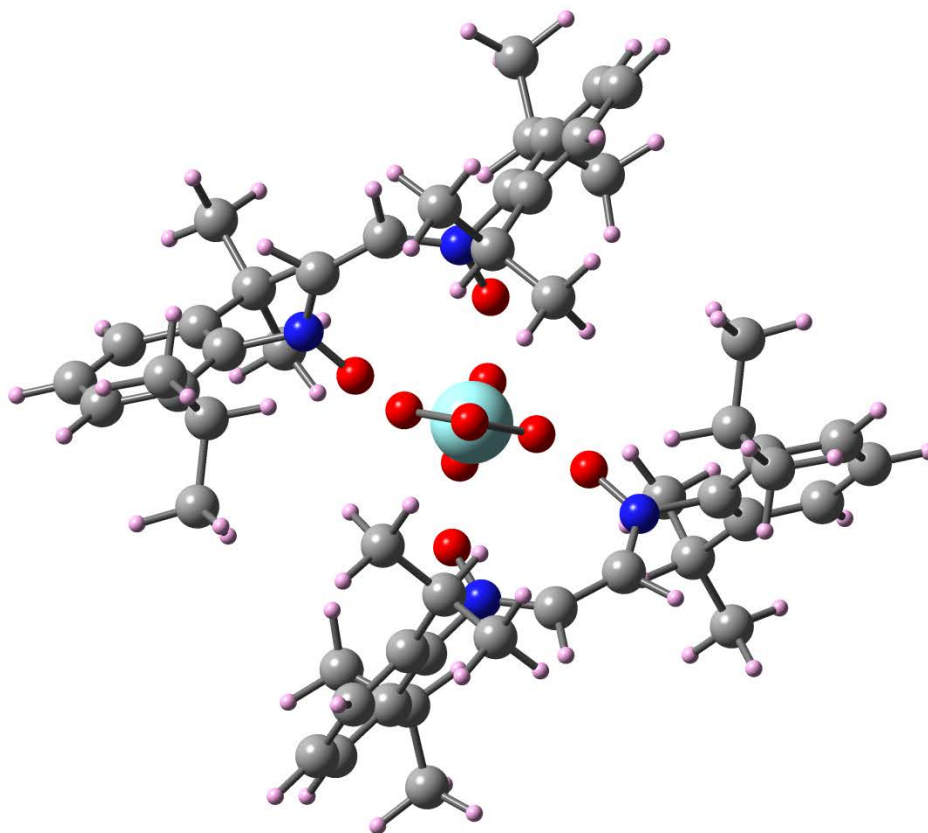
SCF	E <sub>ZP</sub>	H	G
-2891.74093040	-2890.577721	-2890.504492	-2890.690763
O	-2.26187000	1.01212500	-0.59403600
O	1.53670800	-1.15404100	-0.50570500
O	-0.94295900	0.83296100	2.20088700
N	2.88857800	1.86834000	-0.28288700
N	2.53313900	-1.14587400	-1.38947800
N	-1.42555500	-1.37988400	1.68846700
N	-3.31432900	0.74787400	0.20643600
C	3.43920800	1.23215200	-1.30596300
C	3.31023800	-0.12294800	-1.75336800
C	-2.06922700	-0.23835500	2.19411700
C	-3.27785300	0.23285900	1.41574700
C	3.22052900	3.27485000	-0.00889300
C	2.73317800	4.27955100	-0.88123100
C	3.09922800	5.60932300	-0.57544000
C	3.88160000	5.91188900	0.54739900
C	4.31557000	4.88855600	1.40633700
C	3.99277700	3.54169800	1.15077700

C	0.44467400	4.71939900	-1.87346700
C	1.81009800	4.00912500	-2.07520800
C	2.47311400	4.43840600	-3.41010900
C	-0.22979600	-2.19798100	-4.18188200
C	1.18958100	-1.61656000	-3.95620000
C	1.79067800	-1.09692000	-5.28865400
C	2.74849400	-2.44459800	-2.06178400
C	2.10712100	-2.65648900	-3.30417400
C	2.34112200	-3.90032600	-3.92955300
C	3.15122100	-4.87491400	-3.32600400
C	3.74091700	-4.63497600	-2.07411400
C	3.54897800	-3.40785600	-1.40554300
C	3.56777400	2.49506500	3.40757000
C	4.43970300	2.44590800	2.12359700
C	5.94829300	2.53584300	2.46475400
C	3.45016300	-4.08616400	1.02995300
C	4.15234700	-3.17988700	-0.01670200
C	5.68686600	-3.39779900	-0.00614400
C	-1.09582500	-2.59127600	2.38951700
C	-0.20557800	-2.58814100	3.50438300
C	0.05422200	-3.81718100	4.15034900
C	-0.50056500	-5.01873000	3.69023800
C	-1.34979700	-5.00888200	2.57244400
C	-1.67645100	-3.80634400	1.91612100
C	2.02759800	-1.49354400	4.06570500
C	0.48644400	-1.32741100	4.03140900
C	-0.05005700	-0.92898500	5.43261600
C	-3.86306500	-0.75334500	-3.23339600
C	-4.48888600	-0.99299900	-1.83191800
C	-5.44507800	-2.21084300	-1.85029300
C	-4.60330800	1.14763900	-0.38847100
C	-5.17984100	0.28584100	-1.35152600
C	-6.40968200	0.68944600	-1.91111900
C	-7.01511600	1.89912900	-1.53306500
C	-6.39185500	2.74326600	-0.60182200
C	-5.15766000	2.39368500	-0.01143000
C	-1.91438200	-4.42909500	-0.52687200
C	-2.62821800	-3.83832000	0.71807300
C	-3.93605900	-4.60946700	1.03001100
C	-4.03780300	4.65519300	0.16913400
C	-4.46040200	3.37408500	0.93724000
C	-5.34763800	3.72365500	2.15934200
H	4.13026700	1.83487500	-1.88379500
H	3.99375600	-0.38364700	-2.55342100
H	-2.36803200	-0.39952800	3.23256600
H	-4.24536600	0.11437400	1.89137300
H	2.74682000	6.41270800	-1.21606000
H	4.14280800	6.94535600	0.76247900
H	4.90767800	5.13877300	2.28194000
H	1.57614200	2.94176000	-2.14131600
H	1.06458700	-0.75511400	-3.29021000
H	0.55381400	5.81240900	-1.83538900

H	-0.03276500	4.37727700	-0.94843200
H	-0.22174400	4.46964100	-2.70876400
H	2.67734700	5.51748800	-3.43484300
H	1.80352800	4.20393200	-4.24727500
H	3.42547300	3.91614500	-3.58199000
H	-0.22148900	-3.03912900	-4.88872800
H	-0.88432400	-1.41724600	-4.58774200
H	-0.66349700	-2.54424800	-3.23619300
H	2.78486900	-0.65409100	-5.13843900
H	1.13875100	-0.32300800	-5.71259000
H	1.89049400	-1.90164300	-6.02989100
H	1.87632600	-4.10842800	-4.88952800
H	3.31430800	-5.82688400	-3.82570100
H	4.34961200	-5.40670900	-1.61082800
H	4.26434600	1.46746400	1.66271000
H	3.96419700	-2.14308800	0.28622500
H	3.69655000	3.44984500	3.93489000
H	3.85634400	1.68633300	4.09256800
H	2.50891100	2.37797900	3.15439400
H	6.19035500	3.45663500	3.01043800
H	6.56888500	2.50796500	1.55936600
H	6.23683500	1.69107500	3.10395200
H	2.37262800	-3.88991800	1.05783800
H	3.85974600	-3.89728100	2.03088200
H	3.60000500	-5.14884600	0.79794300
H	5.94877300	-4.43610900	-0.24654500
H	6.09153700	-3.17643900	0.98997200
H	6.19125100	-2.74771000	-0.73306400
H	0.71704700	-3.83234500	5.01212600
H	-0.27291100	-5.95456300	4.19576300
H	-1.77754200	-5.94331800	2.21815000
H	0.27336400	-0.49693500	3.35562400
H	-3.65987500	-1.22845400	-1.15535000
H	2.34285400	-2.26981300	4.77590900
H	2.49664800	-0.54853400	4.37057300
H	2.41211300	-1.76090800	3.07370300
H	-1.13512500	-0.75951500	5.41526800
H	0.42952000	-0.00224900	5.77367200
H	0.15226300	-1.71198800	6.17614900
H	-4.63416800	-0.49287100	-3.97139800
H	-3.35266500	-1.66213700	-3.57709400
H	-3.12813800	0.05782300	-3.19152400
H	-5.89990300	-2.38182000	-0.86597900
H	-4.88913900	-3.11437700	-2.13197200
H	-6.25512100	-2.08313700	-2.58007700
H	-6.89211600	0.05633800	-2.65030500
H	-7.96499400	2.18964400	-1.97574000
H	-6.85659600	3.68907100	-0.33724400
H	-2.88990000	-2.80563800	0.46994700
H	-3.53675800	2.92466700	1.31269000
H	-1.59881000	-5.46679300	-0.34934900
H	-1.03222400	-3.82821400	-0.77044400

H	-2.58965800	-4.42494800	-1.39431700
H	-4.62712900	-4.53569300	0.17997200
H	-4.43943000	-4.20277800	1.91733800
H	-3.75061000	-5.67644100	1.21027100
H	-3.36947500	4.40461100	-0.66241300
H	-3.49821900	5.33276400	0.84289100
H	-4.90842200	5.19182500	-0.23212900
H	-5.63408900	2.82427200	2.72101500
H	-6.27008400	4.23805800	1.85852400
H	-4.80067800	4.38890200	2.83948700
O	0.40309700	0.99176100	-1.89668900
O	-1.29711700	2.33967600	1.84481900
O	-0.43806300	2.60522400	0.69366300
O	-1.06891900	-1.27477200	0.29214100
O	2.04371000	1.27886200	0.58768600
Zr	-0.04312100	0.61344000	-0.16293400

## 9.6 Structures with nine oxygen atoms

Peroxo  $\eta^2$ -Ozone ComplexFig. S126: ONCCNO Peroxo  $\eta^2$ -Ozone Complex

SCF	E <sub>ZP</sub>	H	G
-2966.896837	-2965.730543	-2965.655892	-2965.844937

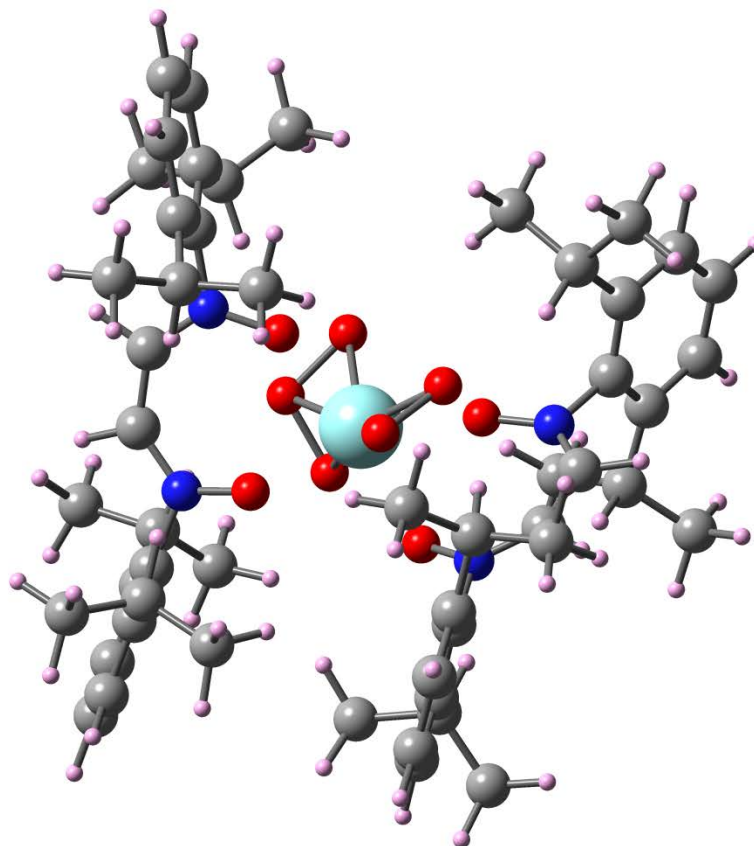
O	0.33839459	2.18833717	-0.33306761
O	-0.33711554	-2.18261190	-0.33321509
O	-1.15182385	0.21174141	1.21321288
N	2.93738278	-1.59464608	-0.52648574
N	0.18683854	-3.08744862	0.50395065
N	-2.93373687	1.58473186	-0.53127008
N	-0.19152019	3.09425087	0.49822479
C	2.67844392	-2.61008949	0.30599294
C	1.48901894	-3.24093655	0.76989728
C	-2.68038289	2.60241298	0.29983861
C	-1.49479013	3.24160550	0.76251837
C	4.33200265	-1.29555562	-0.88655550
C	4.77028842	-1.69111583	-2.17518041
C	6.10640414	-1.38999569	-2.50980720
C	6.94875145	-0.72580861	-1.60238808

C	6.46712093	-0.32674310	-0.34665612
C	5.13396672	-0.58802766	0.03929380
C	3.32201833	-1.30906702	-4.21318450
C	3.83987481	-2.36042890	-3.19176478
C	4.50813833	-3.55780348	-3.91169338
C	-2.29336344	-4.31419858	-2.13540625
C	-1.11521829	-4.94194245	-1.34301594
C	-0.79097209	-6.36707040	-1.85890383
C	-0.78887828	-4.03272286	1.06585185
C	-1.41544750	-4.92776423	0.15995587
C	-2.36351186	-5.82133943	0.69815869
C	-2.66059468	-5.82356107	2.07073105
C	-2.02183100	-4.92211041	2.93428453
C	-1.07444682	-3.99148909	2.45335441
C	4.77922037	1.45258663	1.50758932
C	4.61112323	-0.08458174	1.38952161
C	5.31609496	-0.80701538	2.56817297
C	-1.48934551	-2.15032008	4.16122127
C	-0.42360288	-3.00415039	3.42906514
C	0.48509270	-3.74659057	4.44494773
C	-4.32641959	1.27762880	-0.89168906
C	-5.12620278	0.56899111	0.03524008
C	-6.45784906	0.30081856	-0.35125998
C	-6.94006876	0.69443055	-1.60845833
C	-6.09982959	1.36002252	-2.51679132
C	-4.76540831	1.66801211	-2.18172610
C	-4.76671932	-1.46575045	1.51039629
C	-4.60256997	0.07143505	1.38733910
C	-5.31004678	0.79574611	2.56336774
C	2.27695825	4.31885661	-2.14681069
C	1.09806600	4.94865338	-1.35707103
C	0.77064068	6.37018889	-1.88070376
C	0.77861642	4.04793138	1.05584401
C	1.39916383	4.94295367	0.14579156
C	2.34230559	5.84421258	0.67976051
C	2.64046160	5.85357087	2.05207849
C	2.00778249	4.95180164	2.91974698
C	1.06552766	4.01372237	2.44319510
C	-3.31540577	1.28927256	-4.21923948
C	-3.83754248	2.33972780	-3.19908650
C	-4.51057531	3.53350119	-3.92056481
C	1.49367131	2.18067952	4.15609522
C	0.42166791	3.02592575	3.42301358
C	-0.48970062	3.76630276	4.43794169
H	3.58376852	-3.07005158	0.68607115
H	1.67712666	-4.06377217	1.45024804
H	-3.58829003	3.05776001	0.67938869
H	-1.68793817	4.06594322	1.43962872
H	6.48885229	-1.67523385	-3.48553885
H	7.97725956	-0.50809868	-1.88093696
H	7.12322934	0.20802589	0.33487992
H	2.95715101	-2.74349808	-2.66629078

H	-0.24050580	-4.31342902	-1.53879976
H	4.15869525	-0.84162743	-4.75117606
H	2.73859959	-0.53271003	-3.70894947
H	2.66650338	-1.79324529	-4.94847304
H	5.33402973	-3.23643265	-4.55952466
H	3.77089624	-4.05990379	-4.55115763
H	4.90247640	-4.29436491	-3.19886296
H	-3.22219462	-4.88027910	-1.97980355
H	-2.06711874	-4.31275125	-3.20927421
H	-2.45377428	-3.27686251	-1.82492208
H	0.03878484	-6.82011021	-1.30030383
H	-0.50542560	-6.32034325	-2.91771313
H	-1.65606986	-7.03822722	-1.78148757
H	-2.86788373	-6.52272222	0.03958853
H	-3.39211053	-6.52505193	2.46502710
H	-2.26834895	-4.92875159	3.99261178
H	3.53614065	-0.28224869	1.46254263
H	0.19130774	-2.29145206	2.87338610
H	5.83509660	1.75361645	1.47792999
H	4.35574494	1.80186125	2.45759210
H	4.25144246	1.96663423	0.69592566
H	6.39737199	-0.61388657	2.56815250
H	5.17213983	-1.89516662	2.52147646
H	4.90953147	-0.45326952	3.52445442
H	-2.06490869	-1.56339573	3.43805257
H	-0.99220093	-1.44547504	4.83931641
H	-2.17727015	-2.76791420	4.75461752
H	-0.09365487	-4.43733364	5.07279283
H	0.97844700	-3.02265784	5.10630131
H	1.26644824	-4.33338469	3.94211117
H	-7.11222827	-0.23509685	0.33102878
H	-7.96734166	0.47144248	-1.88738653
H	-6.48268637	1.64114060	-3.49355197
H	-3.52818646	0.27252494	1.46014835
H	0.22433602	4.31748770	-1.54898980
H	-5.82185918	-1.76940125	1.48205945
H	-4.34212678	-1.81101830	2.46131702
H	-4.23803318	-1.98111539	0.70015871
H	-5.16846806	1.88407707	2.51370605
H	-4.90343670	0.44566710	3.52098132
H	-6.39089311	0.60023892	2.56304320
H	3.20504008	4.88679124	-1.99349266
H	2.05068867	4.31256740	-3.22064998
H	2.43840505	3.28301728	-1.83203561
H	-0.05871523	6.82539849	-1.32326745
H	0.48315828	6.31662890	-2.93866334
H	1.63490113	7.04309031	-1.80922953
H	2.84204972	6.54601391	0.01811593
H	3.36815260	6.56093580	2.44294717
H	2.25513000	4.96408255	3.97782288
H	-2.95640889	2.72696883	-2.67406746
H	-0.19000586	2.30806580	2.87042176



H	-4.15010767	0.81795187	-4.75693055
H	-2.72907269	0.51577065	-3.71398475
H	-2.66162465	1.77517681	-4.95493324
H	-3.77539557	4.03752045	-4.56088774
H	-4.90757962	4.26956036	-3.20869447
H	-5.33540167	3.20808980	-4.56773618
H	2.07217667	1.59554327	3.43379048
H	1.00194672	1.47450054	4.83674663
H	2.17846307	2.80427563	4.74682171
H	-1.27565778	4.34638349	3.93447306
H	0.08588740	4.46290301	5.06221513
H	-0.97728560	3.04171581	5.10284769
O	-0.23040456	-0.70171125	-2.60978047
O	0.25618859	0.70997434	-2.60467930
O	0.00613738	0.00875068	2.14884726
O	1.16076208	-0.20308176	1.21090189
O	-2.03925320	0.81512764	-1.15771216
O	2.04794651	-0.82046301	-1.15315796
Zr	0.00423093	0.00188295	-0.64220625

Peroxo  $\eta^3$ -Ozone ComplexFig. S127: ONCCNO Peroxo  $\eta^3$ -Ozone Complex

SCF	E <sub>ZP</sub>	H	G
-2966.887744	-2965.722011	-2965.647317	-2965.837013

O	-1.74123480	-0.90386796	-0.16260104
O	2.48671180	0.68080338	-0.74603158
O	0.26224373	2.06974839	-1.51681499
N	1.92453965	-1.99719346	1.14443856
N	3.57713988	0.54706605	-0.00067147
N	-2.65083946	2.18214595	0.03514053
N	-2.71223839	-0.86271427	-1.10179600
C	3.03528251	-1.39586335	1.54932037
C	3.78908884	-0.30990024	1.00264448
C	-3.46444333	1.52707508	-0.80758604
C	-3.45756696	0.21019414	-1.35721631
C	1.42195666	-3.19489579	1.82806526
C	1.04286945	-3.13158553	3.19632171
C	0.57898275	-4.32985953	3.78291463
C	0.48586878	-5.51926060	3.04841731
C	0.87397756	-5.54545350	1.70017920
C	1.36196560	-4.39050815	1.05732120

C	-0.26234359	-1.54581763	4.70459911
C	1.11150162	-1.86879583	4.06541321
C	2.20584804	-2.01418341	5.15795358
C	2.55195384	4.14074603	0.54734103
C	3.54525275	3.18645796	1.26766379
C	4.10956884	3.83717285	2.55399488
C	4.65001617	1.49957259	-0.34812102
C	4.64511153	2.76116574	0.29079485
C	5.67343068	3.65671247	-0.07503749
C	6.63134580	3.30552875	-1.03896727
C	6.57581193	2.05531661	-1.67793529
C	5.57201471	1.11953831	-1.35246323
C	0.58452536	-4.58276871	-1.34929932
C	1.81298055	-4.48415192	-0.40640602
C	2.78931400	-5.66606337	-0.63796371
C	4.61339773	0.05187603	-3.42645247
C	5.43354696	-0.19479511	-2.12778836
C	6.79297553	-0.86248848	-2.44358752
C	-3.08424925	3.50269495	0.53851048
C	-2.80300364	4.64425573	-0.24599546
C	-3.24086017	5.88477624	0.26775061
C	-3.88957803	5.96624318	1.50935424
C	-4.11068878	4.80951381	2.27593657
C	-3.70917189	3.54099422	1.80905225
C	-0.85158133	5.54183753	-1.61488345
C	-2.05978024	4.57274856	-1.58388920
C	-3.02240715	4.85413912	-2.76848194
C	-2.77427381	-3.76647063	1.46458260
C	-3.79546936	-2.96172135	0.61969845
C	-5.25229024	-3.32487742	1.00863318
C	-3.03588798	-2.15200462	-1.73314333
C	-3.54111622	-3.16823248	-0.87799138
C	-3.83261567	-4.41477070	-1.46585480
C	-3.64254901	-4.63070557	-2.83990897
C	-3.15994629	-3.59841932	-3.65567114
C	-2.83773574	-2.32852215	-3.12678715
C	-2.70813499	2.18457949	3.69431172
C	-3.88081202	2.29064633	2.67816780
C	-5.25016079	2.24375473	3.39863062
C	-1.06863298	-1.71442590	-4.85670604
C	-2.31929108	-1.24055148	-4.07533110
C	-3.44200521	-0.78588522	-5.04808372
H	3.48514466	-1.84301471	2.42808673
H	4.74195971	-0.14844410	1.49432211
H	-4.32009400	2.12265343	-1.10265104
H	-4.24827422	0.02840685	-2.07591473
H	0.27714324	-4.32148198	4.82641889
H	0.11639051	-6.42425234	3.52502845
H	0.81161285	-6.47560063	1.14274036
H	1.34182012	-1.00668856	3.43702966
H	2.96180094	2.31184933	1.57430277
H	-0.61538184	-2.34784833	5.36743674

H	-1.00404110	-1.36817307	3.91995125
H	-0.18180569	-0.62596156	5.29810505
H	1.97495300	-2.83484081	5.85046391
H	2.27545613	-1.08812241	5.74313481
H	3.19749178	-2.21822515	4.72843990
H	3.05005169	5.07023248	0.23624105
H	1.72934441	4.39622171	1.22708152
H	2.12106466	3.66076530	-0.33872685
H	4.81773031	3.17251867	3.06707282
H	3.28568525	4.05406564	3.24546078
H	4.62481612	4.78468843	2.34624727
H	5.71449891	4.63667141	0.39177668
H	7.41381808	4.01247101	-1.30509758
H	7.30942760	1.80935599	-2.43971635
H	2.33779547	-3.56391237	-0.67749465
H	4.85678902	-0.90338489	-1.51977714
H	-0.01434909	-5.47764658	-1.13009152
H	0.91549236	-4.64197651	-2.39460630
H	-0.05074798	-3.69848338	-1.24221973
H	2.30374104	-6.63919742	-0.48911203
H	3.65489739	-5.61421093	0.03584656
H	3.15924156	-5.64010273	-1.67146072
H	3.61856826	0.44478201	-3.19125725
H	4.48916094	-0.88881946	-3.97940760
H	5.12927905	0.76827351	-4.08023709
H	7.38501576	-0.26768604	-3.15096012
H	6.62499149	-1.84330605	-2.90660462
H	7.39454671	-1.00966211	-1.53690244
H	-3.05659693	6.79034658	-0.30341572
H	-4.21309635	6.93324364	1.88745083
H	-4.59537667	4.89326651	3.24408454
H	-1.63661201	3.57146709	-1.70989649
H	-3.64153955	-1.90697480	0.86729643
H	-1.16208314	6.59434583	-1.56086887
H	-0.29333793	5.39834408	-2.54782544
H	-0.16783592	5.33516164	-0.78416072
H	-3.85801169	4.14108459	-2.79300211
H	-2.48062924	4.77036368	-3.71902426
H	-3.44781337	5.86521531	-2.70623592
H	-2.85724953	-4.84435960	1.26956591
H	-2.95361543	-3.60024420	2.53490264
H	-1.75210681	-3.44957085	1.23697016
H	-5.98195329	-2.75681385	0.41637696
H	-5.42076209	-3.09678110	2.06934962
H	-5.46078615	-4.39288077	0.86431982
H	-4.21983439	-5.21755512	-0.84472640
H	-3.87408688	-5.60071130	-3.27359093
H	-3.01809379	-3.77751221	-4.71761737
H	-3.82126610	1.40316030	2.03556563
H	-1.99351687	-0.37390810	-3.49683056
H	-2.67537120	3.07166601	4.34187658
H	-1.74958030	2.08143413	3.17594610

H	-2.84280253	1.29965739	4.33046207
H	-5.36276585	1.28160055	3.91464350
H	-6.08566595	2.35540193	2.69494232
H	-5.33846519	3.03075577	4.15852644
H	-0.26009023	-1.94920148	-4.15848673
H	-0.71454564	-0.90443524	-5.50675540
H	-1.27884201	-2.58951473	-5.48671768
H	-4.32945828	-0.41925242	-4.51218850
H	-3.76701571	-1.60926362	-5.69803753
H	-3.07465049	0.02550038	-5.68923985
O	1.15087846	0.92906308	1.58649076
O	-0.02220060	0.01470235	1.91670813
O	-0.63946964	0.99956796	-2.14707673
O	0.21968675	-0.26334296	-2.26706534
O	-1.49642825	1.77783243	0.53408717
O	1.28304634	-1.64842671	-0.00430689
Zr	0.18380964	0.33359765	-0.16824086

## Catalyst Deformation Product with Oxygen Splitting Ligand Apart

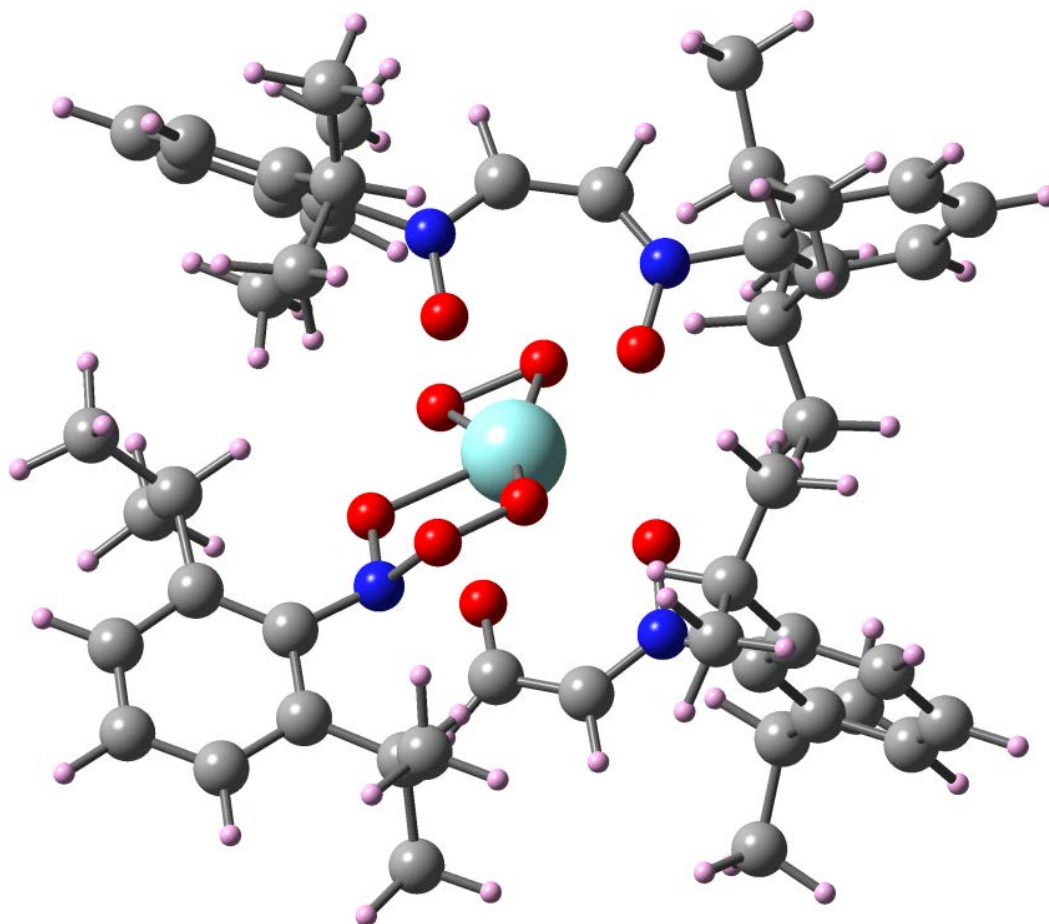


Fig. S128: ONCCNO Catalyst Deformation Product with Oxygen Splitting Ligand Apart

SCF	E <sub>ZP</sub>	H	G
-2966.9301605	-2965.764079	-2965.690083	-2965.875621

Zr	0.16315000	0.00692200	-0.76350100
O	1.65214800	-1.22467600	0.46231400
O	-2.06755100	0.65456100	-0.80671000
O	0.02613900	-1.66564600	-1.98045200
O	1.20680600	-0.75696800	-2.37940300
N	1.49204700	2.60553000	0.04010300
N	-2.48177600	1.93255100	-0.59865200
N	-1.08053700	-2.88244200	0.34331100
N	2.12541800	-2.41570700	0.03967600
C	-0.48867500	2.91211700	-1.61283500
C	-1.70426700	2.98784500	-0.83520500
C	-0.05786400	-3.67326800	0.02132600
C	1.35261400	-3.47441500	-0.15008000
C	2.51737900	3.62554500	0.25829500
C	2.03105300	4.89513800	0.69520700

C	2.95007100	5.95364500	0.82738300
C	4.30781800	5.77449100	0.52869000
C	4.76821000	4.51336800	0.12775300
C	3.90513000	3.40165200	0.00513300
C	0.41448900	5.39376200	2.58502800
C	0.56401500	5.15383000	1.05908000
C	-0.03564800	6.33392300	0.25129500
C	-3.18663200	0.37204300	2.94469900
C	-3.01905500	1.77036600	2.29603200
C	-2.98730100	2.88473400	3.37283300
C	-3.86144800	2.08030000	-0.12713500
C	-4.11956700	2.01209000	1.26232600
C	-5.46280500	2.16385000	1.66942900
C	-6.48672900	2.36794700	0.73196900
C	-6.19378200	2.41581700	-0.64087100
C	-4.87133400	2.26297500	-1.10549100
C	5.88178200	1.78403500	0.28694700
C	4.52209500	2.05501500	-0.40529500
C	4.66902200	1.97807200	-1.94915900
C	-5.47344600	1.34887900	-3.41475000
C	-4.56983300	2.31548100	-2.60766900
C	-4.70501300	3.76608900	-3.14554300
C	-2.40402200	-3.51221700	0.53831400
C	-3.24172200	-3.67434000	-0.58928200
C	-4.49829600	-4.27771600	-0.35965400
C	-4.88421900	-4.68761800	0.92488000
C	-4.02407500	-4.50018900	2.02002800
C	-2.76057600	-3.89775100	1.85413700
C	-3.76201500	-2.05153600	-2.46100300
C	-2.85485500	-3.22209600	-2.00030000
C	-2.90591400	-4.39934800	-3.00815500
C	3.87813900	-0.57063000	2.90439700
C	3.67660400	-2.05238600	2.48933300
C	4.20251400	-3.01581800	3.58448600
C	3.58807400	-2.51885300	-0.07053800
C	4.32804500	-2.32537400	1.12773600
C	5.73147900	-2.40131200	1.03028000
C	6.36037300	-2.67015500	-0.19594800
C	5.59535400	-2.86561700	-1.35402400
C	4.18508100	-2.78738100	-1.32943700
C	-2.53648100	-3.17809200	4.30431800
C	-1.81351700	-3.72000500	3.04687100
C	-1.09431500	-5.05837300	3.37503400
C	3.88712700	-2.01553400	-3.73795500
C	3.40384500	-2.98902500	-2.63377500
C	3.50626700	-4.46231500	-3.11351200
H	-0.05307600	3.86158200	-1.93263800
H	-2.09968400	3.95293700	-0.54360800
H	-0.36303900	-4.70395000	-0.12179800
H	1.89182400	-4.36786500	-0.44209600
H	2.59905500	6.92612000	1.16290100
H	5.00339200	6.60557600	0.61928600

H	5.82550600	4.37977700	-0.07877900
H	-0.00876800	4.25562100	0.82842400
H	-2.04306700	1.75914000	1.80149900
H	0.97386500	6.28094500	2.91054000
H	0.78369700	4.52735500	3.14519000
H	-0.64227400	5.54546600	2.84568900
H	0.46260600	7.28331200	0.48466200
H	-1.10136400	6.45797700	0.49165100
H	0.05961200	6.17020800	-0.83084200
H	-4.14976100	0.27905600	3.46708800
H	-2.38066600	0.20700000	3.67099600
H	-3.11796400	-0.41212300	2.18258000
H	-2.86229100	3.87759100	2.92017500
H	-2.14263300	2.71554600	4.05229600
H	-3.90572300	2.90234700	3.97568200
H	-5.70373600	2.12169100	2.72815400
H	-7.51400100	2.48529800	1.06925300
H	-6.99825100	2.56482100	-1.35591000
H	3.83780000	1.25793200	-0.11247200
H	-3.53606100	1.99145900	-2.77186000
H	6.68161100	2.43997800	-0.08216800
H	6.18779100	0.74995400	0.08132300
H	5.81164000	1.90955600	1.37534700
H	5.31110100	2.78773400	-2.32473200
H	3.68868200	2.04837300	-2.43107300
H	5.12252000	1.01996400	-2.23750300
H	-5.38444900	0.32251700	-3.04227100
H	-5.17654500	1.35610800	-4.47156000
H	-6.53019100	1.64182200	-3.36472000
H	-5.73125800	4.13663800	-3.02253800
H	-4.45644100	3.80146100	-4.21417300
H	-4.03436400	4.45628500	-2.61759000
H	-5.17615900	-4.42210900	-1.19629800
H	-5.85676900	-5.15011300	1.07568000
H	-4.33991400	-4.81687600	3.00977400
H	-1.83030200	-2.83711400	-2.00416500
H	2.59599200	-2.20604100	2.40683900
H	-4.81902100	-2.35108300	-2.49902500
H	-3.46059200	-1.72610600	-3.46492800
H	-3.65781800	-1.19630600	-1.78438500
H	-2.25707600	-5.22830900	-2.69440100
H	-2.56321400	-4.05591100	-3.99203600
H	-3.92375600	-4.79511100	-3.12561000
H	4.94553200	-0.32213800	2.97941800
H	3.41521900	-0.38673400	3.88278200
H	3.40907000	0.09859100	2.17675800
H	4.07395600	-4.06719200	3.29456200
H	3.65215400	-2.84837200	4.51962400
H	5.26669000	-2.85322900	3.79765200
H	6.33501200	-2.25584900	1.92160300
H	7.44514800	-2.72584200	-0.24748400
H	6.09446700	-3.06600000	-2.29762900



H	-1.05044700	-2.98062300	2.77712700
H	2.35314700	-2.73801700	-2.47413100
H	-3.25134000	-3.90543100	4.71065100
H	-3.07634000	-2.25170400	4.08288700
H	-1.80192100	-2.96551100	5.09183100
H	-0.39792200	-4.92169100	4.21263000
H	-0.52288700	-5.43490200	2.51673400
H	-1.82059000	-5.83135900	3.65898100
H	3.74705700	-0.97922400	-3.41561900
H	3.28305000	-2.16064200	-4.64205700
H	4.94177300	-2.17340700	-4.00280600
H	3.14119100	-5.17172500	-2.35635800
H	4.54332500	-4.73793600	-3.34836800
H	2.90631600	-4.60027300	-4.02204000
O	0.95139900	2.15054700	1.40552900
O	-0.05942800	1.14755700	1.06086000
O	1.82076300	1.48638400	-0.67313600
O	-1.06767500	-1.55615800	0.52509600
O	-0.07500400	1.81225200	-2.14501800

## 9.7 Structures with ten oxygen atoms

## Bisozone Complex

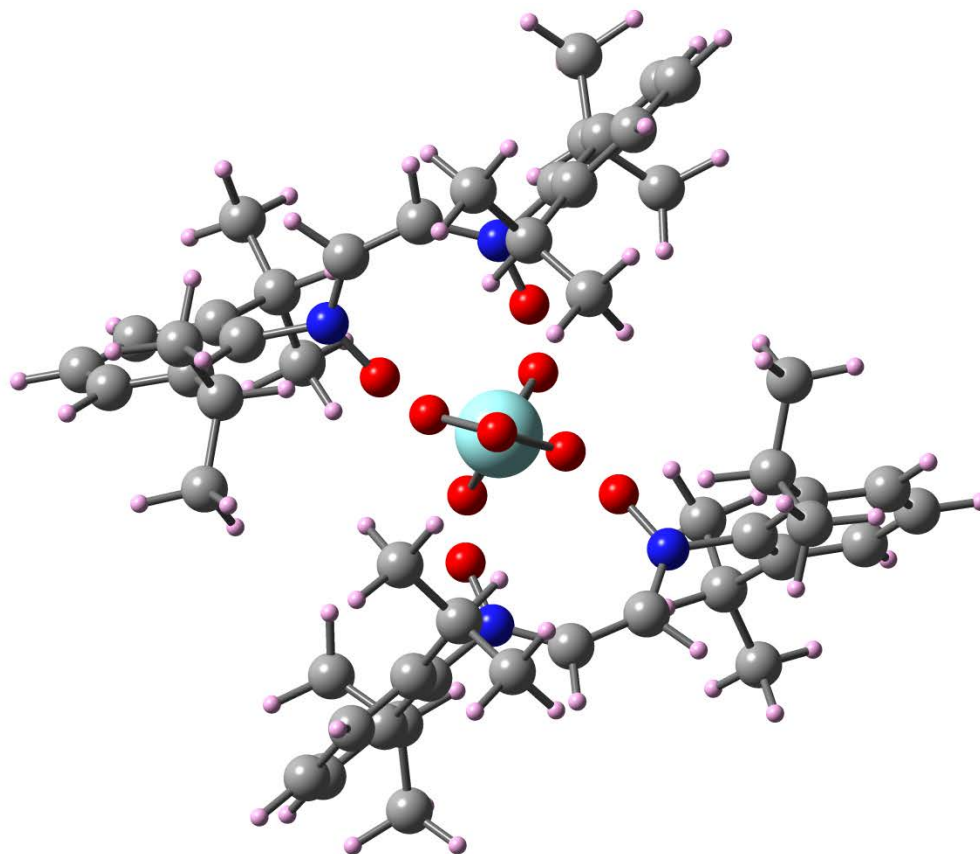


Fig. S129: ONCCNO Bisozone Complex

SCF	E <sub>ZP</sub>	H	G
-3042.041589	-3040.872886	-3040.797459	-3040.988246

O	0.41597868	2.16008176	-0.13592893
O	-0.40971900	-2.12561414	-0.13503583
O	-1.11341890	0.26107701	1.28679494
N	2.90345598	-1.73175640	-0.47572813
N	0.10681517	-3.13669449	0.55003205
N	-2.88685052	1.67906078	-0.51348668
N	-0.13605590	3.17907255	0.50627263
C	2.61574531	-2.81533552	0.24736256
C	1.40669054	-3.41259511	0.70852475
C	-2.63326300	2.78571833	0.18747515
C	-1.44546602	3.42595637	0.64344312
C	4.30741773	-1.43837552	-0.80599554
C	4.75049777	-1.75940104	-2.11262389
C	6.09858406	-1.47241204	-2.41120369
C	6.94467530	-0.89048451	-1.45266474

C	6.45629085	-0.55892653	-0.17955061
C	5.11244169	-0.81074598	0.17325774
C	3.39898417	-1.21669898	-4.17812363
C	3.81854466	-2.33450834	-3.18324980
C	4.44471068	-3.54101379	-3.92625644
C	-2.54236863	-4.09745285	-2.01775209
C	-1.36477218	-4.83095186	-1.32009100
C	-1.14366980	-6.23917164	-1.92769036
C	-0.89633473	-4.05878926	1.10895559
C	-1.59544537	-4.88523877	0.19395355
C	-2.55772605	-5.76027105	0.73888187
C	-2.79969061	-5.80035527	2.12197691
C	-2.09722253	-4.95233990	2.99145871
C	-1.13216344	-4.04366265	2.50465816
C	4.78248417	1.13763362	1.76733480
C	4.58084632	-0.38388976	1.54604981
C	5.24945122	-1.19993780	2.68393856
C	-1.42422906	-2.23221985	4.26807261
C	-0.41355929	-3.09747744	3.47378072
C	0.51557828	-3.88591057	4.43487479
C	-4.27717916	1.33805218	-0.84953173
C	-5.08197976	0.73034682	0.14257890
C	-6.41526987	0.43555897	-0.21719446
C	-6.89325166	0.70656053	-1.50838510
C	-6.04681254	1.26923868	-2.47805071
C	-4.70976857	1.59836014	-2.17355154
C	-4.73630628	-1.15069420	1.81114024
C	-4.55949801	0.36515110	1.53674705
C	-5.25709081	1.20930255	2.63603256
C	2.46200045	4.18478390	-2.09142751
C	1.26407292	4.89200715	-1.40110520
C	0.99190004	6.28012970	-2.03370281
C	0.83661547	4.14602521	1.04297365
C	1.49984855	4.98177416	0.11028443
C	2.43341003	5.89924485	0.63500005
C	2.68272005	5.96957277	2.01556668
C	2.01719608	5.11048827	2.90320369
C	1.08200449	4.16080205	2.43668162
C	-3.31784688	1.01315537	-4.20071168
C	-3.77764236	2.15613081	-3.25327508
C	-4.42344172	3.31838116	-4.04817096
C	1.44861391	2.37955134	4.21547100
C	0.40260415	3.20369753	3.42289723
C	-0.54115101	3.97307890	4.38481436
H	3.50376794	-3.36659557	0.53612566
H	1.56563083	-4.31384640	1.28925758
H	-3.53814927	3.31956368	0.45623092
H	-1.63300772	4.33912831	1.19641239
H	6.48592482	-1.70245405	-3.39952770
H	7.98204078	-0.68216867	-1.70422679
H	7.11623208	-0.08498552	0.54216407
H	2.89686798	-2.68510577	-2.70440001

H	-0.46855289	-4.23640496	-1.52709312
H	4.27953700	-0.78368568	-4.67313871
H	2.84876709	-0.42272841	-3.66421967
H	2.73765556	-1.63153122	-4.94927423
H	5.31624445	-3.24469373	-4.52431821
H	3.70744976	-3.97153827	-4.61590914
H	4.76362343	-4.32804163	-3.22965071
H	-3.49440535	-4.61607754	-1.83770001
H	-2.36822394	-4.05567105	-3.09993186
H	-2.62115139	-3.06743250	-1.65675904
H	-0.31703265	-6.76831148	-1.43499000
H	-0.90329650	-6.14698108	-2.99450588
H	-2.04166430	-6.86515181	-1.84629625
H	-3.11813894	-6.41448240	0.07725340
H	-3.54278393	-6.48708388	2.52061146
H	-2.30844605	-4.98278194	4.05693253
H	3.49992357	-0.55584768	1.58977560
H	0.19850982	-2.39014571	2.90649063
H	5.84474837	1.41651942	1.76299984
H	4.36075347	1.43075327	2.73701013
H	4.26978498	1.71546107	0.98977150
H	6.33521864	-1.03593651	2.71092111
H	5.07860737	-2.27851265	2.56374777
H	4.83781321	-0.89846514	3.65582159
H	-2.02018175	-1.62032860	3.58324038
H	-0.87994277	-1.55090912	4.93393622
H	-2.09818676	-2.84463448	4.88253828
H	-0.05668876	-4.57451203	5.07105868
H	1.05483787	-3.19031151	5.09062572
H	1.25930965	-4.48110002	3.88725903
H	-7.07475966	-0.02493745	0.51357435
H	-7.92235599	0.46572702	-1.76485736
H	-6.42553379	1.45203103	-3.47942325
H	-3.48251351	0.55972359	1.58604418
H	0.38725299	4.26402948	-1.59253479
H	-5.79348634	-1.44784197	1.80713863
H	-4.31919124	-1.40176640	2.79439788
H	-4.20639351	-1.74669916	1.05927685
H	-5.10793208	2.28595751	2.47648377
H	-4.84980477	0.95414125	3.62289693
H	-6.33936294	1.02306285	2.65835679
H	3.39918966	4.73151183	-1.91663815
H	2.28914060	4.12705265	-3.17309032
H	2.56804628	3.16063553	-1.72101385
H	0.15120423	6.79089766	-1.54532348
H	0.74774078	6.15925614	-3.09681027
H	1.86878500	6.93764370	-1.97128978
H	2.96657051	6.56191124	-0.04064419
H	3.40328280	6.68874751	2.39808809
H	2.23445859	5.16518734	3.96652559
H	-2.87124393	2.54673126	-2.77651737
H	-0.19320039	2.47240783	2.86879354

H	-4.18083533	0.54375406	-4.69373999
H	-2.75892043	0.25055444	-3.64979116
H	-2.65285955	1.41491463	-4.97549556
H	-3.68856958	3.74054428	-4.74551789
H	-4.76932118	4.12313269	-3.38542901
H	-5.28066886	2.97867540	-4.64390730
H	2.05752306	1.77996437	3.53097746
H	0.93367016	1.68836681	4.89426164
H	2.10873871	3.02053246	4.81550743
H	-1.31017758	4.53572883	3.83786321
H	0.01502078	4.68846533	5.00551661
H	-1.04953716	3.26860925	5.05565280
O	-0.46983278	-1.01927215	-2.42787277
O	0.58957890	1.05809255	-2.39213978
O	0.02896117	0.03265987	2.22607145
O	1.15893161	-0.22127868	1.27833514
O	-1.98819255	0.83839580	-1.03562493
O	2.03699666	-0.87244083	-1.01453430
O	0.08841098	0.02168662	-3.35154711
Zr	0.02187148	0.01231114	-0.59144603

## 10. ONCCNO Triplet Ground States

### 10.1 Structures with four oxygen atoms

#### Bare Complex

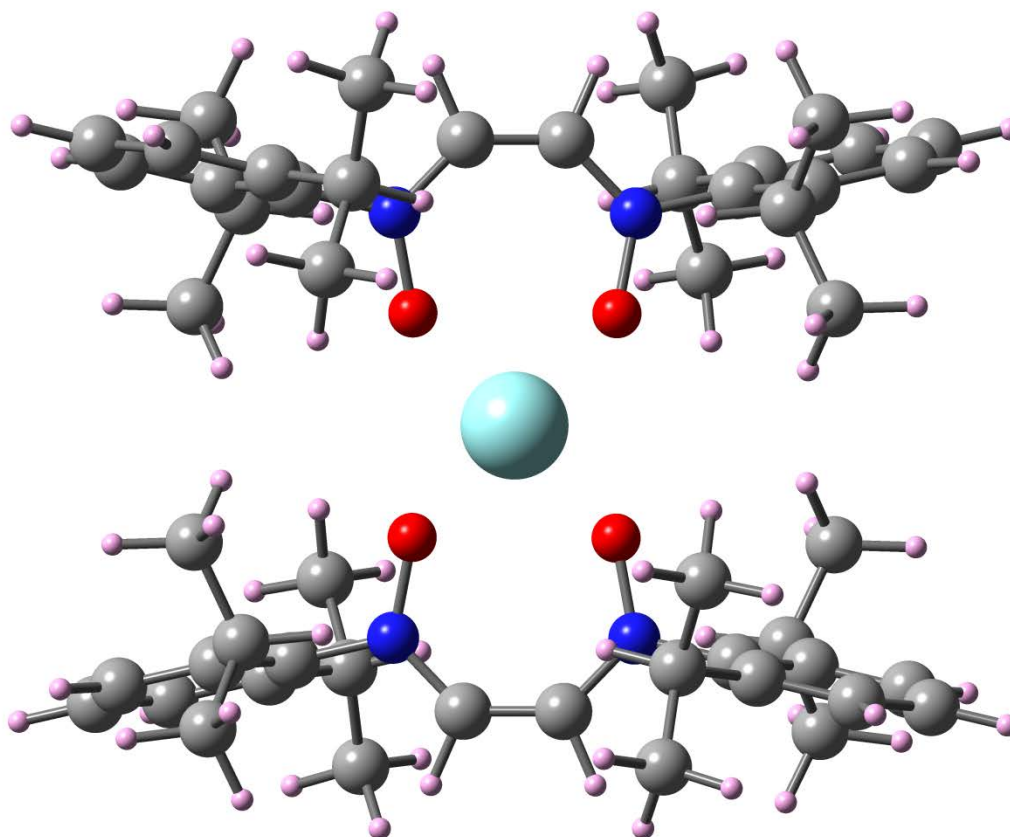


Fig. S130: ONCCNO Bare Complex

SCF	E <sub>ZP</sub>	H	G
-2590.980253	-2589.833472	-2589.763183	-2589.951545

O	1.37418114	1.50042623	-0.17489901
O	-1.37366416	-1.50138432	-0.17680102
N	1.60821134	-2.85739342	0.38946307
N	-1.62911615	-2.84685354	-0.39422205
N	-1.60836135	2.85669034	0.38710407
N	1.62903914	2.84555846	-0.39551805
C	0.65891123	-3.83624161	0.16471503
C	-0.68728897	-3.83191265	-0.16534701
C	-0.65888125	3.83542652	0.16285103
C	0.68732396	3.83089456	-0.16711001
C	2.96603156	-3.17366141	0.77417913
C	3.96772971	-3.23113439	-0.23064603

C	5.28480493	-3.53889238	0.16889403
C	5.59188997	-3.78188342	1.51778125
C	4.58795783	-3.70602043	2.49600639
C	3.25804862	-3.38884344	2.14638934
C	4.28918971	-1.59933712	-2.14124633
C	3.65330466	-2.94492136	-1.70054425
C	4.10232978	-4.10305752	-2.62769239
C	-2.54187631	-2.06496645	-4.18553663
C	-2.22458323	-3.25127462	-3.23672249
C	-2.06332216	-4.57135582	-4.03351561
C	-2.99063635	-3.15394263	-0.77323411
C	-3.28936138	-3.37206668	-2.14357232
C	-4.62355159	-3.67743077	-2.48731337
C	-5.62475674	-3.74023381	-1.50534122
C	-5.31056469	-3.49564777	-0.15842201
C	-3.98925649	-3.19862767	0.23525005
C	2.52687046	-2.08583927	4.19791065
C	2.19028845	-3.25515346	3.23504950
C	1.99718446	-4.57983667	4.01728161
C	-4.29851161	-1.56442544	2.14641533
C	-3.66721046	-2.91124662	1.70331227
C	-4.11406648	-4.06833481	2.63297441
C	-2.96554458	3.17272533	0.77412713
C	-3.25512663	3.38876235	2.14673333
C	-4.58436684	3.70629235	2.49850639
C	-5.59010701	3.78125833	1.52206423
C	-5.28549795	3.53707631	0.17282703
C	-3.96909573	3.22924431	-0.22889203
C	-2.52288046	2.09271419	4.20268065
C	-2.18527245	3.25637038	3.23346551
C	-1.98632348	4.58421859	4.00899361
C	2.54546030	2.07005237	-4.19570163
C	2.22205721	3.24780054	-3.23846548
C	2.05055614	4.57207373	-4.02625761
C	2.99021634	3.15261355	-0.77565711
C	3.28780137	3.36958060	-2.14639233
C	4.62133656	3.67639569	-2.49136837
C	5.62316673	3.74114673	-1.51017222
C	5.31024871	3.49711769	-0.16283501
C	3.98955348	3.19903659	0.23205705
C	-4.29290372	1.59548404	-2.13738731
C	-3.65732368	2.94194927	-1.69913925
C	-4.10912578	4.09903444	-2.62629639
C	4.30183760	1.56670035	2.14428233
C	3.66880445	2.91250454	1.70055027
C	4.11508548	4.07077673	2.62901341
H	1.08481533	-4.82751174	0.28509205
H	-1.12058800	-4.82045882	-0.28166003
H	-1.08468735	4.82674466	0.28325405
H	1.12070899	4.81933974	-0.28393803
H	6.07342507	-3.59046736	-0.57787508
H	6.61265918	-4.02284941	1.80633529

H	4.84126188	-3.88195546	3.53882255
H	2.56797848	-2.83821139	-1.80211527
H	-1.26514609	-3.03379855	-2.75552141
H	5.38442090	-1.63224110	-2.06255131
H	3.92447162	-0.77519701	-1.51787422
H	4.03214566	-1.38128110	-3.18690449
H	5.19177194	-4.23889650	-2.60951439
H	3.81205472	-3.88994750	-3.66517855
H	3.63979074	-5.05359767	-2.33191835
H	-3.48578346	-2.22378751	-4.72414671
H	-1.74340420	-1.94932340	-4.93091474
H	-2.62518736	-1.12702931	-3.62290854
H	-1.80913808	-5.40809597	-3.37024351
H	-1.26288403	-4.47135877	-4.77865672
H	-2.98597528	-4.83452789	-4.56767569
H	-4.88223161	-3.85476980	-3.52855253
H	-6.64878992	-3.97235089	-1.78954927
H	-6.09687181	-3.53714281	0.59144310
H	1.23840529	-3.01253746	2.75077043
H	-2.58125030	-2.80647156	1.79978628
H	3.46097161	-2.27207326	4.74474773
H	1.72387233	-1.95761928	4.93633377
H	2.63859744	-1.14516512	3.64489057
H	2.91280562	-4.86909268	4.55007271
H	1.72602145	-5.40341381	3.34435752
H	1.19735634	-4.47022268	4.76173374
H	-3.93589458	-0.74129731	1.52046724
H	-4.03538858	-1.34602039	3.19049049
H	-5.39421581	-1.59536048	2.07388433
H	-5.20371665	-4.20298187	2.61863241
H	-3.81975045	-3.85500478	3.66928057
H	-3.65361238	-5.01950594	2.33599236
H	-4.83575789	3.88306938	3.54164555
H	-6.61035318	4.02241233	1.81230628
H	-6.07552210	3.58785228	-0.57251008
H	-1.23530831	3.00864237	2.74799643
H	1.26506307	3.02065346	-2.75681941
H	-3.45425561	2.28476219	4.75213973
H	-1.71773234	1.96475920	4.93879976
H	-2.64011045	1.14999404	3.65429556
H	-1.71351246	5.40355071	3.33158651
H	-1.18564135	4.47557260	4.75267673
H	-2.90019563	4.87906260	4.54174070
H	3.48587144	2.23964543	-4.73712071
H	1.74507319	1.95247732	-4.93870975
H	2.63854135	1.12941223	-3.63915455
H	1.79041707	5.40231285	-3.35717050
H	1.25062301	4.47134169	-4.77184571
H	2.97125627	4.84558881	-4.55860169
H	4.87901960	3.85320873	-3.53294953
H	6.64670491	3.97434981	-1.79527027
H	6.09707983	3.54003573	0.58639810



H	-2.57212750	2.83602730	-1.80272227
H	2.58304129	2.80657748	1.79781328
H	-5.38804788	1.62757601	-2.05710331
H	-3.92660164	0.77235794	-1.51358022
H	-4.03720868	1.37637902	-3.18314947
H	-3.82133673	3.88511841	-3.66430455
H	-3.64620875	5.05001060	-2.33251535
H	-5.19856896	4.23447341	-2.60547639
H	3.93988157	0.74275622	1.51900924
H	4.03934956	1.34869231	3.18859349
H	5.39747776	1.59881740	2.07127733
H	3.65332237	5.02122286	2.33172937
H	5.20457263	4.20664179	2.61362441
H	3.82188343	3.85789069	3.66572657
O	1.36298627	-1.51081922	0.16732303
O	-1.36346327	1.51015415	0.16377103
Zr	-0.00004401	-0.00041404	-0.00617499

## 10.2 Structures with five oxygen atoms

### Oxo Complex (conformation 1 lower energy)

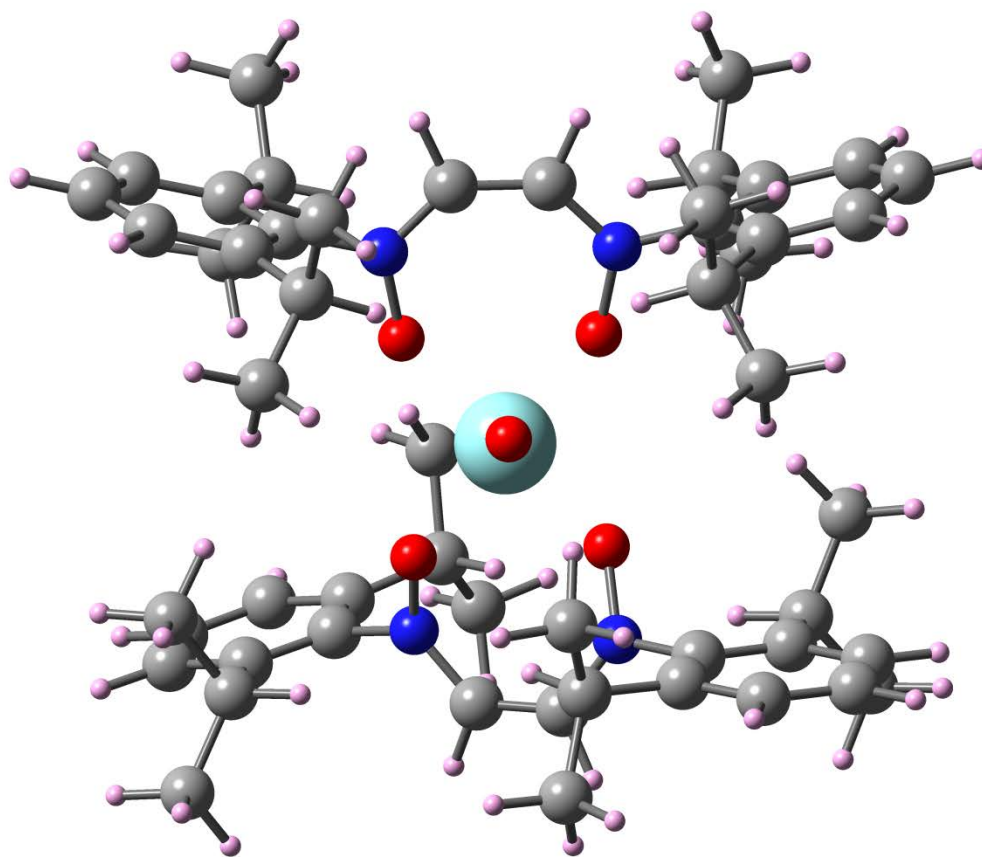


Fig. S131: ONCCNO Oxo Complex (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G
-2666.284443	-2665.133275	-2665.062285	-2665.250380

N	-1.77126114	-2.57797320	-0.51624804
N	1.66161713	2.82103922	0.04463100
C	-0.82563806	-3.55987627	-0.51543204
C	0.52443604	-3.62592928	-0.14897601
C	0.84816507	3.88530930	0.28803602
C	-0.49120504	3.89629830	0.68940505
C	-3.10797324	-2.83025822	-1.03235908
C	-4.12587732	-3.19540124	-0.11591101
C	-5.40995539	-3.45396326	-0.63836705
C	-5.66265145	-3.34390226	-2.01569816
C	-4.64008335	-2.95465523	-2.89535622
C	-3.33985825	-2.67463421	-2.42214518
C	-4.64373735	-2.15290816	2.13233816
C	-3.87165129	-3.27689325	1.39139510

C	-4.22826232	-4.67116036	1.96687015
C	2.51227319	-2.34942318	4.01356531
C	2.20062317	-3.52621727	3.04956224
C	2.18094617	-4.87755637	3.80677329
C	2.81070521	-3.11233024	0.57854904
C	3.18940625	-3.52595827	1.88111914
C	4.53443535	-3.89939630	2.07948016
C	5.45787144	-3.85582430	1.02151108
C	5.05822839	-3.41870926	-0.25091702
C	3.72613029	-3.02269223	-0.49975904
C	-2.67975120	-0.95853207	-4.18482732
C	-2.24571717	-2.21816417	-3.39245026
C	-1.84452014	-3.36410025	-4.35871633
C	4.16436932	-1.26480110	-2.28452917
C	3.32265525	-2.50364719	-1.88348315
C	3.43585826	-3.61832528	-2.95668723
C	2.97215023	2.95139423	-0.56016004
C	3.06408023	3.19037924	-1.95705515
C	4.35783633	3.30450925	-2.51086319
C	5.50378540	3.16183724	-1.71491313
C	5.38177141	2.90716422	-0.33872203
C	4.11548431	2.80146021	0.27033202
C	1.85171214	2.25747517	-3.99885431
C	1.83971914	3.32131325	-2.87003722
C	1.73699913	4.75731336	-3.45099427
C	-1.91128214	0.63380305	3.78900729
C	-1.66490713	2.13484216	3.47409126
C	-1.39476111	2.93695223	4.77155637
C	-2.71765621	3.04151323	1.29605510
C	-2.83532422	2.70796621	2.66920020
C	-4.10211332	2.86495722	3.27045425
C	-5.20266540	3.31855225	2.52625219
C	-5.06223339	3.61395528	1.16024909
C	-3.81673429	3.47748026	0.51298704
C	4.46960634	1.08776909	2.10443016
C	4.00862431	2.53202219	1.77410413
C	4.80226937	3.57444127	2.60329220
C	-4.42021734	2.65838320	-1.80219714
C	-3.68696828	3.75678129	-0.98617608
C	-4.19988432	5.16930840	-1.36499010
H	-1.21589710	-4.48973834	-0.91589607
H	0.97721007	-4.59716735	-0.31961602
H	1.33197810	4.85010137	0.17248901
H	-0.87820007	4.83802137	1.06620608
H	-6.21515848	-3.73929729	0.03410900
H	-6.65826552	-3.55173327	-2.40139318
H	-4.85433837	-2.85546922	-3.95638430
H	-2.80529421	-3.10386223	1.57078712
H	1.19534509	-3.35237426	2.65045320
H	-5.72901943	-2.26405017	2.00508015
H	-4.35312533	-1.16750809	1.75067113
H	-4.42378334	-2.18566617	3.20799325

H	-5.29820840	-4.89203937	1.85829514
H	-3.98757031	-4.71169636	3.03758123
H	-3.66766528	-5.46768641	1.46056611
H	3.51345227	-2.45251819	4.45376134
H	1.78141814	-2.32449118	4.83333137
H	2.46576619	-1.39432011	3.47855627
H	1.95551615	-5.71233341	3.13051124
H	1.41417511	-4.85781437	4.59253435
H	3.14394824	-5.08683439	4.29061533
H	4.86169237	-4.22481032	3.06363723
H	6.49016147	-4.15329232	1.19204509
H	5.78716442	-3.37237626	-1.05583708
H	-1.35543710	-1.93216014	-2.82346921
H	2.27960417	-2.17289417	-1.85394214
H	-3.52801127	-1.16560409	-4.85173737
H	-1.84186914	-0.60247705	-4.79657637
H	-2.96507722	-0.14724601	-3.50464027
H	-2.69248121	-3.67675228	-4.98347238
H	-1.48855511	-4.24581232	-3.80942629
H	-1.03752408	-3.03015323	-5.02356438
H	4.07046931	-0.46644204	-1.53922912
H	3.80653029	-0.86909206	-3.24301225
H	5.22934140	-1.51286612	-2.39244018
H	4.47104834	-3.97057030	-3.06288224
H	3.10754124	-3.23529525	-3.93148630
H	2.81043921	-4.48485634	-2.70387021
H	4.46550934	3.49122727	-3.57616728
H	6.49023249	3.24397825	-2.16576817
H	6.27723949	2.79703221	0.26759602
H	0.93730707	3.13508624	-2.27934017
H	-0.75892206	2.19137317	2.86100522
H	2.76159721	2.32272018	-4.61096035
H	0.98880508	2.41146618	-4.66114536
H	1.76645814	1.25147209	-3.57384427
H	1.69576913	5.51362841	-2.65548820
H	0.82977906	4.85384437	-4.06173131
H	2.59866420	4.99099238	-4.09045031
H	-2.79560622	0.50335004	4.42742034
H	-1.04536808	0.21071802	4.31547733
H	-2.06963316	0.05549400	2.87040622
H	-1.20025709	3.99502031	4.55371935
H	-0.51782204	2.52852419	5.29068541
H	-2.24429117	2.88654622	5.46533040
H	-4.23042333	2.62198620	4.32217833
H	-6.17147648	3.43190126	3.00747223
H	-5.92638344	3.95063730	0.59341704
H	2.95620622	2.60264220	2.06577016
H	-2.62784320	3.69963228	-1.25896009
H	5.51928542	0.93020507	1.82126714
H	3.85221529	0.35603903	1.57258512
H	4.37775834	0.89697407	3.18244024
H	4.65075735	3.39450526	3.67605928

H	4.47511634	4.59824535	2.37884918
H	5.88095246	3.51592927	2.40733218
H	-4.01816931	1.66804813	-1.56111912
H	-4.28692633	2.83254522	-2.87825022
H	-5.49795741	2.65628120	-1.58906712
H	-3.67503428	5.95178146	-0.80134906
H	-5.27477240	5.27764540	-1.16930709
H	-4.03850731	5.35312043	-2.43534119
O	0.45139103	-0.15688401	-2.02657916
O	-1.28533310	1.78076714	-0.15017101
O	1.11176608	-1.44083211	0.74616006
N	-1.42152111	2.89812422	0.65865705
N	1.42573411	-2.73359421	0.34983903
O	-1.58999712	-1.30883110	0.01144900
O	1.35376110	1.56133812	0.55925604
Zr	0.02331700	0.07988501	-0.27726002

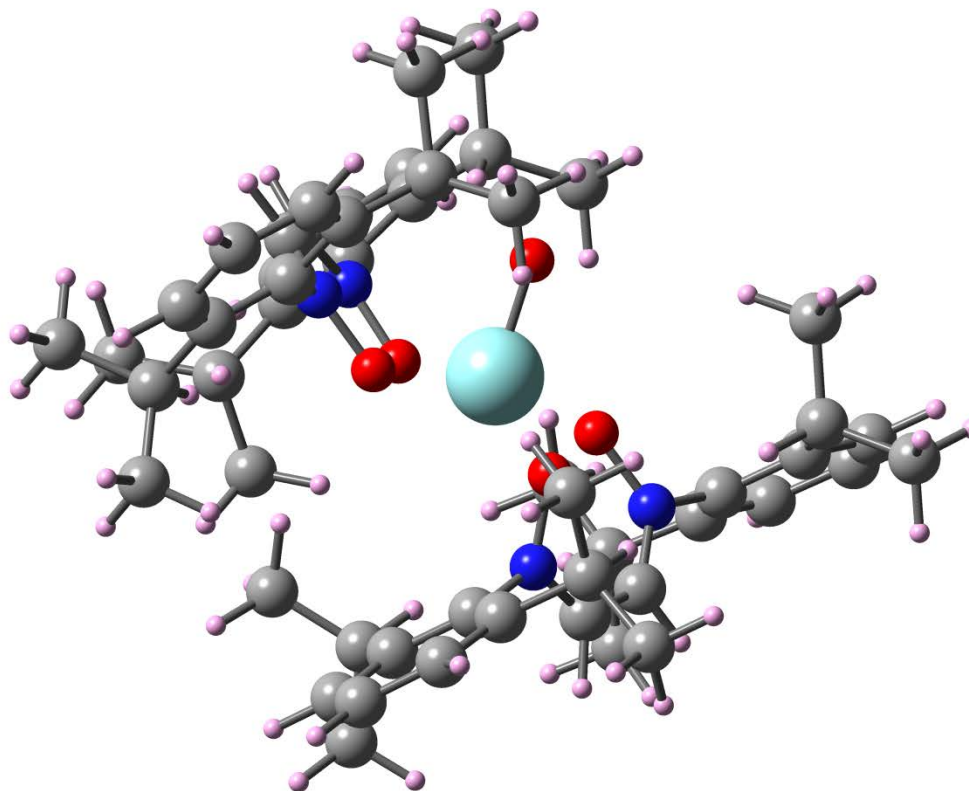
**Oxo Complex (conformation 2 higher energy)**

Fig. S132: ONCCNO Oxo Complex (conformation 2 higher energy)

SCF	$E_{ZP}$	H	G
-2666.253850	-2665.102393	-2665.031645	-2665.215720

Zr	-0.10506125	-0.14509464	-0.65119304
O	-2.01309581	-0.98920312	-0.34416869
O	1.94756449	0.43564589	-0.21543680
N	-0.30734438	2.94582662	-0.00491646
N	2.60948920	1.52899055	-0.73999659
N	0.35989761	-2.75086099	0.91853701
N	-2.71071386	-2.05693126	0.17396591
C	0.85835072	3.37885927	-0.55865950
C	2.09216598	2.77886055	-0.86324487
C	-0.83903542	-3.23211564	1.39034644
C	-2.15792417	-2.98022194	1.01479841
C	-1.42904925	3.85550042	0.17713966
C	-2.32877143	4.04871346	-0.90153932
C	-3.40262769	4.94124001	-0.69162420
C	-3.57683795	5.58915423	0.54096008
C	-2.68392816	5.35333263	1.59978895

C	-1.59045056	4.47764747	1.44141521
C	-3.39913795	2.36474166	-2.46837776
C	-2.19179491	3.31207428	-2.23756099
C	-2.03362616	4.30186016	-3.42056714
C	3.05876244	-0.69886395	-4.14412831
C	3.07684412	0.72221806	-3.52535698
C	3.18247886	1.80125708	-4.63572851
C	3.98015651	1.25913199	-1.15996604
C	4.20889545	0.87371164	-2.50556779
C	5.54647222	0.63739228	-2.88993586
C	6.59948515	0.76615648	-1.97103774
C	6.33753559	1.13052044	-0.64056739
C	5.01955180	1.37845626	-0.20381066
C	-1.36564641	3.25755621	3.64335629
C	-0.65465859	4.17960784	2.61551805
C	-0.12357936	5.46603167	3.29488774
C	5.29707543	0.70039185	2.23427466
C	4.75378168	1.76992297	1.25225338
C	5.34785094	3.16723598	1.57353038
C	1.60030415	-3.07541348	1.59273429
C	1.89788198	-2.44096432	2.82953719
C	3.10972018	-2.78099893	3.46668513
C	3.99859371	-3.70082398	2.89027142
C	3.68441755	-4.30878755	1.66404817
C	2.47931420	-4.01894780	0.99295225
C	1.69279172	-0.00816176	3.53804829
C	0.98603506	-1.38739893	3.46965938
C	0.49493805	-1.83086445	4.87228482
C	-3.23907213	-2.35006310	-3.56831105
C	-3.45750165	-3.29350553	-2.35350668
C	-3.83535180	-4.72227302	-2.81745485
C	-4.11790969	-2.07644787	-0.17834070
C	-4.49363368	-2.69532972	-1.39868235
C	-5.86380791	-2.69482446	-1.73322638
C	-6.81356137	-2.09793140	-0.88800045
C	-6.41070238	-1.47507204	0.30391766
C	-5.05112521	-1.44240524	0.68015756
C	3.11560194	-4.24293245	-1.44981976
C	2.15589212	-4.72087241	-0.32891811
C	2.19336408	-6.26429354	-0.18442796
C	-4.88328774	0.81186342	1.83121558
C	-4.62297377	-0.71269701	1.95621085
C	-5.31768535	-1.29365233	3.21473301
H	0.80518697	4.42788286	-0.82914101
H	2.80404384	3.46285490	-1.31306700
H	-0.71909335	-3.93416654	2.20958790
H	-2.90296097	-3.61561191	1.48327547
H	-4.11027482	5.12026035	-1.49691398
H	-4.41332170	6.27021641	0.68065087
H	-2.83969616	5.85167314	2.55311382
H	-1.30175918	2.67507817	-2.21799836
H	2.11111282	0.85227079	-3.02722634

H	-4.34455321	2.92105711	-2.53477035
H	-3.48403182	1.63161962	-1.65766679
H	-3.25792283	1.80998418	-3.40401785
H	-2.92478790	4.93210543	-3.54509513
H	-1.88294042	3.74387096	-4.35330598
H	-1.16970598	4.96477105	-3.27816026
H	3.96057219	-0.90052790	-4.73910230
H	2.18514558	-0.80178127	-4.79929529
H	2.98326184	-1.46497561	-3.36333963
H	3.15590581	2.81523101	-4.21436940
H	2.33975056	1.70301844	-5.33180602
H	4.11363305	1.69977855	-5.21036345
H	5.76113879	0.34461931	-3.91446425
H	7.62249601	0.57875590	-2.28952752
H	7.16117658	1.21925864	0.06339626
H	0.20998944	3.62481587	2.23446259
H	3.67012783	1.82553914	1.40228824
H	-2.25012120	3.74936636	4.07032782
H	-0.68410941	3.00931969	4.46837937
H	-1.68561503	2.32532497	3.16375075
H	-0.93160277	6.04398361	3.76167297
H	0.38403781	6.11906042	2.57340412
H	0.59377339	5.20581196	4.08443606
H	4.85610748	-0.28177980	2.02909556
H	5.05163774	0.97837255	3.26809592
H	6.38888361	0.60721654	2.16407450
H	6.43942004	3.17140212	1.45492112
H	5.12029424	3.45025267	2.61002961
H	4.93559055	3.93906239	0.91074008
H	3.36585183	-2.31074499	4.41296302
H	4.93228927	-3.94210674	3.39311079
H	4.37781735	-5.02389633	1.22867107
H	0.09843209	-1.26206342	2.84084502
H	-2.49960802	-3.35972747	-1.82601021
H	2.57731635	-0.04481613	4.18767222
H	1.00582153	0.74774699	3.94190584
H	2.01113588	0.31322546	2.53961831
H	-0.03834394	-2.78935466	4.82688944
H	-0.18727758	-1.07938816	5.29160611
H	1.33371045	-1.94782311	5.57084078
H	-4.17068509	-2.21443338	-4.13514261
H	-2.48553143	-2.77374970	-4.24527646
H	-2.88199702	-1.36777986	-3.24054529
H	-3.99237314	-5.39354349	-1.96299253
H	-3.02927468	-5.13864995	-3.43554429
H	-4.75054393	-4.72702586	-3.42407428
H	-6.18887996	-3.15979507	-2.66013538
H	-7.86588553	-2.11040659	-1.16301902
H	-7.15521604	-1.00350471	0.94068845
H	1.14642495	-4.43408999	-0.63609052
H	-3.54258056	-0.84300310	2.08270597
H	4.15954428	-4.49769584	-1.22035679



H	3.04324654	-3.15730229	-1.57422836
H	2.85216332	-4.71867319	-2.40405082
H	1.89573681	-6.73544338	-1.13072031
H	1.50671168	-6.61021242	0.59939168
H	3.19910743	-6.62814571	0.06449358
H	-4.34669454	1.23053326	0.97221785
H	-4.53839418	1.33220712	2.73483394
H	-5.95319293	1.02533399	1.70567567
H	-5.11799691	-2.36772849	3.32383641
H	-6.40632080	-1.15857373	3.17184704
H	-4.95463461	-0.78483385	4.11760548
O	-0.11516071	0.40349957	-2.38050833
O	-0.55139128	1.65765468	0.42529420
O	0.49270791	-2.21639314	-0.37454196

### 10.3 Structures with six oxygen atoms

#### Dioxo Complex (conformation 1 lower energy)

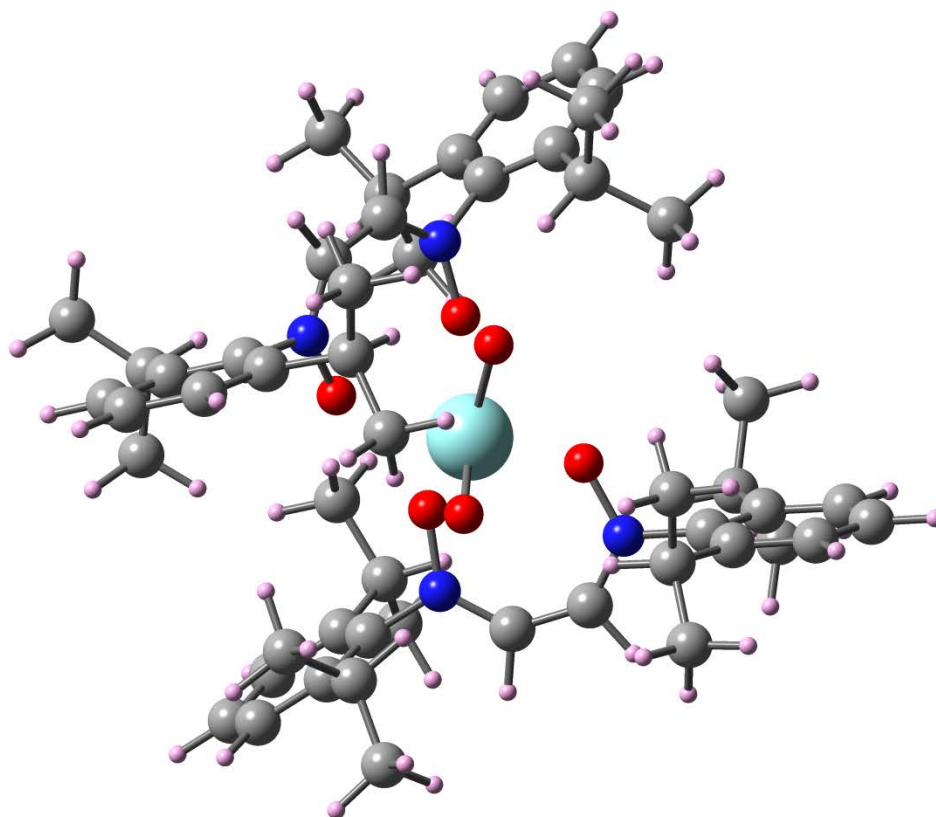


Fig. S133: ONCCNO Dioxo Complex (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G
-2741.425103	-2740.271282	-2740.198744	-2740.388059

O	-0.17049575	1.83097313	0.77831904
O	-2.17980824	-0.47744676	-0.23871104
O	-0.15017880	1.48706910	-1.93868817
N	-0.16865042	-2.77606323	1.17260407
N	-2.91046547	-1.65257074	-0.32887005
N	2.75967942	1.44580967	-0.76221908
N	0.28692847	3.06871315	0.61959702
C	-1.35436459	-3.33505210	0.79579203
C	-2.51014961	-2.85761189	0.16263899
C	2.45684758	2.73644781	-0.67272308
C	1.40349360	3.44681302	-0.00845102
C	0.87949254	-3.59714644	1.76018611
C	1.73755350	-4.32442062	0.89825204
C	2.73408046	-5.12290383	1.50160009

C	2.88132746	-5.16650685	2.89659320
C	2.03638651	-4.40615967	3.72301926
C	1.01620655	-3.60412146	3.17198322
C	2.95256667	-3.81050976	-1.28006712
C	1.62032650	-4.26025360	-0.62809007
C	1.15462327	-5.62127164	-1.20935411
C	-2.82028533	-0.76431069	-4.20118735
C	-3.11096452	-1.94737074	-3.24043927
C	-3.29935273	-3.26919581	-4.02835933
C	-4.21503654	-1.48781354	-0.94929210
C	-4.32144557	-1.64193653	-2.35410520
C	-5.60006264	-1.47484634	-2.92853825
C	-6.71328366	-1.15214815	-2.13652519
C	-6.57040464	-0.97732416	-0.75008408
C	-5.31510360	-1.13545435	-0.12682203
C	0.91423985	-1.47715228	4.53125332
C	0.13082761	-2.73646027	4.07013829
C	-0.43803155	-3.51466025	5.28198238
C	-5.32646233	0.62906678	1.68858711
C	-5.15881253	-0.88181636	1.37496208
C	-6.13618470	-1.73846728	2.21881614
C	3.96695745	1.02194146	-1.49341514
C	3.92334243	0.94838546	-2.90612124
C	5.10327446	0.51178426	-3.54950729
C	6.24447548	0.15626906	-2.81674024
C	6.23817753	0.22357907	-1.41335113
C	5.09400648	0.65636527	-0.71432808
C	2.17474817	0.03513165	-4.50587537
C	2.68402639	1.28678467	-3.74174031
C	2.97308758	2.45999072	-4.71543838
C	-0.16224263	2.67067319	4.39434331
C	0.58792458	3.66966815	3.47161624
C	1.47510379	4.63509310	4.29636730
C	-0.57697345	4.11329036	1.20637507
C	-0.41136639	4.41249236	2.57941617
C	-1.26053031	5.39960156	3.12042721
C	-2.22533730	6.03808974	2.32332515
C	-2.37429236	5.69128173	0.97160005
C	-1.55690243	4.70546755	0.37630700
C	5.00248427	-0.75629583	1.38492008
C	5.08836049	0.68628727	0.81758604
C	6.31254567	1.44246015	1.39289408
C	-3.18225171	3.68535870	-1.28199512
C	-1.77242051	4.30277154	-1.08631811
C	-1.55432932	5.50509363	-2.04133618
H	-1.38776175	-4.39601617	1.02068805
H	-3.26459978	-3.62131484	0.00231998
H	3.16598973	3.37987076	-1.18159112
H	1.52278577	4.52405209	-0.03474503
H	3.40388743	-5.70360495	0.87254704
H	3.65794543	-5.78579501	3.34025323
H	2.16914252	-4.43958969	4.80126735

H	0.87856955	-3.50404244	-0.90374409
H	-2.22102347	-2.05989588	-2.61366722
H	3.76319662	-4.53131193	-1.10299111
H	3.26379783	-2.83325973	-0.89291209
H	2.81447967	-3.70863974	-2.36344820
H	1.87995621	-6.41874583	-0.99627610
H	1.04277327	-5.54510059	-2.29856820
H	0.18680215	-5.92663051	-0.78979009
H	-3.65871136	-0.58580055	-4.88942940
H	-1.92434429	-0.98349584	-4.79502739
H	-2.62691118	0.15592835	-3.63809030
H	-3.47955587	-4.11603385	-3.35272228
H	-2.39508569	-3.48588196	-4.61136237
H	-4.14487779	-3.21041168	-4.72757839
H	-5.72121068	-1.59101233	-4.00256233
H	-7.68959875	-1.02702300	-2.59976822
H	-7.43744770	-0.70999301	-0.15108204
H	-0.71683340	-2.37981212	3.47469224
H	-4.13916249	-1.15461053	1.66732010
H	1.79403288	-1.75595643	5.12783237
H	0.27174990	-0.83443515	5.14884737
H	1.24606296	-0.90144529	3.66043425
H	0.35452847	-3.83195939	5.97250145
H	-0.98572672	-4.41057623	4.96212935
H	-1.12886551	-2.87496210	5.84722741
H	-4.59130717	1.22075272	1.13107506
H	-5.17478028	0.81443878	2.76053518
H	-6.33111037	0.98368996	1.42103108
H	-7.18348675	-1.48232111	2.01120513
H	-5.95942167	-1.56939629	3.28943123
H	-6.00594386	-2.80941438	2.01584813
H	5.11682645	0.43961025	-4.63337338
H	7.13739552	-0.18201709	-3.33710628
H	7.12676054	-0.06378608	-0.85824209
H	1.86297037	1.59370581	-3.08495126
H	1.25481254	3.07354401	2.83748919
H	2.95112917	-0.38777050	-5.15874142
H	1.31794714	0.31468879	-5.13273842
H	1.82948103	-0.73314136	-3.80479232
H	3.32087774	3.35674273	-4.18328434
H	2.05725355	2.72224387	-5.25987943
H	3.73897860	2.19310559	-5.45600545
H	-0.84612260	3.19914533	5.07196436
H	0.55504935	2.10617904	5.00431736
H	-0.74387077	1.95664522	3.80078426
H	2.01410093	5.33926610	3.64918525
H	2.21472176	4.06417695	4.87256835
H	0.88342482	5.22131323	5.01108036
H	-1.16994027	5.66532956	4.17003129
H	-2.86885123	6.79794091	2.76027219
H	-3.13818634	6.17873087	0.37216700
H	4.18855649	1.21097744	1.15917906

H	-1.05859957	3.52130438	-1.37093513
H	5.86802222	-1.35643100	1.07378006
H	4.09073013	-1.25325973	1.03781806
H	4.98223127	-0.73163582	2.48244416
H	6.23205670	1.50709817	2.48587816
H	6.38178782	2.46272022	0.99303205
H	7.25360369	0.92679998	1.16336807
H	-3.31043585	2.79794266	-0.65166408
H	-3.30564776	3.37266770	-2.32600020
H	-3.97884567	4.40282087	-1.04161710
H	-0.54916218	5.93383050	-1.92909417
H	-2.28303926	6.30642780	-1.85882117
H	-1.66829738	5.17716160	-3.08206426
O	0.21303582	-1.35098617	-1.99666218
O	2.08339022	0.45004869	-0.16537204
O	0.12983280	-1.43074417	1.10118406
Zr	-0.12009203	-0.11876803	-0.65927207

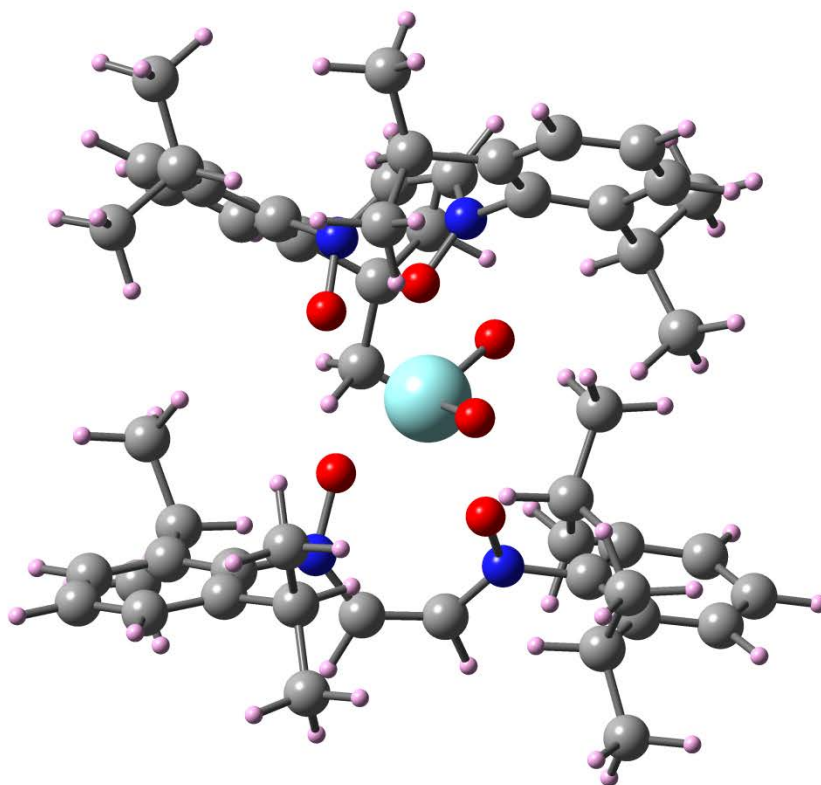
**Dioxo Complex (conformation 2 higher energy)**

Fig. S134: ONCCNO Dioxo Complex (conformation 2 higher energy)

SCF	$E_{ZP}$	H	G
-2741.413097	-2740.257865	-2740.187035	-2740.370078

Zr	-0.26356202	0.31901302	-0.32105802
O	-0.27915602	-1.86806514	-0.35237803
O	1.33113810	1.95761215	-1.06641808
O	-0.95556807	1.57256012	-1.85178914
N	2.70495621	0.16357001	1.09641308
N	1.66695513	2.92614523	-0.19698702
N	-3.21696825	-0.90791607	0.32018302
N	-1.10479408	-2.81878222	-0.94538207
C	2.82242822	1.44414711	1.45374411
C	2.30946617	2.67723820	0.93561007
C	-3.26870625	-2.25981217	0.17412801
C	-2.37224618	-3.08482024	-0.50921704
C	3.53866227	-0.82995306	1.80086314
C	3.03276623	-1.39124610	2.99513523
C	3.85776629	-2.33116818	3.64999228
C	5.10519139	-2.69508720	3.11927624

C	5.55554041	-2.13643216	1.91180215
C	4.77642436	-1.18827909	1.21671109
C	0.73426706	-2.28879717	3.55416827
C	1.65399812	-1.03885408	3.56281027
C	1.76948514	-0.43981603	4.98847938
C	-2.04559416	4.26077432	0.62292105
C	-0.58579504	4.35537433	1.14351609
C	-0.51609004	5.12797639	2.48531719
C	1.34669311	4.30605633	-0.59500105
C	0.30693902	4.99402138	0.07525101
C	0.06461000	6.32403447	-0.33581103
C	0.80304106	6.91300251	-1.37119810
C	1.80154214	6.18181147	-2.03683916
C	2.09649216	4.85501637	-1.66765713
C	5.21481540	-1.74037713	-1.21460409
C	5.25161340	-0.63135305	-0.12870601
C	6.65955651	0.00866800	-0.02983700
C	2.53579319	3.54581527	-3.77917729
C	3.14528824	4.05018931	-2.44159319
C	4.45152834	4.84483237	-2.68659020
C	-4.25175033	-0.15538501	1.00764208
C	-5.24676240	0.48233404	0.21730602
C	-6.23646247	1.22470709	0.89225807
C	-6.24028149	1.32219710	2.29370318
C	-5.24263740	0.68710306	3.04686423
C	-4.21869832	-0.05725000	2.42066619
C	-4.78011636	1.74860413	-1.92618415
C	-5.25523140	0.40397303	-1.31240110
C	-6.64275052	-0.00625300	-1.86853114
C	2.08650516	-4.58186235	0.39576803
C	0.62979305	-4.97404438	0.03257600
C	0.32119302	-6.43344949	0.45250503
C	-0.44767803	-3.67301228	-1.91712414
C	0.37471103	-4.73296236	-1.45697411
C	0.98815708	-5.55186745	-2.42758219
C	0.79325306	-5.31644342	-3.79883029
C	-0.00759600	-4.24588632	-4.22626632
C	-0.63834505	-3.39369926	-3.29458125
C	-2.28517917	0.41101203	3.99130130
C	-3.11655124	-0.68782805	3.27669125
C	-3.70030828	-1.70682013	4.29056433
C	-0.59761104	-1.22084009	-4.61435635
C	-1.46592311	-2.20047217	-3.78156629
C	-2.70517321	-2.66406220	-4.59076835
H	3.48015327	1.57350612	2.30663518
H	2.53852719	3.55464027	1.52865912
H	-4.15311632	-2.72559321	0.59632305
H	-2.71739121	-4.08668431	-0.74791606
H	3.51516927	-2.78463721	4.57611135
H	5.72307243	-3.42213326	3.64087728
H	6.51532649	-2.44154019	1.50366811
H	1.16782909	-0.29087102	2.92557922

H	-0.27445702	3.32218725	1.33122610
H	1.14276709	-3.09800724	4.17510832
H	0.60216505	-2.66218021	2.53256619
H	-0.25436902	-2.02429415	3.94809030
H	2.18932317	-1.16257909	5.70109543
H	0.77682206	-0.14649101	5.35119439
H	2.40856818	0.45343703	5.00017938
H	-2.47692319	5.25371840	0.43251803
H	-2.66974520	3.75133929	1.36756911
H	-2.08241416	3.67625528	-0.30326002
H	0.51163704	5.18198539	2.87214722
H	-1.13297009	4.61809935	3.23602925
H	-0.88977007	6.15641748	2.38694118
H	-0.72481906	6.89056153	0.15008901
H	0.59240104	7.93667161	-1.67181413
H	2.35316618	6.64539450	-2.84947622
H	4.55616235	0.15063501	-0.45489603
H	3.40825226	3.15862724	-1.85971514
H	5.90104447	-2.56147020	-0.96819207
H	5.51420241	-1.32838410	-2.18714417
H	4.20522032	-2.15475216	-1.31417510
H	7.42280356	-0.73247206	0.23969102
H	6.68656852	0.80692306	0.72335206
H	6.94549653	0.44102403	-0.99742708
H	1.64343513	2.94086822	-3.58862427
H	3.26698225	2.93080622	-4.32114133
H	2.25491117	4.38954134	-4.42392634
H	4.28902933	5.70297041	-3.35102425
H	5.19552540	4.19698832	-3.16850924
H	4.88002037	5.22045440	-1.74805314
H	-7.01165951	1.72612613	0.31908402
H	-7.01574952	1.89706415	2.79515721
H	-5.24805640	0.77899506	4.13006832
H	-4.53170734	-0.35553103	-1.62587813
H	-0.03046600	-4.31381633	0.60540905
H	-5.43119942	2.57757920	-1.61487212
H	-4.80143237	1.69234313	-3.02310423
H	-3.75214129	1.96655315	-1.61942912
H	-6.98826554	-0.95344207	-1.43310911
H	-6.58432152	-0.13159101	-2.95790523
H	-7.40684654	0.75603206	-1.66695912
H	2.81138821	-5.18936539	-0.16328901
H	2.26933417	-4.73674036	1.46753211
H	2.26407817	-3.52528127	0.16723701
H	-0.71025405	-6.71386052	0.20170202
H	0.45229703	-6.54917352	1.53665412
H	0.99271008	-7.14905356	-0.03997600
H	1.62143612	-6.37669751	-2.11061516
H	1.27202710	-5.96143243	-4.53236235
H	-0.13679701	-4.06267331	-5.29009541
H	-2.42841319	-1.22864709	2.61836020
H	-1.83041714	-1.64576513	-2.91102922



H	-2.92590822	1.07052908	4.59218135
H	-1.73326013	1.00660008	3.25474325
H	-1.55439812	-0.05227900	4.66897036
H	-2.88969722	-2.18929117	4.85322337
H	-4.27848833	-2.49196719	3.78512429
H	-4.36323333	-1.21723409	5.01636238
H	0.27926302	-0.88856407	-4.04565031
H	-1.18089309	-0.32845603	-4.87168537
H	-0.24660802	-1.68559213	-5.54598342
H	-3.34834926	-3.32315526	-3.99316830
H	-2.41111219	-3.21086224	-5.49697044
H	-3.29991125	-1.79476614	-4.90032437
O	-0.23074302	1.10566708	1.35110410
O	1.89575415	-0.37511403	0.17878701
O	-2.37421118	-0.15437301	-0.48356304

## Distorted Octahedral Complex

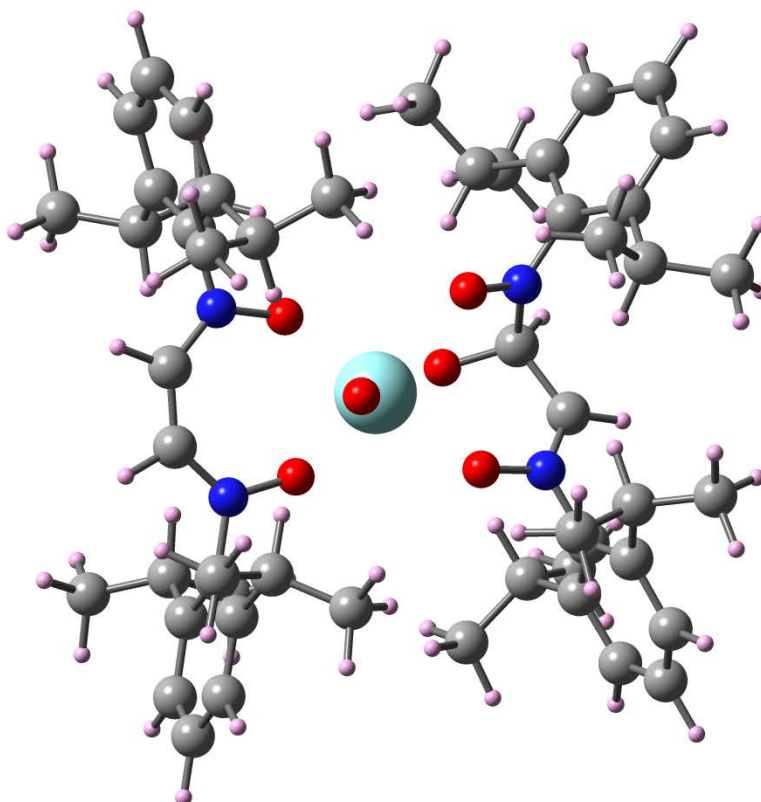


Fig. S135: ONCCNO Distorted Octahedral Complex

SCF	E <sub>ZP</sub>	H	G
-2741.479870	-2740.324113	-2740.252494	-2740.442148

O	1.34812323	1.76300519	0.48593678
O	0.89223193	0.41740918	-1.71982729
N	2.70271538	-1.38393856	-0.49909263
N	2.28589003	1.87654766	-0.46193751
C	3.09981955	-0.38428797	-1.25203592
C	2.19974871	0.80871921	-1.58304391
C	3.44108005	-2.65286173	-0.43652187
C	3.29195118	-3.55309707	-1.51930901
C	4.01108393	-4.76516671	-1.44169513
C	4.80675273	-5.06354607	-0.32559567
C	4.89406638	-4.16162592	0.74770874
C	4.20660724	-2.93077811	0.72196830
C	1.31414415	-4.39929472	-2.87600355
C	2.37812373	-3.28140164	-2.72054045
C	3.20001280	-3.11592235	-4.02625885
C	3.75483258	2.68283581	2.78805663

C	4.45617502	2.25512475	1.46862350
C	5.97119358	2.03395744	1.69328157
C	3.08100611	3.08670253	-0.54651125
C	4.15774075	3.26838831	0.36146818
C	4.91639332	4.45025806	0.24238572
C	4.61562744	5.40740137	-0.74083859
C	3.53379486	5.21095046	-1.61209791
C	2.73249038	4.05268735	-1.52797539
C	3.25734327	-2.46616038	3.01755180
C	4.25273624	-1.98515976	1.92517814
C	5.67856788	-1.82832484	2.50775807
C	0.48021054	5.03536310	-2.15256638
C	1.50678805	3.90701501	-2.43806476
C	1.90345725	3.89215315	-3.93762040
H	4.05195507	-0.51371368	-1.75676687
H	2.63496548	1.30288811	-2.46635035
H	3.93375898	-5.48411249	-2.25268696
H	5.34925125	-6.00501859	-0.28487123
H	5.49881081	-4.41763133	1.61239988
H	1.82765087	-2.34916001	-2.55473297
H	4.01755110	1.29285688	1.17397875
H	1.77479441	-5.37109616	-3.09617567
H	0.63572440	-4.15410041	-3.70293721
H	0.71468693	-4.50204784	-1.96404895
H	3.92739603	-2.29707023	-3.94568413
H	2.53121287	-2.89442527	-4.86767374
H	3.75493415	-4.03200993	-4.26760713
H	4.12413163	3.66050735	3.12682104
H	3.95394253	1.94879616	3.58017651
H	2.67099991	2.74721126	2.64724352
H	6.48484176	1.76454987	0.76090996
H	6.12614706	1.22381630	2.41616273
H	6.45783356	2.92933265	2.10088895
H	5.74751322	4.62396910	0.91930787
H	5.21730580	6.30992211	-0.81897051
H	3.29658983	5.97052560	-2.35240763
H	3.91293385	-0.99255824	1.60540601
H	1.00085385	2.96130974	-2.21800296
H	3.51850867	-3.47429323	3.36785315
H	2.23481813	-2.47788638	2.62926751
H	3.28575436	-1.78526050	3.87806908
H	5.66946624	-1.07797067	3.30847920
H	6.39882489	-1.50768492	1.74388758
H	6.04365002	-2.76509460	2.94766318
H	0.16981477	5.02836753	-1.10107251
H	-0.41537490	4.89281422	-2.77031065
H	0.89641604	6.02557290	-2.38094485
H	2.61996822	3.08992694	-4.15957317
H	2.36147480	4.84262552	-4.24213110
H	1.01424999	3.73205597	-4.56037635
O	-0.52585502	-0.08232655	1.96081633
O	1.57209956	-1.36481712	0.25237469

O	-1.87159288	1.31389223	-0.34179388
N	-2.85938580	-1.85474432	0.17092246
N	-3.06976298	1.45882134	0.34445541
C	-3.79658845	-0.97132961	0.61743958
C	-3.88439105	0.42485077	0.69595028
C	-3.07145450	-3.28918564	0.26772432
C	-2.71617188	-3.94925697	1.47059718
C	-2.94540364	-5.34114938	1.53573781
C	-3.48039109	-6.03909957	0.44177978
C	-3.79518090	-5.36083949	-0.74783933
C	-3.59651534	-3.96942139	-0.86083336
C	-0.70775066	-3.79975869	3.02106480
C	-2.09638310	-3.21181355	2.66110006
C	-3.04095666	-3.23961838	3.89133527
C	-3.35382131	3.37437482	-2.85723980
C	-4.40180417	2.88896269	-1.81878001
C	-5.84400700	3.13677444	-2.32479330
C	-3.46065993	2.83949357	0.58088070
C	-4.13052542	3.53645776	-0.45791218
C	-4.49224442	4.87682283	-0.21277149
C	-4.19403004	5.49065037	1.01578123
C	-3.51532309	4.77976879	2.01748875
C	-3.12084798	3.43819881	1.81932554
C	-2.81218828	-3.57953246	-3.23334300
C	-3.89664643	-3.24316329	-2.17462680
C	-5.31607718	-3.55275160	-2.71215679
C	-1.02842734	3.41445791	3.26626547
C	-2.35180759	2.68876358	2.91092729
C	-3.22855901	2.48951994	4.17512140
H	-4.65933845	-1.48483601	1.02940806
H	-4.79959525	0.77820552	1.15988404
H	-2.69365827	-5.88072936	2.44517666
H	-3.64596776	-7.11195051	0.51262502
H	-4.19883917	-5.91565643	-1.59097466
H	-1.92637226	-2.16429372	2.39252821
H	-4.26771332	1.80612641	-1.71740365
H	-0.78016759	-4.84144134	3.36425923
H	-0.25356059	-3.20428198	3.82266707
H	-0.03477617	-3.76601530	2.15600027
H	-4.01730400	-2.79459161	3.65760666
H	-2.59718757	-2.66754277	4.71619270
H	-3.21459340	-4.26586463	4.24391436
H	-3.41643273	4.46216191	-3.00039410
H	-3.52717657	2.89066535	-3.82812889
H	-2.34295710	3.11995154	-2.52074683
H	-6.58997261	2.80176117	-1.59240279
H	-6.01237326	2.58694411	-3.26031611
H	-6.02798552	4.19920082	-2.53169434
H	-5.00830940	5.44327932	-0.98350196
H	-4.48497236	6.52469616	1.18782756
H	-3.27918535	5.27007352	2.95837759
H	-3.83694311	-2.16458027	-1.99302046

H	-2.06547147	1.69837423	2.54294796
H	-2.80433893	-4.65344910	-3.46575225
H	-1.82092134	-3.29400850	-2.86467041
H	-3.00563814	-3.02979450	-4.16437988
H	-5.51434053	-2.95885837	-3.61431057
H	-6.08718686	-3.31211474	-1.96886749
H	-5.42808363	-4.61080843	-2.98321056
H	-0.39335857	3.52155350	2.37899988
H	-0.47293808	2.82002138	4.00202597
H	-1.20697954	4.41220463	3.69174494
H	-4.14990010	1.93924259	3.94144348
H	-3.51528370	3.45024551	4.62530441
H	-2.67217988	1.91469164	4.92647284
O	-1.67646078	-1.49493984	-0.46594952
Zr	-0.27993666	-0.02189291	0.15157842

## Peroxo Complex

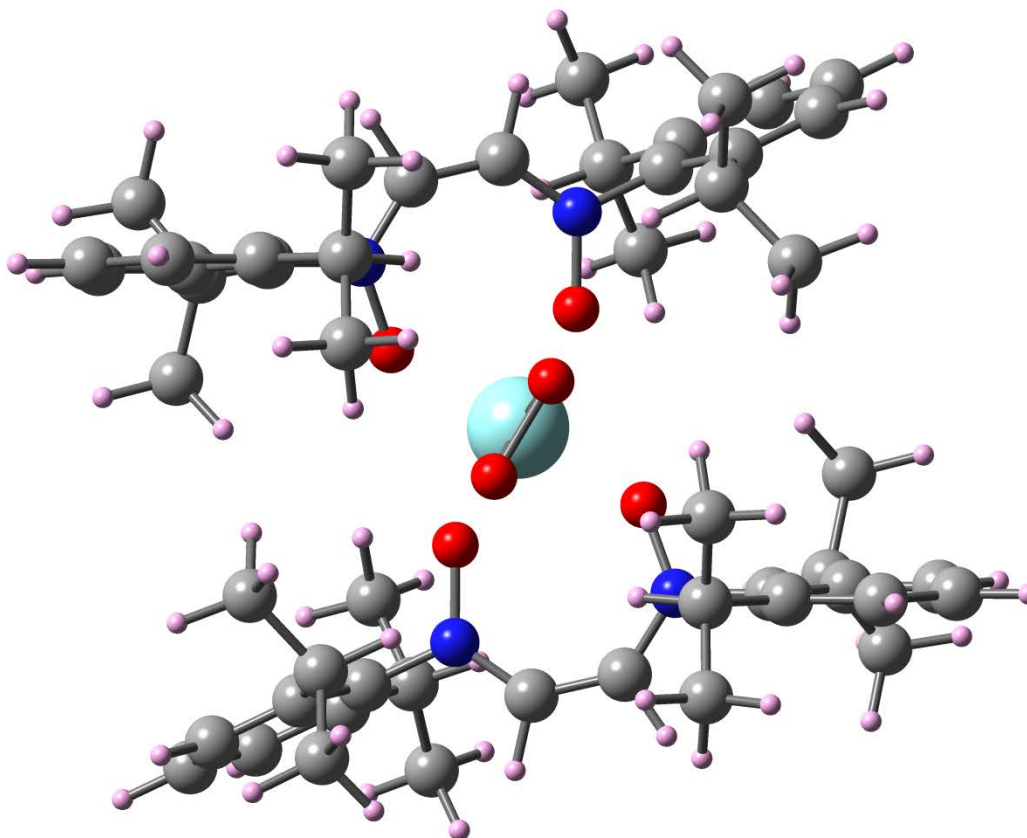


Fig. S136: ONCCNO Peroxo Complex

SCF	E <sub>ZP</sub>	H	G
-2741.437818	-2740.283590	-2740.211385	-2740.400935

O	-1.59379400	-1.36666600	0.15889000
O	1.59328100	1.36687400	0.15844100
O	0.50657500	-0.60333400	-2.08747500
O	-0.50509800	0.59989900	-2.08882800
N	-1.33857700	2.87343100	0.66420000
N	1.82399600	2.66793400	-0.25694400
N	1.33819500	-2.87265800	0.66708100
N	-1.82437800	-2.66834000	-0.25457900
C	-0.39767200	3.78409400	0.29120800
C	0.94096800	3.69447200	-0.11210000
C	0.39739200	-3.78373200	0.29485500
C	-0.94125300	-3.69462400	-0.10853200
C	-2.69194300	3.27610500	1.01119400
C	-3.66568900	3.32457000	-0.01729300
C	-4.97021300	3.72270100	0.34512400
C	-5.28613200	4.03752400	1.67627000

C	-4.30610000	3.94971200	2.67864900
C	-2.98642700	3.56081200	2.36825100
C	-4.19031000	1.72249700	-1.91610000
C	-3.34906700	2.94549400	-1.46678900
C	-3.55800900	4.14664400	-2.42546400
C	2.34112100	1.61763900	-4.14502400
C	2.13121100	2.82197900	-3.19053200
C	1.90184900	4.13315200	-3.98815100
C	3.15256500	2.88676000	-0.80741700
C	3.30346100	2.96978300	-2.21467800
C	4.60849400	3.18316800	-2.71053900
C	5.70682600	3.28278000	-1.84328200
C	5.52730300	3.16716900	-0.45451000
C	4.24491400	2.96585200	0.09467700
C	-2.26040800	2.14338800	4.33108900
C	-1.94293200	3.40075800	3.47685700
C	-1.82613100	4.66403200	4.36586400
C	4.60103300	1.42212900	2.06762000
C	4.06340800	2.80342500	1.60621400
C	4.72507100	3.95456000	2.40505300
C	2.69180200	-3.27481800	1.01369100
C	2.98708100	-3.55837800	2.37082200
C	4.30700000	-3.94676200	2.68080200
C	5.28649700	-4.03519500	1.67794700
C	4.96978900	-3.72149500	0.34672700
C	3.66498600	-3.32389800	-0.01528900
C	2.26160300	-2.13919700	4.33256100
C	1.94414800	-3.39761000	3.47985300
C	1.82836000	-4.65997100	4.37028100
C	-2.33751200	-1.62397400	-4.14360500
C	-2.12965700	-2.82752100	-3.18765600
C	-1.90103500	-4.13979100	-3.98367600
C	-3.15271500	-2.88790800	-0.80529600
C	-3.30276300	-2.97306000	-2.21248800
C	-4.60750600	-3.18712500	-2.70882300
C	-5.70637100	-3.28524100	-1.84206400
C	-5.52767700	-3.16745900	-0.45336000
C	-4.24558800	-2.96546900	0.09629100
C	4.18810300	-1.72296800	-1.91549400
C	3.34749100	-2.94592900	-1.46488700
C	3.55630100	-4.14767200	-2.42284400
C	-4.60261600	-1.41811800	2.06619400
C	-4.06496300	-2.80036400	1.60764400
C	-4.72729300	-3.94990000	2.40822400
H	-0.79419500	4.79407300	0.29043600
H	1.37936200	4.64463300	-0.39864800
H	0.79410000	-4.79363900	0.29468000
H	-1.37949700	-4.64509700	-0.39427700
H	-5.74288500	3.77761800	-0.41742900
H	-6.29807600	4.34119800	1.93476200
H	-4.56973500	4.17894100	3.70793300
H	-2.29831800	2.64560700	-1.53503100

H	1.21770500	2.60435100	-2.62885100
H	-5.26623900	1.94368500	-1.89768500
H	-4.00336000	0.85952200	-1.26698700
H	-3.91746700	1.43776800	-2.93981200
H	-4.60656800	4.47309000	-2.43934400
H	-3.28075900	3.86235100	-3.44865300
H	-2.94212800	5.00688000	-2.13143600
H	3.26201400	1.72002700	-4.73574100
H	1.49375700	1.54554300	-4.83827300
H	2.37556800	0.68143000	-3.57824100
H	1.72743500	4.98785100	-3.32035700
H	1.02612000	4.02646500	-4.64125400
H	2.76594000	4.37481400	-4.62182700
H	4.76401600	3.25718500	-3.78372500
H	6.70365200	3.44166400	-2.24859600
H	6.38853600	3.23466900	0.20503300
H	-0.96601000	3.23131600	3.01066700
H	2.99082300	2.81726600	1.82856800
H	-3.22806700	2.24509000	4.84082600
H	-1.48644100	1.99730900	5.09655500
H	-2.29574600	1.24760600	3.70032200
H	-2.75632900	4.86233100	4.91418400
H	-1.59184300	5.55440600	3.76809800
H	-1.02779000	4.53071900	5.10782000
H	4.07406200	0.61304700	1.55056400
H	4.44985000	1.29681000	3.14850200
H	5.67586200	1.32647000	1.86153500
H	5.81687300	3.95467700	2.29017500
H	4.50677600	3.84243500	3.47537300
H	4.35205300	4.93482200	2.08077400
H	4.57124800	-4.17512100	3.71012100
H	6.29864200	-4.33847200	1.93612500
H	5.74205200	-3.77685800	-0.41620900
H	0.96689400	-3.22905100	3.01403600
H	-1.21635600	-2.61028900	-2.62547000
H	3.22960400	-2.23997300	4.84183800
H	1.48802100	-1.99262000	5.09832200
H	2.29619800	-1.24408900	3.70080300
H	1.59417000	-5.55110100	3.77360400
H	1.03032800	-4.52620000	5.11248900
H	2.75891000	-4.85725900	4.91836600
H	-3.25783800	-1.72614200	-4.73523300
H	-1.48932500	-1.55327600	-4.83599300
H	-2.37178700	-0.68718300	-3.57777900
H	-1.72815700	-4.99395500	-3.31480400
H	-1.02460200	-4.03477800	-4.63610300
H	-2.76483600	-4.38118200	-4.61785600
H	-4.76236400	-3.26298900	-3.78197500
H	-6.70296600	-3.44469700	-2.24772100
H	-6.38932400	-3.23377900	0.20576000
H	2.29661800	-2.64639300	-1.53279700
H	-2.99251100	-2.81398900	1.83066300



H	5.26411600	-1.94378500	-1.89750500
H	4.00120300	-0.85960300	-1.26688500
H	3.91459400	-1.43902900	-2.93924700
H	3.27836900	-3.86417400	-3.44606800
H	2.94087900	-5.00791500	-2.12787700
H	4.60496400	-4.47377500	-2.43709600
H	-4.07523300	-0.61008300	1.54792000
H	-4.45201600	-1.29081700	3.14692600
H	-5.67731500	-1.32268700	1.85932800
H	-4.35428900	-4.93083000	2.08596000
H	-5.81903200	-3.95001500	2.29275300
H	-4.50957100	-3.83584500	3.47845600
O	-1.10908700	1.51489000	0.75671500
O	1.10830900	-1.51413400	0.75927600
Zr	-0.00008100	-0.00019800	-0.21000900

## Octahedral Complex with Transferred Allylic H

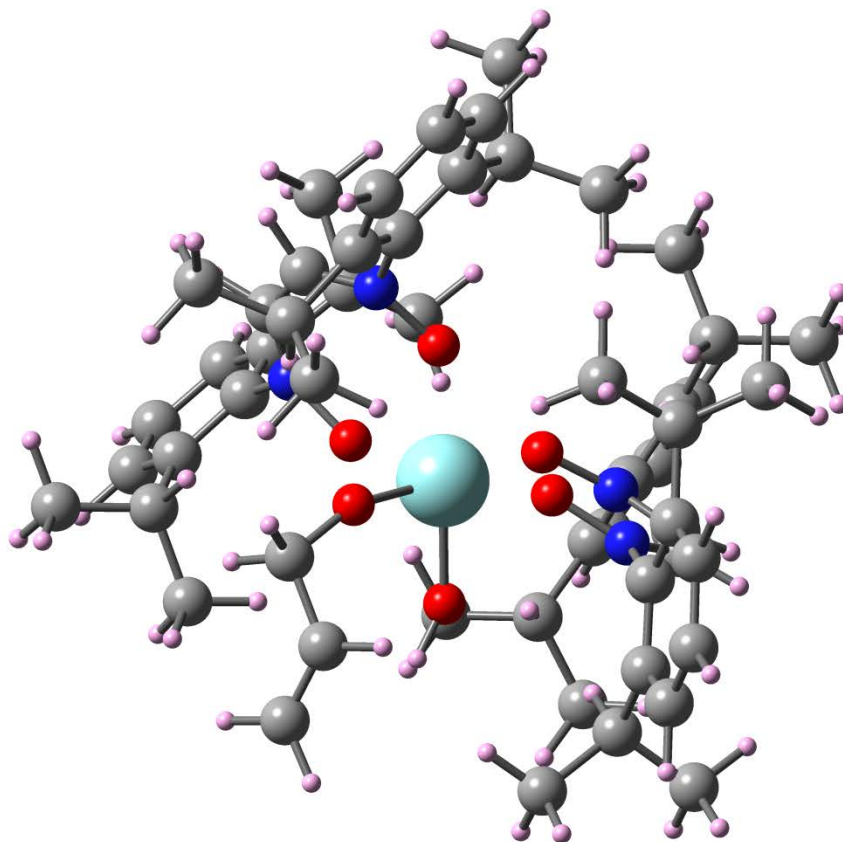


Fig. S137: ONCCNO Octahedral Complex with Transferred Allylic H

SCF	E <sub>ZP</sub>	H	G
-2859.428725	-2858.191821	-2858.114492	-2858.313770

O	0.39290200	-1.42918900	0.72978700
O	1.90339400	0.57110200	-0.88197700
O	-0.03469600	-1.39353200	-2.16204400
N	0.16569600	2.88869200	0.84659700
N	2.80364800	1.57513600	-0.62123300
N	-2.83610800	-1.71792800	-0.04424800
N	0.12194900	-2.74185300	1.02171300
C	1.39322200	3.37466400	0.51385200
C	2.52160200	2.79709600	-0.07751600
C	-2.36238300	-2.87464300	0.50250000
C	-1.11040400	-3.31733800	0.94022100
C	-0.81356800	3.72511900	1.52312000
C	-1.58979400	4.63663800	0.76407500
C	-2.50324300	5.45484700	1.46373500
C	-2.65905200	5.34255700	2.85339000
C	-1.90126700	4.40589500	3.57533800

C	-0.95943500	3.58062100	2.92783000
C	-2.84951800	4.59484900	-1.44742600
C	-1.46993500	4.75281900	-0.75879700
C	-0.80460300	6.09509700	-1.16554000
C	3.03330300	0.52028000	-4.27993800
C	3.45866800	1.77070000	-3.46312000
C	3.95790300	2.90337100	-4.39420600
C	4.16250800	1.25761100	-1.03572300
C	4.49629100	1.37640700	-2.40893300
C	5.81998300	1.07096000	-2.78633400
C	6.76691000	0.66139100	-1.83279300
C	6.40169100	0.53009300	-0.48429200
C	5.08615300	0.81335000	-0.05745000
C	-1.07503000	1.38464400	4.17370000
C	-0.15576000	2.55353600	3.72942200
C	0.56584100	3.19171000	4.94309600
C	4.89651800	-0.86227400	1.84381700
C	4.69737900	0.61315200	1.41039500
C	5.48192400	1.57611600	2.33964400
C	-4.21642500	-1.61918000	-0.48914600
C	-4.61125100	-2.29848600	-1.67189100
C	-5.96186900	-2.18683800	-2.06729400
C	-6.86945000	-1.40719400	-1.33416400
C	-6.44448700	-0.72569100	-0.18202500
C	-5.11241800	-0.82125900	0.26973200
C	-3.63306700	-2.68910100	-3.99843100
C	-3.63874500	-3.13350700	-2.51363400
C	-3.96555900	-4.64738600	-2.40604800
C	1.47277400	-1.85991900	4.76494400
C	0.63243500	-2.84470800	3.91181000
C	-0.13711200	-3.84273200	4.81657700
C	1.26549100	-3.50868000	1.49678200
C	1.50768400	-3.57790000	2.89142900
C	2.60312500	-4.35402900	3.32547900
C	3.43112500	-5.01293700	2.40253300
C	3.18552000	-4.89875900	1.02494300
C	2.10003600	-4.13826100	0.53970800
C	-4.61490200	1.45675700	1.25535500
C	-4.67020100	-0.06949500	1.52803600
C	-5.57615600	-0.38914900	2.74437400
C	3.08013000	-3.39692800	-1.68499500
C	1.85415100	-4.01653100	-0.96626700
C	1.48467300	-5.39208900	-1.58171400
H	1.51248600	4.41946500	0.78110300
H	3.38316900	3.45614000	-0.11849800
H	-3.14143000	-3.62603300	0.57883500
H	-1.09974700	-4.34713200	1.28192900
H	-3.10646900	6.17356100	0.91487000
H	-3.37378800	5.97774100	3.37183600
H	-2.03759500	4.32100300	4.65043200
H	-0.83807700	3.93384200	-1.11741600
H	2.56434800	2.13546100	-2.94588400

H	-3.55147000	5.38260700	-1.14432100
H	-3.29685100	3.62403400	-1.20428800
H	-2.73628000	4.65658800	-2.53800300
H	-1.41019800	6.95270600	-0.84265900
H	-0.69384600	6.15190800	-2.25672200
H	0.19215800	6.20181200	-0.71800400
H	3.88986900	0.08962300	-4.81644600
H	2.26975300	0.79187200	-5.02204300
H	2.61434300	-0.24451300	-3.61697900
H	4.25876500	3.79021800	-3.82140500
H	3.15864700	3.19932800	-5.08665500
H	4.81658700	2.58614900	-5.00030300
H	6.11260700	1.15310300	-3.82980300
H	7.78462400	0.43535100	-2.14302600
H	7.13881800	0.19399600	0.24082300
H	0.60679300	2.12189600	3.07404100
H	3.63118700	0.83658600	1.52008500
H	-1.88105800	1.73985800	4.83076000
H	-0.49274000	0.63373800	4.72362200
H	-1.52006600	0.90054100	3.29765800
H	-0.14467900	3.58920700	5.67966900
H	1.22273400	4.01418800	4.63099400
H	1.18164300	2.43805100	5.45189000
H	4.30402900	-1.53917400	1.21801500
H	4.57471600	-0.99690900	2.88495100
H	5.95002200	-1.16474700	1.77601000
H	6.56292300	1.38951100	2.28786500
H	5.16744100	1.43867300	3.38270400
H	5.30888100	2.62525900	2.06674000
H	-6.30103900	-2.70171500	-2.96269400
H	-7.90354400	-1.32728200	-1.66171700
H	-7.15511800	-0.12129800	0.37568300
H	-2.62490800	-2.97732800	-2.13106400
H	-0.10608200	-2.24670200	3.36749300
H	-4.60590800	-2.85452200	-4.47957600
H	-2.88319000	-3.26424300	-4.55815800
H	-3.38383000	-1.62599100	-4.08912600
H	-3.93856800	-4.99369600	-1.36490600
H	-3.23778800	-5.23729100	-2.97886900
H	-4.96585400	-4.86435600	-2.80422400
H	2.23148800	-2.38451500	5.36071500
H	0.82255100	-1.31260400	5.46017900
H	1.98279500	-1.13055700	4.12416700
H	-0.76962900	-4.51393000	4.22144200
H	-0.78339200	-3.30091300	5.52000600
H	0.55291900	-4.46420900	5.40257200
H	2.81252000	-4.43871200	4.38904000
H	4.27050100	-5.60762700	2.75618600
H	3.84167500	-5.40160900	0.31884300
H	-3.65152400	-0.38230300	1.77665800
H	1.01889200	-3.33184300	-1.14127500
H	-5.60557000	1.85039600	0.98782000

H	-3.91806000	1.66941200	0.43795000
H	-4.26442400	1.99232800	2.14731900
H	-5.18965600	0.11445500	3.64035300
H	-5.60949700	-1.46785200	2.94648900
H	-6.60673500	-0.04315600	2.58960400
H	3.28906000	-2.39370400	-1.29629500
H	2.87273100	-3.30263100	-2.75899300
H	3.98177600	-4.01386900	-1.56738100
H	0.59223600	-5.81773900	-1.10365800
H	2.30290500	-6.11728800	-1.47282600
H	1.27486500	-5.28065400	-2.65397700
O	-0.72291300	1.40086200	-2.09954400
O	-2.12609200	-0.53580500	-0.14858100
O	-0.15475300	1.55002200	0.77607400
Zr	-0.16190800	0.03383800	-0.76253300
C	-0.92513000	1.88826300	-3.42841700
H	-1.47191200	2.84407300	-3.37368100
C	-1.72172800	0.90950800	-4.26745400
H	-2.66896100	0.59688500	-3.82406400
C	-1.33884100	0.43106700	-5.46935500
H	-0.14524600	-1.52917000	-3.11696800
H	-1.96086600	-0.25702200	-6.03821300
H	-0.39154500	0.72110200	-5.92310600
H	0.04671300	2.08800500	-3.90992200

**Oxo Complex with Propylene Oxide Molecule (reaction products of dioxo complex with propene)**

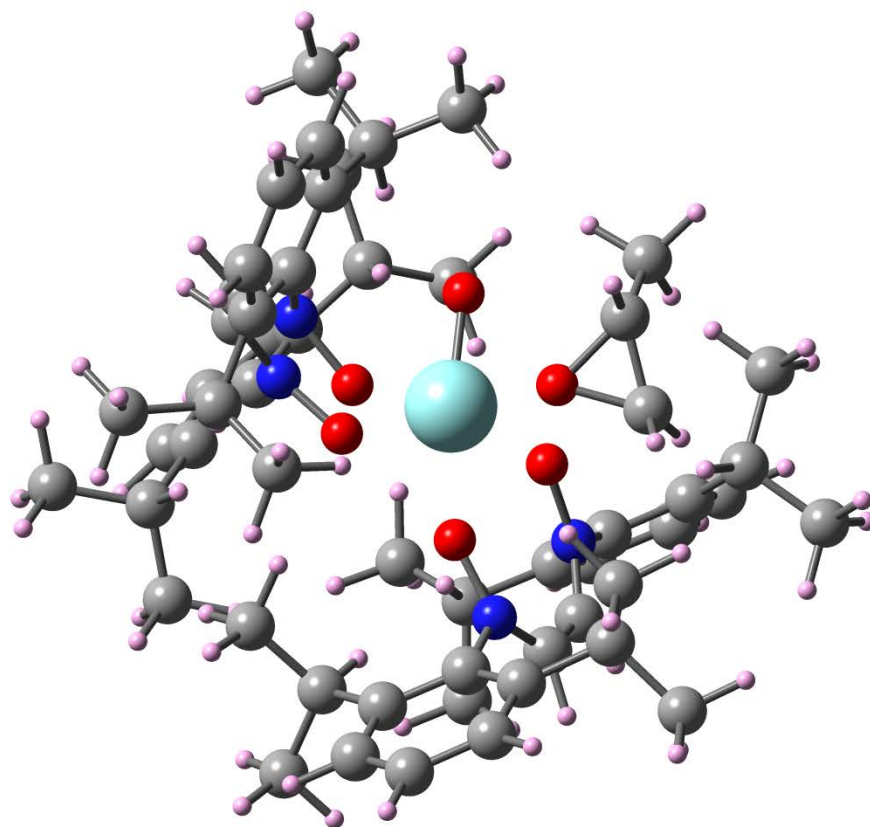


Fig. S138: ONCCNO Oxo Complex with Propylene Oxide Molecule (reaction products of dioxo complex with propene)

SCF	E <sub>ZP</sub>	H	G
-2859.362681	-2858.123493	-2858.047092	-2858.241102

O	0.30645800	-1.40816600	0.79739400
O	1.77677700	0.76565300	-1.09649300
O	-0.17215100	-1.35607500	-2.15699900
N	0.13523500	2.93468200	0.92415900
N	2.76329700	1.52015600	-0.47605600
N	-2.88464000	-1.68749000	-0.28499500
N	0.01836800	-2.76252100	0.90635200
C	1.45046800	3.29327700	0.81436100
C	2.55955700	2.66720400	0.23898100
C	-2.42469900	-2.88665700	0.16916900
C	-1.19809800	-3.33365300	0.67076000
C	-0.78894200	3.75323400	1.69895200
C	-1.34057000	4.92210700	1.11882400
C	-2.22566400	5.69033400	1.90571300

C	-2.56521700	5.29216400	3.20722200
C	-2.02235700	4.11546100	3.74871300
C	-1.11991000	3.32265400	3.01052600
C	-2.31507600	5.45702000	-1.16810000
C	-1.02400900	5.36097800	-0.31399500
C	-0.24543400	6.70284400	-0.33772000
C	3.79086300	1.30003100	-4.43632000
C	3.86610900	2.12825800	-3.12848300
C	4.45309000	3.53941300	-3.39967500
C	4.12431800	1.09731800	-0.77539100
C	4.66828200	1.39444400	-2.05127100
C	6.00240300	1.01494500	-2.30419400
C	6.76444400	0.36050500	-1.32327600
C	6.19809500	0.06230600	-0.07471400
C	4.86355800	0.41252500	0.22376600
C	-1.65130500	0.93496200	3.64989000
C	-0.55554900	2.03374400	3.61386200
C	0.05620600	2.26335600	5.01876200
C	4.52655500	-1.40811800	1.98485200
C	4.26836200	0.06725200	1.59283000
C	4.81592600	1.02133600	2.68958300
C	-4.20871500	-1.56886600	-0.87113400
C	-4.41799000	-2.03910900	-2.19412800
C	-5.72476500	-1.93709600	-2.71933700
C	-6.76400400	-1.35922800	-1.97371300
C	-6.51797000	-0.86949700	-0.68064800
C	-5.23671700	-0.96734700	-0.09958500
C	-3.22823200	-1.98523400	-4.45039600
C	-3.29120100	-2.63604600	-3.04546600
C	-3.44792800	-4.17507800	-3.17705500
C	1.23707700	-2.06002700	4.69333800
C	0.41905500	-3.02171100	3.79330300
C	-0.37075500	-4.04392100	4.65207400
C	1.12507100	-3.58101300	1.37524500
C	1.31695000	-3.72614900	2.77210800
C	2.37302700	-4.55582600	3.20340900
C	3.20685500	-5.20092200	2.27515300
C	3.00655700	-5.01968500	0.89730000
C	1.96420600	-4.19906300	0.41383200
C	-4.97240400	1.14037300	1.27021300
C	-4.98070500	-0.41122100	1.30322300
C	-6.00027900	-0.94366000	2.34138600
C	3.03062000	-3.41798900	-1.76181200
C	1.76329000	-4.00777600	-1.09220400
C	1.35128900	-5.34098400	-1.77065900
H	1.66745100	4.23754200	1.30261800
H	3.49362200	3.19091000	0.41988100
H	-3.17404900	-3.66678100	0.08510200
H	-1.18639300	-4.39365800	0.90440000
H	-2.66091400	6.59716400	1.49296200
H	-3.25449800	5.89307400	3.79600500
H	-2.29776200	3.81346200	4.75579600

H	-0.38359600	4.59807900	-0.77021200
H	2.84268900	2.25026900	-2.75972900
H	-2.99982900	6.22082500	-0.77840900
H	-2.85120200	4.49985100	-1.17809900
H	-2.07090200	5.73409800	-2.20354700
H	-0.83829000	7.51433400	0.10400300
H	-0.00088900	6.98835300	-1.36979600
H	0.69289200	6.62938900	0.22680600
H	4.78541300	1.15291200	-4.87739500
H	3.17216200	1.81771800	-5.18235300
H	3.35386300	0.31270400	-4.24654300
H	4.47145900	4.14608400	-2.48506800
H	3.84919000	4.06872100	-4.14956400
H	5.48084100	3.47663200	-3.78128000
H	6.44800400	1.23574700	-3.27097500
H	7.79372700	0.07868900	-1.53333200
H	6.79264100	-0.45796700	0.67128200
H	0.23959100	1.66190500	2.95999300
H	3.18257000	0.20108600	1.53773100
H	-2.50338300	1.24618500	4.27102600
H	-1.24066300	0.00815500	4.07220100
H	-2.00670000	0.72072600	2.63692100
H	-0.70296100	2.56410600	5.75296500
H	0.83145600	3.04055000	4.99756000
H	0.51470200	1.33367800	5.38100000
H	4.15530400	-2.09592000	1.21767600
H	4.00701300	-1.64232700	2.92211800
H	5.59496900	-1.60952000	2.13998800
H	5.90625400	0.92595800	2.78343900
H	4.36958100	0.77877700	3.66319200
H	4.58672300	2.07029600	2.46369200
H	-5.92498200	-2.29836000	-3.72478200
H	-7.76152900	-1.28475400	-2.40136700
H	-7.32816800	-0.41477500	-0.11628700
H	-2.32881200	-2.42739200	-2.56541200
H	-0.30644400	-2.40974600	3.24716700
H	-4.11637600	-2.21437000	-5.05505600
H	-2.34841500	-2.35970600	-4.98896200
H	-3.14063800	-0.89450800	-4.37174500
H	-3.43691500	-4.66653500	-2.19580800
H	-2.62155500	-4.58943000	-3.76942900
H	-4.39171600	-4.43910000	-3.67447500
H	1.99040200	-2.59971900	5.28284400
H	0.57118300	-1.54135300	5.39624800
H	1.75090200	-1.30469000	4.08669200
H	-0.98644200	-4.69968000	4.02323700
H	-1.03564700	-3.52082000	5.35244100
H	0.30434000	-4.67973300	5.24007400
H	2.54409900	-4.69808900	4.26788300
H	4.01466000	-5.83969600	2.62568600
H	3.66514400	-5.51657900	0.18919000
H	-3.98211500	-0.72685200	1.62241000



H	0.95997000	-3.28478700	-1.26603400
H	-5.94371800	1.53552400	0.94134200
H	-4.19566200	1.50009500	0.58704800
H	-4.76082100	1.54283300	2.26963200
H	-5.73705900	-0.58165400	3.34417900
H	-6.01046900	-2.04120800	2.36621000
H	-7.02102200	-0.60174700	2.12486100
H	3.29262200	-2.45046100	-1.31778700
H	2.83619500	-3.25054800	-2.82852800
H	3.89623100	-4.08943000	-1.67177700
H	0.43263600	-5.74811200	-1.32753600
H	2.13715800	-6.10384300	-1.67875600
H	1.16506400	-5.17233700	-2.83920900
O	-0.99914500	1.44631900	-2.39026800
O	-2.19470100	-0.49152100	-0.14385700
O	-0.35626100	1.73090100	0.51320200
Zr	-0.18315300	-0.09419700	-0.82436400
C	-0.56585400	2.66924000	-3.13469800
H	-1.20456500	3.53011400	-2.96304300
C	-1.06992700	1.48932100	-3.90758700
H	-2.11093100	1.52110100	-4.22641300
C	-0.16284800	0.54781500	-4.66038900
H	-0.38241800	-0.48434200	-4.36657300
H	-0.31849800	0.67411200	-5.74074500
H	0.88956500	0.73038900	-4.42552100
H	0.50649900	2.84431700	-3.09183000

## 10.4 Structures with seven oxygen atoms

### Oxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation)

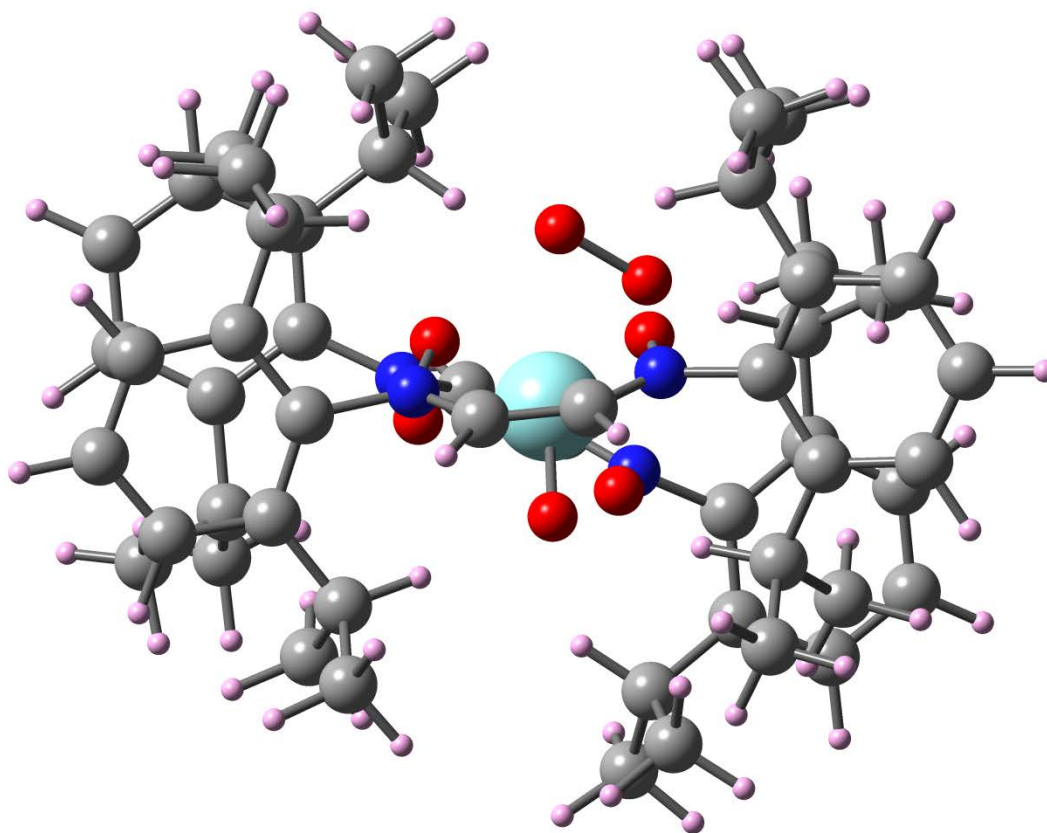


Fig. S139: ONCCNO Oxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation)

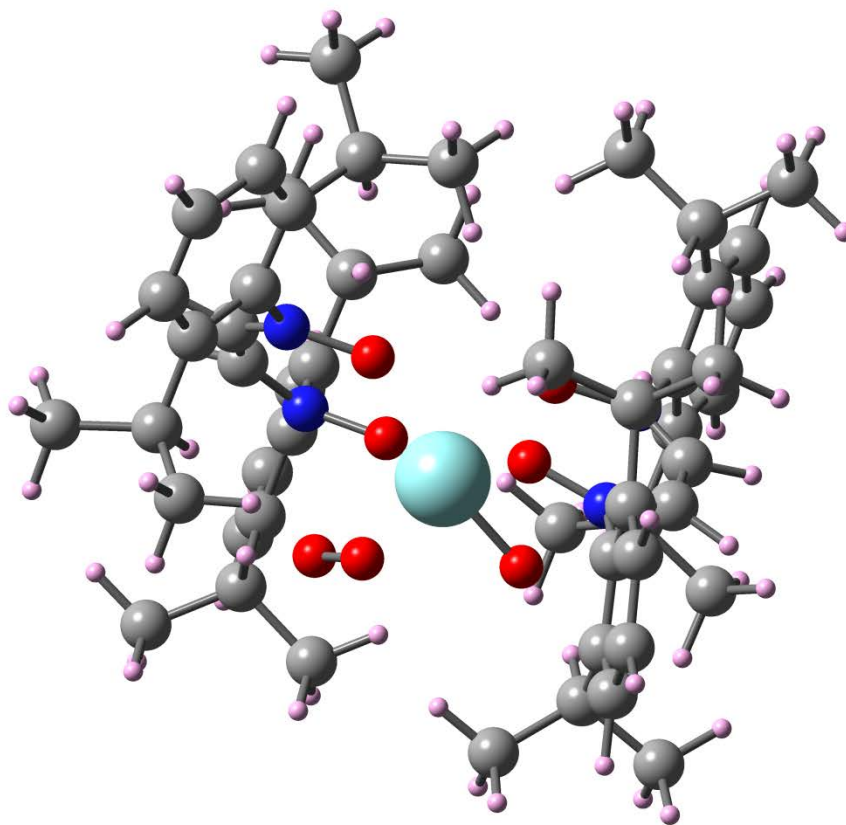
SCF	E <sub>ZP</sub>	H	G
-2816.603173	-2815.444668	-2815.371434	-2815.560405

Zr	0.23490100	0.01289600	-0.01408400
O	1.25709300	-1.77832300	0.60702100
O	-1.31363500	1.70453200	-0.31386500
O	0.02898300	-0.02513000	-2.39657400
O	1.24475100	-0.57624600	-1.99823200
N	1.73591300	2.94344000	-0.09552700
N	-1.46319400	2.68902600	0.58771600
N	-1.81560900	-2.40307900	-0.58845400
N	1.37154500	-3.04397600	0.06809800
C	0.88896500	3.64162100	0.65560100
C	-0.50241600	3.51366100	0.98371500
C	-0.99483200	-3.47784900	-0.77153900
C	0.34656200	-3.75460100	-0.48365900
C	3.13233700	3.40615900	-0.20922000

C	4.02863400	3.06717000	0.83095000
C	5.35727000	3.52508100	0.69035100
C	5.75724300	4.25315500	-0.44050500
C	4.84173100	4.53450700	-1.46889300
C	3.49974500	4.11138300	-1.38060400
C	4.48609800	0.94769900	2.15312600
C	3.61895200	2.22913600	2.04745100
C	3.70704400	3.06215000	3.35333700
C	-2.36532500	0.42405300	3.85758600
C	-1.97834900	1.85417200	3.40012000
C	-1.71899700	2.77563200	4.62099400
C	-2.82013400	2.83809600	1.14080600
C	-3.05533100	2.44627400	2.48249600
C	-4.37463500	2.60449500	2.96200600
C	-5.39470000	3.10669700	2.14068000
C	-5.12305700	3.46310500	0.80960500
C	-3.82566100	3.33493500	0.27459100
C	2.75613800	3.29784500	-3.65341400
C	2.52121100	4.35080400	-2.53450300
C	2.59838300	5.79122500	-3.09666800
C	-4.26586600	2.71160700	-2.13809200
C	-3.55742000	3.71095200	-1.18591600
C	-3.97831100	5.17124400	-1.49307900
C	-3.20403900	-2.45436400	-1.02589300
C	-3.50472500	-2.26594100	-2.39901600
C	-4.86028600	-2.35358700	-2.78688400
C	-5.86929500	-2.60153300	-1.84554700
C	-5.54350400	-2.77073000	-0.48918100
C	-4.20649400	-2.70046800	-0.04974000
C	-2.71477900	-0.66593900	-4.21958400
C	-2.43296500	-1.98443900	-3.45625700
C	-2.29996100	-3.17356100	-4.44502300
C	2.43587100	-2.74060100	3.67139500
C	1.99597100	-3.92860100	2.77343400
C	1.82525800	-5.22524900	3.60356600
C	2.67045100	-3.66135700	0.29522600
C	2.97541800	-4.10422400	1.60924300
C	4.24176600	-4.68616800	1.82113800
C	5.16001600	-4.82423400	0.76661600
C	4.83365700	-4.36766100	-0.51903900
C	3.58526500	-3.76184300	-0.78222000
C	-4.80110000	-2.19756700	2.38984800
C	-3.85777400	-2.95152700	1.42086100
C	-3.87051100	-4.47559400	1.72384800
C	4.30866000	-2.16028300	-2.62064100
C	3.27517800	-3.23059100	-2.18483900
C	3.20308700	-4.38277100	-3.22100800
H	1.35980100	4.50042600	1.12138000
H	-0.84656700	4.25930900	1.69178400
H	-1.50947300	-4.29287600	-1.27012600
H	0.66069900	-4.75103800	-0.77583100
H	6.08262600	3.29521300	1.46600100

H	6.78694800	4.59169500	-0.52838000
H	5.17301200	5.08257600	-2.34612400
H	2.58267100	1.88857800	1.93624400
H	-1.03750100	1.73573500	2.85132000
H	5.54559500	1.18035100	2.32752400
H	4.41040600	0.34645000	1.23949300
H	4.13128100	0.33108000	2.98813100
H	4.73410700	3.39874300	3.55070800
H	3.37977000	2.45353100	4.20561700
H	3.06579400	3.95344300	3.30968100
H	-3.29965100	0.41007500	4.43603100
H	-1.56541400	0.01460800	4.48714400
H	-2.47820200	-0.23763200	2.99181900
H	-1.41281400	3.78543000	4.31275800
H	-0.91674800	2.35411600	5.23984300
H	-2.61278800	2.87838100	5.25159600
H	-4.60155700	2.31812700	3.98513600
H	-6.40276100	3.21391600	2.53420700
H	-5.92365600	3.84319600	0.18105400
H	1.49885400	4.19720600	-2.16718100
H	-2.48404900	3.62566900	-1.38509900
H	3.77076100	3.38529600	-4.06507300
H	2.04033100	3.44984500	-4.47192200
H	2.62045600	2.28295500	-3.26549400
H	3.56251900	5.98815800	-3.58254300
H	2.45685600	6.54245600	-2.30857900
H	1.81697300	5.93693800	-3.85354700
H	-3.93897500	1.68682100	-1.93270700
H	-4.02552600	2.94809100	-3.18296400
H	-5.35701000	2.75613200	-2.02173200
H	-5.05931400	5.31656500	-1.37051000
H	-3.72604000	5.42342000	-2.53137600
H	-3.46668100	5.88491700	-0.83380400
H	-5.12387300	-2.21755300	-3.83268100
H	-6.90717600	-2.66239700	-2.16555900
H	-6.33461600	-2.96253500	0.23053600
H	-1.46864100	-1.85107100	-2.95919000
H	1.01526800	-3.66484700	2.36339300
H	-3.65505200	-0.71362400	-4.78616300
H	-1.89868100	-0.46535300	-4.92437500
H	-2.76784700	0.18009800	-3.52550500
H	-2.05715800	-4.10808100	-3.92188200
H	-1.50080000	-2.97263200	-5.17029200
H	-3.23182000	-3.33527800	-5.00378900
H	3.43665200	-2.91246600	4.09188500
H	1.73146400	-2.61526200	4.50491400
H	2.44591200	-1.81259700	3.09055100
H	1.52153100	-6.07009800	2.97158500
H	1.05384300	-5.07743500	4.37098700
H	2.75205500	-5.50654200	4.12081500
H	4.51025000	-5.03610000	2.81440400
H	6.13014900	-5.28096800	0.94976700

H	5.55745600	-4.46766200	-1.32394400
H	-2.84456700	-2.57836800	1.59799500
H	2.30338300	-2.72938300	-2.16860300
H	-5.82740400	-2.58620400	2.34729800
H	-4.83019100	-1.12605800	2.15938000
H	-4.44707500	-2.31527600	3.42238000
H	-3.59038100	-4.65923600	2.76983400
H	-3.16120100	-5.01490600	1.08343800
H	-4.86937300	-4.90179800	1.55800600
H	4.33083300	-1.32865300	-1.90685600
H	4.03022800	-1.75189800	-3.60012500
H	5.32194200	-2.57792600	-2.69852900
H	2.44669900	-5.12831000	-2.94132400
H	4.16669800	-4.90207500	-3.31258100
H	2.93917300	-3.98479000	-4.20955300
O	0.53897200	0.83908800	1.60702700
O	1.47557300	1.82672300	-0.77653900
O	-1.47819700	-1.27611800	0.15667300

**Oxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)**Fig. S140: ONCCNO Oxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)

SCF	E <sub>ZP</sub>	H	G
-2816.609512	-2815.451430	-2815.378006	-2815.567757

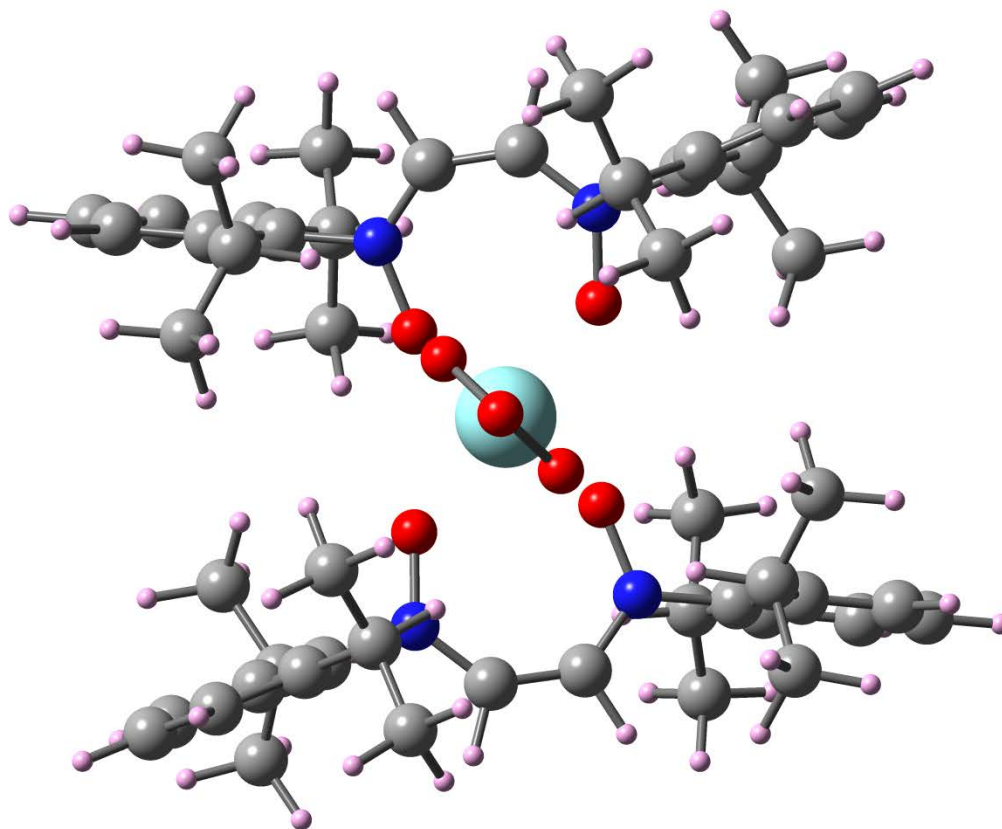
O	-0.31128718	1.62178774	0.74310853
O	-2.29300873	-0.52703418	-0.13659437
O	-1.38473111	1.37698692	-2.17957193
N	-0.06639970	-2.74666994	0.83156035
N	-2.86501358	-1.68925618	-0.48394328
N	2.81056773	1.42501003	-0.48367436
N	0.14931674	2.91000970	0.87001752
C	-1.10774631	-3.35638941	0.27513164
C	-2.33401628	-2.89365603	-0.31293757
C	2.54150963	2.65955285	0.03315831
C	1.43028352	3.29681448	0.59632250
C	1.02260786	-3.56441668	1.39896675
C	1.99066133	-4.09733325	0.51495857
C	3.01694389	-4.87164997	1.10030032
C	3.07318903	-5.07759001	2.48679297
C	2.10639898	-4.50625669	3.33083941

C	1.05488871	-3.72835975	2.80495436
C	3.26147207	-3.10743179	-1.44530523
C	1.97780348	-3.85460020	-0.99834523
C	1.81150028	-5.18724327	-1.77495839
C	-3.00576507	-0.84087049	-4.48543758
C	-3.13264734	-1.96500490	-3.42385588
C	-3.24946884	-3.35499617	-4.10351617
C	-4.20272140	-1.56372182	-1.09050566
C	-4.32346981	-1.70662492	-2.49345521
C	-5.62462329	-1.57613676	-3.02795499
C	-6.72482708	-1.29481885	-2.20480974
C	-6.55420218	-1.12883117	-0.81997342
C	-5.28259040	-1.25649226	-0.22622252
C	0.70229153	-1.89373806	4.50741600
C	0.03726590	-3.06813725	3.74014510
C	-0.60602076	-4.08271053	4.71849460
C	-5.15191618	0.50150445	1.58442902
C	-5.09717483	-1.01975917	1.27581965
C	-6.12556750	-1.80190534	2.13028949
C	4.15024124	1.10130629	-0.95046814
C	4.41946576	1.17794256	-2.34080018
C	5.72340660	0.85288378	-2.77015522
C	6.71343246	0.46831644	-1.85131829
C	6.41387025	0.38479278	-0.48232056
C	5.12114179	0.68700325	-0.00373660
C	2.92208638	0.33130955	-4.20107619
C	3.34335283	1.56493462	-3.35826130
C	3.79624647	2.73205717	-4.27150949
C	-1.66429160	1.57416036	3.97588417
C	-0.58807474	2.65275941	3.68019981
C	0.00315366	3.22822396	4.99170879
C	-0.81281624	3.85954413	1.40911188
C	-1.16918327	3.74459108	2.77834371
C	-2.10920679	4.66209324	3.28936801
C	-2.66778846	5.65685727	2.46956133
C	-2.30629420	5.73988391	1.11691811
C	-1.38009605	4.83619113	0.55098087
C	5.06890258	-0.88657667	1.99772213
C	4.80551137	0.55433398	1.48935610
C	5.60298295	1.58898415	2.32669165
C	-2.32210280	4.73959656	-1.80951139
C	-1.05023937	4.92995996	-0.94273843
C	-0.34509771	6.27001712	-1.28108090
H	-1.01834488	-4.43691703	0.28737320
H	-2.97113356	-3.69425369	-0.67108675
H	3.41628756	3.30019716	-0.02549727
H	1.60824409	4.33349129	0.86243002
H	3.78138237	-5.30506796	0.46130529
H	3.87580138	-5.67543399	2.91215519
H	2.17058074	-4.66335058	4.40404885
H	1.14104850	-3.20108839	-1.27022575
H	-2.19667204	-1.94761361	-2.85349053

H	4.17213519	-3.67887010	-1.21814758
H	3.32808177	-2.12696717	-0.96109751
H	3.22776849	-2.93855660	-2.52888460
H	2.65481052	-5.86965828	-1.60083232
H	1.75963416	-4.98259303	-2.85155637
H	0.89072271	-5.71378489	-1.48691125
H	-3.88288195	-0.79650237	-5.14583938
H	-2.12079995	-1.02589580	-5.10708920
H	-2.87704931	0.13617006	-4.00617413
H	-3.30839390	-4.16670550	-3.36463514
H	-2.36795306	-3.53491246	-4.73148524
H	-4.14056291	-3.42088450	-4.74275759
H	-5.76870624	-1.68040499	-4.09969754
H	-7.71513520	-1.19317541	-2.64237945
H	-7.41364313	-0.89575777	-0.19788414
H	-0.76918599	-2.63313933	3.13863953
H	-4.09811858	-1.36426837	1.56843548
H	1.53211346	-2.24979441	5.13245766
H	-0.03127755	-1.40501507	5.16197570
H	1.08971712	-1.14737435	3.80512086
H	0.13428456	-4.50637446	5.40901012
H	-1.07974815	-4.91503448	4.18184168
H	-1.37384666	-3.58400104	5.32417280
H	-4.37326816	1.03495521	1.02930191
H	-4.99259697	0.67749590	2.65638796
H	-6.12824223	0.92314778	1.31023490
H	-7.15040455	-1.44887767	1.95890943
H	-5.90604694	-1.66338757	3.19693090
H	-6.09843071	-2.87746186	1.91134075
H	5.96477996	0.90221078	-3.82884549
H	7.71444008	0.22755520	-2.20257466
H	7.18541973	0.07319235	0.21779219
H	2.45316133	1.89842070	-2.81667300
H	0.21997173	2.15113581	3.13833832
H	3.77199203	-0.06864195	-4.77191949
H	2.13362124	0.61401640	-4.91035809
H	2.52632533	-0.46232874	-3.55808482
H	4.09359741	3.61022393	-3.68327003
H	2.97092547	3.02737381	-4.93211260
H	4.64562681	2.44801574	-4.90749806
H	-2.52047990	2.00436838	4.51407929
H	-1.23836720	0.77367137	4.59609412
H	-2.02121588	1.13305658	3.03896065
H	0.76807525	3.98791409	4.78491572
H	0.46899287	2.42476925	5.57821984
H	-0.76937329	3.69046702	5.62045427
H	-2.40240126	4.60196697	4.33446601
H	-3.38748273	6.36002229	2.88290150
H	-2.75698701	6.50338534	0.48778064
H	3.73936367	0.75622614	1.63489850
H	-0.36618563	4.11868823	-1.20791812
H	6.12963957	-1.15787769	1.91247332



H	4.48276084	-1.61757001	1.42866934
H	4.78542684	-0.97158877	3.05543700
H	5.34288355	1.50251026	3.39016292
H	5.38522196	2.61561187	2.00528689
H	6.68535432	1.42991069	2.23036900
H	-2.77966220	3.76271840	-1.61830866
H	-2.05780720	4.77931616	-2.87402980
H	-3.06788606	5.52194448	-1.61340249
H	0.57574864	6.39859306	-0.69670897
H	-0.99629333	7.12968900	-1.07327501
H	-0.07984998	6.29827683	-2.34597477
O	-0.20602307	-1.49959395	-1.87420960
O	-0.04265427	1.67753454	-2.40060876
O	1.93055146	0.36131341	-0.58859724
O	0.11633224	-1.42472277	0.93642216
Zr	-0.15770532	0.03061035	-0.83939309

$\eta^2$ -ozone ComplexFig. S141: ONCCNO  $\eta^2$ -ozone Complex

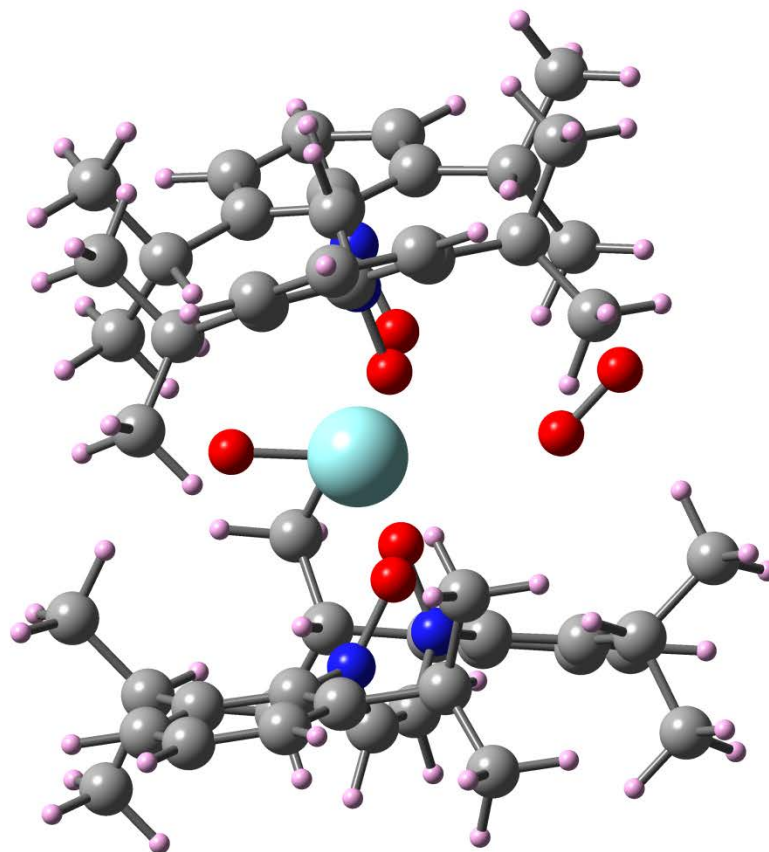
SCF	E <sub>ZP</sub>	H	G
-2816.589395	-2815.431892	-2815.358608	-2815.550471

O	-1.79520700	1.09356900	0.04079300
O	1.79514100	-1.09354500	0.04074800
O	0.51571900	1.03680400	-2.04737700
N	-0.88638500	-2.99802000	0.64807600
N	2.23262000	-2.36870800	-0.24919400
N	0.88634100	2.99804600	0.64794000
N	-2.23266900	2.36872100	-0.24925800
C	0.17761400	-3.77171400	0.30274800
C	1.49752000	-3.50329500	-0.08312500
C	-0.17764900	3.77173500	0.30257200
C	-1.49756900	3.50331400	-0.08325100
C	-2.17454000	-3.57697000	0.99377300
C	-2.46417900	-3.80068100	2.36406900
C	-3.71683300	-4.36574200	2.67939200
C	-4.63735300	-4.68720100	1.66793100
C	-4.33019500	-4.43342500	0.32222200

C	-3.09422100	-3.85961400	-0.04684700
C	-2.00368500	-2.14088400	4.21575400
C	-1.48842100	-3.40493200	3.47543500
C	-1.22222000	-4.56353300	4.46861100
C	4.66920300	-0.82561300	2.29049000
C	4.30886000	-2.25374400	1.79980200
C	5.00685900	-3.33424000	2.66344900
C	3.62185300	-2.43354800	-0.68184200
C	4.63401400	-2.39961500	0.31080700
C	5.97283600	-2.46275000	-0.12609400
C	6.28092500	-2.55236900	-1.49386500
C	5.25629900	-2.56410200	-2.45275800
C	3.89910500	-2.49126300	-2.07021400
C	-3.85420200	-2.59888700	-2.11982200
C	-2.79420800	-3.55635700	-1.51742300
C	-2.69285800	-4.86267900	-2.34873200
C	3.00213600	-1.30511600	-4.13658900
C	2.79875500	-2.47175800	-3.13609100
C	2.72264500	-3.83094900	-3.88142800
C	2.17458600	3.57698100	0.99331100
C	3.09419300	3.85906100	-0.04752200
C	4.33029200	4.43284200	0.32117200
C	4.63763000	4.68711900	1.66674700
C	3.71718500	4.36617500	2.67844200
C	2.46442300	3.80114700	2.36349000
C	3.85372000	2.59711700	-2.11995200
C	2.79398800	3.55511100	-1.51792100
C	2.69279400	4.86102700	-2.34989300
C	-4.66915000	0.82490700	2.29014000
C	-4.30885700	2.25315000	1.79973800
C	-5.00683600	3.33345400	2.66364400
C	-3.62190900	2.43354400	-0.68187600
C	-4.63405300	2.39933400	0.31078100
C	-5.97288600	2.46240100	-0.12609700
C	-6.28099600	2.55229600	-1.49384700
C	-5.25638000	2.56437200	-2.45274700
C	-3.89917700	2.49157100	-2.07022900
C	2.00382100	2.14220900	4.21592100
C	1.48870900	3.40603500	3.47512000
C	1.22282100	4.56510700	4.46782900
C	-3.00203700	1.30616600	-4.13695600
C	-2.79881800	2.47253100	-3.13610500
C	-2.72287700	3.83196100	-3.88102500
H	-0.07196600	-4.82745100	0.31913600
H	2.07640000	-4.39043900	-0.31697300
H	0.07196500	4.82746600	0.31883200
H	-2.07643100	4.39044700	-0.31719000
H	-3.97482200	-4.55421300	3.71829100
H	-5.59724100	-5.12635000	1.93034500
H	-5.05832500	-4.67111500	-0.44893300
H	-0.53102800	-3.13610600	3.01514100
H	3.22761500	-2.37216600	1.93092200

H	-2.96641000	-2.33497900	4.70768400
H	-2.13661000	-1.31107500	3.51238800
H	-1.28445200	-1.83062100	4.98576300
H	-2.13012700	-4.84539600	5.01759600
H	-0.47002600	-4.25971800	5.20851800
H	-0.85092700	-5.45761600	3.95127100
H	5.74504400	-0.63050900	2.18496800
H	4.40564100	-0.70934100	3.35056400
H	4.12248800	-0.07085600	1.71457600
H	4.75084500	-4.34630300	2.32383400
H	4.69575800	-3.23635600	3.71195700
H	6.09975900	-3.23565600	2.63351100
H	6.77720700	-2.43991800	0.60452200
H	7.31986100	-2.60369900	-1.81180600
H	5.51000800	-2.61712400	-3.50820900
H	-1.83430700	-3.03654500	-1.59230500
H	1.83191700	-2.30182300	-2.65184600
H	-4.85357100	-3.05507300	-2.13972400
H	-3.57548200	-2.34184400	-3.14921800
H	-3.90951400	-1.66739800	-1.54478200
H	-3.64311300	-5.41403900	-2.34912100
H	-1.91665200	-5.53179100	-1.95382000
H	-2.43891100	-4.62536200	-3.38978500
H	3.01951900	-0.34288200	-3.61366500
H	2.16626600	-1.27806300	-4.84548100
H	3.93515300	-1.41512300	-4.70658800
H	3.65656400	-4.04570800	-4.41847800
H	1.90697100	-3.81043900	-4.61547200
H	2.53521800	-4.66179900	-3.18800600
H	5.05838300	4.67009300	-0.45015500
H	5.59760800	5.12624000	1.92887800
H	3.97531500	4.55503500	3.71723700
H	1.83397700	3.03544200	-1.59242100
H	-3.22760800	2.37156300	1.93084300
H	4.85317000	3.05310200	-2.14023400
H	3.57482100	2.33957100	-3.14917400
H	3.90893600	1.66592700	-1.54441700
H	1.91675900	5.53049000	-1.95524400
H	2.43869200	4.62322500	-3.39079800
H	3.64315300	5.41220600	-2.35066500
H	-5.74498900	0.62980400	2.18461000
H	-4.40555200	0.70841500	3.35018200
H	-4.12243700	0.07028400	1.71405000
H	-4.75088900	4.34559300	2.32420400
H	-4.69565100	3.23538400	3.71211100
H	-6.09973300	3.23483100	2.63377300
H	-6.77724900	2.43931500	0.60452000
H	-7.31994100	2.60359100	-1.81176700
H	-5.51010100	2.61763800	-3.50818400
H	0.53122100	3.13718300	3.01504000
H	-1.83196300	2.30258000	-2.65190400
H	2.96664600	2.33632600	4.70765000

H	2.13649600	1.31207400	3.51289500
H	1.28462200	1.83241700	4.98615000
H	0.47067000	4.26173500	5.20796200
H	0.85160800	5.45902500	3.95014700
H	2.13084400	4.84706200	5.01657700
H	-3.01925400	0.34377300	-3.61432600
H	-2.16618300	1.27946200	-4.84588200
H	-3.93509000	1.41619900	-4.70689200
H	-2.53561800	4.66262800	-3.18733600
H	-3.65680100	4.04673600	-4.41805900
H	-1.90716000	3.81180400	-4.61502900
O	-0.00027400	0.00012300	-3.01922900
O	-0.51577500	-1.03680100	-2.04737600
O	0.83644800	1.61819800	0.73067100
O	-0.83647200	-1.61816300	0.73074500
Zr	-0.00002600	0.00000900	-0.29060800

**Oxo Complex with weakly adsorbed O<sub>2</sub> molecule**Fig. S142: ONCCNO Oxo Complex with weakly adsorbed O<sub>2</sub> molecule

SCF	E <sub>ZP</sub>	H	G
-2816.604669	-2815.449241	-2815.374298	-2815.572113

Zr	0.01620200	-0.03518800	-0.19227100
O	-0.90642000	-1.84334500	0.51503000
O	1.10547400	1.78325300	0.15706300
O	0.26281600	1.13836700	3.63125100
O	0.36352700	0.24786900	2.72943900
N	-2.17810500	2.31623100	0.32801400
N	0.96811700	3.03520900	-0.41185700
N	2.20431500	-2.50033500	0.41949500
N	-0.92017700	-3.08409000	-0.12023300
C	-1.52876200	3.42712000	-0.11781700
C	-0.19929800	3.73115000	-0.44628700
C	1.49714600	-3.65802700	0.25210100
C	0.16027400	-3.91078900	-0.07040100
C	-3.62008800	2.33990000	0.53684700
C	-4.46263700	2.01770500	-0.55622900
C	-5.85545600	2.07886200	-0.33772900

C	-6.37587400	2.42027400	0.92088500
C	-5.51344600	2.69879500	1.99355600
C	-4.11319900	2.65994600	1.82596600
C	-4.47964500	0.25685200	-2.39774800
C	-3.91105000	1.62029500	-1.92885200
C	-4.19538500	2.72434900	-2.98221500
C	2.19459200	1.85764900	-4.18368800
C	1.48255300	2.91580600	-3.30343300
C	0.78431400	3.98419200	-4.18657200
C	2.20427400	3.61279400	-0.91723600
C	2.45148000	3.57067800	-2.31270200
C	3.65001500	4.15802400	-2.77282600
C	4.56745000	4.72871400	-1.87685500
C	4.30990500	4.72045600	-0.49584400
C	3.12096700	4.16126900	0.01558000
C	-3.33278900	1.80709400	4.08026200
C	-3.18576400	2.92554500	3.01467800
C	-3.43062500	4.32393500	3.63717300
C	3.76874600	3.03583300	2.18430600
C	2.86805800	4.11523500	1.52466000
C	3.06526500	5.49510400	2.20053000
C	3.59681700	-2.53668300	0.84041700
C	3.88764300	-2.61331000	2.22550000
C	5.24608100	-2.67877700	2.60235600
C	6.26551900	-2.64263300	1.63814100
C	5.94715400	-2.53595600	0.27450300
C	4.60510700	-2.47885100	-0.15504200
C	3.01080200	-1.50661700	4.34668800
C	2.79054400	-2.62337500	3.29439100
C	2.69030700	-4.01192800	3.98058300
C	-1.53794000	-2.31667700	-4.07684100
C	-1.19175200	-3.43515600	-3.05993900
C	-0.81024800	-4.75461400	-3.78356500
C	-2.19926700	-3.49892100	-0.66129900
C	-2.33538000	-3.66779500	-2.06534300
C	-3.60129300	-4.06318300	-2.55035700
C	-4.68486600	-4.25751800	-1.68178200
C	-4.52443300	-4.06794900	-0.29896600
C	-3.27963500	-3.69149300	0.24284500
C	4.78576200	-0.98806900	-2.19663400
C	4.27841400	-2.34615300	-1.64475800
C	4.85335300	-3.52982200	-2.46510800
C	-3.84728400	-2.19774100	2.20871700
C	-3.12812300	-3.49561400	1.75445900
C	-3.63384400	-4.72385900	2.55341000
H	-2.21569200	4.25251400	-0.27247500
H	-0.06097100	4.73572500	-0.83168000
H	2.11719000	-4.54025000	0.37473800
H	-0.07313600	-4.94106100	-0.32000900
H	-6.53443900	1.84778300	-1.15442300
H	-7.45281500	2.45956900	1.06837700
H	-5.92966100	2.94433500	2.96747100

H	-2.82540000	1.49837500	-1.85627500
H	0.70929600	2.37654100	-2.74713300
H	-5.56481700	0.30205800	-2.56262500
H	-4.27620700	-0.53070300	-1.66306000
H	-4.00598800	-0.03582200	-3.34287000
H	-5.27476800	2.87593300	-3.11907500
H	-3.76675200	2.43930300	-3.95170900
H	-3.75547000	3.68584200	-2.68624100
H	2.95362300	2.30893600	-4.83716800
H	1.45610300	1.34994100	-4.81612900
H	2.67867100	1.09654000	-3.56144100
H	0.22670000	4.70812800	-3.57769200
H	0.07669600	3.50097900	-4.87259800
H	1.51352700	4.54348200	-4.78864700
H	3.87166600	4.15342900	-3.83681400
H	5.48754300	5.17053300	-2.25283000
H	5.03645300	5.15162800	0.18772800
H	-2.14958100	2.89492700	2.66172000
H	1.83014100	3.80755400	1.69239800
H	-4.34801800	1.78519200	4.49882200
H	-2.62814300	1.97432300	4.90538700
H	-3.12105200	0.82501100	3.64201500
H	-4.44475000	4.41017600	4.04884000
H	-3.30122000	5.12101900	2.89349800
H	-2.72172500	4.50252100	4.45631700
H	3.58222900	2.05485100	1.73368500
H	3.55679000	2.96995800	3.25999000
H	4.83298100	3.27896300	2.06124600
H	4.10618200	5.83760700	2.13258100
H	2.80874000	5.43038200	3.26616800
H	2.42765100	6.26176100	1.74135400
H	5.50703300	-2.74661700	3.65540100
H	7.30666700	-2.69001700	1.94916000
H	6.74636900	-2.49688800	-0.46139500
H	1.83078800	-2.42325100	2.80578000
H	-0.31052200	-3.08794100	-2.51244000
H	3.92682700	-1.67252600	4.92879300
H	2.16846500	-1.48220700	5.05018500
H	3.08507200	-0.52324500	3.86755400
H	2.47549600	-4.80368100	3.25158200
H	1.88589300	-4.01063100	4.72793000
H	3.62732300	-4.27002400	4.49189100
H	-2.45995100	-2.53973000	-4.63110800
H	-0.72227000	-2.21363800	-4.80544600
H	-1.63928300	-1.35642400	-3.56062300
H	-0.53983400	-5.54454700	-3.06970200
H	0.04725200	-4.58636200	-4.44821800
H	-1.64070300	-5.12930800	-4.39669000
H	-3.74001300	-4.20425300	-3.61908900
H	-5.65315200	-4.55196800	-2.08024400
H	-5.37110200	-4.22223600	0.36477600
H	3.19043200	-2.35132000	-1.76446700



H	-2.06586800	-3.36283300	1.98131600
H	5.87900500	-0.90905400	-2.12382300
H	4.34294600	-0.15433700	-1.64014700
H	4.50892400	-0.88192600	-3.25387800
H	4.56358300	-3.43342000	-3.51974100
H	4.47873500	-4.49324900	-2.09524600
H	5.95016800	-3.55666800	-2.42164400
H	-3.42688000	-1.32846600	1.69228100
H	-3.72018700	-2.05295300	3.29046100
H	-4.92456500	-2.24419900	1.99741300
H	-3.12785900	-5.64511900	2.23588500
H	-4.71463900	-4.87479300	2.43341700
H	-3.43889700	-4.57858600	3.62438300
O	-0.33492800	0.06237400	-1.97357900
O	-1.57886400	1.12030600	0.65378000
O	1.75830400	-1.25676500	0.03229500

### 10.5 Structures with eight oxygen atoms

#### Oxo Complex with adsorbed ozone group (conformation 1 lower energy)

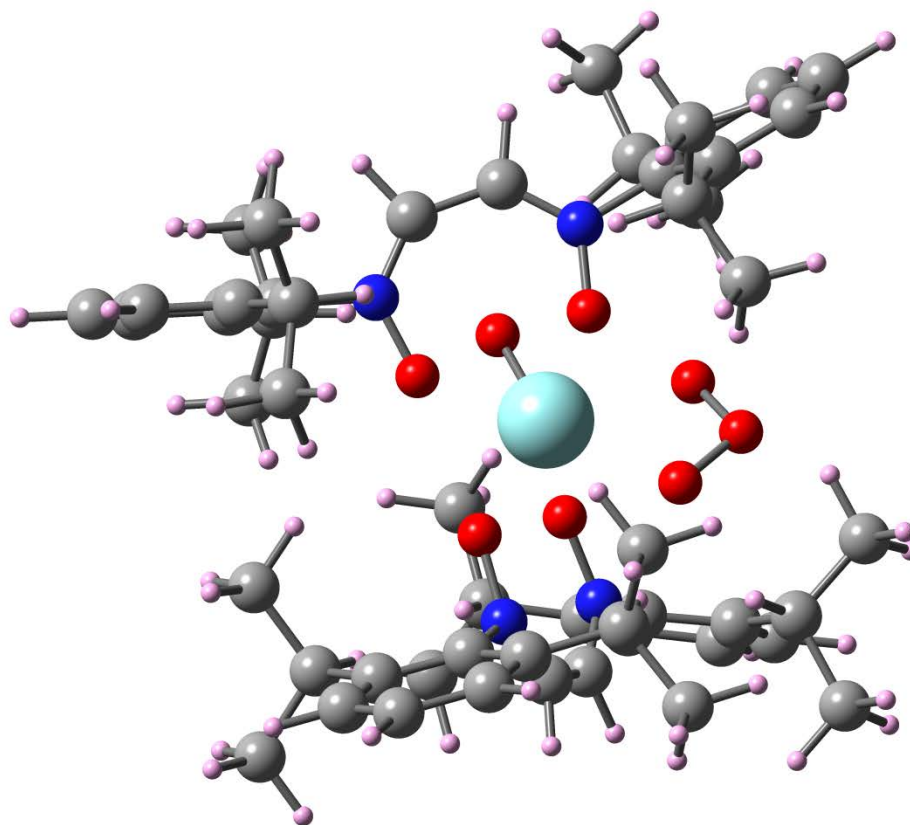


Fig. S143: ONCCNO Oxo Complex with adsorbed ozone group (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G
-2891.748948	-2890.587303	-2890.513003	-2890.704289

O	0.06584578	-1.65904609	0.55993429
O	-1.07419361	1.91116183	0.80471832
O	1.66512317	2.22932680	0.38057256
N	-2.85510920	0.17482018	-1.20942523
N	-1.61699092	2.89513821	0.05449789
N	3.27888754	-1.10366119	-0.22699267
N	0.77617975	-2.49102515	1.40144657
C	-3.07279800	1.47270390	-1.42807055
C	-2.49847508	2.67801992	-0.91004342
C	3.18626504	-2.12187223	0.67190119
C	2.12397286	-2.70162146	1.37106253
C	-3.72333901	-0.79525859	-1.90894933
C	-3.34949296	-1.19332754	-3.21321114
C	-4.20535575	-2.11015470	-3.86125061

C	-5.35294316	-2.60704615	-3.22328477
C	-5.66947825	-2.20760555	-1.91445406
C	-4.85439543	-1.29013023	-1.21913121
C	-1.14125095	-1.86117521	-4.27197007
C	-2.08223989	-0.68350370	-3.90785287
C	-2.43213728	0.15047224	-5.16820496
C	1.57368667	4.58400823	-2.02577667
C	0.03400099	4.46404540	-1.88364722
C	-0.68290559	5.18897322	-3.05461369
C	-1.21012062	4.26440935	0.40012296
C	-0.44084666	5.00875476	-0.53025717
C	-0.08801868	6.32112003	-0.14577077
C	-0.45900833	6.84157014	1.10198778
C	-1.19780316	6.06055183	2.00574861
C	-1.59439265	4.74950381	1.67696138
C	-5.00889520	-2.11813515	1.17081000
C	-5.18501310	-0.90010607	0.22485460
C	-6.60716351	-0.29592807	0.34878629
C	-1.45383473	3.43043063	3.83105877
C	-2.38651935	3.91236551	2.68693097
C	-3.61278254	4.67626733	3.24818954
C	4.55530818	-0.74609359	-0.82766479
C	5.48221280	0.01794605	-0.07554921
C	6.71630653	0.32904722	-0.68713593
C	6.99642032	-0.07666744	-2.00017101
C	6.04466355	-0.80513459	-2.73313046
C	4.80533813	-1.15953031	-2.16271618
C	5.26988603	2.07400431	1.40361548
C	5.18735156	0.52674381	1.33893557
C	6.13551397	-0.12165532	2.38216269
C	-1.82215976	-4.37611796	-0.59669902
C	-0.54899447	-4.78762517	0.19017154
C	-0.20947260	-6.28202145	-0.03521604
C	-0.07261817	-3.31360521	2.25356958
C	-0.71010622	-4.44063343	1.67254346
C	-1.53930936	-5.22051527	2.50439459
C	-1.71899063	-4.89109972	3.85855950
C	-1.08158752	-3.76586946	4.40297877
C	-0.25188223	-2.94363604	3.60925754
C	3.07330821	-0.97075636	-3.99404931
C	3.76503526	-1.92616518	-2.98392543
C	4.36797411	-3.15923098	-3.70181533
C	-0.65360386	-0.72373029	4.78579238
C	0.40594728	-1.70268752	4.21809587
C	1.43782558	-2.09188167	5.30931773
H	-3.86373652	1.64545030	-2.14915738
H	-2.87477298	3.58318983	-1.37229278
H	4.15508797	-2.55726486	0.89317727
H	2.42208938	-3.49191477	2.05214937
H	-3.96364690	-2.44102059	-4.86761889
H	-5.99649911	-3.31336326	-3.74238988
H	-6.55172632	-2.61361784	-1.42698257

H	-1.51535315	-0.03574758	-3.22856784
H	-0.18570719	3.39329567	-1.95388014
H	-1.60021984	-2.54424444	-5.00014987
H	-0.87364008	-2.43733778	-3.37815991
H	-0.21519191	-1.46769395	-4.70828980
H	-2.95826146	-0.45205623	-5.92154083
H	-1.51184579	0.53637895	-5.62395626
H	-3.07023149	1.00963440	-4.92008392
H	1.90767072	5.63069459	-2.04056223
H	1.88952652	4.11466392	-2.96607457
H	2.07294920	4.06254547	-1.20292288
H	-1.77600996	5.08109192	-3.00157687
H	-0.34898318	4.76905142	-4.01189474
H	-0.45745783	6.26409340	-3.05914286
H	0.50254438	6.92883057	-0.82524088
H	-0.16455693	7.85195668	1.37573377
H	-1.47008447	6.47320055	2.97300207
H	-4.47186764	-0.13781027	0.55944449
H	-2.76068608	3.01224437	2.18722357
H	-5.70132965	-2.92919742	0.90871598
H	-5.21089820	-1.82294725	2.20869300
H	-3.98651592	-2.50808494	1.11952194
H	-7.38080520	-1.02602284	0.07846726
H	-6.73086272	0.57954310	-0.30215651
H	-6.79449427	0.01813272	1.38382746
H	-0.62960418	2.83261870	3.42940093
H	-2.01663056	2.81061669	4.54194932
H	-1.03278462	4.28285021	4.38123530
H	-3.31457144	5.55029066	3.84083820
H	-4.19219502	4.01616906	3.90703246
H	-4.27467193	5.02447031	2.44416986
H	7.45302212	0.90771886	-0.13564196
H	7.95012605	0.18096370	-2.45539930
H	6.26899904	-1.10467269	-3.75335443
H	4.16175375	0.25279815	1.60491982
H	0.27858206	-4.19484978	-0.21427525
H	6.28315061	2.43493488	1.18096548
H	4.99937214	2.42155571	2.40900049
H	4.57320156	2.53003858	0.69164325
H	6.05717669	-1.21703912	2.37240412
H	5.88409519	0.22865228	3.39185573
H	7.18383966	0.14026836	2.18569409
H	-2.70515129	-4.91782390	-0.22968514
H	-1.70195099	-4.60951529	-1.66358075
H	-1.99880239	-3.30019976	-0.49586927
H	0.68767693	-6.57917173	0.52342750
H	-0.02425711	-6.46670140	-1.10169804
H	-1.03262927	-6.93966272	0.27363609
H	-2.04335585	-6.09136143	2.09316269
H	-2.35782228	-5.50890064	4.48594602
H	-1.23527190	-3.51622955	5.44988467
H	2.98495941	-2.28573796	-2.30423424

H	0.94226380	-1.16274327	3.43310957
H	3.80473829	-0.53578714	-4.68948907
H	2.56187712	-0.16082766	-3.46368155
H	2.32774777	-1.52100226	-4.58473735
H	3.57149066	-3.72509044	-4.20312024
H	4.87119817	-3.83105075	-2.99404768
H	5.09727720	-2.87005283	-4.46990034
H	-1.37077739	-0.43303041	4.00891901
H	-0.16066869	0.18730637	5.14740486
H	-1.21037619	-1.16728533	5.62278815
H	2.21785709	-2.75089256	4.90574055
H	0.95849181	-2.61407921	6.14855708
H	1.92556003	-1.19147941	5.70485301
O	-0.06622571	1.06646245	-1.84364490
O	1.87404774	1.97592893	1.76227449
O	1.27441254	0.75046392	2.09865089
O	2.19979849	-0.42961339	-0.75961206
O	-1.92617966	-0.38213339	-0.43750900
Zr	0.32755716	0.38821129	-0.18340973

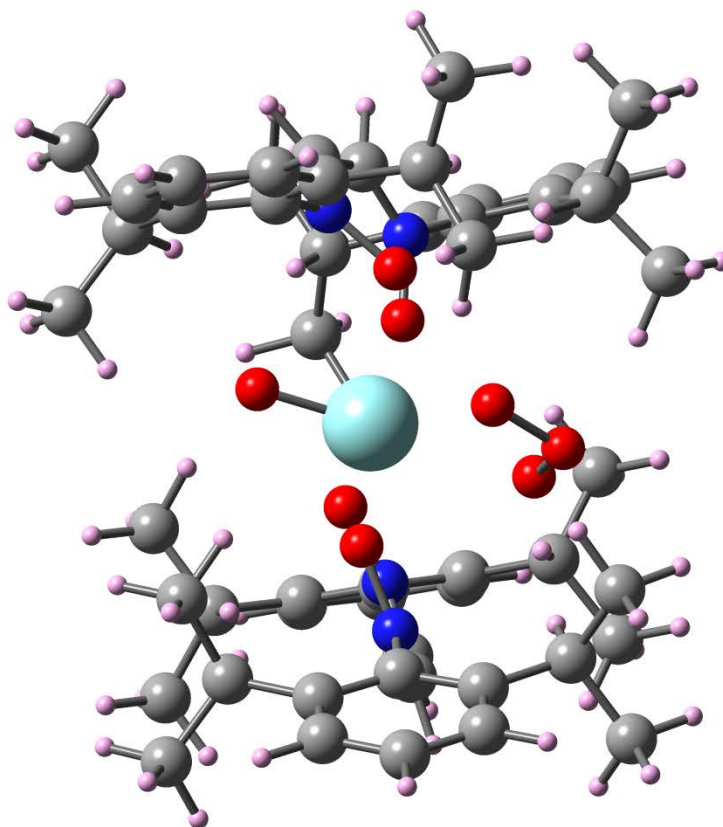
**Oxo Complex with adsorbed ozone group (conformation 2 higher energy)**

Fig. S144: ONCCNO Oxo Complex with adsorbed ozone group (conformation 2 higher energy)

SCF	$E_{ZP}$	H	G
-2891.740131	-2890.578941	-2890.504264	-2890.696996

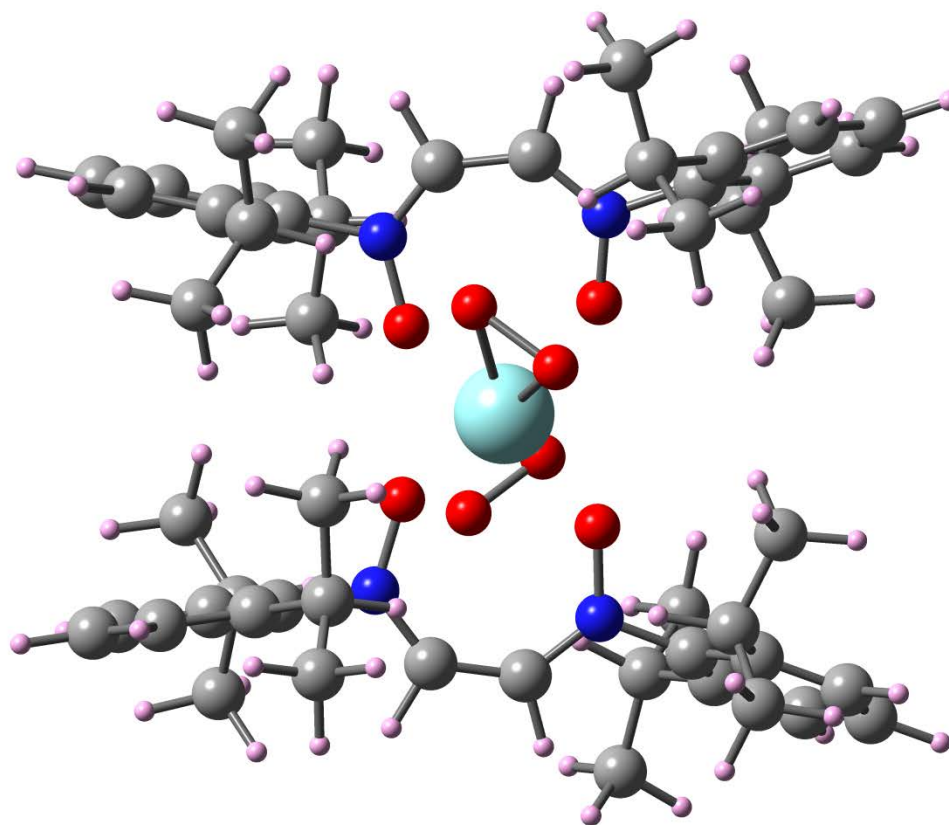
O	2.28300512	-0.86803321	0.15502137
O	-1.73949325	0.74264793	-0.14350497
O	0.03225249	-1.12847331	-2.12264092
N	-0.26342987	3.52256619	0.31497276
N	-2.69967602	1.66216156	-0.20368137
N	-0.29512476	-2.93106423	0.52722255
N	2.80672551	-2.07494689	-0.24030552
C	-1.53210626	3.70426308	0.68123973
C	-2.64243554	2.92146364	0.24101400
C	0.81714515	-3.61291797	0.12238538
C	2.13122228	-3.25855690	-0.19204603
C	0.82093054	4.36510849	0.81983486
C	1.06173512	4.45215740	2.21960499
C	2.13563614	5.27280460	2.62498063
C	2.93441892	5.95052927	1.69378220
C	2.66735725	5.83983597	0.32107657

C	1.60040216	5.05257144	-0.15439976
C	1.16415746	2.90166982	4.24415291
C	0.25087864	3.72146397	3.29861702
C	-0.62162618	4.72624814	4.09979286
C	-4.83808750	-1.07782197	1.96450153
C	-4.70218560	0.40895993	1.54879071
C	-5.67514379	1.30358806	2.36270697
C	-3.95680803	1.18143844	-0.80601788
C	-4.91891267	0.58663417	0.04274166
C	-6.11838440	0.15586672	-0.56215187
C	-6.32092212	0.29708643	-1.94449990
C	-5.32552913	0.86359431	-2.75658996
C	-4.10863855	1.31870023	-2.20598018
C	2.41438099	4.19520998	-2.40374880
C	1.32336709	5.01466720	-1.66381576
C	1.19986876	6.44349693	-2.25565957
C	-2.50945497	0.82936875	-4.11623191
C	-3.01757373	1.89825732	-3.11182521
C	-3.51381939	3.16821761	-3.85121930
C	-1.51608355	-3.65615568	0.84437861
C	-2.38070727	-4.04727524	-0.20876902
C	-3.54327539	-4.77011797	0.13878707
C	-3.83759655	-5.06868668	1.47785297
C	-2.97109928	-4.65177415	2.50210984
C	-1.78966841	-3.94013928	2.20851960
C	-3.25892464	-2.92046260	-2.31559187
C	-2.09422794	-3.71848797	-1.67669719
C	-1.79990788	-5.00617556	-2.49094025
C	4.73677112	-0.21078193	2.44677890
C	4.62823531	-1.69614175	2.00792051
C	5.37312973	-2.62764803	2.99697791
C	4.23445580	-2.03565698	-0.52417420
C	5.12447866	-1.86121887	0.56854667
C	6.50360823	-1.81128049	0.28087679
C	6.97339312	-1.93669097	-1.03714183
C	6.06890198	-2.09981593	-2.09667495
C	4.67623640	-2.13984748	-1.86623315
C	-1.52159619	-2.38190383	4.19060173
C	-0.85697537	-3.49562790	3.33913900
C	-0.41743498	-4.68857919	4.22596024
C	3.87324657	-1.07578964	-4.02931767
C	3.71433694	-2.26892160	-3.05123487
C	3.90435288	-3.62010204	-3.78972726
H	-1.74213398	4.58121413	1.27978286
H	-3.60884313	3.41390893	0.26162632
H	0.61384310	-4.67341932	0.01427126
H	2.76173387	-4.09489959	-0.47471415
H	2.36000862	5.36205824	3.68353649
H	3.76468033	6.56317841	2.03696151
H	3.28814552	6.37680355	-0.39012668
H	-0.39407612	2.98160210	2.81899816
H	-3.67905628	0.71352544	1.79762014

H	1.88508531	3.53082439	4.78287372
H	1.69082262	2.14234094	3.65969863
H	0.54654892	2.38578905	4.99192928
H	0.00332577	5.45145416	4.63765002
H	-1.22792747	4.19039511	4.84196867
H	-1.30267616	5.29875292	3.45312084
H	-5.85220554	-1.45600551	1.78122395
H	-4.62744832	-1.18805494	3.03573093
H	-4.13190739	-1.70901656	1.41480736
H	-5.55749657	2.36628965	2.11105013
H	-5.48796077	1.18572014	3.43778546
H	-6.72073834	1.02953537	2.17096323
H	-6.89081728	-0.30140690	0.05023752
H	-7.25140485	-0.04499549	-2.39115774
H	-5.48954222	0.94668233	-3.82747775
H	0.37435453	4.50096997	-1.84325421
H	-2.15535598	2.18561830	-2.50012268
H	3.41448920	4.61246593	-2.22281978
H	2.22846569	4.21562744	-3.48601161
H	2.39969253	3.14979060	-2.08138530
H	2.15006687	6.99037738	-2.21092805
H	0.44329088	7.03788548	-1.72601805
H	0.90773569	6.38039455	-3.31214371
H	-2.09847227	-0.03900032	-3.59057640
H	-1.71049121	1.25299177	-4.73752375
H	-3.31453856	0.48946290	-4.78157224
H	-4.35207169	2.94089360	-4.52267657
H	-2.70287441	3.58800606	-4.45998676
H	-3.84805049	3.94179465	-3.14684362
H	-4.22458116	-5.09333429	-0.64445653
H	-4.74001953	-5.62418391	1.72377065
H	-3.21018455	-4.88832634	3.53601236
H	-1.20783891	-3.08041289	-1.73074083
H	3.56514292	-1.95581990	2.04282363
H	-4.18948925	-3.50400833	-2.34063828
H	-3.00203490	-2.65101341	-3.34812463
H	-3.44917512	-1.99378264	-1.76168616
H	-0.95142075	-5.56182984	-2.07052392
H	-1.55433487	-4.74763446	-3.52916501
H	-2.66786440	-5.67945759	-2.50512172
H	5.77814607	0.13829147	2.40602941
H	4.37464387	-0.09287561	3.47684696
H	4.12313426	0.42214779	1.79804576
H	5.30541674	-3.67916711	2.68811126
H	4.93168587	-2.53595148	3.99822677
H	6.43667223	-2.36824147	3.08222606
H	7.21389597	-1.67717228	1.09246260
H	8.04201767	-1.90043513	-1.23716425
H	6.44308687	-2.18134294	-3.11402598
H	0.04155880	-3.05600968	2.89627196
H	2.68699425	-2.23660335	-2.67662762
H	-2.44834820	-2.73885102	4.66175712



H	-1.75386567	-1.51381109	3.56404887
H	-0.83893814	-2.05451736	4.98594802
H	0.30166178	-4.34862538	4.98290194
H	0.06256389	-5.47480940	3.62881488
H	-1.26805688	-5.13886493	4.75460272
H	3.69233361	-0.12560772	-3.51479164
H	3.14309385	-1.16073990	-4.84434517
H	4.87770794	-1.04772983	-4.47322498
H	3.75520757	-4.47288354	-3.11393378
H	4.91221195	-3.70495432	-4.21768736
H	3.18163716	-3.70632410	-4.61176441
O	0.79017998	1.12511046	1.65456229
O	0.83722976	-0.23931204	-2.83985565
O	1.27980319	0.82624763	-2.00036232
O	-0.31838761	-1.60139153	0.91612334
O	0.04505547	2.60718342	-0.60811159
Zr	0.45433455	0.22011840	0.11408529

Peroxo Complex with adsorbed O<sub>2</sub> molecule (spiro conformation)Fig. S145: ONCCNO Peroxo Complex with adsorbed O<sub>2</sub> molecule (spiro conformation)

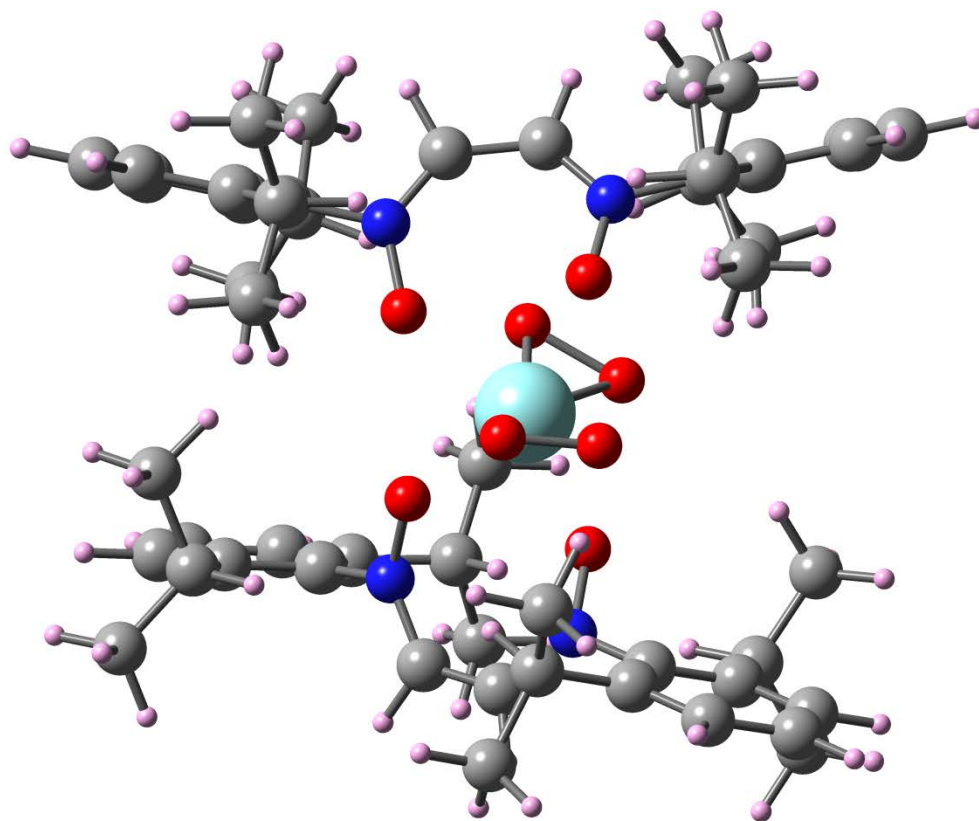
SCF	E <sub>ZP</sub>	H	G
-2891.760878	-2890.599647	-2890.525481	-2890.715226

Zr	0.18095740	-0.02047016	0.12531261
O	1.56739276	1.73786112	-0.38340453
O	-1.30595132	-1.42096943	0.74367617
O	-0.26487084	1.19190341	1.73375095
O	0.89730073	0.22862071	2.04727645
N	1.54311714	-2.91865669	-0.40182965
N	-1.69759566	-2.66355990	0.29959538
N	-1.54386920	2.71467360	-0.36801882
N	1.66493718	2.87887737	0.31827666
C	0.46832472	-3.73780658	-0.54451035
C	-0.89553498	-3.62521896	-0.23297337
C	-0.75028019	3.62401553	0.20406705
C	0.63808975	3.69575712	0.54216007
C	2.87852370	-3.35445482	-0.79005042
C	3.21513127	-3.43580256	-2.16587616
C	4.52426967	-3.85625698	-2.48814320

C	5.45784329	-4.15799663	-1.48631525
C	5.09817697	-4.05496443	-0.13261798
C	3.80045023	-3.65820035	0.24797502
C	2.80262439	-1.96437047	-4.20334561
C	2.23887500	-3.08730415	-3.29517319
C	1.88338737	-4.34533405	-4.13244705
C	-4.38220334	-1.02307601	-2.26931083
C	-3.64955985	-2.33307087	-1.88131339
C	-3.91484819	-3.44500097	-2.93047998
C	-3.10138682	-2.94683575	0.56999357
C	-4.04480292	-2.79259265	-0.47460417
C	-5.39564221	-3.07244907	-0.17316454
C	-5.78121885	-3.46346640	1.11818221
C	-4.82370328	-3.58296398	2.13968477
C	-3.45964015	-3.32883208	1.88894525
C	4.12188928	-2.32935256	2.38144317
C	3.43489388	-3.56038229	1.73257602
C	3.77866705	-4.86177010	2.50150087
C	-2.48414364	-2.15189220	3.90806220
C	-2.42516000	-3.42108420	3.01448531
C	-2.58095797	-4.70838376	3.86133045
C	-2.95708436	3.05812050	-0.59882202
C	-3.86920833	2.91046690	0.47245169
C	-5.21387273	3.25215761	0.20784820
C	-5.61496284	3.69015075	-1.06330225
C	-4.68170837	3.79319676	-2.10855627
C	-3.32360997	3.47682030	-1.90161281
C	-4.26401542	1.12355933	2.23531660
C	-3.46261743	2.39588633	1.85791520
C	-3.64091494	3.49865543	2.93530690
C	4.32893329	2.17413056	-2.36522099
C	3.66933870	3.43315893	-1.74113990
C	4.10217311	4.71952962	-2.48998955
C	3.01611876	3.24048331	0.76690476
C	3.97969800	3.50764282	-0.24174519
C	5.27716281	3.84848021	0.18893044
C	5.59105784	3.92252444	1.55564367
C	4.61399942	3.64497614	2.52191768
C	3.29825143	3.28386124	2.15656750
C	-2.51632605	2.32908470	-4.00681456
C	-2.32102515	3.54311956	-3.05786107
C	-2.40281252	4.87982783	-3.83636021
C	2.80274333	1.83688426	4.19224312
C	2.27736042	2.95166184	3.25247672
C	1.90691377	4.22347511	4.06306582
H	0.73459673	-4.68373332	-1.00350848
H	-1.46501689	-4.51616171	-0.47721792
H	-1.29627493	4.52165947	0.47434223
H	0.91390694	4.60474935	1.06362501
H	4.81551189	-3.93200158	-3.53258442
H	6.46362159	-4.47047410	-1.75806276
H	5.82959168	-4.29190415	0.63536125

H	1.31319503	-2.70047692	-2.86210899
H	-2.57774066	-2.11276706	-1.89439704
H	3.73365561	-2.26907867	-4.70012740
H	2.99558340	-1.05709972	-3.62058907
H	2.06937418	-1.71180559	-4.98004659
H	2.77122058	-4.76098350	-4.62755811
H	1.15301993	-4.08688819	-4.91036964
H	1.44865542	-5.13773280	-3.50806465
H	-5.47132926	-1.16144173	-2.30158779
H	-4.05433117	-0.69127287	-3.26297583
H	-4.15839489	-0.22225939	-1.55484561
H	-3.37529061	-4.36829039	-2.68156094
H	-3.58262320	-3.11494461	-3.92331273
H	-4.98389938	-3.68872736	-2.99521423
H	-6.14801779	-2.97471829	-0.95170404
H	-6.82765262	-3.67031973	1.33136745
H	-5.13860087	-3.87878274	3.13660977
H	2.35662562	-3.39620903	1.81869467
H	-1.42600833	-3.44038642	2.56514618
H	5.21653740	-2.40463478	2.31777073
H	3.84430862	-2.25686785	3.44136300
H	3.79958807	-1.40981443	1.88258091
H	4.86027168	-5.04926520	2.52832493
H	3.29590545	-5.73700551	2.04695692
H	3.43253135	-4.78175947	3.54048741
H	-2.25928649	-1.25912804	3.31631856
H	-1.73913104	-2.22247889	4.71147361
H	-3.47627676	-2.03977514	4.36792679
H	-3.52249532	-4.71598809	4.42614628
H	-1.76250145	-4.77416125	4.58998637
H	-2.55454590	-5.60974721	3.23491994
H	-5.94999046	3.16247704	1.00186992
H	-6.65701196	3.94365264	-1.24338697
H	-5.01035893	4.12096993	-3.09072745
H	-2.40674142	2.10496730	1.85153647
H	2.58923752	3.31846023	-1.87764294
H	-5.34194992	1.32393784	2.30220068
H	-3.92682700	0.75149786	3.21029766
H	-4.10415508	0.32541773	1.50156995
H	-3.05578941	4.39747185	2.69724556
H	-3.30384100	3.12499544	3.91022467
H	-4.69261147	3.80044973	3.03286414
H	5.42219748	2.20751687	-2.26328283
H	4.08712148	2.11104996	-3.43429630
H	3.95983394	1.26651604	-1.87663185
H	3.64360034	5.61562145	-2.05130810
H	3.79433422	4.65779444	-3.54203083
H	5.19103337	4.85638020	-2.47403481
H	6.04504731	4.06119949	-0.54943882
H	6.59845982	4.19002360	1.86573686
H	4.87486495	3.68964617	3.57533677
H	-1.30621126	3.46152491	-2.65142108

H	1.36850851	2.54770652	2.79942166
H	-3.52286689	2.33081852	-4.44697358
H	-2.37087799	1.38983653	-3.46353627
H	-1.78471699	2.36787251	-4.82430281
H	-1.61626604	4.91363909	-4.60124693
H	-2.27149348	5.74380490	-3.17175277
H	-3.36536692	4.99362709	-4.35123607
H	2.99400131	0.92257044	3.62254140
H	2.03547622	1.60084708	4.94007029
H	3.71754888	2.13497301	4.72291124
H	1.50128745	5.01938439	3.42183575
H	2.78048151	4.63519019	4.58658623
H	1.14758116	3.97672892	4.81611236
O	-0.30968110	-1.02252060	-1.92031480
O	0.76435093	-0.15653689	-2.08291067
O	1.51188410	-1.72594132	0.28292091
O	-1.20819863	1.49145640	-0.82209576

Peroxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation)Fig. S146: ONCCNO Peroxo Complex with adsorbed O<sub>2</sub> molecule (planar conformation)

SCF	E <sub>ZP</sub>	H	G
-2891.754894	-2890.593548	-2890.519499	-2890.709371

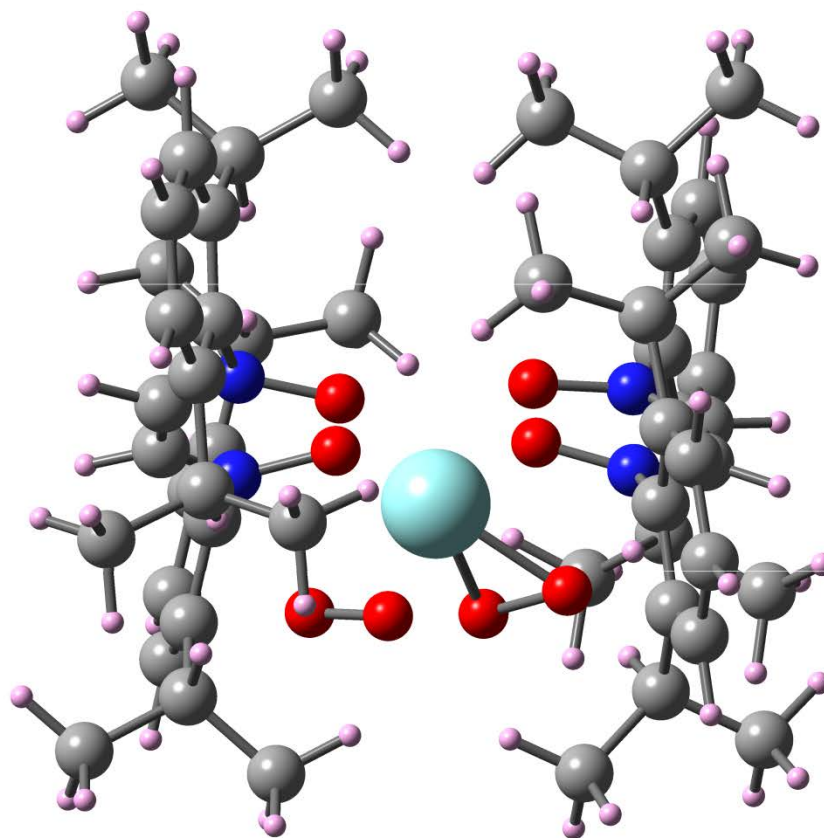
Zr	-0.43080200	-0.02085363	-0.06687941
O	-1.15361940	0.55508815	1.78027192
O	0.33560103	0.96580494	1.56329187
O	-0.88093584	-0.15051861	-2.28869911
O	-2.11934740	0.03052761	-1.66906982
C	-2.06226170	3.88531344	0.70833132
C	-3.02475368	4.35122000	-0.22990383
C	-4.19217326	4.94119946	0.29324332
C	-4.38477992	5.06950666	1.67724078
C	-3.40990786	4.60592093	2.57121857
C	-2.22274498	3.99180016	2.11698331
C	-3.80885209	3.19599394	-2.34718177
C	-2.85072627	4.26208606	-1.75146443
C	-3.05374947	5.64008103	-2.43403712
C	2.60936501	1.06340724	-4.21891906
C	2.80339288	2.40076116	-3.45312734

C	3.15106256	3.55630330	-4.42429307
C	3.51053173	2.08442554	-0.98455204
C	3.85283023	2.22845894	-2.35065988
C	5.22523271	2.16397106	-2.66792456
C	6.19105424	1.96583056	-1.66745763
C	5.80636064	1.81077944	-0.32696535
C	4.44669904	1.85247645	0.05064749
C	-1.87368310	2.55759313	4.19984103
C	-1.20888853	3.48564310	3.15224997
C	-0.50423605	4.68129095	3.85145828
C	4.64187279	0.33907115	2.09118446
C	4.04531350	1.64793754	1.51677560
C	4.46831688	2.86537564	2.38298751
C	2.34319569	-3.12107467	1.04526360
C	2.35619213	-3.09014708	2.46343939
C	3.59123099	-3.32716786	3.10526442
C	4.75780943	-3.56808420	2.36312153
C	4.71793760	-3.57007430	0.95852287
C	3.50893321	-3.34649551	0.26805875
C	1.25199030	-1.44864185	4.06123732
C	1.10377730	-2.78922713	3.29305353
C	0.77136710	-3.95531303	4.25971519
C	-2.74547746	-2.08872248	-4.33538391
C	-2.47640019	-3.11470788	-3.20565184
C	-2.29178248	-4.53936690	-3.79606304
C	-3.33137956	-2.96907275	-0.75350649
C	-3.58426132	-3.10048890	-2.14551120
C	-4.92985058	-3.22430011	-2.55290213
C	-5.97777364	-3.18816394	-1.62196536
C	-5.69878859	-3.04364407	-0.25364410
C	-4.37341902	-2.94317902	0.21479641
C	4.20406350	-2.07675622	-1.81065683
C	3.47976806	-3.33448331	-1.26250134
C	4.07907761	-4.63076486	-1.86502754
C	-4.50766882	-1.40846634	2.22832642
C	-4.10984815	-2.81953521	1.71969943
C	-4.83211968	-3.92837597	2.52747069
H	-4.95277239	5.30753049	-0.38988038
H	-5.29489548	5.52701300	2.05777805
H	-3.57747072	4.70053946	3.63993225
H	-1.83389970	3.92862780	-1.97897233
H	1.83817632	2.63935706	-2.99162689
H	-4.85823942	3.44497717	-2.13744063
H	-3.59066087	2.20618499	-1.93465177
H	-3.68290218	3.14464793	-3.43688384
H	-4.08527836	6.00103198	-2.33235717
H	-2.84057351	5.55467770	-3.50766768
H	-2.38640855	6.40344255	-2.01203003
H	3.54270908	0.75018014	-4.70656891
H	1.83966746	1.18044866	-4.99233280
H	2.28572248	0.27259380	-3.53473482
H	3.30487241	4.50268850	-3.88936352

H	2.33152743	3.69777592	-5.14048132
H	4.05866364	3.34432100	-5.00395557
H	5.53942760	2.26995691	-3.70236193
H	7.24419539	1.92404145	-1.93500659
H	6.56449484	1.64109689	0.43228034
H	-0.45622076	2.86787217	2.65586583
H	2.95616159	1.54873618	1.58461978
H	-2.64575937	3.07259557	4.78771446
H	-1.10889246	2.19146194	4.89729922
H	-2.30807047	1.68736232	3.70000834
H	-1.22255145	5.29412659	4.41252728
H	0.00240122	5.34581667	3.13612545
H	0.24807596	4.31096334	4.56002542
H	4.35284344	-0.52725791	1.48731316
H	4.26769684	0.17767711	3.10952267
H	5.73850953	0.37567133	2.13847616
H	5.55840527	2.99769612	2.37512338
H	4.15243949	2.71480722	3.42299137
H	4.01726271	3.80101587	2.02516295
H	3.63861960	-3.31601254	4.19124461
H	5.69918029	-3.74812288	2.87771120
H	5.63050636	-3.75086855	0.39614008
H	0.25302251	-2.66881538	2.61506186
H	-1.53499430	-2.81925956	-2.73221781
H	2.11880447	-1.46709992	4.73712348
H	0.35282632	-1.26598421	4.66375892
H	1.35249660	-0.60891702	3.36439773
H	0.63818405	-4.90108614	3.71781111
H	-0.15851117	-3.73859214	4.80138251
H	1.56461043	-4.10348678	5.00499719
H	-3.63991255	-2.34775175	-4.91828691
H	-1.89187529	-2.06608275	-5.02549322
H	-2.87189762	-1.08463778	-3.91974791
H	-2.04391222	-5.27408025	-3.01851015
H	-1.48092957	-4.54113694	-4.53675056
H	-3.20815207	-4.88003390	-4.29660536
H	-5.15774403	-3.32794551	-3.61028096
H	-7.00816567	-3.27023310	-1.96069381
H	-6.51802128	-3.02068486	0.46005431
H	2.43632849	-3.26431688	-1.58718932
H	-3.03538690	-2.92088970	1.89570155
H	5.26224264	-2.06499761	-1.51531745
H	3.72670439	-1.16514937	-1.43564333
H	4.15799585	-2.06111472	-2.90793447
H	3.98438202	-4.61590366	-2.95888665
H	3.56247994	-5.52405638	-1.49015333
H	5.14580264	-4.73505899	-1.62625148
H	-3.91372900	-0.64168808	1.72123477
H	-4.31741107	-1.32696217	3.30703346
H	-5.57389016	-1.20744153	2.05245596
H	-4.56073921	-4.92975514	2.16743993
H	-5.92466446	-3.83472937	2.47050537



H	-4.55119559	-3.85837375	3.58688353
O	-1.65074228	-1.73977057	0.48371270
N	-1.96037534	-2.86026343	-0.28845237
O	0.92984273	-1.65318106	-0.21425792
O	-1.06152548	2.19067407	-0.64361220
O	1.41209379	1.03304198	-0.95682541
N	1.08120000	-2.90948681	0.36265048
N	2.07734998	2.14250895	-0.63018114
N	-0.86163294	3.24295392	0.16044296
C	1.62749182	3.26384174	-0.06091005
H	2.42518962	3.97934439	0.10538187
C	0.35031490	3.72768015	0.38943089
H	0.37583488	4.64580634	0.96305371
C	-1.10797226	-3.92082733	-0.28908974
H	-1.54883047	-4.86076648	-0.60231473
C	0.22441027	-3.94426189	0.12549002
H	0.66488483	-4.92172409	0.29740048

Peroxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)Fig. S147: ONCCNO Peroxo Complex with adsorbed O<sub>2</sub> molecule (butterfly conformation)

SCF	E <sub>ZP</sub>	H	G
-2891.763670	-2890.602933	-2890.528493	-2890.720636

O	0.52919000	-1.47557100	0.80872500
O	1.92946100	0.79437800	-0.09899100
O	1.15047900	-1.04869500	-2.21958100
N	-0.38209900	2.90977600	0.71534000
N	2.53496000	1.98854800	-0.45459900
N	-2.53067100	-1.90819100	-0.43899800
N	0.36938400	-2.81085300	0.78155700
C	0.76197500	3.57588900	0.38737100
C	1.99923500	3.19769800	-0.15289400
C	-1.93886000	-3.08669700	-0.26638600
C	-0.67860300	-3.47470000	0.29738300
C	-1.46355500	3.61300700	1.39626400
C	-2.50954700	4.16875200	0.61922200
C	-3.54735900	4.83212400	1.30817600
C	-3.54241900	4.92582900	2.70914300
C	-2.50101200	4.34808000	3.45320100

C	-1.44060200	3.67395300	2.81197400
C	-3.72955600	3.12582400	-1.33954500
C	-2.55453000	4.04156400	-0.90513600
C	-2.63961900	5.42555800	-1.59814000
C	2.88083000	1.22109800	-4.34265600
C	3.08594100	2.39707200	-3.34988900
C	3.40244200	3.71532000	-4.10251500
C	3.89863000	1.85583000	-0.94744700
C	4.17049900	2.05728900	-2.32403300
C	5.50759000	1.89704300	-2.75006900
C	6.51990300	1.53872000	-1.84815400
C	6.21715400	1.33218400	-0.49185900
C	4.90146300	1.48648300	-0.01186400
C	-0.92041000	1.77765900	4.40676400
C	-0.34444100	2.99728400	3.63889000
C	0.35555900	3.98318500	4.60732300
C	4.67029200	-0.27863800	1.78752100
C	4.58853700	1.23742200	1.46654400
C	5.51076200	2.05812400	2.40358000
C	-3.91760200	-1.84352500	-0.93535300
C	-4.16754600	-1.97475600	-2.32337900
C	-5.51857900	-1.90471600	-2.72899500
C	-6.54882800	-1.69117200	-1.80137400
C	-6.25496100	-1.53530200	-0.43652300
C	-4.92748500	-1.60547900	0.03132000
C	-3.13546900	-1.10626200	-4.48496500
C	-3.05997500	-2.17268400	-3.36227300
C	-3.10944600	-3.60428800	-3.95843400
C	1.14015100	-1.77064800	4.36494700
C	0.51745400	-3.02140400	3.69049100
C	-0.05324300	-4.00093000	4.74545900
C	1.49152000	-3.57108900	1.36005200
C	1.54482500	-3.68744600	2.77040400
C	2.62321700	-4.41718500	3.31052500
C	3.59510400	-4.99147600	2.47456600
C	3.51596100	-4.83738400	1.08211400
C	2.46273100	-4.11111300	0.48376100
C	-4.77192300	0.11950600	1.87534300
C	-4.61859400	-1.38327500	1.51604900
C	-5.49248400	-2.27196200	2.43654000
C	3.71142800	-3.28102700	-1.57256500
C	2.41295400	-3.93553300	-1.03741200
C	2.15062100	-5.29455100	-1.74070900
H	0.67563400	4.63811300	0.59215800
H	2.67081000	4.02271300	-0.36600100
H	-2.54991000	-3.92312700	-0.58598100
H	-0.55329900	-4.54999600	0.36030800
H	-4.36459300	5.27304500	0.74328200
H	-4.35158300	5.44218200	3.22082200
H	-2.51426700	4.41653900	4.53821500
H	-1.63449400	3.55834700	-1.24643200
H	2.13386300	2.53594700	-2.83192700

H	-4.69915900	3.55361800	-1.04838500
H	-3.63373000	2.13325000	-0.88516700
H	-3.72142600	2.99771500	-2.42884800
H	-3.56920300	5.95271400	-1.34416600
H	-2.61535600	5.29806100	-2.68808500
H	-1.79820800	6.07062200	-1.31226600
H	3.80163900	1.00324200	-4.90179000
H	2.09496700	1.47886600	-5.06471500
H	2.56308800	0.31367900	-3.81668800
H	3.52849900	4.55738900	-3.40829800
H	2.58072500	3.95890000	-4.78831100
H	4.32106300	3.63195500	-4.69855400
H	5.75051900	2.04262800	-3.79937700
H	7.54153200	1.41540600	-2.20062800
H	7.00872200	1.05051800	0.19799900
H	0.41728100	2.61024700	2.95389000
H	3.55595200	1.54469600	1.65951600
H	-1.68037600	2.08948400	5.13627000
H	-0.11402600	1.26486300	4.94733100
H	-1.37794500	1.06418700	3.71181300
H	-0.34213600	4.38415700	5.35439400
H	0.79169000	4.83222000	4.06552000
H	1.16289400	3.47246800	5.14897200
H	3.95441500	-0.83467600	1.17330000
H	4.42980700	-0.45833700	2.84438500
H	5.67849800	-0.67114400	1.59671100
H	6.56128100	1.75289000	2.31105500
H	5.21394900	1.90630200	3.45011900
H	5.45234800	3.13218200	2.18379400
H	-5.75842500	-2.00424100	-3.78385400
H	-7.58003800	-1.63544300	-2.14213700
H	-7.06116800	-1.35493500	0.26903200
H	-2.08636400	-2.03565500	-2.88225800
H	-0.32374800	-2.66586400	3.08394700
H	-4.06567500	-1.17756400	-5.06550200
H	-2.29461500	-1.24656800	-5.17565600
H	-3.05558700	-0.09591100	-4.06822400
H	-3.02195800	-4.37477800	-3.17973200
H	-2.27874700	-3.74249700	-4.66147600
H	-4.04905100	-3.78184100	-4.49999900
H	2.01381800	-2.04478300	4.97151300
H	0.40607400	-1.29149400	5.02556200
H	1.45471200	-1.04430100	3.60751300
H	-0.49797700	-4.88685000	4.27368400
H	-0.83058200	-3.50080100	5.33787700
H	0.72029200	-4.34523300	5.44351000
H	2.70493400	-4.53469500	4.38757700
H	4.41908500	-5.55187700	2.90999300
H	4.28406300	-5.27312500	0.44924500
H	-3.57114300	-1.64575900	1.70365900
H	1.60004800	-3.25552800	-1.30675000
H	-5.80316800	0.46050800	1.71218000

H	-4.10004300	0.73340300	1.26628000
H	-4.52193500	0.28324000	2.93188800
H	-5.19543200	-2.13011400	3.48393100
H	-5.38474100	-3.33661500	2.19079200
H	-6.55680900	-2.01554900	2.36040700
H	3.88857200	-2.31482500	-1.08747700
H	3.60536400	-3.09328000	-2.64729900
H	4.59223400	-3.92020000	-1.41872500
H	1.20888200	-5.75186800	-1.40656100
H	2.95907100	-6.01245300	-1.54489500
H	2.08405600	-5.14302500	-2.82512200
O	0.01701200	1.72372400	-2.34312900
O	-1.18678100	1.02644900	-2.40942600
O	-0.18394100	-1.76972400	-1.94330700
O	-1.99940600	-0.71857300	-0.09123600
O	-0.66265700	1.58874300	0.46614300
Zr	0.03844800	0.00130800	-0.84495000

## 10.6 Structures with nine oxygen atoms

### Peroxo Complex with adsorbed ozone group

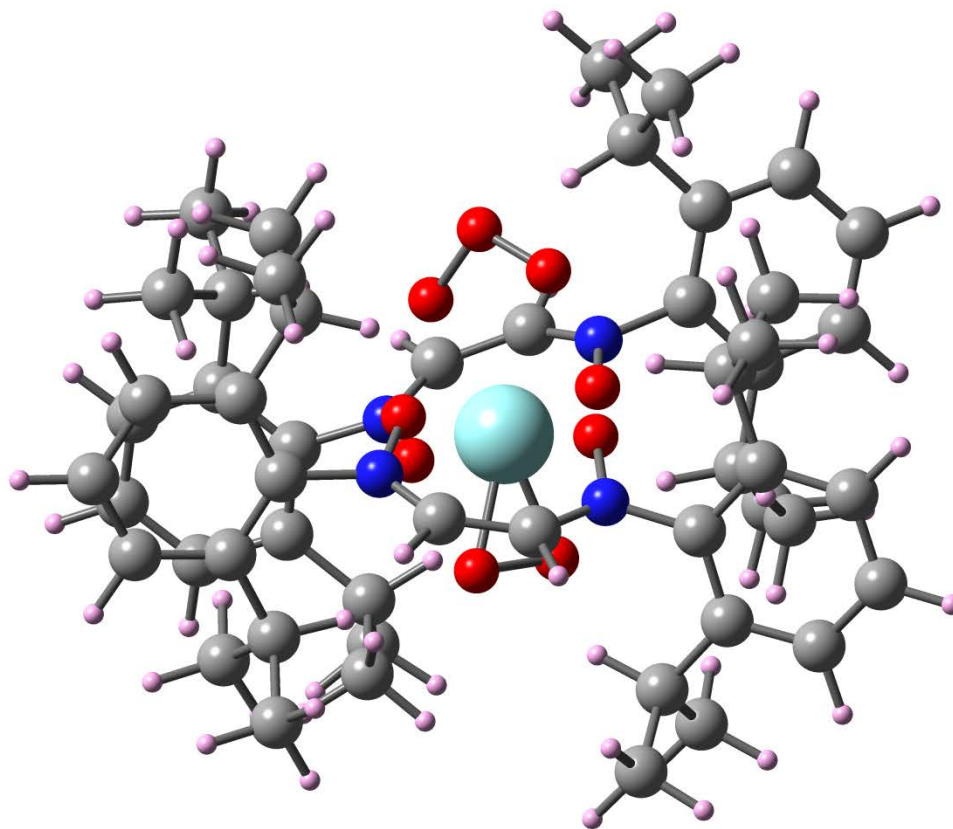


Fig. S148: ONCCNO Peroxo Complex with adsorbed ozone group

SCF	E <sub>ZP</sub>	H	G
-2966.900838	-2965.736557	-2965.660953	-2965.854763

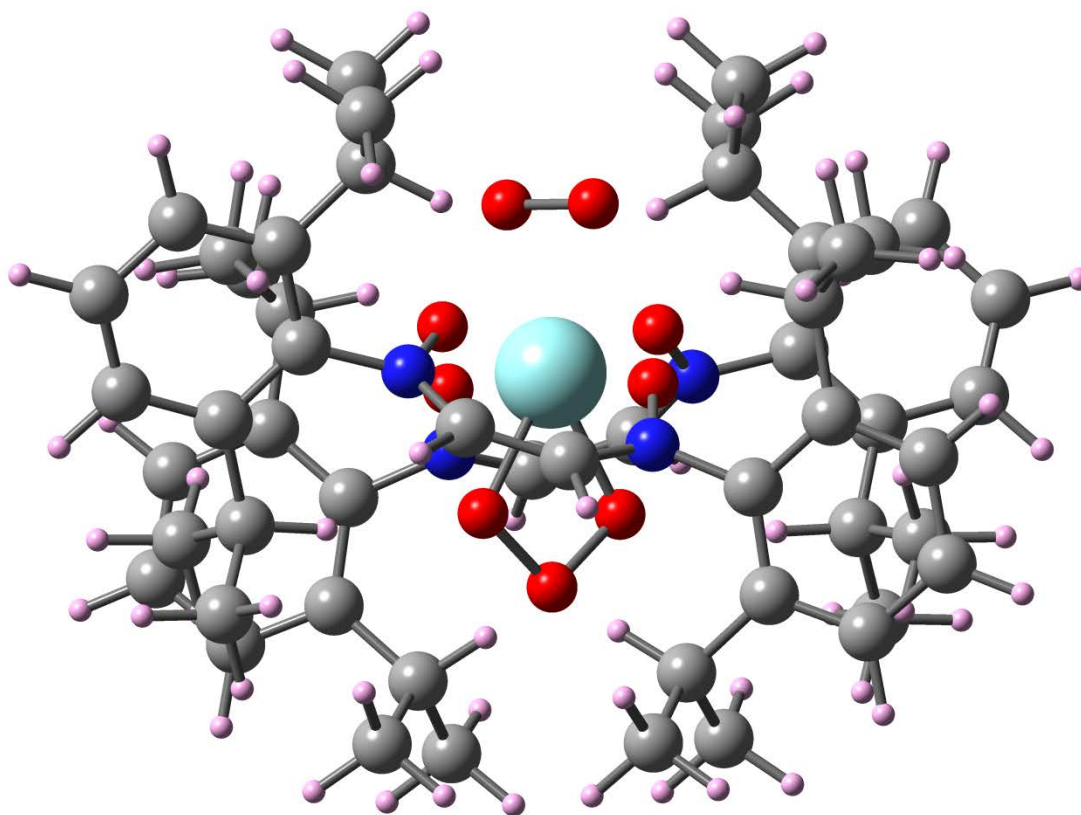
O	1.64944193	1.49558299	0.04293108
O	-1.31841622	-1.44615294	0.91784001
O	-0.61657569	1.21449163	1.79152053
N	1.39093133	-3.08485892	-0.25663906
N	-1.81095920	-2.66887387	0.49227769
N	-1.40377177	2.83019131	-0.44463291
N	1.79755383	2.78143241	0.35067517
C	0.28899083	-3.87974566	-0.30989141
C	-1.06051363	-3.70298661	0.01989186
C	-0.54116978	3.74094965	0.01814484
C	0.84704211	3.72139406	0.34775827
C	2.68406845	-3.54288025	-0.73652934
C	2.92206930	-3.59583721	-2.13395761
C	4.18965879	-4.05502917	-2.55497309

C	5.17817263	-4.41323058	-1.62619762
C	4.91975777	-4.32524077	-0.24817423
C	3.66537612	-3.89330895	0.22788628
C	2.42712641	-2.08473387	-4.12417482
C	1.87721234	-3.18020549	-3.17587199
C	1.38378589	-4.41075970	-3.98333606
C	-4.33518205	-1.24723324	-2.45970862
C	-3.61368899	-2.46536345	-1.82925147
C	-3.77369258	-3.72023585	-2.72839763
C	-3.24105059	-2.82707492	0.70635103
C	-4.11415520	-2.74115352	-0.40724253
C	-5.49376373	-2.91644832	-0.16200254
C	-5.97653663	-3.13465620	1.13750261
C	-5.08831382	-3.18158770	2.22508491
C	-3.69970504	-3.03077029	2.03380543
C	4.19167984	-2.61020973	2.34721706
C	3.40306291	-3.79759449	1.73362074
C	3.73102897	-5.12357093	2.46620543
C	-2.85921383	-1.72081551	4.02648841
C	-2.74367087	-3.04844976	3.22934039
C	-2.96986787	-4.27443078	4.14906012
C	-2.76662493	3.26139772	-0.81169861
C	-3.74057927	3.37283517	0.20715403
C	-5.03126222	3.77977068	-0.19681908
C	-5.32258876	4.03145150	-1.54587965
C	-4.33204728	3.87729620	-2.53049311
C	-3.02230094	3.48392583	-2.18786722
C	-4.38089700	1.91542366	2.18686044
C	-3.45761585	3.05346318	1.67882665
C	-3.59990430	4.31926761	2.56468803
C	4.20006770	1.59502930	-2.38451182
C	3.61839112	2.95937364	-1.92488393
C	3.99836096	4.09171778	-2.91215869
C	3.19408174	3.17342707	0.62332010
C	4.06391145	3.26775101	-0.49184903
C	5.40000527	3.62982219	-0.22481598
C	5.83496156	3.87826549	1.08725614
C	4.94578147	3.75648940	2.16525944
C	3.59810509	3.38776443	1.96207362
C	-2.16536165	1.87700580	-3.94800256
C	-1.96116006	3.26098914	-3.27068103
C	-1.93595725	4.40001656	-4.31983005
C	3.19401229	2.12307383	4.12918885
C	2.66537036	3.21778406	3.16598461
C	2.46006007	4.56268913	3.91241888
H	0.51686934	-4.85852486	-0.71857043
H	-1.67058641	-4.58099475	-0.16536438
H	-0.99442059	4.71962917	0.12632091
H	1.23364757	4.69441873	0.62959173
H	4.40582233	-4.11611692	-3.61837930
H	6.15028569	-4.75568819	-1.97432977
H	5.69555293	-4.59959529	0.46200209

H	1.01748403	-2.73680951	-2.66570483
H	-2.55002242	-2.21078381	-1.79133122
H	3.30240225	-2.42997497	-4.69209020
H	2.69793063	-1.19096698	-3.55281180
H	1.64789413	-1.79387599	-4.84016187
H	2.20330578	-4.87250527	-4.55125434
H	0.60732308	-4.10540821	-4.69696804
H	0.95682504	-5.18139757	-3.32716904
H	-5.40972721	-1.43093532	-2.59622709
H	-3.90169867	-1.03086472	-3.44430727
H	-4.21373302	-0.35424339	-1.83550430
H	-3.22602300	-4.58014198	-2.32068085
H	-3.38250941	-3.51651073	-3.73365515
H	-4.82894933	-4.01025275	-2.82569771
H	-6.19355439	-2.86760108	-0.99219735
H	-7.04403034	-3.26086165	1.30463979
H	-5.47607318	-3.34012919	3.22802269
H	2.34132949	-3.58252089	1.88934024
H	-1.71696824	-3.09991319	2.85211512
H	5.27505915	-2.74445580	2.22072683
H	3.97891009	-2.52883496	3.42139125
H	3.89456969	-1.67077219	1.86954166
H	4.80032017	-5.36721142	2.41095691
H	3.17112558	-5.96633277	2.03993207
H	3.46552237	-5.03943278	3.52841103
H	-2.62081986	-0.86888200	3.38117116
H	-2.15340424	-1.72088647	4.86782719
H	-3.87317018	-1.58879647	4.42987515
H	-3.95696889	-4.24941218	4.62939762
H	-2.21581697	-4.28620456	4.94708780
H	-2.89014300	-5.21606441	3.59015797
H	-5.81349374	3.88451263	0.54991991
H	-6.32549553	4.33793792	-1.83357878
H	-4.57844842	4.06128931	-3.57204603
H	-2.43321893	2.68184596	1.78123349
H	2.52825176	2.85466860	-1.94869634
H	-5.44049670	2.20262737	2.15378409
H	-4.12879237	1.67017849	3.22624621
H	-4.24976220	1.00764616	1.58732283
H	-2.92364535	5.12131623	2.23822713
H	-3.35905275	4.07610474	3.60744197
H	-4.62365362	4.71582359	2.53926519
H	5.29847336	1.61201195	-2.38305379
H	3.86019324	1.36626080	-3.40230022
H	3.85972694	0.78913949	-1.72640435
H	3.59225413	5.06075617	-2.59289053
H	3.59775635	3.86383980	-3.90820734
H	5.08603831	4.19837584	-3.01241215
H	6.10326104	3.71440239	-1.04833440
H	6.86993902	4.15729411	1.26957403
H	5.30126207	3.93352772	3.17654583
H	-0.97180316	3.23185830	-2.79791251



H	1.68478907	2.87848513	2.81802452
H	-3.16418958	1.80758751	-4.40093825
H	-2.04197828	1.06648218	-3.22327747
H	-1.41773343	1.73505796	-4.73897248
H	-1.09677569	4.24684400	-5.01034390
H	-1.81778136	5.38514042	-3.84916848
H	-2.85277643	4.42085683	-4.92292919
H	3.28002039	1.15947310	3.61569918
H	2.49445757	1.99400342	4.96454768
H	4.17484054	2.38921296	4.54479520
H	2.05519154	5.33917735	3.24895707
H	3.40454959	4.93853802	4.32682273
H	1.75851973	4.42658272	4.74518978
O	-0.51550691	-1.02802153	-1.68982043
O	0.69527493	-0.12079176	-1.94980616
O	0.19169136	0.77148871	2.89585564
O	1.08043534	-0.18935912	2.43555678
O	-1.16096844	1.55266885	-0.70730966
O	1.41306415	-1.84734210	0.36286811
Zr	0.15375764	-0.17759212	0.04924453

$\eta^2$ -ozone Complex with adsorbed O<sub>2</sub> moleculeFig. S149: ONCCNO  $\eta^2$ -ozone Complex with adsorbed O<sub>2</sub> molecule

SCF	E <sub>ZP</sub>	H	G
-2966.909914	-2965.746415	-2965.671645	-2965.863149

O	0.81914484	2.01594444	-0.37000122
O	-0.81664045	-2.01157619	-0.36999786
O	-1.04686678	0.47083566	1.28437467
N	2.50313064	-2.12871141	-0.52845521
N	-0.51939965	-3.05818526	0.44350615
N	-2.50168875	2.11965157	-0.53083467
N	0.51694053	3.06380916	0.44015431
C	2.01591828	-3.13574246	0.22142228
C	0.72776010	-3.52559896	0.65624976
C	-2.01878305	3.12989396	0.21769409
C	-0.73244360	3.52627032	0.65158342
C	3.92742534	-2.08516540	-0.86289809
C	4.31254234	-2.53569096	-2.15153942
C	5.68725083	-2.49524571	-2.46155563
C	6.62584389	-2.02640440	-1.52756307
C	6.20583247	-1.56689695	-0.27020927

C	4.84019985	-1.56998412	0.08896625
C	3.12604896	-1.93419765	-4.30319579
C	3.29691290	-3.00915555	-3.19543236
C	3.67617754	-4.38337556	-3.80273852
C	-3.34793693	-3.48013343	-2.12714563
C	-2.33119356	-4.41086941	-1.41372159
C	-2.38784000	-5.84758170	-1.99323890
C	-1.68085459	-3.74296097	1.00797975
C	-2.56056307	-4.39310158	0.10119386
C	-3.68862082	-5.03718329	0.64757277
C	-3.92084803	-5.04342916	2.03247360
C	-3.03149692	-4.39330314	2.89986699
C	-1.89382271	-3.71459086	2.41065166
C	4.85435140	0.46497422	1.60541667
C	4.40177995	-1.00961544	1.44563281
C	4.93802623	-1.87977538	2.61301463
C	-1.75038802	-1.94323119	4.23441834
C	-0.97109707	-2.98985538	3.39843182
C	-0.24320902	-4.00291936	4.32230099
C	-3.92556721	2.06949611	-0.86561676
C	-4.83654370	1.55179577	0.08662517
C	-6.20208558	1.54288649	-0.27280104
C	-6.62366299	1.99905549	-1.53084570
C	-5.68674981	2.47048381	-2.46522393
C	-4.31230275	2.51696427	-2.15488444
C	-4.84797455	-0.47861616	1.60974369
C	-4.39620215	0.99557539	1.44435920
C	-4.93152284	1.86919013	2.60964204
C	3.34193821	3.50201115	-2.13577705
C	2.31726142	4.42387603	-1.42221015
C	2.35862728	5.86012754	-2.00401233
C	1.67521632	3.75637615	1.00159062
C	2.54917176	4.41074113	0.09236080
C	3.67392473	5.06305870	0.63582299
C	3.90840497	5.07284436	2.02034211
C	3.02481509	4.41813861	2.89021832
C	1.89073279	3.73138713	2.40387456
C	-3.12097949	1.91697655	-4.30429528
C	-3.29830905	2.99344606	-3.19899286
C	-3.68414670	4.36428807	-3.80976088
C	1.76167510	1.96084699	4.22927613
C	0.97429331	3.00183410	3.39384508
C	0.24169667	4.01108903	4.31814965
H	2.80291396	-3.79975627	0.56278282
H	0.73218791	-4.41084436	1.28216496
H	-2.80874168	3.79078748	0.55828242
H	-0.74070453	4.41291282	1.27550374
H	6.02434536	-2.83223331	-3.43792934
H	7.68251794	-2.00960492	-1.78461343
H	6.94069584	-1.18749545	0.43493668
H	2.31993371	-3.11864043	-2.71242431
H	-1.33621476	-4.00807892	-1.62613122

H	4.07294563	-1.75760110	-4.83174112
H	2.77923923	-0.98887529	-3.87340156
H	2.38007066	-2.26486916	-5.03757534
H	4.61236765	-4.33240534	-4.37380750
H	2.88881712	-4.71578776	-4.49171425
H	3.79662912	-5.14936576	-3.02522716
H	-4.38079768	-3.81245093	-1.95357961
H	-3.16540672	-3.48034024	-3.20955961
H	-3.24374931	-2.45157639	-1.76673542
H	-1.67190670	-6.51245560	-1.49220811
H	-2.14230817	-5.82500154	-3.06302113
H	-3.38694621	-6.29200258	-1.89441675
H	-4.38506314	-5.54343829	-0.01516019
H	-4.79505906	-5.55131022	2.43313464
H	-3.22746092	-4.39749994	3.96876275
H	3.30831945	-1.00589354	1.49970752
H	-0.21499012	-2.42790242	2.84397894
H	5.94854263	0.56122951	1.59637455
H	4.48879260	0.86695756	2.55869938
H	4.44710787	1.08797685	0.80056015
H	6.03622317	-1.89258534	2.63426993
H	4.59347473	-2.91967473	2.53295756
H	4.58641334	-1.48008955	3.57311078
H	-2.19674212	-1.18860446	3.57852463
H	-1.06100124	-1.42686630	4.91414139
H	-2.54232962	-2.40536316	4.83887336
H	-0.95625041	-4.56646454	4.93863847
H	0.44104300	-3.47274926	4.99738000
H	0.34440366	-4.73142508	3.74675380
H	-6.93560457	1.16158722	0.43271194
H	-7.68021480	1.97774627	-1.78807504
H	-6.02500382	2.80497322	-3.44205985
H	-3.30264077	0.99273008	1.49702255
H	1.32602856	4.01080068	-1.63236242
H	-5.94215599	-0.57529114	1.60381135
H	-4.48001650	-0.87756876	2.56335950
H	-4.44265522	-1.10418581	0.80590290
H	-4.58757765	2.90899352	2.52597843
H	-4.57867751	1.47272254	3.57062339
H	-6.02971741	1.88147564	2.63190754
H	4.37176664	3.84493476	-1.96488398
H	3.15730576	3.49820526	-3.21782207
H	3.24876348	2.47316359	-1.77310307
H	1.63638960	6.51837979	-1.50328233
H	2.11228764	5.83342943	-3.07351866
H	3.35318114	6.31499338	-1.90679189
H	4.36601872	5.57279307	-0.02883110
H	4.77996425	5.58699852	2.41878447
H	3.22260286	4.42502676	3.95877415
H	-2.32234804	3.10906943	-2.71535863
H	0.22066245	2.43482383	2.84113966
H	-4.06676158	1.73387204	-4.83262481

H	-2.76889670	0.97463523	-3.87226612
H	-2.37672207	2.25024512	-5.03925854
H	-2.89740319	4.69968558	-4.49799405
H	-3.81035390	5.13122275	-3.03409866
H	-4.61894917	4.30683420	-4.38249534
H	2.21218664	1.20880108	3.57323291
H	1.07669277	1.44030711	4.91025215
H	2.55144590	2.42856568	4.83232595
H	-0.35159893	4.73524735	3.74294456
H	0.95223508	4.57974644	4.93267077
H	-0.43800746	3.47725963	4.99494352
O	-0.42106228	-0.54306852	-2.72906148
O	0.43903133	0.54553146	-2.72689795
O	0.00624512	0.00283266	2.23254713
O	1.05697228	-0.46809852	1.28316796
O	-1.76534908	1.13977591	-1.12470425
O	1.77176529	-1.14585063	-1.12267324
Zr	0.00463897	0.00116463	-0.54597110

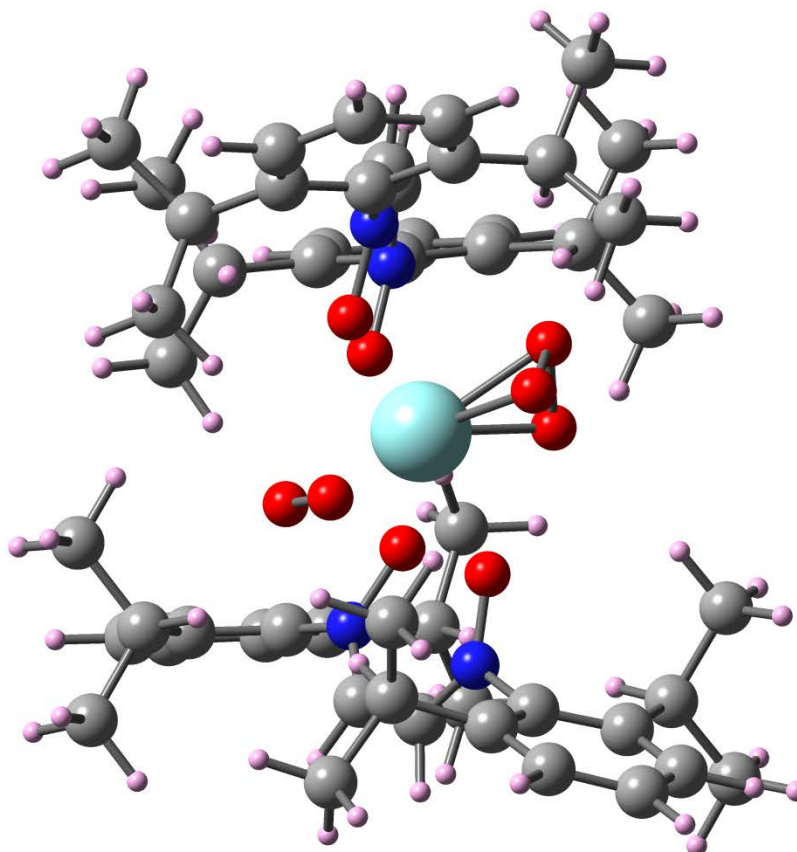
$\eta^3$ -ozone Complex with adsorbed O<sub>2</sub> molecule (conformation 1 lower energy)

Fig. S150: ONCCNO  $\eta^3$ -ozone Complex with adsorbed O<sub>2</sub> molecule (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G
-2966.890476	-2965.726469	-2965.650910	-2965.844032

O	-1.84264214	-0.19310001	-0.03342200
O	2.47628219	-0.16304501	-0.59571704
O	0.96980507	1.97296115	-1.46174511
N	0.97876908	-2.78821421	0.73602106
N	3.46269826	-0.95897807	-0.22780602
N	-1.56349812	3.08829924	0.34654803
N	-2.99770623	0.31216902	-0.61372705
C	2.28923817	-2.87682522	0.94698507
C	3.38843526	-2.10775916	0.45197603
C	-2.76913721	2.81552822	-0.22056402
C	-3.37709826	1.62255812	-0.61954405
C	0.08416401	-3.79297329	1.34043210
C	-0.11864701	-3.79375829	2.74341421
C	-0.96669707	-4.79759037	3.26034325
C	-1.58605512	-5.73222344	2.41892219

C	-1.37120910	-5.68884344	1.03211608
C	-0.52614204	-4.71980836	0.45488403
C	-0.59140404	-1.99033715	4.47432534
C	0.50349804	-2.77158221	3.70258928
C	1.49060411	-3.45518927	4.68533136
C	4.96299738	2.17625017	1.78284714
C	5.09369139	0.63572005	1.65179613
C	6.02076844	0.05809000	2.75234321
C	4.79481937	-0.48723304	-0.66580205
C	5.57637142	0.25462202	0.24843302
C	6.84019550	0.68717905	-0.20874802
C	7.26932258	0.41112003	-1.51574512
C	6.43955651	-0.29101002	-2.40588318
C	5.17012339	-0.75556506	-2.00439015
C	-1.57127912	-4.13387032	-1.77222314
C	-0.31243002	-4.69962736	-1.06230508
C	0.06485100	-6.09657647	-1.61795413
C	3.53680827	-0.36987503	-3.89223230
C	4.23112632	-1.43991311	-3.00255223
C	4.95061338	-2.50598619	-3.86472029
C	-1.16200809	4.44784834	0.67124705
C	-0.79511906	5.33456139	-0.37435103
C	-0.42014903	6.64604449	-0.00874700
C	-0.38692903	7.04611752	1.33484510
C	-0.73779205	6.14014946	2.34905018
C	-1.13874608	4.82468337	2.04114016
C	0.61107405	5.15393340	-2.49028919
C	-0.78524306	4.93587338	-1.85417314
C	-1.88094514	5.70211844	-2.64327720
C	-4.02359731	-2.46940319	2.08582816
C	-4.53551235	-1.20676209	1.34809810
C	-5.88309446	-0.72185106	1.94448215
C	-3.90896330	-0.71051605	-1.10884108
C	-4.65263036	-1.45629411	-0.15788701
C	-5.53550444	-2.44126519	-0.64545205
C	-5.67363944	-2.66731020	-2.02485816
C	-4.92613137	-1.91351114	-2.94195622
C	-4.01904131	-0.92231907	-2.50685219
C	-0.25817402	3.43626926	3.96828730
C	-1.51884612	3.85867530	3.16765724
C	-2.60105420	4.45604834	4.10316831
C	-2.38541818	-1.04032408	-4.46176434
C	-3.22008924	-0.11838701	-3.53754927
C	-4.15815032	0.79617306	-4.37029433
H	2.57606620	-3.71554828	1.57052212
H	4.36156133	-2.53653019	0.66063605
H	-3.35570525	3.70836028	-0.40667603
H	-4.36260033	1.75172013	-1.05428208
H	-1.15272209	-4.83429037	4.33005233
H	-2.24065017	-6.49060651	2.84152922
H	-1.86003514	-6.41626451	0.39074103
H	1.05444508	-2.02056415	3.13094424

H	4.08834931	0.23309502	1.81417414
H	-1.19108409	-2.65098320	5.11458339
H	-1.26254110	-1.47448711	3.77901129
H	-0.12261601	-1.23071209	5.11187739
H	0.97910807	-4.18837632	5.32262241
H	1.95009815	-2.70368721	5.34013643
H	2.29634618	-3.98281631	4.15590632
H	5.93461844	2.67540620	1.66848313
H	4.55956135	2.43289019	2.77008521
H	4.27719133	2.57423920	1.02681708
H	6.09367145	-1.03622008	2.68868221
H	5.63102845	0.31680702	3.74510529
H	7.03758655	0.46497504	2.67597020
H	7.48086759	1.25719110	0.45844904
H	8.24469362	0.75816006	-1.84824614
H	6.77679350	-0.47217604	-3.42203526
H	0.51163004	-4.01822731	-1.29881210
H	3.43366726	-1.95108715	-2.44886919
H	-2.45398119	-4.75590037	-1.57085212
H	-1.41190011	-4.11082731	-2.85802122
H	-1.77828214	-3.11377724	-1.43506111
H	-0.75587406	-6.81702251	-1.50929511
H	0.94718507	-6.51076250	-1.11202608
H	0.29053202	-6.01787744	-2.68925020
H	2.93922322	0.31804602	-3.28612425
H	2.86185122	-0.85904107	-4.60609435
H	4.28072833	0.20653602	-4.45943334
H	5.68968441	-2.05388416	-4.53814535
H	4.21748632	-3.02896523	-4.49189634
H	5.46706843	-3.25144125	-3.24531425
H	-0.13671301	7.35199457	-0.78499606
H	-0.08498801	8.05899659	1.59204412
H	-0.70794005	6.45962048	3.38757226
H	-0.99364407	3.86598129	-1.93519515
H	-3.79291729	-0.42013403	1.51139912
H	0.92126607	6.20716848	-2.45199619
H	0.59074304	4.84424437	-3.54341927
H	1.35787010	4.53843235	-1.97902815
H	-2.88129222	5.52777141	-2.22365717
H	-1.88992214	5.37433943	-3.69108728
H	-1.69883013	6.78521250	-2.63015820
H	-4.72477036	-3.30896725	1.98383815
H	-3.90458130	-2.26027917	3.15751424
H	-3.05262023	-2.78317821	1.68759113
H	-6.23556249	0.18944001	1.44436511
H	-5.76592742	-0.50020404	3.01375023
H	-6.66627049	-1.48519211	1.84414614
H	-6.12328347	-3.02863323	0.05585500
H	-6.36393947	-3.42779726	-2.38344018
H	-5.04036539	-2.09867116	-4.00690331
H	-1.92791215	2.94707222	2.72215021
H	-2.50504519	0.51949404	-3.01186123



H	0.22213902	4.30488833	4.44039134
H	0.46653104	2.94805522	3.30858025
H	-0.53297904	2.72693621	4.76111637
H	-2.89425922	3.71337728	4.85728037
H	-3.49920427	4.74730136	3.54264427
H	-2.23533717	5.34272543	4.63740836
H	-1.66864613	-1.62143512	-3.87312830
H	-1.81095714	-0.43095903	-5.17079940
H	-3.02023323	-1.72756413	-5.03815638
H	-4.73144336	1.47890511	-3.72874929
H	-4.87577437	0.20576602	-4.95636938
H	-3.56850327	1.40294511	-5.06971239
O	1.61011012	0.99664107	1.64302613
O	0.76665506	-0.06905001	1.95773915
O	-0.29551402	1.39717611	-2.10237216
O	0.05260100	-0.08702901	-2.24517117
O	-0.72111706	2.10355816	0.82777406
O	0.39373303	-1.91943915	-0.09911601
Zr	0.20432102	0.44060603	-0.16224101

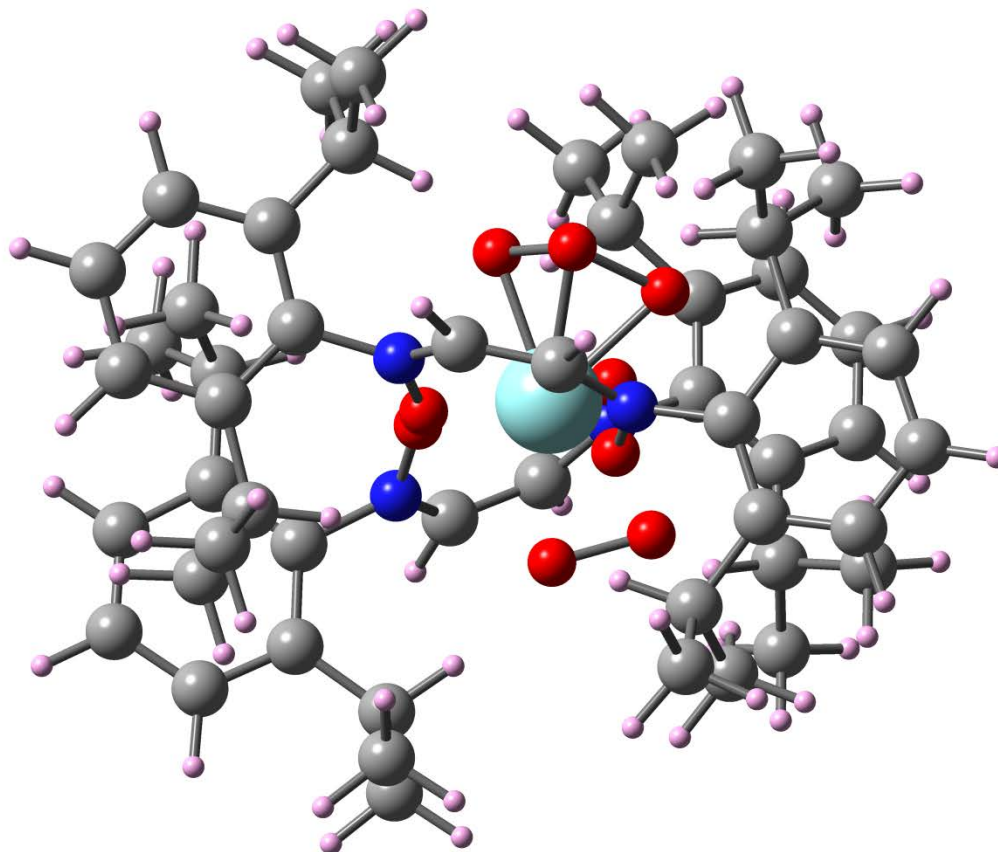
$\eta^3$ -ozone Complex with adsorbed O<sub>2</sub> molecule (conformation 2 higher energy)

Fig. S151: ONCCNO  $\eta^3$ -ozone Complex with adsorbed O<sub>2</sub> molecule (conformation 2 higher energy)

SCF	E <sub>ZP</sub>	H	G
-2966.890307	-2965.726597	-2965.650910	-2965.845550

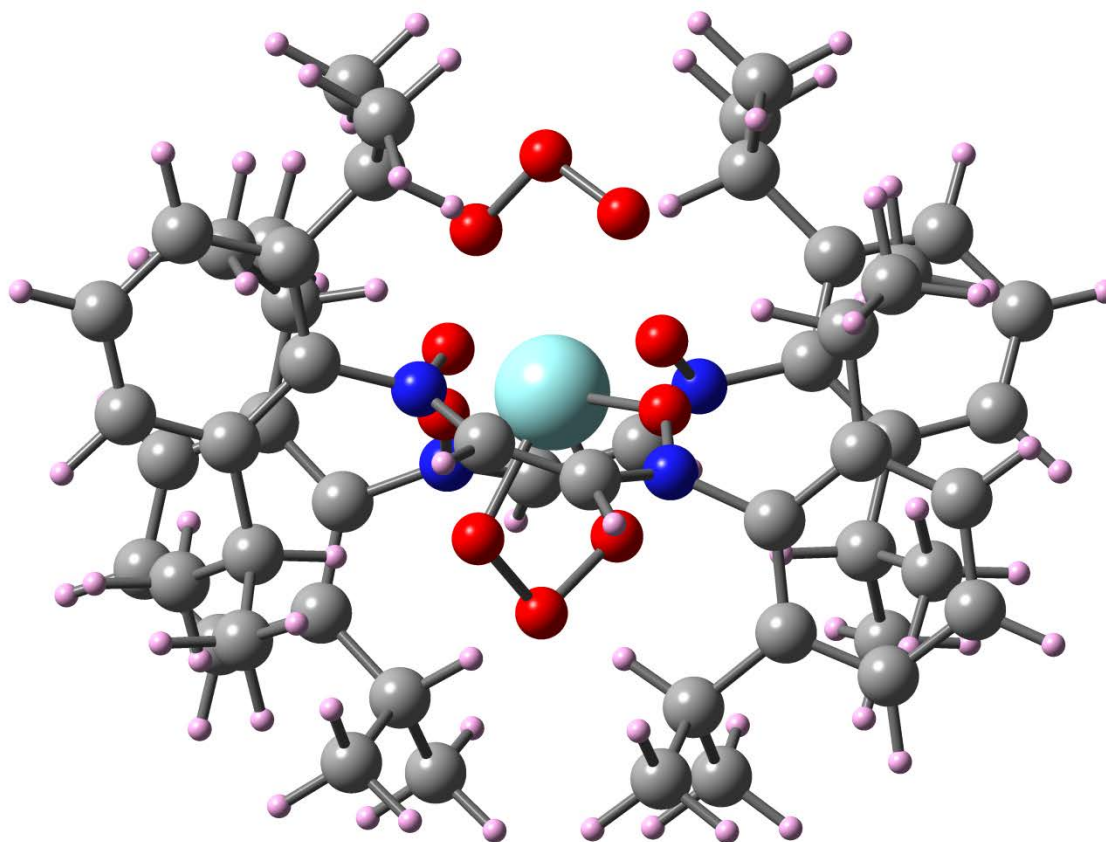
O	-1.85908414	-0.11451001	0.04152500
O	2.45750019	-0.22369802	-0.64456205
O	1.00762008	1.91407015	-1.50833812
N	0.89348207	-2.83922722	0.64892005
N	3.42437526	-1.04561708	-0.27785302
N	-1.45360911	3.14301124	0.39276203
N	-3.00167123	0.41815403	-0.54005804
C	2.20282017	-2.96364023	0.84991007
C	3.31913125	-2.20790817	0.37443803
C	-2.68408721	2.90753022	-0.13776001
C	-3.34050126	1.73872913	-0.53232604
C	-0.01990400	-3.83816129	1.23375909
C	-0.21154402	-3.86981430	2.63831420
C	-1.07732408	-4.86769837	3.13676024
C	-1.72483813	-5.76613846	2.27709517

C	-1.52058111	-5.69197744	0.89012407
C	-0.65761605	-4.72825136	0.33047703
C	-0.62709705	-2.10443216	4.42412034
C	0.44191303	-2.88627122	3.61768827
C	1.42691211	-3.61598928	4.56881735
C	5.12196539	1.86312114	1.97861915
C	5.13032339	0.33502303	1.71056513
C	6.00328046	-0.40942703	2.75409621
C	4.77167736	-0.59188304	-0.68621705
C	5.58924943	0.04035300	0.27821502
C	6.87074755	0.44813203	-0.15159101
C	7.28335054	0.25644802	-1.47888911
C	6.41871249	-0.33264503	-2.41630118
C	5.13030539	-0.76911706	-2.04456616
C	-1.71403913	-4.10339532	-1.88199014
C	-0.45157503	-4.67896336	-1.18714609
C	-0.07393301	-6.06608745	-1.76748313
C	3.52970727	-0.16630501	-3.90111730
C	4.16104132	-1.33209110	-3.08822424
C	4.82837637	-2.37215918	-4.02149431
C	-1.01519008	4.49122634	0.72053606
C	-0.64179905	5.37385143	-0.32536102
C	-0.23498202	6.67555052	0.04145000
C	-0.17685901	7.06770356	1.38661310
C	-0.53141604	6.16352745	2.40129618
C	-0.96345507	4.85815637	2.09192616
C	0.74585505	5.15393940	-2.44769119
C	-0.65387105	4.97776838	-1.80572914
C	-1.72925213	5.77791345	-2.58854920
C	-4.03852731	-2.40547818	2.13036916
C	-4.52307335	-1.11343709	1.42587411
C	-5.84333843	-0.59760205	2.05650516
C	-3.94366130	-0.57605705	-1.03466508
C	-4.67736536	-1.32985710	-0.08183501
C	-5.59057941	-2.28718817	-0.56827204
C	-5.76804143	-2.47986719	-1.94818015
C	-5.03112038	-1.71821813	-2.86715222
C	-4.09544631	-0.75294406	-2.43408818
C	-0.07130501	3.42999526	3.98370730
C	-1.34019410	3.88862029	3.21645125
C	-2.38832818	4.49734734	4.18272732
C	-2.52624320	-0.84732407	-4.44402434
C	-3.31433425	0.06323400	-3.46927627
C	-4.26276533	1.01624508	-4.24573532
H	2.47194119	-3.82545829	1.44929411
H	4.28116133	-2.66340220	0.57778804
H	-3.24913425	3.81938829	-0.29671002
H	-4.32934033	1.90381015	-0.94658207
H	-1.25541109	-4.92837438	4.20675932
H	-2.39302818	-6.52008750	2.68614120
H	-2.03157016	-6.39093550	0.23450402
H	1.00040308	-2.13034716	3.05976123

H	4.09504531	0.00187100	1.83757714
H	-1.23846709	-2.77027121	5.04754238
H	-1.29006510	-1.54987612	3.75132928
H	-0.13395401	-1.37859111	5.08244239
H	0.90801607	-4.35449833	5.19389439
H	1.91091014	-2.89174822	5.23660540
H	2.21415417	-4.14659132	4.01514130
H	6.12984648	2.29280818	1.90512415
H	4.73790736	2.06195016	2.98682723
H	4.47152234	2.38001918	1.26428809
H	5.99228643	-1.49613312	2.59263120
H	5.62967741	-0.21164702	3.76693829
H	7.04898154	-0.07766101	2.71238821
H	7.53854055	0.93515707	0.55370204
H	8.27315261	0.58286504	-1.78884913
H	6.74338051	-0.44809703	-3.44601326
H	0.36982703	-3.99189630	-1.41513711
H	3.33403226	-1.83607114	-2.57333120
H	-2.59537620	-4.73002936	-1.68912113
H	-1.55846112	-4.05985631	-2.96769223
H	-1.92200415	-3.08990524	-1.52586012
H	-0.89096807	-6.79124353	-1.66213013
H	0.81403106	-6.48440048	-1.27485610
H	0.14315101	-5.97091243	-2.83924822
H	2.97510923	0.51334904	-3.24638025
H	2.82422722	-0.56531904	-4.64094736
H	4.30535833	0.40157103	-4.43358234
H	5.60021541	-1.91569214	-4.65417835
H	4.07365331	-2.80483321	-4.69043336
H	5.29381538	-3.18960624	-3.45455226
H	0.05319800	7.37958058	-0.73482805
H	0.14853301	8.07304963	1.64480412
H	-0.47918904	6.47664152	3.44089826
H	-0.89620407	3.91492530	-1.88712615
H	-3.75247029	-0.35445303	1.58922512
H	1.08705908	6.19763647	-2.40968519
H	0.71227505	4.84535137	-3.50072127
H	1.47693612	4.51668735	-1.94026515
H	-2.73268521	5.63067543	-2.16600016
H	-1.75113913	5.45345641	-3.63719028
H	-1.51616812	6.85533251	-2.57334919
H	-4.76940137	-3.21959425	2.03054716
H	-3.88933130	-2.21934517	3.20250524
H	-3.08770324	-2.74472021	1.70528613
H	-6.17568545	0.33358703	1.57976212
H	-5.69943546	-0.39967503	3.12720124
H	-6.65224952	-1.33381710	1.95717115
H	-6.17189750	-2.87875022	0.13487001
H	-6.48105248	-3.21972124	-2.30545518
H	-5.17604239	-1.87692314	-3.93265730
H	-1.77863314	2.99102523	2.76978721
H	-2.57185619	0.67459405	-2.95023123

H	0.43848603	4.28267433	4.45386934
H	0.62780405	2.93366423	3.30276325
H	-0.34391103	2.71806321	4.77491537
H	-2.68106920	3.75141329	4.93369137
H	-3.29171225	4.81527337	3.64574228
H	-1.99134215	5.36856442	4.71997136
H	-1.79484114	-1.44824811	-3.89480030
H	-1.97165415	-0.22853802	-5.16081639
H	-3.18997624	-1.51418411	-5.01129838
H	-4.80004637	1.69295113	-3.56755527
H	-5.01187438	0.45470903	-4.82051237
H	-3.68604828	1.62952913	-4.95033138
O	1.64956113	0.89603907	1.63813113
O	0.76873906	-0.14605301	1.93020115
O	-0.30649302	1.40301011	-2.09908416
O	-0.04103300	-0.09921201	-2.24315017
O	-0.60660505	2.14273317	0.82575606
O	0.32343802	-1.93340215	-0.15657001
Zr	0.20631202	0.42496803	-0.17229201

## 10.7 Structures with ten oxygen atoms

 $\eta^2$ -ozone Complex with adsorbed ozone groupFig. S152: ONCCNO  $\eta^2$ -ozone Complex with adsorbed ozone group

SCF	E <sub>ZP</sub>	H	G
-3042.051659	-3040.883871	-3040.807325	-3041.003191

O	0.84132973	1.93415340	-0.26635814
O	-0.91968998	-2.01291893	-0.12053873
O	-1.13438962	0.40932115	1.38913413
N	2.42452460	-2.09778612	-0.49192172
N	-0.55179230	-3.11286129	0.52128731
N	-2.46095866	2.29485390	-0.51344371
N	0.60485445	3.06558246	0.48658446
C	1.98696459	-3.10712876	0.25715134
C	0.70065147	-3.55349459	0.68934597
C	-1.89974788	3.35145671	0.13460483
C	-0.61032862	3.67325262	0.57371964
C	3.85606215	-2.00554890	-0.82106329
C	4.24874602	-2.40616264	-2.12277736
C	5.62393096	-2.33042810	-2.42353687

C	6.54896709	-1.87338174	-1.47070963
C	6.11573946	-1.45997312	-0.20200579
C	4.74984253	-1.50054813	0.15370452
C	3.10505270	-1.78299009	-4.29034672
C	3.25045566	-2.86796848	-3.18878579
C	3.64141178	-4.23784821	-3.79937764
C	-3.31777801	-3.63590142	-2.13126767
C	-2.21229769	-4.48901104	-1.45310362
C	-2.09830035	-5.88614829	-2.11515420
C	-1.67457248	-3.92573446	1.02358313
C	-2.46765318	-4.59142490	0.05473046
C	-3.54587370	-5.36061797	0.53791572
C	-3.80999412	-5.45458408	1.91384563
C	-3.00887914	-4.76878817	2.83865840
C	-1.92184758	-3.97221739	2.41722931
C	4.75374333	0.47724317	1.74555228
C	4.29915891	-0.98898485	1.52604030
C	4.82491899	-1.90332994	2.66465268
C	-1.99954976	-2.21657674	4.25152892
C	-1.10189015	-3.19859925	3.45568192
C	-0.35162302	-4.16552261	4.40959877
C	-3.88146273	2.28496611	-0.83272136
C	-4.80709624	1.92656791	0.17896184
C	-6.17729018	1.95536272	-0.15910368
C	-6.59615790	2.29684511	-1.45449635
C	-5.65121249	2.61122427	-2.44491248
C	-4.27075835	2.61123317	-2.15673830
C	-4.92728518	0.11432100	1.96043123
C	-4.36858517	1.51116817	1.58658283
C	-4.78991366	2.57107171	2.63904938
C	3.52085930	3.25219858	-2.01866894
C	2.55019784	4.25603945	-1.34134028
C	2.71120756	5.67704057	-1.93958089
C	1.79682600	3.66612906	1.06266979
C	2.74346328	4.24793786	0.17797718
C	3.89888423	4.81902802	0.74903657
C	4.09320307	4.82256876	2.14020826
C	3.14034302	4.23849438	2.98822029
C	1.97558823	3.63179408	2.46966729
C	-3.21829420	1.76998129	-4.29805502
C	-3.25189133	2.92072393	-3.25669590
C	-3.52831377	4.28511542	-3.93785790
C	1.64901883	1.89578090	4.30713905
C	0.97196067	2.97411073	3.42381599
C	0.26260115	4.03916361	4.30271664
H	2.79276723	-3.75405440	0.58678526
H	0.73699533	-4.47758981	1.25473747
H	-2.64224520	4.10458558	0.37664973
H	-0.55145238	4.61335042	1.11164699
H	5.97108484	-2.62961518	-3.40853455
H	7.60594863	-1.82811432	-1.72214675
H	6.84008289	-1.08606017	0.51623297

H	2.26227681	-2.97995409	-2.72970131
H	-1.26849426	-3.96184609	-1.62655365
H	4.05930661	-1.61484060	-4.80788783
H	2.76698072	-0.83483973	-3.85961604
H	2.36331740	-2.09986893	-5.03456705
H	4.59399305	-4.18451257	-4.34201183
H	2.87289970	-4.55938623	-4.51404019
H	3.73678630	-5.01307255	-3.02738883
H	-4.30971945	-4.08747070	-1.99234898
H	-3.12142569	-3.55610471	-3.20749703
H	-3.32910178	-2.62188039	-1.71941815
H	-1.31699596	-6.49589220	-1.64206235
H	-1.84785188	-5.77276535	-3.17764760
H	-3.04211364	-6.44313333	-2.05648307
H	-4.18082910	-5.88857547	-0.16795396
H	-4.64585200	-6.05556354	2.26393253
H	-3.23626445	-4.83673526	3.89885092
H	3.20496629	-0.98251462	1.57337820
H	-0.36038821	-2.57605576	2.94721024
H	5.84803795	0.57011119	1.76087608
H	4.37202361	0.84620316	2.70527197
H	4.36323659	1.13203017	0.95823564
H	5.92279652	-1.91636003	2.69450620
H	4.48258358	-2.94061091	2.54546759
H	4.46494868	-1.53869662	3.63520516
H	-2.47108775	-1.49639702	3.57470843
H	-1.38636223	-1.65145110	4.96445947
H	-2.78358475	-2.74050294	4.81488383
H	-1.05151325	-4.77915983	4.99188347
H	0.26301295	-3.59397233	5.11672362
H	0.31056142	-4.84935532	3.86036002
H	-6.91786221	1.69486654	0.59273270
H	-7.65694232	2.30853471	-1.69510518
H	-5.98735889	2.85849506	-3.44855213
H	-3.27792520	1.42329966	1.60870378
H	1.53657271	3.91163127	-1.56756886
H	-6.02513828	0.10600789	1.99704301
H	-4.55606730	-0.18138252	2.95037941
H	-4.60042453	-0.64185381	1.23700582
H	-4.36670576	3.55770914	2.40781187
H	-4.43580067	2.27642913	3.63574624
H	-5.88234568	2.67794775	2.68543115
H	4.56927584	3.51869671	-1.82394974
H	3.36267963	3.24884471	-3.10478133
H	3.33854272	2.23738706	-1.65017088
H	2.02592298	6.39220536	-1.46578867
H	2.49159065	5.65429632	-3.01501600
H	3.73376379	6.05887709	-1.81931309
H	4.64571268	5.27149984	0.10203634
H	4.98737795	5.27695199	2.56119756
H	3.30682785	4.23997818	4.06234792
H	-2.25466777	2.96780487	-2.80745503



H	0.20936164	2.45534571	2.83618842
H	-4.18999865	1.65855092	-4.79910341
H	-2.96206515	0.82092239	-3.81542020
H	-2.45991022	1.97597122	-5.06459374
H	-2.74648968	4.49846194	-4.67856020
H	-3.53878119	5.10410559	-3.20652338
H	-4.49269728	4.29004346	-4.46289093
H	2.07863865	1.10563688	3.68232636
H	0.90115496	1.43085284	4.96205318
H	2.43952755	2.32044828	4.94079232
H	-0.25212959	4.79158638	3.69038274
H	0.97900763	4.56703411	4.94663893
H	-0.48364785	3.55919133	4.94916589
O	-0.82056849	-0.98480103	-2.45044080
O	0.58458310	0.80657209	-2.70062629
O	-0.12866026	-0.18158855	2.32267623
O	0.94730474	-0.57081544	1.36082692
O	-1.77827586	1.19969043	-0.99853708
O	1.66227425	-1.15454409	-1.07348188
O	-0.16167195	-0.15071551	-3.39800910
Zr	-0.09624545	0.06383775	-0.44320917

## 11. ONCCNO Singlet Transition States

### Spiro Bisperoxo Complex to Oxo Peroxo Complex (conformation 1 lower energy)

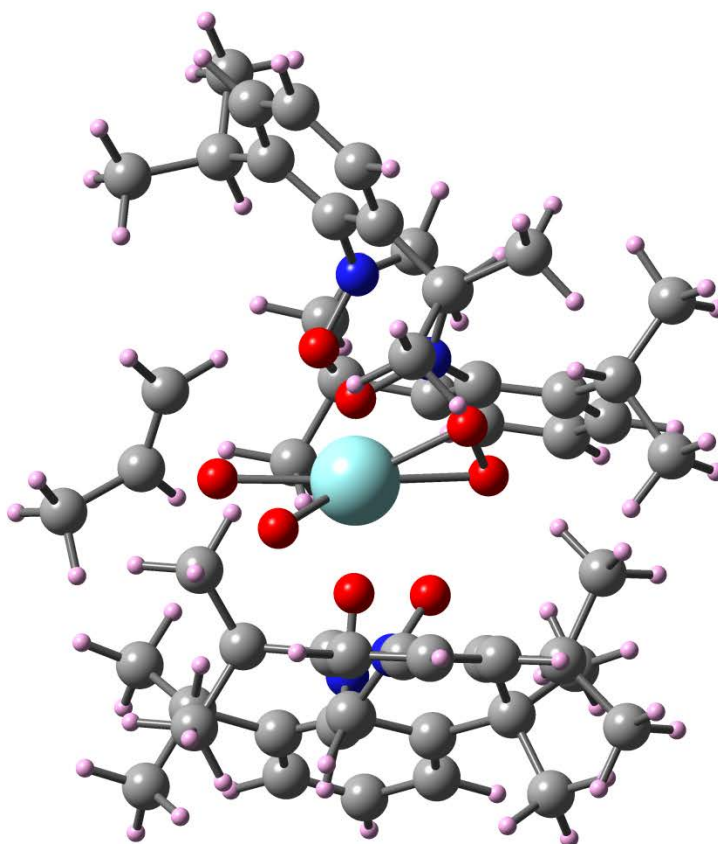


Fig. S153: ONCCNO Spiro Bisperoxo Complex to Oxo Peroxo Complex (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-3009.592624	-3008.348352	-3008.270247	-3008.465555	-488

O	-1.96015315	-0.02790000	-0.54562104
O	2.50543719	-0.49344704	-0.70560606
O	0.45792804	1.55616312	-1.59347512
N	0.65720805	-2.70832321	0.97378807
N	3.38325726	-1.20286709	0.00947900
N	-1.10433408	3.17042024	0.07079801
N	-3.02309123	0.74872106	-0.76380806
C	1.91965515	-2.74793521	1.41050711
C	3.11361024	-2.13965116	0.93117507
C	-2.18192517	3.15736524	-0.71142205
C	-3.09029524	2.07809416	-0.92654707
C	-0.40131203	-3.43779826	1.67590313
C	-0.60857105	-3.22637325	3.07292324

C	-1.64720712	-3.95849630	3.68670028
C	-2.45430219	-4.84654737	2.96374623
C	-2.21254117	-5.04934238	1.59858212
C	-1.17355309	-4.37322333	0.92691207
C	-0.67087105	-1.28596510	4.73769136
C	0.22076502	-2.28777417	3.96361530
C	1.10128908	-3.10854524	4.94696538
C	4.15400232	2.48293219	0.87896507
C	4.45550034	1.08490508	1.48401511
C	5.12262139	1.21495509	2.87624722
C	4.78555736	-0.82667706	-0.22498502
C	5.30686939	0.26583902	0.50980804
C	6.65543649	0.60683805	0.27206802
C	7.43046256	-0.10335101	-0.65907605
C	6.86875451	-1.16257409	-1.38941011
C	5.52373141	-1.54248012	-1.19593109
C	-2.06285516	-4.15449532	-1.43536311
C	-0.92430507	-4.72025436	-0.54730504
C	-0.75821306	-6.24751047	-0.76101106
C	4.93941838	-2.28439417	-3.54937727
C	4.91020238	-2.66008920	-2.04432116
C	5.61487341	-4.01929931	-1.79796514
C	-0.33524303	4.39817633	0.29699602
C	0.27582802	5.06116138	-0.80114606
C	0.99389507	6.24139350	-0.50705404
C	1.11723309	6.71645549	0.80544906
C	0.51933204	6.02010644	1.86789114
C	-0.22594402	4.84554537	1.64410412
C	1.66024212	4.39158334	-2.82868722
C	0.23188502	4.56248935	-2.25220517
C	-0.61482405	5.51197441	-3.14090624
C	-4.30223633	-0.84502806	2.85045922
C	-4.34228733	0.28484302	1.79157914
C	-5.12399439	1.51518211	2.32759618
C	-4.30087933	0.00618200	-0.77966406
C	-4.94081438	-0.19900001	0.46635804
C	-6.18420346	-0.86489306	0.43992703
C	-6.74088253	-1.30983110	-0.76989406
C	-6.05829044	-1.11473208	-1.98096415
C	-4.80861337	-0.45907203	-2.01383115
C	0.20552002	3.28805025	3.59612427
C	-0.86436807	4.11751332	2.83431521
C	-1.60575812	5.08848439	3.78806729
C	-3.99942631	-1.57158112	-4.15985332
C	-4.06876731	-0.25842402	-3.34012626
C	-4.73111336	0.86613206	-4.18252432
H	2.07020116	-3.37464826	2.28026917
H	4.00965531	-2.49176119	1.43142011
H	-2.47139619	4.11322631	-1.12919109
H	-4.07412631	2.39430618	-1.25837409
H	-1.83170814	-3.81617829	4.74759236
H	-3.25710625	-5.38430241	3.46270126

H	-2.82497922	-5.75734845	1.04718408
H	0.86047306	-1.66717613	3.33534826
H	3.48850426	0.59378704	1.63090813
H	-1.38579711	-1.78445114	5.40665941
H	-1.20820509	-0.65643305	4.02300331
H	-0.03698000	-0.63201205	5.35169843
H	0.48542404	-3.69493428	5.64210646
H	1.72928013	-2.43206319	5.54149642
H	1.76354613	-3.81567829	4.42632734
H	5.07674539	3.06120324	0.72789305
H	3.49887627	3.04699123	1.55455012
H	3.64066128	2.38748418	-0.08436801
H	5.33383340	0.23067802	3.31544925
H	4.44975334	1.75225913	3.55649727
H	6.06705447	1.77415114	2.83070321
H	7.09748354	1.43640011	0.81710606
H	8.46851866	0.17616001	-0.82400006
H	7.47362156	-1.68996513	-2.12267116
H	-0.00083400	-4.23829632	-0.87254707
H	3.85720129	-2.77508721	-1.76466114
H	-3.03136723	-4.60106735	-1.17122509
H	-1.86387414	-4.37593034	-2.49302319
H	-2.13698116	-3.06897123	-1.30872210
H	-1.68039513	-6.80102352	-0.54196304
H	0.03854600	-6.65651548	-0.12583201
H	-0.49549904	-6.44703649	-1.80867414
H	4.43291134	-1.32770010	-3.72197728
H	4.43328134	-3.05700924	-4.14315332
H	5.96916043	-2.19575817	-3.91985030
H	6.67449449	-3.97709730	-2.08201216
H	5.13894539	-4.80853137	-2.39487018
H	5.56278141	-4.31194233	-0.74112306
H	1.47804111	6.77862149	-1.31749410
H	1.68485813	7.62292056	1.00281208
H	0.62617205	6.39647048	2.88086822
H	-0.19321901	3.55556827	-2.27484318
H	-3.30391925	0.58965204	1.62445712
H	2.21863617	5.33732740	-2.86192322
H	1.59573912	3.99738531	-3.85092630
H	2.21556417	3.66072928	-2.23261317
H	-1.64296013	5.62454343	-2.76671321
H	-0.66899205	5.11775939	-4.16414632
H	-0.17336101	6.51687651	-3.19070124
H	-5.30975039	-1.18148309	3.12952724
H	-3.80792829	-0.48092804	3.75958729
H	-3.73617229	-1.70890813	2.48485119
H	-5.11804739	2.34313218	1.60631412
H	-4.66945536	1.87412314	3.25999125
H	-6.17140245	1.25920110	2.53711019
H	-6.71510752	-1.04047508	1.37141810
H	-7.70287861	-1.81686314	-0.76788106
H	-6.49366452	-1.48301811	-2.90556922

H	-1.60146312	3.40011326	2.45889919
H	-3.03801223	0.04580800	-3.12282824
H	1.00755407	3.93769830	3.97520530
H	0.63622305	2.52206319	2.94367123
H	-0.25621002	2.78141821	4.45472834
H	-2.12993316	4.51289635	4.56235235
H	-2.34708218	5.69698441	3.25280025
H	-0.91649607	5.77048946	4.30235233
H	-3.57301527	-2.38897218	-3.56684427
H	-3.37126126	-1.42534011	-5.04646639
H	-4.99262038	-1.88524114	-4.50630634
H	-4.73717136	1.82481114	-3.64811028
H	-5.77066345	0.61194105	-4.42854934
H	-4.18374232	1.00905908	-5.12310739
O	1.25051210	0.26068902	1.56755112
O	-0.11128301	-0.30912402	1.80054314
C	-0.21422602	-1.56435912	-3.79936029
H	-1.09159108	-1.95919015	-3.29253525
C	1.03876608	-1.86307314	-3.29255325
H	1.15759709	-2.47294519	-2.40401018
O	0.42181003	-0.10067501	-2.54130619
O	-0.72945706	2.08901916	0.74982606
O	0.36610803	-2.17373017	-0.26231302
Zr	0.29473302	0.11083201	-0.32958202
H	1.93668015	-1.54681512	-3.81334829
C	-0.43169503	-0.82751606	-5.09665039
H	-0.81822606	-1.49997712	-5.87912844
H	-1.15374709	-0.01325600	-4.95959038
H	0.50592804	-0.38430803	-5.44860544

## Spiro Bisperoxo Complex to Oxo Peroxo Complex (conformation 2 higher energy)

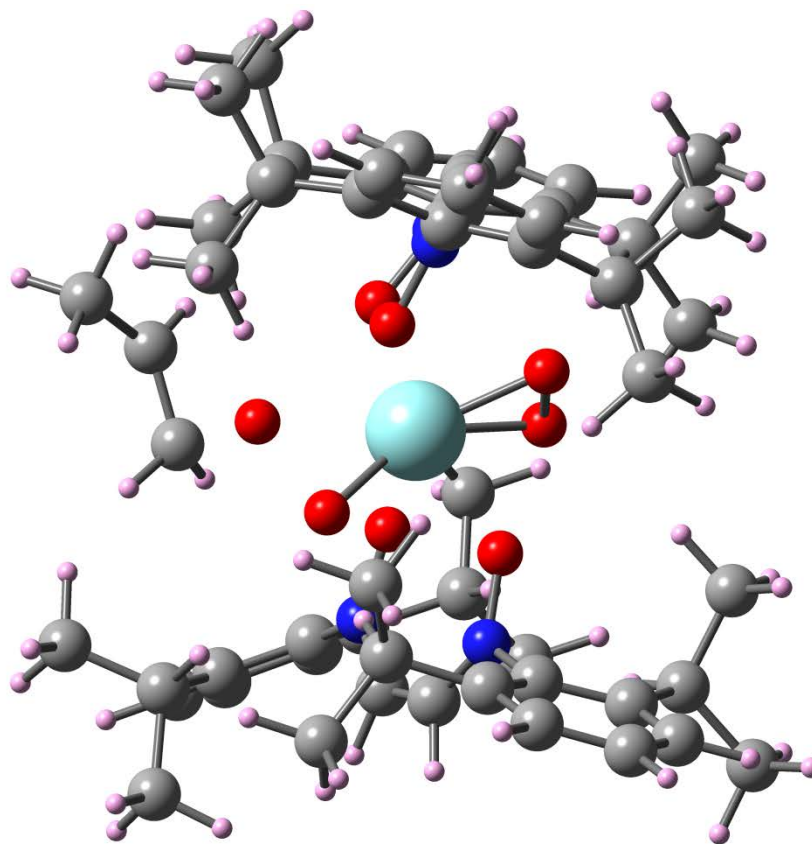


Fig. S154: ONCCNO Spiro Bisperoxo Complex to Oxo Peroxo Complex (conformation 2 higher energy)

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-3009.59076062	-3008.347175	-3008.268853	-3008.466679	-344

O	-2.01904800	0.76749400	-0.01565700
O	1.93092400	-1.01934800	-0.93701000
O	0.27692100	1.26128300	-1.69168900
N	-0.19424400	-3.14082400	0.63170500
N	2.71336200	-1.97535000	-0.40664300
N	0.27506800	3.28012900	0.48908200
N	-2.64076600	1.91331800	-0.37078700
C	1.07986900	-3.52797900	0.79154800
C	2.32429700	-3.04450900	0.30789300
C	-0.88281100	3.74662300	-0.01028100
C	-2.12677800	3.15538200	-0.34488300
C	-1.25561000	-3.83060200	1.37429800
C	-1.29249000	-3.72510700	2.79265800
C	-2.32225200	-4.42613300	3.45846400
C	-3.27063600	-5.18231400	2.75638600

C	-3.20415100	-5.26670600	1.35759500
C	-2.19454200	-4.59932700	0.63539800
C	-0.99741700	-1.92195000	4.57328100
C	-0.28647500	-2.92248600	3.62849000
C	0.63218200	-3.87792200	4.43907000
C	4.68336400	0.73514500	1.90486200
C	4.41939900	-0.77593300	1.67711200
C	5.02383400	-1.62049300	2.82956300
C	4.14199000	-1.79191100	-0.69214200
C	4.96035800	-1.22784400	0.31614000
C	6.32922100	-1.06615200	0.00811800
C	6.83661800	-1.42443400	-1.24987300
C	5.98435600	-1.94546200	-2.23806000
C	4.61129500	-2.13914600	-1.98313700
C	-3.43779400	-4.33209100	-1.56761700
C	-2.12086000	-4.78212000	-0.88402000
C	-1.78513000	-6.25352100	-1.24795200
C	3.29987200	-1.46965000	-4.03397500
C	3.67289000	-2.64156500	-3.08367200
C	4.26077800	-3.83796000	-3.87153100
C	1.35780600	4.22297800	0.80032600
C	2.22613200	4.60486800	-0.24810000
C	3.25627800	5.51333000	0.08065100
C	3.41512900	5.98048800	1.39457800
C	2.55567900	5.54275800	2.41722000
C	1.50319700	4.64459300	2.14480000
C	3.40864300	3.41907300	-2.16525600
C	2.08616900	4.06119800	-1.67439200
C	1.61839700	5.17292600	-2.65050400
C	-4.38438800	-0.55192900	2.08003400
C	-4.35140900	0.97707900	1.81909400
C	-5.12354700	1.74763600	2.92131900
C	-4.07714800	1.75282500	-0.64812800
C	-4.89315500	1.29297000	0.42012300
C	-6.26960100	1.13447800	0.15753000
C	-6.81005300	1.43646500	-1.10159600
C	-5.97821700	1.89821100	-2.13171400
C	-4.58899700	2.05913000	-1.93778800
C	1.29941800	2.87593800	3.94160800
C	0.61328600	4.09722500	3.26530800
C	0.22960800	5.17155600	4.31100700
C	-4.01250400	1.78655000	-4.41784500
C	-3.72752500	2.56299900	-3.10544000
C	-3.95413600	4.08124900	-3.35061300
H	1.17746300	-4.39597000	1.43335500
H	3.16605900	-3.66227600	0.60168800
H	-0.86898900	4.82308400	-0.13796000
H	-2.86549700	3.89359900	-0.63439300
H	-2.38289900	-4.36719900	4.54139600
H	-4.05531900	-5.70700900	3.29652200
H	-3.93497700	-5.86603600	0.82133100
H	0.33343000	-2.31142900	2.96901200

H	3.33228400	-0.89998900	1.70452400
H	-1.64749100	-2.42316100	5.30421400
H	-1.58176200	-1.20877200	3.98506700
H	-0.24379200	-1.34742100	5.12682900
H	0.05725700	-4.47059000	5.16410900
H	1.37754300	-3.29468700	4.99526900
H	1.17077100	-4.58338300	3.79053300
H	5.75736500	0.96411800	1.94403300
H	4.23157400	1.04870700	2.85406900
H	4.22951700	1.33463500	1.10734200
H	4.80575200	-2.68987300	2.70441700
H	4.60030000	-1.29910900	3.78967000
H	6.11506200	-1.50608400	2.88524200
H	6.99521500	-0.64330700	0.75562300
H	7.89372300	-1.28724700	-1.46600000
H	6.38846800	-2.20128300	-3.21339300
H	-1.31849700	-4.14998000	-1.27349500
H	2.73863300	-2.97914000	-2.61904100
H	-4.28938600	-4.94345900	-1.24201800
H	-3.35621400	-4.43042700	-2.65822400
H	-3.66280100	-3.28503800	-1.33256300
H	-2.57049400	-6.94125700	-0.90795600
H	-0.83953200	-6.57173500	-0.78999700
H	-1.69069000	-6.36229100	-2.33675700
H	2.76857400	-0.68625100	-3.48399900
H	2.64283700	-1.83059200	-4.83646600
H	4.19938200	-1.03946600	-4.49568400
H	5.14140200	-3.54737500	-4.45897500
H	3.51249100	-4.22282900	-4.57686800
H	4.55492000	-4.65804800	-3.20329800
H	3.94409800	5.84156600	-0.69387100
H	4.21780300	6.67682600	1.62693600
H	2.70628200	5.89853900	3.43216400
H	1.33868800	3.25899700	-1.69184400
H	-3.30173500	1.27736400	1.87485200
H	4.22173100	4.15396600	-2.24553700
H	3.25342200	2.97266300	-3.15527300
H	3.72887400	2.61924200	-1.48742900
H	0.65479400	5.60090800	-2.34204500
H	1.49613300	4.75747700	-3.65907700
H	2.34715700	5.99349300	-2.70640100
H	-5.41001100	-0.94376600	2.03165700
H	-3.98042600	-0.77224200	3.07610800
H	-3.76894900	-1.07998900	1.34471500
H	-5.11161300	2.83067300	2.74040200
H	-4.65696500	1.56000500	3.89701700
H	-6.17180000	1.42822400	2.98967400
H	-6.92291800	0.78250900	0.95087700
H	-7.87556200	1.31265700	-1.27984200
H	-6.40852300	2.12452400	-3.10313100
H	-0.31828500	3.72536700	2.82019900
H	-2.67038200	2.41326500	-2.85892000



H	2.27187900	3.16349000	4.36576800
H	1.44448700	2.06324000	3.22279400
H	0.66760200	2.49638200	4.75546900
H	-0.49022400	4.75085000	5.02493000
H	-0.22763800	6.05261100	3.84138200
H	1.10018900	5.50809800	4.88915900
H	-3.94168700	0.70347400	-4.27207400
H	-3.28554500	2.07789100	-5.18704100
H	-5.01266000	2.01002900	-4.81001200
H	-3.72867400	4.68612500	-2.46308900
H	-4.99797300	4.27911500	-3.62751200
H	-3.31256800	4.43304700	-4.16894000
O	1.11212600	-0.54925700	1.59512400
O	-0.33192500	-0.22480900	1.95454800
C	-1.56377200	-0.41753700	-3.19430100
H	-2.41342600	-0.16776600	-2.55398500
C	-1.38196500	-1.83174200	-3.49055900
H	-1.74684100	-2.54916200	-2.76406600
O	-0.27277200	-0.31342100	-2.38910200
H	-1.46866700	0.26479000	-4.04395800
C	-0.57280900	-2.31923500	-4.65646600
H	0.20784200	-3.02913700	-4.34560600
H	-1.20835800	-2.85258200	-5.38703700
H	-0.08598200	-1.48642900	-5.17659600
O	0.56228700	2.01368100	0.75720900
O	-0.58071500	-2.18260100	-0.25366600
Zr	0.06887700	-0.02930900	-0.13193300

### Butterfly Bisperoxo Complex to Oxo Peroxo Complex

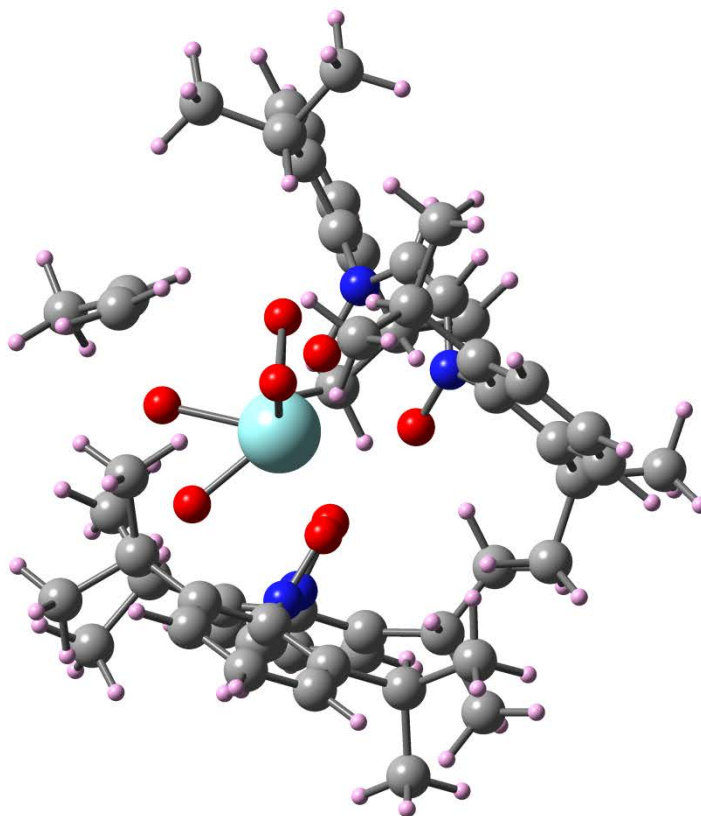


Fig. S155: ONCCNO Butterfly Bisperoxo Complex to Oxo Peroxo Complex

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-3009.60946146	-3008.364592	-3008.286566	-3008.481065	-482

O	0.20432700	-1.01548600	1.26943500
O	2.15433700	0.16372500	-0.30337200
O	0.76201600	-1.88292600	-1.63845400
N	0.34728500	2.85773300	0.34949100
N	2.91198500	1.14223100	-0.81670500
N	-2.83822700	-1.50575100	0.46969100
N	0.16404600	-2.35019600	1.45622700
C	1.47851000	3.16625500	-0.28215200
C	2.57960600	2.42805200	-0.83072500
C	-2.28672000	-2.60793100	0.98515200
C	-0.96309100	-3.03620400	1.31704500
C	-0.52422700	3.96026100	0.79197700
C	-1.25022100	4.68080500	-0.18813600
C	-2.04886000	5.75008600	0.27445700
C	-2.13613100	6.05640100	1.64070300
C	-1.42980200	5.29297400	2.58450300

C	-0.60438300	4.22338900	2.18099500
C	-2.64153900	4.15838300	-2.24949200
C	-1.21133900	4.34013200	-1.68327900
C	-0.45402500	5.43388600	-2.48356200
C	2.73149000	-0.80739700	-4.33592400
C	3.09259600	0.57337200	-3.72597400
C	3.37279100	1.61821200	-4.83745800
C	4.20472000	0.71685000	-1.38401300
C	4.28394200	0.44914500	-2.77211700
C	5.54323000	0.03942600	-3.26507100
C	6.64977900	-0.10213700	-2.41513500
C	6.52443700	0.15441700	-1.03988400
C	5.29246300	0.56216500	-0.48981400
C	-0.87770700	2.53765500	4.04243200
C	0.13504600	3.38628100	3.22856100
C	1.00969200	4.26218800	4.16158900
C	5.63413800	-0.38453200	1.85136500
C	5.17469500	0.83515600	1.01309200
C	5.96775900	2.10975700	1.40896600
C	-4.30575700	-1.47885500	0.31279700
C	-4.93004000	-2.39568200	-0.57718300
C	-6.33495700	-2.30995800	-0.69086600
C	-7.07095900	-1.35638000	0.02727600
C	-6.41733500	-0.46242500	0.88918200
C	-5.01822900	-0.50375300	1.05771600
C	-4.60405100	-3.48164200	-2.88172300
C	-4.17868400	-3.46346500	-1.39074700
C	-4.40551400	-4.87712600	-0.78214500
C	2.13349300	-0.10310400	3.79733000
C	1.29877000	-1.39820800	3.98192200
C	1.14418500	-1.75664200	5.48151200
C	1.38926800	-3.00347400	1.93524600
C	1.92285100	-2.53827700	3.16882000
C	3.09038800	-3.16653700	3.64443600
C	3.69095600	-4.21748300	2.93351100
C	3.13602100	-4.65379000	1.72341500
C	1.97534600	-4.05596700	1.18298300
C	-4.32752400	1.90826400	1.38346200
C	-4.33806200	0.48782600	2.00835400
C	-4.99975300	0.49701400	3.40997700
C	2.53989200	-4.52655100	-1.25298500
C	1.44068700	-4.56432000	-0.16193200
C	0.86184500	-5.99824500	-0.01869300
H	1.60104500	4.23764500	-0.39753900
H	3.31592400	3.05593800	-1.32042800
H	-3.02993800	-3.36745200	1.19505800
H	-0.88749100	-4.08681800	1.56955700
H	-2.61712600	6.33543800	-0.44297200
H	-2.76103500	6.88285900	1.97122900
H	-1.51626100	5.53166400	3.64116200
H	-0.69241100	3.38608200	-1.83736000
H	2.20518500	0.90895000	-3.17766500

H	-3.21756900	5.09393600	-2.23098900
H	-3.19156600	3.40014500	-1.67982700
H	-2.57809500	3.81634200	-3.28863200
H	-0.95007500	6.41082000	-2.39825400
H	-0.41883900	5.15917700	-3.54515700
H	0.58102500	5.55450200	-2.13568000
H	3.57188000	-1.24150200	-4.89687700
H	1.88503100	-0.69002400	-5.02496600
H	2.41943800	-1.50849400	-3.55374700
H	3.61400600	2.60354600	-4.41481300
H	2.47979400	1.73109600	-5.46479500
H	4.20679000	1.31715300	-5.48701300
H	5.64909200	-0.17535400	-4.32484500
H	7.60780400	-0.41865600	-2.82124900
H	7.38611100	0.03078800	-0.38922000
H	0.79650000	2.68074000	2.71581400
H	4.12050500	1.00502300	1.25759500
H	-1.59507000	3.17758500	4.57374000
H	-0.35162200	1.92726200	4.78828400
H	-1.43053100	1.86600500	3.37636200
H	0.40151500	4.94746900	4.76643300
H	1.72604400	4.86552100	3.58887500
H	1.57687000	3.62493900	4.85284800
H	5.05025000	-1.27647000	1.59782900
H	5.49604500	-0.17837200	2.92099000
H	6.69621800	-0.61037700	1.68967900
H	7.03975400	1.98855100	1.20479100
H	5.84925700	2.31619600	2.48106200
H	5.61925100	2.98891200	0.85098100
H	-6.85361400	-2.98902000	-1.36120600
H	-8.15126700	-1.30867600	-0.08681200
H	-6.99779100	0.27084500	1.44179300
H	-3.10430500	-3.24705200	-1.37179400
H	0.30101600	-1.18415400	3.58756100
H	-5.64787600	-3.79828300	-3.00682700
H	-3.97452000	-4.19370500	-3.43050700
H	-4.47994500	-2.49959500	-3.34771600
H	-4.10821900	-4.93823500	0.27316200
H	-3.82441600	-5.62286400	-1.33938100
H	-5.46495900	-5.15990000	-0.83921000
H	3.16500900	-0.24647500	4.14767400
H	1.68949300	0.71953800	4.37346300
H	2.15115200	0.17741600	2.73924400
H	0.57457500	-2.68535400	5.61676700
H	0.61013900	-0.95025500	6.00186500
H	2.11428400	-1.88051900	5.97960400
H	3.52723700	-2.83763900	4.58308700
H	4.58954500	-4.69182500	3.32120600
H	3.61547000	-5.45962300	1.17523500
H	-3.29132900	0.19566900	2.13707900
H	0.65439200	-3.89738100	-0.52162100
H	-5.34899500	2.27373100	1.20930200

H	-3.78853200	1.89796500	0.43086500
H	-3.82135400	2.61540700	2.05305000
H	-4.43191900	1.15335600	4.08240700
H	-5.02212500	-0.50775500	3.85201600
H	-6.03002200	0.87424900	3.37597000
H	2.92445100	-3.50842300	-1.36378500
H	2.10469700	-4.81883500	-2.21667200
H	3.37352700	-5.20870800	-1.03350600
H	0.05053500	-6.04718600	0.72212700
H	1.63381700	-6.71526200	0.29289400
H	0.45829300	-6.33389800	-0.98264800
O	0.38253100	1.35934800	-2.09813000
O	-1.18175200	0.53852600	-2.71496100
O	-0.73458200	-2.16157700	-1.44418100
O	-2.22713000	-0.37887500	0.06733700
O	-0.12631700	1.62949300	0.60723100
Zr	-0.11998500	-0.15304700	-0.92613900
C	-3.16944600	-0.13464200	-3.32035700
H	-3.57052300	-0.49106100	-2.37524900
C	-2.02615200	-0.73735200	-3.83097500
H	-1.62062300	-1.64413600	-3.39045700
H	-1.64396900	-0.43776200	-4.80408600
C	-3.89531900	1.00091600	-3.99014200
H	-3.32341000	1.38679700	-4.84201000
H	-4.88244600	0.67367700	-4.35689400
H	-4.06943800	1.82697500	-3.29058000

## Oxo Peroxo Complex to Peroxo Ozone Complex

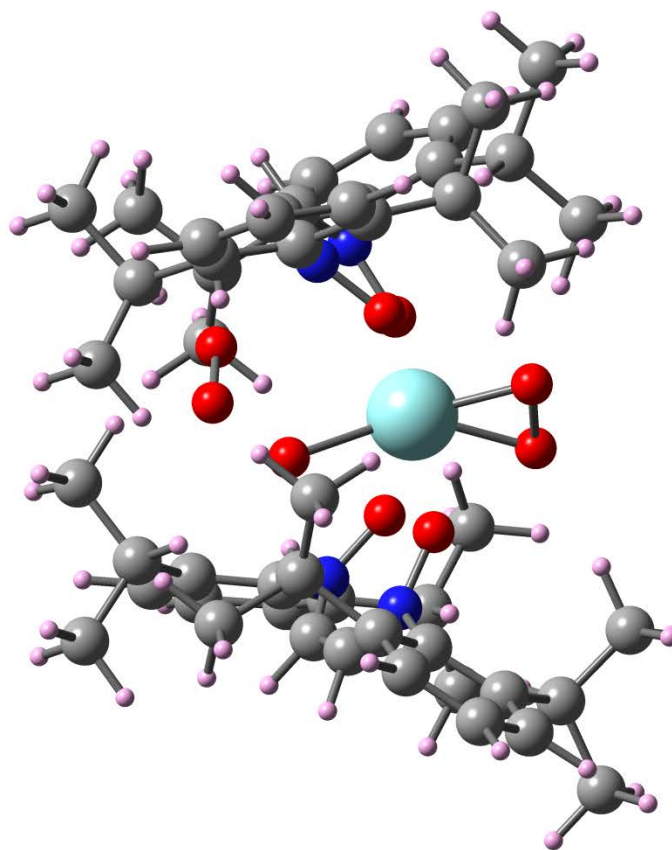


Fig. S156: ONCCNO Oxo Peroxo Complex to Peroxo Ozone Complex

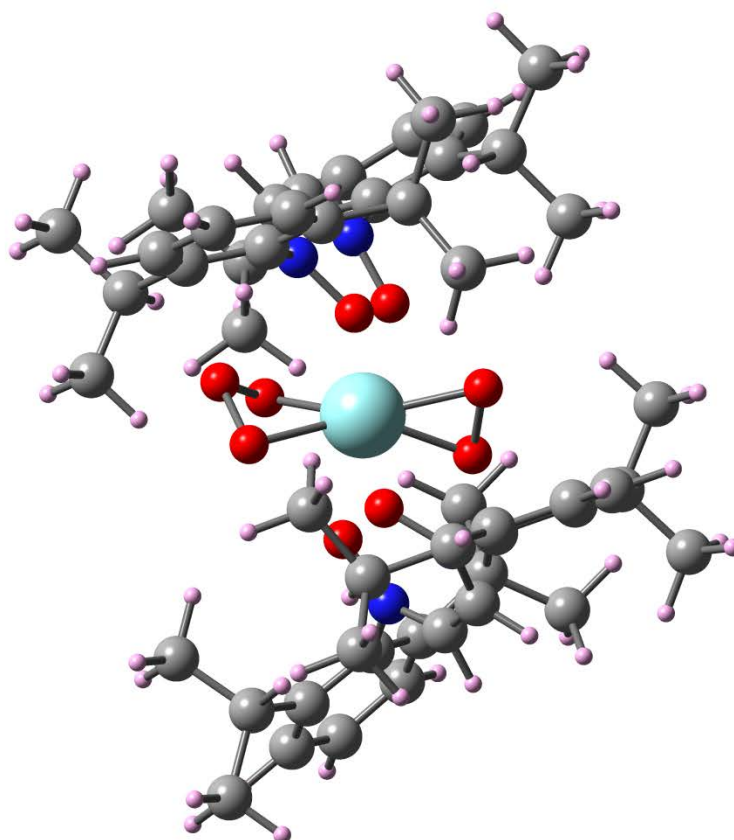
SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2966.876852	-2965.711364	-2965.637093	-2965.824359	-81
O	-0.60604431	-2.10513737	-0.48409152	
O	0.59925550	2.07374192	-0.61981428	
O	0.75653559	-0.16932605	1.09013928	
N	-2.65197778	1.68027701	-0.48519318	
N	0.27432904	2.98025449	0.34254363	
N	2.71637943	-2.04135510	-0.27256732	
N	-0.34459488	-2.94478878	0.52969296	
C	-2.24047483	2.63790686	0.35156982	
C	-0.98552434	3.18504256	0.74895071	
C	2.19756109	-2.95460376	0.55659629	
C	0.87156942	-3.31066424	0.93877396	
C	-4.05632841	1.56494185	-0.87302867	
C	-4.40181923	1.97157682	-2.18803172	
C	-5.75652929	1.85841968	-2.56152987	
C	-6.71667230	1.36830360	-1.66121029	
C	-6.33683379	0.95938424	-0.37424236	
C	-4.99106017	1.03019152	0.04752463	
C	-3.04965880	1.37577695	-4.24444996	

C	-3.36106157	2.47539021	-3.19257602
C	-3.79538725	3.79585637	-3.87680556
C	2.64605661	3.68450891	-2.63933261
C	1.62087295	4.49266214	-1.80140933
C	1.41029770	5.91097237	-2.39477720
C	1.36824591	3.87846810	0.72698404
C	2.04386821	4.55861582	-0.32740912
C	3.14521540	5.36533051	0.02347789
C	3.53949750	5.52369146	1.36022115
C	2.82446545	4.88046553	2.37866713
C	1.72652818	4.03902531	2.09411573
C	-5.03121058	-0.94837212	1.63958673
C	-4.60198790	0.52780504	1.44106108
C	-5.20678131	1.42658284	2.55251264
C	1.94951921	2.51875573	4.13182860
C	0.99434526	3.38443297	3.27245068
C	0.29018618	4.45874089	4.14534561
C	4.17209779	-2.04691757	-0.51163303
C	4.98125234	-1.25366380	0.33159837
C	6.37120242	-1.28520802	0.08498895
C	6.89998120	-2.04603695	-0.96888574
C	6.05235334	-2.78197675	-1.81445623
C	4.65696989	-2.79706511	-1.61097208
C	4.72872885	1.12992131	1.13666770
C	4.40651957	-0.35874446	1.43414919
C	4.92933435	-0.77266889	2.83419883
C	-3.05459571	-3.77389080	-2.06895064
C	-2.06427832	-4.59028959	-1.19566344
C	-2.10044463	-6.09404547	-1.57088686
C	-1.52698799	-3.57239881	1.13935185
C	-2.35127648	-4.36224190	0.29335574
C	-3.48262189	-4.96009081	0.88432470
C	-3.76472120	-4.79141811	2.24898995
C	-2.92531479	-4.00765957	3.05261390
C	-1.78706316	-3.36386454	2.52019038
C	3.41338638	-2.58937484	-3.80131782
C	3.72136039	-3.51528065	-2.58912571
C	4.27305627	-4.88267703	-3.05901755
C	-1.74880495	-1.43771145	4.20319649
C	-0.91491728	-2.50271372	3.44622542
C	-0.14302653	-3.39769773	4.45601225
H	-3.07980715	3.18155479	0.77568540
H	-1.08013857	3.98897625	1.46826982
H	2.96234931	-3.56162053	1.02722242
H	0.84098069	-4.07672651	1.70413589
H	-6.06147747	2.15890667	-3.56000204
H	-7.75822621	1.29741794	-1.96623380
H	-7.08747325	0.56648962	0.30646282
H	-2.42398594	2.67294049	-2.66084013
H	0.67058257	3.95888132	-1.87722142
H	-3.95116288	1.10814073	-4.81329696
H	-2.65458977	0.47639943	-3.76166503

H	-2.28922973	1.73388827	-4.94970495
H	-4.68426439	3.65705847	-4.50597570
H	-2.98803544	4.15924438	-4.52550351
H	-4.02183408	4.57822654	-3.14022068
H	3.64810891	4.13316639	-2.58437727
H	2.33760447	3.66151930	-3.69229497
H	2.69631367	2.64979790	-2.28763439
H	0.69283663	6.49457105	-1.80236813
H	1.02039770	5.82621616	-3.41768450
H	2.34702554	6.48113238	-2.44690229
H	3.68849130	5.88607976	-0.75989929
H	4.39168222	6.15281775	1.60628421
H	3.12537118	5.02141842	3.41333295
H	-3.51244294	0.55658795	1.54316509
H	0.23337939	2.70174951	2.89666946
H	-6.12265459	-1.06534143	1.60254911
H	-4.68760703	-1.30979013	2.61663767
H	-4.59166163	-1.59269622	0.86902192
H	-6.30476618	1.40887590	2.52811341
H	-4.88803021	2.47229570	2.44742931
H	-4.88283397	1.07440249	3.54027544
H	2.38957171	1.72047731	3.52434942
H	1.38806044	2.04638372	4.94824049
H	2.75908858	3.11255594	4.57660148
H	1.01430747	5.14681177	4.60145899
H	-0.27317882	3.97575554	4.95446988
H	-0.41312818	5.06599614	3.55807926
H	7.03694418	-0.69873606	0.71232821
H	7.97326675	-2.05359653	-1.14390005
H	6.47710169	-3.34263618	-2.64149166
H	3.31412860	-0.44501235	1.44405633
H	-1.06317603	-4.21582107	-1.42917790
H	5.81105836	1.31729552	1.13990239
H	4.27005870	1.77443837	1.89611763
H	4.32976035	1.42811710	0.16052103
H	4.67973215	-1.81695603	3.06586478
H	4.47678914	-0.13699066	3.60605707
H	6.01980682	-0.66443074	2.90689085
H	-4.09234467	-4.08826779	-1.89129990
H	-2.82874299	-3.92256240	-3.13254269
H	-2.96793628	-2.70474415	-1.85137468
H	-1.41211222	-6.68286936	-0.95019936
H	-1.80490325	-6.21817717	-2.62065282
H	-3.10506442	-6.52210113	-1.46056356
H	-4.14010944	-5.57177589	0.27348049
H	-4.63967373	-5.26842662	2.68409660
H	-3.16109281	-3.87998428	4.10503018
H	2.76356677	-3.70546540	-2.08805949
H	-0.18678196	-1.94448756	2.85008423
H	4.33973493	-2.31815172	-4.32613742
H	2.90183214	-1.67562822	-3.48323465
H	2.75462743	-3.10790740	-4.50969305



H	3.51596282	-5.39575079	-3.66544488
H	4.53377916	-5.53243008	-2.21291862
H	5.16562095	-4.76692164	-3.68719669
H	-2.20281283	-0.73536178	3.49779722
H	-1.08646065	-0.85586088	4.85651736
H	-2.52845025	-1.89065663	4.83000023
H	0.47348727	-4.15845762	3.95664786
H	-0.83564076	-3.92552648	5.12499491
H	0.51924712	-2.77924859	5.07503556
O	0.72232019	0.55788892	-2.83915696
O	0.16067001	-0.86429780	-2.87538532
O	0.10283074	0.63061918	2.15864740
O	-1.27139573	0.88792523	1.89060488
O	2.06949566	-1.11984125	-0.96514665
O	-1.85292853	0.71692494	-1.03097415
Zr	0.09524437	-0.03092805	-0.97867477

Peroxo  $\eta^2$ -Ozone Complex to Peroxo  $\eta^3$ -Ozone ComplexFig. S157: ONCCNO Peroxo  $\eta^2$ -Ozone Complex to Peroxo  $\eta^3$ -Ozone Complex

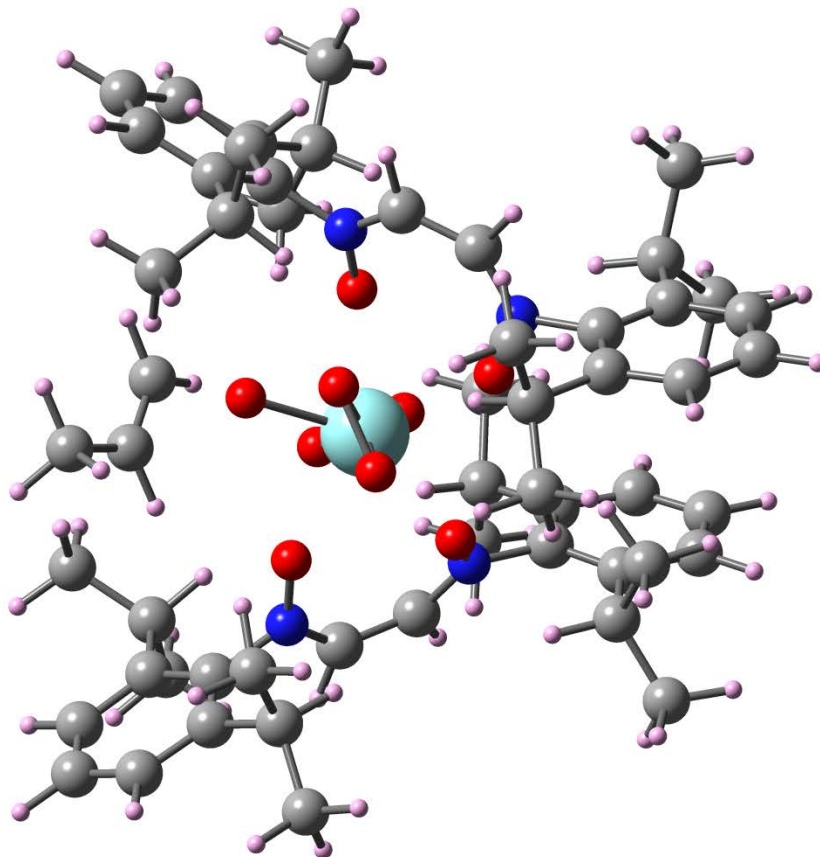
SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2966.884976	-2965.719613	-2965.645439	-2965.834506	-146

O	-2.07389739	0.03488687	-0.08219090
O	2.39010619	-0.38438319	-0.83761953
O	0.66835640	1.57744231	-1.70523912
N	0.91923713	-2.91134561	0.84609514
N	3.36629752	-1.08199795	-0.26708966
N	-1.18081126	3.14995517	0.23191196
N	-2.97770599	0.65477208	-0.86741873
C	2.21451645	-2.88446054	1.12612942
C	3.29033677	-2.12936610	0.55936646
C	-2.29054580	3.06410433	-0.52198710
C	-3.05628129	1.97659431	-1.03322267
C	0.00502836	-3.81124792	1.55819916
C	-0.17603013	-3.66848759	2.96013392
C	-1.07790659	-4.56507938	3.57430883
C	-1.77120973	-5.53147518	2.83276405
C	-1.57021390	-5.63724067	1.44763266

C	-0.67206144	-4.78596636	0.77414434
C	-0.47741443	-1.78289758	4.65162071
C	0.53354431	-2.62104901	3.82963276
C	1.56971710	-3.30283766	4.76533861
C	4.40917239	2.38142405	1.38949542
C	4.66908021	0.85643219	1.51402987
C	5.50643308	0.53746887	2.77917205
C	4.71017524	-0.59008227	-0.63353410
C	5.33833792	0.32490507	0.24177204
C	6.62000918	0.78049763	-0.13703900
C	7.21202247	0.35839883	-1.33760458
C	6.53171517	-0.51872357	-2.19946051
C	5.25262136	-1.01310600	-1.86988468
C	-1.69230057	-4.41541385	-1.51716266
C	-0.46362045	-4.95373148	-0.73639637
C	-0.15860000	-6.42485623	-1.11889358
C	3.80276090	-1.00585942	-3.93665137
C	4.46856905	-1.89369028	-2.84744179
C	5.33703662	-3.00539951	-3.48418621
C	-0.76800691	4.47796251	0.72671673
C	-0.00977995	5.30974938	-0.12907631
C	0.35876761	6.57362526	0.38257938
C	0.00968889	6.95702212	1.68626965
C	-0.71181773	6.08323919	2.51736184
C	-1.11984294	4.81442374	2.05743460
C	1.95404839	5.00350658	-1.71728748
C	0.41873802	4.88709296	-1.53801422
C	-0.32473051	5.71497739	-2.61955299
C	-4.20856575	-1.88955717	1.75456808
C	-4.76798328	-0.61813919	1.06319999
C	-6.11729974	-0.18689906	1.69379459
C	-4.03423385	-0.22092927	-1.40045821
C	-4.88869459	-0.84022697	-0.44891064
C	-5.88821663	-1.69838655	-0.94822565
C	-6.03266149	-1.91966007	-2.32731553
C	-5.17463369	-1.28623571	-3.23623725
C	-4.14503522	-0.42300491	-2.79910641
C	-0.82170272	3.09177043	3.88704267
C	-1.84728878	3.83675638	2.98668026
C	-2.94232704	4.52407838	3.83885921
C	-2.47069735	-0.85536206	-4.66428494
C	-3.22356148	0.22140866	-3.84062570
C	-4.01836566	1.18079900	-4.76632247
H	2.52071403	-3.59134213	1.88818490
H	4.26969962	-2.46282300	0.88472188
H	-2.70880184	4.03737599	-0.74942188
H	-3.90217919	2.28252877	-1.63806765
H	-1.24803115	-4.48960095	4.64433888
H	-2.46743640	-6.20106485	3.33239828
H	-2.10815403	-6.39377760	0.88380131
H	1.04957050	-1.90175097	3.18939049
H	3.68644263	0.38948541	1.63894551

H	-1.07100972	-2.39836895	5.34135301
H	-1.14211040	-1.24107532	3.97279113
H	0.06651121	-1.03777606	5.24673614
H	1.07907086	-3.98384711	5.47382777
H	2.10780303	-2.54231029	5.34601771
H	2.31204911	-3.89150203	4.20697313
H	5.34718227	2.94660864	1.30272232
H	3.87187167	2.74008994	2.27616984
H	3.79139523	2.59840694	0.51036330
H	5.67497905	-0.54220475	2.89075126
H	4.97962248	0.89271373	3.67384639
H	6.48834676	1.02850064	2.75036757
H	7.14720059	1.48019885	0.50595282
H	8.19873653	0.72496431	-1.61095568
H	6.99387905	-0.81513107	-3.13646773
H	0.39100382	-4.34708823	-1.05002754
H	3.65257148	-2.38580516	-2.30398153
H	-2.60636886	-4.96090215	-1.24412199
H	-1.53304155	-4.53398501	-2.59697540
H	-1.83967231	-3.35068969	-1.31192565
H	-1.01381338	-7.08636918	-0.92908032
H	0.70206819	-6.81785321	-0.56141109
H	0.07122825	-6.48625979	-2.19065547
H	3.12053257	-0.27997129	-3.48265228
H	3.22212251	-1.63123176	-4.62703497
H	4.56333150	-0.46579710	-4.51751664
H	6.11326984	-2.59078379	-4.14019205
H	4.70683455	-3.65989413	-4.09996785
H	5.83119398	-3.62277674	-2.72228044
H	0.93507567	7.25154826	-0.24109847
H	0.30846956	7.93335547	2.06090658
H	-0.95888986	6.38910952	3.52973482
H	0.18260449	3.82879556	-1.68962034
H	-4.04469036	0.18115550	1.25163785
H	2.30087424	6.04424481	-1.65606102
H	2.23868832	4.60523452	-2.69865690
H	2.48001128	4.41690601	-0.95477797
H	-1.41459199	5.59896004	-2.54230186
H	-0.02102932	5.38136458	-3.61995923
H	-0.09584520	6.78613073	-2.53394460
H	-4.87682944	-2.74898024	1.60616621
H	-4.10664082	-1.71920130	2.83438697
H	-3.22075701	-2.13972767	1.35510391
H	-6.52208732	0.71056757	1.20749681
H	-5.97386858	0.03666977	2.75916447
H	-6.87471061	-0.97832718	1.62337845
H	-6.56123124	-2.19172521	-0.25240391
H	-6.81195220	-2.58540877	-2.69083375
H	-5.29128967	-1.46972070	-4.30070337
H	-2.34186022	3.07153590	2.37552290
H	-2.44914509	0.80159711	-3.33436177
H	-0.24151053	3.80599035	4.48770630

H	-0.13702612	2.49023409	3.28136899
H	-1.34804317	2.41376616	4.57182717
H	-3.50523018	3.76551557	4.39782204
H	-3.65014249	5.08659388	3.21578539
H	-2.51278828	5.21638891	4.57436022
H	-1.82223802	-1.44291516	-4.00652901
H	-1.82906861	-0.36560918	-5.40805919
H	-3.16103841	-1.52452320	-5.19615381
H	-4.54159476	1.96219019	-4.19664007
H	-4.77163315	0.64118166	-5.35592904
H	-3.33305726	1.67316630	-5.46806667
O	1.31201415	-0.07869224	1.54369372
O	-0.17718588	-0.20729712	1.87797245
O	-0.44271885	0.84070723	-2.45415570
O	-0.21198501	-0.64142404	-2.18693010
O	-0.40128106	2.16176358	0.63770167
O	0.38255936	-2.19969023	-0.16433963
Zr	0.18633624	0.08244150	-0.18512522

Peroxo  $\eta^3$ -Ozone Complex to Spiro Bisperoxo ComplexFig. S158: ONCCNO Peroxo  $\eta^3$ -Ozone Complex to Spiro Bisperoxo Complex

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-3084.759833	-3083.511989	-3083.432900	-3083.630394	-349

O	-2.00455900	-0.35249400	-0.24969800
O	2.45265900	-0.41729100	-0.72834100
O	1.14345200	2.13952600	-0.80950400
N	0.69336100	-2.72846000	0.87264500
N	3.34008800	-1.29126000	-0.25631200
N	-1.69663000	2.91530300	0.42923600
N	-3.06744600	0.24184500	-0.78718500
C	1.97556100	-2.87406400	1.18957500
C	3.13519500	-2.31460100	0.58364700
C	-2.76764300	2.73394900	-0.33701500
C	-3.37993900	1.54085900	-0.82538700
C	-0.33583900	-3.52409200	1.54901300
C	-0.50866400	-3.43217100	2.95942300
C	-1.51584500	-4.23791700	3.53393500
C	-2.31004000	-5.09198700	2.75723400
C	-2.08970300	-5.18524100	1.37550900

C	-1.08819200	-4.42299900	0.74062300
C	-0.54692200	-1.62802900	4.76460400
C	0.33601500	-2.55763700	3.89618400
C	1.24667500	-3.44259300	4.79172700
C	5.82466600	1.21026600	2.04346800
C	5.36647300	-0.21620100	1.64481700
C	6.02742800	-1.26286000	2.58421500
C	4.71336500	-1.04759000	-0.73325800
C	5.67396900	-0.53201700	0.17327700
C	6.97303200	-0.31409400	-0.33462600
C	7.28032600	-0.57447600	-1.67897900
C	6.29328100	-1.06021000	-2.55182600
C	4.98106700	-1.31146200	-2.09985700
C	-2.00719400	-4.08539900	-1.59839600
C	-0.83469500	-4.64648700	-0.75609400
C	-0.58138900	-6.14374400	-1.07270400
C	3.42260000	-0.66315200	-3.98820900
C	3.90885200	-1.81804100	-3.07030500
C	4.40149200	-3.02764700	-3.90405900
C	-1.24234400	4.26808600	0.76592100
C	-0.88327200	5.16176900	-0.27978400
C	-0.41865600	6.43635400	0.11113900
C	-0.30436100	6.79164300	1.46269900
C	-0.66821500	5.88022200	2.46648300
C	-1.15379500	4.59653800	2.14653400
C	0.38335400	5.06415000	-2.49859700
C	-0.96694300	4.83360000	-1.77831200
C	-2.09981800	5.65593900	-2.45203500
C	-5.04936500	-2.26753100	1.84948600
C	-5.04187900	-0.97445100	0.99692200
C	-6.26569300	-0.08105000	1.33825900
C	-4.04977300	-0.69597000	-1.37594800
C	-4.99858800	-1.27977300	-0.50431500
C	-5.94543200	-2.14816300	-1.08656700
C	-5.92677500	-2.41604200	-2.46519500
C	-4.95613000	-1.82823200	-3.29150300
C	-3.98061100	-0.95360200	-2.76534300
C	-0.32522500	3.05026200	3.98467800
C	-1.57173200	3.64450000	3.27499400
C	-2.51611200	4.33614600	4.29197800
C	-2.23089800	-1.34627600	-4.58825700
C	-2.93323700	-0.30823000	-3.67940300
C	-3.57673600	0.81658300	-4.53558100
H	2.17576900	-3.58480000	1.98204200
H	4.05744200	-2.81170000	0.86120200
H	-3.27854100	3.64599900	-0.61830400
H	-4.31115300	1.71971000	-1.35030700
H	-1.67960700	-4.18611800	4.60661100
H	-3.08531700	-5.69246700	3.22764700
H	-2.68573000	-5.87356200	0.78263700
H	0.95638700	-1.88746000	3.30011300
H	4.28237400	-0.25492500	1.80249600

H	-1.22820900	-2.18708800	5.42129100
H	-1.12400700	-0.96288300	4.11563300
H	0.09382300	-1.00197300	5.39999100
H	0.65470700	-4.08860600	5.45434600
H	1.88296100	-2.80698100	5.42161300
H	1.90314300	-4.09774400	4.20045700
H	6.91552700	1.32080500	1.98617900
H	5.52292200	1.41742600	3.07821800
H	5.36584700	1.97041000	1.40255800
H	5.70404600	-2.28692300	2.35580900
H	5.76594000	-1.05115200	3.62900100
H	7.12156200	-1.23422000	2.49524800
H	7.74333700	0.07626500	0.32451800
H	8.28689400	-0.39223900	-2.04813000
H	6.54293400	-1.24970200	-3.59193900
H	0.05514300	-4.08718500	-1.05422800
H	3.03572100	-2.14548100	-2.49586900
H	-2.95670500	-4.57660800	-1.34406100
H	-1.81788200	-4.25084800	-2.66754200
H	-2.11191700	-3.01050300	-1.42576500
H	-1.46964600	-6.76169500	-0.88699200
H	0.24238200	-6.54944300	-0.47030100
H	-0.31688000	-6.25733100	-2.13260200
H	2.95465700	0.12756900	-3.39406500
H	2.66845200	-1.03716600	-4.69245900
H	4.25629800	-0.24107400	-4.56710400
H	5.21062000	-2.74919400	-4.59208600
H	3.57460800	-3.41654100	-4.51210800
H	4.76657200	-3.84094700	-3.26282100
H	-0.13011400	7.15020300	-0.65516400
H	0.06652400	7.77725800	1.73395100
H	-0.58463100	6.17097900	3.50955800
H	-1.17724000	3.76932500	-1.91080300
H	-4.13519300	-0.42446300	1.27170200
H	0.73663200	6.10048100	-2.41032400
H	0.27146800	4.83685700	-3.56693400
H	1.13143800	4.38260500	-2.08885100
H	-3.07578400	5.49725900	-1.97089800
H	-2.19181700	5.37341300	-3.50869600
H	-1.88707600	6.73231300	-2.40834000
H	-5.95671700	-2.86186200	1.67802400
H	-5.01602400	-2.01070700	2.91620900
H	-4.17872700	-2.89283400	1.62499400
H	-6.24645900	0.86240200	0.77667900
H	-6.27276800	0.16039800	2.40918400
H	-7.20741200	-0.59305100	1.09998300
H	-6.69747700	-2.61762500	-0.45810900
H	-6.66698900	-3.08714700	-2.89478600
H	-4.94717300	-2.05484400	-4.35387500
H	-2.11482600	2.79778200	2.84417900
H	-2.13924800	0.13415000	-3.07053300
H	0.31430400	3.84603700	4.39202700



H	0.25733600	2.43759100	3.29063400
H	-0.64034100	2.40626200	4.81644700
H	-2.87879000	3.59594900	5.01707500
H	-3.38736800	4.78566000	3.79699800
H	-2.00530900	5.12495800	4.85952300
H	-1.77342400	-2.13994900	-3.98865200
H	-1.42927600	-0.84985500	-5.14776600
H	-2.92038700	-1.80300800	-5.31210800
H	-4.02699200	1.59916000	-3.90972000
H	-4.36287800	0.41893400	-5.19229900
H	-2.81151800	1.28915800	-5.16417600
O	1.40614700	0.18458200	1.69468200
O	0.02358500	-0.37633200	1.94420000
O	-0.32699100	1.49886200	-1.76005300
O	0.07860900	0.13546000	-2.24172200
O	-1.02255500	1.90962900	0.99695200
O	0.33892400	-2.03360600	-0.25346400
C	3.21881500	2.65149100	-0.34569300
H	3.57829900	1.62794000	-0.36418200
C	2.40523200	3.04376500	0.69037800
H	2.15539200	2.36458400	1.49994600
H	2.01756900	4.05853000	0.74320700
C	3.70096700	3.54069000	-1.46037000
H	3.34564900	4.57100600	-1.34747100
H	4.80090200	3.55374000	-1.49540400
H	3.34783900	3.15160900	-2.42440300
Zr	0.25960200	0.25824500	-0.08463600

## Oxo Peroxo Complex to Dioxo Complex (conformation 1 lower energy)

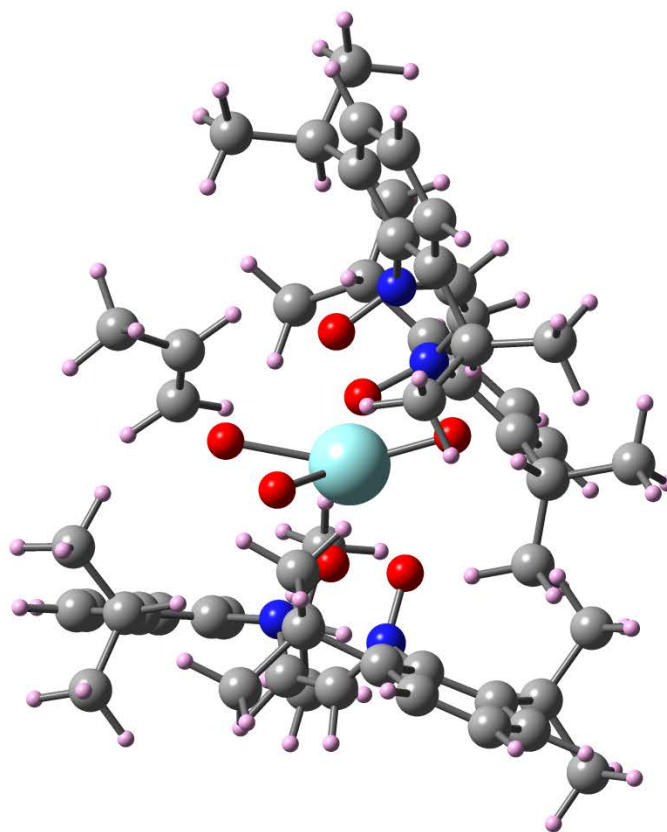


Fig. S159: ONCCNO Oxo Peroxo Complex to Dioxo Complex (conformation 1 lower energy)

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2934.432523	-2933.191623	-2933.114274	-2933.309099	-476

Zr	-0.05093900	0.22064000	-0.21497900
O	1.92206800	-0.93969300	0.27337600
O	-2.20838800	0.57404500	0.78423300
O	0.33118000	1.16239600	1.40379500
N	-1.98021000	-2.33920500	-0.75199500
N	-3.46239100	0.22448400	0.57258900
N	2.47070100	2.36942300	-0.01903400
N	2.63707900	-0.60773500	1.37666400
C	-3.25841800	-1.97719200	-0.66357300
C	-3.91584200	-0.89302300	-0.01858800
C	2.91641500	1.92296000	1.15046400
C	2.98906200	0.61800100	1.74537000
C	-1.58858200	-3.37796600	-1.70898400
C	-1.84670800	-3.16730800	-3.09282900
C	-1.44287900	-4.19335600	-3.97402200
C	-0.80411800	-5.35170800	-3.50814900

C	-0.56401500	-5.52234600	-2.13598500
C	-0.95815000	-4.54436700	-1.20107800
C	-1.72226900	-1.27517600	-4.81802500
C	-2.53684100	-1.92203800	-3.67160300
C	-3.97163500	-2.27605700	-4.15440300
C	-4.05209600	3.55290600	-1.92727200
C	-4.41092900	2.13160200	-1.42668000
C	-5.45652000	1.48076900	-2.37297300
C	-4.45402400	1.23182500	0.99946600
C	-4.91740100	2.14410800	0.02191600
C	-5.87793700	3.08712900	0.44793300
C	-6.31516000	3.12410700	1.78165600
C	-5.78977500	2.23096200	2.73056200
C	-4.83447800	1.26120400	2.36109000
C	0.80339800	-4.68020600	0.61486000
C	-0.71000800	-4.78742700	0.29168400
C	-1.28653900	-6.14984500	0.75659300
C	-3.00793200	1.10557800	4.09090600
C	-4.18340100	0.35098200	3.40634700
C	-5.18796300	-0.18744100	4.45297400
C	2.67826000	3.77990300	-0.38518000
C	1.74003700	4.73671600	0.07049000
C	1.96598800	6.07705100	-0.31273400
C	3.06325700	6.43036300	-1.11337800
C	3.96066800	5.44752800	-1.56186800
C	3.78314000	4.09294200	-1.21232900
C	-0.77130900	4.48335300	0.02523600
C	0.50767800	4.35892300	0.89591400
C	0.38916400	5.21191900	2.18357100
C	4.86048100	-3.48134100	-0.38323400
C	4.91155700	-2.27189100	0.58607200
C	6.37729000	-1.89805700	0.93036600
C	2.99356300	-1.74331300	2.23969100
C	4.09558000	-2.54414600	1.85366000
C	4.42939400	-3.62660000	2.69296300
C	3.68661000	-3.89383100	3.85473200
C	2.58730300	-3.09015600	4.19338600
C	2.20396700	-1.99499600	3.38771800
C	4.69206500	2.94765200	-3.28704500
C	4.75203900	3.03014800	-1.73918500
C	6.20148100	3.28607300	-1.25065100
C	-0.30343400	-2.02789600	3.76472300
C	0.97842100	-1.15395100	3.76217300
C	1.17345800	-0.45903200	5.13499800
H	-3.92736500	-2.62252400	-1.22050700
H	-4.99702400	-0.93204700	-0.07053800
H	3.37063100	2.69761300	1.75894400
H	3.49320000	0.62808900	2.70686800
H	-1.61818900	-4.07281100	-5.03899700
H	-0.49476400	-6.12000200	-4.21290600
H	-0.07649500	-6.42734300	-1.78441000
H	-2.59702200	-1.14666900	-2.90195000

H	-3.48173600	1.55072900	-1.48513700
H	-1.53719600	-1.96951000	-5.64902600
H	-0.77884500	-0.90217200	-4.41400300
H	-2.27649100	-0.41517600	-5.21652100
H	-3.94052000	-2.99125400	-4.98731600
H	-4.48263900	-1.37076100	-4.50658100
H	-4.58629000	-2.72640900	-3.36173700
H	-4.93779800	4.19656300	-2.02248900
H	-3.57999800	3.47900200	-2.91433600
H	-3.33825600	4.03832700	-1.25395600
H	-5.68793000	0.44806700	-2.08014900
H	-5.06768300	1.46091700	-3.39911400
H	-6.39731600	2.04855700	-2.37492000
H	-6.26931700	3.80639200	-0.26566900
H	-7.05426200	3.86125900	2.08684900
H	-6.11953300	2.29194100	3.76346600
H	-1.21251700	-4.00317400	0.86560800
H	-3.74984900	-0.51750900	2.89362100
H	1.38053100	-5.43133000	0.05779900
H	0.97684100	-4.84696400	1.68603200
H	1.18114300	-3.68472500	0.36013900
H	-0.77487500	-6.99616000	0.28039300
H	-2.35762900	-6.23303600	0.52957300
H	-1.15772000	-6.25570700	1.84192000
H	-2.23927300	1.37822600	3.35925500
H	-2.54664000	0.46741800	4.85683200
H	-3.36925500	2.01852000	4.58367700
H	-5.57812000	0.61331300	5.09408900
H	-4.68759900	-0.91246200	5.10784800
H	-6.04142900	-0.68794700	3.97710500
H	1.27075700	6.84492800	0.01528400
H	3.21492700	7.46973600	-1.39568400
H	4.79929400	5.73265400	-2.19201200
H	0.56303300	3.30530200	1.19850400
H	4.46383900	-1.42465200	0.05622700
H	-0.91757500	5.51153200	-0.33746300
H	-1.64581900	4.19754500	0.62364400
H	-0.72294000	3.80707800	-0.83622400
H	1.29309300	5.13601800	2.80360100
H	-0.45969700	4.85437000	2.78011500
H	0.21856800	6.27532100	1.96425000
H	5.32626200	-4.37190900	0.05926000
H	5.39786400	-3.24514400	-1.31068700
H	3.82534400	-3.72947200	-0.64355700
H	6.42331000	-1.01710300	1.58405000
H	6.93763600	-1.67293200	0.01330700
H	6.89024000	-2.72231200	1.44305300
H	5.27236400	-4.26312000	2.43636800
H	3.96176400	-4.73109000	4.49206800
H	2.01474400	-3.31558800	5.08929500
H	4.44197100	2.05107000	-1.35675400
H	0.81814300	-0.36586100	3.01522400

H	5.01373700	3.88996300	-3.74971200
H	3.67272700	2.73181300	-3.62579600
H	5.35355900	2.15025100	-3.65135400
H	6.86968000	2.49141500	-1.60838600
H	6.25602900	3.31193200	-0.15438000
H	6.58811100	4.24212700	-1.62685800
H	-0.47625800	-2.46594000	2.77475400
H	-1.17110800	-1.40356800	4.01123600
H	-0.24534800	-2.83980400	4.50325100
H	2.06934600	0.17647700	5.14101600
H	1.27238200	-1.18641600	5.95285400
H	0.30901700	0.18118600	5.35161000
O	-1.14470400	0.93378100	-1.69844200
O	0.24640400	-0.18003700	-2.38732200
O	-0.99600100	-1.82100500	0.02771300
O	1.78049400	1.64139000	-0.90381500
C	1.70481700	-1.72259700	-2.89053000
H	1.92298100	-2.15325800	-1.91917000
H	1.20802400	-2.35184800	-3.62398300
C	2.01745000	-0.40012900	-3.16782500
H	2.57497500	0.16600300	-2.42601900
C	1.91089500	0.23502400	-4.53352200
H	1.42131300	1.21167500	-4.44650800
H	2.90958900	0.38753400	-4.97170600
H	1.32578900	-0.38457000	-5.22242300

## Oxo Peroxo Complex to Dioxo Complex (conformation 2 higher energy)

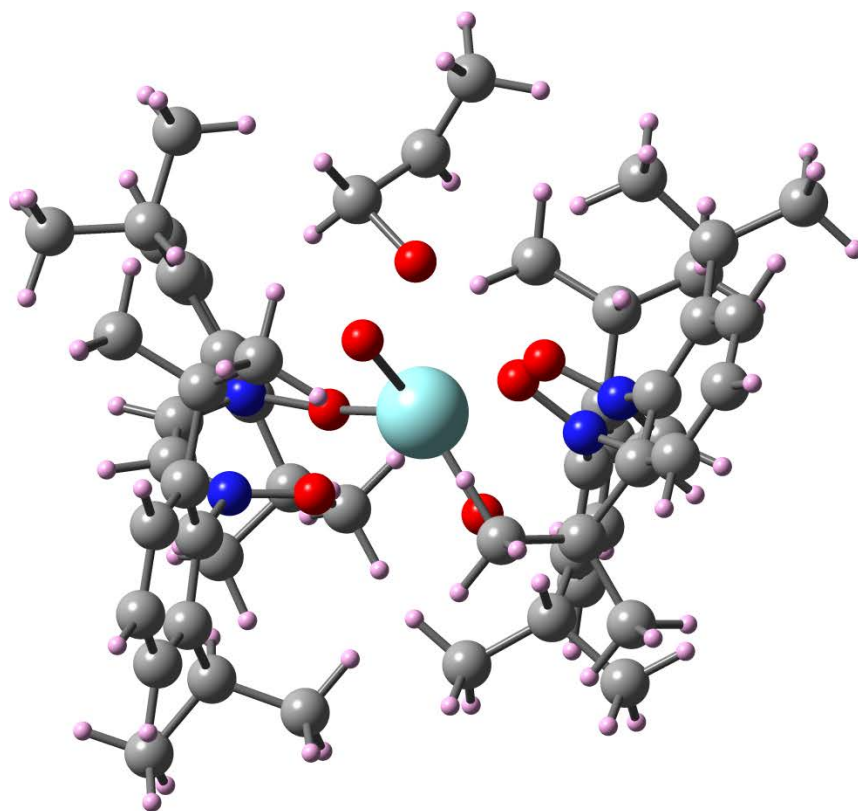


Fig. S160: ONCCNO Oxo Peroxo Complex to Dioxo Complex (conformation 2 higher energy)

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2934.42565380	-2933.185193	-2933.107927	-2933.303477	-362

O	-1.87559500	-0.21434600	-0.11382800
O	2.50293200	-0.37741000	-0.86011400
O	0.47933200	1.48792000	-1.68772200
N	1.04791000	-2.77145400	0.95044200
N	3.48916300	-0.85366900	-0.11618600
N	-1.38760300	3.08565800	0.35526500
N	-3.05853100	0.35979100	-0.52055300
C	2.32858300	-2.62791800	1.28128500
C	3.40233200	-1.81575700	0.80609300
C	-2.63895600	2.84719500	-0.11049900
C	-3.34752000	1.68175300	-0.45221400
C	0.21653700	-3.69869100	1.73018300
C	-0.09417900	-3.36896400	3.07499500
C	-0.85361100	-4.31522700	3.79840700
C	-1.29871400	-5.50389000	3.20171000
C	-1.00103200	-5.77679000	1.85633600
C	-0.23193000	-4.88030100	1.08715600
C	-0.88768100	-1.28334300	4.30221000

C	0.33589200	-2.05881200	3.74943900
C	1.36251200	-2.32608600	4.88179000
C	3.79813400	2.91540200	1.16700300
C	4.20638400	1.46276400	1.52857200
C	4.85229900	1.40122300	2.93640800
C	4.79765600	-0.21475000	-0.35124700
C	5.14217200	0.89111100	0.45848900
C	6.39903500	1.48668900	0.21052500
C	7.23981500	1.00886400	-0.80575400
C	6.84015600	-0.06962100	-1.61383600
C	5.59940300	-0.70697400	-1.40931800
C	-1.20896000	-4.96478000	-1.24066200
C	0.06708600	-5.18497500	-0.38391800
C	0.63842700	-6.61052800	-0.58732700
C	4.44234600	-1.17751200	-3.59973600
C	5.11330400	-1.81423700	-2.34962400
C	6.23319100	-2.80051400	-2.75824600
C	-0.98638600	4.46232700	0.65982000
C	-0.42493600	5.24157300	-0.37796100
C	-0.06316200	6.56830600	-0.05799800
C	-0.22834200	7.06799100	1.24333900
C	-0.74728600	6.24879800	2.26074200
C	-1.13573800	4.91965500	1.99277500
C	1.23149400	4.94328200	-2.29417700
C	-0.20861600	4.68177900	-1.78735100
C	-1.25273800	5.26084700	-2.77926200
C	-4.13919100	-2.88992400	2.20720300
C	-4.03918200	-1.52081700	1.49911400
C	-4.80634300	-0.44220100	2.31760600
C	-4.10903300	-0.58259400	-0.91246200
C	-4.55083500	-1.53604400	0.05276600
C	-5.55598100	-2.44130900	-0.33750400
C	-6.12436600	-2.39449300	-1.62156200
C	-5.69276300	-1.43172300	-2.54075200
C	-4.67289500	-0.50847300	-2.21695800
C	-0.39358200	3.35137600	3.82771800
C	-1.61716000	3.99298000	3.11323600
C	-2.54929600	4.69736800	4.12748700
C	-3.92841300	-0.14069500	-4.64200600
C	-4.26875700	0.52262800	-3.28183600
C	-5.39188600	1.57807400	-3.48391700
H	2.62209900	-3.28060800	2.09620800
H	4.34751400	-2.01067300	1.29981600
H	-3.21701000	3.75862400	-0.21161900
H	-4.37296300	1.88235600	-0.74053900
H	-1.10683500	-4.10897300	4.83489800
H	-1.88521400	-6.21357300	3.78065200
H	-1.36136200	-6.69607400	1.40290000
H	0.79718100	-1.38922100	3.01278100
H	3.27147300	0.88917000	1.56361400
H	-1.40615100	-1.83243200	5.10100400
H	-1.60578800	-1.06846800	3.50223000

H	-0.55206700	-0.32202800	4.71053900
H	0.93336900	-2.94682000	5.68062500
H	1.68225900	-1.37479100	5.32550400
H	2.25918400	-2.84005800	4.50843400
H	4.66381600	3.59274700	1.14313500
H	3.08512200	3.29204300	1.91063900
H	3.30386600	2.94517700	0.18906200
H	5.11976200	0.37190300	3.21278200
H	4.14236200	1.77731900	3.68383000
H	5.76325300	2.01306500	2.99724200
H	6.71056600	2.33700600	0.81124100
H	8.20236300	1.48453800	-0.97966900
H	7.49388700	-0.41237700	-2.41041300
H	0.81518000	-4.47206700	-0.74579000
H	4.33810000	-2.39646000	-1.83475100
H	-2.01107500	-5.65290900	-0.94078300
H	-0.98961000	-5.14262000	-2.30210700
H	-1.57207500	-3.93743900	-1.12821400
H	-0.08983000	-7.38659000	-0.31865400
H	1.54084000	-6.77197700	0.01664800
H	0.90227900	-6.75912400	-1.64263800
H	3.58235700	-0.56447900	-3.30931000
H	4.09446800	-1.96448200	-4.28304500
H	5.15886000	-0.54687200	-4.14341800
H	6.99327100	-2.31714100	-3.38549600
H	5.80626600	-3.62498200	-3.34407200
H	6.73802900	-3.22795100	-1.88197300
H	0.36406300	7.20457100	-0.82827700
H	0.06035100	8.09201800	1.47000400
H	-0.84613100	6.64373700	3.26772700
H	-0.31958300	3.59137400	-1.76187000
H	-2.98363900	-1.23691200	1.47259200
H	1.43589600	6.01385900	-2.43708600
H	1.37749600	4.43632200	-3.25571600
H	1.96834400	4.53586100	-1.59279300
H	-2.27964200	5.02609300	-2.46793000
H	-1.09620600	4.83581900	-3.77947100
H	-1.16632900	6.35374200	-2.85686300
H	-5.18087100	-3.18628700	2.39279500
H	-3.63838400	-2.83476800	3.18114900
H	-3.64965400	-3.68166200	1.62706900
H	-4.69355900	0.55627900	1.87857800
H	-4.41966900	-0.40247100	3.34463600
H	-5.87866300	-0.67738200	2.36515500
H	-5.90885400	-3.18209300	0.37211300
H	-6.90327600	-3.10118400	-1.89793800
H	-6.14175500	-1.39852100	-3.52951700
H	-2.18666400	3.17098500	2.66159500
H	-3.37211200	1.05336800	-2.94498400
H	0.24437900	4.12673900	4.27435100
H	0.20256900	2.76103400	3.12347500
H	-0.73398500	2.68419000	4.63183000



H	-2.94758400	3.96178300	4.83849700
H	-3.39711500	5.18523600	3.62867000
H	-2.01649400	5.45823600	4.71283100
H	-3.16018100	-0.91434500	-4.53348600
H	-3.55376400	0.61779500	-5.34208100
H	-4.81249000	-0.60266000	-5.09930600
H	-5.64100200	2.10150100	-2.55168300
H	-6.31168800	1.10520800	-3.85180600
H	-5.07858500	2.32889000	-4.22093600
O	1.17232600	0.15695300	1.48847400
C	-0.62528900	-0.26478500	-3.49705600
H	-1.57129600	-0.18067000	-2.95461000
C	-0.23673700	-1.62953200	-3.87813300
H	-0.50784500	-2.43610800	-3.19902600
O	0.50756400	-0.06322200	-2.54715300
H	-0.55753800	0.47942400	-4.29837200
C	0.69522000	-1.92689100	-5.01411400
H	1.60580600	-2.44411700	-4.67284200
H	0.22150300	-2.59331500	-5.75778200
H	1.00265800	-1.00885800	-5.52846300
O	-0.44635300	2.17332400	0.61146300
O	0.41846400	-2.13571000	-0.06762100
Zr	0.29462300	0.13937900	-0.15635300

## Butterfly Oxo Peroxo Complex to Dioxo Complex

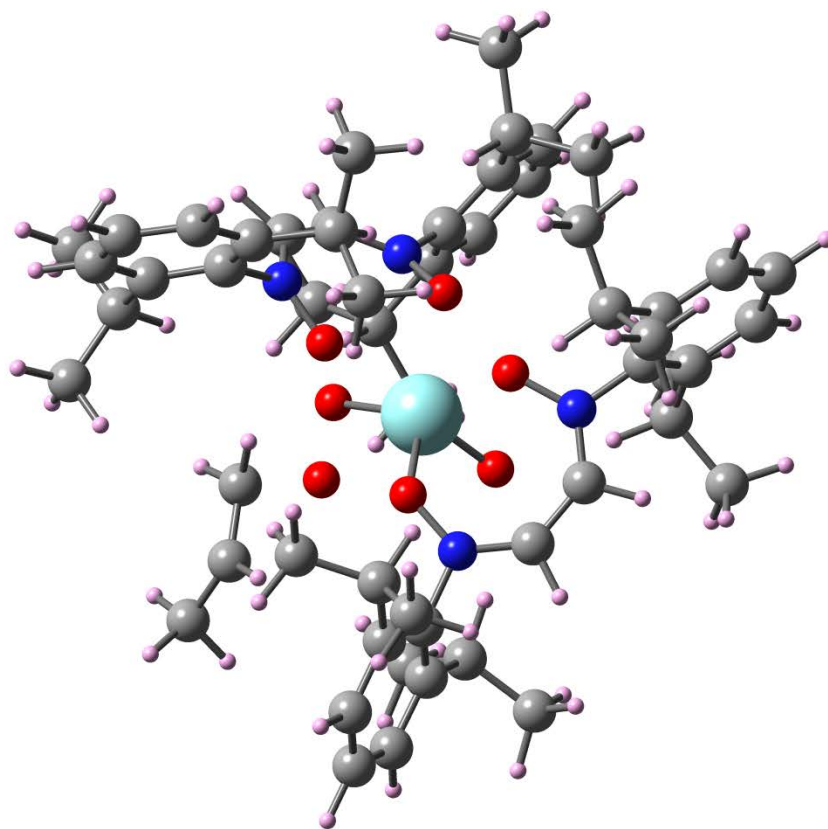


Fig. S161: ONCCNO Butterfly Oxo Peroxo Complex to Dioxo Complex

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2934.44740240	-2933.207491	-2933.130192	-2933.325604	-68

O	-0.52884800	1.78432600	0.65349100
O	-2.05996700	-0.84376900	0.03519300
O	-1.42512700	0.93797200	-2.27706900
N	0.49810300	-2.71746000	1.10658900
N	-2.52439200	-2.11993900	-0.04603100
N	2.53203100	1.67993500	-0.82119800
N	0.03292500	2.98517900	0.85934600
C	-0.55555500	-3.49352800	0.80146600
C	-1.85496900	-3.23318800	0.30018700
C	2.17650100	2.93812300	-0.53740700
C	1.16054800	3.47488400	0.29342200
C	1.73742400	-3.35173000	1.57250500
C	2.59678700	-3.94729000	0.61526500
C	3.75883700	-4.58039500	1.10895000
C	4.05180100	-4.59887100	2.48098000
C	3.18926200	-3.97541300	3.39729600
C	2.01248200	-3.33227900	2.96183700

C	3.50833000	-3.37906600	-1.69749300
C	2.30732000	-3.93232900	-0.88956900
C	1.92441900	-5.35157400	-1.38837000
C	-2.86748900	-1.89704300	-4.09895600
C	-2.85788000	-2.86012800	-2.88335400
C	-2.85766100	-4.34002900	-3.35019400
C	-3.88128000	-2.22737100	-0.58130700
C	-4.03857900	-2.58440700	-1.94445800
C	-5.36301200	-2.67273800	-2.42750400
C	-6.46056700	-2.39579200	-1.59810500
C	-6.26285000	-2.01826900	-0.25908500
C	-4.96373000	-1.92279200	0.28031400
C	1.82674500	-1.57168500	4.78374300
C	1.08089500	-2.66644100	3.97875500
C	0.44425100	-3.71672700	4.92711900
C	-5.18101900	-0.01274500	1.93619700
C	-4.75775300	-1.49191900	1.73566400
C	-5.50639200	-2.42439600	2.72247600
C	3.77216000	1.39422900	-1.54885300
C	3.81030400	1.47063300	-2.96343800
C	5.04105700	1.16660000	-3.58836600
C	6.16847000	0.79842900	-2.84196400
C	6.09489300	0.72871000	-1.44102000
C	4.89720200	1.02598800	-0.76150000
C	2.17599500	0.62212000	-4.70505900
C	2.60085600	1.83025700	-3.82847500
C	2.87858200	3.08205600	-4.70066000
C	-1.08738400	1.15826800	4.00484500
C	-0.03338900	2.25264300	3.68452300
C	0.85333500	2.55655700	4.91806600
C	-0.71942500	3.85738200	1.77455900
C	-0.73242500	3.50498700	3.14841600
C	-1.45375500	4.34191200	4.02409600
C	-2.12862800	5.47805900	3.54995600
C	-2.10840200	5.79012900	2.18291600
C	-1.41430500	4.98072800	1.25739900
C	5.00393400	-0.51655500	1.25125700
C	4.85322200	0.94952800	0.76897000
C	5.92508100	1.86433000	1.41684100
C	-2.90645900	5.47252200	-0.75238000
C	-1.45097100	5.34455000	-0.23289100
C	-0.66558100	6.65555000	-0.50869800
H	-0.35573800	-4.54700100	0.96122800
H	-2.44853900	-4.12856600	0.15120700
H	2.83849000	3.68205300	-0.96886700
H	1.30968000	4.52249600	0.53069700
H	4.44193700	-5.05182800	0.40769300
H	4.95334600	-5.09298700	2.83599500
H	3.43032200	-3.98998800	4.45732600
H	1.46907600	-3.25886500	-1.10238000
H	-1.91258200	-2.67020400	-2.36404600
H	4.39535900	-4.02411500	-1.62339400

H	3.78046200	-2.37344400	-1.35699800
H	3.22891900	-3.30536200	-2.75558600
H	2.74376800	-6.06838200	-1.23659300
H	1.69414000	-5.31787200	-2.46073500
H	1.03899600	-5.74013400	-0.86639700
H	-3.78363900	-1.99847300	-4.69808600
H	-2.00935900	-2.12026500	-4.74493700
H	-2.76481200	-0.85846500	-3.76678700
H	-2.82288300	-5.03514100	-2.49975500
H	-1.97789400	-4.52938300	-3.97803600
H	-3.75294200	-4.57869100	-3.94091200
H	-5.53077300	-2.95058300	-3.46470700
H	-7.47035500	-2.46717000	-1.99590700
H	-7.12176800	-1.79857900	0.36996100
H	0.27168300	-2.16722000	3.43579900
H	-3.68891900	-1.55013000	1.96834100
H	2.66307700	-1.99145500	5.35734400
H	1.14229000	-1.09125800	5.49549400
H	2.22446900	-0.80221300	4.11147500
H	1.20820600	-4.23106800	5.52504900
H	-0.10919200	-4.47920500	4.36373500
H	-0.25444300	-3.22983300	5.62050400
H	-4.60618200	0.64780700	1.27756100
H	-4.99913000	0.29688200	2.97392700
H	-6.24881500	0.12934500	1.72225100
H	-6.59333300	-2.37905000	2.57574100
H	-5.29773700	-2.12413900	3.75781200
H	-5.19474800	-3.46993200	2.60027000
H	5.10592500	1.21083200	-4.67217500
H	7.10194400	0.56377400	-3.34845800
H	6.97575600	0.44450800	-0.87125100
H	1.74140100	2.04632100	-3.18881700
H	0.61555100	1.84593500	2.90218000
H	2.97542700	0.31992500	-5.39667000
H	1.29115100	0.89016500	-5.29603100
H	1.90566100	-0.23605800	-4.07967300
H	3.16121200	3.94921300	-4.08755900
H	1.97595000	3.34566900	-5.26693600
H	3.68705300	2.90594000	-5.42339600
H	-1.77852600	1.49252100	4.79133000
H	-0.58862700	0.24464000	4.35155200
H	-1.66451100	0.91243800	3.10727200
H	1.59792700	3.33182000	4.69503900
H	1.38819700	1.64844600	5.22366500
H	0.26081000	2.89489400	5.77811000
H	-1.48381100	4.10477100	5.08393000
H	-2.67412900	6.11413300	4.24297500
H	-2.64755700	6.66366400	1.82636900
H	3.87181900	1.29078800	1.11215300
H	-0.97421100	4.54285400	-0.80652200
H	5.96496200	-0.94491000	0.93605400
H	4.19676000	-1.13708800	0.84933000

H	4.95588900	-0.56352100	2.34757500
H	5.83297200	1.83494000	2.51082000
H	5.81223900	2.90735800	1.09241600
H	6.94291900	1.54221500	1.16127700
H	-3.47465000	4.55140300	-0.58004200
H	-2.90151800	5.67203800	-1.83199000
H	-3.43940700	6.29882200	-0.26485300
H	0.37920200	6.58459000	-0.17869500
H	-1.12098500	7.50605700	0.01529000
H	-0.66742300	6.88047600	-1.58318400
O	0.19420400	-1.64986500	-1.81508900
O	-0.00507300	1.48863600	-2.18983900
O	1.94890200	0.59472500	-0.21574300
O	0.52468900	-1.36573900	1.04096800
Zr	-0.09847600	-0.15981600	-0.79113400
C	-2.54538300	2.04593000	-1.79245400
H	-2.25723500	2.18223700	-0.74408800
C	-3.86306100	1.51134200	-2.01585000
H	-4.26292400	0.80935500	-1.28619400
C	-4.64463600	1.74094200	-3.27595500
H	-4.22899600	2.56964100	-3.86390200
H	-4.64104300	0.84639900	-3.92621300
H	-5.70424400	1.95651900	-3.06479100
H	-2.27216000	2.89089000	-2.42998700

## Dioxo Complex to Oxo Ozone Complex

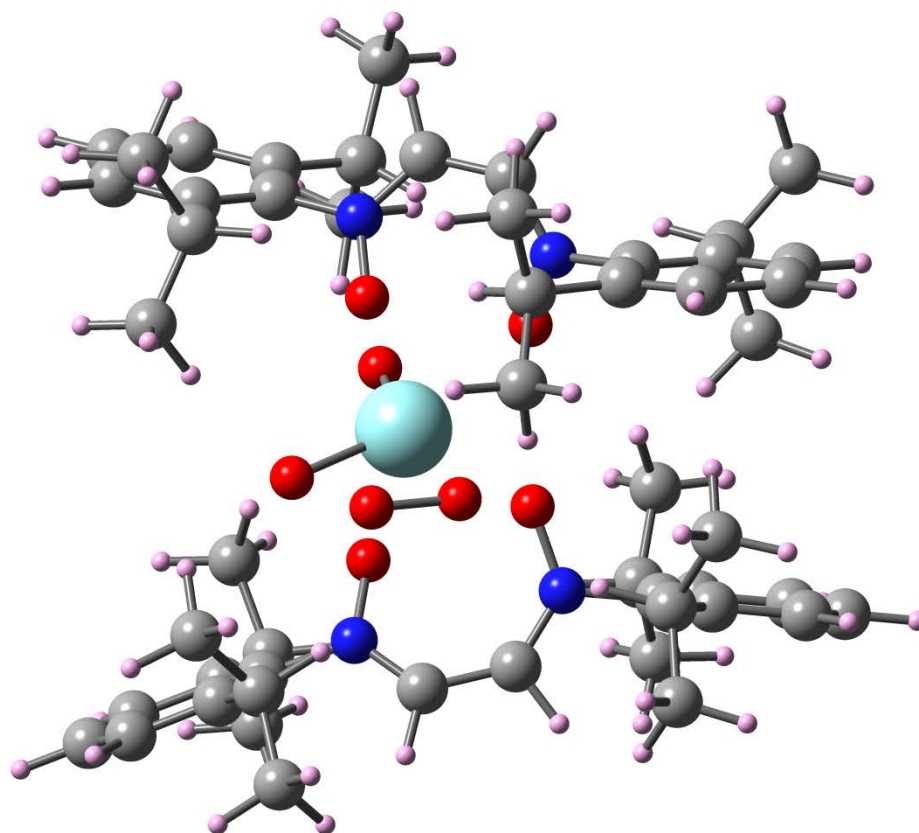


Fig. S162: ONCCNO Dioxo Complex to Oxo Ozone Complex

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2891.709228	-2890.547302	-2890.473985	-2890.659428	-142

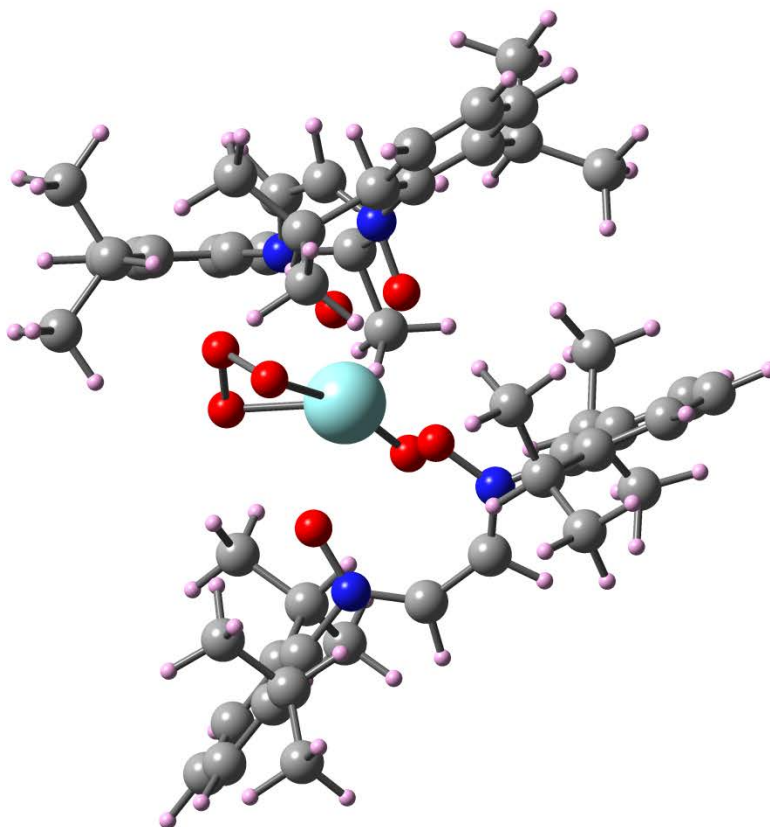
O	2.14623717	-1.44351511	0.66743605
O	-1.79247614	1.00134507	0.37440703
O	-0.30243302	-0.53822004	-1.91038315
N	-0.12605401	3.51501027	0.38289103
N	-2.67977021	1.92697814	0.03962600
N	-0.49292204	-2.89171622	0.21913702
N	2.60686920	-2.28591417	-0.26597602
C	-1.35819810	3.91438230	0.69105305
C	-2.54488719	3.23781625	0.27954402
C	0.47849804	-3.55088827	-0.42575403
C	1.83224614	-3.24710525	-0.76406306
C	1.06243808	4.19568532	0.89617807
C	1.27981310	4.26452333	2.30013718
C	2.43647119	4.94898138	2.72778421
C	3.33445825	5.51383442	1.81111314
C	3.09081124	5.41890939	0.43308103

C	1.94628715	4.76401036	-0.06356400
C	1.14307809	2.73190521	4.33459333
C	0.35842303	3.64339228	3.35848226
C	-0.41761803	4.74703236	4.12931532
C	-4.38561833	-0.81985006	2.06684416
C	-4.68863536	0.67098005	1.75934513
C	-5.88713346	1.18361509	2.59649320
C	-3.92361430	1.44819811	-0.58492905
C	-4.90309337	0.86537406	0.25536202
C	-6.09623145	0.43646103	-0.36169803
C	-6.28761449	0.58591105	-1.74556714
C	-5.28338241	1.15098809	-2.54635920
C	-4.06449931	1.59126112	-1.98615215
C	2.73119721	3.79040229	-2.27145217
C	1.70860613	4.73093436	-1.57866412
C	1.74580613	6.15594249	-2.19126317
C	-2.55052919	1.17309809	-3.99180231
C	-2.97027823	2.17611916	-2.88634122
C	-3.42511626	3.52716127	-3.50029027
C	-1.71770013	-3.64417428	0.55331804
C	-2.68682321	-3.83822329	-0.45826203
C	-3.83303729	-4.58082135	-0.10061801
C	-3.99970230	-5.07355039	1.20331709
C	-3.02535123	-4.83248837	2.18586016
C	-1.85360414	-4.10783531	1.88345414
C	-3.76175529	-2.46139219	-2.31130718
C	-2.52632219	-3.28966025	-1.88077314
C	-2.26608117	-4.44068434	-2.89060522
C	4.62213135	-1.11366308	2.69292021
C	4.54544835	-2.46343019	1.92812815
C	5.39039541	-3.55389227	2.63476320
C	4.02616231	-2.17742317	-0.61401805
C	4.95446638	-2.26607618	0.46253504
C	6.32099948	-2.16551817	0.13678101
C	6.74284149	-1.99456815	-1.19100809
C	5.80009645	-1.90675914	-2.22341117
C	4.41362233	-1.98171915	-1.96645515
C	-1.37212711	-2.81522521	4.00870931
C	-0.81211906	-3.82472029	2.97102522
C	-0.32865203	-5.12538439	3.66156228
C	3.71333228	-0.50150404	-3.91176430
C	3.43981426	-1.81656514	-3.13912024
C	3.50030527	-3.04289323	-4.08953231
H	-1.44714311	4.85712037	1.21620809
H	-3.45036726	3.82171129	0.16197001
H	0.16630601	-4.54480135	-0.72707206
H	2.31881818	-3.94346930	-1.43482411
H	2.64592020	5.01698138	3.79110729
H	4.22548932	6.02356647	2.17028417
H	3.79206629	5.86250545	-0.26762102
H	-0.35687203	2.98257023	2.86146122
H	-3.80459229	1.24174210	2.06698516

H	1.91155015	3.28174025	4.89505038
H	1.59816112	1.91798015	3.76258629
H	0.44826103	2.29308618	5.06455239
H	0.27038502	5.39907641	4.68386136
H	-1.10273709	4.28843733	4.85459937
H	-1.00943108	5.38880344	3.46052327
H	-5.22347440	-1.46387411	1.76758814
H	-4.21878832	-0.95665107	3.14331124
H	-3.48643327	-1.14883809	1.53575312
H	-6.11344347	2.23534017	2.37721918
H	-5.65682245	1.09932008	3.66642128
H	-6.79582954	0.59708105	2.40941618
H	-6.87906251	-0.01250600	0.24319802
H	-7.21746258	0.25305302	-2.20077917
H	-5.43924244	1.24291210	-3.61764728
H	0.71788006	4.31202333	-1.77844513
H	-2.07245516	2.36110318	-2.28790418
H	3.76192429	4.12872532	-2.09284416
H	2.55879420	3.78917329	-3.35679126
H	2.62475020	2.76199921	-1.90824115
H	2.74199521	6.61061052	-2.11371416
H	1.02918108	6.82883750	-1.70051013
H	1.49154212	6.10385345	-3.25821825
H	-2.13722816	0.26411802	-3.54340127
H	-1.76440414	1.61981313	-4.61350535
H	-3.39224326	0.90918507	-4.64693436
H	-4.30618633	3.39775526	-4.14317932
H	-2.61982520	3.95038030	-4.11412632
H	-3.68255028	4.26027332	-2.72362721
H	-4.60267435	-4.76389537	-0.84556707
H	-4.89260938	-5.64060841	1.45618711
H	-3.17441024	-5.20984340	3.19399924
H	-1.66874413	-2.60810820	-1.91269115
H	3.49929327	-2.78332621	1.96693115
H	-4.66753835	-3.07933523	-2.37800918
H	-3.58368828	-2.01932415	-3.29927325
H	-3.95238430	-1.64451713	-1.60726912
H	-1.36717611	-5.01720538	-2.63329120
H	-2.12549116	-4.03158931	-3.89915630
H	-3.11261024	-5.13997339	-2.92144022
H	5.64249942	-0.70620705	2.66848120
H	4.33756433	-1.25937510	3.74389229
H	3.93596130	-0.38491103	2.25128517
H	5.37733040	-4.50161335	2.07998616
H	4.98472538	-3.73875229	3.63824228
H	6.43739647	-3.24922725	2.75961821
H	7.06105556	-2.22878917	0.92886107
H	7.80403058	-1.92258115	-1.41774211
H	6.13791749	-1.75320813	-3.24406025
H	0.06156800	-3.34795925	2.51363519
H	2.42073718	-1.70865413	-2.76130021
H	-2.26499117	-3.21411525	4.50940234



H	-1.63395312	-1.86925414	3.52329927
H	-0.61483805	-2.60465420	4.77462137
H	0.45604203	-4.89001238	4.39198133
H	0.08314801	-5.83792945	2.93490523
H	-1.14301609	-5.62691145	4.20046132
H	3.59744128	0.34758803	-3.23186325
H	2.97366123	-0.39122703	-4.71498236
H	4.71404836	-0.48215304	-4.36503633
H	3.27947825	-3.98665631	-3.56935227
H	4.49440434	-3.14603924	-4.54520035
H	2.76913121	-2.92314823	-4.89938537
O	1.01083907	0.95789207	1.76265814
O	0.77423506	0.00958500	-2.62679320
O	2.09682816	0.58202504	-1.24004809
O	-0.52920104	-1.62041112	0.61512105
O	0.04377400	2.53078419	-0.51753404
Zr	0.59957105	0.33152403	0.09392301

Oxo  $\eta^2$ -Ozone Complex to Oxo  $\eta^3$ -Ozone ComplexFig. S163: ONCCNO Oxo  $\eta^2$ -Ozone Complex to Oxo  $\eta^3$ -Ozone Complex

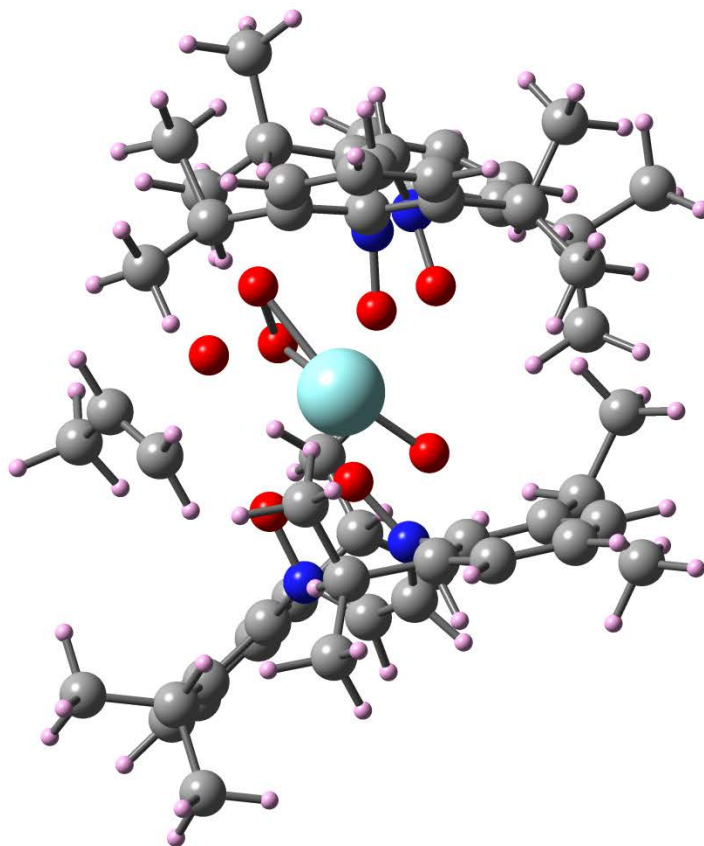
SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-2891.730444	-2890.567614	-2890.494795	-2890.679104	-94

O	-1.84483814	-0.14007401	-0.23777402
O	2.50718619	-0.65708205	-0.78202406
O	1.36132310	1.86115114	-1.22355509
N	0.61515205	-2.79432121	0.91439907
N	3.36235226	-1.30046410	0.00794300
N	-1.22776410	3.11431824	0.08548101
N	-2.87476022	0.47991804	-0.81850406
C	1.85975814	-2.82767321	1.37256911
C	3.07506723	-2.19957817	0.94752807
C	-2.32307718	2.96284223	-0.65810305
C	-3.05880123	1.79376014	-1.01185908
C	-0.42002103	-3.60842527	1.57147612
C	-0.87979807	-3.23098025	2.85820422
C	-1.86929114	-4.05342431	3.44177326
C	-2.38002218	-5.17218640	2.76707621
C	-1.91244614	-5.50060541	1.48393911

C	-0.91787607	-4.72537936	0.85416606
C	-1.53288512	-1.04904208	3.99487930
C	-0.36833503	-1.99877815	3.61455127
C	0.42852903	-2.41650719	4.87878637
C	4.14534232	2.36963118	0.95235307
C	4.42777434	0.95810207	1.53692312
C	5.08085939	1.05434808	2.93817822
C	4.77216636	-0.92073807	-0.20567502
C	5.28583840	0.15337101	0.55583404
C	6.63427353	0.50264104	0.32288002
C	7.40308658	-0.17626801	-0.63474505
C	6.83914550	-1.21149809	-1.39996810
C	5.49889442	-1.60563912	-1.20911109
C	-1.53232712	-4.74040436	-1.59604812
C	-0.43622103	-5.08684739	-0.55400304
C	-0.00586700	-6.57130752	-0.66421005
C	4.33934333	-1.96822215	-3.41926626
C	4.84355137	-2.65178520	-2.11600716
C	5.77059942	-3.84833429	-2.43597319
C	-0.66072705	4.44614134	0.33139503
C	-0.16602301	5.21408640	-0.75597806
C	0.38321403	6.47658548	-0.44079203
C	0.45218103	6.93602352	0.88074407
C	-0.03867200	6.14333849	1.93051915
C	-0.61242205	4.88074637	1.68560813
C	1.26295210	4.75873236	-2.81354421
C	-0.16985101	4.76111336	-2.22182217
C	-1.12444308	5.64582043	-3.06883224
C	-4.99677238	-1.47438011	2.12383516
C	-4.93637738	-0.29197702	1.12302609
C	-6.09613646	0.70724005	1.38080610
C	-3.95275730	-0.42890203	-1.26917409
C	-4.94755638	-0.78447406	-0.32779002
C	-5.98799348	-1.62079412	-0.78400306
C	-6.01361444	-2.08294816	-2.10943716
C	-4.99322338	-1.72695713	-3.00532023
C	-3.92596730	-0.89297207	-2.60630320
C	0.01751500	3.40391626	3.64898628
C	-1.15163009	4.05736031	2.86275622
C	-2.05253716	4.90140438	3.80060029
C	-2.28375617	-1.71783713	-4.38426733
C	-2.82565322	-0.50043704	-3.59604427
C	-3.33480226	0.59170404	-4.57602535
H	1.98801315	-3.49061027	2.22099717
H	3.95120530	-2.52924319	1.49500112
H	-2.73597621	3.88919130	-1.03812408
H	-3.97457331	2.00350215	-1.55178212
H	-2.24776017	-3.80411729	4.42942334
H	-3.14470224	-5.78574442	3.23790925
H	-2.31944618	-6.36642951	0.96906907
H	0.29280102	-1.40941211	2.96788923
H	3.45080526	0.47673604	1.66033713

H	-2.24091817	-1.51472212	4.69499436
H	-2.08235816	-0.73521306	3.09977023
H	-1.12566609	-0.14764701	4.46978934
H	-0.20129902	-2.96454023	5.59350645
H	0.81877706	-1.52401612	5.38440941
H	1.28305610	-3.06065323	4.62836735
H	5.07655739	2.93277722	0.79583806
H	3.51282427	2.93666322	1.64732412
H	3.61314128	2.30084417	-0.00362800
H	5.27981940	0.06012500	3.36119926
H	4.40559634	1.58426812	3.62189528
H	6.03038947	1.60644112	2.91348022
H	7.07610356	1.31867610	0.88795807
H	8.43917663	0.11120701	-0.79847706
H	7.44142256	-1.70779313	-2.15512916
H	0.43445003	-4.46982334	-0.79964106
H	3.95778530	-3.05285323	-1.60684412
H	-2.44481419	-5.32686541	-1.42192311
H	-1.17380209	-4.95970238	-2.61050820
H	-1.78502914	-3.67656028	-1.54047412
H	-0.85037807	-7.25460854	-0.50716404
H	0.77093606	-6.82163254	0.07024001
H	0.39512003	-6.76927950	-1.66686813
H	3.62371728	-1.17157809	-3.19007124
H	3.84036529	-2.70434821	-4.06358931
H	5.17915340	-1.53546912	-3.97990231
H	6.62751953	-3.54657127	-3.05158323
H	5.21514040	-4.60613135	-3.00362223
H	6.15764247	-4.31910033	-1.52261911
H	0.77772306	7.09339057	-1.24311909
H	0.89037807	7.90798062	1.09474808
H	0.01785300	6.51235051	2.95032622
H	-0.51100804	3.72576928	-2.28747018
H	-3.99366431	0.23447202	1.31018410
H	1.72057513	5.75725744	-2.79656421
H	1.22689909	4.41866134	-3.85644530
H	1.89063115	4.05545731	-2.25779117
H	-2.15469316	5.63161541	-2.68356220
H	-1.14445309	5.28645440	-4.10564131
H	-0.79377606	6.69285049	-3.08218924
H	-5.93891446	-2.03051716	2.03345515
H	-4.92816538	-1.09869608	3.15300224
H	-4.16940332	-2.17395017	1.96004115
H	-6.04063646	1.57166912	0.70623306
H	-6.05699248	1.07788708	2.41350318
H	-7.07237651	0.22786302	1.23107609
H	-6.77704550	-1.91395315	-0.09680301
H	-6.82538451	-2.72565521	-2.44210019
H	-5.01691538	-2.10427216	-4.02350931
H	-1.76264814	3.23657425	2.47373319
H	-1.96426715	-0.09879801	-3.05079023
H	0.71171705	4.16740932	4.02674131

H	0.56540404	2.70498020	3.00948123
H	-0.37491903	2.84578322	4.51016634
H	-2.50153519	4.25060432	4.56251535
H	-2.86432522	5.39326440	3.24841025
H	-1.48479911	5.67749746	4.32962733
H	-1.94314415	-2.50545519	-3.70300128
H	-1.42110411	-1.40049011	-4.98183338
H	-3.03288223	-2.14468616	-5.06631939
H	-3.67158728	1.49295311	-4.04594431
H	-4.17503632	0.22521002	-5.18241240
H	-2.52390019	0.88645807	-5.25337640
O	1.11434109	-0.02526200	1.55206212
O	0.20291902	1.59145612	-2.21710317
O	0.14097101	0.09328401	-2.40638618
O	-0.63940305	2.11039316	0.75500506
O	0.19892002	-2.07198116	-0.14363201
Zr	0.44195403	0.26908502	-0.15400901

Oxo  $\eta^3$ -Ozone Complex to Oxo Peroxo ComplexFig. S164: ONCCNO Oxo  $\eta^3$ -Ozone Complex to Oxo Peroxo Complex

SCF	$E_{ZP}$	H	G	imag freq ( $\text{cm}^{-1}$ )
-3009.596990	-3008.352123	-3008.274346	-3008.467672	-430

O	-1.83802100	-0.53270000	-0.38173900
O	2.56660300	-0.22960000	-0.70599900
O	0.83572400	2.14142100	-1.18464000
N	1.05055900	-2.49393800	1.20485900
N	3.47771000	-0.53408900	0.22291800
N	-1.93635900	2.77263500	0.18472800
N	-3.00028700	-0.07938500	-0.86164400
C	2.23407500	-2.17561200	1.71582600
C	3.30068400	-1.32614000	1.27832300
C	-2.95146000	2.46444400	-0.61603500
C	-3.44442200	1.17665900	-0.98984000
C	0.18352500	-3.44026300	1.92218300
C	-0.40592700	-3.03352500	3.14589000
C	-1.22095900	-3.98355800	3.80122000
C	-1.45076100	-5.25256500	3.24993200
C	-0.87170200	-5.60657900	2.02000500

C	-0.03838000	-4.70711100	1.32514500
C	-1.57872600	-0.94094000	3.98854300
C	-0.21462700	-1.64038100	3.75901800
C	0.58539700	-1.72163500	5.08607600
C	3.38166700	3.40704300	0.46441800
C	3.84317800	2.17737600	1.29134200
C	4.29577600	2.59959300	2.71305000
C	4.78675900	0.11811700	0.03612100
C	4.95403900	1.42395400	0.55436100
C	6.21481000	2.02657700	0.35143900
C	7.23954900	1.35695100	-0.33482900
C	7.02701200	0.06701000	-0.84781900
C	5.78571600	-0.58191800	-0.68234900
C	-0.53928800	-5.03592500	-1.12814800
C	0.55737100	-5.09769000	-0.03084400
C	1.24184800	-6.48697600	0.00041900
C	5.87294700	-2.02837500	-2.78215000
C	5.56587900	-1.98325200	-1.26331200
C	6.40729900	-3.04111000	-0.49994200
C	-1.57367600	4.16504100	0.46903200
C	-1.25656100	5.04983400	-0.59912200
C	-0.90651000	6.37099500	-0.24453500
C	-0.85439100	6.78330300	1.09305900
C	-1.15893800	5.87811400	2.12136100
C	-1.52922300	4.54845000	1.84064100
C	0.13585200	4.96939000	-2.73281900
C	-1.24072300	4.66866900	-2.08587000
C	-2.38449800	5.38873000	-2.85065900
C	-4.78931800	-2.27159700	2.17708200
C	-4.86502000	-1.11672200	1.14681600
C	-6.12302600	-0.24088100	1.39514100
C	-3.93207500	-1.15627400	-1.26732600
C	-4.83807000	-1.63864100	-0.29363300
C	-5.74875200	-2.63462200	-0.70547800
C	-5.73392400	-3.12453600	-2.02029800
C	-4.79911700	-2.63907600	-2.94897800
C	-3.86237800	-1.64415200	-2.59438100
C	-0.55489400	3.10259600	3.67950300
C	-1.86122500	3.60628900	3.00562300
C	-2.80758800	4.26536900	4.04178400
C	-2.31516200	-2.21993800	-4.54598700
C	-2.85623800	-1.10564200	-3.61721800
C	-3.49481000	0.02459300	-4.47285400
H	2.44757400	-2.68810400	2.64718700
H	4.16661400	-1.35255800	1.93090100
H	-3.51636500	3.30483200	-0.99833200
H	-4.40892300	1.21323900	-1.48397300
H	-1.68785100	-3.71731700	4.74565900
H	-2.08580000	-5.96353200	3.77352000
H	-1.06597900	-6.58897500	1.59878200
H	0.33382100	-0.99342000	3.06258700
H	2.96660500	1.53010000	1.40950800

H	-2.21062200	-1.48180600	4.70715900
H	-2.12461700	-0.84599300	3.04292100
H	-1.40706700	0.07033200	4.37649700
H	0.05186200	-2.30713200	5.84791500
H	0.74698500	-0.71206200	5.48471000
H	1.57085100	-2.18627600	4.94130600
H	4.21005700	4.10759200	0.28449700
H	2.59181800	3.94063800	1.00807000
H	2.96120900	3.09620500	-0.49819900
H	4.62744300	1.73555500	3.30511100
H	3.45387400	3.06614400	3.23977100
H	5.11925100	3.32665700	2.68405500
H	6.39001700	3.02885700	0.73283200
H	8.20229900	1.84248000	-0.47707200
H	7.82590200	-0.43387400	-1.38828700
H	1.31900200	-4.36045700	-0.30689400
H	4.50926200	-2.25088200	-1.14669500
H	-1.34521500	-5.75334600	-0.92157100
H	-0.10826900	-5.27980400	-2.10839200
H	-0.96946400	-4.03014400	-1.17663300
H	0.52220500	-7.29446700	0.18678100
H	2.01476400	-6.53780300	0.77848900
H	1.71732500	-6.68905200	-0.96827900
H	5.26674000	-1.29637700	-3.32701200
H	5.64673800	-3.02537100	-3.18231500
H	6.93046500	-1.81804300	-2.98680300
H	7.48112900	-2.83310300	-0.59343800
H	6.22089000	-4.04387500	-0.90666800
H	6.16214900	-3.05494100	0.57025500
H	-0.65080200	7.07489900	-1.03102400
H	-0.57120600	7.80494300	1.33537900
H	-1.11560600	6.20907500	3.15458200
H	-1.36634800	3.58831300	-2.19041500
H	-3.98148200	-0.48917800	1.31035600
H	0.39743900	6.03539900	-2.68924100
H	0.11355500	4.67039500	-3.78912400
H	0.90982800	4.37743800	-2.23482200
H	-3.37434600	5.17236100	-2.42215400
H	-2.39180300	5.06873100	-3.90070600
H	-2.25322700	6.47905300	-2.83254800
H	-5.67139500	-2.92284700	2.12267300
H	-4.74087200	-1.86164300	3.19395800
H	-3.89703900	-2.88722900	2.01587000
H	-6.16476600	0.61144000	0.70442600
H	-6.11734000	0.15259100	2.42003900
H	-7.04296000	-0.82527300	1.26171300
H	-6.46605100	-3.03135800	0.00779400
H	-6.44562800	-3.89014100	-2.32026300
H	-4.79060100	-3.04139600	-3.95710300
H	-2.37073200	2.72043000	2.61390500
H	-1.99063500	-0.68298100	-3.09162500
H	0.05592900	3.94699800	4.02946100



H	0.03029500	2.49549400	2.98063700
H	-0.80083500	2.48155000	4.55258900
H	-3.11133700	3.51759800	4.78629400
H	-3.71435300	4.66517100	3.56842100
H	-2.32060300	5.08464900	4.58630400
H	-1.92476500	-3.06710500	-3.96915000
H	-1.49735800	-1.81989200	-5.15664000
H	-3.08427700	-2.59760100	-5.23357000
H	-3.83213500	0.86531800	-3.85418700
H	-4.35817500	-0.34915900	-5.04104000
H	-2.75539500	0.41587900	-5.18262400
O	0.96762800	0.36365000	1.50877100
O	-0.37618500	1.62921200	-1.94837300
O	0.22419300	0.04035600	-2.58157700
O	-1.24212700	1.83449500	0.83592500
O	0.54635400	-2.00003800	0.05875800
Zr	0.32485800	0.31545200	-0.25140100
C	1.26980400	-0.85801800	-3.92718800
H	0.55165100	-0.76680700	-4.74253000
C	1.16094500	-1.95438300	-3.08820100
H	0.31704700	-2.63314500	-3.15068000
H	1.88610600	-2.12738700	-2.29967100
C	2.49393500	0.02066300	-4.04261400
H	3.12037100	-0.29578900	-4.89235700
H	2.18919200	1.06042500	-4.20488300
H	3.08077100	-0.01254100	-3.12053900

## TS for Ligand Cyclization

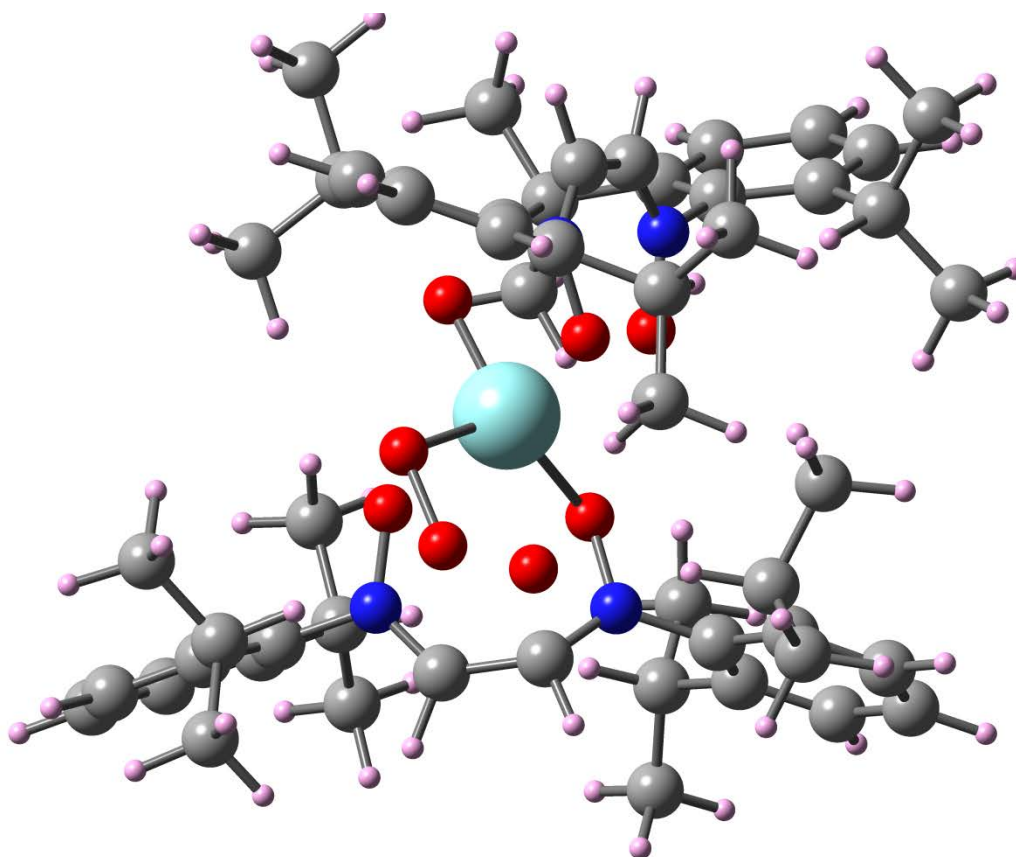


Fig. S165: ONCCNO TS for Ligand Cyclization

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2891.73866196	-2890.576002	-2890.503175	-2890.688530	-152

O	-2.33200224	0.58929400	-0.73076102
O	1.59261013	-1.12883695	-0.61467401
O	-0.87580314	0.83132409	2.14095520
N	2.71147308	1.97421534	-0.22152998
N	2.61956921	-1.01276989	-1.45406007
N	-1.35771907	-1.52772612	1.69571317
N	-3.34680431	0.50809495	0.14664005
C	3.33725215	1.42372133	-1.25169706
C	3.32917721	0.07972022	-1.74916210
C	-2.16825018	-0.53396208	2.13970320
C	-3.29288829	0.04943491	1.38512814
C	2.88768403	3.39924945	0.09012304
C	2.38817595	4.36948751	-0.81613903
C	2.61235690	5.72211763	-0.47662100
C	3.27065994	6.07970270	0.70771609
C	3.71677702	5.08849362	1.59700516

C	3.53334006	3.72138451	1.31257513
C	0.16525676	4.65415842	-1.99632912
C	1.58830890	4.04022444	-2.08230913
C	2.32915093	4.51930951	-3.35809822
C	-0.24008395	-2.35437513	-3.77244226
C	1.13498213	-1.64499401	-3.89719026
C	1.40765712	-1.21334697	-5.36032238
C	2.95513329	-2.26459898	-2.16504213
C	2.24517025	-2.55001803	-3.35470622
C	2.58602633	-3.74746010	-4.01979927
C	3.57138845	-4.60699713	-3.50866123
C	4.23162548	-4.29841407	-2.30845314
C	3.93024741	-3.11725100	-1.59807108
C	3.02411708	2.63875940	3.53248630
C	3.99595215	2.66481645	2.32098021
C	5.45893826	2.88626353	2.78042125
C	4.34967048	-3.94011604	0.76853509
C	4.62735844	-2.81918194	-0.26707799
C	6.15203155	-2.60740986	-0.46003500
C	-0.95702899	-2.68962719	2.46625422
C	0.07671809	-2.61419114	3.43782030
C	0.40731817	-3.79911021	4.13283335
C	-0.24198583	-5.01156733	3.86207633
C	-1.24288990	-5.06729438	2.87887226
C	-1.62076798	-3.91277731	2.16530520
C	2.31506821	-1.47828094	3.16545428
C	0.87263509	-1.33879000	3.72222632
C	0.89115508	-0.97846497	5.22927043
C	-4.25138631	-1.16144822	-3.09640020
C	-4.82852835	-1.24123125	-1.65606109
C	-5.89833736	-2.35455939	-1.54257608
C	-4.62737644	1.00406193	-0.39105399
C	-5.35769146	0.13347883	-1.23646106
C	-6.58237854	0.61586981	-1.74128010
C	-7.03885864	1.90511188	-1.42004407
C	-6.26893564	2.74788198	-0.60495101
C	-5.02972552	2.32293001	-0.07669997
C	-2.10537298	-4.73185640	-0.17753098
C	-2.68469006	-4.01009237	1.06879512
C	-3.98237513	-4.69839248	1.56210016
C	-3.80260354	4.54244823	-0.06238897
C	-4.18416051	3.28530512	0.76207209
C	-4.91076958	3.68133812	2.07379619
H	3.98462917	2.10219340	-1.79478710
H	4.05555827	-0.09690376	-2.53453616
H	-2.40432119	-0.62471910	3.19683828
H	-4.21866937	0.16860788	1.93783919
H	2.24401783	6.49884066	-1.14071505
H	3.42339490	7.12955274	0.94666710
H	4.21070804	5.37913568	2.51981223
H	1.42974093	2.96015835	-2.16196113
H	1.06292108	-0.73248395	-3.29440621

H	0.19312871	5.75245351	-1.96001011
H	-0.35502326	4.27868237	-1.10828005
H	-0.41282327	4.35487937	-2.88001018
H	2.46231690	5.60973361	-3.36534522
H	1.74788590	4.24577647	-4.24780629
H	3.32596303	4.06387652	-3.45133623
H	-0.27544091	-3.27738120	-4.36839430
H	-1.03262404	-1.68364412	-4.12626028
H	-0.45411495	-2.60609216	-2.72700918
H	2.37224918	-0.69641288	-5.45435140
H	0.62181503	-0.52296695	-5.69096841
H	1.41532217	-2.06920803	-6.04917743
H	2.07151531	-4.00781015	-4.94070734
H	3.81782251	-5.52330616	-4.03986828
H	4.97804257	-4.98337509	-1.91476711
H	3.94227219	1.67632537	1.85265817
H	4.21411637	-1.89386789	0.15095605
H	3.02788603	3.60253347	4.05938934
H	3.32877613	1.86102436	4.24618636
H	2.00190300	2.42893634	3.20081828
H	5.57392223	3.82104761	3.34370229
H	6.14954230	2.91967957	1.92735318
H	5.76981428	2.06605448	3.44088830
H	3.27317640	-4.07275510	0.92529711
H	4.80693950	-3.68339400	1.73292917
H	4.76931555	-4.90047609	0.44194007
H	6.63354464	-3.51279890	-0.85156503
H	6.62610356	-2.36331881	0.49955307
H	6.35951756	-1.78870778	-1.16162705
H	1.18877723	-3.76882017	4.88787741
H	0.03476824	-5.91058840	4.40836637
H	-1.73353489	-6.01356147	2.66587424
H	0.40400702	-0.50169896	3.20025828
H	-3.99469527	-1.51745224	-1.00063904
H	2.85686029	-2.29813498	3.65821131
H	2.87151320	-0.54693785	3.33234729
H	2.29435622	-1.67413896	2.08661419
H	-0.12649801	-0.88180701	5.62986045
H	1.40210007	-0.01787888	5.37490946
H	1.41934415	-1.73230501	5.82890650
H	-5.03193738	-0.88686923	-3.81890826
H	-3.83693423	-2.13431528	-3.39202922
H	-3.45063328	-0.41582813	-3.14520721
H	-6.31612243	-2.41086041	-0.52884201
H	-5.44905529	-3.32710744	-1.78269010
H	-6.72894746	-2.19662341	-2.24246814
H	-7.17954957	-0.01763227	-2.39102015
H	-7.98882277	2.25602187	-1.81644010
H	-6.62276371	3.75122805	-0.38392399
H	-2.94164812	-2.99452030	0.75034209
H	-3.24123442	2.80595313	1.03590012
H	-1.80453891	-5.76076948	0.06310804

H	-1.23168594	-4.18887931	-0.55304101
H	-2.85761604	-4.77638843	-0.97739404
H	-4.74259918	-4.67878551	0.76970609
H	-4.39503818	-4.19275746	2.44520022
H	-3.81114706	-5.74968253	1.82753717
H	-3.24656048	4.25964824	-0.96307504
H	-3.15631252	5.19383031	0.53879508
H	-4.68784163	5.11972624	-0.36318099
H	-5.16164556	2.79994304	2.67971824
H	-5.84334367	4.22579911	1.87223118
H	-4.26291856	4.33076920	2.67563224
O	0.34738994	0.97331515	-1.93211711
O	-1.08437222	2.29484419	1.89377518
O	-0.69036220	2.49358322	0.46765707
O	-0.90916604	-1.48128509	0.34948706
O	1.92232805	1.26797225	0.61644608
Zr	-0.09912607	0.52301010	-0.21271598

## 12. ONCCNO Triplet Transition States

### Oxo Peroxo Complex to Dioxo Complex

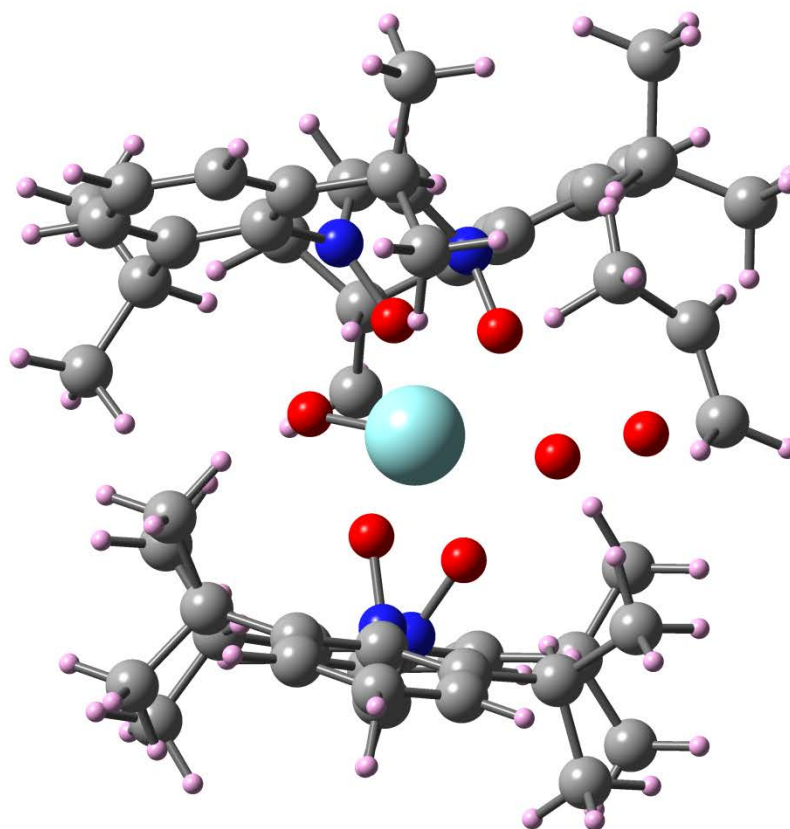


Fig. S166: ONCCNO Oxo Peroxo Complex to Dioxo Complex

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2934.459578	-2933.219375	-2933.142356	-2933.338246	-89

Zr	0.03384203	-0.04094098	0.10720703
O	-1.93186807	-0.95092418	0.05854903
O	1.76348309	1.04054821	0.87443509
O	0.44554705	0.05846305	3.49375629
O	-0.61388703	-0.01226402	2.49484822
N	-0.49461022	2.98908021	-0.73219003
N	2.53552309	1.96593733	0.18067004
N	0.37711626	-3.21066321	-0.20486599
N	-2.58382404	-2.11468132	0.39568305
C	0.77217685	3.45490933	-0.92235505
C	2.04443398	3.02398938	-0.52928102
C	-0.83654379	-3.82851933	-0.23478600
C	-2.10533292	-3.36706038	0.12311403

C	-1.61943534	3.57858218	-1.43957509
C	-1.79458534	3.28676515	-2.81804819
C	-2.88532746	3.89721012	-3.47574425
C	-3.77741758	4.73184113	-2.78642019
C	-3.59670159	4.97770416	-1.41529408
C	-2.51302946	4.41037519	-0.71513903
C	-1.65765618	1.20389900	-4.27846031
C	-0.86586120	2.34746914	-3.59529725
C	-0.02933619	3.13282125	-4.63998733
C	4.38742341	-0.90972876	-2.27724615
C	3.94809929	0.54163232	-1.96467913
C	4.18710225	1.45339741	-3.19946622
C	3.97586721	1.78353442	0.30182005
C	4.66602930	1.10426441	-0.73480103
C	6.06763143	0.98392750	-0.61001502
C	6.74601041	1.50065958	0.50422806
C	6.03379234	2.14840558	1.52636414
C	4.63395922	2.29778650	1.44759014
C	-3.43680050	3.94301309	1.59335015
C	-2.33920347	4.68134122	0.78152508
C	-2.32913657	6.19727631	1.10421111
C	4.17305818	2.40506448	3.94965632
C	3.87584611	3.02607451	2.56055822
C	4.20265904	4.54366764	2.55712922
C	1.55045139	-3.78925617	-0.82367404
C	2.61173850	-4.22734913	0.01617402
C	3.75149463	-4.77778210	-0.60286502
C	3.82719064	-4.90769010	-1.99954413
C	2.76379153	-4.47414814	-2.80372319
C	1.60655340	-3.89369617	-2.24026515
C	3.52795949	-3.04280198	2.06256818
C	2.54721449	-4.12761113	1.54387914
C	2.81969060	-5.49472620	2.22266119
C	-4.93153937	0.16913670	-1.96209412
C	-4.60246225	-1.29633739	-1.57644910
C	-5.33223825	-2.29577251	-2.51214617
C	-3.95752015	-1.94357439	0.84313808
C	-4.93936225	-1.56224243	-0.10686599
C	-6.27121835	-1.44260751	0.34224505
C	-6.60927435	-1.69457355	1.68128215
C	-5.61447330	-2.05472551	2.60392222
C	-4.26473516	-2.17247343	2.20900119
C	0.99655225	-2.26047609	-4.10053329
C	0.49415328	-3.39744221	-3.17286822
C	-0.11208868	-4.56926234	-3.99012128
C	-3.27832912	-1.65137533	4.50080837
C	-3.18904806	-2.54062939	3.23573727
C	-3.27420596	-4.04194351	3.62095330
H	0.78748779	4.33629940	-1.55551709
H	2.84643999	3.65070348	-0.90634505
H	-0.79350872	-4.85360540	-0.58972902
H	-2.87802893	-4.12768449	0.17372504

H	-3.04335446	3.70206910	-4.53338832
H	-4.61480868	5.18418810	-3.31316723
H	-4.29860668	5.61930617	-0.88858204
H	-0.17968612	1.85488515	-2.89973620
H	2.86932821	0.51444025	-1.77411612
H	-2.36357626	1.57713998	-5.03414836
H	-2.21420219	0.62529892	-3.53283525
H	-0.95615709	0.52031599	-4.77260934
H	-0.67101627	3.60068525	-5.39989838
H	0.66333191	2.45294025	-5.15298837
H	0.56434280	3.92719635	-4.16795029
H	5.44228251	-0.96684270	-2.58065117
H	3.78138740	-1.30673583	-3.09939022
H	4.24258445	-1.56660182	-1.41174709
H	3.82735015	2.47499046	-3.02166921
H	3.64763223	1.05405034	-4.06793329
H	5.25502532	1.50850048	-3.45420924
H	6.62874849	0.47462749	-1.38859809
H	7.82625253	1.39641764	0.57813407
H	6.57017937	2.54101465	2.38689220
H	-1.37505037	4.26615825	1.09134311
H	2.80383304	2.91095843	2.36666620
H	-4.43988460	4.29058905	1.31157212
H	-3.30839051	4.12694211	2.66965623
H	-3.38135743	2.86358901	1.41454713
H	-3.29023467	6.67054233	0.86531609
H	-1.54745555	6.72039342	0.53822406
H	-2.14085657	6.35565334	2.17503119
H	3.91412523	1.33863638	3.96517933
H	3.60306810	2.92548248	4.73370939
H	5.23411225	2.49384956	4.21386434
H	5.26949011	4.71914773	2.74830623
H	3.62991096	5.06538565	3.33644828
H	3.95496799	4.99949366	1.59046415
H	4.58006671	-5.11967007	0.01220402
H	4.71319273	-5.34161707	-2.45768017
H	2.83643754	-4.56954314	-3.88421728
H	1.54184939	-3.80334817	1.82703416
H	-3.52537015	-1.42759433	-1.71470011
H	4.56646759	-3.28107393	1.79324916
H	3.46935548	-2.97099498	3.15760826
H	3.27307441	-2.06465793	1.64112615
H	2.12659060	-6.26607232	1.86191217
H	2.69371859	-5.40408920	3.31020628
H	3.84257870	-5.84806018	2.03712118
H	-6.00138447	0.38792965	-1.84155212
H	-4.66726836	0.35339673	-3.01131421
H	-4.36320737	0.87075879	-1.34110608
H	-5.07580315	-3.33443957	-2.26528215
H	-5.04514023	-2.11299648	-3.55618925
H	-6.42333332	-2.19244558	-2.44160216
H	-7.04810543	-1.15679254	-0.36255801



H	-7.64362044	-1.60586961	2.00605218
H	-5.88750029	-2.23545855	3.64050430
H	-0.30681281	-2.96171623	-2.56986618
H	-2.20838299	-2.35591631	2.78554223
H	1.87764734	-2.56564506	-4.68214933
H	1.23072021	-1.37332800	-3.50152624
H	0.20347917	-1.98685312	-4.81069335
H	-0.94523777	-4.20722837	-4.60706233
H	-0.49262866	-5.36545942	-3.33569023
H	0.63103240	-5.01758433	-4.66318333
H	-3.23650518	-0.59049724	4.22582535
H	-2.43784004	-1.87746729	5.17192842
H	-4.20477618	-1.82468640	5.06402641
H	-3.14432291	-4.68653455	2.74304623
H	-4.24636802	-4.27979259	4.07400234
H	-2.48897088	-4.29708848	4.34542235
O	0.53899306	0.01291705	-1.65387710
O	-0.81972517	1.97428311	0.16082803
O	0.57845420	-2.07862610	0.57947006
C	0.49749694	1.71227218	4.26183335
H	1.55785902	1.87298726	4.42352336
C	-0.10106602	0.49928405	4.85756140
H	0.42798306	-0.02999196	5.64738944
H	-1.18304310	0.40395897	4.87467840
C	-0.30387718	2.65868120	3.45894129
H	-0.65255417	2.10698414	2.55384722
H	-1.21251127	2.98301016	3.98239433
H	0.27841381	3.52273830	3.13137526

### Oxo Complex with weakly adsorbed O<sub>2</sub> molecule to Oxo Peroxo Complex

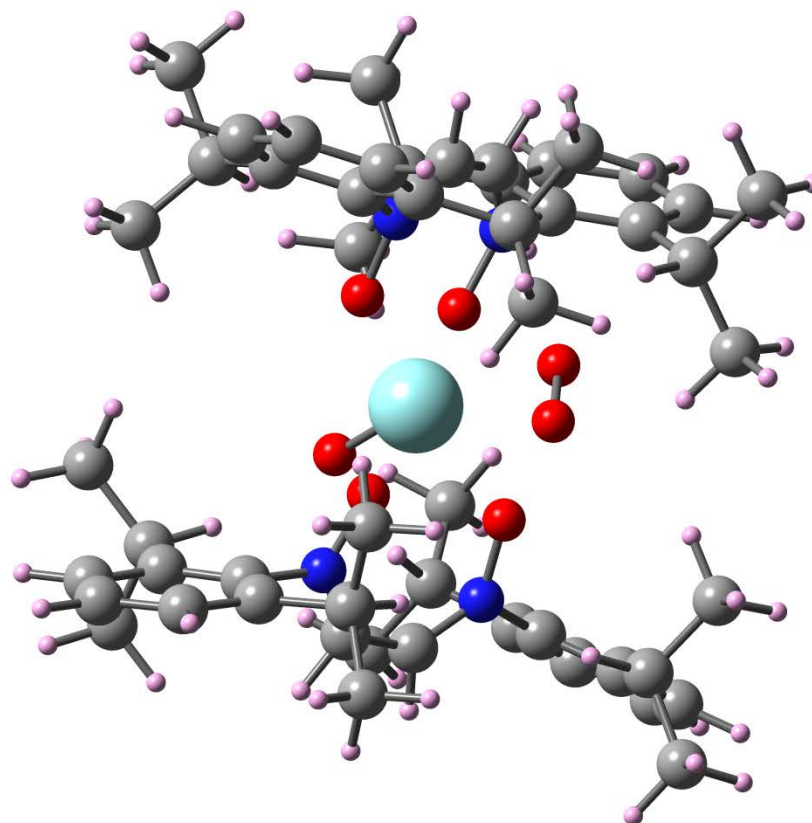


Fig. S167: ONCCNO Oxo Complex with weakly adsorbed O<sub>2</sub> molecule to Oxo Peroxo Complex

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2816.595367	-2815.438353	-2815.365177	-2815.554535	-129

Zr	0.03272346	-0.02922794	-0.23982875
O	1.53965780	1.42954576	-0.65008165
O	-1.67360994	-1.37211737	0.24333776
O	-0.20619028	-0.14550025	2.62426533
O	0.66631756	0.68215524	2.00455349
N	1.27625005	-2.97003709	0.17980048
N	-1.95332505	-2.55009835	-0.35678311
N	-1.35545287	2.86446542	0.34703481
N	1.92399411	2.66361598	-0.17449539
C	0.30774660	-3.72856007	-0.34991945
C	-1.08569892	-3.54952084	-0.57149057
C	-0.29911559	3.71108145	0.51285242
C	1.07912419	3.62983055	0.28636814
C	2.64084127	-3.49743164	0.28624553
C	3.47560626	-3.43045700	-0.85474252

C	4.78108441	-3.95057012	-0.71615408
C	5.22465502	-4.47941372	0.50574474
C	4.37524700	-4.49750424	1.62485819
C	3.05748677	-4.00308006	1.54244670
C	3.95046493	-1.64138003	-2.59600299
C	3.02353340	-2.81367704	-2.18345787
C	2.95956674	-3.88627122	-3.30273498
C	-3.08336685	-1.10499111	-4.10237536
C	-2.64220735	-2.29556382	-3.21426736
C	-2.36298800	-3.54628677	-4.09123753
C	-3.35545091	-2.72329071	-0.75554352
C	-3.68139156	-2.61041169	-2.13050349
C	-5.03618781	-2.80401873	-2.47716389
C	-6.00688373	-3.06813429	-1.49844429
C	-5.64798599	-3.14133977	-0.14269760
C	-4.30853641	-2.96906818	0.26280382
C	2.59141128	-2.82998965	3.73311015
C	2.15440210	-3.97486239	2.77895455
C	2.11942822	-5.33648601	3.51654456
C	-4.50013822	-1.77777906	2.48548104
C	-3.93579941	-3.02067061	1.74720608
C	-4.40848588	-4.33358591	2.42162239
C	-2.69820121	3.27136553	0.73349300
C	-3.05123130	3.27645637	2.10797355
C	-4.35740029	3.69604311	2.44212978
C	-5.27461996	4.07339027	1.44992479
C	-4.90173379	4.04346320	0.09633810
C	-3.60638365	3.64481838	-0.29118864
C	-2.66718665	1.72348270	4.09439854
C	-2.08142763	2.86016312	3.21888522
C	-1.68696077	4.07850867	4.09654323
C	2.99177045	2.24898379	-3.77713923
C	2.83261662	3.46699233	-2.82717127
C	3.01225984	4.80140463	-3.59310532
C	3.34298111	2.94003901	-0.35211940
C	3.78911734	3.34200459	-1.63791372
C	5.16835720	3.58646789	-1.79904959
C	6.05922502	3.43694761	-0.72298195
C	5.58895409	3.02729252	0.53390225
C	4.21897275	2.75883773	0.74611252
C	-4.08215574	2.61352587	-2.55823367
C	-3.22066399	3.63514651	-1.77260717
C	-3.32916569	5.05128360	-2.39593972
C	4.38800319	0.91718719	2.48650915
C	3.73544589	2.27421321	2.11552321
C	3.99909620	3.33448386	3.21664624
H	0.67408316	-4.69718340	-0.67173416
H	-1.56009976	-4.41322608	-1.02327760
H	-0.61346459	4.65902391	0.93724074
H	1.61756745	4.53492195	0.54765674
H	5.45623369	-3.92664786	-1.56725474
H	6.23676076	-4.86832237	0.59032630

H	4.73903318	-4.89564903	2.56803876
H	2.02142641	-2.38473474	-2.07249792
H	-1.70003051	-1.98990824	-2.74499994
H	4.98227413	-1.97539105	-2.77122878
H	3.96372030	-0.86279161	-1.82451633
H	3.57750527	-1.18724821	-3.52222108
H	3.94641655	-4.32877105	-3.49543144
H	2.60430536	-3.43053117	-4.23559250
H	2.27209509	-4.70275310	-3.04223246
H	-3.98336097	-1.33455653	-4.68936546
H	-2.27697014	-0.85640417	-4.80345890
H	-3.28411457	-0.21569077	-3.49511248
H	-1.99993150	-4.39296117	-3.49275467
H	-1.59704801	-3.31243849	-4.84156898
H	-3.26860662	-3.87536069	-4.61917091
H	-5.33317225	-2.73220525	-3.51982872
H	-7.04490459	-3.20794645	-1.79113189
H	-6.41255133	-3.33393611	0.60502193
H	1.13061296	-3.74424691	2.46264486
H	-2.84566264	-2.97198217	1.84024844
H	3.62054207	-2.98232087	4.08617831
H	1.92988680	-2.79371015	4.60846132
H	2.53301078	-1.86278208	3.22377214
H	3.09738567	-5.59414268	3.94323344
H	1.81918793	-6.15175765	2.84517493
H	1.40110334	-5.29322990	4.34537619
H	-4.12344533	-0.85629193	2.02881654
H	-4.19216228	-1.79113772	3.53914646
H	-5.59785110	-1.75893194	2.45099270
H	-5.50301507	-4.41702147	2.42615086
H	-4.07062906	-4.36027295	3.46578571
H	-4.00581865	-5.21717052	1.90913289
H	-4.65905644	3.71576105	3.48620159
H	-6.27757128	4.38794588	1.72963886
H	-5.62016841	4.33727862	-0.66502362
H	-1.16794444	2.46841168	2.76311412
H	1.80472211	3.43836909	-2.44943703
H	-3.57456591	2.04404166	4.62420273
H	-1.92738256	1.41138891	4.84183712
H	-2.91228462	0.84736071	3.48412541
H	-1.23288400	4.87815452	3.49631160
H	-0.96058701	3.77398584	4.86117592
H	-2.56197493	4.50051528	4.60892733
H	4.01490058	2.18686878	-4.17359542
H	2.30069433	2.33889767	-4.62597988
H	2.76048507	1.31993998	-3.24645119
H	2.90158886	5.66632960	-2.92599207
H	2.25629372	4.88157819	-4.38539567
H	3.99776200	4.86884276	-4.07237310
H	5.54750105	3.89570157	-2.76937932
H	7.11926755	3.63405620	-0.86692834
H	6.29004860	2.90498363	1.35564124

H	-2.18093528	3.30673779	-1.85940794
H	2.65643800	2.10053622	2.07164933
H	-5.14623094	2.88591292	-2.54005586
H	-3.97649895	1.61215329	-2.12609182
H	-3.76098290	2.57305364	-3.60760080
H	-3.00085886	5.02864253	-3.44364917
H	-2.70162441	5.77330659	-1.85737828
H	-4.36214551	5.42368886	-2.37706847
H	4.16306730	0.15704924	1.72937114
H	3.99429220	0.56336034	3.44814648
H	5.47965444	1.00277240	2.57605906
H	3.51551650	4.29058111	2.97612514
H	5.07326072	3.52499915	3.34496666
H	3.60190159	2.98522395	4.17862783
O	0.14934987	-0.84182680	-1.87367336
O	1.11782678	-1.72978666	0.69329172
O	-1.28702631	1.64457545	-0.30802796

### Transition State for Forming the Octahedral Complex with Transferred Allylic H from the Adsorbed PO Octahedral Complex

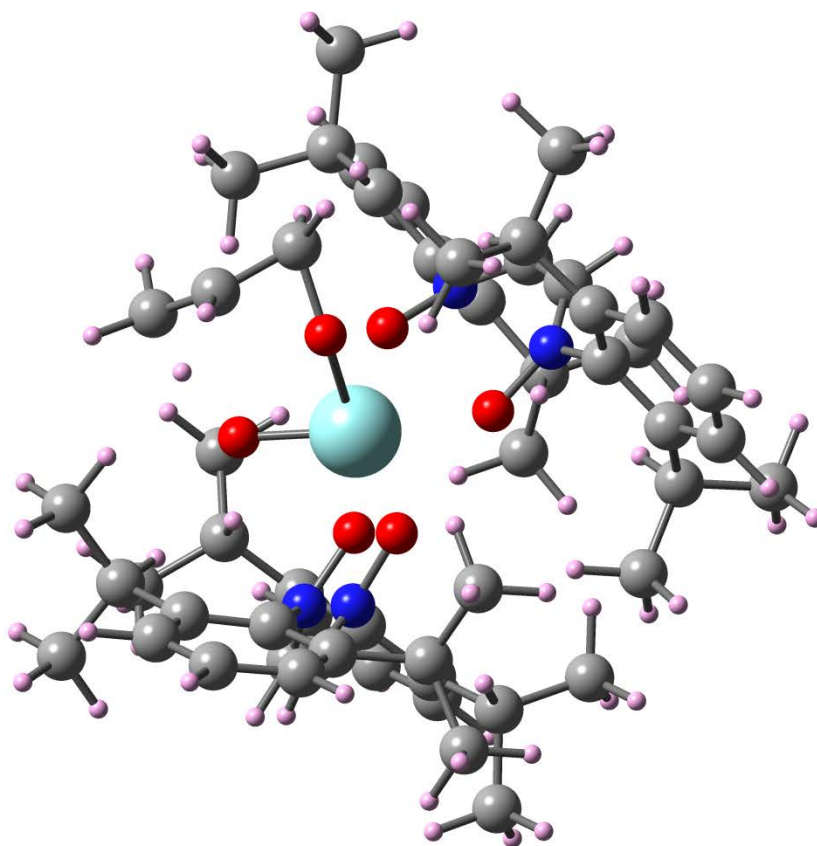


Fig. S168: ONCCNO Transition State for Forming the Octahedral Complex with Transferred Allylic H from the Adsorbed PO Octahedral Complex

SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-2859.350637	-2858.115434	-2858.039771	-2858.234248	-526
O	0.40388986	-1.32701345	0.78825410	
O	1.75955328	0.85977494	-1.13290121	
O	-0.00159073	-1.33379737	-2.18685951	
N	0.04929435	2.97422590	0.78887248	
N	2.71835181	1.67057316	-0.54109707	
N	-2.78531625	-1.80316915	-0.18340551	
N	0.21035990	-2.69022382	0.93179327	
C	1.30685766	3.46412471	0.57930046	
C	2.46084849	2.87087870	0.06146331	
C	-2.24370301	-2.96013091	0.29323260	
C	-0.97589221	-3.33627363	0.74837915	
C	-0.97704744	3.79413261	1.41717945	
C	-1.70330254	4.72459025	0.63400919	
C	-2.68683969	5.50088349	1.28470099	

C	-2.94823819	5.33756130	2.65305888
C	-2.22926878	4.38996495	3.40047880
C	-1.22758793	3.59989482	2.80124874
C	-2.76321637	4.56057076	-1.66783846
C	-1.47562748	4.89638622	-0.87067463
C	-0.96631766	6.32276016	-1.20644339
C	3.41584020	0.76669710	-4.24751606
C	3.77737891	1.91613401	-3.27005862
C	4.48569272	3.07878639	-4.01087688
C	4.09022588	1.25864029	-0.79109438
C	4.61295698	1.37922634	-2.10589266
C	5.94566269	0.97577388	-2.32467970
C	6.73415071	0.48401371	-1.27194185
C	6.19549563	0.37510670	0.01858417
C	4.85960150	0.74499828	0.28576826
C	-1.39500730	1.34047273	3.92376249
C	-0.47329395	2.55338454	3.62568831
C	0.11294974	3.14514748	4.93199898
C	4.53601435	-0.83075019	2.26771364
C	4.29755388	0.59155912	1.70249987
C	4.89709015	1.66213380	2.65468830
C	-4.17241531	-1.75576179	-0.61503700
C	-4.52379154	-2.32573691	-1.86611706
C	-5.88572273	-2.29311202	-2.23669585
C	-6.84649916	-1.68694957	-1.41271057
C	-6.46377934	-1.10016245	-0.19560402
C	-5.12058054	-1.12617821	0.23273211
C	-3.59827527	-2.38971271	-4.24073157
C	-3.48942938	-2.95964515	-2.80349778
C	-3.63183384	-4.50555288	-2.83159202
C	1.28423853	-1.87559379	4.75889549
C	0.56618075	-2.88848590	3.83101430
C	-0.17406691	-3.96915396	4.66302292
C	1.36696764	-3.41625483	1.43336541
C	1.54107905	-3.52582356	2.83606180
C	2.65296299	-4.25973262	3.29961002
C	3.55611659	-4.84542021	2.39744234
C	3.36859519	-4.70197480	1.01325438
C	2.27165673	-3.97799658	0.49772395
C	-4.80860835	1.07143815	1.44578789
C	-4.72241970	-0.47374346	1.55887574
C	-5.57375311	-0.99569050	2.74411581
C	3.32693361	-3.24180638	-1.70275537
C	2.07360964	-3.83761468	-1.01410422
C	1.69529767	-5.20369487	-1.64677343
H	1.42556694	4.48855852	0.91643529
H	3.35813425	3.47390610	0.16647173
H	-2.96280127	-3.77235630	0.28524900
H	-0.90102635	-4.38729535	1.00842902
H	-3.25847549	6.22767606	0.71279313
H	-3.71388883	5.94136259	3.13491886
H	-2.44550829	4.26660504	4.45846845

H	-0.70733402	4.18250471	-1.18479624
H	2.83852463	2.30390053	-2.86072157
H	-3.60112181	5.20526966	-1.37287312
H	-3.05530271	3.51678837	-1.50572429
H	-2.59529877	4.70943996	-2.74398206
H	-1.70633693	7.08642543	-0.93312519
H	-0.77075268	6.41707140	-2.28326583
H	-0.03616060	6.55167621	-0.67021742
H	4.32030494	0.31216660	-4.67374771
H	2.80966942	1.14883509	-5.08147228
H	2.84864876	-0.01236358	-3.72679990
H	4.73991257	3.89576311	-3.32320025
H	3.82970895	3.48228652	-4.79422150
H	5.41245480	2.74745508	-4.49684419
H	6.37177536	1.05440676	-3.32167748
H	7.76278021	0.18361146	-1.45805842
H	6.81182678	-0.01520774	0.82394387
H	0.35942082	2.17375238	3.02527030
H	3.21422087	0.74508736	1.66117965
H	-2.26839190	1.64288894	4.51874298
H	-0.84356198	0.57771489	4.48973729
H	-1.74048004	0.89051176	2.98721313
H	-0.67502204	3.48018426	5.61953366
H	0.76787545	4.00208561	4.72667201
H	0.70359015	2.38171900	5.45570938
H	4.10825942	-1.59642235	1.61158919
H	4.06034240	-0.92716260	3.25183094
H	5.60540415	-1.04562323	2.39528175
H	5.98606738	1.54680022	2.74068790
H	4.46589773	1.56283008	3.65978712
H	4.69372467	2.67959672	2.29722343
H	-6.19335722	-2.73234325	-3.18223301
H	-7.88962420	-1.66691581	-1.72050992
H	-7.21486871	-0.62562591	0.43063218
H	-2.48577108	-2.71658856	-2.43819847
H	-0.18470874	-2.32729236	3.26545328
H	-4.55012597	-2.65778097	-4.71777317
H	-2.78823225	-2.79295841	-4.86211842
H	-3.51729369	-1.29578497	-4.23518246
H	-3.51905470	-4.93995998	-1.83027060
H	-2.86251904	-4.94649774	-3.47906709
H	-4.61559550	-4.80500801	-3.21819313
H	2.06189045	-2.36088475	5.36346193
H	0.56240978	-1.41671420	5.44803218
H	1.75226525	-1.07757094	4.17094146
H	-0.71983122	-4.66651561	4.01462250
H	-0.89720397	-3.49833369	5.34220896
H	0.52721790	-4.55575953	5.27128412
H	2.81421164	-4.37220266	4.36910348
H	4.40727194	-5.40921962	2.77303103
H	4.07986548	-5.15267621	0.32576962
H	-3.67541973	-0.71817975	1.76293244



H	1.25133199	-3.14240154	-1.21148383
H	-5.83517889	1.39816699	1.22881230
H	-4.14930492	1.43159271	0.64901565
H	-4.49270683	1.54126976	2.38635168
H	-5.21457770	-0.55628570	3.68425517
H	-5.51148858	-2.08828881	2.83193661
H	-6.63284941	-0.72580620	2.63660575
H	3.57980082	-2.26377538	-1.27702652
H	3.12396836	-3.09865170	-2.77159188
H	4.20301405	-3.89867471	-1.60824924
H	0.78197018	-5.61396105	-1.19569838
H	2.49741302	-5.94416062	-1.51900000
H	1.51419203	-5.07934242	-2.72234892
O	-0.98833249	1.40813390	-2.30198844
O	-2.13779391	-0.57835330	-0.18422709
O	-0.26730085	1.65136363	0.64701967
Zr	-0.16946113	-0.03428508	-0.83865690
C	-0.46628997	2.14844635	-3.45225195
H	-0.89960484	3.14610733	-3.54603809
C	-1.16322179	1.02019040	-4.12173452
H	-2.24121670	1.13046828	-4.21426543
C	-0.50739553	-0.19323356	-4.56925632
H	-0.27868972	-0.84498753	-3.58618983
H	-1.13974214	-0.81652877	-5.20580080
H	0.48613113	-0.02781176	-4.99974715
H	0.62438309	2.14986173	-3.50982774

### 13. Ground State with Isopropyl Groups Replaced by H Atoms

#### NCCN Bisperoxo Complex

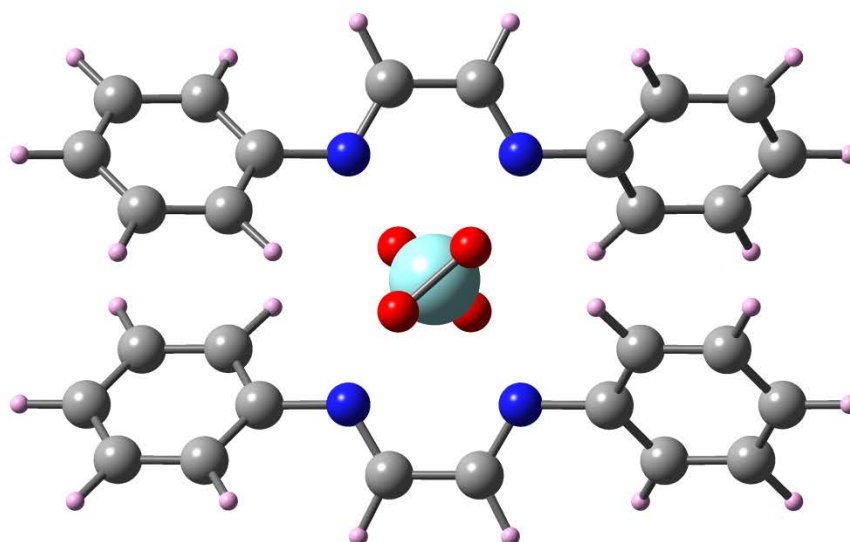


Fig. S169: NCCN Bisperoxo Complex

SCF	$E_{ZP}$	H	G
-1647.703204	-1647.235390	-1647.201535	-1647.301497

Zr	0.00136514	-0.00001783	0.00004505
O	-0.57572846	0.51008626	-1.94817790
O	0.57498123	-0.50660102	-1.95055897
O	0.57490489	0.50638357	1.95069114
O	-0.57591880	-0.51011324	1.94817759
N	-1.36586723	-1.98266952	-0.30880050
N	1.36551270	-1.98407042	0.30622596
N	1.36572705	1.98395972	-0.30627737
N	-1.36569516	1.98272220	0.30867471
C	-0.71552010	-3.10186553	-0.15354083
C	0.71405955	-3.10260036	0.15041408
C	0.71432215	3.10252265	-0.15046373
C	-0.71525515	3.10187610	0.15345676
C	-2.77206438	-1.99299722	-0.58519101

C	-3.64782240	-2.86824595	0.09950613
C	-5.01937213	-2.85471467	-0.20307466
C	-5.51742224	-1.98068873	-1.19023050
C	-4.63873273	-1.10746408	-1.86263118
C	-3.26795207	-1.09717263	-1.55859345
C	2.77173859	-1.99622356	0.58309998
C	3.26823872	-1.10173004	1.55739345
C	4.63891432	-1.11383026	1.86189458
C	5.51683623	-1.98748458	1.18906137
C	5.01816655	-2.86013907	0.20100276
C	3.64671495	-2.87184348	-0.10209376
C	2.77197066	1.99607826	-0.58308499
C	3.26844434	1.10188722	-1.55767434
C	4.63912435	1.11402075	-1.86215742
C	5.51708743	1.98739937	-1.18902310
C	5.01844817	2.85976511	-0.20069388
C	3.64699113	2.87145949	0.10236980
C	-2.77187570	1.99313602	0.58511244
C	-3.26781984	1.09705312	1.55824763
C	-4.63858522	1.10738831	1.86234663
C	-5.51721041	1.98092566	1.19026925
C	-5.01911187	2.85521065	0.20336435
C	-3.64757847	2.86868122	-0.09928370
H	-1.20581132	-4.07099370	-0.27009253
H	1.20350411	-4.07216716	0.26669286
H	1.20379874	4.07206823	-0.26678699
H	-1.20547788	4.07103429	0.27003043
H	-5.69648672	-3.51412372	0.33442909
H	-6.57933276	-1.97372075	-1.42411382
H	-5.02053216	-0.42988624	-2.62195502
H	5.02126260	-0.43731866	2.62189276
H	6.57867224	-1.98186104	1.42331596
H	5.69474472	-3.51987726	-0.33676657
H	5.02142915	0.43780533	-2.62244081
H	6.57892312	1.98181843	-1.42328140
H	5.69505688	3.51927944	0.33731195
H	-5.02042713	0.42958353	2.62144660
H	-6.57911183	1.97398783	1.42419352
H	-5.69617964	3.51486482	-0.33389693
H	-2.56319257	-0.44000131	-2.06496913
H	-3.26723230	-3.51220926	0.88886514
H	2.56424009	0.44469135	-2.06479514
H	3.26589341	3.51412371	0.89254054
H	-2.56312697	0.43959821	2.06434815
H	-3.26695941	3.51284610	-0.88846437
H	3.26556663	-3.51474642	-0.89204615
H	2.56411455	-0.44414388	2.06410931

## 14. Transition State with Isopropyl Groups Replaced by H Atoms

### NCCN Bisperoxo Complex to Oxo Peroxo Complex

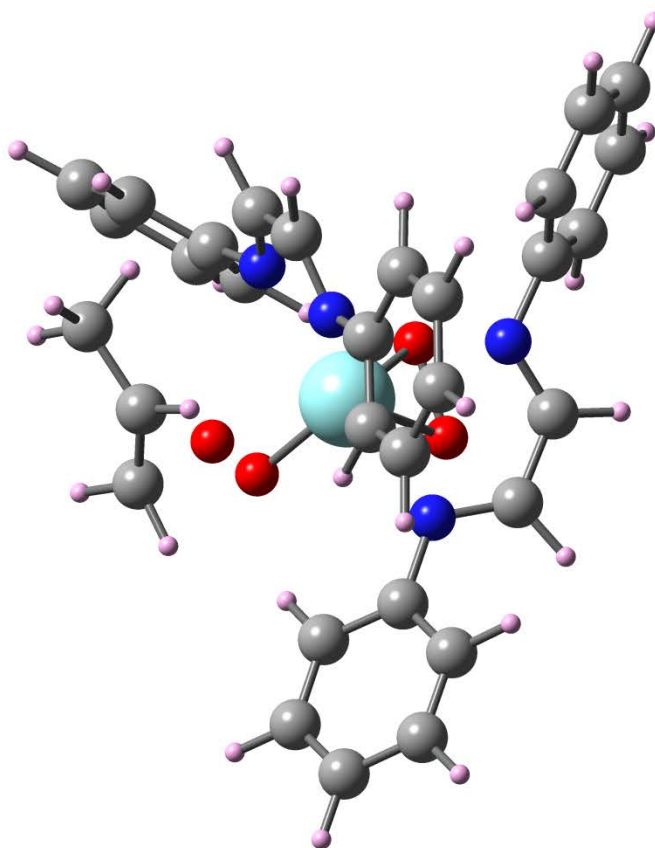


Fig. S170: NCCN Bisperoxo Complex to Oxo Peroxo Complex

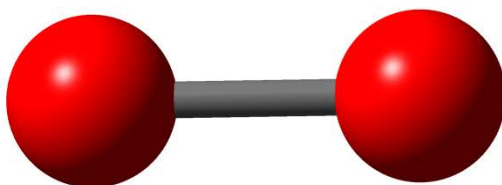
SCF	E <sub>ZP</sub>	H	G	imag freq (cm <sup>-1</sup> )
-1765.542977	-1764.995526	-1764.956349	-1765.069641	-460

Zr	-0.25864003	-0.52045117	-0.67285859
O	-0.20897244	-2.42739703	-1.05014804
N	0.06550936	2.11805338	-1.02973216
N	1.94099725	-0.02755768	-1.49344359
N	-2.23224252	-0.71218942	0.67591930
N	0.11311482	0.55665700	1.54747396
C	0.82460316	2.05584230	-2.09485372
C	1.90802876	1.07329732	-2.20474404
C	-2.19764453	-0.06050717	1.81880463
C	-1.00304410	0.63568021	2.24307530
C	-0.93394924	3.14063494	-0.93507845
C	-1.89236599	3.33851994	-1.95706544
C	-2.85203716	4.35581995	-1.82567897

C	-2.86747196	5.18468867	-0.68524184
C	-1.91634480	4.98155458	0.33341883
C	-0.95716741	3.95972108	0.21434822
C	3.09499341	-0.88203081	-1.54581598
C	2.91299996	-2.28283546	-1.53461143
C	4.03645246	-3.12351314	-1.60871611
C	5.33778630	-2.58573623	-1.67349816
C	5.51612560	-1.18819637	-1.65967073
C	4.40075825	-0.33608239	-1.59371674
C	-3.34598332	-1.55537561	0.36162828
C	-4.06717618	-2.22228597	1.38667198
C	-5.14902419	-3.05270094	1.06094540
C	-5.52456984	-3.23086618	-0.28662455
C	-4.79658591	-2.58352580	-1.30333235
C	-3.70521005	-1.75761906	-0.99103338
C	1.28708184	1.24373360	2.00532131
C	1.22766043	2.41130023	2.80661633
C	2.40899327	3.03903132	3.23354965
C	3.66565170	2.51837679	2.86789212
C	3.72728831	1.36113353	2.06674222
C	2.54993829	0.73113098	1.63614624
H	0.75320807	2.78616388	-2.90528124
H	2.69675967	1.29401089	-2.92838591
H	-3.05858891	-0.03042995	2.48741272
H	-1.05407926	1.16532050	3.19549610
H	-3.59613790	4.49250250	-2.60687297
H	-3.61284755	5.97062885	-0.58969180
H	-1.91779264	5.61933305	1.21483279
H	3.89226671	-4.20096593	-1.61946624
H	6.20072739	-3.24512227	-1.72575620
H	6.51725884	-0.76481159	-1.69095127
H	-5.68492584	-3.57423761	1.85038514
H	-6.36093586	-3.87850790	-0.53840661
H	-5.07051466	-2.72686621	-2.34523822
H	2.34820198	3.93858391	3.84124027
H	4.57830435	3.00721722	3.19868558
H	4.68949694	0.94315101	1.78193521
O	-0.45995353	-0.02611024	-2.76811138
O	-1.70387800	0.23118063	-1.97533611
C	1.01152854	-2.27259808	2.88004328
H	1.67043776	-1.42794786	3.06449356
C	1.28942451	-3.11867594	1.78241313
H	2.28673863	-3.09199984	1.34421972
O	0.32560232	-2.23853233	0.68781465
H	0.80704231	-4.09418937	1.73730131
C	-0.20327607	-2.40442271	3.74401256
H	-0.90338351	-1.56031382	3.57410083
H	-0.74953590	-3.33115730	3.53319897
H	0.05207408	-2.37843612	4.81464371
H	0.26954468	2.84528404	3.07970116
H	2.59990040	-0.17113998	1.03926742
H	-3.75251524	-2.13748409	2.42370772

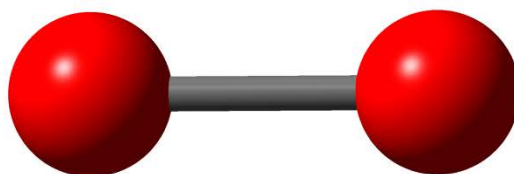
H	-3.14260810	-1.24801867	-1.76720664
H	-0.20573567	3.80886137	0.98232946
H	-1.91121452	2.65310870	-2.79880608
H	4.54282798	0.74157936	-1.54845713
H	1.90280335	-2.68490265	-1.49104867

## 15. Molecules and Ligands

O<sub>2</sub> TripletFig. S171: O<sub>2</sub> Triplet

SCF	E <sub>ZP</sub>	H	G
-150.3147399	-150.311445	-150.308134	-150.331506

O	0.00000000	0.00000000	0.63422700
O	0.00000000	0.00000000	-0.63422700

O<sub>2</sub> SingletFig. S172: O<sub>2</sub> Singlet

SCF	E <sub>ZP</sub>	H	G
-150.2522943	-150.249039	-150.245728	-150.268067

O	0.00000000	0.00000000	0.63532800
O	0.00000000	0.00000000	-0.63532800

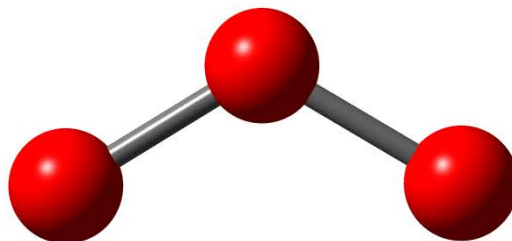
**Ozone**

Fig. S173: Ozone

SCF	E <sub>ZP</sub>	H	G
-225.3954689	-225.389087	-225.385114	-225.412382

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

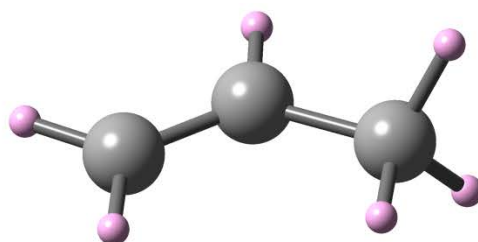
**Propene**

Fig. S174: Propene

SCF	E <sub>ZP</sub>	H	G
-117.8913037	-117.811106	-117.806069	-117.836174

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



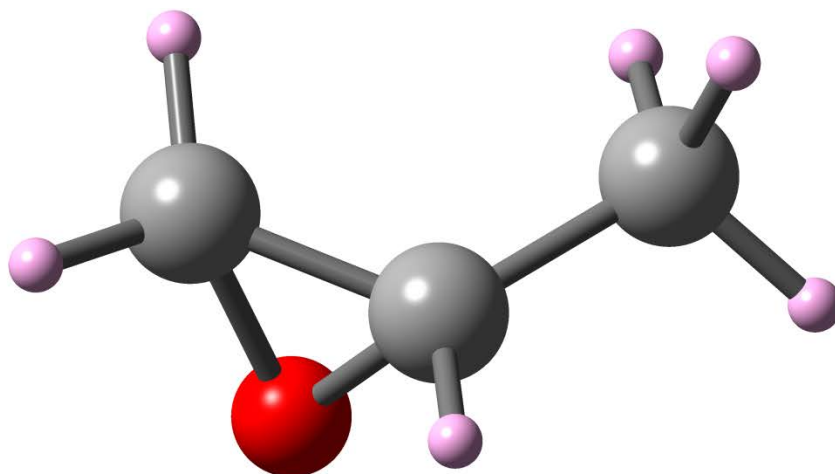
**Propylene Oxide**

Fig. S175: Propylene Oxide

<b>SCF</b>	<b>E<sub>ZP</sub></b>	<b>H</b>	<b>G</b>
-193.0740751	-192.988641	-192.983202	-193.015134

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

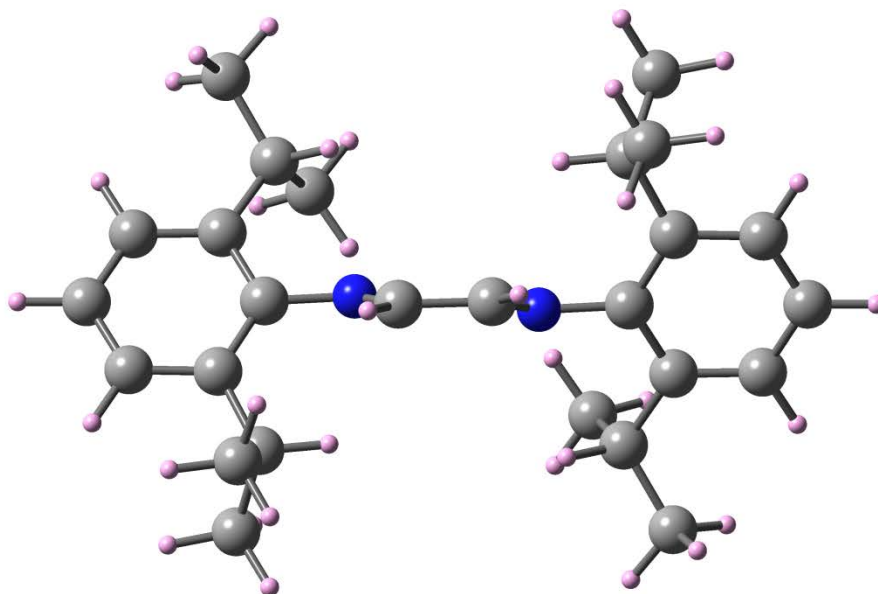


Fig. S176: NCCN Ligand

SCF	E <sub>ZP</sub>	H	G
-1121.7493672	-1121.184542	-1121.153078	-1121.248209

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

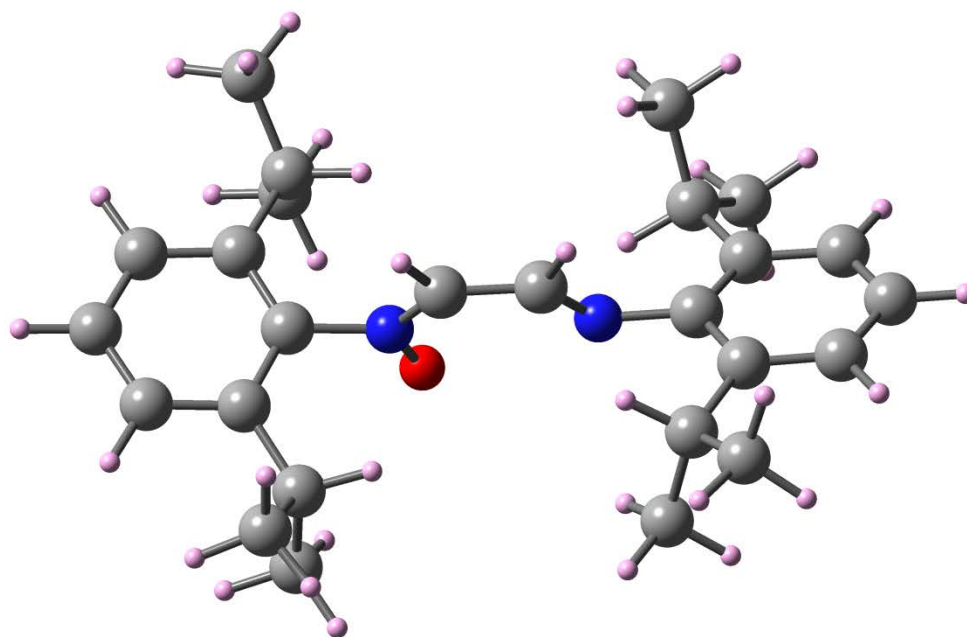


Fig. S177: NCCNO Ligand

SCF	E <sub>ZP</sub>	H	G
-1196.9200136	-1196.350300	-1196.317905	-1196.416154

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

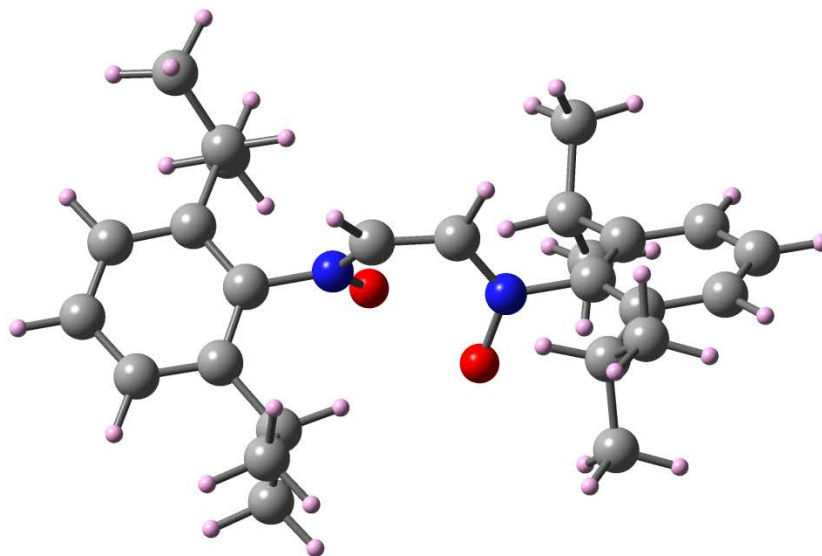


Fig. S178: ONCCNO Ligand

SCF	E <sub>ZP</sub>	H	G
-1272.0941843	-1271.519822	-1271.486587	-1271.585349

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

## 16. Calculations Using 6-311++G\*\* Basis Sets

### NCCN Bare Complex (puckered conformation)

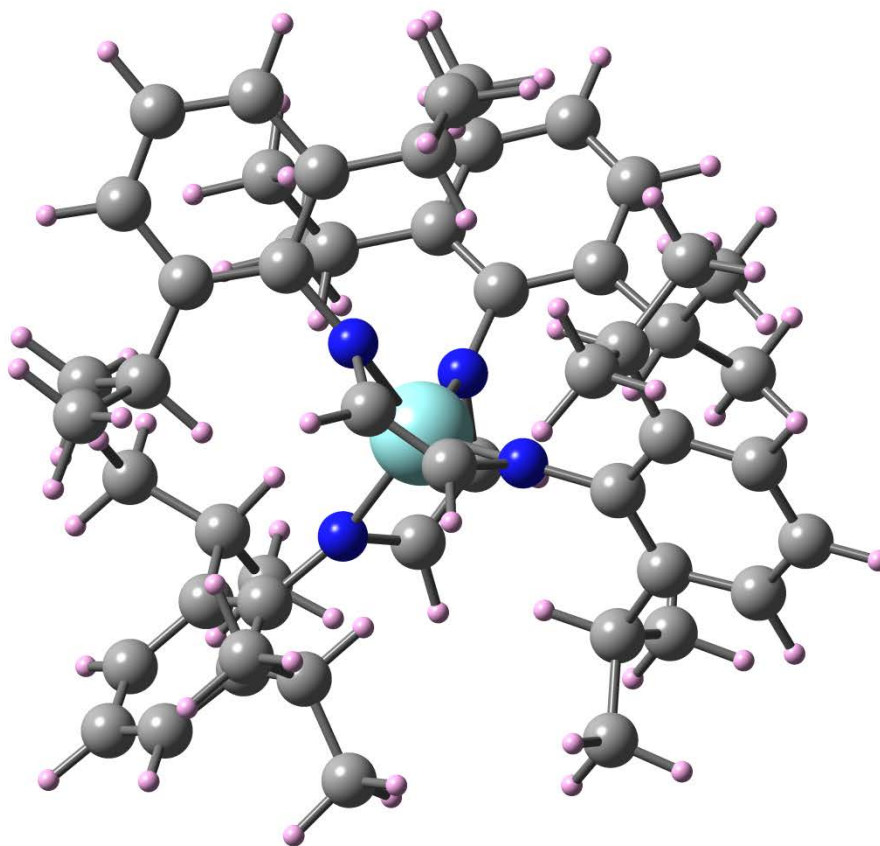


Fig. S179: NCCN Bare Complex (puckered conformation)

<b>SCF</b>
-2291.68050546

Zr	0.00067000	-0.30748500	-0.00049100
N	1.79452400	-1.26557500	0.64042000
N	0.09357500	0.77262900	1.78900600
N	-0.09255300	0.77782000	-1.78672400
N	-1.79641400	-1.25978600	-0.64123900
C	1.31631500	-1.32706800	1.95705300
C	0.50746600	-0.35823600	2.50885300
C	-0.50933400	-0.35071700	-2.50872200
C	-1.31937000	-1.31931000	-1.95832400
C	3.01541700	-1.93754100	0.32734100
C	4.22317700	-1.53677500	0.96251300
C	5.40890900	-2.20202700	0.64405700
C	5.44383800	-3.22109600	-0.29814700
C	4.26610600	-3.59865600	-0.92428600
C	3.04279400	-2.98901200	-0.62429000



C	4.48852700	-0.93069500	3.41067800
C	4.28860300	-0.39813000	1.97796600
C	5.38539200	0.62863300	1.63639200
C	-0.37477100	1.93307600	2.48644200
C	-1.68420000	1.97318100	3.02293500
C	-2.10951300	3.14156100	3.66277600
C	-1.28283300	4.25131200	3.77209300
C	-0.00003800	4.20071300	3.24330300
C	0.48024700	3.05382600	2.60483800
C	1.58286000	-5.02610900	-0.97061400
C	1.79963200	-3.53980500	-1.31478400
C	1.84917400	-3.35116100	-2.84188900
C	0.37514800	1.93915600	-2.48304400
C	-0.48044800	3.05959000	-2.60025900
C	-0.00085800	4.20720700	-3.23797000
C	1.28178200	4.25876300	-3.76704900
C	2.10904700	3.14931200	-3.65880500
C	1.68443500	1.98026000	-3.01977600
C	-2.04805100	4.00993600	-0.85003100
C	-1.90325100	3.06024500	-2.05395300
C	-2.93511300	3.39946200	-3.14529800
C	-3.01604100	-1.93401000	-0.32871000
C	-3.04207600	-2.98385800	0.62475100
C	-4.26346200	-3.59886400	0.92119200
C	-5.44091500	-3.22710200	0.29093800
C	-5.40766200	-2.20809100	-0.65134400
C	-4.22379900	-1.53801300	-0.96680500
C	3.93585500	1.19246000	-2.15432500
C	2.65890100	0.81157600	-2.92512200
C	3.01138300	0.24947800	-4.31562200
C	-3.01250800	0.24209500	4.31698500
C	-2.65855500	0.80449300	2.92697500
C	-3.93470600	1.18602300	2.15514200
C	-1.86096000	-3.35866700	2.84781500
C	-1.79847300	-3.52853300	1.31910800
C	-1.56327100	-5.00802100	0.95827900
C	-4.48824600	-0.93151300	-3.41517700
C	-4.29154300	-0.39919300	-1.98197200
C	-5.39204500	0.62380100	-1.64090000
C	2.93465100	3.39624500	3.14980900
C	1.90305700	3.05573600	2.05861600
C	2.04690800	4.00534600	0.85448600
H	1.48030200	-2.23884900	2.52863500
H	0.06322900	-0.55233700	3.48235000
H	-0.06679100	-0.54318400	-3.48325500
H	-1.48558400	-2.22947200	-2.53178300
H	6.32910700	-1.90537700	1.13414000
H	6.37826800	-3.71553600	-0.53944000
H	4.29041400	-4.40126600	-1.65298600
H	3.33528000	0.12864900	1.95014200
H	3.69440300	-1.62417300	3.69586600
H	4.49301700	-0.10654100	4.13050700

H	5.44172500	-1.46075100	3.50142900
H	6.38726000	0.19647600	1.70696200
H	5.34455600	1.46668000	2.33726700
H	5.26281600	1.02343700	0.62551100
H	-3.11104100	3.18442400	4.07637400
H	-1.63609600	5.14977000	4.26616500
H	0.64406400	5.06844400	3.33146200
H	0.93205800	-2.99235100	-0.93959700
H	2.39528900	-5.64568300	-1.36000900
H	0.64997300	-5.39045400	-1.40962900
H	1.53505400	-5.18224200	0.10924300
H	1.97213400	-2.30181900	-3.11529000
H	0.92704000	-3.71677500	-3.30385900
H	2.68189800	-3.90812600	-3.28106000
H	-0.64540000	5.07470200	-3.32533200
H	1.63453300	5.15773800	-4.26054900
H	3.11040900	3.19296500	-4.07274200
H	-2.11654300	2.04989100	-1.70296700
H	-1.83864100	5.04570900	-1.13441000
H	-1.36423700	3.74212800	-0.04111800
H	-3.06733600	3.97376900	-0.45375900
H	-3.94843600	3.34248500	-2.73852600
H	-2.86598500	2.70632500	-3.98781300
H	-2.79643300	4.41196600	-3.53498500
H	-4.28640200	-4.40108400	1.65037500
H	-6.37383400	-3.72568200	0.52954700
H	-6.32773600	-1.91523500	-1.14396900
H	2.17439100	0.01297100	-2.36038400
H	4.51741500	1.94768200	-2.69078100
H	4.57234900	0.31465600	-2.01453800
H	3.69336100	1.59675300	-1.16898800
H	2.11689600	-0.06031100	-4.86271100
H	3.67238200	-0.61698700	-4.22240400
H	3.52677800	0.99681500	-4.92583300
H	-2.17370400	0.00596800	2.36246900
H	-2.11861600	-0.06825400	4.86474300
H	-3.67387200	-0.62400300	4.22290700
H	-3.52815800	0.98937700	4.92703400
H	-4.51648100	1.94121700	2.69142100
H	-4.57131800	0.30847100	2.01440600
H	-3.69119700	1.59064900	1.17019900
H	-0.93394900	-2.96712200	0.95771700
H	-2.00017600	-2.31436800	3.13254800
H	-0.93691700	-3.71711300	3.31153800
H	-2.68848300	-3.93210500	3.27536200
H	-2.37410000	-5.64004900	1.33081300
H	-0.63146500	-5.36918600	1.40222800
H	-1.50292700	-5.14939800	-0.12294100
H	-3.33999200	0.13071900	-1.95271800
H	-3.69172600	-1.62239900	-3.69998100
H	-4.49452900	-0.10695900	-4.13453400
H	-5.43970900	-1.46443900	-3.50730900

H	-6.39240500	0.18826900	-1.71225400
H	-5.35352500	1.46221600	-2.34150700
H	-5.27146900	1.01873700	-0.62983500
H	2.11727000	2.04549800	1.70783200
H	2.79496000	4.40871200	3.53924100
H	3.94800900	3.34031400	2.74300500
H	2.86632700	2.70327300	3.99251900
H	1.36298100	3.73707300	0.04581800
H	3.06609000	3.96976300	0.45789000
H	1.83694700	5.04101800	1.13882000

## NCCN Spiro Bisperoxo Complex

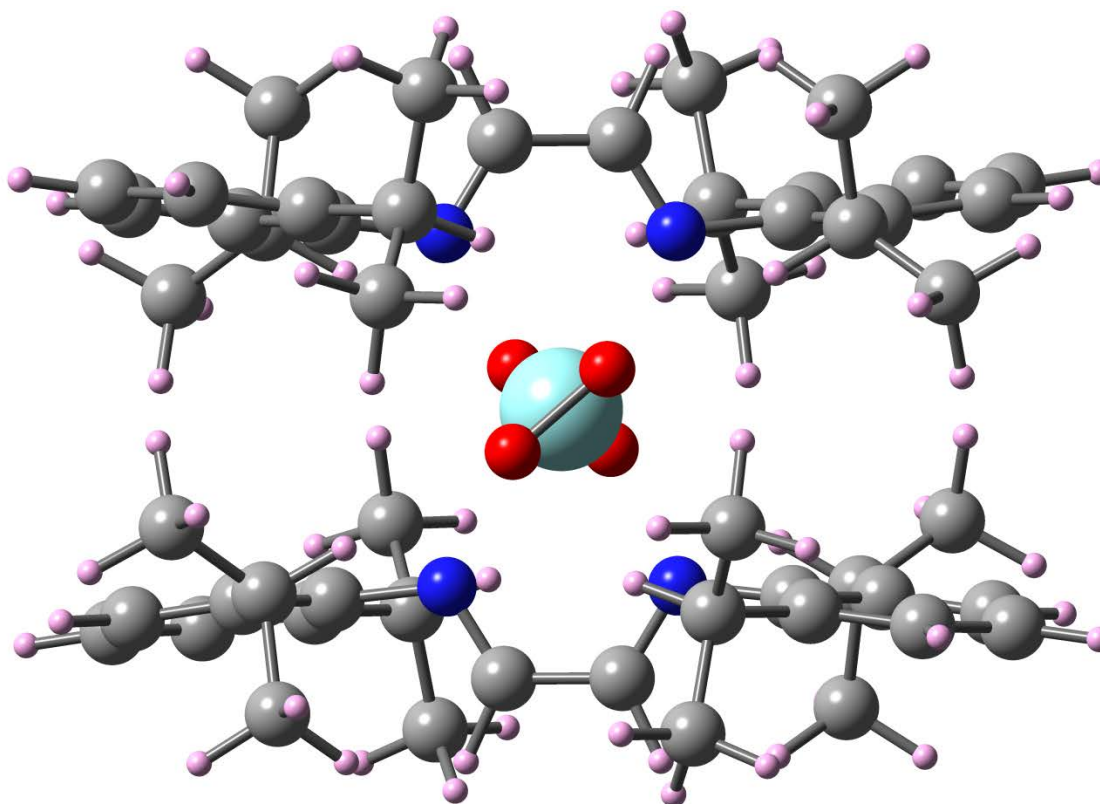


Fig. S180: NCCN Spiro Bisperoxo Complex

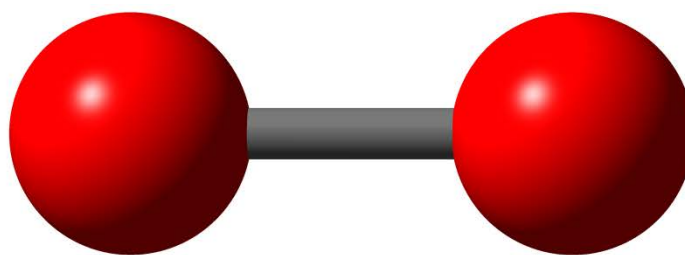
SCF
-2592.55635769

Zr	-0.00190900	-0.00006900	-0.00035700
O	0.55462300	0.44841300	1.94269000
O	-0.56215500	-0.51376200	1.92529000
O	-0.56251400	0.51337000	-1.92593500
O	0.55466400	-0.44834700	-1.94342900
N	1.35921000	-2.07992300	0.34920300
N	-1.35911800	-2.06794700	-0.41325900
N	-1.35998300	2.06726100	0.41320800
N	1.35834400	2.08049800	-0.34934700
C	0.69727900	-3.15771700	0.18130900
C	-0.69832500	-3.15066000	-0.27670700
C	-0.69946600	3.15023900	0.27746200
C	0.69613300	3.15797800	-0.18057100
C	2.71548000	-2.23523900	0.83088500
C	3.76304100	-2.23489600	-0.11217700
C	5.06033600	-2.43378900	0.36855400
C	5.30640100	-2.62227300	1.72446200
C	4.25319200	-2.60663800	2.62972500
C	2.93252800	-2.40860800	2.21168600

C	4.56666800	-1.29812000	-2.35133800
C	3.49123200	-2.10613400	-1.60863200
C	3.33632000	-3.49783400	-2.25667900
C	-2.04545300	-1.29731200	-4.43862900
C	-1.79796700	-2.31315300	-3.31029800
C	-1.55488000	-3.72257300	-3.88648700
C	-2.71449100	-2.20544800	-0.90316000
C	-2.93252700	-2.33138800	-2.28908100
C	-4.25451600	-2.50776300	-2.71255300
C	-5.30758100	-2.54921700	-1.80784500
C	-5.06008700	-2.40921200	-0.44638600
C	-3.76163900	-2.23234000	0.03969600
C	2.05370200	-1.43449800	4.39128400
C	1.79720300	-2.41280400	3.23221800
C	1.53945000	-3.83679200	3.76401300
C	-4.56655200	-1.38990500	2.31757100
C	-3.48564900	-2.15594500	1.53923000
C	-3.30915600	-3.56784600	2.13609900
C	-2.71551600	2.20404900	0.90288400
C	-2.93395400	2.32746500	2.28897600
C	-4.25605200	2.50308900	2.71242300
C	-5.30887200	2.54622700	1.80752400
C	-5.06100200	2.40879200	0.44587600
C	-3.76242400	2.23284300	-0.04020800
C	-2.04789900	1.28873200	4.43660700
C	-1.79976900	2.30695500	3.31056000
C	-1.55668100	3.71511900	3.88980400
C	2.05248600	1.44177900	-4.39281000
C	1.79595900	2.41785800	-3.23188200
C	1.53778900	3.84277200	-3.76100300
C	2.71456100	2.23668400	-0.83098300
C	2.93144000	2.41210500	-2.21155200
C	4.25200700	2.61111200	-2.62942200
C	5.30530800	2.62565500	-1.72424200
C	5.05942700	2.43502800	-0.36860800
C	3.76222100	2.23514400	0.11196100
C	-4.56644200	1.39484100	-2.32001000
C	-3.48611800	2.15985700	-1.53985800
C	-3.31048700	3.57319700	-2.13355900
C	4.56618800	1.29399900	2.34914300
C	3.49068600	2.10358400	1.60822800
C	3.33604200	3.49402400	2.25904200
H	1.14737100	-4.13367500	0.37211100
H	-1.14925500	-4.12010400	-0.49635900
H	-1.15068000	4.11942900	0.49765400
H	1.14593100	4.13418800	-0.37077300
H	5.88915800	-2.44714500	-0.32857500
H	6.32106400	-2.77802900	2.07455100
H	4.45634400	-2.74853100	3.68493400
H	2.54577600	-1.57300600	-1.73796000
H	-0.88710900	-1.98119200	-2.81072500
H	5.52874700	-1.81911900	-2.37568000

H	4.71944200	-0.31834900	-1.89595300
H	4.25755000	-1.14159000	-3.38802400
H	4.26130800	-4.07554600	-2.16297600
H	3.10284900	-3.39817600	-3.32064000
H	2.53583000	-4.08099500	-1.79328200
H	-2.92766700	-1.54439000	-5.03773300
H	-1.18256400	-1.27988700	-5.11043800
H	-2.16204400	-0.29450700	-4.02587400
H	-1.31855600	-4.44922700	-3.10276000
H	-0.71765300	-3.70489200	-4.59064800
H	-2.43478600	-4.09455700	-4.42117100
H	-4.45871400	-2.61242600	-3.77192000
H	-6.32311900	-2.68749200	-2.16269800
H	-5.88839200	-2.44347400	0.25049300
H	0.89036500	-2.05656100	2.74202100
H	-2.54644300	-1.61519700	1.68309400
H	2.93193200	-1.70923800	4.98428900
H	1.18964200	-1.42644900	5.06188100
H	2.18274800	-0.42130700	4.00890900
H	2.41401900	-4.23303200	4.28990900
H	1.29959100	-4.53661400	2.95737700
H	0.69981700	-3.83330000	4.46540100
H	-4.73159900	-0.39430200	1.90255500
H	-4.25394100	-1.27105800	3.35820200
H	-5.52283500	-1.92200700	2.32576500
H	-4.22857900	-4.15268700	2.03151900
H	-3.06624700	-3.50253000	3.20059200
H	-2.50681700	-4.12591100	1.64600600
H	-4.46053400	2.60577800	3.77192800
H	-6.32450300	2.68387900	2.16235700
H	-5.88911500	2.44447800	-0.25116000
H	-0.88877500	1.97587200	2.81066000
H	0.88929600	2.06053600	-2.74215200
H	-2.93035900	1.53462700	5.03584200
H	-1.18532200	1.26971800	5.10877500
H	-2.16444200	0.28683500	4.02161400
H	-1.32016500	4.44343500	3.10767600
H	-0.71958800	3.69588800	4.59408100
H	-2.43666200	4.08602000	4.42511600
H	2.93044100	1.71793000	-4.98556900
H	1.18823200	1.43465900	-5.06316500
H	2.18200900	0.42793200	-4.01234700
H	1.29795200	4.54105100	-2.95302400
H	0.69800500	3.84040000	-4.46221500
H	2.41216700	4.24016900	-4.28634900
H	4.45501600	2.75467300	-3.68443100
H	6.31990000	2.78216700	-2.07420100
H	5.88832500	2.44744200	0.32844700
H	-2.54652700	1.62009300	-1.68484400
H	2.54522600	1.57025200	1.73670200
H	-5.52307000	1.92633800	-2.32710200
H	-4.73089300	0.39820400	-1.90724100

H	-4.25367000	1.27852800	-3.36087800
H	-3.06736800	3.51042200	-3.19815600
H	-2.50860400	4.13067200	-1.64205700
H	-4.23031700	4.15718000	-2.02780000
H	4.71866500	0.31505600	1.89187000
H	4.25731100	1.13556200	3.38560900
H	5.52836300	1.81478500	2.37422100
H	2.53549800	4.07818000	1.79699800
H	4.26105700	4.07184600	2.16628300
H	3.10280600	3.39228800	3.32285800

**O<sub>2</sub> Triplet**Fig. S181: O<sub>2</sub> Triplet

<b>SCF</b>
-150.37041717

O	0.00000000	0.00000000	0.60287800
O	0.00000000	0.00000000	-0.60287800