

Exploring the Reducing Role of Boron: Added Insights from Theory

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Supporting Information File

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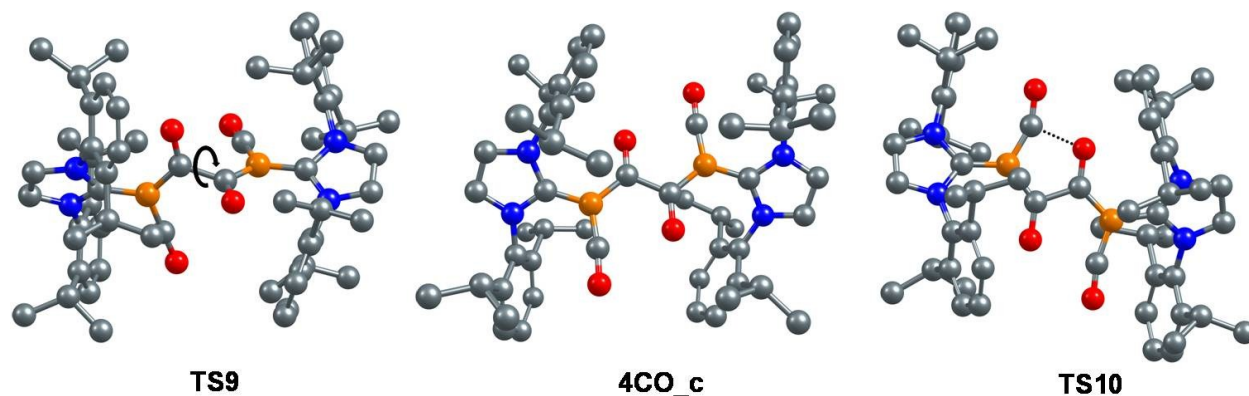


Fig S1. Structures obtained and discussed in the recently published by Brauschweig and coworkers (10.1002/anie.201506368). The color scheme is as follows: boron: yellow, carbon: gray, oxygen: red and nitrogen: blue; all the hydrogens have been removed for the purpose of clarity.

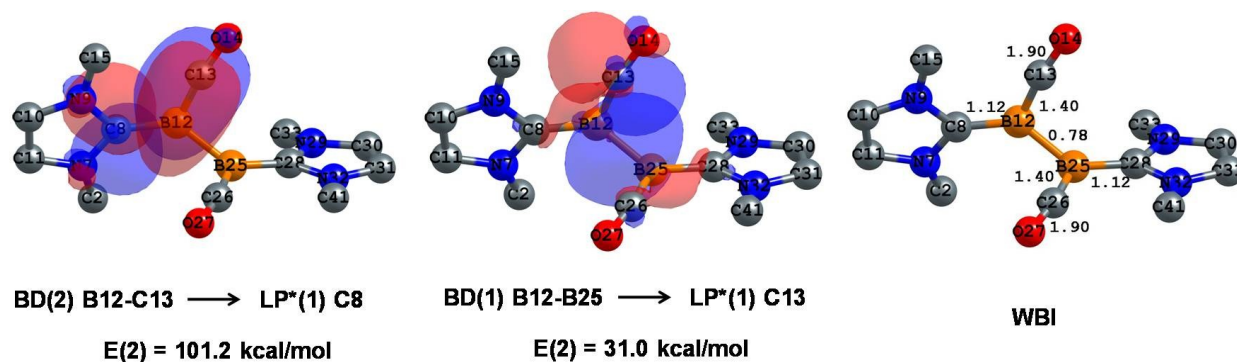


Fig S2. The NBO plots for the intra-molecular donor-acceptor interactions and WBI index values for **2CO_a**. Here BD(1), BD(2), LP, BD*(1), BD*(2) means σ bonding, π bonding, lone pair, σ^* anti-bonding, π^* anti-bonding atomic orbitals respectively. The color scheme is as follows: boron: yellow, carbon: gray, oxygen: red and nitrogen: blue; only one carbon of the Dip group attached to nitrogen has been shown; the rest of the carbons of the Dip group and all the

hydrogens have been removed for the purpose of clarity. Thus the methyl group attached to the nitrogen represents the Dip group.

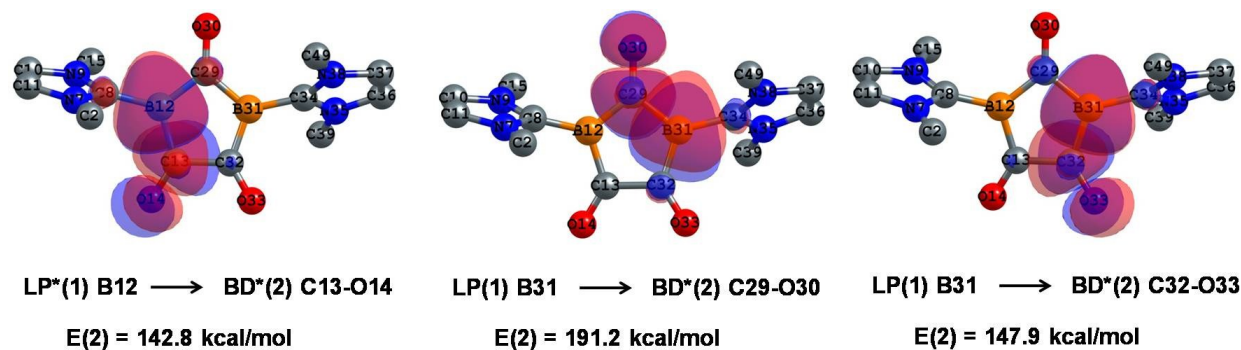


Fig S3. The NBO plots for the intra-molecular donor-acceptor interactions for **3CO_c**. Here BD(1), BD(2), LP, BD*(1), BD*(2) means σ bonding, π bonding, lone pair, σ^* anti-bonding, π^* anti-bonding atomic orbitals respectively. The color scheme is as follows: boron: yellow, carbon: gray, oxygen: red and nitrogen: blue; only one carbon of the Dip group attached to nitrogen has been shown; the rest of the carbons of the Dip group and all the hydrogens have been removed for the purpose of clarity. Thus the methyl group attached to the nitrogen represents the Dip group.

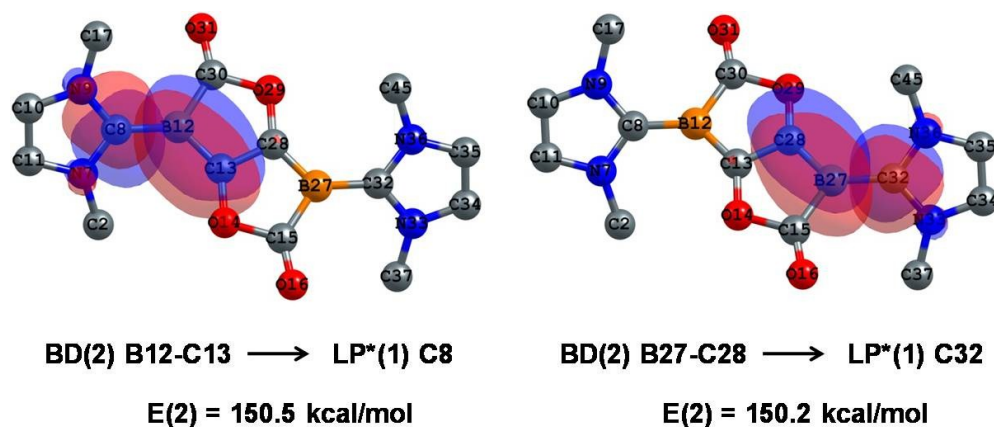


Fig S4. The NBO plots for the intra-molecular donor-acceptor interactions for **3**. Here BD(1), BD(2), LP, BD*(1), BD*(2) means σ bonding, π bonding, lone pair, σ^* anti-bonding, π^* anti-bonding atomic orbitals respectively. The color scheme is as follows: boron: yellow, carbon: gray, oxygen: red and nitrogen: blue; only one carbon of the Dip group attached to nitrogen has been shown; the rest of the carbons of the Dip group and all the hydrogens have been removed for the purpose of clarity. Thus the methyl group attached to the nitrogen represents the Dip group.

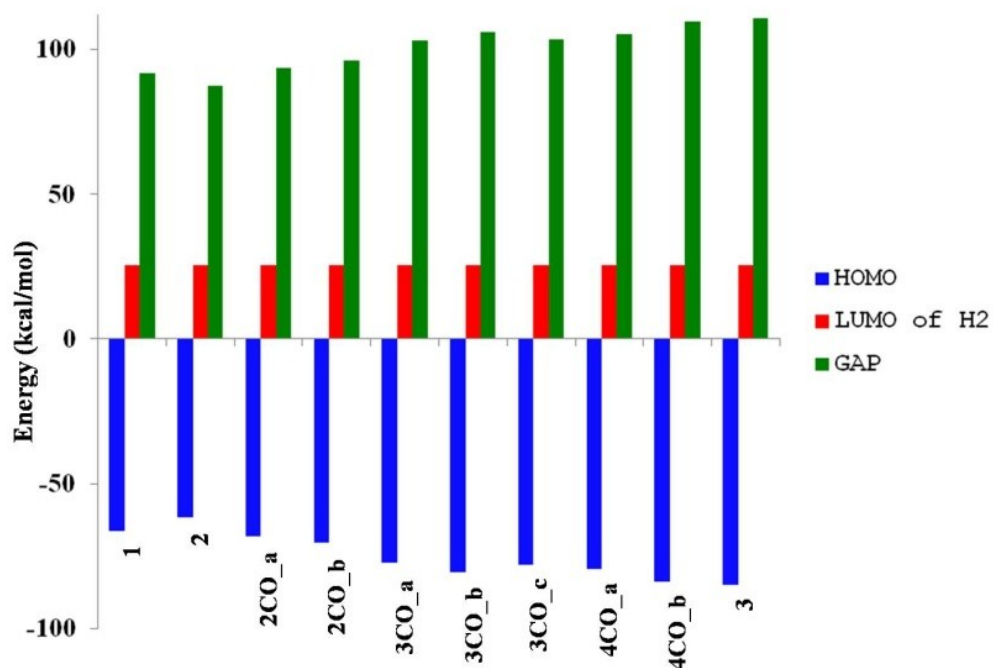
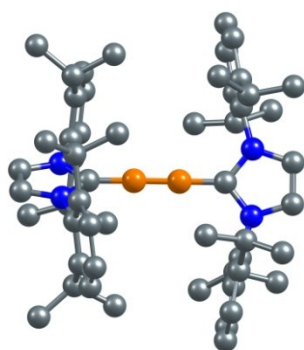


Fig S5. The HOMO energy values for the different B₂ complexes, compared to the LUMO energy value of H₂.

Cartesian Coordinates for investigated structures.



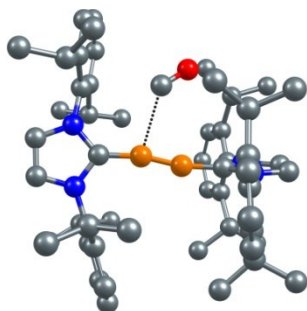
1

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C 8.686 5.819 4.318
C 8.821 6.492 5.531

C 9.253 5.810 6.668
N 9.665 2.377 5.305
C 8.738 1.326 5.400
N 9.537 0.193 5.179
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C 10.944 1.898 5.042
C 9.091 -1.168 5.230
C 8.789 -1.833 4.023
C 8.374 -3.170 4.104
C 8.290 -3.822 5.334
C 8.641 -3.154 6.507
C 9.050 -1.814 6.483
C 8.977 -1.164 2.667
C 9.514 -1.126 7.760

B 7.267 1.396 5.668
B 5.806 1.468 5.923
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C 2.264 1.477 7.205
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C 5.262 -0.094 10.995
C 4.931 -1.002 9.989
C 4.395 -0.567 8.769
C 3.476 2.335 3.938

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C	3.863	4.098	2.349	C	2.521	5.653	4.730	H	9.856	-2.885	1.634
C	3.720	3.702	3.686	H	3.706	4.191	5.761	H	7.873	-0.636	0.870
C	4.154	3.233	9.472	C	7.523	3.899	2.190	H	7.300	-2.135	1.634
C	3.950	-1.574	7.717	C	10.029	4.241	1.952	H	6.906	-0.555	2.362
C	2.913	-0.051	3.180	H	9.047	2.673	3.040	H	3.625	-2.085	2.880
C	3.754	4.734	4.805	C	9.171	3.805	9.062	H	4.114	-0.966	1.587
C	8.892	3.747	2.866	H	10.202	2.660	7.589	H	4.920	-0.901	3.178
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H	11.627	-0.199	4.779	H	9.274	-0.122	2.852	H	1.527	-0.274	1.494
H	8.369	6.369	3.429	C	10.113	-1.843	1.879	H	2.519	6.362	5.573
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H	8.123	-3.708	3.188	H	8.989	4.846	9.372	H	5.179	6.132	3.893
H	1.567	1.320	8.020	H	8.204	3.334	8.842	H	5.117	5.186	9.473
H	1.148	2.105	5.387	H	11.930	3.693	9.036	H	5.895	4.012	10.558
H	5.088	-2.070	10.155	H	12.198	4.165	7.341	H	6.121	3.880	8.794
H	5.689	-0.455	11.933	H	11.468	5.317	8.481	H	2.799	4.709	10.337
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H	4.059	5.147	2.119	H	9.928	5.316	1.734	H	3.448	3.556	11.522
H	3.881	3.503	0.275	H	11.013	4.088	2.418	H	2.320	-2.995	7.406
H	3.362	1.129	0.760	H	7.508	3.353	1.235	H	2.884	-2.907	9.093
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H	3.689	-1.012	6.808	H	11.241	-1.179	9.101	H	5.941	-2.028	6.947
C	5.398	4.126	9.582	H	10.771	-2.777	8.471	H	5.370	-3.183	8.184
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C	3.079	3.656	10.491	H	8.826	-0.647	9.768				
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TS1

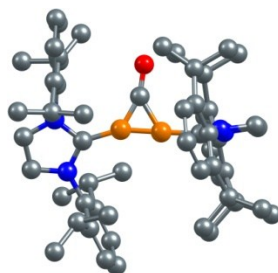
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2

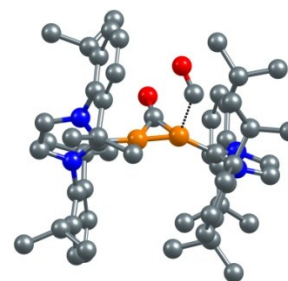
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H	5.109	-2.362	11.054
H	4.991	0.081	11.416
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H	3.937	5.202	1.085
H	3.377	2.802	0.826
C	4.861	-2.849	5.992
C	2.431	-2.910	6.716
H	3.474	-1.224	5.897
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C	4.179	0.182	1.961
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C	1.702	0.713	2.103
C	5.244	5.984	5.827
C	2.800	5.518	6.278
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C	9.677	3.111	1.028
H	8.926	1.963	2.675
C	9.486	5.233	8.015
H	10.014	3.389	7.081
C	11.690	4.725	6.875
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C	8.460	0.088	9.539
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H	0.906	1.192	2.691
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H	5.117	-3.718	6.617
H	2.141	-3.311	5.733
H	2.595	-3.763	7.392
H	1.582	-2.330	7.110
H	5.225	3.686	10.638
H	5.238	2.200	11.609
H	6.315	2.373	10.183
H	2.730	3.462	10.381
H	2.017	2.052	9.566
H	2.676	1.886	11.210
H	11.188	0.500	9.715
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H	11.900	5.788	6.681
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H	6.553	2.709	2.551
H	6.950	3.788	1.195
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H	10.722	3.125	1.371

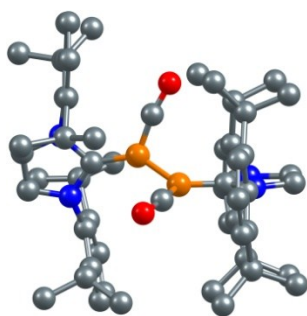


TS2

C	4.714	-1.198	8.485
C	4.378	0.171	8.466
C	4.527	1.009	9.594
C	5.043	0.427	10.760
C	5.400	-0.919	10.802
C	5.240	-1.722	9.675
N	3.759	0.703	7.277
C	4.410	1.246	6.171
N	3.360	1.592	5.319
C	2.129	1.276	5.894
C	2.379	0.718	7.103
C	3.483	2.036	3.957
C	3.703	3.408	3.698
C	3.799	3.798	2.355
C	3.666	2.873	1.319

C	3.407	1.535	1.604	C	7.503	4.375	1.994	H	9.577	3.292	7.625
C	3.298	1.086	2.928	C	8.636	0.084	2.512	H	9.004	1.059	2.860
C	3.734	4.432	4.825	C	7.161	0.271	2.133	H	10.199	-0.045	7.345
C	4.624	5.646	4.540	C	10.313	-1.132	7.215	H	9.229	4.166	9.842
C	2.916	-0.364	3.207	C	9.664	-1.794	8.440	H	9.208	5.847	9.281
C	3.910	-1.380	2.624	C	11.264	4.587	7.943	H	7.887	4.734	8.808
B	5.878	1.637	6.089	C	9.966	4.922	1.760	H	11.609	4.064	8.848
C	6.487	2.962	6.597	C	9.482	-0.304	1.286	H	11.848	4.211	7.091
O	6.253	4.067	7.121	C	11.816	-1.463	7.153	H	11.492	5.658	8.063
C	4.117	2.476	9.575	C	2.678	2.649	10.101	H	10.004	4.372	0.808
C	5.074	3.381	10.363	C	3.559	-3.270	7.600	H	9.763	5.979	1.529
C	4.508	-2.103	7.279	C	1.489	-0.650	2.700	H	10.962	4.871	2.225
C	5.849	-2.608	6.725	C	2.299	4.891	5.155	H	7.541	3.845	1.030
B	7.468	1.876	6.130	H	11.634	3.399	4.461	H	6.734	3.897	2.614
C	8.867	1.880	5.408	H	11.730	0.612	4.368	H	7.184	5.409	1.791
N	9.630	2.999	5.160	H	8.261	6.925	3.190	H	12.314	-1.153	8.084
C	10.894	2.649	4.711	H	8.306	8.140	5.350	H	11.978	-2.545	7.026
C	10.943	1.291	4.672	H	8.955	6.962	7.429	H	12.315	-0.951	6.316
N	9.703	0.828	5.096	H	9.527	-3.607	6.387	H	10.128	-1.410	9.360
C	9.213	4.387	5.238	H	8.515	-4.274	4.230	H	8.589	-1.574	8.491
C	9.275	5.058	6.476	H	8.092	-2.578	2.471	H	9.797	-2.887	8.436
C	8.937	6.417	6.484	H	1.710	0.326	7.859	H	9.399	0.468	0.507
C	8.570	7.081	5.315	H	1.196	1.474	5.380	H	10.545	-0.415	1.545
C	8.541	6.396	4.103	H	5.517	-2.778	9.719	H	9.142	-1.254	0.848
C	8.869	5.035	4.032	H	5.807	-1.345	11.721	H	7.060	1.044	1.356
C	9.334	-0.559	4.908	H	5.181	1.046	11.647	H	6.734	-0.659	1.733
C	8.816	-0.918	3.644	H	3.976	4.848	2.118	H	6.567	0.585	3.002
C	8.509	-2.269	3.433	H	3.750	3.203	0.281	H	3.567	-2.404	2.835
C	8.755	-3.225	4.416	H	3.277	0.824	0.784	H	4.001	-1.278	1.531
C	9.320	-2.847	5.632	H	4.036	-1.503	6.487	H	4.907	-1.257	3.064
C	9.628	-1.507	5.909	H	4.150	2.818	8.530	H	1.184	-1.672	2.970
C	9.750	4.372	7.747	H	2.911	-0.510	4.297	H	0.758	0.049	3.130
C	8.967	4.812	8.992	H	4.152	3.947	5.718	H	1.431	-0.559	1.605
C	8.878	4.335	2.677	H	9.124	3.276	2.841	H	2.315	5.604	5.993

H	1.838	5.392	4.288
H	1.652	4.050	5.443
H	4.688	6.266	5.445
H	5.648	5.345	4.286
H	4.225	6.277	3.728
H	4.813	4.434	10.182
H	5.007	3.205	11.449
H	6.112	3.234	10.043
H	2.386	3.709	10.062
H	1.947	2.077	9.512
H	2.604	2.315	11.148
H	3.379	-3.876	6.699
H	3.983	-3.936	8.368
H	2.588	-2.910	7.970
H	5.687	-3.224	5.827
H	6.503	-1.769	6.449
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C	8.119	1.300	7.947
O	7.684	1.450	9.019



2CO_a

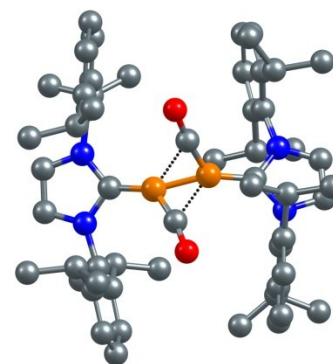
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N	3.303	2.043	5.501
C	4.183	1.691	6.525
N	3.328	1.384	7.592
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C	1.978	1.953	5.934
B	5.705	1.547	6.536
C	6.392	1.385	7.808
O	7.118	1.309	8.741
C	3.701	0.852	8.877
C	3.864	1.744	9.960
C	4.124	1.197	11.224
C	4.225	-0.180	11.403
C	4.064	-1.040	10.318
C	3.791	-0.550	9.034
C	3.739	3.252	9.785
C	3.548	-1.512	7.879
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C	3.580	4.935	5.651
B	6.899	0.886	5.466
C	6.318	-0.426	5.225
O	5.668	-1.395	5.021
C	8.395	1.090	5.231
N	9.165	2.254	5.190
C	10.519	1.947	5.035
C	10.628	0.599	4.969
N	9.347	0.071	5.096
C	8.721	3.606	4.953
C	8.705	4.520	6.027
C	8.442	5.865	5.731
C	8.196	6.282	4.425
C	8.211	5.358	3.382
C	8.493	4.005	3.618
C	9.010	4.094	7.455
C	8.623	3.044	2.444

C	9.118	-1.348	5.193
C	8.927	-2.088	4.006
C	8.813	-3.480	4.116
C	8.879	-4.110	5.356
C	9.065	-3.357	6.515
C	9.198	-1.963	6.463
C	8.867	-1.416	2.640
C	9.471	-1.169	7.734
H	11.267	2.727	4.967
H	11.495	-0.039	4.865
H	8.027	5.695	2.360
H	7.989	7.335	4.219
H	8.430	6.597	6.541
H	9.116	-3.862	7.481
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H	8.662	-4.079	3.216
H	1.190	1.350	7.920
H	1.154	2.202	5.276
H	4.145	-2.118	10.471
H	4.435	-0.587	12.394
H	4.257	1.862	12.079
H	3.898	5.950	3.148
H	3.892	4.753	0.978
H	3.685	2.285	0.916
C	4.532	-2.691	7.861
C	2.096	-2.030	7.902
H	3.697	-0.955	6.943
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H	3.889	3.471	8.717
C	2.331	3.741	10.175
C	4.450	-0.117	2.070
H	3.591	0.146	4.007
C	1.987	0.164	2.575
C	4.730	5.932	5.848

C	2.216	5.644	5.748
H	3.642	4.208	6.474
C	7.380	3.042	1.546
C	9.892	3.352	1.626
H	8.726	2.028	2.851
C	7.982	4.642	8.454
H	8.949	2.997	7.496
C	10.437	4.505	7.862
C	7.782	-2.015	1.732
H	8.609	-0.359	2.807
C	10.239	-1.461	1.939
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C	10.971	-1.208	8.087
H	9.192	-0.123	7.542
H	8.773	-0.955	9.777
H	7.563	-1.657	8.692
H	8.931	-2.649	9.267
H	11.165	-0.610	8.991
H	11.299	-2.240	8.285
H	11.594	-0.805	7.276
H	7.665	-1.399	0.828
H	8.045	-3.032	1.400
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H	10.190	-0.953	0.964
H	11.019	-0.971	2.537
H	10.550	-2.503	1.764
H	10.654	4.168	8.887
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H	8.166	4.215	9.451
H	8.042	5.738	8.545
H	6.961	4.372	8.152
H	10.010	2.622	0.811
H	9.838	4.355	1.176

H	10.797	3.312	2.250
H	7.491	2.292	0.747
H	6.476	2.803	2.120
H	7.226	4.019	1.061
H	4.785	5.091	10.285
H	4.638	3.977	11.654
H	5.816	3.641	10.362
H	2.245	4.828	10.025
H	1.549	3.255	9.573
H	2.124	3.526	11.234
H	4.392	-3.277	6.942
H	5.573	-2.345	7.873
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H	1.900	-2.598	8.825
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H	2.105	6.396	4.951
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H	5.704	5.431	5.791
H	4.713	6.732	5.091
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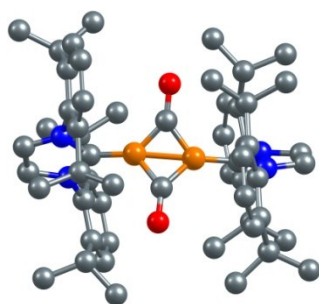


TS3

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N	9.904	2.551	5.591
C	10.604	1.736	4.711
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B	11.951	2.044	4.016
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O	12.634	4.324	2.888
C	9.780	-0.283	3.387
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C	9.421	-0.899	1.095
C	9.670	-2.230	1.417
C	9.975	-2.584	2.728
C	10.036	-1.621	3.743
C	9.150	1.543	1.678
C	7.668	1.702	1.291
C	10.353	-2.041	5.171
C	9.151	-2.749	5.824
C	11.011	2.186	8.253

C	10.017	2.004	9.414	C	11.606	-2.927	5.245	H	13.439	-0.813	6.850
C	9.587	5.168	4.313	C	12.453	1.935	8.722	H	14.220	-2.279	7.494
C	8.053	5.295	4.408	C	10.168	6.359	3.539	H	16.901	-0.890	8.335
B	13.696	1.767	3.796	H	18.175	0.540	4.574	H	16.858	-2.427	7.440
C	15.160	1.875	4.227	H	18.069	3.295	4.921	H	17.784	-1.054	6.798
N	16.057	0.806	4.224	H	15.246	-3.437	5.809	H	17.450	4.362	8.515
C	17.344	1.233	4.524	H	15.231	-4.387	3.521	H	18.078	4.545	6.860
C	17.289	2.574	4.709	H	15.551	-2.916	1.556	H	17.369	5.941	7.696
N	15.968	2.974	4.513	H	15.171	6.871	2.175	H	14.946	4.344	8.963
C	15.752	-0.588	4.021	H	15.117	8.212	4.252	H	14.848	5.970	8.261
C	15.573	-1.404	5.158	H	15.427	7.116	6.453	H	13.794	4.681	7.645
C	15.388	-2.778	4.949	H	7.687	0.208	5.012	H	17.190	3.376	0.585
C	15.382	-3.314	3.664	H	7.947	2.540	6.515	H	17.612	4.940	1.323
C	15.563	-2.485	2.558	H	9.187	-0.629	0.063	H	17.668	3.449	2.294
C	15.762	-1.107	2.708	H	9.633	-2.996	0.639	H	14.915	4.133	-0.169
C	15.608	-0.849	6.576	H	10.175	-3.630	2.969	H	13.851	5.043	0.929
C	16.862	-1.332	7.328	H	11.537	4.616	9.358	H	15.386	5.760	0.342
C	16.041	-0.225	1.497	H	11.269	6.866	8.356	H	11.867	-3.127	6.295
C	17.546	-0.233	1.162	H	10.433	7.110	6.040	H	11.442	-3.900	4.757
C	15.646	4.383	4.438	H	9.338	2.183	2.551	H	12.465	-2.447	4.758
C	15.505	4.990	3.166	H	10.561	-1.127	5.751	H	9.383	-3.026	6.864
C	15.304	6.376	3.137	H	9.822	4.262	3.736	H	8.255	-2.111	5.835
C	15.273	7.133	4.306	H	10.780	1.424	7.495	H	8.897	-3.670	5.277
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C	15.640	5.130	5.636	H	15.757	0.802	1.769	H	11.129	1.920	0.840
C	15.630	4.197	1.871	H	15.831	3.406	6.882	H	9.905	1.490	-0.382
C	17.113	3.975	1.506	H	15.161	3.214	2.046	H	7.446	2.753	1.050
C	15.878	4.498	7.003	H	15.360	0.141	-0.527	H	7.420	1.095	0.407
C	17.276	4.854	7.545	H	15.527	-1.580	-0.154	H	7.000	1.391	2.109
C	14.898	4.831	0.680	H	14.144	-0.655	0.509	H	7.618	5.399	3.402
C	14.801	4.897	8.022	H	17.749	0.424	0.304	H	7.591	4.419	4.883
C	15.213	-0.610	0.263	H	18.159	0.115	2.005	H	7.773	6.186	4.992
C	14.334	-1.192	7.363	H	17.879	-1.249	0.898	H	9.782	6.348	2.509
C	10.076	2.040	0.556	H	14.375	-0.739	8.365	H	9.873	7.322	3.984

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H	8.977	2.139	9.082
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H	13.161	2.021	7.887
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C	12.982	0.798	3.007
O	12.604	-0.096	2.278



2CO_b

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C	9.372	-2.021	4.377
C	9.147	-3.370	4.689
C	9.105	-3.806	6.010
C	9.280	-2.898	7.054
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N	9.742	2.402	4.861
C	11.069	2.039	4.649
C	11.153	0.695	4.843
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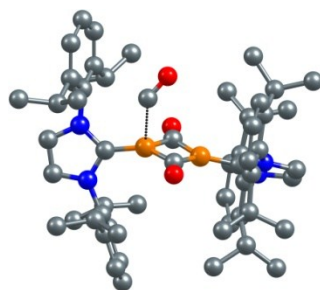
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B	5.591	1.322	6.210
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O	7.236	2.177	8.096
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C	3.719	3.076	1.842
C	3.498	2.315	2.998
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C	3.210	0.822	2.904
C	3.782	0.565	8.540
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H	8.205	7.390	3.916
H	8.852	6.722	6.208
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H	8.924	-4.860	6.231
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H	1.197	1.299	7.852
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H	4.544	-2.566	9.601
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C	4.015	0.120	1.803
H	3.523	0.360	3.852
C	1.701	0.569	2.706
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C	2.657	6.204	5.714
H	3.541	4.402	6.459
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C	9.842	3.558	1.029
H	9.307	2.146	2.544
C	8.898	5.000	8.209
H	9.485	3.206	7.242
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H	9.480	-0.477	2.909

C	10.625	-2.141	2.186
C	8.785	-0.819	9.139
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H	7.819	4.846	8.083
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H	11.808	3.955	6.577
H	11.446	5.586	7.187
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H	6.836	2.457	2.447
H	7.035	3.735	1.229
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H	5.284	3.252	11.342
H	5.919	3.225	9.671
H	2.421	4.260	10.700
H	1.642	2.705	10.314
H	2.717	2.836	11.722

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H	5.838	-2.271	6.986
H	4.744	-3.518	7.655
H	2.177	-2.767	6.206
H	2.219	-2.940	7.979
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H	2.829	6.991	4.965
H	1.662	5.773	5.524
H	5.137	6.211	6.958
H	5.920	4.958	5.964
H	5.417	6.494	5.224

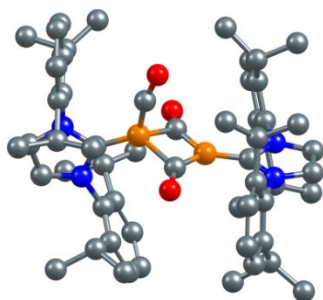
C	10.979	1.180	4.458
C	10.785	2.525	4.466
B	7.457	1.275	5.844
C	6.581	2.033	6.909
O	6.651	3.074	7.599
C	9.712	-0.830	5.164
C	10.210	-1.322	6.389
C	10.156	-2.708	6.592
C	9.651	-3.558	5.610
C	9.195	-3.042	4.399
C	9.215	-1.664	4.142
C	10.854	-0.421	7.436
C	8.788	-1.118	2.786
C	9.690	4.183	7.496
C	8.445	3.935	2.512
C	6.399	0.135	5.619
O	6.275	-0.909	4.945
B	5.450	0.933	6.627
C	3.903	1.052	6.892
N	3.168	0.848	8.049
C	1.841	1.215	7.853
C	1.725	1.656	6.575
N	2.981	1.544	5.992
C	3.580	0.260	9.306
C	3.211	-1.079	9.555
C	3.527	-1.615	10.811
C	4.184	-0.851	11.772
C	4.531	0.470	11.499
C	4.231	1.068	10.266
C	2.492	-1.948	8.528
C	4.568	2.530	10.007
C	3.210	1.911	4.613
C	3.361	3.279	4.309
C	3.460	3.629	2.954



TS4

C	8.487	4.681	3.840
C	8.966	4.094	5.029
C	9.061	4.798	6.251
C	8.616	6.126	6.253
C	8.123	6.730	5.097
C	8.061	6.015	3.904
N	9.503	2.753	4.947
C	8.867	1.557	5.228
N	9.811	0.594	4.918

C	3.416	2.658	1.957	H	3.370	3.871	6.364	H	3.464	-2.567	3.413
C	3.268	1.311	2.291	C	7.017	3.843	1.953	H	3.187	-1.512	2.016
C	3.149	0.902	3.626	C	9.400	4.573	1.486	H	4.676	-1.340	3.008
C	3.388	4.362	5.380	H	8.788	2.905	2.686	H	9.499	4.143	9.652
C	2.893	-0.558	3.977	C	9.095	4.718	8.805	H	9.359	5.773	8.978
C	5.966	-0.957	8.122	H	9.481	3.103	7.470	H	8.005	4.600	8.798
O	6.906	-1.146	8.757	C	11.220	4.388	7.487	H	11.669	3.924	8.378
H	11.432	3.342	4.171	C	7.623	-1.897	2.163	H	11.697	3.946	6.601
H	11.841	0.585	4.182	H	8.439	-0.086	2.942	H	11.466	5.461	7.504
H	7.679	6.499	3.002	C	9.985	-1.083	1.813	H	9.399	3.995	0.550
H	7.784	7.768	5.129	C	10.336	-0.678	8.859	H	9.095	5.603	1.246
H	8.658	6.698	7.180	C	12.389	-0.560	7.390	H	10.433	4.611	1.863
H	10.519	-3.126	7.533	H	10.606	0.621	7.188	H	7.009	3.258	1.021
H	9.613	-4.635	5.790	H	6.057	4.027	10.453	H	6.339	3.355	2.667
H	8.801	-3.720	3.641	H	5.567	3.100	11.887	H	6.609	4.840	1.725
H	1.109	1.120	8.645	H	6.651	2.373	10.662	H	9.676	-0.667	0.842
H	0.876	2.039	6.024	H	3.598	4.480	10.072	H	10.815	-0.471	2.193
H	3.261	-2.650	11.033	H	2.480	3.159	9.669	H	10.369	-2.100	1.638
H	4.430	-1.288	12.742	H	3.046	3.362	11.345	H	7.254	-1.366	1.273
H	5.046	1.056	12.260	H	2.732	-3.822	7.451	H	7.930	-2.903	1.835
H	3.578	4.679	2.682	H	4.273	-3.031	7.863	H	6.805	-1.985	2.889
H	3.500	2.950	0.908	H	3.339	-3.887	9.119	H	12.860	0.127	8.108
H	3.238	0.562	1.500	H	0.527	-2.844	8.212	H	12.694	-1.585	7.652
C	3.259	-3.246	8.227	H	1.051	-2.847	9.912	H	12.792	-0.338	6.391
C	1.054	-2.259	8.982	H	0.475	-1.342	9.167	H	10.789	0.042	9.556
H	2.432	-1.385	7.586	H	2.142	6.004	6.095	H	9.246	-0.576	8.915
C	5.779	3.025	10.808	H	2.115	5.805	4.328	H	10.603	-1.686	9.212
H	4.851	2.644	8.949	H	1.210	4.677	5.360				
C	3.348	3.430	10.288	H	4.668	5.955	6.122				
C	3.599	-1.542	3.037	H	5.564	4.571	5.473				
H	3.306	-0.736	4.981	H	4.774	5.726	4.363				
C	1.377	-0.845	4.010	H	1.196	-1.892	4.298				
C	4.676	5.197	5.324	H	0.846	-0.202	4.726				
C	2.140	5.260	5.284	H	0.931	-0.685	3.016				



3CO_a

C 3.188 -0.304 9.445
 C 3.202 1.054 9.064
 C 3.407 2.107 9.982
 C 3.608 1.758 11.324
 C 3.610 0.424 11.729
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 C 3.893 1.496 6.689
 N 3.160 1.780 5.555
 C 1.802 1.837 5.852
 C 1.665 1.588 7.180
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 O 6.597 0.867 9.170
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 C 3.890 3.282 3.751
 C 4.262 3.437 2.408
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 C 4.099 1.056 2.027
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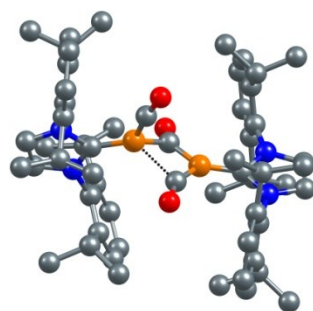
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 C 10.458 4.962 1.983
 H 9.544 3.229 2.851
 C 8.932 3.938 9.104
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 C 11.271 3.513 8.237
 C 7.669 -0.253 1.542
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 C 11.190 -1.477 7.437
 H 9.488 -0.192 7.141
 H 11.432 -1.082 8.436
 H 11.447 -2.548 7.424
 H 11.833 -0.966 6.706
 H 8.975 -1.393 9.170

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H	9.069	-2.973	8.369
H	10.085	-0.208	0.169
H	11.080	-1.041	1.389
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H	7.678	0.451	0.696
H	7.251	-1.206	1.183
H	6.994	0.144	2.312
H	9.004	3.144	9.862
H	9.282	4.871	9.573
H	7.876	4.059	8.831
H	11.439	2.827	9.081
H	11.884	3.165	7.393
H	11.634	4.511	8.532
H	7.988	4.069	1.125
H	7.182	3.976	2.710
H	7.698	5.552	2.063
H	10.481	4.533	0.969
H	10.301	6.047	1.883
H	11.446	4.810	2.441
H	4.593	6.404	5.157
H	5.767	5.186	4.635
H	4.730	6.024	3.432
H	2.129	5.973	5.064
H	2.180	5.452	3.363
H	1.485	4.382	4.600
H	1.558	-1.841	3.837
H	1.169	-0.106	3.903
H	1.709	-0.836	2.375
H	3.927	-2.639	3.692
H	4.142	-1.762	2.169
H	5.279	-1.504	3.535
H	1.481	-2.999	8.059
H	1.779	-2.730	9.790

H	0.792	-1.571	8.872
H	3.955	-3.179	7.632
H	5.048	-1.826	7.973
H	4.414	-2.822	9.313
H	2.088	5.309	9.653
H	1.211	3.761	9.575
H	1.998	4.261	11.089
H	4.638	5.353	9.673
H	4.620	4.415	11.180
H	5.564	3.841	9.781

C	9.198	-1.973	3.886
C	8.725	-2.944	2.995
C	8.415	-2.622	1.675
C	8.584	-1.319	1.213
C	9.069	-0.309	2.057
C	9.551	-2.335	5.323
C	9.277	1.099	1.517
C	10.092	1.508	8.445
C	9.842	4.749	4.471
C	6.706	0.051	5.156
O	6.310	-0.907	4.555
B	5.489	1.045	6.668
C	5.941	-0.000	7.583
O	6.453	-0.828	8.246
C	3.996	1.420	6.619
N	2.980	0.890	7.399
C	1.761	1.481	7.098
C	1.993	2.393	6.120
N	3.353	2.354	5.825
C	3.138	-0.118	8.414
C	2.923	-1.468	8.064
C	3.033	-2.423	9.084
C	3.340	-2.050	10.390
C	3.544	-0.708	10.707
C	3.449	0.289	9.730
C	2.570	-1.903	6.648
C	3.654	1.751	10.101
C	3.913	3.135	4.744
C	4.244	4.485	4.986
C	4.690	5.240	3.892
C	4.798	4.679	2.623
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C	3.990	2.542	3.463
C	4.074	5.140	6.351



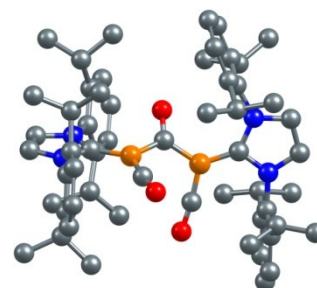
TS5

C	9.889	4.478	5.968
C	9.974	3.176	6.500
C	9.983	2.919	7.885
C	9.911	4.022	8.746
C	9.836	5.322	8.248
C	9.822	5.544	6.874
N	10.149	2.073	5.584
C	9.179	1.212	5.086
N	9.897	0.353	4.262
C	11.248	0.682	4.258
C	11.404	1.753	5.077
B	7.692	1.155	5.490
C	6.796	2.065	6.358
O	6.822	3.240	6.761
C	9.358	-0.662	3.391

C	3.510	1.119	3.196
H	12.284	2.318	5.356
H	11.964	0.124	3.666
H	9.749	6.566	6.493
H	9.780	6.167	8.938
H	9.911	3.859	9.825
H	8.580	-3.967	3.347
H	8.037	-3.394	1.001
H	8.340	-1.078	0.176
H	0.849	1.195	7.607
H	1.322	3.061	5.595
H	2.878	-3.478	8.847
H	3.423	-2.812	11.168
H	3.787	-0.429	11.734
H	4.962	6.286	4.044
H	5.155	5.286	1.788
H	4.534	2.920	1.411
C	3.589	-2.906	6.083
C	1.139	-2.470	6.587
H	2.599	-1.012	6.004
C	4.949	1.975	10.897
H	3.749	2.325	9.168
C	2.435	2.297	10.867
C	4.340	0.374	2.142
H	3.603	0.551	4.133
C	2.024	1.126	2.782
C	5.260	6.036	6.741
C	2.758	5.943	6.405
H	4.022	4.337	7.100
C	8.492	5.363	4.067
C	11.018	5.627	4.011
H	9.928	3.784	3.949
C	9.118	1.262	9.607
H	9.813	0.810	7.642

C	11.540	1.194	8.867
C	7.944	1.773	1.154
H	9.737	1.702	2.313
C	10.247	1.107	0.322
C	8.544	-3.305	5.961
C	10.981	-2.904	5.405
H	9.522	-1.407	5.913
H	11.244	-3.131	6.449
H	11.063	-3.834	4.823
H	11.726	-2.195	5.016
H	8.762	-3.415	7.033
H	7.516	-2.935	5.857
H	8.602	-4.308	5.510
H	8.122	2.792	0.775
H	7.411	1.211	0.372
H	7.287	1.848	2.032
H	10.442	2.140	-0.003
H	11.211	0.643	0.582
H	9.833	0.559	-0.537
H	8.434	5.474	2.973
H	7.658	4.732	4.401
H	8.360	6.361	4.513
H	10.986	5.771	2.920
H	10.983	6.622	4.480
H	11.988	5.173	4.266
H	9.114	0.197	9.878
H	9.402	1.831	10.507
H	8.095	1.546	9.327
H	11.616	0.163	9.246
H	12.241	1.298	8.026
H	11.871	1.874	9.667
H	5.112	3.052	11.054
H	4.908	1.498	11.888
H	5.820	1.575	10.360

H	2.574	3.364	11.100
H	1.509	2.196	10.282
H	2.293	1.759	11.816
H	3.318	-3.178	5.052
H	4.602	-2.481	6.062
H	3.613	-3.833	6.677
H	0.874	-2.730	5.551
H	1.047	-3.382	7.196
H	0.399	-1.745	6.957
H	3.995	-0.668	2.075
H	4.228	0.819	1.141
H	5.403	0.351	2.405
H	1.666	0.096	2.625
H	1.383	1.591	3.544
H	1.888	1.680	1.841
H	5.113	6.414	7.764
H	6.197	5.465	6.716
H	5.345	6.913	6.081
H	2.622	6.385	7.403
H	2.772	6.764	5.671
H	1.880	5.318	6.189

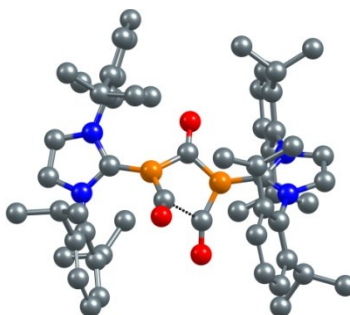


3CO_b

C	2.891	3.125	0.752
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C	1.848	2.046	2.718
C	1.324	3.293	3.086
C	1.577	4.434	2.326
C	2.352	4.348	1.173

N	3.271	0.748	1.197	C	-4.379	-2.748	-0.549	C	-2.816	-0.980	-4.686
C	2.727	-0.376	0.591	C	-4.438	1.555	2.252	C	-0.991	4.671	-0.892
N	3.781	-1.284	0.583	C	-1.789	1.579	-2.688	C	-2.987	4.939	-2.438
C	4.921	-0.735	1.157	C	-1.455	2.947	-2.690	H	-2.683	3.372	-1.000
C	4.606	0.528	1.535	C	-0.529	3.384	-3.646	C	2.899	3.497	-1.747
B	1.298	-0.638	0.106	C	0.043	2.495	-4.552	C	5.017	3.878	-0.396
C	0.101	0.405	-0.123	C	-0.307	1.146	-4.527	H	4.003	2.009	-0.685
O	0.345	1.584	-0.471	C	-1.240	0.657	-3.603	C	0.188	0.730	4.133
C	3.737	-2.604	0.015	C	-2.067	3.940	-1.712	H	1.782	-0.068	2.970
C	3.393	-3.691	0.847	C	-1.689	-0.798	-3.651	C	2.643	0.782	4.750
C	3.389	-4.968	0.270	H	5.195	1.297	2.019	C	3.579	-1.419	-3.433
C	3.710	-5.152	-1.072	H	5.844	-1.297	1.235	H	4.426	-0.675	-1.619
C	4.055	-4.061	-1.868	H	2.536	5.246	0.578	C	5.975	-1.733	-2.659
C	4.085	-2.763	-1.343	H	1.162	5.396	2.634	C	1.719	-4.170	2.702
C	3.057	-3.514	2.322	H	0.714	3.372	3.987	C	4.202	-4.041	3.207
C	4.506	-1.592	-2.220	H	3.124	-5.831	0.883	H	2.956	-2.435	2.514
C	1.622	0.821	3.595	H	3.692	-6.156	-1.503	H	3.974	-3.872	4.271
C	3.720	3.059	-0.523	H	4.311	-4.220	-2.918	H	4.348	-5.122	3.060
C	0.915	-1.983	-0.313	H	-5.966	0.554	-1.021	H	5.154	-3.540	2.980
O	0.496	-3.012	-0.702	H	-4.472	1.841	-2.988	H	1.484	-3.956	3.755
B	-1.412	-0.082	0.095	H	-5.230	-3.803	1.816	H	0.894	-3.788	2.086
C	-1.518	-1.036	1.195	H	-5.631	-2.650	3.970	H	1.757	-5.264	2.588
O	-1.478	-1.782	2.105	H	-5.247	-0.214	4.178	H	3.891	-0.547	-4.028
C	-2.683	0.395	-0.614	H	-0.244	4.438	-3.672	H	3.605	-2.301	-4.091
N	-3.995	0.126	-0.238	H	0.769	2.855	-5.285	H	2.541	-1.258	-3.113
C	-4.897	0.669	-1.146	H	0.144	0.460	-5.245	H	6.285	-0.855	-3.245
C	-4.169	1.295	-2.103	C	-3.440	-3.955	-0.392	H	6.649	-1.822	-1.794
N	-2.822	1.126	-1.786	C	-5.718	-3.169	-1.183	H	6.120	-2.624	-3.289
C	-4.399	-0.633	0.914	H	-3.891	-2.044	-1.239	H	3.491	3.365	-2.666
C	-4.609	-2.021	0.768	C	-3.724	1.965	3.548	H	1.979	2.903	-1.825
C	-5.059	-2.727	1.893	H	-3.802	1.879	1.415	H	2.620	4.561	-1.682
C	-5.286	-2.080	3.105	C	-5.793	2.279	2.128	H	5.618	3.787	-1.313
C	-5.068	-0.708	3.221	C	-0.542	-1.777	-3.929	H	4.800	4.946	-0.243
C	-4.623	0.048	2.130	H	-2.090	-1.055	-2.660	H	5.633	3.540	0.450

H	0.035	-0.234	4.637
H	-0.029	1.523	4.864
H	-0.540	0.801	3.313
H	2.497	-0.120	5.362
H	3.678	0.776	4.377
H	2.524	1.659	5.404
H	-3.509	3.043	3.531
H	-4.343	1.769	4.438
H	-2.773	1.429	3.667
H	-5.653	3.369	2.184
H	-6.292	2.050	1.175
H	-6.471	1.981	2.943
H	-3.242	-4.407	-1.376
H	-2.477	-3.662	0.045
H	-3.885	-4.735	0.244
H	-5.545	-3.658	-2.154
H	-6.254	-3.882	-0.538
H	-6.379	-2.306	-1.350
H	-0.902	-2.812	-3.836
H	-0.137	-1.663	-4.947
H	0.277	-1.644	-3.212
H	-3.164	-2.025	-4.696
H	-3.681	-0.337	-4.467
H	-2.459	-0.733	-5.698
H	-1.468	5.318	-0.139
H	-0.343	3.947	-0.381
H	-0.365	5.312	-1.531
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H	-2.420	5.545	-3.161
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TS6

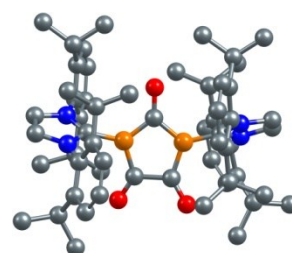
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C	7.718	5.223	11.409
C	8.145	5.967	10.356
B	5.262	4.134	8.747
C	4.556	4.933	7.680
O	4.059	5.950	7.272
C	5.857	3.667	11.894
C	7.483	6.275	7.977
C	4.714	2.655	8.674
O	4.746	1.778	9.573
B	4.099	2.520	7.219
C	4.747	3.572	6.359
O	5.214	3.967	5.322
C	2.954	1.603	6.742
N	1.929	1.920	5.864
C	1.051	0.853	5.731
C	1.512	-0.147	6.524
N	2.669	0.310	7.146
C	1.814	3.143	5.099
C	3.482	-0.572	7.955
H	8.962	6.672	10.264
H	8.071	5.162	12.431
H	0.187	0.907	5.081
H	1.139	-1.149	6.700

C	2.416	3.168	3.819
C	2.314	4.347	3.070
C	1.643	5.458	3.571
C	1.034	5.395	4.821
C	1.081	4.236	5.612
C	3.113	1.951	3.220
H	2.781	4.396	2.085
H	1.593	6.379	2.986
H	0.499	6.265	5.207
C	0.240	4.258	6.891
C	3.031	-0.901	9.250
C	3.774	-1.841	9.975
C	4.927	-2.416	9.444
C	5.352	-2.067	8.164
C	4.634	-1.151	7.383
C	1.801	-0.263	9.880
H	3.453	-2.109	10.983
H	5.499	-3.137	10.031
H	6.256	-2.522	7.754
C	5.114	-0.837	5.972
C	7.038	7.600	7.792
C	7.276	8.191	6.544
C	7.921	7.493	5.528
C	8.345	6.181	5.739
C	8.147	5.542	6.968
C	6.337	8.398	8.886
H	6.939	9.214	6.365
H	8.086	7.968	4.559
H	8.838	5.642	4.930
C	8.678	4.134	7.212
C	6.359	2.405	12.274
C	5.649	1.696	13.251
C	4.481	2.211	13.810
C	4.003	3.456	13.407

C	4.686	4.221	12.451
C	7.618	1.807	11.663
H	6.008	0.713	13.562
H	3.936	1.636	14.562
H	3.086	3.851	13.849
C	4.154	5.596	12.069
C	5.003	8.995	8.408
H	6.107	7.708	9.712
C	7.261	9.499	9.440
H	4.491	9.486	9.250
H	5.158	9.756	7.629
H	4.347	8.213	8.003
H	6.761	10.047	10.253
H	8.201	9.088	9.836
H	7.521	10.224	8.654
C	10.090	4.184	7.831
H	8.005	3.649	7.936
C	8.682	3.259	5.950
H	10.454	3.165	8.031
H	10.797	4.669	7.140
H	10.106	4.741	8.778
H	8.932	2.222	6.222
H	7.701	3.260	5.458
H	9.440	3.592	5.224
C	4.127	6.547	13.279
H	4.835	6.032	11.324
C	2.769	5.497	11.406
H	3.790	7.548	12.970
H	3.437	6.188	14.057
H	5.123	6.646	13.735
H	2.425	6.493	11.089
H	2.806	4.849	10.520
H	2.022	5.086	12.103
C	7.360	0.405	11.087

H	7.921	2.450	10.824
C	8.775	1.784	12.680
H	8.256	0.046	10.557
H	7.137	-0.322	11.883
H	6.513	0.428	10.389
H	9.687	1.380	12.215
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H	8.527	1.146	13.542
C	2.144	0.423	11.213
H	1.443	0.521	9.198
C	0.663	-1.285	10.058
H	4.421	-0.108	5.529
C	6.505	-0.180	5.987
C	5.097	-2.090	5.079
C	0.845	3.660	8.167
H	0.092	5.332	7.096
C	-1.159	3.667	6.622
C	4.447	2.290	2.537
H	3.338	1.254	4.040
C	2.172	1.226	2.237
H	2.658	0.323	1.835
H	1.231	0.919	2.717
H	1.917	1.881	1.390
H	4.953	1.361	2.231
H	4.298	2.890	1.626
H	5.106	2.845	3.217
H	0.259	3.998	9.035
H	0.815	2.561	8.166
H	1.887	3.972	8.313
H	-1.812	3.826	7.494
H	-1.633	4.133	5.747
H	-1.103	2.582	6.445
H	1.268	0.973	11.589
H	2.426	-0.312	11.982

H	2.979	1.123	11.080
H	-0.226	-0.798	10.484
H	0.373	-1.749	9.103
H	0.963	-2.094	10.742
H	5.398	-1.831	4.052
H	5.795	-2.857	5.447
H	4.094	-2.541	5.038
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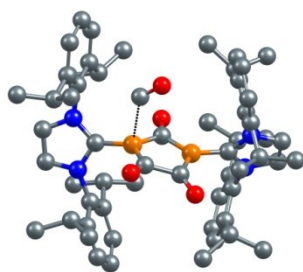


3CO_c

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C	13.803	7.256	1.345
C	13.000	7.558	0.235
C	11.849	8.332	0.362
C	11.471	8.828	1.608
N	14.203	7.510	3.762
C	13.934	6.569	4.723
N	14.894	6.752	5.681
C	15.747	7.790	5.319
C	15.306	8.271	4.126
B	12.818	5.481	4.649
C	12.935	4.314	3.611
O	13.897	3.919	2.928
C	15.059	5.989	6.901
C	15.655	4.710	6.830
C	15.884	4.047	8.045

C	15.539	4.627	9.264	C	6.807	7.737	3.459	H	13.883	8.340	7.173
C	14.941	5.884	9.298	C	7.274	6.733	2.612	H	7.731	5.216	7.159
C	14.684	6.597	8.118	C	7.742	5.512	3.116	H	8.867	3.730	2.697
C	16.094	4.075	5.518	C	7.284	6.193	6.920	H	10.135	3.548	7.601
C	15.806	2.567	5.457	C	8.163	7.260	7.595	H	9.303	1.003	3.592
C	14.025	7.969	8.198	C	8.185	4.408	2.164	H	8.160	-1.170	3.161
C	12.629	7.883	8.839	C	8.979	4.937	0.961	H	9.222	-1.986	4.333
C	15.080	6.445	1.169	C	5.852	6.203	7.485	H	8.050	-0.775	4.892
C	14.905	5.246	0.226	C	6.971	3.582	1.698	H	10.118	-0.368	1.764
C	11.834	9.175	4.093	C	8.748	-1.025	4.080	H	11.482	0.480	2.517
C	10.336	9.033	4.393	C	9.714	2.264	9.277	H	11.215	-1.268	2.825
C	11.478	5.396	5.456	C	17.588	4.357	5.260	H	9.427	3.093	9.941
O	11.089	6.107	6.430	C	14.926	8.976	8.936	H	8.793	1.827	8.862
B	10.725	4.219	4.747	C	16.228	7.352	0.682	H	10.206	1.492	9.888
C	11.540	3.664	3.532	C	12.270	10.652	4.151	H	11.591	4.334	9.344
O	11.225	2.863	2.633	H	6.118	3.338	5.523	H	12.436	2.778	9.471
C	9.374	3.563	5.165	H	7.556	1.091	6.339	H	12.597	3.772	7.998
N	9.224	2.300	5.676	H	6.464	8.348	5.495	H	9.421	4.090	0.417
C	7.881	2.032	5.914	H	6.441	8.677	3.039	H	8.344	5.496	0.256
C	7.181	3.131	5.527	H	7.273	6.895	1.533	H	9.804	5.589	1.281
N	8.105	4.068	5.075	H	11.877	-1.386	4.882	H	7.302	2.757	1.048
C	10.309	1.401	6.014	H	13.141	-1.035	6.981	H	6.423	3.147	2.546
C	11.013	1.632	7.217	H	12.606	0.877	8.458	H	6.267	4.206	1.125
C	12.035	0.729	7.541	H	15.666	9.083	3.505	H	8.164	7.107	8.685
C	12.336	-0.348	6.710	H	16.581	8.082	5.945	H	9.198	7.184	7.234
C	11.622	-0.547	5.531	H	13.281	7.168	-0.744	H	7.782	8.275	7.402
C	10.591	0.322	5.149	H	11.238	8.547	-0.516	H	5.870	6.044	8.574
C	10.662	2.768	8.171	H	10.568	9.434	1.696	H	5.355	7.167	7.296
C	11.898	3.443	8.778	H	14.660	6.323	10.257	H	5.227	5.416	7.036
C	9.813	0.068	3.864	H	15.731	4.091	10.196	H	12.169	8.883	8.868
C	10.723	-0.294	2.680	H	16.345	3.059	8.029	H	11.980	7.219	8.249
C	7.725	5.350	4.521	H	15.352	6.031	2.151	H	12.685	7.513	9.874
C	7.279	6.353	5.406	H	12.363	8.634	4.891	H	14.460	9.973	8.938
C	6.815	7.549	4.838	H	15.520	4.523	4.694	H	15.082	8.679	9.984

H	15.917	9.063	8.464
H	17.895	3.925	4.296
H	17.801	5.436	5.231
H	18.214	3.912	6.049
H	15.984	2.204	4.436
H	16.454	1.993	6.138
H	14.758	2.349	5.705
H	17.159	6.772	0.592
H	15.997	7.778	-0.306
H	16.417	8.190	1.369
H	15.830	4.652	0.217
H	14.095	4.590	0.570
H	14.709	5.562	-0.810
H	12.021	11.086	5.132
H	13.353	10.767	3.994
H	11.754	11.242	3.378
H	10.122	9.408	5.404
H	9.718	9.609	3.687
H	10.021	7.983	4.357



TS7

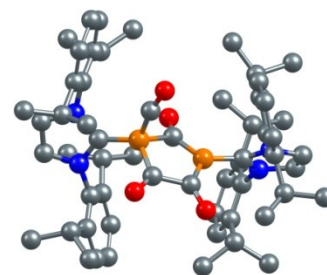
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C	3.174	2.947	1.816
N	2.919	2.119	5.431
C	3.838	1.594	6.302

N	3.089	0.990	7.281
C	1.732	1.138	7.016
C	1.626	1.849	5.863
B	5.398	1.754	6.310
C	6.053	2.772	7.299
C	7.564	2.466	7.311
O	8.332	2.925	8.172
C	3.576	0.180	8.381
C	3.849	-1.182	8.126
C	4.194	-1.981	9.223
C	4.266	-1.449	10.509
C	4.003	-0.099	10.724
C	3.644	0.751	9.669
C	3.735	-1.794	6.734
C	3.306	2.210	9.947
C	3.550	4.969	5.645
C	2.704	0.701	2.885
C	6.482	0.981	5.489
O	6.314	0.159	4.539
B	7.846	1.488	6.110
C	9.287	1.416	5.478
N	9.869	2.493	4.847
C	11.138	2.168	4.391
C	11.370	0.880	4.746
N	10.234	0.420	5.405
C	9.244	3.765	4.541
C	8.459	3.843	3.369
C	7.924	5.095	3.040
C	8.175	6.215	3.830
C	8.969	6.108	4.969
C	9.532	4.883	5.354
C	8.246	2.648	2.448
C	10.455	4.812	6.564
C	10.212	-0.916	5.969

C	10.908	-1.127	7.179
C	10.948	-2.437	7.677
C	10.322	-3.481	7.002
C	9.651	-3.240	5.804
C	9.586	-1.954	5.246
C	11.609	-0.007	7.940
C	8.895	-1.715	3.909
O	5.555	3.669	8.007
C	7.970	-0.291	7.957
O	7.233	-0.703	8.730
H	11.746	2.883	3.850
H	12.231	0.240	4.601
H	7.301	5.191	2.150
H	7.745	7.182	3.557
H	9.157	6.993	5.579
H	11.470	-2.636	8.614
H	10.356	-4.493	7.412
H	9.166	-4.068	5.286
H	0.979	0.718	7.671
H	0.761	2.188	5.306
H	4.417	-3.037	9.065
H	4.543	-2.090	11.348
H	4.076	0.309	11.733
H	3.832	6.011	3.138
H	3.566	4.882	0.950
H	3.066	2.457	0.846
C	4.843	-2.813	6.434
C	2.348	-2.436	6.532
H	3.851	-0.987	5.995
C	4.324	2.889	10.877
H	3.349	2.757	8.994
C	1.882	2.334	10.523
C	3.844	-0.082	2.211
H	2.603	0.303	3.905

C	1.362	0.471	2.166
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C	2.184	5.588	6.002
H	3.808	4.243	6.431
C	6.815	2.555	1.909
C	9.261	2.678	1.287
H	8.421	1.731	3.028
C	9.940	5.623	7.763
H	10.500	3.764	6.892
C	11.877	5.272	6.179
C	7.801	-2.741	3.591
H	8.376	-0.744	3.965
C	9.922	-1.677	2.759
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C	13.139	-0.132	7.807
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H	5.838	-2.381	6.599
H	4.749	-3.721	7.050
H	2.260	-2.844	5.513
H	2.196	-3.262	7.244
H	1.534	-1.712	6.677
H	1.627	3.393	10.682
H	1.124	1.902	9.853
H	1.805	1.817	11.492
H	4.074	3.955	10.975
H	4.314	2.453	11.888
H	5.339	2.830	10.465
H	2.237	6.078	6.986
H	1.890	6.345	5.258
H	1.388	4.831	6.046
H	4.766	6.402	6.713
H	5.622	5.622	5.373
H	4.418	6.900	5.042

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H	4.027	0.278	1.187
H	4.772	0.002	2.797
H	1.113	-0.600	2.161
H	0.537	1.011	2.655
H	1.405	0.807	1.119
H	9.131	1.794	0.645
H	9.113	3.575	0.665
H	10.300	2.686	1.646
H	6.690	1.615	1.352
H	6.081	2.558	2.725
H	6.577	3.381	1.222
H	12.551	5.189	7.044
H	12.304	4.673	5.361
H	11.871	6.324	5.853
H	10.601	5.454	8.626
H	9.940	6.705	7.559
H	8.931	5.302	8.051
H	7.253	-2.416	2.695
H	8.213	-3.742	3.382
H	7.074	-2.818	4.409
H	9.410	-1.483	1.803
H	10.678	-0.892	2.897
H	10.446	-2.642	2.671
H	11.689	0.906	9.908
H	10.119	0.171	9.535
H	11.510	-0.858	9.965
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H	13.463	-0.125	6.755

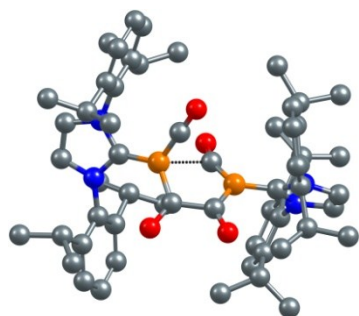


4CO_a

C	9.811	-1.990	5.180
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C	11.033	-2.386	7.695
C	10.518	-3.466	6.984
C	9.911	-3.268	5.744
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C	9.327	1.334	5.435
N	9.807	2.431	4.758
C	11.084	2.178	4.270
C	11.415	0.913	4.635
B	7.957	1.145	6.205
C	6.412	1.073	5.370
O	6.341	0.531	4.254
C	9.137	3.685	4.454
C	8.386	3.755	3.259
C	7.821	4.994	2.931
C	8.023	6.115	3.733
C	8.801	6.021	4.884
C	9.391	4.809	5.271
C	8.247	2.575	2.304
C	9.335	2.642	1.211
C	10.317	4.771	6.480
C	11.731	5.247	6.086
C	11.533	0.081	7.985
C	13.069	-0.004	8.060
C	9.167	-1.786	3.815

C	10.195	-2.008	2.688	C	3.715	0.044	2.070	H	2.269	-2.684	5.573
B	5.406	1.689	6.347	C	6.861	2.480	1.656	H	2.110	-3.033	7.312
C	6.081	2.539	7.435	C	9.796	5.597	7.667	H	1.620	-1.447	6.673
O	5.621	3.345	8.278	C	10.917	0.172	9.391	H	1.302	3.231	10.736
C	3.847	1.586	6.328	C	7.930	-2.669	3.596	H	0.959	1.695	9.906
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N	3.081	1.025	7.325	H	12.310	0.327	4.467	H	5.049	3.046	10.547
C	3.213	2.895	4.266	H	7.217	5.080	2.027	H	2.438	6.015	7.203
C	3.019	2.294	3.006	H	7.571	7.070	3.459	H	2.109	6.398	5.494
C	3.181	3.108	1.875	H	8.960	6.907	5.500	H	1.518	4.874	6.196
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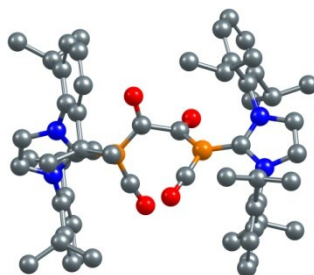
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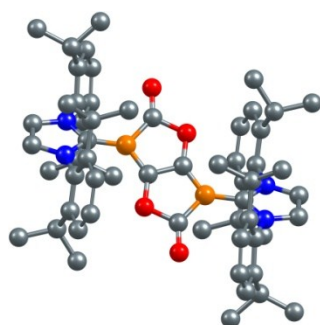
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4CO_b

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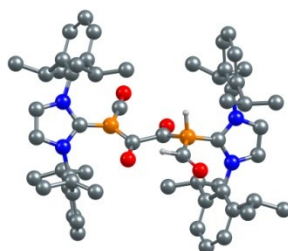
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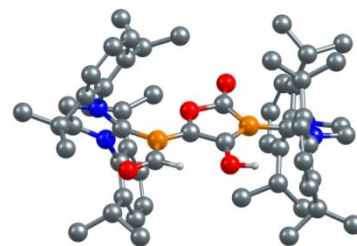


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 C -0.428 3.872 20.153
 B -1.618 0.289 20.715

C -2.641 -0.256 19.578
 O -3.193 0.483 18.753
 C -5.260 -0.844 18.441
 O -5.959 -0.053 17.927
 C 1.069 0.866 18.860
 C 2.303 0.531 19.463
 C 3.103 -0.407 18.798
 C 2.709 -0.969 17.587
 C 1.512 -0.581 16.994
 C 0.670 0.359 17.605
 C 2.824 1.193 20.735
 C 3.819 2.318 20.382
 C -0.564 0.861 16.869
 C -0.175 1.998 15.902
 C -3.803 3.854 19.568
 C -3.683 5.319 19.106
 C -0.797 2.585 23.556
 C 0.072 3.736 24.095
 C -0.696 -0.749 21.519
 O 0.491 -0.588 21.816
 O -2.311 -2.616 20.006
 C -3.083 -1.750 19.556
 B -4.523 -1.974 19.010
 C -5.264 -3.316 19.163
 N -4.776 -4.590 18.950
 C -5.750 -5.537 19.256
 C -6.857 -4.865 19.668
 N -6.556 -3.510 19.613
 C -3.552 -4.943 18.261
 C -2.507 -5.550 18.990
 C -1.368 -5.941 18.275
 C -1.266 -5.731 16.902
 C -2.317 -5.138 16.208
 C -3.491 -4.743 16.865

C	-2.591	-5.816	20.487	H	-2.980	3.454	24.925	H	-3.840	-2.173	15.845
C	-2.912	-7.298	20.766	H	-5.109	4.365	24.044	H	-3.479	-3.230	14.455
C	-4.651	-4.190	16.045	H	-5.481	4.525	21.601	H	4.155	2.830	21.297
C	-5.267	-5.292	15.164	H	-2.236	-4.990	15.129	H	4.708	1.907	19.880
C	-7.462	-2.475	20.052	H	1.965	1.632	21.260	H	3.382	3.074	19.714
C	-8.534	-2.117	19.208	H	-1.268	1.271	17.605	H	3.743	0.723	22.642
C	-9.444	-1.163	19.686	H	-0.239	2.096	22.745	H	2.801	-0.618	21.948
C	-9.286	-0.585	20.942	H	-3.038	3.261	19.046	H	4.422	-0.206	21.300
C	-8.211	-0.951	21.751	H	-7.840	-3.324	17.589	H	-1.070	2.386	15.392
C	-7.276	-1.906	21.332	H	-5.410	-2.889	21.671	H	0.304	2.838	16.427
C	-8.737	-2.733	17.829	H	-5.431	-3.848	16.740	H	0.526	1.637	15.135
C	-9.941	-3.692	17.825	H	-3.411	-5.202	20.886	H	-2.274	0.142	15.750
C	-6.147	-2.328	22.263	H	-5.852	-3.602	24.010	H	-0.746	-0.603	15.239
C	-6.678	-3.263	23.366	H	-7.414	-2.746	24.002	H	-1.524	-1.106	16.763
C	-8.887	-1.666	16.730	H	-7.167	-4.153	22.943	H	-0.061	1.065	24.922
C	-5.405	-1.126	22.867	H	-4.537	-1.475	23.446	H	-1.480	1.936	25.543
C	-4.241	-2.970	15.205	H	-5.035	-0.453	22.081	H	-1.672	0.709	24.263
C	-1.313	-5.402	21.234	H	-6.045	-0.546	23.549	H	1.029	3.347	24.474
C	3.485	0.203	21.707	H	-10.053	-4.166	16.838	H	0.291	4.480	23.314
C	-1.312	-0.246	16.114	H	-9.832	-4.490	18.574	H	-0.433	4.257	24.923
C	-5.164	3.270	19.159	H	-10.874	-3.152	18.048	H	-5.257	3.271	18.064
C	-1.023	1.514	24.635	H	-8.936	-2.149	15.743	H	-5.272	2.232	19.496
H	-7.823	-5.220	20.005	H	-9.813	-1.085	16.857	H	-6.002	3.861	19.562
H	-5.566	-6.597	19.134	H	-8.042	-0.965	16.733	H	-3.832	5.391	18.018
H	-8.096	-0.489	22.733	H	-1.465	-5.508	22.319	H	-4.443	5.948	19.594
H	-10.004	0.159	21.294	H	-0.458	-6.041	20.964	H	-2.696	5.747	19.341
H	-10.284	-0.864	19.056	H	-1.060	-4.357	21.018	H	-1.216	-1.653	21.930
H	-0.362	-6.034	16.369	H	-3.007	-7.471	21.849	H	-2.454	0.594	21.568
H	-0.538	-6.406	18.811	H	-3.848	-7.623	20.288				
H	1.330	3.585	18.818	H	-2.107	-7.948	20.390				
H	-0.572	4.925	20.357	H	-6.138	-4.902	14.615				
H	1.221	-1.007	16.033	H	-4.541	-5.662	14.424				
H	3.347	-1.708	17.096	H	-5.599	-6.151	15.765				
H	4.054	-0.703	19.244	H	-5.114	-2.571	14.666				



5

C	-1.957	1.719	23.068	C	-2.803	-1.912	19.809	C	-0.567	-0.240	23.900
C	-2.303	2.378	21.868	B	-4.217	-1.964	19.318	H	-8.284	-4.381	19.016
C	-3.578	2.944	21.644	C	-5.243	-3.097	19.205	H	-6.219	-6.244	18.868
C	-4.526	2.813	22.669	N	-5.008	-4.462	19.082	H	-8.548	-0.010	22.114
C	-4.222	2.152	23.857	C	-6.203	-5.166	18.980	H	-9.824	1.090	20.298
C	-2.952	1.615	24.050	C	-7.208	-4.257	19.042	H	-9.572	0.323	17.955
N	-1.286	2.558	20.851	N	-6.629	-3.000	19.180	H	-0.382	-7.060	18.963
C	-0.746	1.589	20.046	C	-3.727	-5.119	19.059	H	-1.725	-7.028	21.043
N	0.180	2.245	19.279	C	-3.301	-5.800	20.225	H	0.867	4.288	19.088
C	0.211	3.595	19.600	C	-2.085	-6.499	20.159	H	-0.977	4.679	21.139
C	-0.697	3.788	20.592	C	-1.328	-6.517	18.990	H	0.468	0.583	14.995
B	-0.990	0.027	20.085	C	-1.771	-5.835	17.857	H	2.920	0.276	15.175
C	-2.318	-0.557	19.762	C	-2.979	-5.126	17.859	H	4.104	0.902	17.257
O	-3.322	0.286	19.268	C	-4.104	-5.795	21.521	H	-2.718	1.108	24.988
C	-4.485	-0.470	18.920	C	-4.659	-7.197	21.830	H	-4.979	2.058	24.638
O	-5.388	0.147	18.367	C	-3.467	-4.430	16.597	H	-5.522	3.233	22.526
C	0.929	1.677	18.177	C	-4.100	-5.448	15.629	H	-1.165	-5.851	16.950
C	2.329	1.540	18.301	C	-7.442	-1.839	19.475	H	2.386	2.098	20.359
C	3.022	1.030	17.193	C	-8.149	-1.226	18.421	H	-1.727	1.716	17.796
C	2.358	0.679	16.021	C	-9.013	-0.173	18.749	H	0.022	1.178	22.432
C	0.979	0.846	15.923	C	-9.152	0.261	20.065	H	-3.163	3.543	19.633
C	0.229	1.357	16.991	C	-8.432	-0.356	21.085	H	-7.158	-2.368	16.919
C	3.107	1.959	19.542	C	-7.569	-1.429	20.818	H	-6.187	-2.887	21.551
C	3.841	3.292	19.294	C	-8.001	-1.662	16.970	H	-4.246	-3.712	16.892
C	-1.258	1.628	16.807	C	-9.262	-2.393	16.475	H	-4.961	-5.120	21.384
C	-1.465	2.964	16.066	C	-6.846	-2.113	21.971	H	-7.305	-3.346	23.712
C	-3.943	3.725	20.386	C	-7.842	-2.813	22.913	H	-8.517	-2.087	23.392
C	-3.979	5.238	20.685	C	-7.655	-0.480	16.049	H	-8.465	-3.542	22.373
C	-0.557	1.199	23.363	C	-5.945	-1.133	22.740	H	-5.398	-1.663	23.535
C	0.167	2.146	24.338	C	-2.358	-3.624	15.906	H	-5.208	-0.665	22.074
C	0.269	-0.821	20.480	C	-3.283	-5.256	22.706	H	-6.533	-0.334	23.216
O	1.347	-0.344	20.892	C	4.101	0.885	20.011	H	-9.129	-2.729	15.435
O	-1.952	-2.850	20.338	C	-1.996	0.487	16.094	H	-9.497	-3.276	17.089
				C	-5.277	3.281	19.767	H	-10.138	-1.727	16.503

H	-7.445	-0.846	15.032	H	-5.273	2.218	19.496
H	-8.492	0.231	15.973	H	-6.123	3.471	20.446
H	-6.775	0.053	16.429	H	-4.180	5.804	19.763
H	-3.913	-5.206	23.607	H	-4.778	5.472	21.405
H	-2.428	-5.910	22.938	H	-3.035	5.608	21.112
H	-2.893	-4.248	22.505	H	0.198	-1.932	20.393
H	-5.274	-7.172	22.742	H	-2.330	-3.733	20.166
H	-5.284	-7.577	21.009	*****			
H	-3.845	-7.919	21.994				
H	-4.488	-4.935	14.736				
H	-3.357	-6.190	15.298				
H	-4.934	-5.990	16.098				
H	-2.783	-3.039	15.077				
H	-1.882	-2.924	16.606				
H	-1.578	-4.275	15.482				
H	4.355	3.622	20.209				
H	4.600	3.180	18.504				
H	3.158	4.096	18.981				
H	4.582	1.212	20.946				
H	3.579	-0.059	20.211				
H	4.901	0.715	19.275				
H	-2.540	3.185	15.975				
H	-0.989	3.802	16.596				
H	-1.038	2.922	15.052				
H	-3.078	0.682	16.108				
H	-1.685	0.382	15.043				
H	-1.824	-0.468	16.608				
H	0.464	-0.611	23.983				
H	-1.030	-0.304	24.897				
H	-1.111	-0.910	23.219				
H	1.195	1.796	24.513				
H	0.220	3.172	23.942				
H	-0.348	2.188	25.310				
H	-5.464	3.858	18.849				