

DFT study on the enantioselectivity of spiroacetalization reaction catalysed by an imidodiphosphoric acid catalyst: how confinement works.

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Full citation 39

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Energies of TS structures of the reaction of 1 with cat I

TS	dist C-O	$\Delta\Delta G$	rmsd	$\Delta\Delta E$ HL	H+ probe	MeOH probe
R-anti-ev(-,+)	2.641	1.8	0.460	0.54	4.5	-0.5
R-anti-ev(-,-)	2.670	0.9	0.235	2.58	0.9	-0.61
R-anti-hc(-,+)	2.607	5.2	0.496	3.02	2.7	-2.5
R-anti-hc(-,-)	2.762	4.3	0.340	3.05	0.9	-1.4
R-anti-ev(+,+)	2.607	6.2	0.737	4.49	0.6	6.8
R-anti-hc(+,+)	2.959	2.6	0.463	0.42	-2.6	-2.6
R-anti-hc(+,+) intermediate		-0.2				
R-anti-hc(+,+) 2 nd step		0.0				
R-gau-ev(-,+)	2.593	0.0	0.358	0.0	0.0	0.0
R-gau-ev(-,-)	2.603	1.3	0.733	0.2	0.0	-0.3
R-gau-hc(-,+)	3.180	4.2	0.311	3.0	-0.6	-4.6
R-gau-hc(-,+) intermediate		-0.7				
R-gau-hc(-,+) 2 nd step		2.0				
R-gau-hc(-,-)	3.94	1.9	0.339	0.1	-3.0	-3.0
R-gau-hc(-,-) intermediate		-14.3	Anomeric P intermediate			
R-gau-hc(-,-) 2 nd step		-0.1	Lead to R-gau-hc(-,+) intermediate			
R-gau-ev(+,+)	2.603	1.3	0.409	0.5	1.4	-1.2
R-gau-hc(+,+)	3.372	4.7	1.644	2.6	-0.2	-3.5
R-gau-hc(+,+) intermediate		-13.2	Anomeric intermediate; Lead to R-gau-hc(-,+) intermediate by R-gau-hc(-,-) 2 nd step			

S-anti-ev(-,+)	2.737	2.4	0.344	-0.1	1.6	-0.4
S-anti-ev(-,-)	3.089	0.7	0.377	-0.4	-2.7	-2.1
S-anti-ev(-,-) intermediate		-4.2				
S-anti-ev(-,-) 2 nd step		-2.4				
S-anti-hc(-,+)	2.744	2.4	0.193	1.4	2.6	-3.2
S-anti-hc(-,-)	3.289	0.3	0.298	-0.4	-2.1	-3.1
S-anti-hc(-,-) intermediate		-14.6	Anomeric P intermediate			
S-anti-hc(-,-) 2 nd step		-2.0	Lead to S-anti-ev(-,-) intermediate			
S-anti-ev(+,+)	2.689	2.3	0.964	0.4	0.2	-0.9
S-anti-ev(+,-)	2.661	0.7	0.469	0.4	2.9	-1.7
S-anti-hc(+,+)	2.746	4.5	0.275	2.8	2.9	-2.6
S-anti-hc(+,-)	2.718	3.2	0.422	2.7	3.4	-2.8
S-gau-ev(-,+)	2.590	0.6	0.599	0.3	3.2	2.9
S-gau-ev(-,-)	2.688	3.2	0.377	1.8	0.0	7.3
S-gau-hc(-,+)	3.071	1.6	0.323	2.08	5.2	-1.8
S-gau-hc(-,+)		0.2				
S-gau-hc(-,+)		0.6				
S-gau-hc(-,-)	3.738	-0.3	0.236	-2.38	-2.2	-2.5
S-gau-hc(-,-) intermediate		-2.7				
S-gau-hc(-,-) 2 nd step		0.6	The same that S-gau-hc(-,-) 2 nd step			
S-gau-ev(+,+)	2.631	2.7	0.702	0.1	-0.9	-0.2
S-gau-ev(+,-)	2.576	1.7	0.514	0.7	3.2	-1.1
S-gau-hc(+,+)	3.836	1.0	0.900	-1.1	-2.9	-2.2
S-gau-hc(+,+)		-2.1				
S-gau-hc(+,+)		0.6	The same that S-gau-hc(-,-) 2 nd step			
S-gau-hc(+,-)	3.725	0.2	0.291	-1.4	-2.1	-0.3
S-gau-hc(+,-) intermediate		-13.5	Anomeric P intermediate;			
S-gau-hc(+,-) 2 nd step		-1.4	Lead to S-gau-hc(-,+)			

Analysis and justification of the relative energies of the TS structures for Cat I.

We discuss the geometric features of these TS structures adopting the perspective of the catalyst as presented in **Figure 2**. Assuming that the catalyst protonates the furan C3 atom via the *pro*-Rp oxygen (C2 symmetry assures identical results for the other oxygen), the alcohol side chain of the substrate is preferentially directed downward to interact with *pro*-Sp O. In TS structures yielding (*R*)-spirocyclic products O, C2 and C4 atoms lie toward the left. For TS structures involving the *pro*-Rp(+) region these atoms clash with the anthryl ring to the right. The solution in **R-gau-ev(+,+)** (+1.3 kcal/mol, **Figure 3b**) and **R-anti-hc(+,+)** (+2.6 kcal/mol) is to rotate the furan so C3' is directed sideways to the right. **R-anti-ev(+,+)** (+6.2 kcal/mol) also rotates the furan, but in doing so it harms the H-bond interactions with the catalyst (the energy of the structure in which the substrate is substituted by a MeOH molecule (see computational methods) is 7.1 kcal/mol higher than for **R-gau-ev(-,+)** structure). **R-gau-hc(+,+)** (+4.7 kcal/mol, **Figure 3c**) cannot rotate the furan and has a higher energy as a consequence of steric interactions.

R-anti-ev(-,-) (+0.9 kcal/mol, **Figure 3d**) and **R-anti-hc(-,-)** (4.3 kcal/mol) are more stable than **R-anti-ev(-,+)** (1.8 kcal/mol, **Figure 3e**) and **R-anti-hc(-,+)** (5.2 kcal/mol), respectively. A plausible explanation is the proximity of C2' to the left anthryl ring. These steric effects are supported by larger RMSD values with respect to the structures in which the anthryl groups are not present. In anti-hc TS structures the substrate adopts a less stable conformation than in anti-ev TS structures.

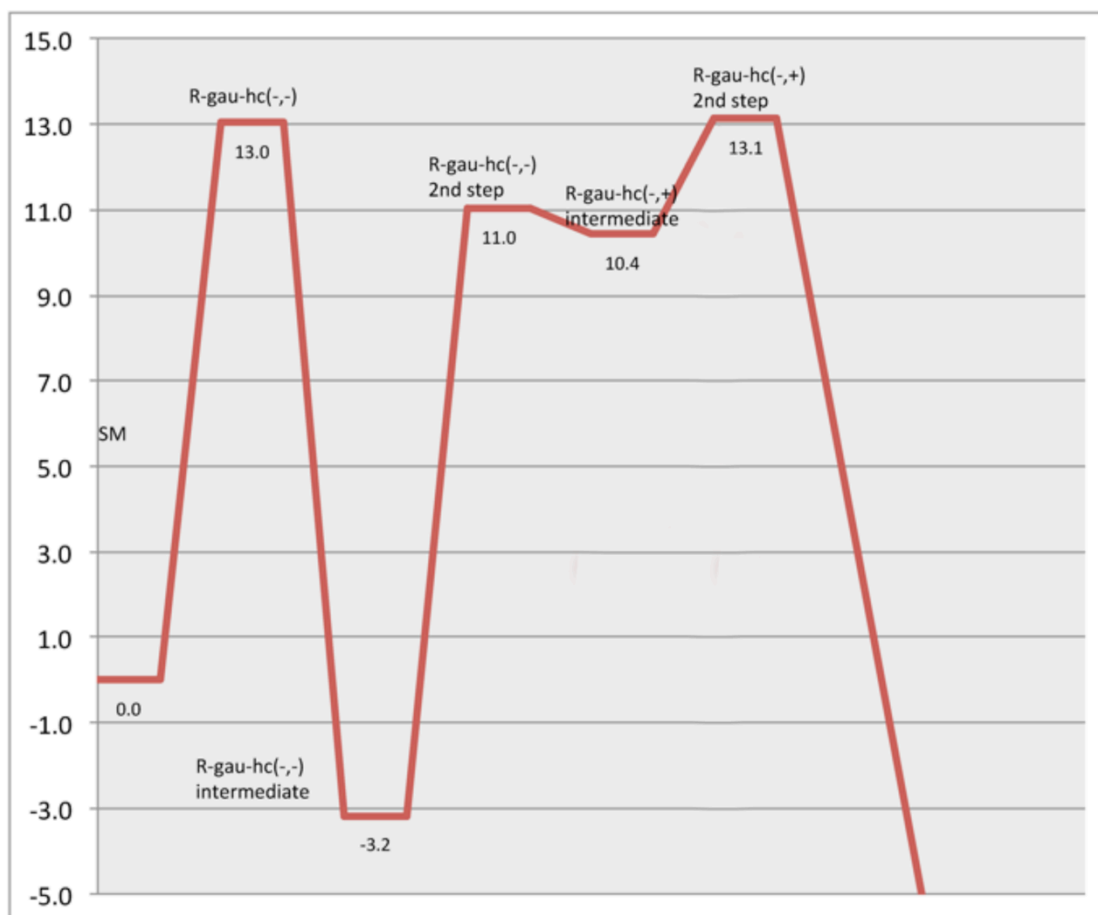
The more stable R TS structure is **R-gau-ev(-,+)** (**Figure 3a**). The steric interactions with C2' are reduced by the change in the 2-3' torsion angle with respect to anti TS structures. In **R-gau-ev(-,-)** (+1.3 kcal/mol, **Figure 3f**) and **R-gau-hc(-,-)** (+1.9 kcal/mol) there are steric interactions (large RMSD) between the furan and the left anthryl catalyst ring. **R-gau-hc(-,+)** (+4.2 kcal/mol) is handicapped by a less stable substrate conformation.

S-anti-ev(-,-) (0.7 kcal/mol, **Figure 4a**) and **S-anti-hc(-,-)** (0.3 kcal/mol, **Figure 4b**) are, respectively, more stable than **S-anti-ev(-,+)** (2.4 kcal/mol) and **S-anti-hc(-,+)** (2.4 kcal/mol, **Figure 4c**). The calculations in which all substrate atoms except H⁺ is maintained –see computational methods- show that the main advantage is in the position occupied by the H⁺ (see supporting information). In **S-anti-hc(-,+)** the C1'-C2' is almost eclipsed. For similar reasons, **S-gau-hc(-,-)** (-0.32 kcal/mol, **Figure 4d**) is more stable than **S-gau-hc(-,+)** (+1.6 kcal/mol, **Figure 4e**). On the contrary, **S-gau-ev(-,+)** (+0.6 kcal/mol) is more stable than **S-gau-ev(-,-)** (+3.2, **Figure 4f**); in this case, the main difference is also in the energy of the QM region, which can be attributed to the poor alignment of the H-bond with C1'-OH group (see results for the H-bond positioning study described in the computational methods section of the SI).

Calculation of energy barriers for step-wise reaction paths

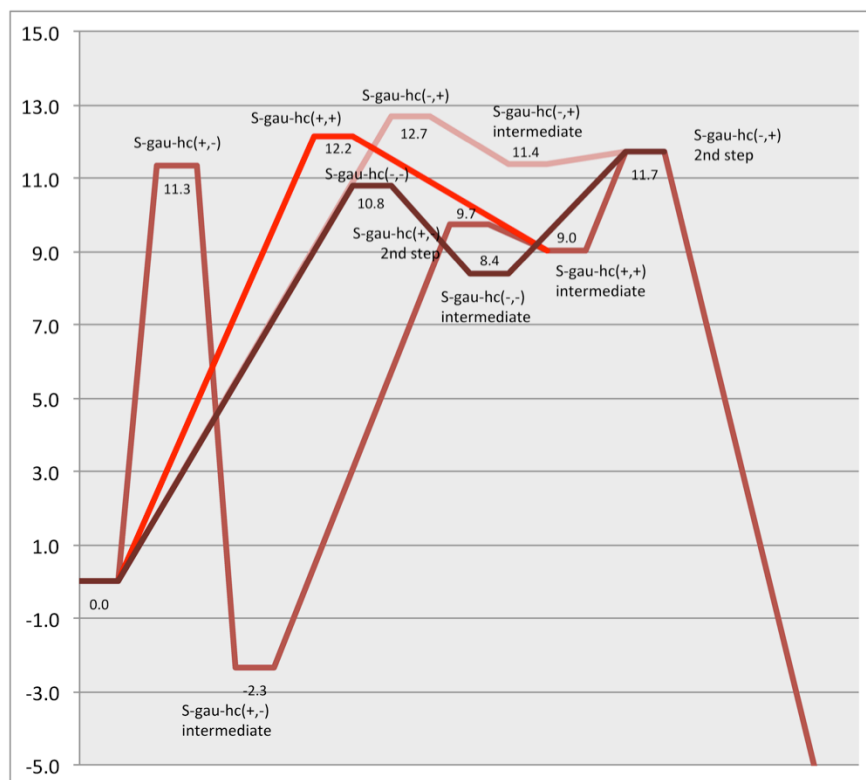
Calculation of energy barriers of reaction paths involving concerted TS structures is straight forward. For reaction paths involving a high energy intermediate in which the C-O bond is formed in a second step, the reaction barrier is defined by one of the two TS in the path: the one with higher energy. This corresponds to the energy of the first TS structure for paths initiated by **R-anti-hc(+,+)**, **R-gau-hc(-,+)** and **S-anti-ev(-,-)**, but the second step for **S-gau-hc(-,+)** and **S-gau-hc(-,+)**. For TS structures leading to anomeric P intermediate the calculation is more complicated because the processes have a higher number of steps.

For the path involving **R-gau-hc(-,-)**:

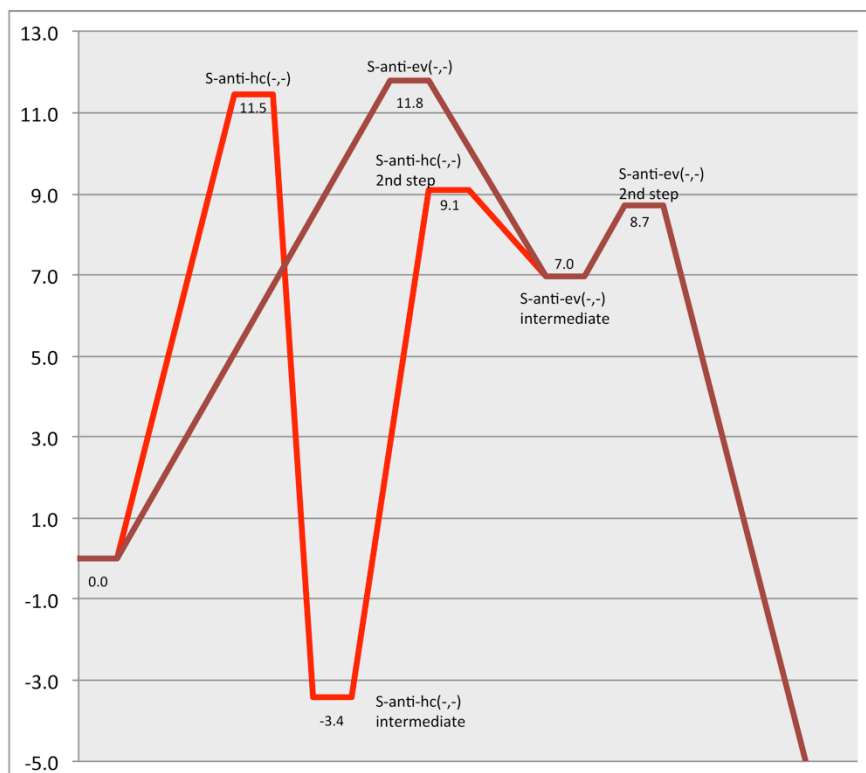


The energy of any of the limiting TS structures (13.1 kcal/mol) is high enough to prevent any contribution from this path to the product distribution – compared with an energy barrier of 11.3 kcal/mol for the path involving **R-gau-ev(-,+)**.

For multi-step reaction paths leading to S product:



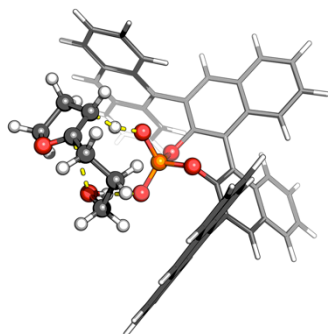
In some cases the first TS structure has a lower energy, so that the rate limiting step corresponds (in the best cases) to S-gau-hc(-,+)^{2nd} step TS (11.7 kcal/mol).



For the paths involving S-anti TS structures, the rate limiting step corresponds to the first TS structure.

Cartesian coordinates for TS structures and intermediates for the reaction of 1 with cat I

R-anti-ev(-,+)

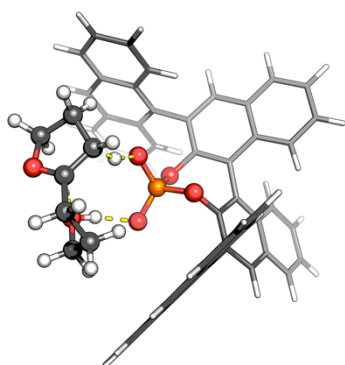


E(RM062X) = -2913.00924692

C	-1.48192	1.45249	-0.09284	C	1.03906	-3.91989	-1.31385
C	-2.83097	1.57562	0.28014	C	-0.01574	-4.80795	-1.00484
C	-0.62216	2.56980	-0.03001	C	2.24884	-4.46902	-0.55701
C	-3.30653	2.79121	0.78439	H	1.12954	-3.63346	-2.36188
C	-1.08168	3.77157	0.56864	C	-1.40043	-4.80487	-1.54412
C	-2.44195	3.87822	0.95630	O	0.27583	-5.69426	-0.10476
C	0.76094	2.42611	-0.56997	H	2.82992	-3.67530	-0.08552
C	1.25831	3.24631	-1.61582	H	2.90835	-5.05928	-1.20112
C	1.58245	1.41391	-0.03183	H	-0.83917	-2.75234	1.43013
C	2.61874	3.13118	-2.00142	C	-2.19087	-3.59909	-0.98163
C	2.93144	1.31876	-0.41238	H	-1.34893	-4.73306	-2.63492
C	3.44560	2.18808	-1.38039	H	-1.89014	-5.74318	-1.26755
H	4.48748	2.10421	-1.67004	C	1.55792	-5.33678	0.49719
H	-4.34824	2.87469	1.07478	O	-1.04090	-3.68155	1.15341
C	-2.91903	5.07033	1.52444	H	-3.18644	-3.60624	-1.43924
C	-2.05498	6.14610	1.73226	H	-1.69790	-2.66364	-1.27334
H	-3.95808	5.16655	1.81664	H	2.06060	-6.26750	0.75511
H	-2.42758	7.06082	2.17494	H	1.29334	-4.76936	1.39355
C	-0.70888	6.04002	1.38408	C	-2.30919	-3.66302	0.54006
C	-0.22030	4.86328	0.81235	H	-2.88404	-2.80109	0.89126
H	-0.03936	6.87184	1.56142	H	-2.84965	-4.57422	0.83084
H	0.83417	4.81357	0.57658	O	-0.66114	-1.12471	1.55799
C	3.13395	3.95575	-3.01428	C	3.81895	0.28863	0.18773
C	2.30760	4.87468	-3.66204	C	4.23226	-0.83329	-0.58098
H	4.17369	3.88320	-3.31092	C	4.28006	0.43154	1.52428
H	2.70966	5.50480	-4.44485	C	5.12208	-1.78219	-0.01564
C	0.96117	4.97300	-3.31265	C	3.77347	-1.04395	-1.90173
C	0.43482	4.16398	-2.30325	C	5.14568	-0.54744	2.07625
H	0.32083	5.67681	-3.82861	C	3.91300	1.53595	2.32742
H	-0.61880	4.25595	-2.07664	C	5.55949	-2.87876	-0.77723
O	0.75155	-1.46047	-0.60869	C	5.56190	-1.63488	1.30276
P	0.02594	-0.54249	0.36684	C	4.21234	-2.14317	-2.64257
H	0.74207	-2.76993	-0.83942	H	3.06875	-0.37083	-2.37103
O	1.08469	0.56710	0.92635	C	5.59861	-0.42109	3.39999
O	-1.02393	0.26445	-0.60457	C	4.37130	1.64549	3.64191
				H	3.27428	2.32365	1.95132
				C	5.10915	-3.05280	-2.08567
				H	6.24461	-3.60592	-0.35755
				H	6.23397	-2.37203	1.73009
				H	3.85329	-2.29094	-3.65288
				H	6.25751	-1.16477	3.83271
				C	5.20834	0.66872	4.17779
				H	4.07723	2.49358	4.24688
				H	5.44620	-3.90268	-2.66488
				H	5.56089	0.75937	5.19714
				C	-3.75872	0.41892	0.17304
				C	-4.21271	-0.02199	-1.09933
				C	-4.21392	-0.24056	1.34694
				C	-5.11782	-1.11114	-1.18263
				C	-3.79898	0.60280	-2.29824
				C	-5.14299	-1.30701	1.23802

C	-3.74976	0.11918	2.63314
C	-5.55937	-1.56580	-2.43602
C	-5.58113	-1.73165	-0.01923
C	-4.24723	0.13781	-3.53621
H	-3.13092	1.45331	-2.29364
C	-5.60361	-1.96076	2.39276
C	-4.21516	-0.54354	3.77058
H	-3.01758	0.90290	2.77320
C	-5.12088	-0.94556	-3.60539
H	-6.24617	-2.40069	-2.51114
H	-6.27977	-2.55867	-0.09324
H	-3.91700	0.62216	-4.44615
H	-6.31432	-2.77567	2.32093
C	-5.14277	-1.57652	3.65156
H	-3.85189	-0.25611	4.74890
H	-5.46532	-1.30126	-4.56785
H	-5.49964	-2.08671	4.53694

R-anti-ev(-,-)



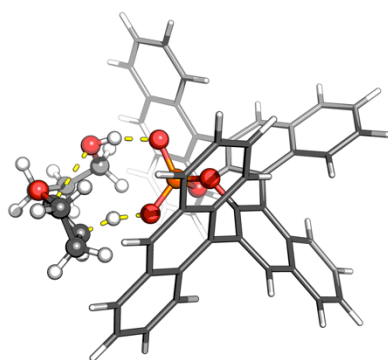
E(RM062X) = -2913.00662210

C	-1.41656	1.48643	-0.06995
C	-2.77574	1.63938	0.24667
C	-0.52998	2.57569	0.04607
C	-3.23739	2.85414	0.76464
C	-0.97846	3.77606	0.65528
C	-2.34904	3.91118	0.99766
C	0.85930	2.40817	-0.47427
C	1.39193	3.24597	-1.48952
C	1.64783	1.35454	0.03914
C	2.75491	3.11016	-1.85894
C	2.99807	1.23498	-0.33239
C	3.54871	2.12648	-1.25918
H	4.59213	2.02583	-1.53771
H	-4.28771	2.96115	1.01299
C	-2.81369	5.10307	1.57616
C	-1.92891	6.14994	1.83793
H	-3.85961	5.22165	1.83358
H	-2.29239	7.06469	2.28808
C	-0.57475	6.01518	1.53287
C	-0.09767	4.83833	0.95150
H	0.10970	6.82481	1.75109
H	0.96239	4.76446	0.74898
C	3.30557	3.95354	-2.83722
C	2.51165	4.91148	-3.46853

H	4.34779	3.86508	-3.12056
H	2.94086	5.55576	-4.22499
C	1.16234	5.03010	-3.13784
C	0.60115	4.20297	-2.16249
H	0.54672	5.76387	-3.64206
H	-0.45403	4.31234	-1.95199
O	0.63754	-1.59710	-0.38860
P	-0.00863	-0.53463	0.49553
H	-0.03513	-2.71287	-0.88748
O	1.13807	0.51424	0.99699
O	-0.96245	0.28902	-0.55873
C	-0.18038	-3.73947	-1.59856
C	-0.15209	-4.79665	-0.65443
C	1.21975	-3.76463	-2.22343
H	-1.07102	-3.62985	-2.21260
C	-1.26798	-5.57115	-0.05750
O	1.05015	-5.15504	-0.32659
H	1.54781	-2.76221	-2.49736
H	1.27879	-4.42695	-3.09348
H	-0.89269	-2.66357	1.87704
C	-2.56737	-4.77731	0.11995
H	-1.43270	-6.42353	-0.73206
H	-0.91860	-5.96328	0.89910
C	2.01554	-4.30458	-1.03894
O	-1.15205	-3.57614	1.61301
H	-3.24043	-5.40245	0.71347
H	-3.05971	-4.60712	-0.84380
H	2.86656	-4.93970	-1.27770
H	2.29021	-3.50840	-0.34297
C	-2.31026	-3.43926	0.82616
H	-2.18153	-2.63262	0.08878
H	-3.17611	-3.17373	1.44239
O	-0.75819	-0.95596	1.71433
C	3.84581	0.15361	0.23722
C	4.25863	-0.93647	-0.57769
C	4.24693	0.20082	1.60020
C	5.06240	-1.96417	-0.02084
C	3.88551	-1.03800	-1.93791
C	5.02902	-0.85296	2.13870
C	3.90200	1.28204	2.44388
C	5.49292	-3.03489	-0.82197
C	5.42743	-1.91881	1.32728
C	4.33222	-2.10284	-2.72319
H	3.24460	-0.30482	-2.40765
C	5.41681	-0.82368	3.48855
C	4.29645	1.29590	3.78329
H	3.33256	2.12647	2.07972
C	5.13485	-3.09685	-2.16809
H	6.10820	-3.82435	-0.40672
H	6.03360	-2.71541	1.74642
H	4.04290	-2.16371	-3.76444
H	6.00995	-1.62611	3.91135
C	5.04730	0.24453	4.30534
H	4.02049	2.12786	4.41840
H	5.47047	-3.92434	-2.77964
H	5.35042	0.26082	5.34428
C	-3.72883	0.51697	0.04583

C	-4.13919	0.15372	-1.26530
C	-4.23896	-0.19678	1.16329
C	-5.05160	-0.91762	-1.44353
C	-3.67315	0.83930	-2.41082
C	-5.17346	-1.24437	0.95999
C	-3.82854	0.09292	2.48461
C	-5.45329	-1.29300	-2.73611
C	-5.56322	-1.59744	-0.33476
C	-4.08291	0.45343	-3.68872
H	-2.99448	1.67798	-2.33316
C	-5.69447	-1.94666	2.05947
C	-4.34882	-0.62143	3.56563
H	-3.09774	0.86208	2.69524
C	-4.96702	-0.61136	-3.85135
H	-6.14690	-2.11246	-2.88382
H	-6.26717	-2.41027	-0.48080
H	-3.71451	0.98486	-4.55681
H	-6.41103	-2.74679	1.91579
C	-5.28274	-1.63397	3.35464
H	-4.02475	-0.38897	4.57189
H	-5.28166	-0.90541	-4.84437
H	-5.68287	-2.18383	4.19666

R-anti-hc(-,+)



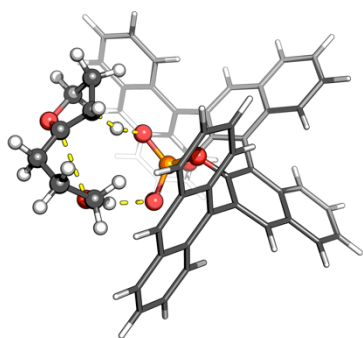
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C	-2.83480	1.52022	0.29799
C	-0.62544	2.53015	0.05659
C	-3.31751	2.71119	0.85153
C	-1.09390	3.70370	0.70334
C	-2.45797	3.79069	1.08086
C	0.75640	2.42283	-0.49473
C	1.24339	3.30857	-1.49135
C	1.59322	1.39447	-0.01108
C	2.61040	3.25066	-1.86416
C	2.94956	1.35523	-0.38076
C	3.45417	2.29766	-1.28385
H	4.50197	2.25936	-1.56162
H	-4.36315	2.78141	1.13143
C	-2.94538	4.95704	1.69199
C	-2.08754	6.02614	1.95245
H	-3.98815	5.03850	1.97542
H	-2.46840	6.92132	2.42693

C	-0.73737	5.93804	1.61528
C	-0.23865	4.78677	1.00171
H	-0.07279	6.76410	1.83329
H	0.81854	4.74956	0.77620
C	3.11577	4.14273	-2.82344
C	2.27287	5.07313	-3.43227
H	4.16067	4.11383	-3.10921
H	2.66724	5.75500	-4.17459
C	0.92013	5.11665	-3.09665
C	0.40386	4.24070	-2.13925
H	0.26718	5.83000	-3.58284
H	-0.65466	4.29223	-1.92258
O	0.73478	-1.52073	-0.62465
P	0.02866	-0.58335	0.35121
H	0.49504	-2.81613	-0.91911
O	1.11701	0.49728	0.91276
O	-1.00832	0.24914	-0.61248
C	0.74518	-3.99060	-1.35743
C	0.10745	-4.93402	-0.51653
C	2.22589	-4.09187	-0.97917
H	0.43545	-3.97115	-2.40097
C	-1.22724	-5.56643	-0.66673
O	0.84365	-5.32691	0.47717
H	2.70814	-3.11811	-1.02366
H	2.77390	-4.80911	-1.59899
H	-1.28851	-2.70933	1.33106
C	-2.31305	-4.57160	-1.10547
H	-1.12012	-6.36180	-1.41615
H	-1.48386	-6.02421	0.28947
C	2.09540	-4.56410	0.46479
O	-1.57550	-3.56565	0.93067
H	-3.27699	-5.07099	-0.97492
H	-2.21868	-4.33685	-2.17091
H	2.87462	-5.23247	0.82683
H	1.94420	-3.72959	1.15566
C	-2.24784	-3.27951	-0.27315
H	-1.72373	-2.49396	-0.83515
H	-3.26103	-2.91717	-0.08188
O	-0.66323	-1.15556	1.54324
C	3.85514	0.30835	0.16321
C	4.34433	-0.72415	-0.68384
C	4.24574	0.33768	1.52987
C	5.20927	-1.71594	-0.15377
C	3.98437	-0.80642	-2.04963
C	5.09184	-0.68019	2.04006
C	3.83030	1.36848	2.40442
C	5.71031	-2.73185	-0.98489
C	5.56231	-1.69153	1.19806
C	4.49663	-1.81930	-2.86335
H	3.29951	-0.10184	-2.50054
C	5.47243	-0.66803	3.39227
C	4.21934	1.36650	3.74552
H	3.21046	2.18657	2.06333
C	5.35960	-2.77673	-2.33388
H	6.37270	-3.49324	-0.59015
H	6.21585	-2.46097	1.59621
H	4.21448	-1.86732	-3.90719

H	6.11468	-1.44336	3.79335
C	5.03371	0.34930	4.23918
H	3.89006	2.16002	4.40402
H	5.74854	-3.56299	-2.96782
H	5.33278	0.35347	5.27944
C	-3.76961	0.37827	0.12215
C	-4.24528	0.03182	-1.17113
C	-4.24485	-0.33198	1.25744
C	-5.20858	-1.00057	-1.31095
C	-3.79782	0.69756	-2.33526
C	-5.22652	-1.34259	1.09400
C	-3.75685	-0.07042	2.55821
C	-5.67450	-1.36101	-2.58595
C	-5.70320	-1.65954	-0.18144
C	-4.26968	0.32491	-3.59557
H	-3.08198	1.50669	-2.28669
C	-5.70915	-2.04275	2.21187
C	-4.24488	-0.77805	3.65848
H	-2.98878	0.67034	2.73661
C	-5.20160	-0.70352	-3.72115
H	-6.40530	-2.15239	-2.70460
H	-6.44706	-2.44098	-0.29788
H	-3.91142	0.83763	-4.47900
H	-6.46037	-2.81554	2.09864
C	-5.22077	-1.75794	3.48679
H	-3.86238	-0.56657	4.64875
H	-5.56327	-0.98824	-4.70078
H	-5.59556	-2.30296	4.34355

R-anti-hc(-,-)



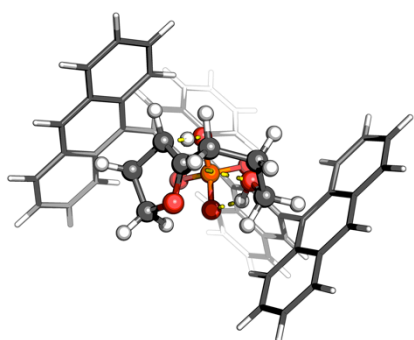
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C	-0.52998	2.57569	0.04607
C	-3.23739	2.85414	0.76464
C	-0.97846	3.77606	0.65528
C	-2.34904	3.91118	0.99766
C	0.85930	2.40817	-0.47427
C	1.39193	3.24597	-1.48952
C	1.64783	1.35454	0.03914
C	2.75491	3.11016	-1.85894
C	2.99807	1.23498	-0.33239
C	3.54871	2.12648	-1.25918
H	4.59213	2.02583	-1.53771

H	-4.28771	2.96115	1.01299
C	-2.81369	5.10307	1.57616
C	-1.92891	6.14994	1.83793
H	-3.85961	5.22165	1.83358
H	-2.29239	7.06469	2.28808
C	-0.57475	6.01518	1.53287
C	-0.09767	4.83833	0.95150
H	0.10970	6.82481	1.75109
H	0.96239	4.76446	0.74898
C	3.30557	3.95354	-2.83722
C	2.51165	4.91148	-3.46853
H	4.34779	3.86508	-3.12056
H	2.94086	5.55576	-4.22499
C	1.16234	5.03010	-3.13784
C	0.60115	4.20297	-2.16249
H	0.54672	5.76387	-3.64206
H	-0.45403	4.31234	-1.95199
O	0.63754	-1.59710	-0.38860
P	-0.00863	-0.53463	0.49553
H	-0.03513	-2.71287	-0.88748
O	1.13807	0.51424	0.99699
O	-0.96245	0.28902	-0.55873
C	-0.18038	-3.73947	-1.59856
C	-0.15209	-4.79665	-0.65443
C	1.21975	-3.76463	-2.22343
H	-1.07102	-3.62985	-2.21260
C	-1.26798	-5.57115	-0.05750
O	1.05015	-5.15504	-0.32659
H	1.54781	-2.76221	-2.49736
H	1.27879	-4.42695	-3.09348
H	-0.89269	-2.66357	1.87704
C	-2.56737	-4.77731	0.11995
H	-1.43270	-6.42353	-0.73206
H	-0.91860	-5.96328	0.89910
C	2.01554	-4.30458	-1.03894
O	-1.15205	-3.57614	1.61301
H	-3.24043	-5.40245	0.71347
H	-3.05971	-4.60712	-0.84380
H	2.86656	-4.93970	-1.27770
H	2.29021	-3.50840	-0.34297
C	-2.31026	-3.43926	0.82616
H	-2.18153	-2.63262	0.08878
H	-3.17611	-3.17373	1.44239
O	-0.75819	-0.95596	1.71433
C	3.84581	0.15361	0.23722
C	4.25863	-0.93647	-0.57769
C	4.24693	0.20082	1.60020
C	5.06240	-1.96417	-0.02084
C	3.88551	-1.03800	-1.93791
C	5.02902	-0.85296	2.13870
C	3.90200	1.28204	2.44388
C	5.49292	-3.03489	-0.82197
C	5.42743	-1.91881	1.32728
C	4.33222	-2.10284	-2.72319
H	3.24460	-0.30482	-2.40765
C	5.41681	-0.82368	3.48855
C	4.29645	1.29590	3.78329

H	3.33256	2.12647	2.07972
C	5.13485	-3.09685	-2.16809
H	6.10820	-3.82435	-0.40672
H	6.03360	-2.71541	1.74642
H	4.04290	-2.16371	-3.76444
H	6.00995	-1.62611	3.91135
C	5.04730	0.24453	4.30534
H	4.02049	2.12786	4.41840
H	5.47047	-3.92434	-2.77964
H	5.35042	0.26082	5.34428
C	-3.72883	0.51697	0.04583
C	-4.13919	0.15372	-1.26530
C	-4.23896	-0.19678	1.16329
C	-5.05160	-0.91762	-1.44353
C	-3.67315	0.83930	-2.41082
C	-5.17346	-1.24437	0.95999
C	-3.82854	0.09292	2.48461
C	-5.45329	-1.29300	-2.73611
C	-5.56322	-1.59744	-0.33476
C	-4.08291	0.45343	-3.68872
H	-2.99448	1.67798	-2.33316
C	-5.69447	-1.94666	2.05947
C	-4.34882	-0.62143	3.56563
H	-3.09774	0.86208	2.69524
C	-4.96702	-0.61136	-3.85135
H	-6.14690	-2.11246	-2.88382
H	-6.26717	-2.41027	-0.48080
H	-3.71451	0.98486	-4.55681
H	-6.41103	-2.74679	1.91579
C	-5.28274	-1.63397	3.35464
H	-4.02475	-0.38897	4.57189
H	-5.28166	-0.90541	-4.84437
H	-5.68287	-2.18383	4.19666

R-anti-ev(+,+)



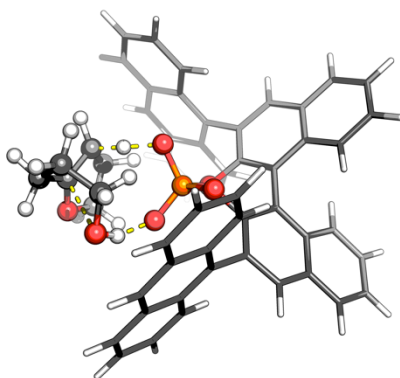
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C	-3.02003	2.91495	1.18181
C	-0.72802	3.75611	1.07037
C	-2.06743	3.88297	1.52449
C	0.98611	2.49933	-0.35017
C	1.56269	3.44933	-1.23314

C	1.69530	1.31632	-0.04731
C	2.89471	3.25910	-1.68568
C	3.01493	1.14548	-0.49409
C	3.61326	2.12251	-1.29519
H	4.63104	1.97628	-1.64013
H	-4.04131	3.00619	1.53513
C	-2.43346	4.96860	2.33602
C	-1.48120	5.91395	2.71869
H	-3.45408	5.08034	2.68269
H	-1.76890	6.74642	3.34779
C	-0.15610	5.77995	2.30534
C	0.22369	4.70852	1.49392
H	0.58175	6.50748	2.61824
H	1.26498	4.62906	1.21256
C	3.48727	4.20228	-2.54041
C	2.76467	5.31665	-2.96804
H	4.50598	4.07198	-2.88618
H	3.22549	6.03760	-3.63092
C	1.44467	5.49547	-2.55564
C	0.84234	4.56961	-1.70101
H	0.88341	6.35333	-2.90305
H	-0.18972	4.73349	-1.42219
O	0.53045	-1.36645	-1.10929
P	-0.06564	-0.51598	-0.00552
H	0.62008	-2.77211	-0.85000
O	1.11765	0.35085	0.73887
O	-0.98840	0.57715	-0.79322
C	1.05028	-3.85655	-0.45894
C	-0.07114	-4.65585	-0.09775
C	1.74266	-3.53433	0.87208
H	1.64260	-4.22297	-1.29630
C	-0.89822	-5.57564	-0.93381
O	-0.32448	-4.66015	1.17079
H	2.07125	-2.49303	0.90900
H	2.60163	-4.18651	1.05622
H	-1.89928	-2.36593	0.30206
C	-2.36993	-5.14134	-1.18727
H	-0.38077	-5.72610	-1.88287
H	-0.88949	-6.52788	-0.39147
C	0.61470	-3.77331	1.87962
O	-2.02665	-2.96957	-0.45936
H	-3.01314	-6.02510	-1.16386
H	-2.43118	-4.70714	-2.18888
H	0.89955	-4.30768	2.78512
H	0.05841	-2.85981	2.09802
C	-2.85795	-4.07437	-0.22039
H	-3.90921	-3.84480	-0.43966
H	-2.79513	-4.41689	0.82180
O	-0.81156	-1.19329	1.10831
C	3.77026	-0.08521	-0.14741
C	3.91411	-1.12748	-1.10190
C	4.32237	-0.24142	1.15147
C	4.61309	-2.31020	-0.74930
C	3.35821	-1.03408	-2.39817
C	5.01305	-1.43545	1.48146
C	4.20796	0.76636	2.13603
C	4.74554	-3.35367	-1.67999

C	5.15627	-2.45056	0.53109
C	3.49578	-2.08232	-3.31009
H	2.80283	-0.16143	-2.71482
C	5.55344	-1.60338	2.76697
C	4.75061	0.58300	3.40956
H	3.70292	1.70150	1.93316
C	4.18830	-3.23763	-2.95309
H	5.27444	-4.26302	-1.42000
H	5.68429	-3.36150	0.79352
H	3.06054	-1.99880	-4.29759
H	6.07968	-2.51310	3.03134
C	5.41942	-0.59844	3.72482
H	4.65272	1.36176	4.15498
H	4.29046	-4.04749	-3.66380
H	5.83777	-0.73496	4.71371
C	-3.65120	0.73079	0.14954
C	-4.01496	-0.18502	1.17359
C	-4.20342	0.58497	-1.15085
C	-4.93443	-1.22660	0.88900
C	-3.46639	-0.10788	2.47458
C	-5.11251	-0.47163	-1.41278
C	-3.87480	1.46880	-2.20400
C	-5.29232	-2.14367	1.89098
C	-5.47399	-1.35704	-0.39368
C	-3.83065	-1.02946	3.45815
H	-2.74512	0.65238	2.74200
C	-5.65100	-0.63423	-2.69977
C	-4.41769	1.29185	-3.47837
H	-3.20002	2.30126	-2.05491
C	-4.74221	-2.04262	3.16832
H	-5.99281	-2.94409	1.68374
H	-6.17119	-2.16172	-0.60350
H	-3.40148	-0.95851	4.44934
H	-6.34218	-1.44141	-2.91232
C	-5.30067	0.24243	-3.72635
H	-4.15257	1.97263	-4.27704
H	-5.02045	-2.75441	3.93478
H	-5.71751	0.10958	-4.71636

R-anti-hc(+,+)



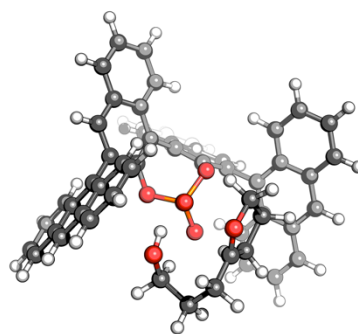
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C	1.62048	1.31355	-0.06512
C	2.96323	1.24482	-0.47104
C	0.83697	2.44238	-0.38394
C	3.50655	2.26380	-1.26012
C	1.36049	3.42938	-1.25866
C	2.71313	3.33892	-1.67820
C	-0.53101	2.53554	0.20510
C	-0.92343	3.61123	1.04500
C	-1.43704	1.48096	-0.04037
C	-2.26166	3.67561	1.51231
C	-2.75655	1.55559	0.43371
C	-3.16690	2.65901	1.18813
H	-4.18736	2.70286	1.55307
H	4.54287	2.19802	-1.57321
C	3.25405	4.32320	-2.52070
C	2.46069	5.38057	-2.96760
H	4.28810	4.26994	-2.84040
H	2.88239	6.13406	-3.62024
C	1.12175	5.46129	-2.58597
C	0.57013	4.49351	-1.74352
H	0.50694	6.27565	-2.94711
H	-0.47701	4.58030	-1.48630
C	-2.67385	4.74844	2.31891
C	-1.76649	5.74293	2.68513
H	-3.69555	4.81238	2.67439
H	-2.08938	6.56548	3.31018
C	-0.44020	5.67038	2.26128
C	-0.01564	4.61231	1.45468
H	0.26401	6.43530	2.56232
H	1.02649	4.58187	1.16756
O	0.65730	-1.33177	-1.26283
C	0.08997	-4.48684	-0.03421
C	1.06449	-3.72084	1.86605
C	-0.94215	-5.23811	-0.79874
H	0.60718	-2.80545	2.23989
H	1.44342	-4.34356	2.67633
C	-1.63352	-4.41873	-1.90260
H	-1.68195	-5.60072	-0.08470
H	-0.43261	-6.09668	-1.25461
C	2.05606	-3.46164	0.72347
H	-0.92697	-4.17770	-2.70522
H	-2.39833	-5.07185	-2.33453
H	2.94105	-4.10012	0.79419
H	2.37443	-2.41745	0.73388
C	-2.26697	-3.12154	-1.35872
O	-2.60109	-3.25757	0.00418
H	-3.17022	-2.89218	-1.93629
H	-1.57149	-2.28987	-1.50664
H	-2.07096	-2.61327	0.50991
O	-0.02933	-4.47895	1.25186
C	1.21622	-3.77897	-0.51987
H	0.81391	-2.65147	-0.93825
H	1.69087	-4.18501	-1.41327
O	-0.66374	-1.48384	0.94068
C	3.80857	0.08556	-0.08579

C	4.28197	-0.04136	1.24783
C	4.13017	-0.91420	-1.04309
C	5.07324	-1.16212	1.60798
C	3.99072	0.92452	2.23846
C	4.93514	-2.01813	-0.66139
C	3.64772	-0.85944	-2.37073
C	5.53043	-1.30604	2.92834
C	5.39935	-2.12899	0.65255
C	4.45155	0.76512	3.54696
H	3.40802	1.80810	2.01490
C	5.24932	-3.01746	-1.59695
C	3.96688	-1.86313	-3.28742
H	3.01233	-0.05258	-2.71011
C	5.21605	-0.34783	3.89179
H	6.13034	-2.16149	3.21593
H	6.00644	-2.98212	0.93740
H	4.21499	1.50923	4.29673
H	5.86260	-3.86545	-1.31567
C	4.76721	-2.93707	-2.90298
H	3.58941	-1.80844	-4.30042
H	5.56953	-0.46653	4.90798
H	5.01120	-3.71218	-3.61801
C	-3.71131	0.44434	0.19212
C	-4.32325	0.28686	-1.07922
C	-4.02241	-0.46423	1.23894
C	-5.24956	-0.76736	-1.28582
C	-4.04292	1.15956	-2.15496
C	-4.96357	-1.50063	1.01233
C	-3.40065	-0.38326	2.50626
C	-5.85264	-0.93797	-2.54265
C	-5.56679	-1.64018	-0.24082
C	-4.65062	0.97511	-3.39868
H	-3.35579	1.98828	-2.04755
C	-5.27511	-2.40577	2.04038
C	-3.71760	-1.29453	3.51540
H	-2.65749	0.37158	2.72598
C	-5.55051	-0.07138	-3.59280
H	-6.55840	-1.74256	-2.71291
H	-6.27843	-2.44218	-0.40783
H	-4.42325	1.64814	-4.21536
H	-5.99290	-3.20128	1.87842
C	-4.65435	-2.30012	3.28484
H	-3.23205	-1.22154	4.48009
H	-6.01847	-0.20936	-4.55898
H	-4.89581	-3.00374	4.07107

R-anti-hc(+,+) intermediate



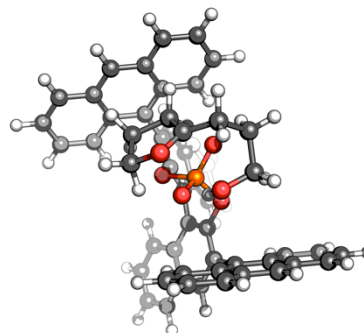
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P	-0.03619	-0.62863	-0.33838
O	-1.09467	0.49610	-0.88642
O	1.09392	0.20339	0.54638
C	1.61004	1.29301	-0.10884
C	2.93836	1.27065	-0.56395
C	0.82203	2.44994	-0.27181
C	3.45615	2.36591	-1.26191
C	1.31851	3.52832	-1.04846
C	2.65280	3.48113	-1.53008
C	-0.52477	2.47376	0.36874
C	-0.88270	3.43897	1.34616
C	-1.44643	1.46304	0.02142
C	-2.20610	3.45200	1.85797
C	-2.75544	1.49458	0.52841
C	-3.13242	2.49409	1.43042
H	-4.14465	2.50392	1.81988
H	4.48055	2.33414	-1.61682
C	3.16587	4.55054	-2.28117
C	2.36260	5.65294	-2.57572
H	4.18553	4.52989	-2.64741
H	2.76256	6.47226	-3.15903
C	1.04156	5.69580	-2.13071
C	0.51762	4.64270	-1.37769
H	0.41886	6.54725	-2.37338
H	-0.51702	4.70423	-1.06790
C	-2.58372	4.41705	2.80522
C	-1.65634	5.35260	3.26492
H	-3.59387	4.44200	3.19674
H	-1.95248	6.09171	3.99806
C	-0.34459	5.32798	2.79271
C	0.04558	4.37759	1.84676
H	0.37505	6.04615	3.16409
H	1.07746	4.37918	1.52299
O	0.58682	-1.25413	-1.54589
C	0.12641	-4.38977	0.59859
C	1.02207	-3.13479	2.27450
C	-0.80496	-5.37212	-0.00054
H	0.47321	-2.21115	2.45169
H	1.42656	-3.56221	3.19171
C	-1.32151	-4.97460	-1.39442
H	-1.63282	-5.52017	0.69277
H	-0.22920	-6.30652	-0.07774
C	2.00408	-3.03697	1.10420

H	-0.51263	-5.00390	-2.13351
H	-2.04696	-5.74222	-1.68025
H	2.95628	-3.51307	1.34575
H	2.17675	-1.99197	0.84927
C	-1.97357	-3.57749	-1.37220
O	-2.53573	-3.32420	-0.10599
H	-2.75446	-3.53181	-2.14022
H	-1.22364	-2.81666	-1.62005
H	-2.04365	-2.56968	0.28342
O	-0.00366	-4.09750	1.82328
C	1.29206	-3.76558	-0.04977
H	0.94313	-3.05334	-0.82617
H	1.88616	-4.53177	-0.56029
O	-0.68312	-1.53633	0.68414
C	3.79865	0.08808	-0.31244
C	4.39138	-0.10123	0.96399
C	4.00079	-0.87958	-1.33171
C	5.17587	-1.25711	1.20879
C	4.22049	0.83308	2.01081
C	4.78445	-2.03026	-1.06086
C	3.42522	-0.74197	-2.61499
C	5.75521	-1.45955	2.47210
C	5.36674	-2.20409	0.19817
C	4.80335	0.61639	3.26108
H	3.63960	1.73583	1.87489
C	4.96820	-3.00612	-2.05401
C	3.61625	-1.72239	-3.59055
H	2.81490	0.11338	-2.87270
C	5.56699	-0.52652	3.49162
H	6.35265	-2.34134	2.67181
H	5.96305	-3.08866	0.39671
H	4.66248	1.33906	4.05454
H	5.56079	-3.89164	-1.85653
C	4.38421	-2.85121	-3.31100
H	3.16402	-1.60691	-4.56715
H	6.01587	-0.68930	4.46299
H	4.52751	-3.60868	-4.07071
C	-3.74045	0.45465	0.13897
C	-4.36965	0.50608	-1.13281
C	-4.05388	-0.60074	1.03608
C	-5.30440	-0.49763	-1.49398
C	-4.09812	1.54005	-2.05763
C	-5.00246	-1.58491	0.65747
C	-3.42455	-0.71982	2.29656
C	-5.92534	-0.46032	-2.75336
C	-5.61441	-1.52505	-0.59794
C	-4.72443	1.56229	-3.30551
H	-3.40524	2.33847	-1.82726
C	-5.31165	-2.63821	1.53404
C	-3.73704	-1.77799	3.15204
H	-2.67740	-0.01033	2.62625
C	-5.63308	0.56437	-3.65340
H	-6.63856	-1.22372	-3.04136
H	-6.33191	-2.28778	-0.88254
H	-4.50475	2.35839	-4.00528
H	-6.03396	-3.39626	1.25492
C	-4.67976	-2.73209	2.77389

H	-3.24312	-1.85958	4.11173
H	-6.11543	0.58694	-4.62211
H	-4.91723	-3.55057	3.44109

R-anti-hc(+,+) 2nd step



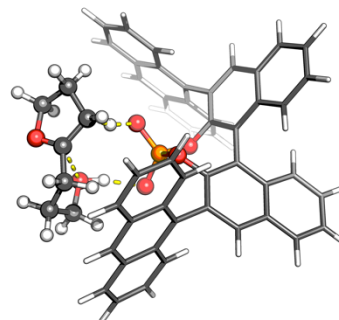
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P	-0.07291	-0.55673	-0.26617
O	-1.14180	0.52859	-0.86657
O	1.05183	0.32786	0.55389
C	1.54575	1.39137	-0.15494
C	0.74617	2.53499	-0.35866
C	3.37573	2.41832	-1.36769
C	1.23222	3.58143	-1.18397
C	2.56395	3.51887	-1.67481
C	-0.60099	2.57111	0.28811
C	-0.96967	3.56588	1.23176
C	-1.50208	1.52318	0.00437
C	-2.28132	3.55573	1.77734
C	-3.18284	2.54408	1.42229
H	-4.18084	2.52855	1.84637
H	4.39758	2.37523	-1.72811
C	3.06600	4.55859	-2.47342
C	2.25546	5.64471	-2.80637
H	4.08287	4.52726	-2.84661
H	2.64733	6.44119	-3.42570
C	0.93756	5.70043	-2.35325
C	0.42387	4.67734	-1.55324
H	0.30940	6.53874	-2.62577
H	-0.60840	4.74732	-1.23732
C	-2.66811	4.54651	2.69379
C	-1.76203	5.53013	3.09138
H	-3.66814	4.55348	3.11117
H	-2.06507	6.28843	3.80178
C	-0.46147	5.52831	2.58861
C	-0.06173	4.55296	1.67249
H	0.24253	6.28354	2.91365
H	0.96215	4.57411	1.32533
O	0.50279	-1.24737	-1.46409
C	0.36099	-4.54789	0.22040
C	0.65242	-3.72293	2.30683
C	-0.27157	-5.30191	-0.88584
H	-0.12855	-2.97629	2.46113
H	0.91252	-4.24486	3.22601

C	-0.83248	-4.31156	-1.93755
H	-1.04950	-5.95671	-0.48774
H	0.51943	-5.90457	-1.35024
C	1.82277	-3.17047	1.49191
H	-0.07587	-3.55944	-2.18541
H	-1.06478	-4.86714	-2.85116
H	2.77369	-3.59687	1.81953
H	1.86450	-2.08277	1.57706
C	-2.08670	-3.62069	-1.37219
O	-1.97362	-3.47772	0.02004
H	-2.97018	-4.24122	-1.56729
H	-2.23054	-2.65395	-1.87136
H	-1.59445	-2.59196	0.27994
O	0.02869	-4.73782	1.43084
C	1.47975	-3.59876	0.05593
H	1.16725	-2.75754	-0.59400
H	2.28740	-4.11221	-0.47949
O	-0.68058	-1.40554	0.82738
C	2.86805	1.35348	-0.61837
C	3.72573	0.18314	-0.30408
C	4.30904	0.05915	0.98460
C	3.89249	-0.85886	-1.25364
C	5.04367	-1.10827	1.31346
C	4.17731	1.07202	1.96199
C	4.62868	-2.01857	-0.90015
C	3.32442	-0.78785	-2.54544
C	5.61429	-1.24413	2.58979
C	5.19553	-2.13104	0.37279
C	4.75187	0.92160	3.22574
H	3.63615	1.98707	1.75968
C	4.77595	-3.06697	-1.82303
C	3.47471	-1.84204	-3.44876
H	2.75043	0.07204	-2.86427
C	5.46689	-0.23294	3.53930
H	6.17454	-2.13348	2.85348
H	5.75294	-3.02414	0.63578
H	5.33125	-3.96008	-1.56160
C	4.19726	-2.97811	-3.08878
H	5.90997	-0.34386	4.52063
H	4.30886	-3.79291	-3.79243
C	-2.79184	1.52078	0.55490
C	-3.72173	0.40239	0.25593
C	-4.39743	0.35130	-0.99141
C	-3.87187	-0.66546	1.18064
C	-5.20893	-0.76879	-1.30472
C	-4.28438	1.39085	-1.94220
C	-4.68883	-1.77496	0.84429
C	-3.20343	-0.67339	2.42646
C	-5.87139	-0.83343	-2.54155
C	-5.34689	-1.81540	-0.38830
C	-4.94984	1.31087	-3.16729
H	-3.68686	2.27202	-1.74841
C	-4.82186	-2.84848	1.74037
C	-3.34103	-1.75176	3.30255
H	-2.55813	0.14056	2.72845
C	-5.73952	0.20202	-3.46677
H	-6.49091	-1.68620	-2.79336

H	-5.96483	-2.67135	-0.63937
H	-5.43981	-3.70323	1.49177
C	-4.14803	-2.83530	2.96137
H	-6.25251	0.14532	-4.41817
H	-4.24962	-3.66906	3.64398
H	3.02642	-1.77812	-4.43187
H	4.64288	1.70515	3.96466
H	-4.85308	2.11336	-3.88723
H	-2.81622	-1.74805	4.24921

R-gau-ev(-,+)



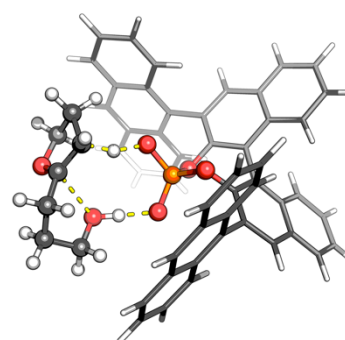
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C	-0.95030	1.69201	-0.06099
C	-2.25292	2.09203	0.27920
C	0.11955	2.60968	0.01726
C	-2.47890	3.37951	0.77747
C	-0.09574	3.88235	0.60666
C	-1.41274	4.26621	0.96883
C	1.45129	2.18381	-0.50545
C	2.11593	2.87610	-1.55193
C	2.03358	1.01681	0.03155
C	3.41474	2.46011	-1.94546
C	3.31509	0.61074	-0.37346
C	4.00782	1.34583	-1.34034
H	4.99628	1.02137	-1.64691
H	-3.48740	3.67636	1.04430
C	-1.64634	5.53288	1.52767
C	-0.58461	6.41038	1.75081
H	-2.64904	5.84075	1.79994
H	-0.77055	7.38387	2.18587
C	0.71750	6.03045	1.42692
C	0.96579	4.77626	0.86483
H	1.53928	6.70926	1.61539
H	1.99159	4.51124	0.64660
C	4.09760	3.15269	-2.95807
C	3.49593	4.23632	-3.59865
H	5.09281	2.84933	-3.26113
H	4.02599	4.76370	-4.38125
C	2.20646	4.63101	-3.24410
C	1.51560	3.95579	-2.23551
H	1.73771	5.46172	-3.75580
H	0.50939	4.27951	-2.00692
O	0.58196	-1.68345	-0.41856
P	0.10209	-0.55911	0.48501

H	-0.43960	-2.43132	-1.05921
O	1.37692	0.31294	1.00897
O	-0.73278	0.42609	-0.54368
C	-1.13457	-3.09239	-1.82985
C	-2.08838	-3.78022	-1.02785
C	-0.22735	-4.20012	-2.37028
H	-1.54244	-2.33561	-2.50039
C	-3.37226	-3.25455	-0.50239
O	-1.78699	-5.01712	-0.80161
H	0.81414	-3.88420	-2.42577
H	-0.54883	-4.55967	-3.35315
H	-0.97113	-2.59481	1.63229
C	-3.73505	-3.80468	0.87864
H	-3.27809	-2.16404	-0.48328
H	-4.14010	-3.50577	-1.24721
C	-0.42711	-5.26075	-1.29052
O	-1.44456	-3.44255	1.46164
H	-3.68832	-4.89812	0.86010
H	-4.76184	-3.52067	1.12777
H	-0.39106	-6.29823	-1.61776
H	0.22196	-5.09719	-0.42550
C	-2.76586	-3.24794	1.91801
H	-2.94379	-2.17483	2.05837
H	-2.92347	-3.74946	2.88202
O	-0.71859	-0.90288	1.68636
C	3.91909	-0.62701	0.18219
C	3.95050	-1.81574	-0.59617
C	4.43634	-0.63958	1.50466
C	4.49311	-3.00305	-0.04175
C	3.43988	-1.85990	-1.91422
C	4.96686	-1.84152	2.03906
C	4.44688	0.52065	2.31213
C	4.52573	-4.18420	-0.80168
C	4.99038	-3.00538	1.26476
C	3.48928	-3.03958	-2.65901
H	2.99385	-0.99159	-2.37981
C	5.47262	-1.86608	3.34930
C	4.95341	0.47887	3.61283
H	4.06999	1.46725	1.94804
C	4.02777	-4.19866	-2.10427
H	4.93659	-5.09744	-0.38751
H	5.39952	-3.91985	1.68191
H	3.09734	-3.05725	-3.66790
H	5.87718	-2.77964	3.76910
C	5.46242	-0.71079	4.13070
H	4.95256	1.37419	4.22117
H	4.05581	-5.11217	-2.68411
H	5.85373	-0.73712	5.13954
C	-3.39740	1.15511	0.13377
C	-3.98849	0.56683	1.28398
C	-3.91974	0.85686	-1.15349
C	-5.11277	-0.28555	1.13776
C	-3.47770	0.79169	2.58291
C	-5.03346	-0.01354	-1.27453
C	-3.36690	1.41125	-2.33065
C	-5.70694	-0.86781	2.26952
C	-5.62455	-0.56260	-0.13291

C	-4.07710	0.20059	3.69697
H	-2.60746	1.41211	2.75000
C	-5.54589	-0.32918	-2.54350
C	-3.88839	1.08661	-3.58462
H	-2.53126	2.09717	-2.29647
C	-5.18993	-0.62370	3.54145
H	-6.56596	-1.52069	2.16913
H	-6.47781	-1.22511	-0.23544
H	-3.67383	0.38005	4.68527
H	-6.39125	-0.99915	-2.64774
C	-4.97158	0.21637	-3.69123
H	-3.45072	1.51353	-4.47785
H	-5.64910	-1.08071	4.40845
H	-5.37093	-0.03214	-4.66606

R-gau-ev(-,-)



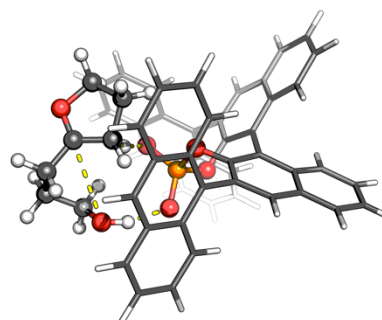
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C	1.85950	1.19684	0.00710
C	3.18824	0.91159	-0.34497
C	1.25891	2.40860	-0.39132
C	3.90364	1.80319	-1.14990
C	1.95355	3.27006	-1.27972
C	3.29290	2.96499	-1.63874
C	-0.11335	2.70852	0.11571
C	-0.40383	3.86830	0.88120
C	-1.13855	1.77017	-0.13586
C	-1.74647	4.13675	1.25420
C	-2.46247	2.04428	0.24610
C	-2.76261	3.23663	0.91325
H	-3.78817	3.43975	1.20197
H	4.92790	1.57063	-1.42003
C	4.00181	3.82121	-2.49634
C	3.38832	4.96073	-3.01814
H	5.02731	3.60375	-2.77085
H	3.93871	5.61440	-3.68245
C	2.06261	5.25133	-2.69752
C	1.34519	4.41313	-1.84127
H	1.58667	6.12811	-3.11746
H	0.31299	4.66155	-1.63441
C	-2.05457	5.29589	1.98421
C	-1.04226	6.17606	2.36777
H	-3.07723	5.51546	2.26753
H	-1.28563	7.06557	2.93440

C	0.28452	5.90362	2.03667
C	0.60691	4.75799	1.30589
H	1.06804	6.58111	2.35091
H	1.65003	4.57245	1.08885
O	-0.86111	-1.15694	1.00775
P	0.00787	-0.50639	-0.06051
H	-0.87148	-2.51356	1.15325
O	-0.86643	0.62883	-0.84719
O	1.15268	0.30708	0.77608
C	-1.19145	-3.63820	1.64502
C	-1.18399	-4.64104	0.64404
C	-2.67556	-3.41816	1.94768
H	-0.47032	-3.76187	2.45182
C	-0.05130	-5.50716	0.22288
O	-2.35079	-4.87319	0.12604
H	-2.88162	-2.36978	2.15853
H	-3.03571	-4.03862	2.77513
H	-0.27760	-2.63706	-1.55615
C	0.01448	-5.75376	-1.28764
H	0.87396	-5.04937	0.58790
H	-0.18292	-6.45492	0.76339
C	-3.27770	-3.84929	0.61377
O	-0.71015	-3.52500	-1.65957
H	-0.93720	-6.17071	-1.63273
H	0.80008	-6.48621	-1.49845
H	-4.26482	-4.30673	0.65280
H	-3.24528	-3.04783	-0.13069
C	0.29317	-4.44482	-2.01469
H	1.28029	-4.05905	-1.72057
H	0.30704	-4.61627	-3.10015
O	0.60875	-1.37812	-1.11601
C	3.83058	-0.34444	0.11783
C	3.94749	-1.45471	-0.76076
C	4.29074	-0.45627	1.45649
C	4.50452	-2.66942	-0.28540
C	3.50753	-1.39452	-2.10288
C	4.84853	-1.67988	1.90692
C	4.21630	0.62616	2.36279
C	4.60747	-3.77897	-1.14076
C	4.94670	-2.77008	1.03713
C	3.61689	-2.50689	-2.93979
H	3.06618	-0.49672	-2.51438
C	5.30374	-1.80055	3.23039
C	4.67382	0.48939	3.67502
H	3.81139	1.58516	2.06743
C	4.16524	-3.69511	-2.46077
H	5.02827	-4.71291	-0.78718
H	5.37157	-3.70351	1.39184
H	3.26986	-2.44819	-3.96334
H	5.73017	-2.73117	3.58608
C	5.21464	-0.72000	4.10795
H	4.61035	1.32637	4.35851
H	4.24411	-4.55516	-3.11309
H	5.56839	-0.81976	5.12603
C	-3.54333	1.05676	-0.01898
C	-4.12018	0.32261	1.05430
C	-3.99526	0.82737	-1.34698

C	-5.14301	-0.62360	0.78780
C	-3.69678	0.49507	2.39286
C	-4.99778	-0.14654	-1.58914
C	-3.48268	1.55370	-2.44658
C	-5.73541	-1.33794	1.84255
C	-5.56082	-0.85629	-0.52509
C	-4.30073	-0.21840	3.43051
H	-2.89608	1.17349	2.65269
C	-5.43713	-0.39428	-2.90014
C	-3.93094	1.29538	-3.74353
H	-2.73836	2.32784	-2.31742
C	-5.32020	-1.12820	3.15713
H	-6.51857	-2.06161	1.64958
H	-6.33372	-1.59272	-0.71987
H	-3.97002	-0.07101	4.45055
H	-6.19852	-1.13997	-3.09687
C	-4.90140	0.32147	-3.97039
H	-3.52510	1.85543	-4.57620
H	-5.78061	-1.68259	3.96465
H	-5.24514	0.12567	-4.97789

R-gau-hc(-,+)



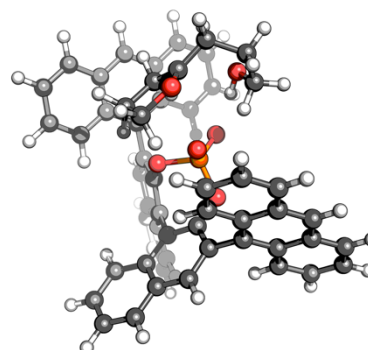
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C	0.90202	1.69425	-0.10969
C	2.16875	2.13278	-0.52167
C	-0.20333	2.56566	-0.14115
C	2.32155	3.41570	-1.05625
C	-0.06797	3.83645	-0.75587
C	1.21235	4.26013	-1.20121
C	-1.47826	2.09489	0.47809
C	-2.08274	2.76898	1.57266
C	-2.04933	0.89153	0.00634
C	-3.31907	2.29508	2.08506
C	-3.27255	0.43775	0.52239
C	-3.90869	1.14657	1.54463
H	-4.85070	0.78053	1.93823
H	3.30313	3.74300	-1.38084
C	1.36604	5.52517	-1.79013
C	0.26175	6.36167	-1.95916
H	2.33895	5.86388	-2.12626
H	0.38619	7.33433	-2.41739
C	-1.00403	5.94276	-1.54938
C	-1.17354	4.68950	-0.95671

H	-1.85888	6.59068	-1.69438
H	-2.17313	4.39236	-0.66850
C	-3.94220	2.96558	3.14971
C	-3.34002	4.08424	3.72600
H	-4.89015	2.61782	3.54316
H	-3.82334	4.59411	4.54939
C	-2.10841	4.53662	3.25454
C	-1.47789	3.88422	2.19285
H	-1.63703	5.39441	3.71672
H	-0.51275	4.25367	1.87485
O	-0.34021	-1.77869	0.26507
P	-0.07955	-0.58531	-0.64044
H	1.09169	-2.20638	0.57300
O	-1.45708	0.20023	-1.02052
O	0.75066	0.42446	0.38101
C	2.17853	-2.25599	1.07870
C	2.41354	-3.65585	1.14722
C	1.86123	-1.84841	2.51808
H	2.83077	-1.67172	0.43895
C	3.07467	-4.54066	0.16160
O	1.91979	-4.19618	2.21691
H	1.14719	-1.02364	2.54255
H	2.76093	-1.57611	3.07832
H	1.84093	-2.08220	-2.09793
C	2.10196	-5.05755	-0.92793
H	3.85117	-3.95703	-0.33707
H	3.51327	-5.38634	0.69773
C	1.24720	-3.15150	3.01813
O	2.33913	-2.91688	-1.94807
H	1.36556	-5.73800	-0.48795
H	2.71567	-5.63634	-1.62501
H	1.42258	-3.40799	4.06109
H	0.18696	-3.22357	2.76525
C	1.39407	-3.92230	-1.66263
H	0.94418	-4.32240	-2.58219
H	0.57474	-3.52323	-1.04870
C	-3.87754	-0.81714	0.01228
C	-4.59824	-0.81577	-1.21051
C	-3.70419	-2.03256	0.72593
C	-5.13404	-2.03008	-1.71008
C	-4.80391	0.36965	-1.95231
C	-4.24892	-3.23434	0.20614
C	-2.98744	-2.08719	1.94345
C	-5.84516	-2.03918	-2.92147
C	-4.95521	-3.22180	-1.00068
C	-5.51297	0.34296	-3.15508
H	-4.42367	1.32368	-1.61124
C	-4.07405	-4.44352	0.89938
C	-2.82507	-3.29722	2.62085
H	-2.54114	-1.20275	2.37846
C	-6.03110	-0.85728	-3.63870
H	-6.25754	-2.96131	-3.31398
H	-5.36730	-4.14650	-1.39150
H	-5.66212	1.25796	-3.71386
H	-4.48462	-5.36818	0.51100
C	-3.36526	-4.47164	2.10039
H	-2.27574	-3.32418	3.55309

H	-6.58000	-0.87170	-4.57150
H	-3.23380	-5.40701	2.62889
C	3.34423	1.23458	-0.39161
C	3.83690	0.53157	-1.52280
C	3.93636	1.01939	0.88166
C	4.91256	-0.38028	-1.36835
C	3.26923	0.69363	-2.80687
C	5.01264	0.10452	1.01001
C	3.47764	1.68814	2.03955
C	5.39021	-1.09928	-2.47622
C	5.49049	-0.58024	-0.11116
C	3.75503	-0.03040	-3.89746
H	2.44092	1.36780	-2.97882
C	5.59025	-0.13049	2.26844
C	4.06193	1.44142	3.28344
H	2.66784	2.40438	1.99667
C	4.81173	-0.92392	-3.73300
H	6.20799	-1.80216	-2.36879
H	6.30911	-1.28410	-0.00203
H	3.30689	0.09975	-4.87408
H	6.40810	-0.83271	2.37928
C	5.11362	0.53425	3.39806
H	3.69718	1.95695	4.16252
H	5.18237	-1.48423	-4.58160
H	5.56154	0.34604	4.36522
O	0.66486	-0.79444	-1.91681

R-gau-hc(-,+) intermediate



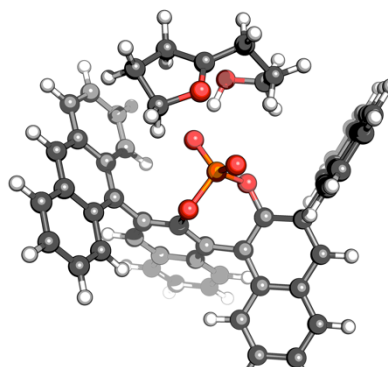
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C	-1.15900	1.58958	0.08690
C	-2.45292	1.86785	0.55114
C	-0.14581	2.56429	0.16181
C	-2.72567	3.09709	1.15900
C	-0.39940	3.78001	0.84701
C	-1.70805	4.04496	1.33064
C	1.17203	2.24625	-0.46238
C	1.72220	3.02254	-1.51573
C	1.85086	1.08677	-0.02880
C	3.00766	2.69605	-2.02189
C	3.12710	0.78456	-0.52838
C	3.70445	1.59478	-1.51012
H	4.68823	1.34624	-1.89312
H	-3.72743	3.30019	1.52128
C	-1.98016	5.25382	1.99053

C	-0.96465	6.18942	2.19270
H	-2.97638	5.47133	2.35725
H	-1.17997	7.11789	2.70557
C	0.33024	5.92530	1.74684
C	0.61684	4.72977	1.08415
H	1.11693	6.64863	1.91846
H	1.63705	4.55338	0.77065
C	3.57519	3.46808	-3.04812
C	2.87134	4.54326	-3.59158
H	4.55921	3.23368	-3.43674
H	3.31242	5.13181	-4.38567
C	1.59441	4.85197	-3.12416
C	1.01791	4.09756	-2.10001
H	1.04621	5.67725	-3.56013
H	0.01718	4.35640	-1.78188
O	0.45787	-1.70513	-0.52718
P	0.03757	-0.63438	0.43800
H	-2.12887	-2.06025	-0.18800
O	1.29666	0.28895	0.94050
O	-0.89409	0.38092	-0.50123
C	-2.37000	-2.59413	-1.11966
C	-1.58372	-3.84508	-1.13299
C	-1.93078	-1.87187	-2.40434
H	-3.43433	-2.84667	-1.06602
C	-1.78130	-5.03521	-0.27373
O	-0.72495	-3.89883	-2.05993
H	-1.66450	-0.83731	-2.18991
H	-2.72333	-1.90297	-3.15548
H	-1.34854	-2.55742	2.04612
C	-0.60413	-5.32088	0.68458
H	-2.68273	-4.87417	0.31772
H	-1.91782	-5.88829	-0.94900
C	-0.69900	-2.65491	-2.86522
O	-1.52706	-3.51835	1.95623
H	0.28778	-5.60692	0.11943
H	-0.91216	-6.17990	1.28995
H	-0.71586	-2.99532	-3.89961
H	0.23658	-2.16933	-2.59271
C	-0.30612	-4.10745	1.56432
H	0.27770	-4.43206	2.43683
H	0.29627	-3.38955	0.99539
C	3.86162	-0.40540	-0.03257
C	4.54801	-0.35173	1.20882
C	3.85269	-1.61268	-0.78002
C	5.21110	-1.50751	1.69420
C	4.59663	0.83032	1.98250
C	4.51861	-2.75692	-0.27160
C	3.18322	-1.71688	-2.02053
C	5.89150	-1.46426	2.92240
C	5.18883	-2.69361	0.95398
C	5.27733	0.85610	3.20151
H	4.11515	1.74207	1.65395
C	4.50100	-3.96067	-0.99541
C	3.17362	-2.92176	-2.72622
H	2.65354	-0.87703	-2.45022
C	5.92200	-0.28725	3.67043
H	6.40058	-2.34152	3.30397

H	5.69637	-3.57396	1.33475
H	5.30574	1.76781	3.78440
H	5.00491	-4.84181	-0.61582
C	3.82952	-4.04011	-2.21537
H	2.65181	-2.98875	-3.67218
H	6.44828	-0.26109	4.61592
H	3.81771	-4.97160	-2.76640
C	-3.52815	0.85329	0.41173
C	-3.90785	0.05600	1.52413
C	-4.13854	0.63263	-0.85137
C	-4.89120	-0.95292	1.36087
C	-3.31598	0.22084	2.79713
C	-5.12113	-0.38058	-0.98861
C	-3.79149	1.39484	-1.99017
C	-5.25619	-1.76284	2.44875
C	-5.49075	-1.15542	0.11457
C	-3.68815	-0.59490	3.86745
H	-2.55353	0.96728	2.97487
C	-5.71495	-0.62029	-2.23858
C	-4.38934	1.14150	-3.22623
H	-3.05754	2.18807	-1.93866
C	-4.65489	-1.58344	3.69418
H	-6.00403	-2.53879	2.33444
H	-6.23969	-1.93206	-0.00142
H	-3.22161	-0.46159	4.83503
H	-6.46215	-1.39625	-2.35633
C	-5.34635	0.13614	-3.35075
H	-4.10944	1.72874	-4.09128
H	-4.93845	-2.21365	4.52726
H	-5.80633	-0.05567	-4.31148
O	-0.72464	-1.00536	1.67443

R-gau-hc(-,+)^{2nd} step



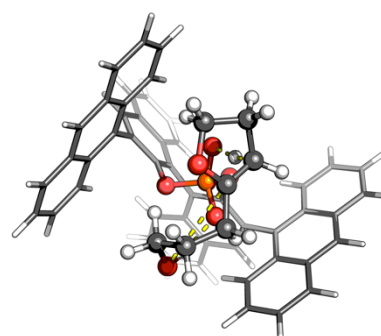
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C	-0.57924	2.53447	0.29980
C	-3.19580	2.52661	1.34357
C	-0.96321	3.51326	1.25423
C	-2.29244	3.51461	1.75231
C	0.78601	2.49718	-0.30201
C	1.30888	3.56010	-1.08226
C	1.56638	1.34070	-0.09590
C	2.65758	3.50157	-1.52098

C	2.90689	1.30625	-0.50975
C	3.44922	2.38893	-1.20921
H	4.48376	2.34848	-1.53212
H	-4.20754	2.51872	1.73430
C	-2.69584	4.49199	2.67609
C	-1.78868	5.45103	3.12744
H	-3.71012	4.50744	3.05729
H	-2.10467	6.19936	3.84277
C	-0.47097	5.43685	2.67196
C	-0.05498	4.47431	1.74950
H	0.23344	6.17244	3.03853
H	0.98110	4.48498	1.44019
C	3.19676	4.55706	-2.27350
C	2.40599	5.65602	-2.61175
H	4.22744	4.52818	-2.60690
H	2.82632	6.46469	-3.19563
C	1.07155	5.70902	-2.20971
C	0.52144	4.66998	-1.45579
H	0.45902	6.55753	-2.48622
H	-0.52214	4.73871	-1.17913
O	0.56756	-1.24428	-1.51330
P	-0.06199	-0.58428	-0.33712
H	-1.64394	-4.12185	1.40252
O	1.03034	0.26423	0.56403
O	-1.11202	0.53463	-0.93377
C	-1.59433	-4.79740	0.54135
C	-0.31909	-4.48284	-0.17347
C	-2.64543	-4.47130	-0.53093
H	-1.59836	-5.82396	0.91408
C	1.06527	-4.95827	0.05899
O	-0.51509	-3.79013	-1.21484
H	-3.57453	-4.09612	-0.10780
H	-2.87018	-5.35414	-1.13648
H	-0.02293	-2.42243	1.56613
C	2.03277	-3.76568	0.21823
H	1.08119	-5.60843	0.93652
H	1.33786	-5.53764	-0.83222
C	-1.93020	-3.41021	-1.36074
O	0.45276	-3.22040	1.96036
H	1.82902	-3.02988	-0.56947
H	3.05896	-4.12597	0.10105
H	-2.12884	-3.41544	-2.43010
H	-2.00321	-2.40630	-0.94017
C	1.81446	-3.15635	1.61118
H	2.37430	-3.73003	2.35987
H	2.17904	-2.12169	1.62742
C	3.75227	0.12188	-0.21534
C	4.27053	-0.07561	1.09213
C	4.02492	-0.83262	-1.23061
C	5.05488	-1.22410	1.36994
C	4.02812	0.84491	2.13729
C	4.81922	-1.96850	-0.93026
C	3.50912	-0.69722	-2.53950
C	5.55847	-1.43634	2.66379
C	5.32559	-2.15142	0.35985
C	4.53624	0.61872	3.41809
H	3.44820	1.74417	1.97724

C	5.08304	-2.92553	-1.92386
C	3.77733	-1.66014	-3.51438
H	2.88675	0.14241	-2.81883
C	5.29681	-0.51906	3.68132
H	6.15446	-2.31305	2.88856
H	5.92503	-3.02817	0.58222
H	4.33973	1.33021	4.20984
H	5.68560	-3.79907	-1.70436
C	4.56250	-2.77002	-3.20822
H	3.37190	-1.54581	-4.51145
H	5.68759	-0.68923	4.67625
H	4.76594	-3.51389	-3.96766
C	-3.73462	0.41673	0.13278
C	-3.99421	-0.61133	1.07867
C	-4.36603	0.37754	-1.13813
C	-4.90023	-1.65196	0.75264
C	-3.35789	-0.64272	2.34108
C	-5.25249	-0.68531	-1.44825
C	-4.14296	1.37694	-2.11238
C	-5.16974	-2.66831	1.68437
C	-5.51537	-1.68062	-0.50232
C	-3.62477	-1.66915	3.24903
H	-2.64033	0.11223	2.63319
C	-5.87381	-0.73861	-2.70681
C	-4.76875	1.30879	-3.35888
H	-3.48838	2.21712	-1.92199
C	-4.53093	-2.67631	2.92381
H	-5.86304	-3.46659	1.44688
H	-6.19854	-2.48741	-0.74702
H	-3.12566	-1.68321	4.20939
H	-6.55038	-1.54770	-2.95593
C	-5.62927	0.25347	-3.65624
H	-4.58622	2.07919	-4.09701
H	-4.73496	-3.46883	3.63211
H	-6.11157	0.20609	-4.62407
O	-0.79904	-1.43325	0.68488

R-gau-hc(-,-)



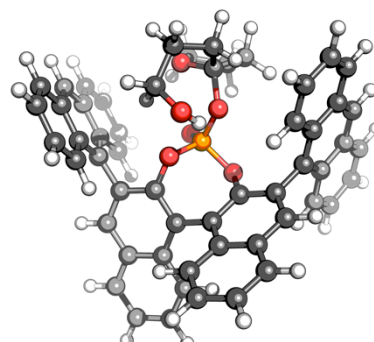
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C	-1.91067	1.12633	-0.08915
C	-3.19834	0.81262	0.37179
C	-1.27739	2.32164	0.30706

C	-3.85910	1.68251	1.24324
C	-1.91301	3.16199	1.25912
C	-3.22514	2.84451	1.70102
C	0.08307	2.60723	-0.24116
C	0.37991	3.78549	-0.97407
C	1.09684	1.64331	-0.04417
C	1.72096	4.04382	-1.36217
C	2.42190	1.92027	-0.41219
C	2.73085	3.12345	-1.05430
H	3.75743	3.32464	-1.34035
H	-4.85317	1.42861	1.59466
C	-3.87797	3.68080	2.62060
C	-3.23464	4.81214	3.12328
H	-4.88198	3.45320	2.95898
H	-3.74201	5.45074	3.83484
C	-1.93253	5.11197	2.72474
C	-1.27034	4.29302	1.80750
H	-1.43152	5.98089	3.13169
H	-0.25332	4.54825	1.54339
C	2.03426	5.21866	-2.06414
C	1.02907	6.12490	-2.40398
H	3.05536	5.43141	-2.35807
H	1.27642	7.02656	-2.94928
C	-0.29574	5.86475	-2.05463
C	-0.62347	4.70382	-1.35079
H	-1.07351	6.56400	-2.33346
H	-1.66472	4.52845	-1.11585
O	0.70751	-1.14341	-1.46632
P	-0.08142	-0.59600	-0.28093
H	0.38257	-2.50842	-1.45723
O	0.81303	0.45814	0.58633
O	-1.27687	0.27936	-0.96133
C	0.34548	-3.75632	-1.58326
C	0.96738	-4.09997	-0.35940
C	1.43495	-3.94272	-2.64235
H	-0.68481	-4.05979	-1.74546
C	0.35344	-4.46188	0.94331
O	2.26573	-4.06625	-0.43241
H	1.34873	-3.21797	-3.45411
H	1.44639	-4.95522	-3.05907
H	-0.05578	-1.89110	2.37413
C	1.29603	-4.35459	2.14431
H	-0.53299	-3.82871	1.06430
H	-0.00863	-5.49265	0.81196
C	2.66415	-3.65528	-1.78544
O	0.45002	-2.28898	3.10721
H	2.23346	-4.88109	1.93294
H	0.82026	-4.84989	2.99607
H	3.56832	-4.21052	-2.02731
H	2.85531	-2.58339	-1.71857
C	1.58352	-2.90618	2.55232
H	2.36912	-2.90505	3.31630
H	1.96381	-2.33354	1.69126
O	-0.58673	-1.61380	0.69010
C	-3.83008	-0.47454	-0.01239
C	-3.78134	-1.58343	0.87490
C	-4.40669	-0.62979	-1.29985

C	-4.28833	-2.83969	0.45556
C	-3.21190	-1.48307	2.16550
C	-4.91684	-1.89348	-1.69240
C	-4.48827	0.44558	-2.21318
C	-4.21133	-3.95103	1.31145
C	-4.85131	-2.98126	-0.81631
C	-3.13918	-2.59872	3.00177
H	-2.80094	-0.55245	2.53303
C	-5.48127	-2.05844	-2.96800
C	-5.05219	0.26436	-3.47780
H	-4.12277	1.43201	-1.95924
C	-3.63587	-3.82890	2.57605
H	-4.59044	-4.91700	0.99924
H	-5.23637	-3.94652	-1.12870
H	-2.68996	-2.50933	3.98253
H	-5.87098	-3.02023	-3.28029
C	-5.54615	-0.98345	-3.85453
H	-5.10706	1.09614	-4.16829
H	-3.57392	-4.69092	3.22762
H	-5.98160	-1.11806	-4.83626
C	3.49475	0.92996	-0.13268
C	4.04531	0.15341	-1.18752
C	3.94210	0.72045	1.20001
C	5.04830	-0.80823	-0.90118
C	3.60679	0.29152	-2.52450
C	4.92568	-0.26671	1.46345
C	3.43743	1.47491	2.28430
C	5.60709	-1.57351	-1.93830
C	5.47144	-1.01258	0.41509
C	4.16764	-0.48252	-3.54255
H	2.82421	0.98700	-2.79562
C	5.35857	-0.49576	2.78003
C	3.87876	1.23463	3.58703
H	2.70397	2.25661	2.13853
C	5.16872	-1.40742	-3.25181
H	6.37508	-2.30937	-1.73100
H	6.22886	-1.76059	0.62576
H	3.82131	-0.36655	-4.56142
H	6.10563	-1.25126	2.99331
C	4.83306	0.24995	3.83488
H	3.48018	1.81712	4.40775
H	5.59809	-2.00601	-4.04470
H	5.17161	0.06844	4.84680

R-gau-hc(-,-) intermediate

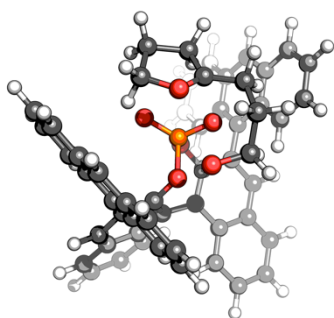


E(RM062X) = ant55-R-gau2-13-min

C	-1.52673	1.30692	-0.12271
C	-2.84265	1.25964	0.36485
C	-0.64918	2.33977	0.29031
C	-3.28470	2.21355	1.28528
C	-1.07028	3.24236	1.30462
C	-2.40862	3.18800	1.77430
C	0.72806	2.39011	-0.28904
C	1.25081	3.52969	-0.95238
C	1.53360	1.24529	-0.15627
C	2.61801	3.54266	-1.33989
C	2.88623	1.27263	-0.52024
C	3.42898	2.42485	-1.09620
H	4.47496	2.43474	-1.38184
H	-4.30421	2.16450	1.65215
C	-2.84898	4.09461	2.75194
C	-1.96885	5.03468	3.28784
H	-3.87114	4.06765	3.11089
H	-2.31309	5.72738	4.04493
C	-0.64136	5.07064	2.86415
C	-0.18931	4.18005	1.88810
H	0.04287	5.78883	3.29738
H	0.85416	4.22623	1.60913
C	3.15525	4.67401	-1.97389
C	2.34704	5.77900	-2.24536
H	4.19823	4.70038	-2.26670
H	2.76640	6.64669	-2.73806
C	0.99701	5.76322	-1.89472
C	0.44748	4.64806	-1.25829
H	0.37206	6.61779	-2.11998
H	-0.60745	4.66496	-1.01873
O	0.63751	-1.15670	-1.93949
P	0.01816	-0.65655	-0.70613
H	-2.34718	-3.25703	-0.69864
O	0.99305	0.09290	0.34787
O	-1.14849	0.39950	-1.08384
C	-1.41291	-3.81688	-0.63728
C	-0.42952	-3.15513	0.33045
C	-0.62528	-3.88279	-1.95091
H	-1.63397	-4.82325	-0.26908
C	-0.58134	-3.54592	1.79610
O	0.83995	-3.44775	-0.12678
H	-0.75256	-2.97212	-2.53729
H	-0.91608	-4.73965	-2.56225
H	-0.31026	-0.76935	2.28701
C	0.65459	-3.34364	2.67685
H	-1.43211	-2.99794	2.20616
H	-0.84458	-4.60840	1.81680
C	0.82285	-3.99046	-1.46342
O	0.17533	-0.97786	3.09352
H	1.46299	-3.99240	2.32197
H	0.38702	-3.66881	3.68852
H	1.16254	-5.02910	-1.39077
H	1.51576	-3.40556	-2.06888
C	1.18052	-1.91358	2.73976
H	1.95143	-1.84821	3.51368

H	1.64360	-1.63843	1.78667
O	-0.66624	-1.68242	0.29273
C	-3.75504	0.16480	-0.05695
C	-4.04578	-0.90441	0.83358
C	-4.30146	0.15416	-1.36802
C	-4.86505	-1.97707	0.39772
C	-3.53103	-0.94285	2.15005
C	-5.10921	-0.93517	-1.78301
C	-4.07090	1.20907	-2.28037
C	-5.15566	-3.04050	1.26822
C	-5.37973	-1.98580	-0.90173
C	-3.84439	-1.99873	3.00822
H	-2.88229	-0.16583	2.52964
C	-5.64366	-0.96042	-3.08178
C	-4.61072	1.16891	-3.56755
H	-3.47949	2.07340	-2.00873
C	-4.64959	-3.04668	2.56751
H	-5.77694	-3.86701	0.94385
H	-5.99976	-2.81441	-1.22820
H	-3.44570	-2.01226	4.01447
H	-6.25876	-1.78972	-3.41094
C	-5.39198	0.08658	-3.96817
H	-4.42364	1.98242	-4.25668
H	-4.87930	-3.86833	3.23352
H	-5.80784	0.06099	-4.96716
C	3.72521	0.06707	-0.30374
C	3.99362	-0.81993	-1.37964
C	4.15309	-0.26996	1.00788
C	4.67276	-2.03985	-1.12975
C	3.57804	-0.53774	-2.70071
C	4.82845	-1.49616	1.23284
C	3.91399	0.58151	2.11089
C	4.92029	-2.93596	-2.18261
C	5.08154	-2.36454	0.16717
C	3.82992	-1.44075	-3.73546
H	3.04783	0.37272	-2.94537
C	5.23347	-1.84844	2.53085
C	4.32293	0.21601	3.39490
H	3.41306	1.53337	1.99296
C	4.49898	-2.63566	-3.47768
H	5.43481	-3.87254	-2.00257
H	5.59458	-3.30319	0.34956
H	3.50163	-1.21357	-4.74153
H	5.74484	-2.78583	2.71547
C	4.97880	-0.99563	3.60476
H	4.12945	0.87565	4.23095
H	4.68967	-3.33264	-4.28349
H	5.29170	-1.27461	4.60261

R-gau-hc(-,-) 2nd step



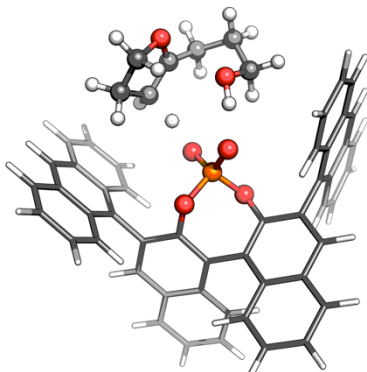
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C	-1.81423	1.04482	0.05968
C	-3.10709	0.78833	0.54019
C	-1.09973	2.17637	0.50697
C	-3.66350	1.60650	1.52689
C	-1.63048	2.96040	1.56512
C	-2.93124	2.67523	2.05750
C	0.21632	2.47761	-0.13071
C	0.48389	3.70385	-0.79295
C	1.21433	1.48411	-0.08915
C	1.79424	3.96195	-1.27513
C	2.51215	1.75965	-0.54484
C	2.80001	2.99886	-1.12430
H	3.80446	3.19828	-1.48126
H	-4.66179	1.39359	1.89338
C	-3.48224	3.46087	3.08234
C	-2.74775	4.50897	3.63794
H	-4.47838	3.25958	3.45858
H	-3.17704	5.10922	4.42976
C	-1.45638	4.77614	3.18464
C	-0.89564	4.00747	2.16220
H	-0.88528	5.58080	3.62959
H	0.11607	4.23386	1.85410
C	2.08056	5.18028	-1.91120
C	1.07677	6.13244	-2.09264
H	3.07877	5.39237	-2.27575
H	1.30287	7.06801	-2.58776
C	-0.22040	5.87582	-1.64934
C	-0.52070	4.67120	-1.00948
H	-0.99835	6.61203	-1.80554
H	-1.54291	4.50140	-0.69908
O	0.63154	-1.15149	-1.71596
P	-0.04389	-0.71418	-0.45904
H	-0.82570	-3.36985	-1.13695
O	0.93637	0.26222	0.46529
O	-1.29042	0.24475	-0.92364
C	-0.05592	-4.13497	-1.02559
C	0.67865	-3.86566	0.24864
C	1.04219	-4.05818	-2.10315
H	-0.54616	-5.11146	-0.95326
C	0.19299	-4.19248	1.60996
O	1.90587	-3.60839	0.06882
H	0.75233	-3.37164	-2.89806

H	1.25670	-5.04552	-2.51892
H	1.70478	-0.98467	1.68901
C	1.07546	-3.78618	2.79251
H	-0.81149	-3.77218	1.68501
H	0.07924	-5.28877	1.58886
C	2.25276	-3.49328	-1.35768
O	2.12546	-1.68353	2.20894
H	2.08981	-4.17984	2.66174
H	0.65206	-4.27268	3.67861
H	3.18135	-4.05255	-1.46926
H	2.38051	-2.42885	-1.53922
C	1.17584	-2.28420	3.06017
H	0.19073	-1.81875	2.94033
H	1.50453	-2.14706	4.09930
O	-0.47123	-1.76213	0.54151
C	-3.88803	-0.35177	0.00191
C	-3.92009	-1.58758	0.69905
C	-4.56912	-0.22432	-1.23703
C	-4.61160	-2.69100	0.13750
C	-3.27073	-1.75873	1.94268
C	-5.26039	-1.33933	-1.77519
C	-4.58482	0.99246	-1.95649
C	-4.63331	-3.92347	0.81084
C	-5.27023	-2.55781	-1.08907
C	-3.31110	-2.98772	2.60376
H	-2.72316	-0.95173	2.41130
C	-5.93684	-1.22258	-3.00089
C	-5.26376	1.09198	-3.17270
H	-4.08077	1.87558	-1.58607
C	-3.98469	-4.06830	2.03721
H	-5.15269	-4.77548	0.38813
H	-5.79748	-3.40730	-1.51088
H	-2.80504	-3.10610	3.55328
H	-6.46767	-2.06801	-3.42258
C	-5.93692	-0.01172	-3.69371
H	-5.26924	2.03035	-3.71238
H	-4.00361	-5.02151	2.54945
H	-6.46212	0.07179	-4.63649
C	3.57822	0.73414	-0.42207
C	3.95983	-0.03894	-1.55008
C	4.17863	0.48027	0.83952
C	4.93484	-1.05887	-1.40384
C	3.37207	0.15535	-2.82091
C	5.14030	-0.55445	0.96350
C	3.83907	1.22792	1.99047
C	5.30587	-1.84145	-2.50971
C	5.51064	-1.30734	-0.15451
C	3.74781	-0.63590	-3.90827
H	2.61091	0.90641	-2.98424
C	5.71865	-0.83133	2.21325
C	4.42233	0.93850	3.22565
H	3.12186	2.03699	1.94900
C	4.71271	-1.62951	-3.75402
H	6.04670	-2.62581	-2.40875
H	6.24647	-2.09798	-0.04988
H	3.28538	-0.47966	-4.87436
H	6.44953	-1.62412	2.32113

C	5.35665	-0.08950	3.33757
H	4.14794	1.51450	4.10004
H	4.99803	-2.24126	-4.60007
H	5.80438	-0.31018	4.29798

R-gau-ev(+,-)



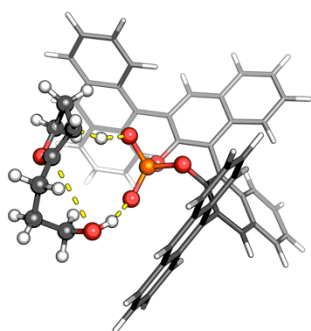
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C	1.74189	1.28761	-0.07998
C	3.07725	1.13865	-0.48394
C	1.03337	2.46831	-0.37505
C	3.68419	2.12922	-1.26247
C	1.61815	3.43427	-1.23317
C	2.96022	3.26014	-1.66260
C	-0.31976	2.63707	0.23192
C	-0.62648	3.71337	1.10662
C	-1.29729	1.64754	-0.01939
C	-1.94823	3.84967	1.60475
C	-2.60109	1.79905	0.47850
C	-2.92363	2.90323	1.27255
H	-3.93326	3.00506	1.65560
H	4.71438	2.00177	-1.57643
C	3.56069	4.21998	-2.49267
C	2.83713	5.33563	-2.91629
H	4.58702	4.10317	-2.82018
H	3.30438	6.06995	-3.55970
C	1.50933	5.50058	-2.52231
C	0.89886	4.55807	-1.69186
H	0.94891	6.36104	-2.86456
H	-0.13789	4.71085	-1.42297
C	-2.27495	4.92412	2.44757
C	-1.29895	5.84879	2.81985
H	-3.28326	5.04308	2.82639
H	-1.55617	6.67274	3.47290
C	0.01117	5.70411	2.36558
C	0.35119	4.64379	1.52267
H	0.76864	6.41438	2.67123
H	1.38350	4.55579	1.21321
O	-0.68421	-1.36749	0.85348
P	0.01866	-0.53614	-0.21091
H	-1.35838	-2.50713	0.55143
O	-1.00895	0.57949	-0.83167
O	1.13542	0.29510	0.64578

C	-2.15696	-3.49129	0.53025
C	-1.36668	-4.65666	0.39649
C	-3.08736	-3.50489	-0.68268
H	-2.56427	-3.33450	1.53041
C	-0.35214	-5.17537	1.35142
O	-1.56175	-5.31890	-0.69922
H	-3.17029	-2.52357	-1.15432
H	-4.09107	-3.85699	-0.42477
H	0.72958	-2.83152	-1.24840
C	1.01689	-5.39628	0.67905
H	-0.27107	-4.45950	2.17469
H	-0.72820	-6.12323	1.75578
C	-2.36083	-4.49189	-1.60206
O	0.64899	-3.79703	-1.02554
H	0.92355	-6.17993	-0.07998
H	1.72254	-5.74439	1.43972
H	-2.99595	-5.16669	-2.17357
H	-1.62895	-3.99854	-2.24712
C	1.53897	-4.13126	0.01035
H	1.61167	-3.31309	0.74482
H	2.54711	-4.32559	-0.38067
O	0.60876	-1.23333	-1.39517
C	3.84680	-0.06791	-0.08744
C	4.06932	-1.11528	-1.02043
C	4.33238	-0.19591	1.24134
C	4.77640	-2.27640	-0.61589
C	3.59041	-1.04593	-2.34831
C	5.02743	-1.37123	1.62445
C	4.14907	0.82357	2.20382
C	4.99947	-3.31905	-1.53028
C	5.24321	-2.39413	0.69650
C	3.81264	-2.09551	-3.24196
H	3.03348	-0.19004	-2.70536
C	5.50359	-1.51050	2.93871
C	4.62886	0.66903	3.50603
H	3.63996	1.74699	1.96141
C	4.51676	-3.22726	-2.83535
H	5.53865	-4.21049	-1.23200
H	5.77700	-3.28938	0.99848
H	3.43609	-2.03061	-4.25464
H	6.03338	-2.40546	3.24332
C	5.30197	-0.49475	3.87311
H	4.47918	1.45682	4.23318
H	4.68631	-4.03756	-3.53255
H	5.67185	-0.60869	4.88396
C	-3.63990	0.77511	0.20096
C	-3.99159	-0.17088	1.20029
C	-4.29735	0.74522	-1.05697
C	-5.01674	-1.11604	0.94215
C	-3.33822	-0.20948	2.45321
C	-5.30864	-0.21995	-1.29700
C	-3.97991	1.66079	-2.08592
C	-5.37579	-2.05153	1.92649
C	-5.66444	-1.12951	-0.29665
C	-3.70488	-1.14834	3.41952
H	-2.53559	0.47469	2.69454
C	-5.95968	-0.26240	-2.54079

C	-4.63645	1.60429	-3.31711
H	-3.22596	2.42500	-1.95124
C	-4.72293	-2.06375	3.15889
H	-6.15721	-2.77865	1.73969
H	-6.44214	-1.86167	-0.48798
H	-3.19482	-1.16741	4.37399
H	-6.73154	-0.99753	-2.73634
C	-5.62139	0.64476	-3.54479
H	-4.38051	2.30902	-4.09783
H	-5.00179	-2.79014	3.91122
H	-6.12688	0.60594	-4.50109

R-gau-hc(+,+)



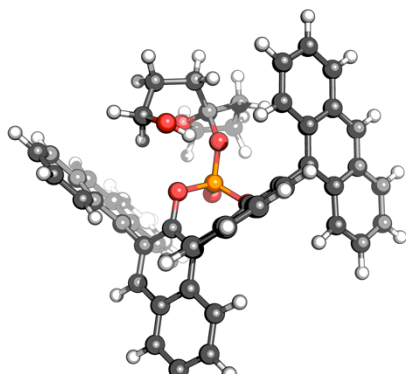
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C	-1.62713	1.40154	-0.06710
C	-2.99317	1.33577	0.25265
C	-0.85770	2.51834	0.31994
C	-3.58634	2.36023	0.99730
C	-1.43803	3.50926	1.15561
C	-2.82031	3.43294	1.46718
C	0.55615	2.59668	-0.15307
C	1.03923	3.69105	-0.91764
C	1.42595	1.52541	0.14946
C	2.42337	3.77289	-1.21597
C	2.79591	1.61850	-0.15354
C	3.28996	2.75508	-0.80355
H	4.34858	2.81840	-1.03120
H	-4.64225	2.29937	1.23769
C	-3.41841	4.42655	2.25870
C	-2.65433	5.47944	2.76284
H	-4.47551	4.38469	2.49354
H	-3.12084	6.24145	3.37384
C	-1.28766	5.54363	2.49379
C	-0.67863	4.56552	1.70438
H	-0.69620	6.35358	2.90097
H	0.38732	4.64008	1.53759
C	2.92248	4.86550	-1.94294
C	2.05824	5.86158	-2.39846
H	3.97936	4.94245	-2.16970
H	2.44806	6.69792	-2.96420
C	0.69077	5.77300	-2.14066
C	0.18003	4.69660	-1.41198
H	0.02215	6.53954	-2.51075
H	-0.88898	4.65342	-1.25308

O	0.77573	-1.25030	-1.10732
P	-0.02965	-0.56229	-0.01409
H	0.50669	-2.64190	-1.42570
O	0.95962	0.43095	0.83466
O	-1.05923	0.41366	-0.83097
C	0.82695	-3.76475	-1.81402
C	0.62159	-4.60126	-0.68229
C	2.34612	-3.57256	-1.86165
H	0.26002	-3.99684	-2.71235
C	-0.54149	-5.46537	-0.36939
O	1.61959	-4.59896	0.14003
H	2.59727	-2.57958	-2.22999
H	2.84895	-4.33675	-2.46267
H	-1.86131	-2.72392	0.92616
C	-0.83588	-5.64935	1.12030
H	-1.41359	-5.04999	-0.88016
H	-0.30748	-6.43001	-0.84607
C	2.67227	-3.70304	-0.37676
O	-2.14789	-3.65769	0.99473
H	0.01023	-6.11944	1.63224
H	-1.69273	-6.32570	1.20094
H	3.62223	-4.17413	-0.13017
H	2.54590	-2.75603	0.15307
C	-1.17510	-4.31095	1.77367
H	-1.54367	-4.48862	2.79346
H	-0.27655	-3.68358	1.84948
O	-0.72848	-1.40858	0.99716
C	3.72340	0.49998	0.16863
C	4.29213	-0.27880	-0.87763
C	4.05137	0.20298	1.51998
C	5.18585	-1.33398	-0.56141
C	3.98366	-0.04547	-2.23848
C	4.92168	-0.87936	1.80950
C	3.54730	0.96723	2.59772
C	5.76642	-2.09810	-1.58737
C	5.48157	-1.62916	0.77181
C	4.57600	-0.80897	-3.24649
H	3.27779	0.71591	-2.53948
C	5.23522	-1.19482	3.14190
C	3.86956	0.64043	3.91664
H	2.90684	1.82342	2.43544
C	5.46662	-1.83010	-2.92242
H	6.45035	-2.90615	-1.35606
H	6.15397	-2.44877	1.00362
H	4.33324	-0.61501	-4.28332
H	5.89370	-2.02370	3.37408
C	4.70615	-0.44027	4.18834
H	3.47039	1.23030	4.73175
H	5.91708	-2.42338	-3.70755
H	4.95247	-0.68897	5.21259
C	-3.81048	0.16752	-0.16315
C	-4.19353	-0.81057	0.79398
C	-4.21130	0.01940	-1.51767
C	-4.98020	-1.91877	0.38836
C	-3.79797	-0.72506	2.14907
C	-4.98503	-1.10585	-1.90105
C	-3.87050	0.97190	-2.50524

C	-5.36928	-2.88783	1.32815
C	-5.36337	-2.05685	-0.94874
C	-4.19032	-1.69895	3.06947
H	-3.17629	0.08366	2.50867
C	-5.37990	-1.26541	-3.23961
C	-4.27006	0.79725	-3.83181
H	-3.29800	1.85773	-2.26464
C	-4.97682	-2.77448	2.66168
H	-5.97336	-3.73658	1.02992
H	-5.96004	-2.91148	-1.25073
H	-3.88043	-1.61992	4.10355
H	-5.96910	-2.12245	-3.54417
C	-5.02009	-0.31866	-4.19848
H	-3.99820	1.53238	-4.57837
H	-5.27801	-3.52616	3.37979
H	-5.32767	-0.44823	-5.22812

R-gau-hc(+,+) intermediate



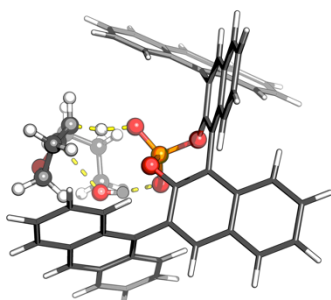
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C	0.69026	2.22650	-0.41190
C	3.31952	2.00541	-1.40268
C	1.12051	3.06570	-1.47384
C	2.45334	2.95844	-1.95015
C	-0.66481	2.35778	0.20447
C	-1.11519	3.54432	0.83882
C	-1.51636	1.24023	0.15743
C	-2.45957	3.62316	1.29282
C	-2.84541	1.33150	0.59027
C	-3.31785	2.52455	1.14387
H	-4.34609	2.58315	1.48312
H	4.34163	1.93029	-1.75753
C	2.90150	3.80042	-2.98046
C	2.03453	4.72772	-3.55906
H	3.91970	3.73398	-3.34539
H	2.38463	5.37045	-4.35647
C	0.71336	4.81742	-3.12273
C	0.25384	3.99197	-2.09425
H	0.04015	5.52704	-3.58625
H	-0.78392	4.07763	-1.80228
C	-2.92614	4.79976	1.89988
C	-2.06931	5.88653	2.07969
H	-3.95134	4.87582	2.24259

H	-2.43421	6.78957	2.55182
C	-0.74010	5.80724	1.66450
C	-0.26072	4.64609	1.05415
H	-0.07648	6.64818	1.81949
H	0.78111	4.61569	0.76451
O	-0.61069	-1.29369	1.85481
P	-0.03799	-0.72696	0.62829
H	2.21593	-3.47299	0.32686
O	-1.05445	0.05900	-0.35622
O	1.13599	0.31765	1.01802
C	1.24178	-3.95620	0.23864
C	0.29041	-3.13720	-0.63572
C	0.47702	-4.08836	1.55977
H	1.38015	-4.93674	-0.22715
C	0.39987	-3.39179	-2.13642
O	-0.98897	-3.39081	-0.18026
H	0.67557	-3.24258	2.21898
H	0.72233	-5.01228	2.08765
H	0.26741	-0.62034	-2.34143
C	-0.83468	-3.06186	-2.97997
H	1.26567	-2.84192	-2.51194
H	0.62022	-4.45666	-2.26154
C	-0.98337	-4.05976	1.09971
O	-0.23650	-0.69295	-3.16122
H	-1.66928	-3.70067	-2.67103
H	-0.58901	-3.31432	-4.01769
H	-1.39024	-5.06349	0.93697
H	-1.62702	-3.49352	1.77296
C	-1.29197	-1.60859	-2.91547
H	-2.04195	-1.43074	-3.69185
H	-1.75947	-1.40577	-1.94708
O	0.62505	-1.69551	-0.44584
C	-3.73451	0.14913	0.47223
C	-3.94927	-0.69674	1.59205
C	-4.26850	-0.21090	-0.79313
C	-4.68360	-1.89948	1.43156
C	-3.42719	-0.38993	2.86912
C	-4.99598	-1.42014	-0.92966
C	-4.08638	0.60091	-1.93605
C	-4.88086	-2.75492	2.52798
C	-5.19707	-2.24805	0.17871
C	-3.63048	-1.25259	3.94804
H	-2.85168	0.50908	3.04450
C	-5.50613	-1.79621	-2.18313
C	-4.60050	0.21250	-3.17471
H	-3.54801	1.53818	-1.88438
C	-4.35507	-2.43087	3.77845
H	-5.43711	-3.67820	2.41628
H	-5.75152	-3.17378	0.06397
H	-3.22146	-1.00696	4.91962
H	-6.05820	-2.72126	-2.30074
C	-5.30551	-0.98330	-3.29871
H	-4.44923	0.84115	-4.04273
H	-4.50794	-3.09650	4.61812
H	-5.69939	-1.28054	-4.26201
C	3.78790	0.08146	0.11641
C	4.11743	-1.06239	-0.65936

C	4.30732	0.20994	1.43280
C	4.94704	-2.07067	-0.10474
C	3.63199	-1.23850	-1.97501
C	5.12747	-0.81612	1.96733
C	4.03748	1.34342	2.23395
C	5.27473	-3.20820	-0.86077
C	5.43577	-1.94167	1.19833
C	3.97954	-2.36882	-2.71786
H	2.97966	-0.51289	-2.44109
C	5.63574	-0.70336	3.27205
C	4.55125	1.44008	3.52874
H	3.43551	2.16499	1.86906
C	4.79385	-3.35259	-2.16145
H	5.90460	-3.98608	-0.44543
H	6.06487	-2.72125	1.61563
H	3.60401	-2.48787	-3.72609
H	6.26016	-1.48325	3.69191
C	5.34530	0.41902	4.04735
H	4.33410	2.31250	4.13161
H	5.05155	-4.23090	-2.73903
H	5.74100	0.49959	5.05159

S-anti-ev(-,+)



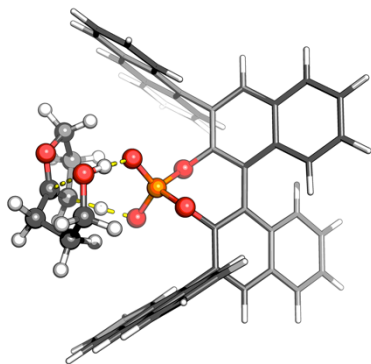
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C	-0.99906	1.68840	0.07690
C	-2.29491	2.03292	0.48960
C	0.04770	2.63201	0.14570
C	-2.53658	3.29070	1.05085
C	-0.17783	3.87430	0.79227
C	-1.48811	4.20239	1.22925
C	1.36615	2.25791	-0.44790
C	1.96062	2.99291	-1.50791
C	1.99259	1.08020	0.01334
C	3.23255	2.59812	-2.00053
C	3.23967	0.69000	-0.49854
C	3.86387	1.46067	-1.48314
H	4.82627	1.14681	-1.87238
H	-3.53999	3.54377	1.37536
C	-1.73169	5.43815	1.84944
C	-0.68640	6.33858	2.05922

H	-2.72894	5.70379	2.17995
H	-0.87984	7.28782	2.54198
C	0.60959	6.01264	1.66007
C	0.86785	4.78992	1.03646
H	1.41902	6.70895	1.83777
H	1.88911	4.56553	0.75900
C	3.84653	3.33145	-3.02844
C	3.20199	4.43515	-3.58767
H	4.82049	3.04421	-3.40692
H	3.67902	4.99410	-4.38238
C	1.93649	4.80877	-3.13730
C	1.31368	4.09266	-2.11276
H	1.43302	5.65490	-3.58701
H	0.32281	4.40202	-1.81017
O	0.56261	-1.65863	-0.36313
C	-1.41817	-4.26313	-1.13505
C	-3.19148	-3.01913	-1.70170
C	-0.71527	-5.25346	-0.28496
H	-3.34115	-2.37002	-0.83717
H	-4.13009	-3.24164	-2.20617
C	-0.32315	-4.59645	1.06699
H	-1.37678	-6.10701	-0.11070
H	0.18946	-5.58803	-0.79989
C	-2.04014	-2.54138	-2.58973
H	0.39121	-3.78624	0.88389
H	0.17782	-5.36628	1.66433
H	-2.16103	-2.87569	-3.62499
H	-1.96250	-1.45216	-2.57444
C	-1.52400	-4.03848	1.83130
O	-2.11384	-2.94723	1.16175
H	-2.29110	-4.81613	1.94710
H	-1.19548	-3.74095	2.83534
H	-1.65470	-2.12389	1.46555
O	-2.71136	-4.27084	-1.11459
C	-0.84992	-3.21731	-1.90547
H	-0.28701	-2.46109	-1.07682
H	0.02807	-3.49539	-2.48928
O	-0.63604	-0.86906	1.80395
C	-3.40879	1.06055	0.35096
C	-3.86772	0.33354	1.48133
C	-4.00049	0.83041	-0.91956
C	-4.92232	-0.60303	1.33234
C	-3.28864	0.49932	2.76005
C	-5.05714	-0.10762	-1.04197
C	-3.56644	1.51261	-2.07907
C	-5.36972	-1.34133	2.44023
C	-5.51215	-0.80473	0.08122
C	-3.74307	-0.24513	3.85033
H	-2.47414	1.19131	2.92754
C	-5.63781	-0.35404	-2.29688
C	-4.15163	1.25242	-3.31987
H	-2.77390	2.24803	-2.04057
C	-4.78018	-1.16221	3.69136
H	-6.17270	-2.06171	2.33724
H	-6.31656	-1.52544	-0.02359
H	-3.28641	-0.11169	4.82257
H	-6.43967	-1.07514	-2.40331

C	-5.18217	0.32068	-3.42907
H	-3.80438	1.77699	-4.20070
H	-5.12751	-1.73725	4.53999
H	-5.63090	0.12211	-4.39378
C	3.86564	-0.57817	-0.04770
C	4.52527	-0.64343	1.20728
C	3.75099	-1.74948	-0.84407
C	5.05761	-1.87889	1.65644
C	4.67076	0.49504	2.03193
C	4.28759	-2.97407	-0.37141
C	3.09136	-1.74064	-2.09509
C	5.70523	-1.95476	2.90054
C	4.93468	-3.02634	0.86681
C	5.31624	0.40190	3.26679
H	4.29170	1.46307	1.73157
C	4.15876	-4.14252	-1.14066
C	2.97071	-2.91133	-2.84601
H	2.65100	-0.83841	-2.49774
C	5.83085	-0.81884	3.70029
H	6.11325	-2.89393	3.25539
H	5.34124	-3.96813	1.22084
H	5.41846	1.28112	3.88983
H	4.56261	-5.08428	-0.78810
C	3.50163	-4.10852	-2.37044
H	2.45768	-2.89042	-3.79895
H	6.32985	-0.88502	4.65850
H	3.40247	-5.01341	-2.95594

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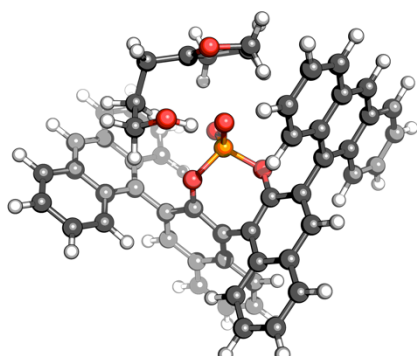
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C	-1.60426	1.35692	0.02966
C	-0.75951	2.43973	0.34926
C	-3.37457	2.30658	1.38862
C	-1.19619	3.40846	1.29054
C	-2.52331	3.34314	1.79062
C	0.58942	2.49132	-0.28851
C	1.01046	3.58121	-1.09413
C	1.45701	1.39387	-0.10175
C	2.34529	3.61480	-1.57584
C	3.22372	2.56476	-1.28199

H	4.24794	2.59524	-1.63734
H	-4.38848	2.25497	1.77013
C	-2.97894	4.30984	2.70116
C	-2.12567	5.32441	3.13634
H	-3.99248	4.27540	3.08309
H	-2.48184	6.06463	3.84115
C	-0.81028	5.37811	2.67656
C	-0.34278	4.42706	1.76691
H	-0.14792	6.15812	3.02940
H	0.68984	4.49139	1.45181
C	2.78376	4.69811	-2.35385
C	1.90609	5.73381	-2.67647
H	3.80295	4.73938	-2.71969
H	2.24891	6.56401	-3.28044
C	0.58431	5.69502	-2.23359
C	0.13396	4.62754	-1.45370
H	-0.09622	6.49385	-2.49886
H	-0.90351	4.62420	-1.14762
O	0.57924	-1.27080	-1.43724
C	0.11013	-4.39880	-0.35809
C	-2.10386	-3.98843	-0.16671
C	1.45698	-4.81785	0.11900
H	-2.27445	-3.07890	0.40617
H	-2.90369	-4.71401	-0.02225
C	2.33851	-3.59439	0.47735
H	1.34032	-5.47386	0.98499
H	1.92627	-5.37190	-0.70023
C	-1.73150	-3.69836	-1.62840
H	2.10552	-2.76084	-0.19330
H	3.38406	-3.86283	0.29632
H	-2.15198	-4.44258	-2.31120
H	-2.09153	-2.71055	-1.92919
C	2.18199	-3.17769	1.94625
O	0.85835	-3.24418	2.40749
H	2.75518	-3.86921	2.57464
H	2.61207	-2.17496	2.08011
H	0.31429	-2.56465	1.96322
O	-0.90111	-4.57633	0.42562
C	-0.20218	-3.76447	-1.58204
H	0.24138	-2.56100	-1.46228
H	0.36329	-4.09040	-2.45452
O	-0.63870	-1.57723	0.80297
C	-2.91612	1.30744	0.52490
C	-3.81030	0.17847	0.16263
C	-4.04493	-0.87128	1.09015
C	-4.40581	0.12358	-1.12539
C	-4.88429	-1.95511	0.72561
C	-3.44124	-0.88629	2.36847
C	-5.22796	-0.97894	-1.47191
C	-4.20724	1.14461	-2.08262
C	-5.11623	-3.00199	1.63306
C	-5.46280	-1.99944	-0.54595
C	-3.67647	-1.93853	3.25553
H	-2.77472	-0.09725	2.68988
C	-5.81059	-1.04861	-2.74805
C	-4.79382	1.05970	-3.34700
H	-3.60239	2.01495	-1.86515

C	-4.51372	-2.99110	2.89075
H	-5.75450	-3.83555	1.36465
H	-6.09422	-2.83844	-0.81970
H	-6.43715	-1.88832	-3.02504
C	-5.59072	-0.03423	-3.67972
H	-4.69151	-3.80441	3.58238
H	-6.04257	-0.09468	-4.66142
C	2.78283	1.45356	-0.55743
C	3.72181	0.33816	-0.27904
C	4.01127	-0.62093	-1.28492
C	4.31583	0.21159	1.00452
C	4.90036	-1.68862	-1.00072
C	3.41996	-0.55819	-2.56694
C	5.19833	-0.86730	1.26592
C	4.05526	1.13684	2.04105
C	5.17777	-2.65364	-1.98273
C	5.48670	-1.79791	0.26374
C	3.70217	-1.52892	-3.53001
H	2.72685	0.22893	-2.83261
C	5.78128	-1.00774	2.53605
C	4.64290	0.98237	3.29827
H	3.39965	1.98461	1.89217
C	4.57854	-2.57280	-3.23941
H	5.85174	-3.47635	-1.77486
H	6.16047	-2.62212	0.47395
H	6.45319	-1.83102	2.74841
C	5.50141	-0.08722	3.54581
H	4.79253	-3.32315	-3.98949
H	5.95370	-0.20187	4.52246
H	-4.63030	1.84706	-4.07157
H	-3.20475	-1.93840	4.22975
H	3.23679	-1.47220	-4.50558
H	4.43196	1.69663	4.08381

S-anti-ev(-,+) intermediate



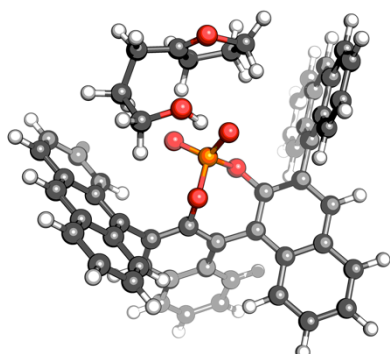
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P	0.07389	-0.67729	0.54266
O	-1.02400	0.10942	-0.41213
O	1.18467	0.44855	0.98108
C	1.56153	1.32297	-0.00695
C	0.67240	2.33126	-0.43606
C	3.27916	2.18638	-1.48911
C	1.05911	3.20145	-1.48912

C	2.38231	3.13303	-1.99659
C	-0.67111	2.40808	0.20648
C	-1.12758	3.56674	0.88602
C	-1.50159	1.27143	0.13935
C	-2.46425	3.61214	1.36040
C	-3.31014	2.51125	1.17851
H	-4.33795	2.55127	1.52245
H	4.29166	2.13481	-1.87459
C	2.78926	4.00571	-3.01842
C	1.89062	4.92775	-3.55590
H	3.79995	3.96845	-3.40756
H	2.20922	5.59529	-4.34610
C	0.57846	4.98095	-3.08722
C	0.15959	4.12334	-2.06765
H	-0.11917	5.68740	-3.51834
H	-0.87203	4.18213	-1.74836
C	-2.93829	4.76065	2.01407
C	-2.09384	5.85246	2.21958
H	-3.95966	4.81085	2.37265
H	-2.46393	6.73348	2.72788
C	-0.77043	5.80640	1.78186
C	-0.28515	4.67360	1.12465
H	-0.11600	6.65090	1.95552
H	0.75222	4.66854	0.81781
O	-0.55292	-1.16975	1.80557
C	-0.10570	-4.25662	-0.17885
C	2.14285	-4.09382	0.03977
C	-1.39398	-4.43077	-0.88418
H	2.52005	-3.16958	-0.38628
H	2.83975	-4.92150	-0.08901
C	-2.14872	-3.08336	-1.04912
H	-1.21237	-4.88841	-1.85920
H	-1.99461	-5.09933	-0.25746
C	1.58142	-3.90131	1.45289
H	-1.94649	-2.42442	-0.19904
H	-3.21915	-3.30355	-1.03705
H	1.97224	-4.64811	2.14580
H	1.82568	-2.90447	1.82246
C	-1.78608	-2.40509	-2.37787
O	-0.42151	-2.50619	-2.69223
H	-2.32656	-2.90372	-3.19092
H	-2.11571	-1.35963	-2.33725
H	0.08644	-2.04115	-1.99361
O	0.98239	-4.41807	-0.80402
C	0.05939	-4.02859	1.27238
H	-0.47444	-3.11575	1.58759
H	-0.38942	-4.88400	1.79342
O	0.69247	-1.69544	-0.39382
C	2.87126	1.27378	-0.51117
C	3.82435	0.23909	-0.03569
C	4.14111	-0.87137	-0.86295
C	4.42218	0.35214	1.24772
C	5.06159	-1.84820	-0.40395
C	3.54532	-1.05031	-2.13301
C	5.32458	-0.64801	1.69171
C	4.15265	1.44524	2.10281
C	5.38317	-2.94886	-1.21562

C	5.63776	-1.73021	0.86402
C	3.87129	-2.15363	-2.92428
H	2.81529	-0.35250	-2.52051
C	5.91254	-0.55092	2.96373
C	4.74576	1.52638	3.36437
H	3.48745	2.24551	1.80708
C	4.79051	-3.09728	-2.46950
H	6.08559	-3.70060	-0.87545
H	6.33289	-2.48800	1.21060
H	6.60044	-1.31119	3.31474
C	5.62032	0.53035	3.79485
H	5.03782	-3.95136	-3.08657
H	6.07711	0.59872	4.77375
C	-2.83327	1.34179	0.57832
C	-3.74696	0.18644	0.40161
C	-4.01776	-0.68530	1.48861
C	-4.34949	-0.05569	-0.86091
C	-4.88701	-1.79018	1.30168
C	-3.43441	-0.49295	2.76119
C	-5.21586	-1.16649	-1.02321
C	-4.11092	0.78291	-1.97378
C	-5.14792	-2.66802	2.36649
C	-5.48128	-2.01449	0.05627
C	-3.70256	-1.37634	3.80872
H	-2.76098	0.33119	2.95605
C	-5.80164	-1.42505	-2.27323
C	-4.70025	0.51067	-3.20996
H	-3.46701	1.64951	-1.90255
C	-4.55606	-2.46048	3.61225
H	-5.80803	-3.51722	2.23427
H	-6.14311	-2.86382	-0.07808
H	-6.45967	-2.27501	-2.41054
C	-5.54071	-0.59086	-3.36009
H	-4.75976	-3.14231	4.42779
H	-5.99377	-0.79745	-4.32110
H	4.52707	2.36704	4.01027
H	3.40498	-2.27926	-3.89296
H	-3.24461	-1.21991	4.77691
H	-4.50369	1.15736	-4.05540

S-anti-ev(-,+)^{2nd} step



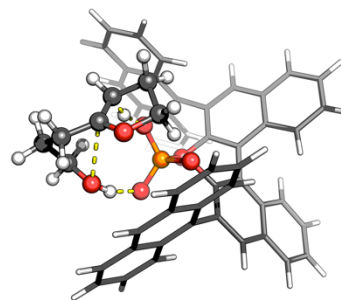
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P	0.03186	-0.60789	0.24770
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O	-1.05191	0.27987	-0.61857
O	1.09789	0.46908	0.88129
C	1.51625	1.44336	0.01128
C	0.64113	2.49036	-0.34746
C	3.28562	2.44349	-1.31390
C	1.06520	3.45999	-1.29334
C	2.40663	3.43912	-1.75609
C	-0.72587	2.50117	0.25115
C	-1.20914	3.58397	1.03065
C	-1.54472	1.36989	0.05336
C	-2.55514	3.56995	1.48056
C	-3.38246	2.48001	1.18402
H	-4.41401	2.47222	1.51889
H	4.31099	2.42698	-1.66702
C	2.84920	4.40770	-2.67112
C	1.96917	5.37993	-3.14763
H	3.87337	4.40672	-3.02524
H	2.31526	6.12127	-3.85626
C	0.64058	5.38927	-2.72431
C	0.18602	4.43616	-1.81028
H	-0.04198	6.13609	-3.10902
H	-0.85657	4.46501	-1.52404
C	-3.05568	4.64572	2.23112
C	-2.22892	5.72146	2.55718
H	-4.08413	4.65058	2.57254
H	-2.61965	6.54607	3.13931
C	-0.89639	5.73016	2.14601
C	-0.38447	4.67027	1.39426
H	-0.25551	6.56029	2.41391
H	0.65921	4.70501	1.11224
O	-0.62607	-1.28013	1.41366
C	0.25906	-4.65514	0.11025
C	2.30761	-4.08163	-0.65156
C	-1.12238	-5.18152	0.05341
H	2.15940	-3.24468	-1.33595
H	3.14083	-4.71540	-0.94939
C	-2.13103	-4.00587	0.12266
H	-1.25201	-5.77293	-0.85546
H	-1.25882	-5.81772	0.93674
C	2.28635	-3.63703	0.81059
H	-1.86268	-3.32661	0.93897
H	-3.12047	-4.41775	0.34335
H	2.97717	-4.22564	1.41813
H	2.54205	-2.57984	0.88587
C	-2.14422	-3.24362	-1.21433
O	-0.87647	-3.25984	-1.82010
H	-2.84177	-3.72940	-1.90713
H	-2.49006	-2.21781	-1.04440
H	-0.33242	-2.48190	-1.53094
O	1.09324	-4.90485	-0.81266
C	0.82465	-3.87058	1.22442
H	0.24931	-2.93194	1.35453
H	0.68906	-4.43911	2.15260
O	0.72888	-1.47440	-0.77881
C	2.84266	1.43710	-0.44961
C	3.77411	0.34937	-0.05251
C	4.12997	-0.66173	-0.98573

C	4.31046	0.31059	1.26241
C	5.03043	-1.68749	-0.59990
C	3.59802	-0.69014	-2.29546
C	5.19025	-0.73933	1.63073
C	4.00213	1.30029	2.22380
C	5.39815	-2.68434	-1.51861
C	5.54450	-1.71956	0.69934
C	3.97107	-1.69062	-3.19526
H	2.88484	0.04914	-2.63406
C	5.71597	-0.79334	2.93215
C	4.53381	1.23181	3.51318
H	3.35403	2.13450	1.99082
C	4.87183	-2.68162	-2.81006
H	6.08631	-3.47176	-1.23465
H	6.22332	-2.51519	0.98871
H	6.38579	-1.59317	3.22551
C	5.38508	0.18686	3.86746
H	5.15524	-3.45611	-3.51093
H	5.79442	0.13926	4.86833
C	-2.88119	1.37830	0.48423
C	-3.76819	0.21963	0.21243
C	-4.02589	-0.73744	1.22932
C	-4.35202	0.05527	-1.07143
C	-4.86449	-1.84714	0.95212
C	-3.45488	-0.62850	2.51748
C	-5.18568	-1.06395	-1.32507
C	-4.12756	0.98060	-2.11606
C	-5.11266	-2.80738	1.94664
C	-5.43538	-1.99790	-0.31508
C	-3.70690	-1.59527	3.49282
H	-2.80108	0.19289	2.77908
C	-5.75816	-1.24125	-2.59525
C	-4.70481	0.78944	-3.37310
H	-3.50841	1.85644	-1.97344
C	-4.53310	-2.68097	3.20875
H	-5.74847	-3.66131	1.74464
H	-6.07081	-2.85338	-0.51956
H	-6.39295	-2.09496	-2.80164
C	-5.51595	-0.31838	-3.61263
H	-4.72389	-3.42790	3.96843
H	-5.96017	-0.46147	-4.58922
H	4.28571	1.99439	4.24026
H	3.55560	-1.69959	-4.19468
H	-3.25736	-1.50255	4.47306
H	-4.52243	1.50463	-4.16488

S-anti-hc(-,+)



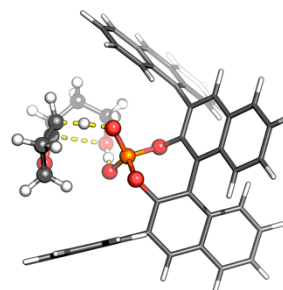
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P	-0.14029	-0.62242	-0.67203
O	-1.47410	0.23613	-1.04778
O	0.75768	0.35856	0.31962
C	0.94145	1.62433	-0.17630
C	2.21078	2.01810	-0.62623
C	-0.13143	2.53858	-0.17564
C	2.39535	3.29489	-1.16480
C	0.03359	3.80427	-0.79406
C	1.31512	4.18042	-1.27638
C	-1.41096	2.11181	0.46513
C	-1.97319	2.79817	1.57405
C	-2.03026	0.93406	-0.00557
C	-3.21321	2.35872	2.10836
C	-3.25169	0.50731	0.53796
C	-3.84612	1.22904	1.57635
H	-4.78799	0.88594	1.99037
H	3.37858	3.58593	-1.51776
C	1.49873	5.43931	-1.87008
C	0.42180	6.31609	-2.00851
H	2.47345	5.74187	-2.23425
H	0.56893	7.28357	-2.47098
C	-0.84647	5.94387	-1.56325
C	-1.04516	4.69758	-0.96510
H	-1.68078	6.62263	-1.68504
H	-2.04682	4.43769	-0.64960
C	-3.79534	3.04272	3.18748
C	-3.14931	4.14090	3.75576
H	-4.74533	2.72139	3.59812
H	-3.60153	4.66161	4.58997
C	-1.91403	4.55860	3.26216
C	-1.32347	3.89208	2.18628
H	-1.40891	5.40049	3.71791
H	-0.35450	4.23433	1.84989
O	-0.51705	-1.76786	0.25451
C	2.22531	-3.49982	1.34851
C	2.17024	-1.59535	2.55658
C	2.87126	-4.56783	0.54605
H	1.95308	-0.77487	1.86880
H	2.78468	-1.26239	3.39127
C	1.98770	-5.11693	-0.58389
H	3.80161	-4.16061	0.14760

H	3.12118	-5.37247	1.25167
C	0.91174	-2.38092	2.91902
H	1.18941	-5.75102	-0.18320
H	2.62584	-5.75965	-1.19694
H	1.00446	-2.88106	3.88850
H	0.03551	-1.73034	2.92478
C	1.38716	-3.98174	-1.42749
O	2.24757	-2.87049	-1.32260
H	1.28161	-4.30998	-2.46978
H	0.38395	-3.71897	-1.06423
H	1.76902	-2.08912	-1.68635
O	2.98671	-2.55456	1.79771
C	0.87113	-3.37317	1.75221
H	0.31864	-2.68014	0.86739
H	0.28431	-4.28776	1.81789
O	0.56499	-0.90797	-1.95314
C	3.35744	1.08127	-0.52766
C	3.74503	0.30350	-1.64981
C	4.02647	0.90790	0.71223
C	4.77020	-0.66665	-1.51008
C	3.12406	0.45290	-2.91028
C	5.05291	-0.06380	0.82601
C	3.69457	1.67681	1.85103
C	5.13964	-1.46253	-2.60675
C	5.40838	-0.84296	-0.27881
C	3.50266	-0.34715	-3.99019
H	2.33618	1.17688	-3.07037
C	5.70935	-0.25306	2.05319
C	4.35832	1.47708	3.06317
H	2.92431	2.43608	1.81625
C	4.50558	-1.30297	-3.83873
H	5.91690	-2.21138	-2.50989
H	6.18855	-1.59068	-0.18017
H	3.01324	-0.22707	-4.94810
H	6.49157	-0.99629	2.15319
C	5.36140	0.51467	3.16452
H	4.09263	2.07123	3.92801
H	4.79306	-1.92192	-4.67879
H	5.87120	0.36319	4.10716
C	-3.89165	-0.73767	0.04582
C	-3.72980	-1.95291	0.76339
C	-4.61785	-0.73229	-1.17359
C	-4.28382	-3.15142	0.24614
C	-3.00744	-2.01246	1.97757
C	-5.16808	-1.94240	-1.66755
C	-4.81299	0.45286	-1.91860
C	-4.10660	-4.36294	0.93484
C	-4.99651	-3.13444	-0.95684
C	-2.83549	-3.22597	2.64621
H	-2.55595	-1.13058	2.41195
C	-5.88241	-1.94783	-2.87707
C	-5.52507	0.42978	-3.11961
H	-4.42210	1.40391	-1.58131
C	-3.38296	-4.39737	2.12688
H	-4.52282	-5.28542	0.54734
H	-5.41646	-4.05655	-1.34536
H	-2.27095	-3.25812	3.56924

H	-6.30481	-2.86693	-3.26595
C	-6.05717	-0.76643	-3.59795
H	-5.66541	1.34441	-3.68126
H	-3.24520	-5.33544	2.64892
H	-6.60783	-0.77816	-4.52972

S-anti-hc(-,-)



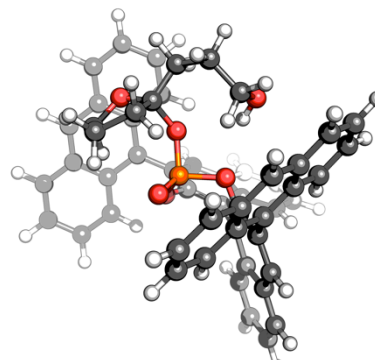
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O	1.17386	0.37251	0.78843
C	1.60463	1.36720	-0.05145
C	2.90723	1.31544	-0.56923
C	0.76583	2.46609	-0.33268
C	3.36265	2.32849	-1.41785
C	1.19849	3.45208	-1.25759
C	2.51648	3.38354	-1.78143
C	-0.57708	2.51034	0.31892
C	-0.98196	3.57577	1.16419
C	-1.45080	1.42237	0.11092
C	-2.30659	3.59329	1.67494
C	-2.76455	1.46185	0.60388
C	-3.18994	2.54958	1.37173
H	-4.20490	2.56588	1.75351
H	4.36935	2.27416	-1.81757
C	2.96742	4.36527	-2.67810
C	2.11821	5.39828	-3.07636
H	3.97380	4.32820	-3.07826
H	2.47054	6.14980	-3.77107
C	0.81152	5.45616	-2.59290
C	0.34881	4.49041	-1.69640
H	0.15204	6.25085	-2.91723
H	-0.67743	4.55916	-1.36198
C	-2.72892	4.65265	2.49381
C	-1.84526	5.67960	2.82788
H	-3.73994	4.68163	2.88277
H	-2.17565	6.49125	3.46317
C	-0.53309	5.65544	2.35628
C	-0.09859	4.61183	1.53616
H	0.15238	6.44702	2.63042
H	0.93210	4.61897	1.20811
O	-0.60074	-1.26235	1.36760
C	0.04716	-4.39519	0.17591
C	2.09091	-3.66864	0.79818

C	-0.92414	-5.04748	-0.74055
H	2.21540	-2.65555	0.41371
H	3.04169	-4.19794	0.84061
C	-2.28283	-4.34673	-0.86473
H	-0.45869	-5.13244	-1.72407
H	-1.06952	-6.05920	-0.33594
C	1.23797	-3.72318	2.06790
H	-2.79224	-4.29246	0.10511
H	-2.89751	-4.97694	-1.51502
H	1.49180	-4.58785	2.68922
H	1.35144	-2.81094	2.65714
C	-2.15921	-2.93748	-1.46567
O	-1.18367	-2.89344	-2.47828
H	-3.12628	-2.65092	-1.89288
H	-1.93290	-2.21744	-0.67114
H	-0.43257	-2.37011	-2.13829
O	1.27832	-4.35490	-0.21268
C	-0.16778	-3.84030	1.46441
H	-0.49825	-2.64382	1.29259
H	-0.98447	-4.26554	2.04633
O	0.61129	-1.54620	-0.88145
C	3.79276	0.16878	-0.24482
C	3.97195	-0.88200	-1.18340
C	4.42248	0.09116	1.02541
C	4.78764	-1.99225	-0.84602
C	3.33568	-0.87133	-2.44566
C	5.22623	-1.03339	1.34259
C	4.27346	1.10953	1.99438
C	4.95814	-3.04415	-1.76091
C	5.40554	-2.05590	0.40638
C	3.51258	-1.92726	-3.34184
H	2.68894	-0.05831	-2.74731
C	5.84257	-1.12502	2.60143
C	4.89221	1.00220	3.24158
H	3.68218	1.99449	1.79939
C	4.32268	-3.00900	-3.00182
H	5.57717	-3.89825	-1.51268
H	6.02110	-2.91321	0.65860
H	3.01672	-1.90718	-4.30377
H	6.45557	-1.98159	2.85622
C	5.67253	-0.11202	3.54506
H	4.76630	1.78768	3.97567
H	4.45556	-3.82493	-3.70044
H	6.14927	-0.18990	4.51367
C	-3.70439	0.34841	0.31997
C	-3.91549	-0.67375	1.28277
C	-4.36489	0.27880	-0.93467
C	-4.76748	-1.76431	0.97266
C	-3.28455	-0.64902	2.54695
C	-5.22716	-0.81184	-1.21434
C	-4.19079	1.27319	-1.92401
C	-4.95314	-2.79919	1.90382
C	-5.41806	-1.81885	-0.26340
C	-3.47686	-1.68778	3.45995
H	-2.62678	0.16031	2.83499
C	-5.88109	-0.89147	-2.45480
C	-4.84849	1.17874	-3.15217

H	-3.55071	2.12997	-1.75905
C	-4.30597	-2.76078	3.13858
H	-5.59558	-3.64114	1.67429
H	-6.06965	-2.65613	-0.49106
H	-2.97782	-1.66140	4.42005
H	-6.53869	-1.72255	-2.68110
C	-5.69027	0.09995	-3.41717
H	-4.70520	1.94680	-3.90133
H	-4.44974	-3.56414	3.84947
H	-6.19714	0.03203	-4.37112

S-anti-hc(-,+) intermediate



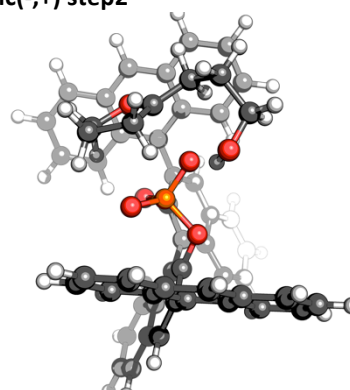
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P	-0.05941	-0.70660	0.59950
O	-1.12204	0.00048	-0.40679
O	1.05308	0.40945	0.97185
C	1.39515	1.31002	-0.01020
C	2.71664	1.32548	-0.48677
C	0.46896	2.28410	-0.45625
C	3.10088	2.25294	-1.45952
C	0.83565	3.15937	-1.51351
C	2.17028	3.14940	-1.99438
C	-0.89079	2.31928	0.16043
C	-1.41930	3.47031	0.79961
C	-1.66814	1.14944	0.09901
C	-2.76917	3.46166	1.24185
C	-3.00400	1.15379	0.52260
C	-3.55494	2.31274	1.07753
H	-4.58723	2.30461	1.40959
H	4.12310	2.24940	-1.82218
C	2.55592	4.02928	-3.01843
C	1.62515	4.89923	-3.58665
H	3.57510	4.03663	-3.38664
H	1.92738	5.57165	-4.37914
C	0.30231	4.89270	-3.14665
C	-0.09545	4.02817	-2.12455
H	-0.42014	5.55752	-3.60241
H	-1.13605	4.03875	-1.83058
C	-3.31374	4.60218	1.85291
C	-2.52826	5.73915	2.04770
H	-4.34449	4.61129	2.18716
H	-2.95294	6.61402	2.52287
C	-1.19337	5.74637	1.64339
C	-0.63730	4.62198	1.02928

H	-0.58506	6.62609	1.80967
H	0.40663	4.65890	0.74787
O	-0.60773	-1.28589	1.83260
C	0.91864	-3.10325	-0.42815
C	2.28452	-3.07791	1.38632
C	0.76151	-3.57895	-1.86140
H	2.26835	-2.01604	1.66680
H	3.23058	-3.50991	1.71426
C	-0.67867	-3.83066	-2.31927
H	1.23364	-2.83825	-2.51253
H	1.33785	-4.50588	-1.94373
C	1.03514	-3.81848	1.89034
H	-1.12198	-4.65754	-1.74902
H	-0.63476	-4.15957	-3.36337
H	1.29057	-4.82546	2.22708
H	0.55426	-3.27813	2.70559
C	-1.62917	-2.63624	-2.24290
O	-1.14946	-1.52028	-2.96675
H	-2.58580	-2.92580	-2.69128
H	-1.83634	-2.36162	-1.19990
H	-0.72064	-0.92290	-2.34306
O	2.24214	-3.19338	-0.03988
C	0.13051	-3.87202	0.64144
H	-0.86517	-3.46290	0.81433
H	0.02751	-4.89840	0.27879
O	0.57145	-1.66499	-0.48221
C	3.71209	0.34552	0.01895
C	4.11769	-0.74505	-0.79625
C	4.25798	0.48860	1.32267
C	5.06728	-1.67555	-0.30166
C	3.58344	-0.95042	-2.08909
C	5.19394	-0.46420	1.79991
C	3.90320	1.56624	2.16624
C	5.46972	-2.76113	-1.09695
C	5.59116	-1.52856	0.98574
C	3.99699	-2.03328	-2.86760
H	2.83503	-0.28984	-2.50541
C	5.72949	-0.33871	3.09233
C	4.44549	1.67647	3.44825
H	3.21042	2.33278	1.84571
C	4.93673	-2.93554	-2.37369
H	6.19260	-3.47921	-0.72805
H	6.30955	-2.25119	1.35889
H	3.57819	-2.17866	-3.85505
H	6.44188	-1.06341	3.46877
C	5.35301	0.72561	3.91121
H	4.16175	2.50481	4.08467
H	5.24857	-3.77637	-2.97962
H	5.77022	0.81639	4.90582
C	-3.81924	-0.08136	0.40574
C	-4.04062	-0.90123	1.54395
C	-4.31227	-0.49071	-0.86169
C	-4.75521	-2.11826	1.40315
C	-3.54733	-0.55269	2.82207
C	-5.02130	-1.71333	-0.97739
C	-4.11303	0.28676	-2.02542
C	-4.96879	-2.94231	2.52045

C	-5.23737	-2.50989	0.15072
C	-3.76598	-1.38477	3.92179
H	-2.98243	0.35558	2.98324
C	-5.50090	-2.13294	-2.22914
C	-4.59218	-0.14735	-3.26295
H	-3.58875	1.23261	-1.99173
C	-4.47586	-2.57460	3.77223
H	-5.51313	-3.87444	2.42445
H	-5.77856	-3.44527	0.05195
H	-3.38053	-1.10618	4.89414
H	-6.04027	-3.06739	-2.33003
C	-5.28305	-1.35336	-3.36496
H	-4.42790	0.45565	-4.14668
H	-4.64160	-3.21592	4.62825
H	-5.65199	-1.68477	-4.32698

S-anti-hc(-,+)-step2



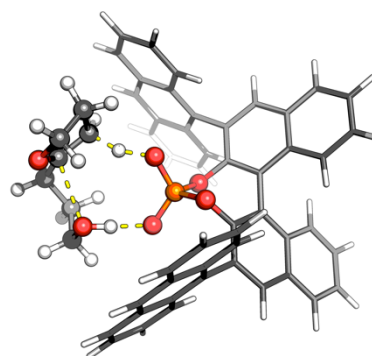
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P	-0.10414	-0.66961	0.22839
O	-1.22887	0.06716	-0.69945
O	0.84649	0.53981	0.82792
C	1.12126	1.57308	-0.03270
C	2.44421	1.77313	-0.45941
C	0.10896	2.49248	-0.39266
C	2.75455	2.85478	-1.28976
C	0.40824	3.53008	-1.31479
C	1.74907	3.71766	-1.73979
C	-1.25957	2.30325	0.17575
C	-1.91639	3.29753	0.94660
C	-1.89769	1.06678	-0.04252
C	-3.25495	3.07916	1.36777
C	-3.22072	0.86132	0.37756
C	-3.90017	1.87410	1.06113
H	-4.92102	1.70399	1.38523
H	3.77961	2.99831	-1.61390
C	2.06630	4.75929	-2.62627
C	1.06415	5.59896	-3.11321
H	3.08813	4.91756	-2.95054
H	1.31445	6.39739	-3.79980
C	-0.26169	5.40162	-2.72948
C	-0.59285	4.37384	-1.84379
H	-1.03773	6.04552	-3.12290
H	-1.63555	4.24127	-1.58914
C	-3.92720	4.06482	2.10778

C	-3.27842	5.25114	2.45247
H	-4.95135	3.91340	2.42792
H	-3.80086	6.00540	3.02665
C	-1.95323	5.46072	2.07196
C	-1.27164	4.49263	1.33116
H	-1.44984	6.37603	2.35556
H	-0.23854	4.68375	1.07407
O	-0.66869	-1.34600	1.43065
C	1.90170	-3.27408	0.28227
C	2.08265	-2.28768	2.32799
C	2.44056	-3.65577	-1.05221
H	1.64120	-1.29043	2.30047
H	2.93427	-2.32052	3.00658
C	1.64848	-4.65896	-1.89427
H	2.58219	-2.71641	-1.59293
H	3.44192	-4.05050	-0.83017
C	1.05428	-3.40485	2.50293
H	1.29933	-5.49646	-1.27885
H	2.34487	-5.07785	-2.63004
H	1.45271	-4.20965	3.12557
H	0.13855	-3.00447	2.93551
C	0.45802	-4.06112	-2.64428
O	-0.58036	-3.65964	-1.78785
H	0.80570	-3.21839	-3.26112
H	0.05242	-4.82186	-3.31984
H	-0.34638	-2.76595	-1.46671
O	2.64729	-2.51799	0.98828
C	0.79682	-3.89145	1.06503
H	-0.16193	-3.54891	0.66478
H	0.83755	-4.97804	0.93643
O	0.69783	-1.51183	-0.75160
C	3.51547	0.82199	-0.06101
C	4.05976	-0.08059	-1.01510
C	3.98730	0.79425	1.27927
C	5.07540	-0.98943	-0.62165
C	3.60547	-0.11770	-2.35401
C	4.98674	-0.14048	1.65239
C	3.49383	1.68139	2.26339
C	5.62456	-1.88107	-1.55791
C	5.52325	-1.01355	0.70203
C	4.16433	-1.00855	-3.27288
H	2.81109	0.52786	-2.70241
C	5.44264	-0.19171	2.97994
C	3.95756	1.61678	3.57878
H	2.75110	2.43201	2.02908
C	5.17241	-1.88542	-2.87710
H	6.40004	-2.57998	-1.26737
H	6.29115	-1.72154	0.99632
H	3.80666	-1.02516	-4.29431
H	6.20034	-0.90703	3.27752
C	4.92528	0.68045	3.93719
H	3.56578	2.29822	4.32299
H	5.59739	-2.57803	-3.59197
H	5.28072	0.63490	4.95851
C	-3.88451	-0.44416	0.13245
C	-3.99819	-1.39555	1.18163
C	-4.34791	-0.77455	-1.16853

C	-4.56225	-2.66932	0.91511
C	-3.54236	-1.12112	2.49167
C	-4.90829	-2.05479	-1.40985
C	-4.27067	0.14196	-2.24200
C	-4.66143	-3.62399	1.94085
C	-5.00957	-2.98505	-0.37122
C	-3.64500	-2.08272	3.49875
H	-3.09172	-0.17184	2.74801
C	-5.36020	-2.39401	-2.69586
C	-4.72454	-0.21137	-3.51447
H	-3.86540	1.13644	-2.10920
C	-4.20346	-3.32962	3.22489
H	-5.08892	-4.60095	1.74795
H	-5.43685	-3.96335	-0.56620
H	-3.28657	-1.86024	4.49561
H	-5.78671	-3.37065	-2.89264
C	-5.26579	-1.47555	-3.74134
H	-4.65748	0.49964	-4.32790
H	-4.27943	-4.07146	4.00941
H	-5.61586	-1.74384	-4.72979

S-anti-ev(+,+)



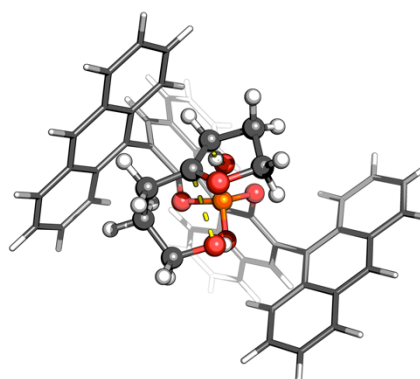
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P	-0.01176	-0.51826	0.09007
O	0.84086	0.66818	0.82817
O	-1.18454	0.23560	-0.76205
C	-1.87416	1.17803	-0.04310
C	-3.19248	0.91649	0.35974
C	-1.27191	2.42075	0.24044
C	-3.90169	1.87363	1.09140
C	-1.95959	3.35690	1.05590
C	-3.29264	3.08014	1.45936
C	0.09966	2.67059	-0.29473
C	0.39326	3.75350	-1.16415
C	1.12186	1.75585	0.04055
C	1.73603	3.97816	-1.56576
C	2.44662	1.99291	-0.35836
C	2.74987	3.11075	-1.14183
H	3.77612	3.28189	-1.44815
H	-4.91841	1.65901	1.40185
C	-3.99544	4.00857	2.24375
C	-3.38197	5.19415	2.65007
H	-5.01604	3.81264	2.55081
H	-3.92774	5.90398	3.25820

C	-2.06182	5.45946	2.28744
C	-1.35036	4.54899	1.50301
H	-1.58552	6.37320	2.61886
H	-0.32218	4.78193	1.26139
C	2.04674	5.06136	-2.40322
C	1.03718	5.90705	-2.86398
H	3.06934	5.24783	-2.70957
H	1.28263	6.73780	-3.51292
C	-0.28948	5.67497	-2.50269
C	-0.61464	4.60519	-1.66582
H	-1.07077	6.32454	-2.87586
H	-1.65755	4.44695	-1.42700
O	0.82977	-1.17701	-0.99639
C	1.86116	-4.47584	-0.29897
C	0.94547	-4.59245	-2.33924
C	2.13379	-4.90946	1.09552
H	-0.03129	-4.11297	-2.22631
H	0.91700	-5.36132	-3.10942
C	1.40299	-4.03028	2.13132
H	1.83309	-5.95559	1.20394
H	3.21595	-4.83376	1.24911
C	2.07823	-3.57371	-2.43653
H	1.63021	-2.97164	1.95876
H	1.77259	-4.29490	3.12798
H	2.96381	-3.99774	-2.92184
H	1.76247	-2.67717	-2.97317
C	-0.10561	-4.23880	2.04314
O	-0.56623	-3.96643	0.73862
H	-0.35179	-5.28290	2.27504
H	-0.60718	-3.59422	2.77530
H	-0.72574	-2.99433	0.73017
O	1.19212	-5.27513	-1.06727
C	2.30468	-3.29429	-0.94673
H	1.51110	-2.33180	-0.74565
H	3.25670	-2.90255	-0.59572
O	-0.54666	-1.37564	1.18955
C	3.52653	1.04399	0.01916
C	4.07297	0.16117	-0.95136
C	4.00659	1.00104	1.35574
C	5.10930	-0.73389	-0.58146
C	3.60057	0.13063	-2.28363
C	5.02437	0.07743	1.70650
C	3.50335	1.86216	2.35786
C	5.66452	-1.60209	-1.53632
C	5.56864	-0.77078	0.73795
C	4.15946	-0.74273	-3.21874
H	2.79211	0.76893	-2.61337
C	5.49349	0.01532	3.02909
C	3.97995	1.78643	3.66821
H	2.74221	2.59979	2.14161
C	5.19083	-1.60310	-2.84789
H	6.45772	-2.28870	-1.26494
H	6.35226	-1.46874	1.01437
H	3.78629	-0.75624	-4.23464
H	6.26715	-0.68998	3.30919
C	4.96904	0.86385	4.00376
H	3.58081	2.44773	4.42654

H	5.61770	-2.28011	-3.57645
H	5.33423	0.80943	5.02123
C	-3.82220	-0.39043	0.04435
C	-3.89599	-1.40468	1.03632
C	-4.30263	-0.65265	-1.26577
C	-4.44428	-2.67021	0.70592
C	-3.41781	-1.19947	2.35089
C	-4.84743	-1.92586	-1.57155
C	-4.25703	0.32510	-2.28564
C	-4.50736	-3.68481	1.67538
C	-4.91404	-2.91683	-0.58754
C	-3.48508	-2.21983	3.30153
H	-2.97853	-0.25844	2.65361
C	-5.31836	-2.19689	-2.86691
C	-4.72764	0.03846	-3.56880
H	-3.86203	1.31576	-2.10278
C	-4.02868	-3.45807	2.96553
H	-4.92419	-4.65553	1.43395
H	-5.33083	-3.88867	-0.83137
H	-3.11132	-2.04963	4.30298
H	-5.73436	-3.16694	-3.11263
C	-5.25548	-1.21844	-3.85901
H	-4.68365	0.79550	-4.34123
H	-4.07814	-4.24523	3.70673
H	-5.61875	-1.43480	-4.85540

S-anti-ev(+,-)



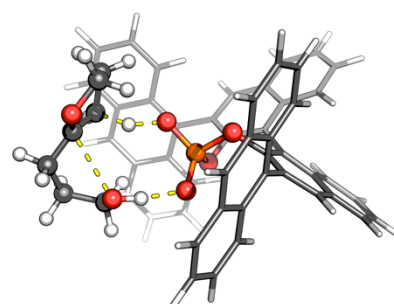
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P	-0.08654	-0.60945	-0.01474
O	0.66251	0.64052	0.73984
O	-1.34605	0.03879	-0.82322
C	-2.11583	0.88252	-0.06364
C	-3.38873	0.47130	0.36205
C	-1.64214	2.17408	0.24317
C	-4.17929	1.33100	1.13064
C	-2.40654	3.01174	1.09718
C	-3.69397	2.58613	1.51765
C	-0.31663	2.58264	-0.30867
C	-0.15893	3.72105	-1.14138
C	0.80716	1.77948	-0.01257
C	1.14494	4.11958	-1.53382
C	2.09372	2.19202	-0.39670
C	2.25698	3.36865	-1.13585

H	3.25438	3.67685	-1.43015
H	-5.15940	1.00130	1.45763
C	-4.47373	3.41499	2.33997
C	-3.97991	4.64806	2.76718
H	-5.46113	3.10444	2.66073
H	-4.58423	5.28066	3.40447
C	-2.70275	5.05998	2.38820
C	-1.91631	4.24959	1.56647
H	-2.31794	6.01000	2.73606
H	-0.92319	4.59559	1.31426
C	1.31998	5.26085	-2.33276
C	0.21421	5.99432	-2.76424
H	2.31157	5.57989	-2.63155
H	0.35536	6.87054	-3.38380
C	-1.07346	5.59240	-2.41088
C	-1.26407	4.46310	-1.61160
H	-1.92870	6.15612	-2.76074
H	-2.27928	4.17270	-1.37708
O	0.81004	-1.13656	-1.12859
C	2.93462	-3.82390	-0.36688
C	1.55265	-5.14555	-1.52996
C	3.73899	-3.43261	0.81896
H	0.57637	-5.00934	-1.05584
H	1.64840	-6.14530	-1.95007
C	2.91901	-2.51934	1.75845
H	4.05136	-4.33701	1.34881
H	4.62765	-2.90077	0.46715
C	1.91785	-3.98603	-2.45919
H	2.58075	-1.62868	1.21410
H	3.57804	-2.18190	2.56582
H	2.62928	-4.29833	-3.23095
H	1.03285	-3.56806	-2.94261
C	1.71070	-3.25700	2.33112
O	0.86409	-3.71685	1.30167
H	2.04974	-4.12884	2.90641
H	1.16581	-2.58871	3.00918
H	0.20339	-2.99525	1.15346
O	2.51594	-5.04856	-0.43553
C	2.54646	-3.01442	-1.45913
H	1.65560	-2.16388	-1.09791
H	3.29904	-2.30597	-1.79777
O	-0.51984	-1.53316	1.07471
C	3.28603	1.37489	-0.04626
C	3.98058	0.65493	-1.05652
C	3.74087	1.30983	1.29902
C	5.13274	-0.09856	-0.71522
C	3.55066	0.65343	-2.40380
C	4.87791	0.52421	1.61815
C	3.09827	2.01758	2.34090
C	5.83917	-0.79578	-1.70936
C	5.56519	-0.15950	0.61203
C	4.26549	-0.04342	-3.38034
H	2.65917	1.18007	-2.71569
C	5.32156	0.43391	2.94771
C	3.55177	1.91625	3.65762
H	2.24533	2.65511	2.15202
C	5.40944	-0.76077	-3.03566

H	6.72205	-1.37223	-1.45943
H	6.43955	-0.75026	0.86515
H	3.92655	-0.03188	-4.40822
H	6.18403	-0.17039	3.20331
C	4.65636	1.12296	3.96110
H	3.04486	2.45777	4.44596
H	5.95750	-1.30178	-3.79614
H	5.00294	1.04771	4.98370
C	-3.88053	-0.89245	0.04202
C	-3.84272	-1.91355	1.02938
C	-4.35358	-1.19353	-1.26235
C	-4.27511	-3.22358	0.70042
C	-3.36540	-1.66993	2.33799
C	-4.77784	-2.51199	-1.56772
C	-4.42104	-0.21058	-2.27589
C	-4.23185	-4.24258	1.66648
C	-4.73626	-3.50876	-0.58818
C	-3.32579	-2.69497	3.28513
H	-3.00816	-0.69423	2.63880
C	-5.24062	-2.82115	-2.85742
C	-4.88296	-0.53504	-3.55319
H	-4.12236	0.81309	-2.09241
C	-3.75926	-3.97655	2.95146
H	-4.56018	-5.24700	1.42625
H	-5.06244	-4.51480	-0.83137
H	-2.95476	-2.49430	4.28202
H	-5.56453	-3.82579	-3.10286
C	-5.28983	-1.83610	-3.84368
H	-4.92677	0.22691	-4.32076
H	-3.72627	-4.76715	3.68999
H	-5.64696	-2.08168	-4.83550

S-anti-hc(+,+)



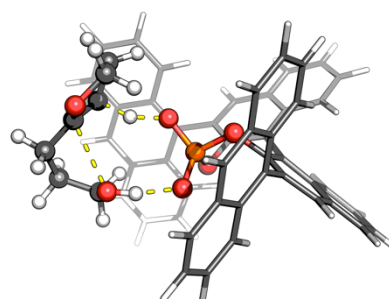
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O	0.70664	0.71151	0.86487
O	-1.26558	0.02858	-0.71191
C	-2.05829	0.91392	-0.02626
C	-3.34844	0.53165	0.37408
C	-1.58490	2.21506	0.23698
C	-4.15166	1.42657	1.08751
C	-2.36459	3.09183	1.03540
C	-3.66505	2.69151	1.44025

C	-0.24739	2.59480	-0.30606
C	-0.07149	3.68998	-1.19168
C	0.86705	1.80073	0.04490
C	1.23968	4.05897	-1.58870
C	2.16039	2.17863	-0.35329
C	2.34103	3.31758	-1.14572
H	3.34354	3.60094	-1.44755
H	-5.14452	1.11885	1.39692
C	-4.45816	3.55743	2.20990
C	-3.96558	4.80343	2.59969
H	-5.45526	3.26626	2.51855
H	-4.58015	5.46460	3.19692
C	-2.67724	5.19252	2.23438
C	-1.87738	4.34516	1.46455
H	-2.29426	6.15360	2.55264
H	-0.87648	4.67477	1.22089
C	1.43254	5.15864	-2.44025
C	0.33752	5.87854	-2.91934
H	2.42977	5.45491	-2.74365
H	0.49240	6.72235	-3.57931
C	-0.95707	5.50366	-2.56186
C	-1.16543	4.41612	-1.71084
H	-1.80394	6.05572	-2.94878
H	-2.18561	4.14507	-1.47506
O	0.87286	-1.20601	-0.85811
C	2.31096	-4.26073	-0.61044
C	1.20965	-3.96926	-2.55426
C	2.73889	-5.01635	0.59318
H	0.27629	-3.45265	-2.31680
H	1.09694	-4.61046	-3.42673
C	3.04383	-4.13560	1.81291
H	1.95262	-5.73724	0.82223
H	3.63641	-5.57618	0.29444
C	2.39377	-3.00759	-2.56941
H	4.00400	-3.62051	1.69949
H	3.14188	-4.80789	2.67024
H	3.22446	-3.38491	-3.17525
H	2.08767	-2.02469	-2.92916
C	1.92005	-3.11911	2.05117
O	0.72865	-3.68007	1.55700
H	1.84401	-2.88371	3.12080
H	2.14556	-2.17396	1.53328
H	0.06999	-2.94507	1.50875
O	1.48649	-4.85603	-1.41634
C	2.72484	-2.98801	-1.07205
H	1.82901	-2.17351	-0.69379
H	3.68101	-2.62186	-0.70869
O	-0.53402	-1.40875	1.32607
C	-3.85184	-0.83217	0.07368
C	-3.85090	-1.83219	1.08276
C	-4.29960	-1.15441	-1.23457
C	-4.28510	-3.14539	0.76897
C	-3.41008	-1.56433	2.39916
C	-4.73115	-2.47420	-1.52320
C	-4.33598	-0.19072	-2.26809
C	-4.27240	-4.14552	1.75536
C	-4.71879	-3.45226	-0.52422

C	-3.40072	-2.57083	3.36680
H	-3.05753	-0.58394	2.69024
C	-5.17223	-2.80331	-2.81558
C	-4.77756	-0.53462	-3.54745
H	-4.03000	0.83321	-2.09843
C	-3.83098	-3.85695	3.04654
H	-4.60061	-5.15261	1.52639
H	-5.04835	-4.46008	-0.75515
H	-3.05529	-2.35236	4.36911
H	-5.50224	-3.80902	-3.04810
C	-5.19303	-1.83663	-3.82089
H	-4.79934	0.21313	-4.32980
H	-3.82073	-4.63332	3.80065
H	-5.53489	-2.09714	-4.81427
C	3.33998	1.36002	0.03635
C	4.03245	0.59285	-0.94070
C	3.77994	1.33414	1.38784
C	5.16085	-0.17705	-0.55831
C	3.62381	0.55954	-2.29411
C	4.88876	0.52694	1.74986
C	3.15222	2.10533	2.39322
C	5.86644	-0.91980	-1.51976
C	5.56733	-0.21304	0.77795
C	4.33849	-0.18127	-3.23762
H	2.74920	1.09484	-2.63692
C	5.31868	0.47874	3.08620
C	3.59325	2.04705	3.71674
H	2.32274	2.76234	2.16933
C	5.45742	-0.91644	-2.85267
H	6.73107	-1.50932	-1.23847
H	6.42148	-0.81860	1.06312
H	4.01573	-0.19359	-4.27071
H	6.16116	-0.13898	3.37442
C	4.66944	1.23261	4.06331
H	3.09936	2.63910	4.47649
H	6.00330	-1.49389	-3.58748
H	5.00722	1.19188	5.09080

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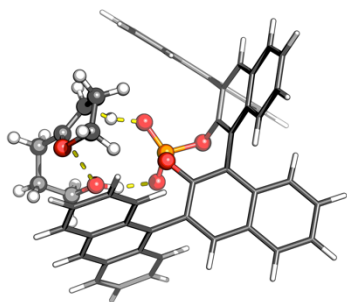


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P	-0.02564	-0.56114	0.21444
O	0.69896	0.74779	0.88093
O	-1.26460	0.01760	-0.68142

C	-2.06042	0.90996	-0.00898	C	-4.22467	-3.15769	0.87012
C	-3.34656	0.52453	0.39922	C	-3.38082	-1.52785	2.46851
C	-1.59907	2.22166	0.22416	C	-4.67340	-2.54334	-1.43739
C	-4.15921	1.42740	1.09130	C	-4.31782	-0.26899	-2.22865
C	-2.38850	3.10913	1.00090	C	-4.19565	-4.13691	1.87691
C	-3.68568	2.70550	1.41373	C	-4.64739	-3.49969	-0.41790
C	-0.26406	2.60092	-0.32678	C	-3.35531	-2.51387	3.45675
C	-0.09538	3.67298	-1.24179	H	-3.04601	-0.53561	2.73964
C	0.85450	1.81995	0.03875	C	-5.09898	-2.90864	-2.72524
C	1.21277	4.03011	-1.66045	C	-4.74343	-0.64885	-3.50324
C	2.14343	2.18238	-0.38465	H	-4.03297	0.76413	-2.07901
C	2.31776	3.29772	-1.21076	C	-3.76214	-3.81379	3.16257
H	3.31728	3.56863	-1.53315	H	-4.50436	-5.15449	1.66802
H	-5.14927	1.11703	1.40690	H	-4.95597	-4.51842	-0.62910
C	-4.48894	3.58214	2.16033	H	-3.01546	-2.26869	4.45478
C	-4.00989	4.84251	2.51951	H	-5.40707	-3.92554	-2.93838
H	-5.48374	3.28867	2.47424	C	-5.13123	-1.96439	-3.75136
H	-4.63251	5.51219	3.09866	H	-4.77398	0.08134	-4.30172
C	-2.72483	5.23553	2.14682	H	-3.73918	-4.57419	3.93251
C	-1.91481	4.37748	1.39975	H	-5.46028	-2.25294	-4.74131
H	-2.35249	6.20827	2.44136	C	3.32294	1.36526	0.00670
H	-0.91702	4.71123	1.14893	C	3.97901	0.55063	-0.95652
C	1.39861	5.10643	-2.54280	C	3.79778	1.38688	1.34598
C	0.29980	5.81402	-3.03134	C	5.11451	-0.20975	-0.57637
H	2.39324	5.39348	-2.86314	C	3.52547	0.45966	-2.29282
H	0.44931	6.63974	-3.71499	C	4.91113	0.58635	1.70898
C	-0.99182	5.44925	-2.65329	C	3.19941	2.19770	2.33776
C	-1.19338	4.38485	-1.77190	C	5.78968	-0.99238	-1.52805
H	-1.84177	5.99095	-3.04802	C	5.55911	-0.19472	0.74818
H	-2.21168	4.12037	-1.52136	C	4.20338	-0.32917	-3.22444
O	0.89421	-1.16627	-0.84090	H	2.64268	0.98562	-2.62964
C	2.25961	-4.26203	-0.60600	C	5.37606	0.58598	3.03440
C	0.88625	-4.07505	-2.38033	C	3.67516	2.18676	3.65049
C	2.85791	-4.92628	0.57840	H	2.36582	2.84865	2.11113
H	0.00471	-3.52495	-2.04105	C	5.33569	-1.04728	-2.84558
H	0.63359	-4.76821	-3.18079	H	6.66163	-1.57232	-1.24951
C	3.29881	-3.94599	1.67586	H	6.41775	-0.79402	1.03310
H	2.12697	-5.63819	0.96390	H	3.84459	-0.38824	-4.24391
H	3.72406	-5.49117	0.20617	H	6.22249	-0.02584	3.32362
C	2.06746	-3.14345	-2.63794	C	4.75664	1.38006	3.99902
H	4.21567	-3.41940	1.38894	H	3.20396	2.80923	4.40027
H	3.53909	-4.54535	2.55853	H	5.85520	-1.65908	-3.57163
H	2.79155	-3.58047	-3.33365	H	5.12125	1.37600	5.01811
H	1.72832	-2.17718	-3.01388				
C	2.18351	-2.93756	1.99147				
O	0.95819	-3.54821	1.67051				
H	2.22740	-2.64608	3.04902				
H	2.32518	-2.01812	1.40192				
H	0.27204	-2.83642	1.63191				
O	1.32011	-4.89386	-1.23917				
C	2.61953	-3.03650	-1.21188				
H	1.80842	-2.16889	-0.75998				
H	3.62475	-2.67532	-1.01885				
O	-0.48833	-1.40054	1.35679				
C	-3.83351	-0.85147	0.12848				
C	-3.81582	-1.83041	1.15771				
C	-4.26934	-1.20958	-1.17453				

S-gau-ev(-,+)



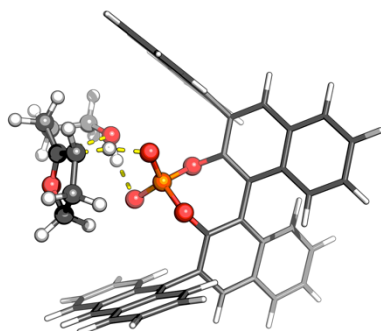
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C	-0.85898	1.61935	0.02775
C	-2.12074	2.07902	0.43882
C	0.23678	2.50591	-0.03242
C	-2.27913	3.40464	0.85528
C	0.09546	3.82545	0.46932
C	-1.18176	4.27322	0.89603
C	1.52121	1.99249	-0.59166
C	2.13563	2.56276	-1.73731
C	2.09693	0.85333	0.00947
C	3.38576	2.05687	-2.17987
C	3.32947	0.35739	-0.44507
C	3.97743	0.97335	-1.51995
H	4.92713	0.57869	-1.86434
H	-3.25663	3.74715	1.17700
C	-1.34317	5.58440	1.37141
C	-0.24763	6.44527	1.44766
H	-2.31503	5.94042	1.69240
H	-0.37772	7.45364	1.81887
C	1.01733	6.00477	1.05954
C	1.19373	4.70517	0.57946
H	1.86637	6.67197	1.13424
H	2.19372	4.39532	0.30727
C	4.01915	2.62714	-3.29561
C	3.41415	3.67604	-3.98872
H	4.97727	2.25427	-3.63809
H	3.90548	4.10856	-4.85072
C	2.16986	4.15723	-3.58317
C	1.52891	3.60432	-2.47236
H	1.69710	4.95987	-4.13445
H	0.55527	3.99152	-2.20477
O	0.58451	-1.80216	-0.16398
O	-0.61811	-0.85098	1.94438
H	-0.21280	-2.75966	-0.79009
C	-0.66863	-3.45934	-1.71040
C	-2.03836	-3.67347	-1.40422
C	-0.69005	-2.46770	-2.87623
H	-0.03019	-4.34058	-1.73793
C	-2.64512	-4.77951	-0.61663
O	-2.83616	-2.81650	-1.95242

H	0.13476	-1.75569	-2.80996
H	-0.67321	-2.96465	-3.85192
C	-2.02423	-1.77870	-2.60465
C	-3.70274	-4.31501	0.39348
H	-1.83626	-5.32011	-0.11582
H	-3.09170	-5.46193	-1.35243
H	-2.58412	-1.45114	-3.47840
H	-1.91929	-0.97931	-1.86624
H	-4.47597	-3.73790	-0.12404
H	-4.17637	-5.19296	0.84276
C	-3.05917	-3.44823	1.46365
O	-2.44902	-2.37379	0.79760
H	-2.31882	-4.03719	2.02768
H	-3.82346	-3.10688	2.17367
H	-1.86324	-1.84902	1.39941
C	3.92372	-0.85428	0.17281
C	3.81610	-2.11186	-0.48006
C	4.56827	-0.77023	1.43486
C	4.34797	-3.27122	0.13958
C	3.17026	-2.25177	-1.73052
C	5.09254	-1.94388	2.03412
C	4.71046	0.45877	2.11848
C	4.23165	-4.52178	-0.48992
C	4.97923	-3.17647	1.38359
C	3.05757	-3.50294	-2.33934
H	2.73323	-1.40426	-2.24100
C	5.72602	-1.87167	3.28581
C	5.34206	0.51274	3.36277
H	4.33993	1.38531	1.70011
C	3.58778	-4.63412	-1.72223
H	4.63410	-5.41434	-0.02546
H	5.38176	-4.06934	1.85089
H	2.55244	-3.59552	-3.29228
H	6.12774	-2.76228	3.75471
C	5.84682	-0.64851	3.94536
H	5.44146	1.46019	3.87672
H	3.49727	-5.60164	-2.19889
H	6.33530	-0.60047	4.91006
C	-3.28747	1.16142	0.45982
C	-3.74088	0.61070	1.68794
C	-3.95098	0.82328	-0.74877
C	-4.84767	-0.27603	1.69282
C	-3.11005	0.90863	2.91736
C	-5.03582	-0.08971	-0.72176
C	-3.56603	1.37822	-1.99058
C	-5.31025	-0.81759	2.90349
C	-5.47269	-0.62669	0.49264
C	-3.57650	0.35384	4.11070
H	-2.24967	1.56233	2.96890
C	-5.68201	-0.44984	-1.91552
C	-4.22532	1.01638	-3.16716
H	-2.75547	2.09100	-2.06515
C	-4.67528	-0.50320	4.10463
H	-6.15643	-1.49437	2.91912
H	-6.30748	-1.31986	0.50438
H	-3.08271	0.58986	5.04457
H	-6.50594	-1.15367	-1.90783

C	-5.27533	0.10046	-3.13085
H	-3.91604	1.44386	-4.11218
H	-5.03287	-0.92960	5.03297
H	-5.77864	-0.18075	-4.04681

S-gau-ev(-,-)



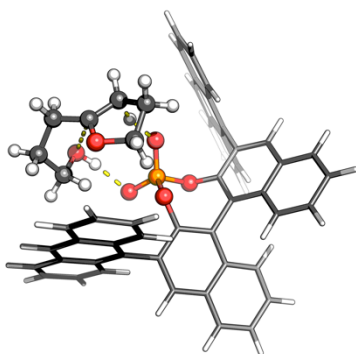
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O	0.92883	0.56124	0.69665
O	-1.19162	0.34886	-0.80597
C	-1.75810	1.28156	0.02399
C	-3.05871	1.06851	0.50331
C	-1.06666	2.47547	0.32804
C	-3.66611	2.02377	1.32300
C	-1.64959	3.40248	1.23199
C	-2.96938	3.17676	1.70577
C	0.29385	2.67278	-0.26012
C	0.62632	3.78205	-1.08012
C	1.26451	1.67939	-0.02027
C	1.96442	3.93696	-1.53189
C	2.58254	1.84051	-0.47195
C	2.93256	2.97710	-1.20663
H	3.95315	3.09094	-1.55506
H	-4.67037	1.84570	1.69166
C	-3.56929	4.09833	2.57873
C	-2.86590	5.22547	3.00454
H	-4.57859	3.94096	2.94051
H	-3.33250	5.92982	3.68109
C	-1.55679	5.43760	2.57391
C	-0.94704	4.53347	1.70145
H	-1.00959	6.30461	2.92105
H	0.07696	4.72314	1.41012
C	2.31370	5.04332	-2.32244
C	1.34699	5.98121	-2.68726
H	3.33242	5.17710	-2.66680
H	1.62188	6.82959	-3.30062
C	0.02408	5.81970	-2.27646
C	-0.33949	4.72780	-1.48524
H	-0.72469	6.54182	-2.57566
H	-1.37926	4.62701	-1.20480
O	0.78397	-1.03572	-1.35424
C	0.72981	-4.39222	-0.53377
C	-1.50000	-3.96412	-0.41830

C	1.99128	-5.04761	-0.09142
H	-1.70455	-3.08879	0.19629
H	-2.29291	-4.70886	-0.35308
C	2.19886	-4.99614	1.42730
H	1.90718	-6.08924	-0.43224
H	2.82371	-4.58554	-0.62981
C	-1.05236	-3.60243	-1.83940
H	2.96010	-5.72622	1.71969
H	1.26633	-5.27662	1.92645
H	-1.41562	-4.32580	-2.57506
H	-1.40638	-2.60617	-2.11658
C	2.63713	-3.58086	1.82914
O	1.99305	-2.61644	1.03896
H	2.47286	-3.41579	2.90093
H	3.71047	-3.47000	1.63788
H	1.11687	-2.33553	1.37181
O	-0.31490	-4.58951	0.19570
C	0.47746	-3.62987	-1.71098
H	0.79714	-2.48542	-1.43902
H	1.08709	-3.88419	-2.57776
O	-0.45462	-1.51184	0.87003
C	3.58957	0.78129	-0.20295
C	3.93979	-0.14660	-1.22080
C	4.12805	0.62675	1.10223
C	4.81218	-1.22344	-0.91845
C	3.42008	-0.04897	-2.53202
C	5.00010	-0.45692	1.37849
C	3.81728	1.52622	2.14745
C	5.14030	-2.16375	-1.90885
C	5.33494	-1.36451	0.36987
C	3.75510	-0.99336	-3.50434
H	2.74152	0.74404	-2.81539
C	5.52216	-0.62844	2.67105
C	4.34510	1.34144	3.42700
H	3.16991	2.37830	1.98698
C	4.61196	-2.04740	-3.19406
H	5.80174	-2.99300	-1.68703
H	5.99844	-2.19390	0.59239
H	3.34480	-0.90885	-4.50240
H	6.18394	-1.45690	2.89492
C	5.19271	0.26648	3.68878
H	4.09593	2.03605	4.21890
H	4.86654	-2.77750	-3.95144
H	5.59782	0.12761	4.68283
C	-3.76979	-0.19622	0.18286
C	-3.86002	-1.22885	1.15471
C	-4.29975	-0.40851	-1.11759
C	-4.49172	-2.45406	0.82018
C	-3.30907	-1.08647	2.44905
C	-4.91194	-1.64852	-1.43237
C	-4.23535	0.58595	-2.12008
C	-4.57675	-3.48504	1.77036
C	-5.00798	-2.65134	-0.46353
C	-3.39907	-2.12281	3.38038
H	-2.79601	-0.18352	2.75108
C	-5.42114	-1.87481	-2.72166
C	-4.74554	0.34426	-3.39729

H	-3.79408	1.55509	-1.92851
C	-4.03342	-3.31688	3.04358
H	-5.05590	-4.42550	1.52489
H	-5.47844	-3.59668	-0.71367
H	-2.97207	-1.99968	4.36738
H	-5.88586	-2.82054	-2.97479
C	-5.33393	-0.88281	-3.69814
H	-4.68472	1.11297	-4.15692
H	-4.09929	-4.11697	3.76955
H	-5.72677	-1.06481	-4.69015

S-gau-hc(-,+)



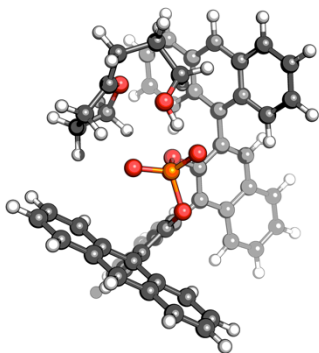
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P	0.14732	-0.66947	0.64407
O	1.41498	0.27898	1.04813
O	-0.79030	0.25790	-0.37426
C	-0.96996	1.55763	0.02519
C	-2.24499	1.98853	0.42347
C	0.09743	2.47665	-0.06275
C	-2.44175	3.31588	0.81757
C	-0.08182	3.80007	0.41700
C	-1.37031	4.21673	0.84142
C	1.39227	1.99987	-0.63199
C	1.98069	2.58118	-1.78543
C	2.01769	0.89595	-0.01838
C	3.25454	2.12863	-2.21903
C	3.27949	0.46038	-0.45369
C	3.89957	1.08942	-1.53737
H	4.87217	0.74173	-1.86807
H	-3.42939	3.63625	1.13098
C	-1.56977	5.53101	1.29321
C	-0.50075	6.42610	1.34857
H	-2.55091	5.86343	1.61128
H	-0.66011	7.43684	1.70147
C	0.77542	6.01724	0.96267
C	0.98945	4.71499	0.50568
H	1.60398	6.71128	1.02105
H	1.99747	4.43093	0.23507
C	3.86151	2.71139	-3.34289
C	3.20805	3.71969	-4.05222
H	4.83719	2.38006	-3.67845
H	3.67946	4.16202	-4.92036
C	1.94217	4.14819	-3.65406
C	1.32682	3.58265	-2.53510

H	1.43296	4.91962	-4.21728
H	0.33596	3.92758	-2.27249
O	0.61184	-1.77451	-0.28334
O	-0.57988	-0.99513	1.90307
H	-0.05255	-2.95427	-0.87138
C	-0.46894	-3.64228	-1.77517
C	-1.85614	-3.70599	-1.45856
C	-0.39419	-2.68452	-2.96838
H	0.08682	-4.57702	-1.76755
C	-2.57859	-4.69107	-0.61886
O	-2.53813	-2.73150	-1.95860
H	0.50266	-2.06643	-2.92390
H	-0.43569	-3.21264	-3.92595
C	-1.64201	-1.83884	-2.72469
C	-3.52466	-4.03763	0.40181
H	-1.83296	-5.30254	-0.10931
H	-3.14152	-5.33172	-1.31170
H	-2.20015	-1.54581	-3.61215
H	-1.44820	-0.98408	-2.07221
H	-4.38304	-3.58243	-0.10163
H	-3.89913	-4.83387	1.05192
C	-2.78709	-2.98624	1.22301
O	-1.53466	-3.51220	1.58975
H	-3.38431	-2.72270	2.10495
H	-2.65493	-2.06710	0.63172
H	-1.00637	-2.74892	1.90490
C	3.94444	-0.68850	0.21133
C	3.92516	-1.97335	-0.39488
C	4.55983	-0.51920	1.47974
C	4.50598	-3.07648	0.28118
C	3.32197	-2.19611	-1.65399
C	5.13702	-1.63708	2.13437
C	4.62106	0.74173	2.11591
C	4.47225	-4.35512	-0.29980
C	5.10396	-2.89861	1.53244
C	3.29260	-3.47420	-2.21510
H	2.85751	-1.39275	-2.20931
C	5.74163	-1.48054	3.39266
C	5.22561	0.87984	3.36709
H	4.20881	1.62934	1.65436
C	3.86573	-4.55028	-1.54060
H	4.91084	-5.20556	0.20889
H	5.54486	-3.74883	2.04271
H	2.81956	-3.63084	-3.17606
H	6.18291	-2.32820	3.90370
C	5.78258	-0.22758	4.00425
H	5.26346	1.85095	3.84376
H	3.83901	-5.53908	-1.97997
H	6.24976	-0.11439	4.97405
C	-3.38826	1.04035	0.44296
C	-3.87393	0.53270	1.67740
C	-3.99663	0.62917	-0.77309
C	-4.97691	-0.35907	1.68409
C	-3.27537	0.87397	2.91161
C	-5.07469	-0.29179	-0.74191
C	-3.56476	1.11944	-2.02674
C	-5.47025	-0.85957	2.90033

C	-5.55943	-0.76567	0.48035
C	-3.77316	0.36112	4.11110
H	-2.41558	1.52844	2.96271
C	-5.66505	-0.72529	-1.94023
C	-4.16706	0.68307	-3.20846
H	-2.76119	1.83911	-2.10766
C	-4.86984	-0.49874	4.10623
H	-6.31268	-1.54098	2.91710
H	-6.39022	-1.46358	0.49458
H	-3.30450	0.63086	5.04878
H	-6.48278	-1.43627	-1.92843
C	-5.20858	-0.24181	-3.16609
H	-3.82063	1.06071	-4.16183
H	-5.25091	-0.89337	5.03925
H	-5.66823	-0.58014	-4.08569

S-gau-hc(-,+) intermediate



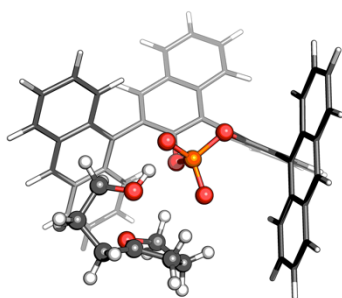
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P	0.12201	-0.67960	0.52890
O	1.39102	0.24523	0.99650
O	-0.79568	0.30945	-0.45655
C	-0.92950	1.60761	-0.03785
C	-2.19337	2.07747	0.35301
C	0.16753	2.49211	-0.11707
C	-2.35108	3.41137	0.74323
C	0.02593	3.82093	0.36070
C	-1.25238	4.27841	0.77373
C	1.45368	1.97455	-0.67107
C	2.07678	2.53714	-1.81510
C	2.03848	0.85538	-0.04637
C	3.34634	2.05108	-2.22478
C	3.30118	0.39318	-0.44987
C	3.95581	1.00215	-1.52476
H	4.92851	0.63401	-1.83215
H	-3.33024	3.76296	1.04978
C	-1.41446	5.59893	1.22235
C	-0.31855	6.46026	1.28583
H	-2.38734	5.96225	1.53190
H	-0.44924	7.47595	1.63627
C	0.94746	6.01103	0.91169
C	1.12455	4.70205	0.45813
H	1.79685	6.67880	0.97672
H	2.12568	4.38640	0.19728
C	3.98631	2.61348	-3.34064

C	3.36991	3.63437	-4.06515
H	4.95910	2.25682	-3.65807
H	3.86647	4.06074	-4.92722
C	2.10908	4.09694	-3.68941
C	1.46137	3.55234	-2.57838
H	1.62902	4.87869	-4.26389
H	0.47565	3.92359	-2.33252
O	0.53054	-1.77216	-0.41443
O	-0.63295	-1.00721	1.78351
H	0.00477	-3.76873	-0.75471
C	-0.60775	-4.07055	-1.62137
C	-2.00354	-3.83735	-1.19747
C	-0.41774	-3.06541	-2.76968
H	-0.42610	-5.12114	-1.85944
C	-2.89082	-4.73559	-0.42573
O	-2.49803	-2.76555	-1.66560
H	0.55162	-2.57741	-2.69357
H	-0.52911	-3.55080	-3.74292
C	-1.52751	-2.04520	-2.52778
C	-3.81760	-3.97993	0.54119
H	-2.25402	-5.43866	0.11224
H	-3.46967	-5.29923	-1.17196
H	-2.10246	-1.75989	-3.40816
H	-1.20946	-1.17621	-1.95406
H	-4.66090	-3.53244	0.00704
H	-4.22168	-4.71534	1.24181
C	-3.01372	-2.89863	1.27262
O	-1.68203	-3.34094	1.35500
H	-3.44415	-2.71279	2.26449
H	-3.04889	-1.95574	0.71187
H	-1.14674	-2.53831	1.61980
C	3.93760	-0.75027	0.25190
C	3.92024	-2.04662	-0.32907
C	4.52545	-0.56151	1.53094
C	4.47383	-3.14149	0.38274
C	3.34848	-2.28840	-1.59903
C	5.07477	-1.67166	2.22166
C	4.58718	0.71175	2.14235
C	4.44454	-4.43069	-0.17449
C	5.04226	-2.94466	1.64477
C	3.32717	-3.57640	-2.13818
H	2.90474	-1.49204	-2.18117
C	5.65240	-1.49566	3.49002
C	5.16513	0.86927	3.40375
H	4.19658	1.59440	1.65333
C	3.87197	-4.64417	-1.42811
H	4.86217	-5.27478	0.36168
H	5.46229	-3.78868	2.18222
H	2.88250	-3.74751	-3.11010
H	6.07249	-2.33727	4.02821
C	5.69443	-0.23073	4.07626
H	5.20413	1.84977	3.86070
H	3.85026	-5.64059	-1.85019
H	6.14136	-0.10245	5.05369
C	-3.36560	1.16285	0.37352
C	-3.89907	0.71366	1.61185
C	-3.95185	0.72115	-0.84365

C	-5.03393	-0.13767	1.62019
C	-3.31358	1.06722	2.84910
C	-5.06459	-0.15789	-0.80833
C	-3.46204	1.13686	-2.10315
C	-5.56879	-0.58678	2.83877
C	-5.60329	-0.56202	0.41632
C	-3.85434	0.60698	4.05136
H	-2.42944	1.68807	2.90128
C	-5.63153	-0.62482	-2.00542
C	-4.03810	0.66401	-3.28378
H	-2.63330	1.82629	-2.19029
C	-4.98081	-0.21328	4.04675
H	-6.43450	-1.23834	2.85627
H	-6.45931	-1.22871	0.43274
H	-3.39496	0.88548	4.99106
H	-6.47534	-1.30458	-1.98966
C	-5.11504	-0.21881	-3.23541
H	-3.64606	0.98326	-4.24082
H	-5.39447	-0.56816	4.98186
H	-5.55573	-0.58407	-4.15399

S-gau-hc(-,+)^{2nd} step



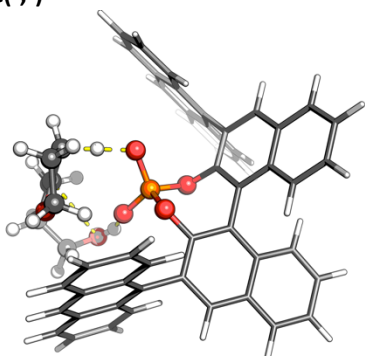
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P	0.14920	-0.65689	0.51971
O	1.40985	0.25745	1.02279
O	-0.73795	0.33401	-0.48693
C	-0.90497	1.62225	-0.04546
C	-2.18863	2.07372	0.30532
C	0.18588	2.51853	-0.05479
C	-2.36953	3.39400	0.73276
C	0.01763	3.82763	0.46544
C	-1.27826	4.26339	0.84317
C	1.49136	2.03510	-0.59139
C	2.13551	2.64514	-1.69910
C	2.06851	0.89641	0.00408
C	3.41436	2.17926	-2.10205
C	3.33503	0.44579	-0.40133
C	4.00960	1.10033	-1.43686
H	4.98582	0.74209	-1.74491
H	-3.36277	3.73183	1.00810
C	-1.46584	5.56498	1.33520
C	-0.37819	6.42770	1.47605
H	-2.45238	5.91193	1.61921
H	-0.52845	7.42834	1.86033

C	0.90416	5.99893	1.13486
C	1.10641	4.70936	0.63831
H	1.74646	6.66731	1.25896
H	2.11860	4.40804	0.40416
C	4.07581	2.78859	-3.18021
C	3.47178	3.83733	-3.87470
H	5.05571	2.44689	-3.49216
H	3.98488	4.30002	-4.70786
C	2.20163	4.28049	-3.50740
C	1.53246	3.68870	-2.43392
H	1.73089	5.08373	-4.05954
H	0.54019	4.04673	-2.19534
O	0.57812	-1.76785	-0.38837
O	-0.64934	-0.96920	1.75648
H	0.00277	-3.84018	-0.49081
C	-0.61701	-4.20700	-1.32234
C	-2.02471	-3.97224	-0.92012
C	-0.44929	-3.29130	-2.54640
H	-0.42418	-5.26939	-1.49049
C	-2.92571	-4.85310	-0.13930
O	-2.54535	-2.95971	-1.49245
H	0.51542	-2.78861	-2.51774
H	-0.56649	-3.85047	-3.47885
C	-1.57008	-2.26961	-2.36940
C	-3.87293	-4.04824	0.76799
H	-2.29934	-5.52715	0.44566
H	-3.48569	-5.45023	-0.87232
H	-2.13123	-2.02471	-3.27070
H	-1.26028	-1.37303	-1.83396
H	-4.73322	-3.67632	0.20442
H	-4.24891	-4.72665	1.53761
C	-3.08611	-2.87928	1.38015
O	-1.72742	-3.23874	1.36434
H	-3.43690	-2.66260	2.39619
H	-3.22368	-1.97600	0.77371
H	-1.20476	-2.39657	1.58838
C	3.94889	-0.74380	0.24143
C	3.95729	-1.99525	-0.43201
C	4.50195	-0.64419	1.54578
C	4.51450	-3.13196	0.20757
C	3.40798	-2.15184	-1.72556
C	5.04769	-1.79680	2.16635
C	4.53331	0.58076	2.25097
C	4.52203	-4.37512	-0.44676
C	5.05017	-3.02271	1.49428
C	3.42392	-3.39478	-2.36178
H	2.95300	-1.32409	-2.25260
C	5.58888	-1.71006	3.45976
C	5.07431	0.64936	3.53650
H	4.14593	1.49361	1.81825
C	3.97944	-4.50258	-1.72521
H	4.94580	-5.24991	0.03233
H	5.47101	-3.89885	1.97690
H	2.99889	-3.49973	-3.35180
H	6.00537	-2.58500	3.94500
C	5.59831	-0.49240	4.13997
H	5.08844	1.59324	4.06623

H	3.98735	-5.46377	-2.22286
H	6.01626	-0.43311	5.13666
C	-3.36156	1.16064	0.24277
C	-3.98337	0.71427	1.44086
C	-3.88081	0.74298	-1.01322
C	-5.13940	-0.10538	1.36956
C	-3.46643	1.03871	2.71616
C	-5.01448	-0.10899	-1.05586
C	-3.30782	1.16141	-2.23641
C	-5.76299	-0.54842	2.54751
C	-5.64018	-0.50777	0.12841
C	-4.09518	0.58485	3.87734
H	-2.56793	1.62992	2.83028
C	-5.51929	-0.54892	-2.29048
C	-3.82194	0.71430	-3.45507
H	-2.46253	1.83507	-2.26672
C	-5.24272	-0.20120	3.79373
H	-6.64584	-1.17536	2.50406
H	-6.51279	-1.15138	0.08459
H	-3.68758	0.84106	4.84682
H	-6.38001	-1.20596	-2.33386
C	-4.92022	-0.14262	-3.48218
H	-3.36697	1.03601	-4.38300
H	-5.72470	-0.55136	4.69737
H	-5.31439	-0.48586	-4.42996

S-gau-hc(-,-)



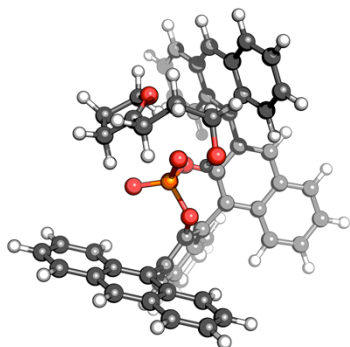
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P	0.14920	-0.65689	0.51971
O	1.40985	0.25745	1.02279
O	-0.73795	0.33401	-0.48693
C	-0.90497	1.62225	-0.04546
C	-2.18863	2.07372	0.30532
C	0.18588	2.51853	-0.05479
C	-2.36953	3.39400	0.73276
C	0.01763	3.82763	0.46544
C	-1.27826	4.26339	0.84317
C	1.49136	2.03510	-0.59139
C	2.13551	2.64514	-1.69910
C	2.06851	0.89641	0.00408
C	3.41436	2.17926	-2.10205
C	3.33503	0.44579	-0.40133
C	4.00960	1.10033	-1.43686
H	4.98582	0.74209	-1.74491

H	-3.36277	3.73183	1.00810
C	-1.46584	5.56498	1.33520
C	-0.37819	6.42770	1.47605
H	-2.45238	5.91193	1.61921
H	-0.52845	7.42834	1.86033
C	0.90416	5.99893	1.13486
C	1.10641	4.70936	0.63831
H	1.74646	6.66731	1.25896
H	2.11860	4.40804	0.40416
C	4.07581	2.78859	-3.18021
C	3.47178	3.83733	-3.87470
H	5.05571	2.44689	-3.49216
H	3.98488	4.30002	-4.70786
C	2.20163	4.28049	-3.50740
C	1.53246	3.68870	-2.43392
H	1.73089	5.08373	-4.05954
H	0.54019	4.04673	-2.19534
O	0.57812	-1.76785	-0.38837
O	-0.64934	-0.96920	1.75648
H	0.00277	-3.84018	-0.49081
C	-0.61701	-4.20700	-1.32234
C	-2.02471	-3.97224	-0.92012
C	-0.44929	-3.29130	-2.54640
H	-0.42418	-5.26939	-1.49049
C	-2.92571	-4.85310	-0.13930
O	-2.54535	-2.95971	-1.49245
H	0.51542	-2.78861	-2.51774
H	-0.56649	-3.85047	-3.47885
C	-1.57008	-2.26961	-2.36940
C	-3.87293	-4.04824	0.76799
H	-2.29934	-5.52715	0.44566
H	-3.48569	-5.45023	-0.87232
H	-2.13123	-2.02471	-3.27070
H	-1.26028	-1.37303	-1.83396
H	-4.73322	-3.67632	0.20442
H	-4.24891	-4.72665	1.53761
C	-3.08611	-2.87928	1.38015
O	-1.72742	-3.23874	1.36434
H	-3.43690	-2.66260	2.39619
H	-3.22368	-1.97600	0.77371
H	-1.20476	-2.39657	1.58838
C	3.94889	-0.74380	0.24143
C	3.95729	-1.99525	-0.43201
C	4.50195	-0.64419	1.54578
C	4.51450	-3.13196	0.20757
C	3.40798	-2.15184	-1.72556
C	5.04769	-1.79680	2.16635
C	4.53331	0.58076	2.25097
C	4.52203	-4.37512	-0.44676
C	5.05017	-3.02271	1.49428
C	3.42392	-3.39478	-2.36178
H	2.95300	-1.32409	-2.25260
C	5.58888	-1.71006	3.45976
C	5.07431	0.64936	3.53650
H	4.14593	1.49361	1.81825
C	3.97944	-4.50258	-1.72521
H	4.94580	-5.24991	0.03233

H	5.47101	-3.89885	1.97690
H	2.99889	-3.49973	-3.35180
H	6.00537	-2.58500	3.94500
C	5.59831	-0.49240	4.13997
H	5.08844	1.59324	4.06623
H	3.98735	-5.46377	-2.22286
H	6.01626	-0.43311	5.13666
C	-3.36156	1.16064	0.24277
C	-3.98337	0.71427	1.44086
C	-3.88081	0.74298	-1.01322
C	-5.13940	-0.10538	1.36956
C	-3.46643	1.03871	2.71616
C	-5.01448	-0.10899	-1.05586
C	-3.30782	1.16141	-2.23641
C	-5.76299	-0.54842	2.54751
C	-5.64018	-0.50777	0.12841
C	-4.09518	0.58485	3.87734
H	-2.56793	1.62992	2.83028
C	-5.51929	-0.54892	-2.29048
C	-3.82194	0.71430	-3.45507
H	-2.46253	1.83507	-2.26672
C	-5.24272	-0.20120	3.79373
H	-6.64584	-1.17536	2.50406
H	-6.51279	-1.15138	0.08459
H	-3.68758	0.84106	4.84682
H	-6.38001	-1.20596	-2.33386
C	-4.92022	-0.14262	-3.48218
H	-3.36697	1.03601	-4.38300
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H	-5.31439	-0.48586	-4.42996

S-gau-hc(-,-) intermediate



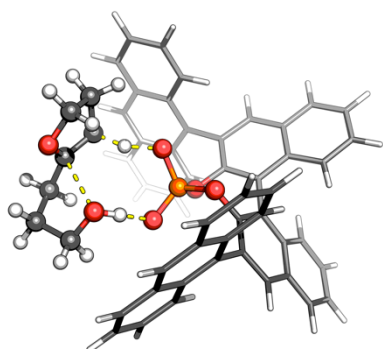
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O	1.21828	-0.01942	0.58391
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C	-1.07980	1.57079	-0.03526
C	-2.38774	1.84477	0.40222
C	-0.02358	2.45634	0.29336
C	-2.63962	2.95863	1.20890
C	-0.26660	3.52302	1.20089
C	-1.59246	3.78173	1.63270
C	1.33262	2.21326	-0.28241
C	2.02648	3.17993	-1.05490

C	1.94113	0.97219	-0.02481
C	3.37415	2.93397	-1.42873
C	3.28096	0.74647	-0.37663
C	3.99643	1.73328	-1.06198
H	5.02945	1.54815	-1.33518
H	-3.65402	3.15764	1.53752
C	-1.85410	4.85433	2.50040
C	-0.81051	5.65538	2.96404
H	-2.86487	5.06637	2.82867
H	-1.01795	6.47770	3.63658
C	0.50142	5.38795	2.57612
C	0.77701	4.32889	1.70855
H	1.30999	6.00127	2.95256
H	1.81111	4.14225	1.45344
C	4.08200	3.89296	-2.17041
C	3.46032	5.07968	-2.56137
H	5.11359	3.72117	-2.45427
H	4.01022	5.81340	-3.13651
C	2.12815	5.31726	-2.22317
C	1.41139	4.37615	-1.48073
H	1.64710	6.23351	-2.54047
H	0.37468	4.58724	-1.25449
O	0.74401	-1.18918	-1.69945
O	-0.63971	-1.68971	0.41939
H	0.35588	-3.16758	-1.53691
C	-0.53316	-3.77988	-1.74637
C	-1.36051	-3.87611	-0.52070
C	-1.45676	-3.06372	-2.74572
H	-0.21269	-4.78202	-2.04810
C	-1.00907	-4.64767	0.68858
O	-2.51119	-3.35041	-0.63841
H	-0.91908	-2.25101	-3.23543
H	-1.85815	-3.75560	-3.48969
C	-2.56885	-2.51550	-1.85214
C	-2.02023	-4.62773	1.83040
H	-0.04972	-4.23094	1.02603
H	-0.79046	-5.66782	0.34385
H	-3.58181	-2.61553	-2.23778
H	-2.37643	-1.50085	-1.49619
H	-3.00713	-4.95246	1.48012
H	-1.67888	-5.34963	2.57890
C	-2.12550	-3.24747	2.48476
O	-0.86665	-2.77450	2.89695
H	-2.76987	-3.32718	3.36714
H	-2.58450	-2.54474	1.78106
H	-0.54168	-2.19918	2.17934
C	3.93475	-0.54063	-0.02909
C	4.11188	-1.54518	-1.01766
C	4.33107	-0.79597	1.31081
C	4.66511	-2.79904	-0.65183
C	3.73414	-1.34239	-2.36458
C	4.88467	-2.05647	1.65103
C	4.19474	0.17771	2.32694
C	4.82486	-3.80667	-1.61741
C	5.04393	-3.04145	0.67193
C	3.89668	-2.35576	-3.31124
H	3.30194	-0.40832	-2.69726

C	5.27221	-2.32066	2.97519
C	4.58512	-0.10124	3.63830
H	3.79260	1.16059	2.11948
C	4.44015	-3.58381	-2.93929
H	5.24411	-4.76914	-1.34856
H	5.46494	-4.00438	0.94241
H	3.59764	-2.18790	-4.33791
H	5.69331	-3.28145	3.24715
C	5.12042	-1.34664	3.96198
H	4.47347	0.65314	4.40651
H	4.56318	-4.36586	-3.67739
H	5.42138	-1.55709	4.98017
C	-3.51106	0.94120	0.03812
C	-4.09364	0.09511	1.02121
C	-4.00437	0.91111	-1.29436
C	-5.15020	-0.77865	0.65778
C	-3.64757	0.08923	2.36350
C	-5.04980	0.01527	-1.63551
C	-3.48703	1.75746	-2.30172
C	-5.74068	-1.61046	1.62350
C	-5.60864	-0.81707	-0.66176
C	-4.25885	-0.72958	3.31512
H	-2.82458	0.70848	2.69216
C	-5.52810	-0.03917	-2.95498
C	-3.97460	1.69130	-3.60844
H	-2.70776	2.47773	-2.09188
C	-5.30087	-1.57790	2.94630
H	-6.54722	-2.28290	1.35590
H	-6.41042	-1.49647	-0.93212
H	-3.91047	-0.71879	4.33985
H	-6.32107	-0.72542	-3.22813
C	-4.98853	0.79300	-3.93526
H	-3.56503	2.34166	-4.37064
H	-5.76265	-2.21925	3.68576
H	-5.36207	0.74579	-4.95002

S-gau-ev(+,+)



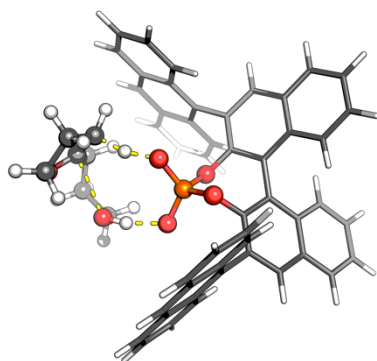
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O	-1.09280	0.40188	-0.80083
C	-1.69943	1.38421	-0.06021
C	-3.04252	1.23758	0.31877
C	-0.98718	2.55670	0.26744

C	-3.66995	2.23810	1.06702
C	-1.59669	3.53107	1.10040
C	-2.95629	3.37119	1.47707
C	0.41206	2.68905	-0.23710
C	0.82649	3.76382	-1.06639
C	1.33368	1.67006	0.08680
C	2.19278	3.86914	-1.43674
C	2.68228	1.78604	-0.28532
C	3.10895	2.89392	-1.02449
H	4.15253	2.97232	-1.30923
H	-4.70713	2.11235	1.35797
C	-3.58141	4.34019	2.27799
C	-2.86574	5.45062	2.72707
H	-4.62091	4.23348	2.56499
H	-3.35223	6.19205	3.34766
C	-1.52048	5.59912	2.39126
C	-0.88508	4.64702	1.59109
H	-0.96561	6.45401	2.75584
H	0.16453	4.78785	1.37163
C	2.62363	4.94180	-2.23362
C	1.70992	5.89473	-2.68510
H	3.66548	5.03720	-2.51607
H	2.04756	6.71675	-3.30302
C	0.35983	5.78153	-2.35505
C	-0.08412	4.72371	-1.55851
H	-0.34739	6.51454	-2.72131
H	-1.14213	4.66003	-1.34327
O	0.79521	-1.18685	-1.05228
O	-0.63596	-1.33446	1.09555
H	1.32322	-2.41386	-0.66350
C	2.03008	-3.44186	-0.62562
C	1.28997	-4.50780	-0.04745
C	2.17273	-3.83189	-2.09929
H	2.89730	-3.11466	-0.05332
C	1.13907	-4.84102	1.39249
O	0.77083	-5.31520	-0.91670
H	2.09736	-2.96482	-2.75749
H	3.10847	-4.36284	-2.30269
C	0.95939	-4.74565	-2.25231
C	-0.22376	-5.44370	1.74015
H	1.33257	-3.92766	1.96575
H	1.94914	-5.54848	1.62051
H	1.06884	-5.58277	-2.93959
H	0.04353	-4.18521	-2.46007
H	-0.42904	-6.28638	1.07223
H	-0.20188	-5.82784	2.76490
C	-1.31212	-4.38213	1.59695
O	-1.20663	-3.76921	0.33213
H	-1.19724	-3.62600	2.38565
H	-2.29807	-4.85024	1.71251
H	-1.12248	-2.79834	0.49989
C	3.65260	0.71730	0.06909
C	4.12331	-0.17955	-0.92825
C	4.09360	0.56780	1.41141
C	5.03654	-1.20562	-0.57468
C	3.69500	-0.09391	-2.27307
C	4.98963	-0.48046	1.74317

C	3.67088	1.44341	2.43787
C	5.51431	-2.09193	-1.55417
C	5.45340	-1.34950	0.75154
C	4.18381	-0.97972	-3.23526
H	2.97728	0.64863	-2.59394
C	5.41892	-0.64615	3.07037
C	4.10707	1.26441	3.75227
H	3.00576	2.27264	2.23723
C	5.09289	-1.97337	-2.87803
H	6.21138	-2.87995	-1.29466
H	6.14315	-2.14501	1.01425
H	3.84872	-0.90038	-4.26139
H	6.09955	-1.44658	3.33587
C	4.97528	0.22117	4.06838
H	3.77115	1.93951	4.52887
H	5.46321	-2.66128	-3.62703
H	5.30982	0.08722	5.08903
C	-3.78853	0.00430	-0.03798
C	-3.99755	-1.00985	0.93482
C	-4.26084	-0.18568	-1.36351
C	-4.67671	-2.20073	0.57170
C	-3.53159	-0.87786	2.26311
C	-4.93012	-1.38879	-1.70415
C	-4.08863	0.79784	-2.36417
C	-4.88812	-3.20947	1.52602
C	-5.13172	-2.37906	-0.73804
C	-3.74759	-1.89152	3.19862
H	-2.99056	0.00015	2.58935
C	-5.39398	-1.58899	-3.01484
C	-4.55552	0.58256	-3.66251
H	-3.59765	1.73897	-2.15449
C	-4.42741	-3.05150	2.83288
H	-5.40598	-4.12333	1.25971
H	-5.64616	-3.29571	-1.00770
H	-3.38311	-1.77764	4.21139
H	-5.90431	-2.50542	-3.28715
C	-5.20435	-0.60738	-3.98747
H	-4.41462	1.34327	-4.41959
H	-4.58998	-3.83483	3.56181
H	-5.56427	-0.76850	-4.99547

S-gau-ev(+,-)



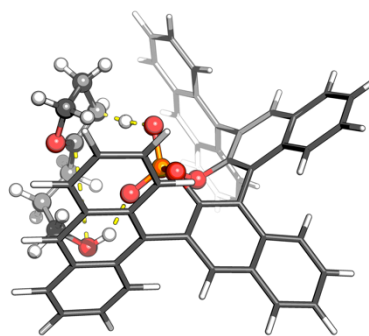
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O	-1.38643	0.01417	-0.82030
C	-2.16131	0.81013	-0.01611
C	-3.42283	0.36019	0.40466
C	-1.70843	2.09693	0.33608
C	-4.21576	1.17034	1.22311
C	-2.47430	2.88329	1.23612
C	-3.74629	2.41560	1.65837
C	-0.40867	2.56123	-0.23186
C	-0.30481	3.73536	-1.02243
C	0.74492	1.78064	0.00615
C	0.97675	4.19077	-1.42482
C	2.01049	2.25323	-0.38180
C	2.11989	3.46290	-1.07663
H	3.10066	3.81684	-1.37549
H	-5.18675	0.81090	1.54595
C	-4.52850	3.19485	2.52561
C	-4.05183	4.41949	2.99462
H	-5.50486	2.85244	2.84777
H	-4.65812	5.01401	3.66581
C	-2.78944	4.87214	2.61242
C	-2.00088	4.11131	1.74651
H	-2.41791	5.81539	2.99172
H	-1.01925	4.48726	1.49193
C	1.09876	5.36674	-2.18226
C	-0.03850	6.07967	-2.56329
H	2.07326	5.72905	-2.48787
H	0.06173	6.98276	-3.15144
C	-1.30498	5.62315	-2.19997
C	-1.44267	4.45889	-1.44101
H	-2.18489	6.17154	-2.51085
H	-2.44305	4.12700	-1.19796
O	0.77951	-1.11976	-1.20379
O	-0.49779	-1.58707	1.01911
H	1.71902	-2.08068	-1.17138
C	2.69623	-2.83509	-1.49343
C	3.10287	-3.57393	-0.35837
C	2.24974	-3.88833	-2.50634
H	3.38699	-2.05232	-1.80003
C	3.82412	-3.07081	0.84017
O	2.83884	-4.84190	-0.42541
H	1.35486	-3.58733	-3.05409
H	3.04078	-4.12623	-3.22530
C	1.96513	-5.06836	-1.57577
C	3.30205	-3.66774	2.15179
H	3.71857	-1.98200	0.84530
H	4.88763	-3.30262	0.69620
H	2.20409	-6.05619	-1.96638
H	0.95007	-5.04347	-1.16932
H	3.35140	-4.76021	2.10174
H	3.94176	-3.33841	2.97643
C	1.86370	-3.22531	2.38891
O	1.10081	-3.59054	1.26327
H	1.82686	-2.13448	2.53383
H	1.47524	-3.69832	3.30188
H	0.37007	-2.92280	1.16696
C	3.24060	1.47167	-0.08214

C	3.95449	0.83395	-1.13344
C	3.72496	1.37697	1.25121
C	5.15732	0.13915	-0.84549
C	3.49412	0.85630	-2.47045
C	4.91352	0.64899	1.51627
C	3.06374	2.00198	2.33364
C	5.87952	-0.47867	-1.87997
C	5.62249	0.05379	0.46926
C	4.22395	0.23656	-3.48703
H	2.56584	1.33964	-2.74291
C	5.38742	0.52852	2.83293
C	3.54860	1.87249	3.63669
H	2.17171	2.59563	2.18771
C	5.41548	-0.42401	-3.19398
H	6.80062	-1.00986	-1.67098
H	6.53592	-0.49235	0.68126
H	3.86014	0.26407	-4.50607
H	6.28926	-0.03290	3.04717
C	4.70315	1.13349	3.88652
H	3.02692	2.34971	4.45633
H	5.97544	-0.90483	-3.98560
H	5.07376	1.03596	4.89878
C	-3.90729	-0.98729	0.01349
C	-3.84662	-2.06360	0.93871
C	-4.40704	-1.21354	-1.29611
C	-4.28184	-3.35405	0.54282
C	-3.34626	-1.89353	2.25014
C	-4.83452	-2.51345	-1.66893
C	-4.49984	-0.17305	-2.24850
C	-4.21725	-4.42690	1.44739
C	-4.76899	-3.56560	-0.75048
C	-3.28565	-2.97135	3.13562
H	-2.98790	-0.93469	2.60008
C	-5.32613	-2.74803	-2.96371
C	-4.99047	-0.42359	-3.53169
H	-4.19946	0.83924	-2.01222
C	-3.72120	-4.23346	2.73653
H	-4.54764	-5.41697	1.15589
H	-5.09809	-4.55688	-1.04492
H	-2.89697	-2.82690	4.13549
H	-5.65352	-3.73762	-3.26028
C	-5.40088	-1.70681	-3.88880
H	-5.05408	0.38207	-4.25180
H	-3.67208	-5.06518	3.42746
H	-5.78073	-1.89485	-4.88475

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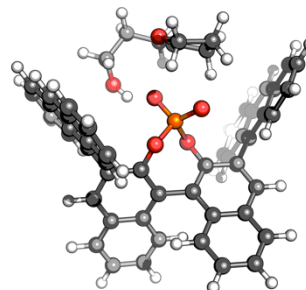
E(RM062X) = -2913.01003960

P	0.04624	-0.57707	-0.19403
O	1.05440	0.30143	0.74481
O	-0.97133	0.49292	-0.89171
C	-1.37775	1.53918	-0.10084
C	-2.72393	1.62120	0.28999
C	-0.47498	2.57592	0.23004
C	-3.16885	2.71280	1.04218
C	-0.90772	3.63356	1.07339
C	-2.27310	3.70614	1.45300
C	0.92980	2.47891	-0.26653
C	1.53093	3.47733	-1.07564
C	1.66603	1.32533	0.06722
C	2.90470	3.36212	-1.41579
C	3.02531	1.22358	-0.26873
C	3.64335	2.25103	-0.98848
H	4.69289	2.16197	-1.24665
H	-4.21099	2.76398	1.33840
C	-2.72322	4.76322	2.26022
C	-1.82861	5.73289	2.71382
H	-3.76531	4.83352	2.54905
H	-2.18096	6.54310	3.33908
C	-0.47813	5.65083	2.37727
C	-0.01550	4.60863	1.57100
H	0.21507	6.39594	2.74600
H	1.04298	4.56981	1.35320
C	3.51986	4.35486	-2.19494
C	2.78143	5.44489	-2.65740
H	4.56938	4.28234	-2.45481
H	3.26034	6.20437	-3.26186
C	1.42407	5.55043	-2.35490
C	0.79819	4.57467	-1.57598
H	0.85264	6.39019	-2.72892
H	-0.26035	4.68146	-1.38037
O	0.81527	-1.14999	-1.38060
O	-0.64137	-1.56291	0.69097
H	1.15383	-2.46592	-1.10726
C	1.27151	-3.71257	-1.21729
C	0.18341	-4.15786	-0.42437
C	0.78816	-3.87270	-2.66182
H	2.27127	-4.01292	-0.91727
C	0.19283	-4.55329	1.00548
O	-0.93614	-4.20310	-1.07504

H	1.16256	-3.07636	-3.30765
H	1.05862	-4.84477	-3.08669
C	-0.72007	-3.73838	-2.45221
C	-1.13832	-5.05544	1.56476
H	0.52178	-3.66769	1.56707
H	0.99069	-5.29864	1.11256
H	-1.34965	-4.35822	-3.08819
H	-1.04413	-2.69518	-2.47220
H	-1.59221	-5.78581	0.88483
H	-0.92841	-5.56751	2.50912
C	-2.12024	-3.91831	1.85432
O	-1.57368	-3.01714	2.78958
H	-3.03382	-4.34578	2.28320
H	-2.38808	-3.39643	0.92771
H	-1.21442	-2.26917	2.28247
C	3.79887	0.01335	0.11210
C	4.11090	-0.97382	-0.86186
C	4.17938	-0.19121	1.46537
C	4.79071	-2.15547	-0.46994
C	3.74313	-0.82779	-2.21927
C	4.85346	-1.38371	1.83261
C	3.90955	0.76751	2.46892
C	5.09181	-3.14371	-1.42184
C	5.15167	-2.34881	0.86647
C	4.04462	-1.82258	-3.15139
H	3.20865	0.04390	-2.57137
C	5.22269	-1.60008	3.17057
C	4.28294	0.53640	3.79443
H	3.41429	1.70209	2.24117
C	4.71784	-2.97605	-2.75472
H	5.60950	-4.05079	-1.13287
H	5.66678	-3.25856	1.15740
H	3.75036	-1.69973	-4.18572
H	5.73439	-2.50946	3.46318
C	4.93514	-0.64430	4.14479
H	4.06674	1.27777	4.55294
H	4.94699	-3.74468	-3.48143
H	5.22203	-0.81797	5.17392
C	-3.67419	0.53135	-0.05212
C	-4.10453	-0.37981	0.95039
C	-4.15333	0.38955	-1.38174
C	-5.01033	-1.41770	0.61312
C	-3.65076	-0.29011	2.28663
C	-5.04327	-0.66879	-1.69764
C	-3.77979	1.28603	-2.40901
C	-5.45831	-2.31034	1.60098
C	-5.46109	-1.55724	-0.70251
C	-4.11370	-1.17947	3.25836
H	-2.93590	0.46081	2.59430
C	-5.51756	-0.82128	-3.01096
C	-4.26146	1.12073	-3.70923
H	-3.12049	2.12245	-2.21898
C	-5.01699	-2.18413	2.91780
H	-6.15183	-3.10571	1.35472
H	-6.14840	-2.35899	-0.95235
H	-3.76161	-1.09513	4.27841
H	-6.19633	-1.62734	-3.26394

C	-5.12510	0.06913	-4.01010
H	-3.96564	1.81375	-4.48632
H	-5.36658	-2.87510	3.67393
H	-5.49651	-0.05302	-5.01939

S-gau-hc(+,+) intermediate



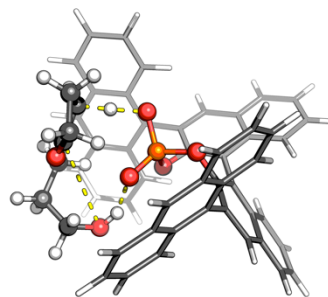
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P	0.10395	-0.62635	-0.45217
O	1.04800	0.20181	0.60759
O	-1.04110	0.42948	-0.96566
C	-1.43471	1.42740	-0.10807
C	-2.78801	1.49692	0.26797
C	-0.54183	2.46443	0.26043
C	-3.24383	2.56194	1.05130
C	-0.98621	3.48139	1.14831
C	-2.35492	3.53560	1.51604
C	0.86050	2.43167	-0.25435
C	1.43546	3.49526	-0.99682
C	1.63676	1.29435	0.02943
C	2.82046	3.45605	-1.30940
C	3.00899	1.27213	-0.26320
C	3.59894	2.35967	-0.91455
H	4.65900	2.33241	-1.14154
H	-4.29117	2.60558	1.33018
C	-2.81715	4.55722	2.36131
C	-1.93043	5.50834	2.86614
H	-3.86278	4.61354	2.64034
H	-2.29196	6.29055	3.52111
C	-0.57615	5.44280	2.54237
C	-0.10218	4.43681	1.69765
H	0.11120	6.17237	2.95095
H	0.95919	4.40898	1.49276
C	3.40876	4.51414	-2.02009
C	2.63401	5.59583	-2.44115
H	4.46609	4.50048	-2.25704
H	3.09269	6.40652	-2.99243
C	1.26735	5.62883	-2.16428
C	0.66742	4.58728	-1.45299
H	0.66880	6.46374	-2.50525
H	-0.39845	4.63890	-1.27490
O	0.86265	-1.01909	-1.68088
O	-0.49401	-1.74363	0.37540
H	1.85419	-2.67107	-0.52118
C	1.60167	-3.70266	-0.78600

C	0.33052	-4.06807	-0.10221
C	1.24197	-3.81371	-2.27680
H	2.40739	-4.36170	-0.45022
C	0.19188	-4.43548	1.32106
O	-0.64059	-4.22728	-0.90195
H	1.63222	-2.96075	-2.82992
H	1.60449	-4.75248	-2.70326
C	-0.28206	-3.76574	-2.25870
C	-1.20225	-4.85533	1.77756
H	0.53615	-3.56149	1.89059
H	0.93709	-5.22469	1.49433
H	-0.79301	-4.44065	-2.94325
H	-0.66112	-2.74475	-2.32647
H	-1.60180	-5.64181	1.12643
H	-1.09931	-5.27759	2.78204
C	-2.17745	-3.67593	1.84479
O	-1.65330	-2.63580	2.63394
H	-3.10776	-4.02466	2.30598
H	-2.40912	-3.31243	0.83634
H	-1.21864	-2.02104	2.01257
C	3.82729	0.09000	0.11100
C	4.20656	-0.86150	-0.87347
C	4.16576	-0.13549	1.47219
C	4.89823	-2.03688	-0.48283
C	3.89220	-0.68805	-2.24056
C	4.85862	-1.31772	1.83707
C	3.83357	0.79207	2.48640
C	5.25407	-2.99700	-1.44427
C	5.21388	-2.25348	0.86152
C	4.25532	-1.65142	-3.18372
H	3.35586	0.18245	-2.59281
C	5.18679	-1.55452	3.18228
C	4.16775	0.54156	3.81882
H	3.32075	1.71792	2.26149
C	4.93200	-2.80300	-2.78700
H	5.77703	-3.90127	-1.15601
H	5.73921	-3.15785	1.15092
H	4.00303	-1.50746	-4.22637
H	5.71242	-2.45652	3.47298
C	4.84013	-0.62867	4.16620
H	3.90547	1.25975	4.58506
H	5.20538	-3.54908	-3.52184
H	5.09651	-0.81752	5.20068
C	-3.74281	0.43151	-0.14239
C	-4.26841	-0.46933	0.82517
C	-4.13518	0.30465	-1.50313
C	-5.16938	-1.48738	0.42003
C	-3.91684	-0.38932	2.19281
C	-5.01412	-0.74087	-1.88586
C	-3.68768	1.20515	-2.49743
C	-5.71446	-2.36623	1.37084
C	-5.51925	-1.62198	-0.92604
C	-4.47798	-1.26261	3.12688
H	-3.20518	0.33905	2.55558
C	-5.39258	-0.88643	-3.23081
C	-4.07482	1.04719	-3.82970
H	-3.04331	2.04018	-2.25781

C	-5.37698	-2.24513	2.71821
H	-6.40540	-3.14569	1.07191
H	-6.19988	-2.41166	-1.22747
H	-4.20408	-1.18433	4.17110
H	-6.05907	-1.68508	-3.53479
C	-4.92007	0.00186	-4.19633
H	-3.71977	1.74126	-4.58063
H	-5.80255	-2.92426	3.44559
H	-5.21723	-0.11532	-5.23051

S-gau-hc(+,-)



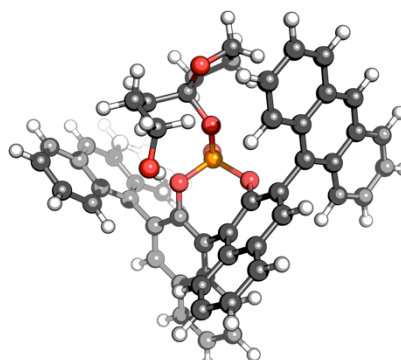
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P	-0.06624	-0.59003	-0.49076
O	0.88251	0.36374	0.44541
O	-1.28977	0.35535	-0.99452
C	-1.82208	1.16945	-0.02644
C	-3.09164	0.87842	0.49411
C	-1.11757	2.31686	0.40066
C	-3.65955	1.71080	1.46156
C	-1.65820	3.11417	1.44461
C	-2.95128	2.81521	1.95077
C	0.22362	2.58596	-0.20191
C	0.53930	3.79426	-0.87477
C	1.20001	1.57354	-0.11301
C	1.86960	4.01390	-1.32267
C	2.51313	1.80481	-0.54430
C	2.84775	3.02798	-1.13258
H	3.86463	3.19476	-1.47031
H	-4.63983	1.47141	1.85894
C	-3.51002	3.60994	2.96444
C	-2.79056	4.67979	3.49745
H	-4.49887	3.39621	3.35281
H	-3.22515	5.28584	4.28192
C	-1.50524	4.95849	3.03471
C	-0.93664	4.18096	2.02351
H	-0.94407	5.77814	3.46478
H	0.07145	4.41659	1.71170
C	2.20233	5.21557	-1.96767
C	1.22680	6.18820	-2.19087
H	3.21510	5.39871	-2.30689
H	1.48899	7.11096	-2.69215
C	-0.08836	5.96850	-1.78171
C	-0.43549	4.78077	-1.13415
H	-0.84372	6.72053	-1.97011

H	-1.46942	4.63919	-0.84912
O	0.65393	-0.98024	-1.77561
O	-0.45888	-1.70704	0.42257
H	1.08508	-2.24589	-1.61097
C	1.44745	-3.47101	-1.49925
C	1.41362	-3.69510	-0.10150
C	0.33264	-4.35459	-2.06380
H	2.43175	-3.45067	-1.96484
C	2.37883	-3.20203	0.91439
O	0.38184	-4.36650	0.30119
H	-0.22300	-3.86396	-2.86531
H	0.71501	-5.31110	-2.43487
C	-0.54162	-4.53886	-0.82065
C	2.09971	-3.60384	2.36184
H	2.35733	-2.10402	0.83450
H	3.37919	-3.50902	0.58817
H	-1.00071	-5.51902	-0.70210
H	-1.27509	-3.73791	-0.69844
H	1.97623	-4.69022	2.44330
H	2.97828	-3.32464	2.95257
C	0.87764	-2.89602	2.95396
O	1.02730	-1.49505	2.89480
H	0.78254	-3.18416	4.00724
H	-0.02996	-3.20655	2.42731
H	0.52082	-1.18289	2.12934
C	3.53433	0.73493	-0.40035
C	3.90482	-0.05462	-1.52171
C	4.06749	0.42816	0.88044
C	4.81164	-1.13209	-1.35227
C	3.37193	0.18119	-2.80965
C	4.96776	-0.65808	1.02460
C	3.71859	1.17196	2.03088
C	5.16781	-1.93207	-2.45031
C	5.33781	-1.41674	-0.08919
C	3.73294	-0.62675	-3.88962
H	2.66446	0.97839	-2.99325
C	5.47640	-0.98766	2.29157
C	4.23186	0.82972	3.28356
H	3.04938	2.02031	1.97531
C	4.62881	-1.67884	-3.71121
H	5.85702	-2.75980	-2.33130
H	6.02414	-2.24852	0.03181
H	3.31305	-0.43764	-4.86913
H	6.15747	-1.82156	2.41452
C	5.10510	-0.24842	3.41424
H	3.95155	1.40431	4.15699
H	4.90318	-2.30270	-4.55194
H	5.49826	-0.51008	4.38812
C	-3.80404	-0.34964	0.06322
C	-3.70911	-1.53527	0.83947
C	-4.51386	-0.36838	-1.16521
C	-4.30502	-2.73211	0.36690
C	-3.01476	-1.56739	2.07075
C	-5.11134	-1.57454	-1.61169
C	-4.64431	0.78824	-1.96660
C	-4.18954	-3.91729	1.11203
C	-4.99869	-2.73999	-0.84711

C	-2.91178	-2.75339	2.80000
H	-2.53523	-0.68546	2.47412
C	-5.81157	-1.60353	-2.82899
C	-5.34394	0.74216	-3.17431
H	-4.21302	1.73470	-1.66757
C	-3.49354	-3.92534	2.32073
H	-4.63494	-4.83929	0.75733
H	-5.45194	-3.66036	-1.20070
H	-2.37160	-2.76454	3.73798
H	-6.27042	-2.51983	-3.18151
C	-5.92529	-0.44953	-3.60444
H	-5.43635	1.63538	-3.77869
H	-3.40544	-4.84292	2.88790
H	-6.46626	-0.47917	-4.54148

S-gau-hc(+,-) intermediate



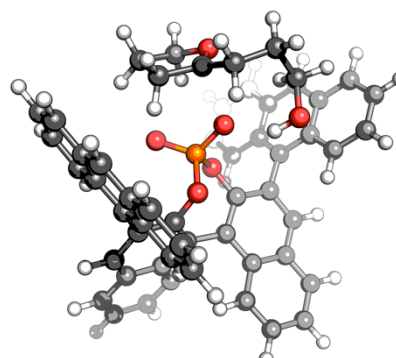
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P	-0.08997	-0.69829	0.79441
O	-1.10900	-0.05876	-0.30968
O	1.04351	0.40982	1.08637
C	1.42283	1.23442	0.05193
C	2.76473	1.21657	-0.36611
C	0.52222	2.18175	-0.49751
C	3.19158	2.06675	-1.39040
C	0.93346	2.96512	-1.60917
C	2.28550	2.91422	-2.03521
C	-0.85542	2.29024	0.07240
C	-1.38956	3.50112	0.58297
C	-1.65154	1.13389	0.08188
C	-2.75854	3.55263	0.96042
C	-3.00487	1.19329	0.43843
C	-3.55933	2.40601	0.85955
H	-4.60616	2.44358	1.13986
H	4.22887	2.03853	-1.70620
C	2.71436	3.70632	-3.11235
C	1.80981	4.52637	-3.78705
H	3.74727	3.68288	-3.43931
H	2.14534	5.13055	-4.62007
C	0.47079	4.55696	-3.40038
C	0.03031	3.78084	-2.32625
H	-0.23088	5.18174	-3.93791
H	-1.02113	3.81571	-2.07593
C	-3.30753	4.75145	1.44208
C	-2.50935	5.88895	1.57184

H	-4.35197	4.80641	1.72559
H	-2.93775	6.80921	1.94752
C	-1.15778	5.83963	1.23045
C	-0.59663	4.65654	0.74459
H	-0.54065	6.72133	1.34596
H	0.45929	4.65166	0.50902
O	-0.73500	-1.12181	2.04387
O	0.61388	-1.78608	-0.10853
H	-0.79940	-3.31688	1.61660
C	-0.18141	-3.88194	0.92009
C	0.08667	-3.15819	-0.39820
C	1.24424	-4.13817	1.41230
H	-0.68059	-4.82269	0.66674
C	-1.07320	-3.07473	-1.38572
O	1.16084	-3.82044	-0.95230
H	1.60789	-3.27652	1.97789
H	1.31658	-5.02073	2.05012
C	2.02370	-4.30213	0.09584
C	-0.67066	-2.96058	-2.86110
H	-1.72674	-2.24941	-1.08628
H	-1.66166	-3.98946	-1.25973
H	2.25410	-5.34389	-0.14014
H	2.94582	-3.71963	0.08615
H	-0.11640	-3.86284	-3.14023
H	-1.58646	-2.93180	-3.46235
C	0.18194	-1.74813	-3.21693
O	-0.51405	-0.52057	-3.09638
H	0.48541	-1.81710	-4.26532
H	1.08874	-1.75049	-2.60247
H	-0.73779	-0.37835	-2.16860
C	-3.82999	-0.04172	0.38952
C	-4.17562	-0.71891	1.58992
C	-4.17406	-0.61645	-0.86421
C	-4.87096	-1.95366	1.52323
C	-3.81907	-0.21499	2.86200
C	-4.84870	-1.86296	-0.90397
C	-3.84933	0.01326	-2.08797
C	-5.21237	-2.63444	2.70352
C	-5.19803	-2.51104	0.28380
C	-4.16350	-0.90616	4.02530
H	-3.26597	0.70749	2.97273
C	-5.15650	-2.45789	-2.13865
C	-4.15699	-0.59458	-3.30651
H	-3.35427	0.97476	-2.11668
C	-4.86130	-2.10967	3.94688
H	-5.74456	-3.57766	2.66405
H	-5.71729	-3.46306	0.24320
H	-3.88471	-0.50746	4.99226
H	-5.66432	-3.41427	-2.18060
C	-4.80522	-1.82768	-3.33211
H	-3.89183	-0.10592	-4.23520
H	-5.12463	-2.64144	4.85211
H	-5.04058	-2.29455	-4.27977
C	3.74080	0.29157	0.26903
C	4.21166	-0.84820	-0.43744
C	4.20250	0.53714	1.59048
C	5.13219	-1.72979	0.18494

C	3.78139	-1.14245	-1.75084
C	5.10998	-0.36890	2.19679
C	3.79375	1.67414	2.32510
C	5.60784	-2.85585	-0.50785
C	5.56408	-1.48712	1.49171
C	4.25536	-2.27117	-2.42204
H	3.07852	-0.50759	-2.27111
C	5.56301	-0.14096	3.50680
C	4.25435	1.88608	3.62614
H	3.12265	2.41047	1.90366
C	5.16892	-3.12310	-1.80456
H	6.31267	-3.53483	-0.04258
H	6.26233	-2.17169	1.96229
H	3.91259	-2.48485	-3.42629
H	6.25315	-0.82883	3.98112
C	5.13310	0.97994	4.21657
H	3.92989	2.75906	4.17783
H	5.53384	-3.99614	-2.32991
H	5.48716	1.14977	5.22521

S-gau-hc(+,-) intermediate



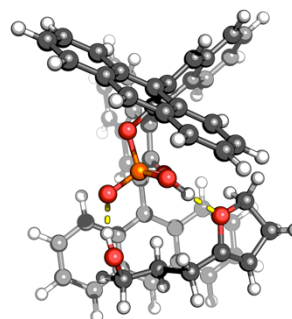
E(RM062X) = -2913.01921540

P	0.14558	-0.66790	-0.45865
O	1.09841	0.14179	0.60027
O	-1.01582	0.38153	-0.93800
C	-1.37423	1.41267	-0.10348
C	-2.72974	1.54153	0.25205
C	-0.45120	2.43184	0.24615
C	-3.15554	2.63979	1.00604
C	-0.86797	3.47790	1.11373
C	-2.23698	3.58696	1.46631
C	0.94690	2.36591	-0.27828
C	1.53667	3.41054	-1.03659
C	1.70566	1.22062	0.01686
C	2.91949	3.34409	-1.35479
C	3.07551	1.17059	-0.28313
C	3.68103	2.23925	-0.95067
H	4.73912	2.19033	-1.18312
H	-4.20448	2.72981	1.26729
C	-2.67111	4.63913	2.28872
C	-1.75632	5.56720	2.78621
H	-3.71687	4.73741	2.55542
H	-2.09637	6.37313	3.42368

C	-0.40227	5.44881	2.47690
C	0.04381	4.41222	1.65427
H	0.30637	6.16129	2.87919
H	1.10538	4.34394	1.45957
C	3.52248	4.38343	-2.08068
C	2.76432	5.47294	-2.51158
H	4.57838	4.34900	-2.32189
H	3.23425	6.26901	-3.07460
C	1.39959	5.53223	-2.22983
C	0.78521	4.50962	-1.50355
H	0.81368	6.37273	-2.57891
H	-0.27905	4.58113	-1.32300
O	0.87055	-1.05964	-1.70192
O	-0.44806	-1.79102	0.38126
H	1.79095	-2.81192	-0.55302
C	1.33641	-3.77851	-0.77296
C	0.05368	-3.94520	-0.01809
C	0.89590	-3.88678	-2.24462
H	2.02420	-4.56942	-0.45597
C	-0.03737	-4.33232	1.41090
O	-0.95059	-4.13236	-0.78522
H	1.32502	-3.07756	-2.83366
H	1.16653	-4.85755	-2.66751
C	-0.62035	-3.73170	-2.16074
C	-1.43880	-4.59865	1.95329
H	0.46578	-3.54774	1.98591
H	0.59066	-5.23115	1.49735
H	-1.20414	-4.38252	-2.80952
H	-0.93415	-2.68975	-2.24874
H	-1.94660	-5.35631	1.34479
H	-1.31904	-5.01076	2.96049
C	-2.30170	-3.33905	2.04173
O	-1.65159	-2.31908	2.76357
H	-3.22406	-3.59292	2.57336
H	-2.56873	-2.98912	1.03720
H	-1.14206	-1.81444	2.10519
C	3.87353	-0.02242	0.09869
C	4.20007	-1.00771	-0.87108
C	4.23830	-0.22556	1.45628
C	4.86241	-2.19562	-0.46810
C	3.86105	-0.85487	-2.23462
C	4.90697	-1.41799	1.83291
C	3.95474	0.73374	2.45547
C	5.15955	-3.19128	-1.41320
C	5.20810	-2.38807	0.87264
C	4.16212	-1.85524	-3.16091
H	3.35134	0.02791	-2.59603
C	5.26291	-1.63138	3.17497
C	4.31542	0.50586	3.78506
H	3.45959	1.66678	2.22054
C	4.80738	-3.02039	-2.75160
H	5.65987	-4.10519	-1.11529
H	5.71336	-3.30076	1.17146
H	3.88901	-1.72774	-4.20044
H	5.77098	-2.54042	3.47479
C	4.96595	-0.67321	4.14415
H	4.09069	1.24844	4.53992

H	5.03527	-3.79381	-3.47359
H	5.24308	-0.84430	5.17638
C	-3.72197	0.50903	-0.15821
C	-4.32888	-0.32972	0.81830
C	-4.06797	0.35015	-1.52894
C	-5.25979	-1.32028	0.41207
C	-4.02944	-0.21586	2.19612
C	-4.97305	-0.67312	-1.91084
C	-3.54831	1.19738	-2.53525
C	-5.88679	-2.13458	1.36987
C	-5.55655	-1.49358	-0.94212
C	-4.67224	-1.02369	3.13637
H	-3.29573	0.48771	2.56321
C	-5.29960	-0.85636	-3.26480
C	-3.88471	1.00287	-3.87640
H	-2.88586	2.01897	-2.29895
C	-5.60187	-1.97632	2.72540
H	-6.60128	-2.89209	1.06987
H	-6.25797	-2.26486	-1.24356
H	-4.43764	-0.91900	4.18783
H	-5.98377	-1.64030	-3.56783
C	-4.75201	-0.02480	-4.24100
H	-3.47290	1.65486	-4.63601
H	-6.09074	-2.60532	3.45804
H	-5.00915	-0.17101	-5.28218

Complex between the substrate and the catalyst (starting material)



More than 20 initial geometries for this complex were evaluated. The one shown here is the most stable

E(RM062X) = -2913.03217893

C	1.00961	1.43971	-0.16579
C	2.29418	1.81453	-0.58843
C	-0.01742	2.40214	-0.07248
C	2.53362	3.12438	-1.01594
C	0.20286	3.70813	-0.58048
C	1.49660	4.06483	-1.04144
C	-1.30768	1.99256	0.55520
C	-1.81155	2.61835	1.72626
C	-2.00957	0.90332	-0.00576
C	-3.07706	2.22621	2.23484

C	-3.25968	0.52593	0.51066	C	-5.34729	-2.82108	-1.21790
C	-3.79524	1.19929	1.61222	C	-3.22068	-3.36157	2.36638
H	-4.75915	0.89363	2.00434	H	-2.70556	-1.30168	2.25192
H	3.52738	3.40068	-1.35120	C	-6.10018	-1.43126	-3.05662
C	1.73648	5.36061	-1.52572	C	-5.50038	0.90767	-3.14989
C	0.70202	6.29590	-1.57577	H	-4.30356	1.66352	-1.56026
H	2.72223	5.64755	-1.87250	C	-3.89609	-4.43200	1.78321
H	0.89224	7.29203	-1.95402	H	-5.12157	-5.09478	0.15781
C	-0.57934	5.94635	-1.15025	H	-5.86370	-3.66732	-1.65925
C	-0.83309	4.66319	-0.66056	H	-2.66584	-3.50962	3.28402
H	-1.38101	6.67170	-1.20315	H	-6.61643	-2.27501	-3.49934
H	-1.84393	4.42441	-0.35799	C	-6.15261	-0.19459	-3.69978
C	-3.60100	2.85341	3.37652	H	-5.54687	1.86610	-3.65083
C	-2.87228	3.84707	4.03069	H	-3.86728	-5.40781	2.25063
H	-4.56984	2.56764	3.76895	H	-6.70257	-0.08998	-4.62617
H	-3.27976	4.32384	4.91283	O	0.87600	-2.47257	2.01281
C	-1.61282	4.21578	3.55976	C	2.00418	-3.28161	1.89609
C	-1.07977	3.60525	2.42245	C	1.09035	-1.57619	3.12489
H	-1.04430	4.97544	4.08065	C	2.79079	-3.19177	2.96713
H	-0.09037	3.90446	2.10473	C	2.09406	-4.00726	0.59960
O	-0.70861	-1.82867	0.11372	C	2.16539	-2.26039	3.98197
P	-0.20696	-0.67583	-0.81779	H	0.13044	-1.43441	3.62258
H	-0.07669	-2.12013	0.83895	H	1.44024	-0.62699	2.70730
O	-1.50276	0.24464	-1.10021	H	3.70754	-3.74682	3.10784
O	0.76782	0.14283	0.21193	C	2.68196	-3.10466	-0.49533
O	0.43074	-1.04509	-2.09459	H	2.71130	-4.90207	0.72464
C	3.40635	0.83164	-0.58966	H	1.09156	-4.33161	0.29549
C	3.83617	0.24053	-1.80670	H	2.86709	-1.53323	4.39709
C	4.05590	0.48890	0.62579	H	1.73026	-2.81832	4.82012
C	4.93355	-0.65781	-1.80109	H	3.75888	-3.00263	-0.32675
C	3.19011	0.50954	-3.03438	H	2.25108	-2.09819	-0.42362
C	5.13805	-0.42743	0.60861	C	2.43178	-3.65120	-1.89824
C	3.66163	1.04392	1.86445	O	1.05967	-3.82327	-2.16870
C	5.36598	-1.24781	-3.00000	H	2.89810	-2.98379	-2.63528
C	5.57761	-0.97338	-0.60098	H	2.89761	-4.63868	-2.00136
C	3.62881	-0.09023	-4.21651	H	0.67760	-2.94150	-2.31061
H	2.33746	1.17316	-3.09154				
C	5.77335	-0.78873	1.80794				
C	4.30615	0.67662	3.04713				
H	2.85312	1.75936	1.93355				
C	4.71491	-0.96351	-4.20024				
H	6.20249	-1.93662	-3.00733				
H	6.41091	-1.66838	-0.60525				
H	3.12257	0.12225	-5.14932				
H	6.59491	-1.49533	1.80775				
C	5.35437	-0.24119	3.02014				
H	3.98707	1.10214	3.98982				
H	5.04995	-1.42601	-5.11962				
H	5.84625	-0.52636	3.94106				
C	-3.99754	-0.62087	-0.07423				
C	-3.96465	-1.88902	0.56520				
C	-4.71628	-0.46354	-1.28813				
C	-4.64444	-2.98709	-0.02052				
C	-3.25384	-2.09998	1.76958				
C	-5.38913	-1.57642	-1.85389				
C	-4.78929	0.78072	-1.95477				
C	-4.60600	-4.24855	0.59651				

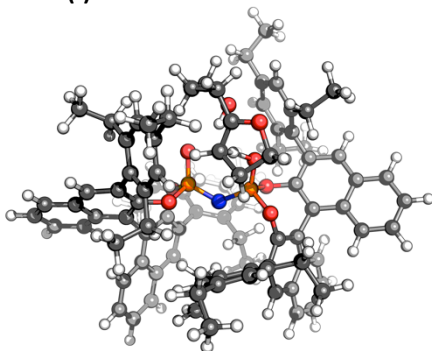
Energies of TS structures of the reaction of 1 with cat II

TS	dist C-O	$\Delta\Delta G$	rmsd	$\Delta\Delta E$ HL	H+ probe	MeOH probe
R-anti-ev(-)	2.966	2.7	0.724	0.68	-0.44	5.16
R-anti-ev(+)	2.8	13.1	0.779	2.58		
R-anti-hc(-)	3.489	2.5	0.354	3.90	2.21	0.12
R-anti-hc(-)-intermediate		-3.6				
R-anti-hc(-) 2 nd step		6.7				
R-anti-hc(+)	2.801	12.2	0.94	2.64		
R-gau-ev(-)	2.754	4.1	0.697	0.29	-0.04	7.21
R-gau-ev(+)	2.853	15.6	0.940	6.57		
R-gau-hc(-)	3.237	0.0	0.221	0.00	0.00	0.00
R-gau-hc(-) intermediate		-4.7				
R-gau-hc(-) 2 nd step		1.1				
R-gau-hc(+)*	3.138	15.8	0.301	2.62		
R-gau-hc(+) intermediate		-1.52				
S-anti-ev(-)	2.616	5.5	0.376	1.97	7.73	5.38
S-anti-ev(+)*	3.169	7.6	0.667	1.86		
S-anti-ev(+) intermediate		1.4				
S-anti-hc(-)	2.597	4.4	0.248	3.55	7.79	1.33
S-anti-hc(+)*	3.924	4.5	0.400	0.59		
S-anti-hc(+) intermediate		3.6				
S-gau-ev(-)	2.618	2.4	0.411	1.52	8.1	3.88
S-gau-ev(+)	3.007	10.2	0.534	3.35		
S-gau-hc(-)	2.779	4.4	0.682	2.40	8.99	4.11
S-gau-hc(+)	3.912	7.3	0.152	0.62		
S-gau-hc(+)* intermediate		-0.6				

*These TS structures correspond to the first step of an stepwise mechanism; however, since the high energy of them prevent that these stepwise paths contribute to the product distribution, none of the other points in the path have been calculated.

Cartesian coordinates of the TS structures and intermediates for the reaction of 1 with cat II.

R-anti-ev(-)



E(RM062X) = -5019.78786483

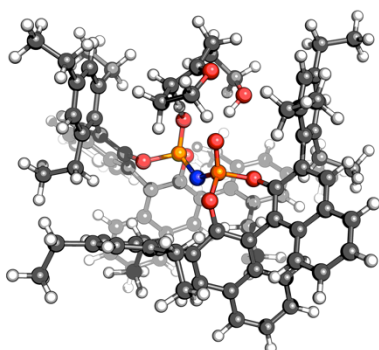
C	-1.90521	0.10575	2.58908
C	-1.14681	0.68318	3.61906
C	-3.22981	0.53699	2.36748
C	-1.63184	1.80985	4.29341
C	-3.68994	1.72422	2.98981
C	-2.87764	2.35498	3.96478
C	-4.11929	-0.31995	1.53390
C	-5.30176	-0.90921	2.05649
C	-3.71946	-0.61505	0.21473
C	-6.13345	-1.67350	1.19957
C	-4.54465	-1.39389	-0.61756
C	-5.75532	-1.89364	-0.12773
H	-6.38722	-2.48706	-0.77912
H	-1.03866	2.25424	5.08389
C	-3.33276	3.51334	4.61426
C	-4.57263	4.06315	4.28449
H	-2.72590	3.99809	5.36982
H	-4.91518	4.96074	4.78283
C	-5.36710	3.46394	3.30681
C	-4.93321	2.30424	2.66094
H	-6.32230	3.90105	3.04618
H	-5.56755	1.87630	1.89570
C	-7.32206	-2.23737	1.69017
C	-7.67842	-2.07363	3.02877
H	-7.96871	-2.81623	1.04121
H	-8.59318	-2.51524	3.40256
C	-6.84771	-1.35954	3.89089
C	-5.66535	-0.78769	3.41634
H	-7.11779	-1.25290	4.93365
H	-5.03797	-0.26755	4.12664
C	3.66125	0.53155	-0.74731
C	1.42155	2.63331	-1.22213
C	3.79260	1.91090	-1.01465
C	4.77825	-0.31631	-0.90387

C	0.48220	3.68178	-1.20907
C	2.68621	2.82936	-0.63438
C	4.97386	2.39773	-1.63645
C	5.98450	0.19840	-1.39272
C	0.73890	4.83786	-0.46102
C	2.90568	3.95271	0.20264
C	6.08194	1.53142	-1.79392
C	5.07879	3.72228	-2.11767
H	6.84208	-0.45689	-1.48943
C	1.92093	4.96658	0.27229
H	0.01908	5.64729	-0.46627
C	4.08347	4.09488	0.96706
C	7.27446	2.00723	-2.36240
C	6.26792	4.17957	-2.68954
H	4.24336	4.40790	-2.07353
C	2.14542	6.11227	1.05228
C	4.28737	5.23298	1.75036
H	4.84366	3.32463	0.97560
C	7.36560	3.32764	-2.80315
H	8.13184	1.35437	-2.47674
H	6.33663	5.19797	-3.04976
C	3.32524	6.24237	1.78670
H	1.40497	6.90188	1.10101
H	5.19447	5.33172	2.33241
H	8.28521	3.68748	-3.24625
H	3.48984	7.12362	2.39303
C	-0.75876	3.62458	-2.01916
C	-0.69949	3.81163	-3.42736
C	-2.02360	3.52018	-1.38175
C	-1.89205	3.89805	-4.16232
C	-3.19457	3.62420	-2.14799
C	-3.13694	3.82848	-3.53003
H	-4.15958	3.55537	-1.65939
C	4.69932	-1.76841	-0.61328
C	4.64929	-2.23141	0.72764
C	4.73840	-2.71143	-1.67733
C	4.58272	-3.61023	0.98059
C	4.68264	-4.08339	-1.38457
C	4.59279	-4.53756	-0.06545
H	4.69094	-4.80213	-2.19554
C	-4.11577	-1.77767	-1.98313
C	-4.20403	-0.84827	-3.05016
C	-3.66778	-3.10062	-2.24251
C	-3.82771	-1.24190	-4.34403
C	-3.32911	-3.46845	-3.55356
C	-3.39614	-2.54681	-4.60278
H	-2.97397	-4.47303	-3.75275
C	0.14994	0.09397	4.03179
C	0.17757	-1.09605	4.80826

C	1.36702	0.75302	3.72075	C	1.42029	1.99021	2.85057
C	1.40577	-1.58140	5.28235	H	0.46951	2.15849	2.30496
C	2.57495	0.24904	4.22721	C	1.73800	3.23051	3.68149
C	2.59972	-0.90237	5.02111	H	2.78004	3.18614	4.06254
H	3.50232	0.76415	4.00528	H	1.62851	4.13657	3.05434
H	4.52683	-3.96823	2.00195	H	1.03992	3.31788	4.53924
H	1.43173	-2.48128	5.88576	C	-4.72961	0.55564	-2.85270
H	-3.89350	-0.53235	-5.16060	H	-4.36248	0.98897	-1.90150
H	-1.85347	4.05354	-5.23424	C	-6.25416	0.58456	-2.87777
C	4.48757	-6.01197	0.22981	H	-6.67293	-0.02256	-2.04948
H	3.61067	-6.19440	0.88832	H	-6.60669	1.63059	-2.75906
C	5.75389	-6.53314	0.90351	H	-6.62948	0.19034	-3.84614
H	5.90944	-6.03599	1.88424	C	-3.49132	-4.13519	-1.14693
H	5.65992	-7.62620	1.07451	H	-3.53107	-3.68487	-0.13407
H	6.63685	-6.34905	0.25477	C	-4.55450	-5.22615	-1.23700
C	4.70919	-1.29211	1.91233	H	-4.40957	-5.95358	-0.41077
H	4.07021	-0.40239	1.75577	H	-5.56948	-4.78601	-1.14756
C	6.14127	-0.85315	2.19983	H	-4.47629	-5.76969	-2.20219
H	6.77904	-1.73857	2.40784	C	-2.98684	-2.95558	-5.99480
H	6.56249	-0.29346	1.34014	H	-2.91286	-2.06781	-6.66014
H	6.15383	-0.18860	3.08902	C	-3.99180	-3.93141	-6.60069
C	4.80437	-2.29993	-3.13803	H	-3.68160	-4.18895	-7.63524
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C	6.16958	-2.61700	-3.74404	H	-5.00148	-3.46915	-6.63649
H	6.19669	-2.27015	-4.79845	H	-0.83611	-2.90427	5.44200
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H	6.35786	-3.71129	-3.72953	H	4.31285	-1.79964	2.81541
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H	-5.53485	5.49814	-5.38407	H	-5.29168	3.70264	-3.72505
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H	1.33392	5.70922	-3.03465	P	-1.19869	-0.78547	0.29045
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C	-2.16866	3.29947	0.10958	O	-2.55099	-0.08371	-0.27312
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H	4.92506	-1.58374	7.49270	O	2.50663	0.04343	-0.18201
H	3.82069	-0.16149	7.37070	O	1.16959	1.49278	-1.94607
H	3.14241	-1.82629	7.59560	C	1.15869	-5.25896	-1.81833
C	-1.08121	-1.84842	5.19351	O	0.05713	-5.34093	0.28145
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C	-1.75525	-1.21688	6.40789	H	1.82411	-3.88117	2.07908
H	-1.05130	-1.18943	7.26687	H	-0.21870	-2.32645	-2.43204
H	-2.09364	-0.18600	6.18055	C	1.60989	-4.27932	-2.90537
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C	-0.17294	-4.58855	1.52748
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H	-0.15149	-5.31908	2.33460
H	-1.16061	-4.13448	1.42401
C	0.41435	-3.70013	-3.65325
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R-anti-ev(+)



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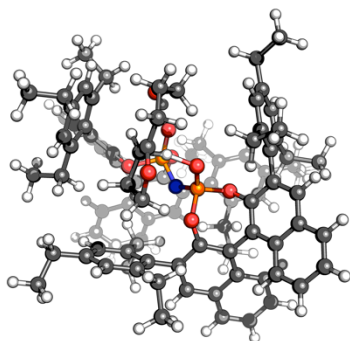
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H	5.53860	-5.09856	2.14398
H	5.06189	-2.75817	1.60727
C	7.29989	0.70494	2.92360
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H	8.34712	0.23125	4.74153
C	6.37379	-0.62106	4.71814

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H	6.47089	-1.06314	5.70140
H	4.38500	-1.33272	4.46517
N	0.00775	-0.21499	0.01777
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O	-1.05959	1.64199	-1.53974
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C	-5.20686	-2.59872	-3.21225
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C	-4.37253	-3.99295	-0.37352
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C	-7.38523	-1.79211	-3.88995
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H	-6.49046	-3.60671	-4.61394
C	-3.72715	-6.31867	-0.19020
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H	-4.01453	-1.48365	3.64523	H	-2.33949	-4.57422	1.80426
H	-4.81321	3.59311	2.94160	H	-1.81123	-4.24335	3.48731
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H	4.70932	1.77666	-4.36575	H	4.21379	-0.65484	-1.67900
H	1.74299	-2.46899	-6.14524	C	6.22962	-0.54015	-2.44403
C	-4.50884	6.03255	1.80693	H	6.70697	-0.29813	-1.47146
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H	-5.88432	7.40653	2.76426	H	4.26010	3.41363	1.33345
H	-6.61416	6.43346	1.43071	C	5.81706	4.83185	0.86013
C	-4.95686	1.04674	2.10861	H	5.71663	5.31364	1.85544
H	-4.39055	0.16756	1.74393	H	6.66363	4.11665	0.89903
C	-6.44367	0.71252	2.16081	H	6.04180	5.61944	0.11036
H	-7.01695	1.57203	2.56899	C	4.68123	4.49165	-4.48889
H	-6.82525	0.46592	1.14864	H	4.50401	3.88588	-5.40424
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C	-4.13044	3.33971	-2.41622	H	6.00897	5.82429	-5.56460
H	-3.88728	2.32462	-2.79252	H	6.19667	5.88769	-3.77311
C	-5.35468	3.86616	-3.16107	H	6.84636	4.47634	-4.70468
H	-5.16698	3.82732	-4.25477	H	0.49828	1.28212	6.17016
H	-6.24685	3.24771	-2.93449	H	-4.36833	1.30317	5.81674
H	-5.56137	4.91971	-2.87733	H	-4.60167	1.24142	3.14082
C	4.27634	-2.83431	-5.24517	H	-3.26228	3.98070	-2.66792
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H	5.77050	-4.23933	-5.94348	H	5.02613	-2.15508	-4.78999
C	-0.73132	-2.53798	-5.12299	H	-0.55536	-1.99502	-6.07737
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C	-1.32247	-3.90485	-5.45598	H	-2.71796	-2.06847	1.48980
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H	-2.23594	-3.77241	-6.07315	C	1.12201	3.77923	-1.50926
C	1.97523	-3.25812	-0.80166	C	0.04344	4.65287	-1.40990
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C	2.41984	-4.68423	-0.48408	H	2.05419	4.14843	-1.09856
H	2.30723	-4.87648	0.60077	C	-0.21057	5.67897	-0.35474
H	1.79973	-5.42417	-1.02953	O	-0.80195	4.58662	-2.39812
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R-anti-hc(-)



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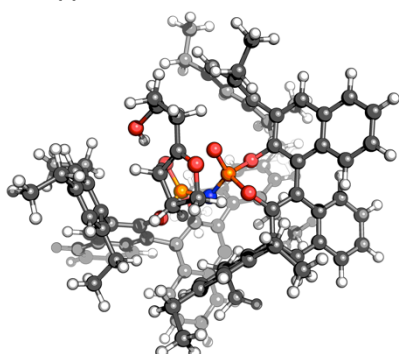
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C	-7.38695	-2.63316	0.63815
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H	4.65062	3.33265	1.56865
C	7.20528	3.94557	-2.21315
H	8.04013	1.97364	-2.17581
H	6.11150	5.79494	-2.18712
C	3.01506	6.07521	2.70277
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C	4.76655	-4.31639	-0.58981
H	4.72926	-4.27498	-2.73862
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C	-3.67445	-0.60256	-3.45935
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C	6.05492	-6.37788	0.00921	H	-6.00490	0.41368	-4.52679
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H	6.00763	-7.48702	0.03010	H	-3.52014	-3.82563	-0.87425
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C	6.26152	-0.89168	2.12026	H	-3.99589	-5.55345	-3.38670
H	6.96050	-1.75439	2.15490	C	-1.71149	-2.24693	-6.29441
H	6.60548	-0.17353	1.34906	H	-1.53803	-1.27290	-6.80185
H	6.27845	-0.38081	3.10601	C	-2.49875	-3.15089	-7.23906
C	4.71306	-1.66180	-3.31741	H	-1.94960	-3.25272	-8.19870
H	4.43852	-0.58755	-3.29442	H	-2.62658	-4.16199	-6.79770
C	6.06079	-1.81326	-4.01862	H	-3.49823	-2.71190	-7.44575
H	6.01603	-1.32853	-5.01654	H	-1.13611	-3.47158	5.13811
H	6.86589	-1.33096	-3.42746	H	3.72005	-2.94929	5.04249
H	6.30810	-2.88664	-4.15995	H	4.52035	-2.02163	2.66253
C	-4.37209	4.39612	-4.03282	H	3.93722	-2.16246	-3.93314
H	-4.26701	3.81744	-4.97590	H	4.52061	-6.26894	-1.49728
C	-4.57545	5.87318	-4.35843	H	-0.71525	-2.69645	-6.09173
H	-4.67978	6.46147	-3.42168	H	-2.26804	-4.59512	-1.86147
H	-3.71838	6.26673	-4.94484	H	-3.85986	1.51198	-3.86785
H	-5.50014	5.99646	-4.96061	H	-5.28201	4.02440	-3.51413
C	0.61978	4.54252	-3.56405	H	0.55467	4.42693	-4.66812
H	1.39875	3.82797	-3.23374	H	-3.05754	2.34108	0.42712
C	1.06562	5.97004	-3.26102	H	1.81713	1.69457	2.29358
H	0.29978	6.69445	-3.61151	O	-1.03672	-2.29043	-0.49931
H	1.23066	6.11073	-2.17407	P	-1.19707	-0.92256	0.13028
H	2.02038	6.17931	-3.78781	H	0.30423	-2.87214	-0.37699
C	-2.36701	3.20867	0.41240	O	-2.50068	-0.16422	-0.46823
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C	-2.96857	4.34210	1.23984	N	-0.01045	0.11111	0.10783
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H	-4.00964	4.54990	0.91426	C	0.80634	-4.67310	0.08066
C	3.58440	-1.90681	5.40338	C	1.39281	-2.91982	1.51475
H	4.43043	-1.30318	5.00889	H	2.09361	-3.11424	-0.68721
C	3.65143	-1.87816	6.92798	O	1.18749	-0.66847	-2.15538
H	4.64618	-2.24094	7.26226	O	2.48804	0.15906	-0.06064
H	3.50828	-0.84058	7.29863	O	1.09531	1.76757	-1.63995
H	2.87185	-2.53539	7.36777	C	0.62862	-5.69261	-0.98917
C	-1.39662	-2.39728	5.01788	O	0.25639	-4.98057	1.21738
H	-2.13081	-2.35367	4.18827	H	1.13933	-1.86336	1.63095
C	-2.04826	-1.91127	6.30842	H	2.37770	-3.09029	1.95336
H	-1.33228	-1.99184	7.15403	H	1.52870	-2.22296	-2.75051
H	-2.37797	-0.85704	6.20936	C	1.15514	-5.37796	-2.39096
H	-2.93683	-2.53763	6.53389	H	1.08004	-6.61533	-0.60054
C	1.00393	1.69724	3.04857	H	-0.45018	-5.89249	-1.01270
H	0.06310	1.88160	2.49369	C	0.34108	-3.83528	2.13761
C	1.22646	2.83969	4.03547	O	1.82350	-3.14819	-2.88798
H	2.25553	2.79781	4.45091	H	0.81857	-6.19930	-3.03127
H	1.09019	3.81007	3.52038	H	2.24899	-5.39680	-2.40262
H	0.49421	2.78568	4.86767	H	0.59181	-4.24813	3.11358
C	-4.31117	0.74561	-3.20370	H	-0.65252	-3.38316	2.14504
H	-4.12473	1.08156	-2.16442	C	0.73085	-4.02622	-2.98711

H	0.45272	-4.16672	-4.04058
H	-0.14705	-3.61784	-2.46629

R-anti-hc(-)-intermediate



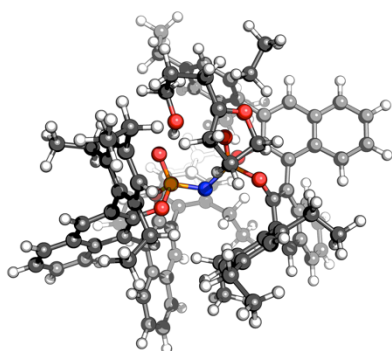
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C	-2.18949	0.14358	4.52083
C	-4.09031	0.33830	3.00468
C	-3.45186	0.66814	4.22726
C	-4.16900	-1.12737	0.92119
C	-5.38618	-1.84756	1.04486
C	-3.60617	-0.93881	-0.35788
C	-6.10217	-2.20783	-0.12493
C	-4.32727	-1.29631	-1.51402
C	-5.58283	-1.89991	-1.38648
H	-6.14670	-2.14775	-2.27705
H	-1.71505	0.36944	5.46905
C	-4.08706	1.52073	5.14431
C	-5.33017	2.07777	4.84217
H	-3.61466	1.76885	6.08741
H	-5.81011	2.74299	5.54821
C	-5.94791	1.79217	3.62507
C	-5.33663	0.93248	2.71014
H	-6.90396	2.24062	3.38784
H	-5.83759	0.75269	1.76830
C	-7.32886	-2.88258	-0.01874
C	-7.83592	-3.22783	1.23434
H	-7.88979	-3.15307	-0.90562
H	-8.77929	-3.75308	1.30957
C	-7.12155	-2.91189	2.38934
C	-5.90423	-2.23326	2.30055
H	-7.51064	-3.19707	3.35831
H	-5.37036	-2.02826	3.21862
C	3.61987	0.84947	-0.49399
C	1.20215	2.80002	-0.15577
C	3.62276	2.24421	-0.30566
C	4.78126	0.20903	-0.97008
C	0.24738	3.77637	0.18947
C	2.48743	2.87367	0.41634
C	4.70553	3.02019	-0.79830
C	5.89309	0.97002	-1.34976

C	0.48702	4.63453	1.27106
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C	5.85400	2.36460	-1.30260
C	4.67020	4.43261	-0.81798
H	6.78760	0.46790	-1.69943
C	1.68483	4.56350	1.98628
H	-0.25077	5.38369	1.53241
C	3.90287	3.61453	2.30099
C	6.95089	3.11362	-1.75781
C	5.76466	5.16495	-1.28264
H	3.79577	4.98134	-0.49533
C	1.89797	5.39977	3.09375
C	4.09378	4.43719	3.41324
H	4.69163	2.92403	2.03070
C	6.90497	4.50794	-1.74310
H	7.83913	2.62052	-2.13498
H	5.72613	6.24666	-1.28950
C	3.09694	5.33112	3.80518
H	1.13339	6.09694	3.41537
H	5.01879	4.38211	3.97246
H	7.75087	5.08051	-2.10101
H	3.25226	5.96995	4.66490
C	-0.96376	4.01126	-0.63472
C	-0.85343	4.69043	-1.87947
C	-2.25078	3.72233	-0.11149
C	-2.01847	5.08545	-2.55526
C	-3.39297	4.15011	-0.80496
C	-3.28471	4.84445	-2.01369
H	-4.37495	3.93292	-0.40093
C	4.85872	-1.26310	-1.11379
C	5.07179	-2.08216	0.02591
C	4.84373	-1.85198	-2.40747
C	5.26071	-3.46282	-0.14321
C	5.01956	-3.23823	-2.53632
C	5.23793	-4.04501	-1.41499
H	4.99069	-3.69001	-3.52096
C	-3.75937	-1.06680	-2.86912
C	-3.63699	0.25293	-3.37868
C	-3.32566	-2.16081	-3.66721
C	-3.00942	0.46326	-4.61728
C	-2.71807	-1.91362	-4.90768
C	-2.54214	-0.61066	-5.37964
H	-2.36246	-2.74534	-5.50507
C	-0.19768	-1.22891	3.94608
C	-0.09529	-2.53661	4.48565
C	0.97685	-0.45673	3.76255
C	1.16923	-3.05589	4.80376
C	2.22650	-1.00597	4.08622
C	2.33043	-2.30039	4.60548
H	3.12267	-0.41332	3.94246
H	5.42235	-4.09357	0.72315
H	1.25091	-4.05945	5.20444
H	-2.90359	1.47063	-5.00272
H	-1.94028	5.61061	-3.50008
C	5.41021	-5.53451	-1.56778
H	4.71059	-6.05991	-0.88211
C	6.84403	-5.95760	-1.26104

H	7.10557	-5.72035	-0.20808	C	-3.46689	-3.60482	-3.23483
H	6.94800	-7.05278	-1.41143	H	-3.63630	-3.70356	-2.14325
H	7.55139	-5.43625	-1.94094	C	-4.59670	-4.30099	-3.98950
C	5.13160	-1.51947	1.43188	H	-4.69324	-5.34687	-3.62950
H	4.35826	-0.74110	1.58616	H	-5.56113	-3.77966	-3.82490
C	6.51092	-0.95033	1.74699	H	-4.37995	-4.32216	-5.07870
H	7.28882	-1.73197	1.61296	C	-1.85660	-0.37087	-6.70058
H	6.74191	-0.08809	1.08963	H	-1.62044	0.70780	-6.83117
H	6.53463	-0.60243	2.80122	C	-2.73388	-0.81869	-7.86643
C	4.63710	-1.04070	-3.67365	H	-2.21724	-0.60064	-8.82476
H	4.25235	-0.02243	-3.45979	H	-2.92950	-1.91059	-7.81239
C	5.92970	-0.92370	-4.47816	H	-3.70084	-0.27172	-7.85093
H	5.74822	-0.30607	-5.38282	H	-1.04142	-4.47832	4.61009
H	6.72482	-0.44027	-3.87521	H	3.79957	-3.86095	4.43714
H	6.27978	-1.92658	-4.80206	H	4.91082	-2.31868	2.17108
C	-4.52110	5.30096	-2.74631	H	3.87278	-1.53291	-4.30974
H	-4.48371	4.94040	-3.79703	H	5.16190	-5.85549	-2.60299
C	-4.64209	6.82224	-2.72936	H	-0.89352	-0.92557	-6.72343
H	-4.67609	7.19252	-1.68237	H	-2.52431	-4.14180	-3.46006
H	-3.78320	7.28969	-3.25572	H	-3.77551	2.38488	-3.07460
H	-5.57774	7.12576	-3.24443	H	-5.43532	4.87295	-2.28109
C	0.48255	5.06648	-2.49192	H	0.37589	5.19366	-3.59149
H	1.23176	4.26256	-2.35671	H	-3.16325	2.12368	0.99110
C	1.01526	6.37287	-1.91059	H	1.76153	1.13400	2.54434
H	0.28008	7.19103	-2.06598	O	-0.97800	-2.45795	-0.83830
H	1.22172	6.26859	-0.82679	P	-1.11647	-1.21228	-0.00953
H	1.96359	6.64505	-2.42001	H	1.50089	-2.45988	-1.17889
C	-2.44743	2.95163	1.17449	O	-2.39248	-0.31251	-0.47624
H	-1.50735	2.48050	1.51920	O	-1.47854	-1.80565	1.49237
C	-2.98522	3.85207	2.28425	N	0.08103	-0.19192	0.16094
H	-2.96499	3.30734	3.24825	C	1.68194	-3.35643	-0.58462
H	-2.36130	4.76267	2.39058	P	1.13923	0.32920	-0.91503
H	-4.03235	4.15158	2.06828	C	0.55419	-4.30256	-0.72008
C	3.67989	-2.88003	4.94590	C	1.78828	-3.11928	0.93252
H	4.49561	-2.21602	4.58638	H	2.54748	-3.84224	-1.04676
C	3.84170	-3.05878	6.45306	O	1.20969	-0.29625	-2.26708
H	4.85793	-3.44822	6.67325	O	2.54307	0.10688	-0.07776
H	3.71451	-2.08393	6.97066	O	0.94951	1.93452	-1.19332
H	3.09582	-3.78208	6.84496	C	-0.05693	-4.95754	-1.90362
C	-1.31020	-3.40622	4.73197	O	0.14593	-4.76093	0.39742
H	-2.11072	-3.20577	3.99058	H	1.59798	-2.06862	1.16222
C	-1.85534	-3.19113	6.13966	H	2.77151	-3.38960	1.31590
H	-1.08061	-3.44307	6.89498	H	1.62782	-1.71182	-3.15907
H	-2.17033	-2.13597	6.27792	C	0.44952	-4.64384	-3.31170
H	-2.73631	-3.84727	6.30111	H	0.00455	-6.03493	-1.70078
C	0.93397	0.96809	3.26481	H	-1.11324	-4.69244	-1.79139
H	-0.00375	1.18195	2.71797	C	0.70720	-4.02378	1.53098
C	1.06448	1.94405	4.43032	O	1.72849	-2.64103	-3.44878
H	2.09267	1.90878	4.84887	H	-0.19254	-5.21757	-3.98846
H	0.85347	2.97332	4.08271	H	1.46901	-5.02158	-3.45037
H	0.33588	1.69852	5.23079	H	1.06614	-4.77991	2.22894
C	-4.20711	1.45333	-2.65565	H	-0.13966	-3.47694	1.93781
H	-3.93900	1.43857	-1.58157	C	0.44892	-3.16851	-3.71583
C	-5.72288	1.53030	-2.81110	H	0.22773	-3.09214	-4.78957
H	-6.21409	0.64274	-2.36458	H	-0.32152	-2.61689	-3.16117
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R-anti-hc(-)-2nd step



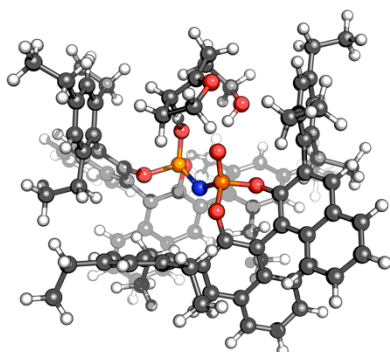
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C	-2.04340	0.95198	4.43139
C	-4.01868	0.95310	2.99809
C	-3.31211	1.45484	4.12099
C	-4.19778	-0.80308	1.15573
C	-5.38008	-1.53752	1.43989
C	-3.66742	-0.82578	-0.14970
C	-6.07780	-2.16961	0.37790
C	-4.35536	-1.47649	-1.18860
C	-5.56719	-2.12096	-0.92358
H	-6.09240	-2.61757	-1.73163
H	-1.52252	1.30151	5.31519
C	-3.88971	2.44930	4.92609
C	-5.14575	2.96891	4.60941
H	-3.36480	2.83259	5.79309
H	-5.58242	3.74147	5.22892
C	-5.83405	2.50404	3.48877
C	-5.27845	1.50607	2.68533
H	-6.80138	2.92061	3.23948
H	-5.83298	1.18363	1.81395
C	-7.26449	-2.87397	0.63645
C	-7.74992	-2.98058	1.93986
H	-7.80952	-3.35343	-0.16819
H	-8.66261	-3.52925	2.13349
C	-7.05037	-2.39925	2.99638
C	-5.87148	-1.69056	2.75515
H	-7.41994	-2.50260	4.00850
H	-5.34701	-1.28049	3.60691
C	3.59783	0.91195	-0.48263
C	1.23149	2.89456	-0.65144
C	3.64503	2.32015	-0.51082
C	4.73817	0.16766	-0.83621
C	0.22657	3.86998	-0.50706
C	2.47220	3.08383	-0.01051
C	4.78375	2.97613	-1.05178
C	5.89952	0.82247	-1.25880
C	0.38583	4.90042	0.42893
C	2.59794	4.06651	1.00259
C	5.92525	2.21173	-1.39578

C	4.81074	4.37006	-1.28287
H	6.77486	0.23756	-1.51947
C	1.54081	4.98362	1.21080
H	-0.38617	5.65356	0.52988
C	3.75097	4.16121	1.81000
C	7.07419	2.84531	-1.89580
C	5.95788	4.98568	-1.78806
H	3.94674	4.99250	-1.09494
C	1.66781	5.99453	2.17679
C	3.85708	5.16135	2.77899
H	4.56688	3.45750	1.70742
C	7.08947	4.22736	-2.08451
H	7.95569	2.26981	-2.15293
H	5.96698	6.05508	-1.95527
C	2.82195	6.07947	2.95731
H	0.87108	6.71174	2.33470
H	4.74547	5.22448	3.39393
H	7.97576	4.70983	-2.47595
H	2.91123	6.85488	3.70706
C	-0.97357	3.88814	-1.37857
C	-0.86551	4.32136	-2.72878
C	-2.25688	3.62010	-0.83318
C	-2.02989	4.49053	-3.49406
C	-3.39918	3.81311	-1.62483
C	-3.29493	4.26312	-2.94442
H	-4.37880	3.61625	-1.20490
C	4.72931	-1.31171	-0.84770
C	4.97785	-2.03638	0.34401
C	4.64599	-2.00321	-2.08449
C	5.19197	-3.42145	0.27748
C	4.84441	-3.39183	-2.11347
C	5.13855	-4.10218	-0.94462
H	4.77682	-3.91990	-3.05729
C	-3.75757	-1.57588	-2.54171
C	-3.77181	-0.45916	-3.41494
C	-3.14747	-2.78654	-2.96497
C	-3.14496	-0.55208	-4.66738
C	-2.54479	-2.84990	-4.23072
C	-2.53051	-1.73899	-5.07944
H	-2.07531	-3.77220	-4.55245
C	-0.10648	-0.54849	3.97538
C	0.00217	-1.84083	4.55472
C	1.06506	0.22542	3.77188
C	1.26367	-2.32187	4.93729
C	2.31163	-0.28958	4.16075
C	2.41608	-1.54991	4.75809
H	3.20528	0.30434	4.00726
H	5.38775	-3.97711	1.18732
H	1.34997	-3.30284	5.38974
H	-3.14125	0.30319	-5.33314
H	-1.95493	4.83267	-4.51973
C	5.33906	-5.59565	-0.98794
H	4.66455	-6.08093	-0.24964
C	6.78699	-5.96699	-0.68103
H	7.06396	-5.64766	0.34597
H	6.91055	-7.06813	-0.75239
H	7.46993	-5.48391	-1.41220

C	5.04973	-1.36824	1.69866	H	-3.98794	-5.98166	-1.90979
H	4.51536	-0.39769	1.71301	H	-5.08836	-4.71801	-2.57762
C	6.49693	-1.14037	2.11991	H	-3.77751	-5.42008	-3.60952
H	7.03741	-2.10804	2.19075	C	-1.85121	-1.81387	-6.42309
H	7.01128	-0.48524	1.38502	H	-1.15768	-0.95263	-6.53616
H	6.52082	-0.64702	3.11431	C	-2.87160	-1.80288	-7.55785
C	4.34433	-1.29505	-3.39127	H	-2.34470	-1.88925	-8.53143
H	3.96336	-0.26563	-3.22937	H	-3.56995	-2.66074	-7.45378
C	5.57979	-1.22521	-4.28511	H	-3.45136	-0.85559	-7.55387
H	5.32866	-0.68587	-5.22260	H	-0.89923	-3.78532	4.87658
H	6.39961	-0.68035	-3.77295	H	3.92415	-3.08378	4.77246
H	5.92948	-2.24555	-4.54926	H	4.54287	-2.01127	2.44768
C	-4.53323	4.49612	-3.77304	H	3.54072	-1.83942	-3.92832
H	-4.43229	3.97291	-4.74847	H	5.07779	-5.99980	-1.99019
C	-4.76246	5.98560	-4.01303	H	-1.24269	-2.74104	-6.50504
H	-4.86494	6.51881	-3.04370	H	-2.05161	-4.42366	-2.10260
H	-3.91784	6.42442	-4.58527	H	-4.07781	1.66013	-3.68195
H	-5.69564	6.12792	-4.59767	H	-5.43032	4.08063	-3.26477
C	0.46213	4.67745	-3.37043	H	0.38266	4.60871	-4.47748
H	1.25613	3.96123	-3.08297	H	-3.12140	2.24157	0.56622
C	0.89146	6.09731	-3.01212	H	1.82085	1.67055	2.37339
H	0.10842	6.82413	-3.31648	O	-0.94404	-2.24667	-0.59318
H	1.07462	6.19262	-1.92318	P	-1.15707	-0.94623	0.10191
H	1.83309	6.34499	-3.54582	H	2.61406	-4.16035	-0.09816
C	-2.45133	3.12494	0.58400	O	-2.49659	-0.16329	-0.41313
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H	4.57740	-1.41575	4.85225	H	2.15749	-5.52749	0.96445
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H	4.84600	-2.50629	7.03054	O	2.48910	0.27396	0.01479
H	3.66256	-1.15146	7.17610	O	1.06815	1.86338	-1.54659
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C	-1.20549	-2.71788	4.81777	O	-0.44154	-4.85639	0.07175
H	-1.93599	-2.65900	3.98655	H	1.08886	-2.64488	1.01618
C	-1.88517	-2.33968	6.12995	H	1.50861	-3.66543	2.41714
H	-1.16893	-2.43315	6.97405	H	1.14122	-2.24436	-1.81705
H	-2.26749	-1.29950	6.08983	C	1.55697	-5.26005	-2.84877
H	-2.74203	-3.02148	6.31354	H	1.18308	-6.81399	-1.37364
C	1.02951	1.60284	3.14791	H	-0.28593	-6.04629	-1.99288
H	0.06958	1.80310	2.63184	C	-0.34019	-4.21611	1.39762
C	1.25687	2.68299	4.20157	O	1.39482	-3.20921	-1.79751
H	2.29392	2.62889	4.59511	H	1.37915	-5.85868	-3.74621
H	1.10067	3.68242	3.75062	H	2.62614	-5.30151	-2.62007
H	0.54099	2.56623	5.04143	H	-0.50336	-5.02879	2.11254
C	-4.46835	0.83332	-3.05413	H	-1.12956	-3.47323	1.43925
H	-4.26511	1.11279	-2.00118	C	1.14955	-3.80955	-3.04020
C	-5.97316	0.73376	-3.28211	H	1.73694	-3.34458	-3.83989
H	-6.41968	-0.04795	-2.63474	H	0.08645	-3.73088	-3.30558
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H	-6.18443	0.49205	-4.34561				
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R-anti-hc(+)



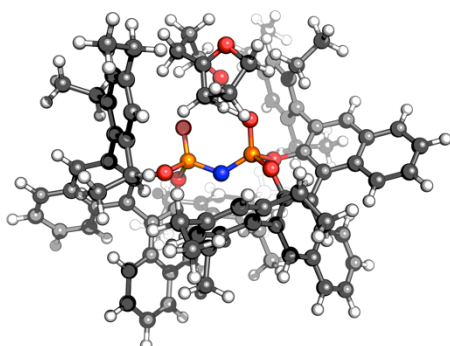
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C	0.65934	-1.66193	3.35870
C	2.83703	-1.38403	2.31336
C	0.98201	-2.98973	3.66835
C	3.12981	-2.75114	2.54870
C	2.18793	-3.55098	3.23892
C	3.88669	-0.41506	1.90090
C	5.06617	-0.24069	2.67556
C	3.69422	0.35924	0.73277
C	6.12462	0.54292	2.15944
C	4.75639	1.15046	0.24575
C	5.97201	1.19631	0.93721
H	6.78991	1.78377	0.53594
H	0.29661	-3.58018	4.26384
C	2.48164	-4.89397	3.52410
C	3.69367	-5.45135	3.11318
H	1.77336	-5.51243	4.06260
H	3.91320	-6.48830	3.33194
C	4.61844	-4.67723	2.41198
C	4.34153	-3.33856	2.12580
H	5.55102	-5.11731	2.08341
H	5.07224	-2.77401	1.56146
C	7.31961	0.68173	2.88379
C	7.45952	0.07594	4.13238
H	8.13990	1.27062	2.49041
H	8.38031	0.19140	4.68944
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C	5.21688	-0.81503	3.95860
H	6.51128	-1.11191	5.65122
H	4.41648	-1.37045	4.42809
N	0.01158	-0.21989	0.01248
P	-1.15261	0.26353	-0.98346
O	-1.05374	1.64065	-1.54022
O	-2.52404	0.06743	-0.11954
O	-1.20998	-0.78799	-2.23645
C	-3.67341	-0.11268	-0.85227
C	-1.54515	-2.08238	-1.91559
C	-3.88176	-1.33038	-1.53253

C	-4.69673	0.85738	-0.82788
C	-0.65555	-3.12991	-2.21177
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C	-5.05026	-1.50832	-2.32063
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C	-0.97749	-4.44222	-1.84197
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C	-6.07335	-0.53134	-2.27216
C	-5.22101	-2.62245	-3.17312
H	-6.68720	1.36410	-1.46177
C	-2.18731	-4.72785	-1.20254
H	-0.29055	-5.24621	-2.07649
C	-4.35094	-4.00834	-0.35166
C	-7.25466	-0.70946	-3.01007
C	-6.39763	-2.78254	-3.90800
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C	-2.48049	-6.04127	-0.80252
C	-4.62649	-5.31820	0.04700
H	-5.08678	-3.24344	-0.14041
C	-7.41563	-1.83429	-3.81924
H	-8.04763	0.02816	-2.97144
H	-6.51807	-3.64367	-4.55268
C	-3.69634	-6.33244	-0.18169
H	-1.76859	-6.84134	-0.96757
H	-5.56273	-5.54640	0.53966
H	-8.32565	-1.96349	-4.39079
H	-3.91522	-7.34577	0.12908
C	0.59625	-2.88985	-2.97008
C	0.54476	-2.65383	-4.37125
C	1.85631	-3.02561	-2.33110
C	1.74020	-2.58567	-5.10384
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C	2.97937	-2.76708	-4.48214
H	3.99257	-3.08642	-2.61503
C	-4.52449	2.16734	-0.15673
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H	-4.19895	5.49273	-0.89569
C	4.61252	2.01002	-0.95329
C	4.64926	1.44414	-2.25315
C	4.58797	3.42415	-0.80730
C	4.65618	2.28692	-3.37557
C	4.60754	4.23611	-1.95180
C	4.64861	3.67785	-3.23260
H	4.57168	5.31400	-1.84471
C	-0.60278	-1.09332	3.88979
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C	-1.77762	0.24221	5.55924
C	-3.03812	-1.11832	4.01331
C	-3.00761	-0.23733	5.09902
H	-3.99182	-1.48067	3.64782
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C	-4.51730	6.05939	1.74529	H	6.72164	-0.24668	-1.55384
H	-3.81830	6.05386	2.60912	H	6.27994	-1.57898	-2.68411
C	-5.91875	6.42763	2.22484	H	6.76056	0.03118	-3.34331
H	-6.27501	5.70173	2.98632	C	4.49360	4.10637	0.54629
H	-5.90111	7.43877	2.68319	H	4.24129	3.39318	1.35764
H	-6.62702	6.43723	1.36879	C	5.79274	4.82422	0.90541
C	-4.92512	1.07521	2.12824	H	5.69406	5.28717	1.90979
H	-4.36943	0.19017	1.76136	H	6.64161	4.11111	0.92841
C	-6.41088	0.74448	2.21689	H	6.01262	5.62622	0.16963
H	-6.97287	1.60758	2.63307	C	4.66824	4.57175	-4.44600
H	-6.81566	0.49309	1.21481	H	4.49535	3.98180	-5.37243
H	-6.55611	-0.13027	2.88510	C	6.00706	5.29346	-4.57449
C	-4.15258	3.30384	-2.43799	H	6.00477	5.92061	-5.49071
H	-3.90554	2.28477	-2.80084	H	6.18267	5.95177	-3.69732
C	-5.38896	3.80925	-3.17735	H	6.83463	4.55591	-4.65018
H	-5.21271	3.75544	-4.27227	H	0.54611	1.24226	6.17474
H	-6.27365	3.18733	-2.93212	H	-4.31844	1.30427	5.82984
H	-5.60112	4.86526	-2.90711	H	-4.54488	1.28168	3.14948
C	4.24788	-2.76947	-5.29913	H	-3.29270	3.94762	-2.71000
H	4.05047	-2.41185	-6.33321	H	-4.16698	6.84503	1.04081
C	4.84631	-4.17092	-5.37885	H	3.84765	5.31768	-4.37029
H	5.12873	-4.53312	-4.36759	H	3.67043	4.85192	0.52718
H	4.11510	-4.87531	-5.83006	H	4.28172	-0.30717	-3.44923
H	5.75777	-4.14984	-6.01264	H	4.99031	-2.07853	-4.84968
C	-0.76194	-2.53615	-5.13296	H	-0.60083	-1.98811	-6.08705
H	-1.50674	-1.94147	-4.56894	H	2.73212	-2.53244	-0.42828
C	-1.33976	-3.90890	-5.46518	H	-2.70754	-2.07854	1.49335
H	-0.60574	-4.50387	-6.04934	O	1.02089	2.20110	0.58359
H	-1.60477	-4.46112	-4.54148	H	0.95029	2.86793	-0.42966
H	-2.26101	-3.78541	-6.07257	C	1.09153	3.82821	-1.45491
C	1.98965	-3.24866	-0.83928	C	-0.00762	4.67233	-1.32835
H	1.03891	-3.05336	-0.30128	C	1.02586	3.23344	-2.85807
C	2.44496	-4.67479	-0.53736	H	2.01771	4.20719	-1.03845
H	2.33820	-4.87835	0.54602	C	-0.28159	5.66544	-0.24687
H	1.82745	-5.41370	-1.08716	O	-0.85623	4.61022	-2.31401
H	3.50955	-4.80941	-0.82311	H	1.81574	3.63016	-3.50156
C	-4.28718	0.19479	5.77077	H	1.08954	2.14325	-2.84912
H	-5.17147	-0.13195	5.18157	C	0.12137	5.14462	1.13804
C	-4.40187	-0.39678	7.17309	H	-1.34128	5.93101	-0.28314
H	-5.36764	-0.09026	7.62719	H	0.30294	6.55935	-0.50133
H	-4.36739	-1.50625	7.12520	C	-0.36569	3.68575	-3.33862
H	-3.57720	-0.03216	7.82136	C	-0.92995	4.15245	1.67138
C	0.72389	0.30453	5.60411	H	1.10473	4.66692	1.08207
H	1.47161	0.56340	4.82956	H	0.21540	5.98705	1.83078
C	1.30765	-0.72897	6.56344	H	-1.07668	2.86422	-3.37499
H	0.56793	-0.98170	7.35277	H	-0.35952	4.25234	-4.27148
H	1.59572	-1.65309	6.02367	H	-1.69164	4.70542	2.23032
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C	-1.96903	-2.48871	2.21327	H	-1.12399	2.77844	0.23886
H	-1.01286	-2.58267	1.65807	O	-1.62732	3.50396	0.63570
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H	-3.48672	-3.85263	2.97757				
H	-2.32627	-4.58786	1.81105				
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R-gau-ev(-)



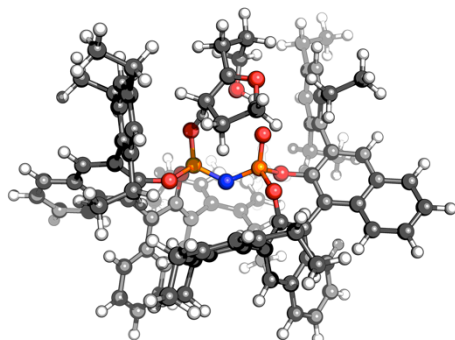
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H	6.42841	2.47689	-0.24454
H	0.84508	-2.82022	4.87776
C	3.16702	-3.99948	4.34304
C	4.42217	-4.49906	3.99200
H	2.54134	-4.57317	5.01649
H	4.75788	-5.44653	4.39321
C	5.24113	-3.78450	3.11749
C	4.81634	-2.55984	2.59781
H	6.20863	-4.18190	2.83923
H	5.47057	-2.04129	1.90915
C	7.21409	2.03333	2.24981
C	7.50195	1.74447	3.58388
H	7.89670	2.66063	1.68863
H	8.39919	2.14095	4.04134
C	6.62704	0.95975	4.33384
C	5.46750	0.44446	3.75054
H	6.84530	0.75326	5.37373
H	4.80395	-0.13694	4.37581
C	-3.67326	-0.37417	-0.87363
C	-1.44002	-2.44277	-1.51160
C	-3.80824	-1.70889	-1.30965
C	-4.77869	0.49843	-0.95557
C	-0.51673	-3.50335	-1.58396
C	-2.72909	-2.68290	-0.99774
C	-4.97151	-2.10176	-2.02422
C	-5.97233	0.06221	-1.54260
C	-0.81804	-4.73239	-0.98341
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C	-6.06635	-1.20924	-2.11019

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C	-4.20391	-4.09711	0.39672
C	-7.24275	-1.59740	-2.77128
C	-6.24379	-3.72635	-3.32779
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C	-2.30005	-6.14687	0.31820
C	-4.45329	-5.31307	1.03671
H	-4.95273	-3.31888	0.46679
C	-7.32965	-2.85305	-3.37299
H	-8.09045	-0.92507	-2.83252
H	-6.30881	-4.69259	-3.81130
C	-3.50814	-6.33793	0.99065
H	-1.57332	-6.95044	0.30234
H	-5.38281	-5.46064	1.57112
H	-8.23657	-3.14480	-3.88670
H	-3.70809	-7.27951	1.48539
C	0.75289	-3.38341	-2.34033
C	0.74154	-3.43244	-3.76110
C	1.99503	-3.37992	-1.65199
C	1.95765	-3.49498	-4.45872
C	3.19009	-3.46100	-2.38286
C	3.17873	-3.53647	-3.77925
H	4.13726	-3.47508	-1.85631
C	-4.70068	1.89945	-0.47561
C	-4.68003	2.18321	0.91572
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C	-4.60891	3.51697	1.34773
C	-4.68014	4.29451	-0.93651
C	-4.60422	4.57256	0.43117
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C	4.25856	1.84042	-1.65434
C	4.44568	0.94296	-2.73624
C	3.86762	3.18007	-1.91824
C	4.22888	1.38618	-4.05026
C	3.67631	3.59426	-3.24581
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C	-0.39032	0.51471	4.97654
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C	-1.63604	0.92760	5.47315
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H	-3.67410	-1.23464	3.82960
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H	-1.68687	1.73828	6.19067
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H	1.95452	-3.54691	-5.54130
C	-4.49948	5.99588	0.91564
H	-3.64412	6.08507	1.61974
C	-5.78439	6.43815	1.60993
H	-5.97665	5.81714	2.51035
H	-5.68886	7.49794	1.92702
H	-6.64582	6.35121	0.91368

C	-4.77744	1.09818	1.96656	H	4.50823	5.95718	0.06098
H	-4.13132	0.23508	1.71783	H	5.70187	4.77461	-0.59239
C	-6.21734	0.62824	2.14712	H	4.74768	5.81958	-1.71969
H	-6.86405	1.48073	2.44547	C	3.65628	3.17699	-5.73161
H	-6.60855	0.18374	1.20967	H	3.64977	2.31484	-6.43371
H	-6.25799	-0.14490	2.94271	C	4.76447	4.13678	-6.15574
C	-4.73897	2.75806	-2.91139	H	4.60834	4.44037	-7.21231
H	-4.51574	1.70836	-3.18981	H	4.75571	5.04900	-5.52225
C	-6.08618	3.15355	-3.51209	H	5.75492	3.64064	-6.07059
H	-6.08082	2.94579	-4.60280	H	0.59525	2.23220	5.85677
H	-6.90910	2.57414	-3.04626	H	-4.25513	1.81363	5.56174
H	-6.27704	4.23716	-3.36252	H	-4.41395	1.48298	2.94149
C	4.46955	-3.66164	-4.54953	H	-3.94727	3.37298	-3.38809
H	4.50394	-2.88582	-5.34476	H	-4.30098	6.68653	0.06713
C	4.60465	-5.04593	-5.17776	H	2.67217	3.68318	-5.82303
H	4.56880	-5.82927	-4.39067	H	2.64034	4.69055	-0.99652
H	3.78957	-5.22501	-5.91049	H	4.61554	-1.09979	-3.39514
H	5.57725	-5.11922	-5.70838	H	5.34381	-3.49374	-3.88323
C	-0.54171	-3.49397	-4.56692	H	-0.36291	-3.12113	-5.59922
H	-1.32088	-2.83286	-4.14046	H	2.81329	-2.49688	0.12824
C	-1.07113	-4.92207	-4.65953	H	-2.30822	-2.06688	1.82190
H	-0.30521	-5.58751	-5.11193	O	1.09612	2.24877	0.14213
H	-1.34348	-5.30803	-3.65660	P	1.14862	0.77272	0.48115
H	-1.97923	-4.93964	-5.29817	H	-0.12304	2.87279	0.03719
C	2.08909	-3.29247	-0.14262	O	2.51979	0.13824	-0.12370
H	1.12225	-3.00642	0.31913	O	1.28336	0.76371	2.11530
C	2.55607	-4.61432	0.46288	N	-0.02659	-0.17401	0.03530
H	2.48378	-4.56379	1.56724	C	-1.13043	3.56587	0.33224
H	1.92325	-5.45473	0.11302	P	-1.13524	0.06041	-1.09191
H	3.61261	-4.81614	0.18743	C	-0.91610	4.61774	-0.57784
C	-4.13779	0.71396	5.67293	C	-0.69312	4.11466	1.68889
H	-4.98266	0.23284	5.13453	H	-1.98938	2.91655	0.20091
C	-4.23368	0.33459	7.14812	O	-1.07790	1.28322	-1.95097
H	-5.22862	0.62953	7.54307	O	-2.53126	0.02874	-0.22256
H	-4.11359	-0.76319	7.27025	O	-1.14555	-1.23264	-2.09282
H	-3.45172	0.85684	7.73895	C	-1.53664	4.83100	-1.90785
C	0.85088	1.21063	5.49949	O	-0.12075	5.54140	-0.11794
H	1.60303	1.35135	4.69818	H	-0.22036	3.34920	2.30895
C	1.47065	0.43844	6.66024	H	-1.52490	4.56643	2.23955
H	0.73186	0.32105	7.48156	H	0.32795	2.45290	-2.16692
H	1.81133	-0.56368	6.33024	C	-0.57883	5.16475	-3.05546
H	2.34883	0.99565	7.04895	H	-2.08804	3.91868	-2.14231
C	-1.54643	-2.29514	2.59658	H	-2.25214	5.64964	-1.75348
H	-0.57835	-2.38630	2.06350	C	0.32821	5.15456	1.22682
C	-1.87475	-3.63268	3.25453	O	0.73216	3.31914	-2.36234
H	-2.92847	-3.64478	3.60467	H	0.16614	5.89701	-2.72684
H	-1.73499	-4.45179	2.52279	H	-1.14491	5.60502	-3.88281
H	-1.20220	-3.82173	4.11634	H	0.37606	6.07203	1.81113
C	4.92408	-0.47666	-2.53227	H	1.31816	4.71294	1.10145
H	4.45949	-0.93212	-1.63548	C	0.10894	3.87768	-3.49158
C	6.44324	-0.54084	-2.41680	H	-0.63194	3.18237	-3.90869
H	6.79469	0.02198	-1.52836	H	0.85503	4.08985	-4.26598
H	6.76099	-1.59947	-2.31051				
H	6.91598	-0.11767	-3.32867				
C	3.61534	4.18954	-0.81608				
H	3.54117	3.70919	0.18096				
C	4.71377	5.24796	-0.76824				

R-gau-ev(+)



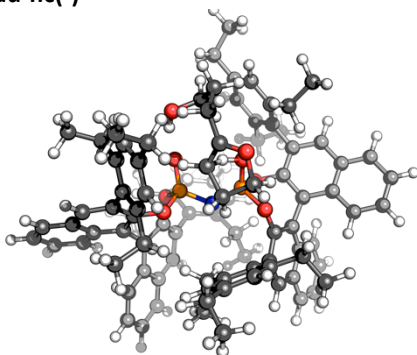
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C	-1.48623	-1.88799	-2.09310
C	-0.56858	-2.90157	-2.42873
C	-2.78066	-2.24300	-1.66751
C	-0.88266	-4.24098	-2.15958
C	-3.06720	-3.58573	-1.31571
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C	-4.98396	-1.37878	-2.56252
C	-3.69072	-0.02622	-0.97589
C	-6.05022	-0.45489	-2.47050
C	-4.76092	0.89532	-0.91307
C	-5.94128	0.64729	-1.62384
H	-6.76492	1.34872	-1.54780
H	-0.18184	-5.01887	-2.43517
C	-2.38447	-5.92915	-1.27135
C	-3.61326	-6.28050	-0.71010
H	-1.65618	-6.70585	-1.47257
H	-3.82543	-7.31639	-0.47932
C	-4.56586	-5.29800	-0.43953
C	-4.29793	-3.95924	-0.73379
H	-5.51282	-5.57332	0.00634
H	-5.05102	-3.22128	-0.49009
C	-7.20769	-0.63184	-3.24573
C	-7.30117	-1.70188	-4.13561
H	-8.03396	0.06567	-3.17368
H	-8.19278	-1.82994	-4.73573
C	-6.23912	-2.59504	-4.26755
C	-5.08633	-2.43579	-3.49566
H	-6.30675	-3.41220	-4.97416
H	-4.27601	-3.13501	-3.65067
N	-0.00138	-0.10608	-0.04743
P	1.21261	0.67141	0.62894
O	1.29674	2.16128	0.54187
O	2.58516	0.01726	0.02022
O	1.16942	0.27947	2.23343
C	3.69497	0.14467	0.82469
C	1.42271	-1.04203	2.53214

C	3.80666	-0.64747	1.98362
C	4.76415	0.98396	0.45301
C	0.46767	-1.81321	3.22198
C	2.70390	-1.58378	2.30387
C	4.92507	-0.49378	2.84608
C	5.91621	1.04506	1.24563
C	0.72395	-3.16732	3.48290
C	2.93407	-2.96865	2.49187
C	5.99739	0.33765	2.44547
C	4.99591	-1.12501	4.10869
H	6.73810	1.68382	0.94071
C	1.92454	-3.76033	3.08514
H	-0.00619	-3.75342	4.02662
C	4.14932	-3.58145	2.11767
C	7.12939	0.47418	3.26501
C	6.12455	-0.97450	4.91721
H	4.17986	-1.72318	4.49009
C	2.14808	-5.12703	3.31634
C	4.35747	-4.94283	2.34989
H	4.93612	-3.01858	1.63249
C	7.19241	-0.18535	4.49259
H	7.95915	1.10204	2.96227
H	6.16852	-1.46814	5.87952
C	3.36080	-5.71305	2.94955
H	1.38553	-5.74116	3.78057
H	5.29249	-5.40316	2.05803
H	8.06467	-0.07185	5.12329
H	3.52676	-6.76776	3.12671
C	-0.78245	-1.22272	3.75926
C	-0.73711	-0.38211	4.90625
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C	-3.21519	-1.27263	3.92554
C	-3.16977	-0.47353	5.07231
H	-4.17485	-1.61458	3.55628
C	4.69119	1.88318	-0.71803
C	4.99524	1.39279	-2.01099
C	4.52341	3.27866	-0.51886
C	5.15273	2.29458	-3.07361
C	4.70486	4.15504	-1.59906
C	5.03284	3.67307	-2.87138
H	4.58468	5.22118	-1.44724
C	-4.67377	2.17714	-0.17425
C	-4.83392	2.20707	1.23319
C	-4.63596	3.40067	-0.89721
C	-4.94510	3.44067	1.89354
C	-4.77364	4.61638	-0.20771
C	-4.92341	4.64389	1.18199
H	-4.72196	5.55128	-0.75336
C	0.70835	-2.60145	-3.12134
C	0.70510	-2.22507	-4.49327
C	1.94680	-2.83150	-2.46378
C	1.92548	-2.08913	-5.17318
C	3.14452	-2.71279	-3.18501
C	3.14136	-2.35690	-4.53730
H	4.08710	-2.91154	-2.68882
H	5.39404	1.92171	-4.06243

H	1.92964	-1.81010	-6.22039	C	-4.95486	0.95016	2.05975
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C	5.22931	4.62624	-4.02271	H	-6.91588	0.39432	1.30028
H	4.60518	4.30166	-4.88324	H	-6.47810	-0.35031	2.88393
C	6.69478	4.68402	-4.44500	H	-6.94866	1.39039	2.81387
H	7.03933	3.68981	-4.80045	C	-4.36160	3.45639	-2.38801
H	6.81415	5.41459	-5.27256	H	-4.03803	2.47401	-2.78969
H	7.32750	5.00726	-3.59082	C	-5.58651	3.92680	-3.16885
C	5.21768	-0.07582	-2.28263	H	-5.35201	3.93604	-4.25405
H	4.63263	-0.71035	-1.58789	H	-6.44338	3.24298	-2.99942
C	6.69446	-0.43825	-2.17372	H	-5.87526	4.95457	-2.86371
H	7.29103	0.14849	-2.90434	C	-5.03579	5.96165	1.90484
H	7.06834	-0.23542	-1.14819	H	-4.94848	5.81666	3.00380
H	6.82730	-1.51877	-2.39226	C	-6.37197	6.63826	1.61107
C	4.14379	3.86653	0.82736	H	-6.43963	7.58933	2.18005
H	3.81326	3.08724	1.54461	H	-6.46464	6.86812	0.52843
C	5.30295	4.64125	1.44917	H	-7.21160	5.97891	1.91891
H	4.99463	5.03594	2.44011	H	-0.37165	-1.42451	-6.19772
H	6.18176	3.97894	1.59097	H	4.49965	-1.27759	-5.80986
H	5.59227	5.49802	0.80494	H	4.86022	-0.31568	-3.30414
C	-4.43879	-0.13784	5.81668	H	3.27986	4.54997	0.69794
H	-4.25105	0.64908	6.57932	H	4.90220	5.65197	-3.74465
C	-5.00262	-1.36857	6.52123	H	-4.20285	6.62773	1.59166
H	-5.27496	-2.15146	5.78191	H	-3.51955	4.15788	-2.57514
H	-4.25477	-1.78002	7.23248	H	-4.46601	1.11618	3.04088
H	-5.91504	-1.08679	7.08778	H	-5.19811	0.26170	5.11306
C	0.56469	0.06868	5.54270	H	0.39276	0.97449	6.16442
H	1.30655	0.37017	4.77881	H	-2.89983	-2.04422	1.32252
C	1.15515	-1.01569	6.44018	H	2.76914	-2.54831	-0.49634
H	0.41885	-1.31648	7.21572	O	-1.15434	1.81031	-1.52770
H	1.44648	-1.90607	5.84818	H	-1.02360	2.80939	-0.64089
H	2.06310	-0.62399	6.94521	C	-1.27045	3.74281	0.23579
C	-2.17155	-2.51186	2.01747	C	-0.28137	4.71889	0.06890
H	-1.21529	-2.58822	1.45932	C	-1.16460	3.27118	1.68652
C	-2.65501	-3.91797	2.37018	H	-2.22591	4.02738	-0.18253
H	-2.51227	-4.58990	1.50090	C	-0.13853	5.69004	-1.05181
H	-2.08430	-4.33618	3.22330	O	0.54457	4.83383	1.06223
H	-3.73349	-3.90052	2.63396	H	-2.03951	3.57025	2.26929
C	4.43478	-2.26767	-5.30894	H	-1.05735	2.18635	1.76187
H	5.30821	-2.35411	-4.62647	C	1.25212	5.72761	-1.69898
C	4.53477	-3.37773	-6.35188	H	-0.37446	6.66966	-0.61634
H	5.51203	-3.30863	-6.87445	H	-0.90073	5.45803	-1.80182
H	4.46299	-4.37212	-5.86155	C	0.10704	3.98560	2.18229
H	3.72562	-3.28178	-7.10634	C	1.43014	4.52889	-2.62369
C	-0.57301	-2.03280	-5.28886	H	1.35672	6.65396	-2.27373
H	-1.32848	-1.46517	-4.71281	H	2.02029	5.74329	-0.91938
C	-1.15946	-3.36892	-5.73625	H	0.92929	3.30701	2.38991
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H	-1.47476	-3.97588	-4.86421	H	2.43756	4.52432	-3.05393
H	-2.05115	-3.18700	-6.37242	H	0.73120	4.62112	-3.46386
C	2.03426	-3.21039	-0.99880	H	1.59854	3.11831	-1.19161
H	1.06993	-3.06243	-0.46990	O	1.09724	3.32000	-2.00096
C	2.48079	-4.66102	-0.82516				
H	3.55529	-4.76807	-1.08402				
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R-gau-hc(-)



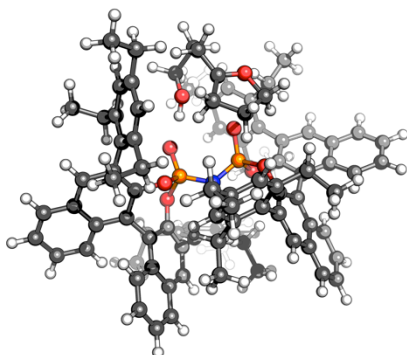
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C	-6.18409	-1.89222	0.79796
C	-4.50721	-1.48831	-0.91103
C	-5.74161	-2.01643	-0.52178
H	-6.33345	-2.56990	-1.24237
H	-1.31218	1.82782	5.16802
C	-3.63446	3.04005	4.71962
C	-4.87877	3.57747	4.38661
H	-3.07079	3.48188	5.53275
H	-5.26774	4.42250	4.93975
C	-5.61664	3.03585	3.33406
C	-5.12241	1.94429	2.61679
H	-6.57441	3.46538	3.07030
H	-5.71347	1.56299	1.79453
C	-7.39235	-2.49124	1.18864
C	-7.81035	-2.43039	2.51793
H	-8.00633	-3.01904	0.46833
H	-8.73999	-2.89889	2.81426
C	-7.02149	-1.78642	3.46982
C	-5.82007	-1.18084	3.09557
H	-7.33886	-1.76114	4.50437
H	-5.22613	-0.71987	3.87235
C	3.60425	0.74217	-0.67614
C	1.26987	2.77332	-0.99733
C	3.66982	2.14058	-0.84657
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C	0.29875	3.78887	-0.92786
C	2.52581	2.97615	-0.39431
C	4.81743	2.72325	-1.44791
C	5.92432	0.55754	-1.38359
C	0.50516	4.89458	-0.09315
C	2.69996	4.04305	0.52238
C	5.95655	1.91881	-1.69034
C	4.85740	4.08320	-1.82971

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C	1.67636	5.01078	0.66023
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C	3.87022	4.17408	1.29956
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C	6.01378	4.63158	-2.38849
H	3.99593	4.72769	-1.71850
C	1.85345	6.10221	1.52543
C	4.02642	5.25646	2.16815
H	4.66085	3.43640	1.25195
C	7.14253	3.83771	-2.58695
H	7.99653	1.88031	-2.42277
H	6.03271	5.67585	-2.67270
C	3.02458	6.22137	2.27564
H	1.08309	6.85730	1.62782
H	4.92766	5.34686	2.76056
H	8.03651	4.26812	-3.01945
H	3.15264	7.06000	2.94767
C	-0.91865	3.75340	-1.77417
C	-0.82994	4.04573	-3.16281
C	-2.19325	3.54714	-1.18498
C	-2.00510	4.13475	-3.92505
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C	-3.26212	3.96504	-3.33702
H	-4.32049	3.50853	-1.52250
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C	4.81911	-2.02669	0.64140
C	4.80771	-2.39879	-1.78362
C	4.91286	-3.41394	0.83466
C	4.90483	-3.77944	-1.55168
C	4.96374	-4.29171	-0.25174
H	4.92963	-4.46360	-2.39192
C	-3.97641	-1.81542	-2.25358
C	-3.97267	-0.84165	-3.28322
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C	-3.45057	-1.17086	-4.54381
C	-2.97446	-3.41692	-3.79174
C	-2.95557	-2.45306	-4.80545
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C	0.04628	-1.43910	4.69249
C	1.18450	0.51558	3.74409
C	1.28598	-1.91813	5.14256
C	2.40453	0.01462	4.22377
C	2.46034	-1.18729	4.93697
H	3.31632	0.57298	4.04673
H	4.96961	-3.81215	1.84103
H	1.33582	-2.85679	5.68183
H	-3.44981	-0.42902	-5.33385
H	-1.94477	4.36822	-4.98169
C	5.08770	-5.77741	-0.02607
H	4.90360	-6.02971	1.04103
C	6.47809	-6.27554	-0.40940
H	7.25243	-5.74974	0.18923
H	6.55103	-7.36490	-0.20729
H	6.67050	-6.10355	-1.48970
C	4.83147	-1.13572	1.86446

H	4.12122	-0.29337	1.75845	H	-5.47581	-4.86468	-1.76000
C	6.23020	-0.59962	2.14943	H	-4.24097	-5.79162	-2.70484
H	6.94180	-1.44052	2.29266	C	-2.40030	-2.79490	-6.16484
H	6.58383	0.04085	1.31609	H	-2.28433	-1.87885	-6.78426
H	6.20982	0.01078	3.07678	C	-3.31518	-3.76628	-6.90562
C	4.74408	-1.92334	-3.22313	H	-2.89833	-3.97315	-7.91374
H	4.41705	-0.86628	-3.30102	H	-3.39512	-4.72686	-6.35393
C	6.09287	-2.07819	-3.92226	H	-4.32819	-3.32533	-7.02294
H	6.01728	-1.69540	-4.96176	H	-0.91536	-3.31779	5.18594
H	6.87852	-1.50348	-3.39113	H	3.93549	-2.73922	5.14458
H	6.39104	-3.14715	-3.96267	H	4.49252	-1.71124	2.74942
C	-4.51221	4.11391	-4.16714	H	3.99127	-2.52124	-3.77678
H	-4.43068	3.48369	-5.07898	H	4.32407	-6.31451	-0.62740
C	-4.73680	5.56901	-4.56888	H	-1.39148	-3.24658	-6.05150
H	-4.81755	6.20854	-3.66392	H	-2.41185	-4.64849	-1.43443
H	-3.90087	5.93413	-5.20230	H	-4.12511	1.24322	-3.82791
H	-5.68012	5.65248	-5.14859	H	-5.40332	3.76682	-3.60113
C	0.48891	4.33152	-3.85559	H	0.39300	4.15631	-4.94952
H	1.28508	3.64334	-3.51074	H	-3.04965	2.34084	0.36875
C	0.92738	5.77752	-3.64265	H	2.00398	1.76303	2.19688
H	0.14336	6.47462	-4.00801	O	-1.03338	-2.29903	-0.38080
H	1.12291	5.97790	-2.57019	P	-1.19991	-0.89765	0.18968
H	1.86369	5.96753	-4.20840	H	0.24838	-2.75931	-0.33565
C	-2.36621	3.20948	0.27997	O	-2.54350	-0.20390	-0.39467
H	-1.41110	2.90610	0.75503	O	-1.48293	-1.19549	1.78093
C	-2.95375	4.38858	1.05222	N	-0.02856	0.13886	0.04665
H	-2.92534	4.17366	2.13854	C	1.41423	-3.14624	0.05112
H	-2.36952	5.31275	0.86806	P	1.11698	0.21711	-1.07504
H	-4.00891	4.56114	0.75240	C	1.17146	-4.51867	-0.08855
C	3.77189	-1.69339	5.48357	C	1.32964	-2.87633	1.55354
H	4.61947	-1.08196	5.10453	H	2.12284	-2.65735	-0.60645
C	3.79340	-1.63861	7.00883	O	1.16105	-0.79589	-2.16418
H	4.78365	-1.97898	7.37822	O	2.47454	0.16565	-0.14714
H	3.62242	-0.59761	7.35752	O	1.05811	1.67938	-1.80040
H	3.01200	-2.30152	7.43670	C	1.45269	-5.41628	-1.23933
C	-1.19093	-2.25460	5.01191	O	0.59472	-5.04782	0.96013
H	-1.89943	-2.26324	4.16026	H	0.92592	-1.88987	1.78424
C	-1.89077	-1.73120	6.26238	H	2.30694	-2.97160	2.03549
H	-1.19435	-1.74843	7.12775	H	1.58338	-2.36279	-2.89519
H	-2.25390	-0.69525	6.10712	C	0.47869	-5.30084	-2.43147
H	-2.76375	-2.37633	6.49575	H	2.43554	-5.13700	-1.62047
C	1.20488	1.81354	2.96601	H	1.47167	-6.44409	-0.86918
H	0.25660	1.98717	2.41805	C	0.37920	-3.99610	1.96930
C	1.46468	3.00007	3.89018	O	1.66034	-3.32260	-3.05702
H	2.49958	2.96084	4.29084	H	-0.50760	-5.69012	-2.16634
H	1.33871	3.94527	3.32723	H	0.88550	-5.95809	-3.20704
H	0.74625	3.00302	4.73563	H	0.57408	-4.45315	2.93823
C	-4.55206	0.54048	-3.08211	H	-0.66773	-3.69427	1.88230
H	-4.28436	0.94106	-2.08408	C	0.36742	-3.87811	-2.97403
C	-6.06881	0.52947	-3.24345	H	-0.09859	-3.92101	-3.96778
H	-6.54040	-0.13274	-2.48908	H	-0.27600	-3.26360	-2.33416
H	-6.46543	1.55640	-3.10330				
H	-6.34329	0.17759	-4.26072				
C	-3.42489	-4.20115	-1.45601				
H	-3.59795	-3.80529	-0.43498				
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H	-4.40817	-6.05860	-0.93053				

R-gau-hc(-)-intermediate



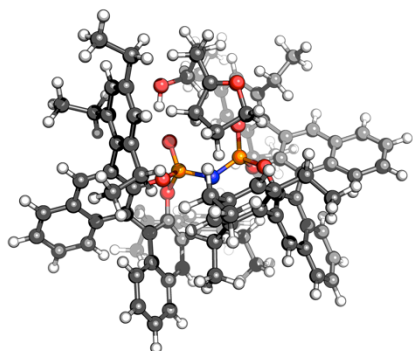
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C	-1.88782	1.37199	4.33556
C	-3.89573	1.32210	2.95422
C	-3.14275	1.89556	4.00910
C	-4.20243	-0.59960	1.31214
C	-5.40400	-1.23931	1.72103
C	-3.73167	-0.78564	-0.00304
C	-6.18614	-1.92835	0.75919
C	-4.50061	-1.50224	-0.93660
C	-5.73648	-2.03683	-0.55985
H	-6.32136	-2.58710	-1.28849
H	-1.33664	1.77345	5.17782
C	-3.66476	2.97607	4.73791
C	-4.91315	3.50751	4.41077
H	-3.10365	3.41466	5.55457
H	-5.30753	4.34499	4.97151
C	-5.64802	2.96988	3.35420
C	-5.14653	1.88832	2.62694
H	-6.60889	3.39508	3.09474
H	-5.73563	1.51096	1.80154
C	-7.39289	-2.53784	1.13812
C	-7.81600	-2.49510	2.46657
H	-8.00136	-3.06033	0.40931
H	-8.74429	-2.97183	2.75381
C	-7.03392	-1.85858	3.42912
C	-5.83423	-1.24248	3.06667
H	-7.35530	-1.84721	4.46268
H	-5.24536	-0.78730	3.85076
C	3.60285	0.76318	-0.66333
C	1.21065	2.74438	-0.95339
C	3.62312	2.16466	-0.82251
C	4.78533	0.02449	-0.88837
C	0.22976	3.75148	-0.88618
C	2.46256	2.96303	-0.34929
C	4.74837	2.79073	-1.42295
C	5.93371	0.66904	-1.36243
C	0.42085	4.85583	-0.04541
C	2.62250	4.02778	0.57242
C	5.91598	2.03020	-1.66692

C	4.73877	4.15278	-1.79998
H	6.84142	0.09634	-1.51340
C	1.58757	4.98221	0.71261
H	-0.33274	5.63268	-0.00466
C	3.79233	4.17227	1.34794
C	7.05433	2.64104	-2.21713
C	5.87477	4.74540	-2.35538
H	3.85385	4.76464	-1.68802
C	1.75165	6.07421	1.57972
C	3.93599	5.25486	2.21844
H	4.59224	3.44478	1.29711
C	7.03219	3.99431	-2.55502
H	7.95723	2.06906	-2.39606
H	5.85552	5.79065	-2.63594
C	2.92204	6.20676	2.32900
H	0.97238	6.81991	1.68337
H	4.83685	5.35562	2.80975
H	7.91036	4.45880	-2.98462
H	3.04033	7.04580	3.00230
C	-0.97626	3.71830	-1.74856
C	-0.87001	4.01953	-3.13435
C	-2.25902	3.51916	-1.17481
C	-2.03602	4.12101	-3.90907
C	-3.40318	3.64407	-1.97732
C	-3.30068	3.95813	-3.33582
H	-4.38260	3.50063	-1.53575
C	4.85726	-1.43870	-0.66308
C	4.96602	-1.95537	0.65483
C	4.94148	-2.32646	-1.77105
C	5.13694	-3.33642	0.84538
C	5.10176	-3.70217	-1.54235
C	5.20327	-4.21199	-0.24362
H	5.13662	-4.38443	-2.38373
C	-3.95508	-1.82433	-2.27486
C	-3.93381	-0.84408	-3.29794
C	-3.45153	-3.12544	-2.53855
C	-3.38959	-1.16458	-4.55130
C	-2.92255	-3.41470	-3.80533
C	-2.88745	-2.44405	-4.81227
H	-2.52366	-4.40223	-4.00598
C	-0.02988	-0.24616	3.99735
C	0.02941	-1.48753	4.68597
C	1.16782	0.47271	3.75038
C	1.26931	-1.97047	5.13142
C	2.38803	-0.03169	4.22593
C	2.44397	-1.23858	4.93048
H	3.29950	0.52870	4.05381
H	5.22158	-3.73205	1.85078
H	1.31873	-2.91247	5.66482
H	-3.37748	-0.41818	-5.33694
H	-1.96242	4.36022	-4.96357
C	5.35496	-5.69532	-0.02277
H	5.21616	-5.94972	1.05067
C	6.73455	-6.17895	-0.46032
H	7.52614	-5.64238	0.10526
H	6.82792	-7.26668	-0.25791
H	6.88201	-6.00909	-1.54792

C	4.92428	-1.06755	1.87885	H	-4.44734	-6.08247	-1.01886
H	4.17820	-0.25743	1.76546	H	-5.48223	-4.87442	-1.86925
C	6.29399	-0.46914	2.17900	H	-4.22123	-5.79666	-2.78364
H	7.04101	-1.27700	2.33161	C	-2.31401	-2.77752	-6.16625
H	6.62730	0.18527	1.34782	H	-2.18493	-1.85702	-6.77642
H	6.23553	0.14085	3.10501	C	-3.22310	-3.73832	-6.92766
C	4.84123	-1.85337	-3.20918	H	-2.79270	-3.93995	-7.93113
H	4.46130	-0.81375	-3.28248	H	-3.31625	-4.70246	-6.38429
C	6.19003	-1.94000	-3.91976	H	-4.23194	-3.29100	-7.05642
H	6.08555	-1.56503	-4.95960	H	-0.93559	-3.36642	5.17218
H	6.94905	-1.32316	-3.39720	H	3.92442	-2.78751	5.12104
H	6.54313	-2.99215	-3.95966	H	4.59927	-1.65996	2.75810
C	-4.54042	4.11914	-4.17904	H	4.11476	-2.48818	-3.75733
H	-4.45327	3.49183	-5.09237	H	4.57137	-6.23775	-0.59439
C	-4.75045	5.57741	-4.57710	H	-1.30928	-3.23523	-6.04312
H	-4.83676	6.21374	-3.67041	H	-2.42985	-4.67578	-1.44193
H	-3.90504	5.93931	-5.19972	H	-4.09008	1.24176	-3.83836
H	-5.68669	5.66988	-5.16683	H	-5.44019	3.77614	-3.62438
C	0.45768	4.30530	-3.81059	H	0.37259	4.13976	-4.90691
H	1.24729	3.61081	-3.46396	H	-3.13925	2.30843	0.36118
C	0.90065	5.74750	-3.58133	H	1.99084	1.73808	2.22134
H	0.12297	6.45129	-3.94740	O	-1.10989	-2.39176	-0.36517
H	1.08809	5.93788	-2.50568	P	-1.22200	-1.00022	0.17254
H	1.84273	5.93810	-4.13722	H	1.04928	-2.50682	-0.64768
C	-2.45117	3.17470	0.28616	O	-2.54037	-0.22006	-0.38332
H	-1.50313	2.86468	0.77166	O	-1.49323	-1.24472	1.79065
C	-3.04485	4.35162	1.05749	N	-0.02077	0.02934	0.04532
H	-3.02160	4.13512	2.14357	C	1.62346	-3.15407	0.03113
H	-2.46236	5.27769	0.87833	P	1.11551	0.18191	-1.06253
H	-4.09877	4.52254	0.75247	C	1.07289	-4.50203	-0.15561
C	3.75548	-1.74747	5.47476	C	1.34860	-2.85426	1.50930
H	4.60206	-1.12686	5.10884	H	2.64767	-3.09637	-0.31512
C	3.77179	-1.71450	7.00082	O	1.21220	-0.80008	-2.18341
H	4.76288	-2.05432	7.36846	O	2.48970	0.14456	-0.14258
H	3.59352	-0.67969	7.36393	O	1.01969	1.65517	-1.76787
H	2.99326	-2.38818	7.41684	C	1.34179	-5.43919	-1.26891
C	-1.20871	-2.30127	5.00665	O	0.33500	-4.88221	0.80500
H	-1.92258	-2.30197	4.15954	H	1.04214	-1.81771	1.65682
C	-1.89974	-1.78357	6.26431	H	2.23658	-3.04881	2.11680
H	-1.19910	-1.81026	7.12602	H	1.76046	-2.33120	-2.83442
H	-2.25851	-0.74474	6.11812	C	0.46498	-5.21277	-2.52795
H	-2.77465	-2.42617	6.49748	H	2.37840	-5.26673	-1.56898
C	1.18746	1.77849	2.98638	H	1.21140	-6.45936	-0.90023
H	0.24149	1.95503	2.43482	C	0.22421	-3.83102	1.84994
C	1.43938	2.95482	3.92584	O	1.79439	-3.29998	-2.97040
H	2.47506	2.91780	4.32471	H	-0.55127	-5.56818	-2.34900
H	1.30526	3.90642	3.37620	H	0.90352	-5.84713	-3.30468
H	0.72244	2.94158	4.77238	H	0.33160	-4.36091	2.79569
C	-4.52104	0.53482	-3.09883	H	-0.77127	-3.40787	1.73178
H	-4.26488	0.93231	-2.09665	C	0.45994	-3.75843	-2.98015
C	-6.03613	0.51816	-3.27543	H	0.03370	-3.70389	-3.99033
H	-6.51289	-0.14874	-2.52856	H	-0.16929	-3.14957	-2.31683
H	-6.43843	1.54282	-3.13525				
H	-6.29886	0.16917	-4.29679				
C	-3.43953	-4.22375	-1.49119				
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C	-4.46206	-5.30910	-1.81543				

R-gau-hc(-)-2nd step



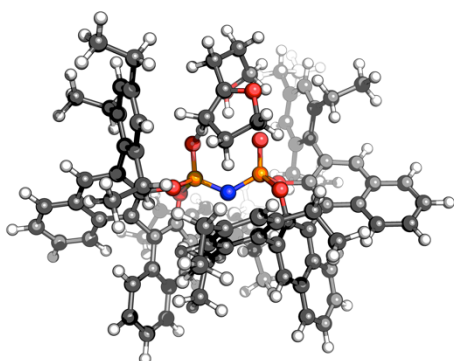
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C	-1.94211	1.11561	4.40559
C	-3.92257	1.16550	2.98299
C	-3.19079	1.66202	4.09115
C	-4.19127	-0.62600	1.18987
C	-5.41106	-1.28457	1.50112
C	-3.67816	-0.70626	-0.11945
C	-6.16275	-1.88479	0.45783
C	-4.42012	-1.32600	-1.13866
C	-5.66967	-1.88337	-0.85112
H	-6.23417	-2.35972	-1.64466
H	-1.40317	1.46330	5.27931
C	-3.72330	2.69584	4.87779
C	-4.95786	3.26080	4.55466
H	-3.17900	3.07517	5.73451
H	-5.35938	4.06364	5.15929
C	-5.66899	2.80259	3.44575
C	-5.15884	1.76554	2.66194
H	-6.61872	3.25447	3.19034
H	-5.72966	1.44986	1.79872
C	-7.38579	-2.51243	0.74295
C	-7.85616	-2.57400	2.05480
H	-7.97116	-2.96770	-0.04727
H	-8.79707	-3.06418	2.26909
C	-7.10627	-2.02354	3.09324
C	-5.89053	-1.39074	2.82533
H	-7.46549	-2.09216	4.11201
H	-5.32835	-1.00304	3.66357
C	3.63364	0.75096	-0.53758
C	1.37526	2.85781	-0.72381
C	3.75750	2.15211	-0.60773
C	4.72931	-0.06669	-0.86292
C	0.42512	3.88550	-0.58127
C	2.63639	2.99286	-0.10953
C	4.92558	2.72612	-1.17749
C	5.91756	0.50645	-1.32732
C	0.65187	4.92183	0.33331
C	2.83041	3.98583	0.88258
C	6.01750	1.88753	-1.51225

C	5.02946	4.10932	-1.44595
H	6.75705	-0.13461	-1.57261
C	1.82471	4.95955	1.09253
H	-0.08175	5.71229	0.43662
C	4.00006	4.03395	1.66987
C	7.19349	2.44013	-2.04418
C	6.20293	4.64367	-1.98233
H	4.20528	4.78507	-1.26282
C	2.01952	5.97741	2.03967
C	4.17306	5.04217	2.62062
H	4.77707	3.28761	1.56661
C	7.28479	3.81338	-2.27221
H	8.03767	1.80829	-2.29421
H	6.27132	5.70593	-2.17873
C	3.18925	6.01479	2.80038
H	1.26305	6.73668	2.19888
H	5.07357	5.06908	3.22042
H	8.19178	4.23323	-2.68766
H	3.33049	6.79598	3.53600
C	-0.78812	3.94196	-1.43271
C	-0.68582	4.35000	-2.79081
C	-2.07019	3.71567	-0.86749
C	-1.85488	4.53853	-3.54417
C	-3.21744	3.92708	-1.64720
C	-3.11848	4.35364	-2.97510
H	-4.19616	3.76200	-1.21170
C	4.63855	-1.54152	-0.78531
C	4.80037	-2.20193	0.45798
C	4.51027	-2.30556	-1.97429
C	4.88197	-3.60150	0.49034
C	4.58179	-3.70562	-1.90455
C	4.79224	-4.35658	-0.68360
H	4.48516	-4.29040	-2.81170
C	-3.82890	-1.50980	-2.48468
C	-3.72705	-0.41554	-3.38018
C	-3.31128	-2.77601	-2.86421
C	-3.06918	-0.58690	-4.60805
C	-2.66913	-2.91521	-4.10390
C	-2.53613	-1.82776	-4.97314
H	-2.26254	-3.87870	-4.38840
C	-0.06976	-0.46706	3.98286
C	-0.01146	-1.73981	4.61076
C	1.12959	0.25971	3.76615
C	1.22973	-2.25242	5.01807
C	2.35298	-0.28067	4.19198
C	2.40850	-1.52293	4.83232
H	3.26703	0.28008	4.03434
H	5.02365	-4.10863	1.43776
H	1.27805	-3.21987	5.50404
H	-2.97534	0.24974	-5.29057
H	-1.78355	4.86085	-4.57648
C	4.90635	-5.85923	-0.62565
H	4.19276	-6.25620	0.12845
C	6.32512	-6.29170	-0.26589
H	6.60288	-5.92392	0.74451
H	6.38611	-7.40037	-0.26547
H	7.04736	-5.89583	-1.01160

C	4.93613	-1.44925	1.76238	H	-4.47246	-5.86640	-1.80149
H	4.35366	-0.50664	1.75281	H	-5.42533	-4.52683	-2.54430
C	6.39725	-1.14025	2.06832	H	-4.13196	-5.36037	-3.49749
H	6.98354	-2.08126	2.13815	C	-1.81932	-1.98619	-6.28971
H	6.83187	-0.49584	1.27571	H	-1.05396	-1.18680	-6.39311
H	6.46727	-0.60476	3.03850	C	-2.79574	-1.91574	-7.46057
C	4.29355	-1.66343	-3.33147	H	-2.24483	-2.06547	-8.41289
H	4.01701	-0.59240	-3.24816	H	-3.56583	-2.71102	-7.36604
C	5.53857	-1.77921	-4.20697	H	-3.29523	-0.92438	-7.49497
H	5.35427	-1.27954	-5.18122	H	-0.98379	-3.64012	4.98456
H	6.40479	-1.28882	-3.71627	H	3.86854	-3.10004	4.93088
H	5.78382	-2.84499	-4.39939	H	4.51653	-2.06143	2.58704
C	-4.36078	4.60649	-3.79165	H	3.44329	-2.15788	-3.84336
H	-4.29282	4.05360	-4.75341	H	4.64140	-6.31268	-1.60562
C	-4.54406	6.09598	-4.06911	H	-1.28677	-2.96141	-6.33287
H	-4.61117	6.65860	-3.11338	H	-2.40375	-4.48253	-1.92248
H	-3.69590	6.49036	-4.66777	H	-3.88177	1.71369	-3.71891
H	-5.48232	6.25406	-4.64144	H	-5.26327	4.23728	-3.25848
C	0.64340	4.65405	-3.45503	H	0.54922	4.56262	-4.55928
H	1.42065	3.92266	-3.15919	H	-2.95712	2.38578	0.56456
C	1.11544	6.06887	-3.13286	H	1.94532	1.62615	2.32075
H	0.35152	6.81049	-3.44996	O	-0.97520	-2.24268	-0.54598
H	1.30744	6.18412	-2.04728	P	-1.16030	-0.91750	0.11520
H	2.06041	6.27683	-3.67751	H	1.55982	-3.08028	0.13011
C	-2.25773	3.24653	0.55870	O	-2.47973	-0.11087	-0.41578
H	-1.31062	2.88331	1.00466	O	-1.50552	-1.32059	1.69213
C	-2.82484	4.35942	1.43680	N	-0.01296	0.17409	0.11581
H	-2.81513	4.03844	2.49696	C	1.31411	-4.04282	0.58774
H	-2.21415	5.28087	1.34931	P	1.14630	0.31329	-0.96651
H	-3.87167	4.58821	1.14562	C	0.62456	-4.86149	-0.44821
C	3.72388	-2.07134	5.32620	C	0.27902	-3.93182	1.71996
H	4.57128	-1.45036	4.96246	H	2.24571	-4.53480	0.87994
C	3.77471	-2.09626	6.85153	O	1.21602	-0.60232	-2.14809
H	4.76721	-2.46728	7.18348	O	2.49188	0.18873	-0.02690
H	3.62383	-1.07287	7.25698	O	1.14025	1.82615	-1.60030
H	2.99284	-2.77113	7.25942	C	1.20642	-5.64436	-1.57540
C	-1.25135	-2.56470	4.89225	O	-0.58990	-5.09414	-0.16609
H	-1.97439	-2.50476	4.05441	H	0.13092	-2.89568	2.01789
C	-1.92389	-2.12370	6.18846	H	0.58208	-4.51855	2.59009
H	-1.21544	-2.21590	7.03922	H	1.05354	-2.21471	-2.19175
H	-2.27013	-1.07286	6.11489	C	0.55812	-5.31608	-2.93138
H	-2.80460	-2.76978	6.38760	H	2.27648	-5.44963	-1.61876
C	1.14778	1.61417	3.09224	H	1.04147	-6.69827	-1.31958
H	0.19833	1.82862	2.56324	C	-1.01194	-4.48013	1.10806
C	1.40731	2.72436	4.10668	O	1.16638	-3.20535	-2.12825
H	2.43968	2.64919	4.50881	H	-0.52750	-5.38426	-2.84115
H	1.28887	3.71105	3.61784	H	0.87661	-6.05874	-3.66822
H	0.68333	2.66442	4.94551	H	-1.47609	-5.29690	1.66183
C	-4.33279	0.93507	-3.06909	H	-1.72340	-3.70430	0.83926
H	-4.11814	1.23370	-2.02378	C	1.00557	-3.90420	-3.32872
C	-5.83971	0.93182	-3.30655	H	1.95760	-3.97273	-3.87604
H	-6.34300	0.20044	-2.64224	H	0.26865	-3.42873	-3.98501
H	-6.25214	1.93946	-3.09158				
H	-6.05995	0.67570	-4.36478				
C	-3.39508	-3.99464	-1.96660				
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C	-4.42079	-4.99600	-2.48892				

R-gau-hc(+)



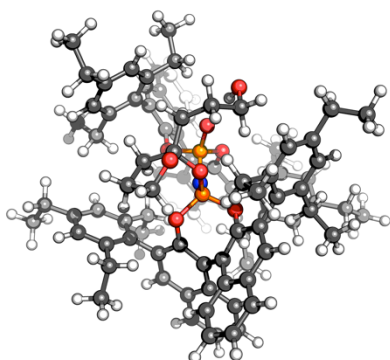
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C	1.31620	2.69520	-0.91820
C	0.35946	3.71196	-0.73372
C	2.58929	2.84240	-0.33992
C	0.60922	4.74439	0.18276
C	2.81242	3.83297	0.64834
C	1.80294	4.78760	0.90662
C	3.70476	2.05988	-0.91938
C	4.81280	2.71508	-1.52346
C	3.65152	0.64847	-0.87650
C	5.95187	1.96004	-1.88086
C	4.80167	-0.08657	-1.25388
C	5.94694	0.57839	-1.70748
H	6.82887	0.00282	-1.96718
H	-0.12059	5.53377	0.30981
C	2.02296	5.80636	1.84736
C	3.23400	5.87587	2.53828
H	1.26028	6.55022	2.04516
H	3.39793	6.66214	3.26371
C	4.23200	4.93094	2.29870
C	4.02578	3.91256	1.36535
H	5.16562	4.98237	2.84373
H	4.81214	3.18308	1.22059
C	7.08076	2.59536	-2.42328
C	7.07400	3.97249	-2.64437
H	7.96350	2.02486	-2.68737
H	7.94464	4.45676	-3.06740
C	5.93967	4.72267	-2.33884
C	4.81454	4.10391	-1.78997
H	5.92999	5.78786	-2.53089
H	3.94707	4.71941	-1.59432
N	-0.02067	0.11023	0.05158
P	-1.19948	-0.97554	0.17549
O	-1.14063	-2.21728	-0.64551
O	-2.59749	-0.17520	-0.10263
O	-1.20877	-1.43517	1.75766
C	-3.72046	-0.67749	0.51907
C	-1.50136	-0.43686	2.65799
C	-3.86361	-0.54123	1.91645

C	-4.79346	-1.20097	-0.23775
C	-0.57334	-0.08818	3.65562
C	-2.78774	0.13468	2.68171
C	-5.00413	-1.07911	2.57043
C	-5.97768	-1.58582	0.40340
C	-0.86513	0.96023	4.53998
C	-3.05360	1.24644	3.51889
C	-6.08015	-1.56591	1.79378
C	-5.09790	-1.15857	3.97864
H	-6.81140	-1.94255	-0.19002
C	-2.07384	1.65626	4.45266
H	-0.15490	1.21712	5.31569
C	-4.27700	1.94838	3.46237
C	-7.23972	-2.05200	2.41923
C	-6.25219	-1.65451	4.58821
H	-4.28000	-0.85677	4.61867
C	-2.33480	2.72959	5.31928
C	-4.52384	3.01378	4.33089
H	-5.04045	1.68965	2.74029
C	-7.32455	-2.08986	3.81115
H	-8.07371	-2.41731	1.83156
H	-6.31313	-1.70491	5.66775
C	-3.55619	3.40266	5.25739
H	-1.59536	3.04616	6.04529
H	-5.46519	3.54528	4.27869
H	-8.21741	-2.47256	4.28846
H	-3.75140	4.23076	5.92630
C	0.69281	-0.83850	3.84178
C	0.67294	-2.14694	4.40015
C	1.93877	-0.19423	3.61900
C	1.88415	-2.76694	4.74635
C	3.12577	-0.83433	4.00463
C	3.10580	-2.10711	4.58362
H	4.07513	-0.33182	3.86260
C	-4.70409	-1.43199	-1.69998
C	-4.84121	-0.34984	-2.60569
C	-4.67491	-2.76284	-2.20378
C	-4.91932	-0.60346	-3.98355
C	-4.77988	-2.97960	-3.58645
C	-4.90416	-1.91054	-4.47787
H	-4.77117	-3.99324	-3.96979
C	4.85028	-1.56529	-1.24876
C	5.06251	-2.27130	-0.03856
C	4.88105	-2.27105	-2.48384
C	5.29426	-3.65530	-0.07452
C	5.12318	-3.65409	-2.48345
C	5.33674	-4.34816	-1.28832
H	5.12655	-4.19882	-3.42036
C	-0.88597	3.77286	-1.53444
C	-0.83282	4.13184	-2.91032
C	-2.14757	3.64366	-0.89432
C	-2.02920	4.34522	-3.61246
C	-3.31893	3.90661	-1.61936
C	-3.26843	4.25867	-2.97165
H	-4.27955	3.83326	-1.12369
H	-5.03199	0.22210	-4.67699
H	-1.99703	4.61927	-4.66052

H	5.45981	-4.19240	0.85235	H	4.53976	-0.62165	1.29511
H	1.87151	-3.75182	5.19826	C	6.50847	-1.34047	1.77959
C	-5.04574	-2.16172	-5.95731	H	7.04145	-0.68417	1.05887
H	-4.32629	-1.52306	-6.51373	H	6.49026	-0.83966	2.77052
C	-6.46738	-1.86496	-6.42898	H	7.05694	-2.30121	1.87810
H	-6.71812	-0.79490	-6.26835	C	4.58223	-1.60225	-3.81127
H	-6.55427	-2.08813	-7.51313	H	4.16826	-0.58122	-3.68000
H	-7.19503	-2.49750	-5.87649	C	5.82930	-1.51740	-4.68863
C	-5.00009	1.07697	-2.13896	H	5.57690	-1.00918	-5.64290
H	-4.37701	1.27911	-1.24759	H	6.62513	-0.93555	-4.17975
C	-6.45800	1.39811	-1.82684	H	6.21433	-2.53234	-4.92226
H	-7.08718	1.24499	-2.72941	C	5.59908	-5.83185	-1.31191
H	-6.83379	0.75426	-1.00528	H	5.52631	-6.26058	-0.28856
H	-6.54426	2.45842	-1.50932	C	6.98978	-6.13256	-1.86452
C	-4.53735	-3.97860	-1.30350	H	7.16866	-7.22820	-1.84561
H	-4.23229	-3.70248	-0.27321	H	7.07904	-5.77825	-2.91340
C	-5.83437	-4.78400	-1.23932	H	7.76509	-5.63511	-1.24303
H	-5.70139	-5.64517	-0.55121	H	0.30942	4.30659	-4.74668
H	-6.66941	-4.16025	-0.86265	H	-4.54957	3.92559	-4.66721
H	-6.10161	-5.17643	-2.24304	H	-4.64838	1.76670	-2.93300
C	4.38750	-2.74898	5.05540	H	-3.73771	-4.64023	-1.69585
H	4.22012	-3.81700	5.31499	H	-4.80765	-3.22014	-6.20101
C	4.93741	-2.03360	6.28637	H	4.83060	-6.33534	-1.93753
H	5.19103	-0.97950	6.04502	H	3.80048	-2.18643	-4.34373
H	4.18897	-2.05183	7.10737	H	4.55087	-2.22978	2.03833
H	5.85888	-2.54658	6.63362	H	5.14667	-2.72325	4.24661
C	-0.61471	-2.88498	4.71716	H	-0.41719	-3.97473	4.81710
H	-1.34818	-2.79155	3.89379	H	2.77431	1.14546	2.15539
C	-1.23482	-2.39691	6.02383	H	-3.00636	2.39103	0.63307
H	-0.50433	-2.49152	6.85537	O	1.05659	-0.86764	-2.16976
H	-1.55850	-1.34039	5.94026	H	1.21801	-2.03211	-1.64091
H	-2.12684	-3.01340	6.26272	C	1.68108	-3.15450	-1.01144
C	2.04268	1.18046	2.98982	C	0.93382	-4.21093	-1.52134
H	1.08129	1.50866	2.54324	C	1.50250	-3.18846	0.50472
C	2.49808	2.22302	4.01004	H	2.65799	-3.04973	-1.45582
H	2.31353	3.24006	3.61125	C	0.95359	-4.72913	-2.91711
H	1.93965	2.12318	4.96247	O	0.16043	-4.80105	-0.65632
H	3.58326	2.11117	4.21728	H	2.42163	-3.51149	1.00199
C	-4.53753	4.53561	-3.73814	H	1.21976	-2.22182	0.92802
H	-5.42968	4.24723	-3.14084	C	-0.43711	-5.00010	-3.49994
C	-4.65618	6.01495	-4.09404	H	1.55171	-5.64971	-2.90613
H	-5.61407	6.19257	-4.62672	H	1.47588	-3.98997	-3.52858
H	-4.64196	6.63353	-3.17127	C	0.37667	-4.22704	0.67765
H	-3.82189	6.32687	-4.75734	C	-1.36580	-3.80484	-3.29544
C	0.47243	4.36905	-3.64847	H	-0.31226	-5.20743	-4.56775
H	1.21867	3.58601	-3.41462	H	-0.88486	-5.88715	-3.03878
C	1.05077	5.74713	-3.33745	H	-0.57006	-3.78554	0.97989
H	0.30980	6.53861	-3.57951	H	0.63978	-5.06912	1.32023
H	1.33545	5.82755	-2.26956	H	-1.67144	-3.75199	-2.24718
H	1.96125	5.91321	-3.95094	H	-2.25409	-3.94280	-3.92146
C	-2.28614	3.23249	0.55874	H	-0.69024	-2.01375	-2.89130
H	-1.33053	2.85712	0.97987	O	-0.71208	-2.60685	-3.65787
C	-2.78776	4.39126	1.41934				
H	-3.86964	4.56487	1.23940				
H	-2.63884	4.15086	2.49078				
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C	5.08015	-1.58699	1.30717				

R-gau-hc(+)-intermediate



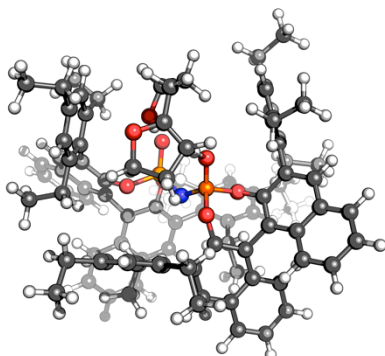
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C	1.17559	3.79783	-0.33628
C	3.24076	2.51645	-0.22189
C	1.67428	4.68692	0.62239
C	3.71299	3.36609	0.80972
C	2.91797	4.46425	1.22098
C	4.11984	1.51311	-0.88373
C	5.31942	1.87934	-1.54851
C	3.70593	0.16695	-0.88444
C	6.16235	0.86404	-2.06595
C	4.55489	-0.83223	-1.39716
C	5.78397	-0.47789	-1.96327
H	6.43644	-1.25443	-2.34610
H	1.09591	5.56392	0.88814
C	3.38787	5.33840	2.21403
C	4.62425	5.11300	2.82119
H	2.79442	6.18900	2.52776
H	4.97784	5.78503	3.59236
C	5.40058	4.01724	2.44372
C	4.95269	3.14742	1.44717
H	6.35283	3.83957	2.92648
H	5.57342	2.29840	1.19252
C	7.36967	1.20508	-2.69631
C	7.73370	2.54403	-2.84159
H	8.02610	0.43634	-3.08680
H	8.66306	2.80115	-3.33321
C	6.89396	3.55227	-2.36999
C	5.69332	3.22848	-1.73440
H	7.17189	4.59012	-2.50133
H	5.05957	4.04133	-1.40721
N	0.06363	0.18213	-0.05522
P	-1.16532	-0.75040	0.09137
O	-1.31915	-2.01745	-0.81638
O	-2.49972	0.10116	-0.23965
O	-1.26266	-1.35574	1.61275
C	-3.65518	-0.39127	0.31166
C	-1.52483	-0.38362	2.54254

C	-3.85955	-0.33356	1.70856
C	-4.72466	-0.76696	-0.52716
C	-0.62503	-0.14661	3.60173
C	-2.78943	0.23629	2.56645
C	-5.06034	-0.84578	2.26897
C	-5.95602	-1.13507	0.02744
C	-0.91027	0.84085	4.55298
C	-3.04048	1.29722	3.47214
C	-6.12217	-1.21461	1.41013
C	-5.22934	-1.01439	3.66192
H	-6.77840	-1.39437	-0.62862
C	-2.08888	1.58648	4.47807
H	-0.22041	1.00795	5.37175
C	-4.21677	2.07364	3.40424
C	-7.33553	-1.67605	1.94535
C	-6.43798	-1.48394	4.18046
H	-4.42953	-0.80389	4.35879
C	-2.34543	2.59695	5.41861
C	-4.45160	3.08732	4.33575
H	-4.95154	1.91232	2.62618
C	-7.49155	-1.80437	3.32561
H	-8.15813	-1.95048	1.29541
H	-6.55614	-1.60357	5.24974
C	-3.52284	3.34307	5.34474
H	-1.63133	2.81609	6.20355
H	-5.35709	3.67698	4.27446
H	-8.42657	-2.16702	3.73271
H	-3.71173	4.12723	6.06636
C	0.57186	-0.99351	3.81324
C	0.43605	-2.25208	4.45751
C	1.86874	-0.48165	3.54975
C	1.58452	-2.98057	4.80253
C	2.99603	-1.23188	3.91912
C	2.86277	-2.47137	4.55367
H	3.98770	-0.83646	3.73171
C	-4.56732	-0.85077	-1.99803
C	-4.52129	0.32918	-2.78550
C	-4.56266	-2.12111	-2.63749
C	-4.43613	0.22353	-4.18207
C	-4.49582	-2.18700	-4.03714
C	-4.43224	-1.02455	-4.81249
H	-4.48284	-3.15445	-4.52527
C	4.15781	-2.26058	-1.39415
C	4.25898	-3.02818	-0.20633
C	3.75943	-2.89293	-2.60180
C	3.97338	-4.40189	-0.24211
C	3.46610	-4.26497	-2.59854
C	3.57366	-5.02364	-1.42919
H	3.13619	-4.74419	-3.51305
C	-0.10452	4.11329	-1.01559
C	-0.09882	4.65226	-2.33024
C	-1.33754	3.94743	-0.33504
C	-1.31264	5.02122	-2.93001
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C	-2.52591	4.88381	-2.24835
H	-3.47248	4.21867	-0.43563
H	-4.39664	1.12113	-4.78826

H	-1.31247	5.44300	-3.92839	C	4.69896	-2.42729	1.10865
H	4.05982	-4.99029	0.66397	H	4.33937	-1.38605	1.22188
H	1.48000	-3.93182	5.31131	C	6.21636	-2.45980	1.24894
C	-4.34375	-1.11284	-6.31478	H	6.69379	-1.85717	0.44833
H	-3.49615	-0.48943	-6.67312	H	6.50596	-2.03463	2.23302
C	-5.63919	-0.64404	-6.97143	H	6.58587	-3.50577	1.19046
H	-5.83504	0.42293	-6.73349	C	3.60307	-2.13873	-3.90674
H	-5.55586	-0.74945	-8.07361	H	3.58219	-1.03997	-3.75524
H	-6.49307	-1.26108	-6.61846	C	4.72574	-2.48037	-4.88265
C	-4.63986	1.71264	-2.18207	H	4.59045	-1.90136	-5.82031
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C	-6.09821	2.07552	-1.92079	H	4.71059	-3.56253	-5.13179
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H	-6.55620	1.36867	-1.19904	H	3.17028	-6.89251	-0.40983
H	-6.15596	3.09799	-1.49268	C	4.26964	-7.29368	-2.21875
C	-4.62046	-3.42844	-1.86636	H	4.00543	-8.37167	-2.18735
H	-4.42695	-3.28796	-0.78365	H	4.30367	-6.97017	-3.28066
C	-5.96815	-4.12468	-2.04307	H	5.27370	-7.15983	-1.76229
H	-5.98674	-5.05434	-1.43621	H	0.97504	4.91045	-4.19462
H	-6.79722	-3.46886	-1.70885	H	-3.89613	4.87309	-3.90720
H	-6.12969	-4.39745	-3.10727	H	-4.20909	2.46606	-2.87441
C	4.08603	-3.22803	5.00830	H	-3.82715	-4.11024	-2.23042
H	3.82029	-4.26979	5.29167	H	-4.14403	-2.15835	-6.63632
C	4.73295	-2.54819	6.21157	H	2.22793	-6.62983	-1.90965
H	5.07644	-1.52622	5.94439	H	2.63102	-2.41031	-4.36967
H	4.00837	-2.48365	7.05139	H	4.24792	-3.00012	1.94412
H	5.61169	-3.13971	6.54440	H	4.82460	-3.28991	4.18228
C	-0.91114	-2.81549	4.86633	H	-0.88856	-3.92588	4.81143
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C	2.09266	0.88160	2.93218	C	-0.55822	-3.30341	-0.89228
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H	1.90208	1.89131	4.85882	O	-1.50678	-4.28776	-0.69302
H	3.60483	1.62214	4.31526	H	0.13548	-5.20036	1.51265
C	-3.81243	5.32896	-2.89699	H	-0.40350	-3.70549	2.29002
H	-4.68942	4.98968	-2.30489	C	-0.86246	-3.40316	-3.47566
C	-3.87416	6.84945	-3.01394	H	0.55443	-4.43069	-2.22044
H	-4.84541	7.14793	-3.46167	H	0.85728	-2.69542	-2.36145
H	-3.78766	7.31510	-2.00888	C	-1.72689	-4.41367	0.71092
H	-3.05645	7.22623	-3.66406	C	-1.08311	-2.02020	-4.08851
C	1.18182	4.90253	-3.10205	H	-0.41698	-4.02104	-4.26323
H	1.91842	4.09089	-2.93998	H	-1.82226	-3.86121	-3.22393
C	1.80174	6.24332	-2.72073	H	-2.42274	-3.63362	1.04499
H	1.08389	7.06816	-2.91695	H	-2.17645	-5.39253	0.88100
H	2.08621	6.25499	-1.64905	H	-1.46200	-1.31578	-3.33508
H	2.71546	6.41526	-3.32764	H	-1.83592	-2.11523	-4.87673
C	-1.42115	3.37335	1.06140	H	0.58130	-1.03038	-4.04255
H	-0.48437	2.86029	1.36005	O	0.07665	-1.51782	-4.71186
C	-1.73339	4.46687	2.07967				
H	-2.76990	4.84067	1.94139				
H	-1.63628	4.06098	3.10495				
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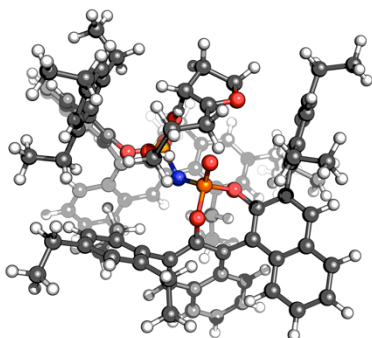
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C	-3.24687	0.18679	2.28477
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C	-3.70584	1.28255	3.05914
C	-2.90135	1.76693	4.11993
C	-4.13938	-0.54513	1.34217
C	-5.34852	-1.15637	1.77167
C	-3.72872	-0.68652	0.00136
C	-6.20175	-1.75643	0.81164
C	-4.56478	-1.32649	-0.93050
C	-5.81234	-1.81469	-0.52905
H	-6.45863	-2.28622	-1.26005
H	-1.07630	1.50136	5.23259
C	-3.35979	2.82323	4.92317
C	-4.59676	3.41659	4.66621
H	-2.75883	3.19376	5.74517
H	-4.94245	4.23461	5.28480
C	-5.38307	2.96557	3.60600
C	-4.94404	1.90997	2.80393
H	-6.33485	3.43850	3.40156
H	-5.57111	1.60041	1.97821
C	-7.42069	-2.32742	1.21100
C	-7.78582	-2.33623	2.55722
H	-8.08361	-2.78110	0.48360
H	-8.72373	-2.78359	2.86004
C	-6.93393	-1.79007	3.51603
C	-5.72179	-1.21186	3.13319
H	-7.21098	-1.81930	4.56199
H	-5.07924	-0.82706	3.91288
N	-0.04458	0.19754	-0.02820
P	1.12663	0.34650	-1.10849
O	1.18164	-0.56930	-2.28443
O	2.46331	0.20971	-0.16772
O	1.10620	1.85988	-1.72216
C	3.60699	0.78135	-0.66698
C	1.33883	2.88496	-0.83824
C	3.72367	2.18535	-0.72140

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C	0.38719	3.91008	-0.69726
C	2.59732	3.01792	-0.21811
C	4.88936	2.77208	-1.28337
C	5.89807	0.56189	-1.44763
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C	2.78702	4.01098	0.77531
C	5.98945	1.94498	-1.61773
C	4.98336	4.15780	-1.54367
H	6.74498	-0.06939	-1.69272
C	1.77628	4.97960	0.98757
H	-0.12892	5.73096	0.32596
C	3.95962	4.06776	1.55804
C	7.16513	2.51084	-2.13652
C	6.15619	4.70552	-2.06764
H	4.15207	4.82561	-1.36364
C	1.96716	5.99775	1.93517
C	4.13084	5.07938	2.50563
H	4.74056	3.32580	1.45346
C	7.24723	3.88632	-2.35404
H	8.01605	1.88757	-2.38519
H	6.21696	5.76955	-2.25690
C	3.14071	6.04486	2.68953
H	1.20674	6.75270	2.09628
H	5.03384	5.11319	3.10127
H	8.15394	4.31642	-2.75950
H	3.27983	6.82780	3.42369
C	-0.81408	3.96920	-1.56558
C	-0.69046	4.37437	-2.92317
C	-2.10408	3.73442	-1.02229
C	-1.84714	4.55430	-3.69757
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C	-3.11916	4.36073	-3.15096
H	-4.22548	3.76412	-1.40914
C	4.63614	-1.50575	-0.95398
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C	4.81447	-4.32311	-0.90251
H	4.60258	-4.21705	-3.03834
C	-4.09002	-1.60514	-2.30584
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C	-3.53548	-0.84644	-4.55451
C	-3.23188	-3.17054	-3.96633
C	-3.14646	-2.14228	-4.91056
H	-2.92463	-4.17245	-4.24349
C	0.11095	-0.50110	3.91257
C	0.11692	-1.76788	4.55513
C	1.33915	0.16812	3.67653
C	1.33859	-2.34253	4.93666
C	2.54105	-0.42668	4.09068
C	2.54804	-1.67260	4.72688
H	3.47726	0.09358	3.92574
H	4.98662	-4.11531	1.22787
H	1.34781	-3.31021	5.42439

H	-3.48753	-0.05575	-5.29411	H	-4.15160	1.17162	-1.96588
H	-1.75704	4.88821	-4.72467	C	-6.01003	0.94332	-3.05441
C	4.91499	-5.82670	-0.87030	H	-6.49454	0.26096	-2.32701
H	4.20318	-6.23208	-0.11948	H	-6.32846	1.98061	-2.82094
C	6.33216	-6.27402	-0.52318	H	-6.35253	0.68640	-4.07936
H	6.61768	-5.91786	0.48938	C	-3.77719	-4.09529	-1.70438
H	6.38493	-7.38302	-0.53445	H	-3.87386	-3.76777	-0.64949
H	7.05352	-5.87572	-1.26848	C	-4.93983	-5.02315	-2.04646
C	4.88185	-1.46247	1.59973	H	-4.98096	-5.85287	-1.30976
H	4.28573	-0.52905	1.59737	H	-5.90233	-4.47291	-2.01372
C	6.33237	-1.13699	1.93677	H	-4.80508	-5.45802	-3.05949
H	6.93166	-2.07018	2.00030	C	-2.65182	-2.43548	-6.30368
H	6.77069	-0.47174	1.16368	H	-2.44290	-1.49185	-6.85348
H	6.37718	-0.61791	2.91731	C	-3.68358	-3.23692	-7.09331
C	4.34568	-1.59066	-3.51023	H	-3.30910	-3.41251	-8.12369
H	4.03393	-0.53050	-3.41144	H	-3.86668	-4.22095	-6.61185
C	5.60617	-1.65322	-4.36902	H	-4.64071	-2.67563	-7.15389
H	5.41904	-1.14634	-5.33895	H	-0.94888	-3.60794	4.97443
H	6.44906	-1.14161	-3.86012	H	3.93134	-3.31874	4.78057
H	5.88942	-2.70751	-4.57216	H	4.45789	-2.09741	2.40466
C	-4.35158	4.62870	-3.97800	H	3.51805	-2.10656	-4.04221
H	-4.08589	4.75865	-5.04978	H	4.63845	-6.26060	-1.85596
C	-5.06829	5.88862	-3.50111	H	-1.69876	-3.00474	-6.24772
H	-5.41486	5.76777	-2.45282	H	-2.83816	-4.68066	-1.75252
H	-4.38725	6.76426	-3.56369	H	-4.04800	1.55600	-3.69443
H	-5.95258	6.07902	-4.14504	H	-5.04416	3.76477	-3.91405
C	0.64850	4.68579	-3.56540	H	0.57056	4.60536	-4.67178
H	1.42175	3.95149	-3.26663	H	-3.01564	2.42113	0.41488
C	1.11628	6.09756	-3.22404	H	2.20174	1.50412	2.22818
H	0.35515	6.84192	-3.54123	O	-1.09451	-2.19865	-0.64619
H	1.29801	6.20223	-2.13580	H	-0.64976	-3.30984	-0.16390
H	2.06651	6.31145	-3.75717	C	-0.40845	-4.45236	0.43379
C	-2.31300	3.28014	0.40651	C	0.64510	-5.02664	-0.30133
H	-1.37266	2.91921	0.87212	C	0.20254	-4.10456	1.79110
C	-2.89005	4.40659	1.26073	H	-1.38580	-4.92503	0.35754
H	-2.87479	4.11020	2.32777	C	0.57252	-5.73827	-1.60694
H	-2.29027	5.33286	1.15219	O	1.80993	-4.89917	0.26164
H	-3.93939	4.61791	0.96505	C	1.67118	-3.98540	1.39314
C	3.84445	-2.28903	5.18998	H	0.04530	-4.89576	2.53255
H	4.71405	-1.70619	4.81611	H	-0.18069	-3.16291	2.18108
C	3.92339	-2.33368	6.71374	C	0.14565	-4.78718	-2.74658
H	4.90370	-2.75412	7.02212	H	1.55015	-6.17999	-1.82217
H	3.82811	-1.30912	7.13283	H	-0.16593	-6.54068	-1.50445
H	3.11920	-2.97629	7.13018	H	1.91064	-2.99291	0.99549
C	-1.15827	-2.51964	4.88302	H	2.40076	-4.28880	2.14240
H	-1.90489	-2.42322	4.06962	H	-0.75539	-4.24135	-2.45791
C	-1.76215	-2.03433	6.19696	H	-0.08112	-5.38379	-3.63628
H	-1.03280	-2.16199	7.02513	C	1.23687	-3.76763	-3.03506
H	-2.05087	-0.96608	6.12682	O	1.58223	-3.12486	-1.83315
H	-2.67109	-2.62836	6.42874	H	2.11686	-4.28024	-3.45228
C	1.40925	1.52266	3.00508	H	0.88423	-3.04282	-3.77898
H	0.46518	1.77981	2.48203	H	1.42864	-2.15541	-1.94842
C	1.72626	2.61641	4.02164				
H	2.76641	2.50816	4.39526				
H	1.62200	3.61030	3.54498				
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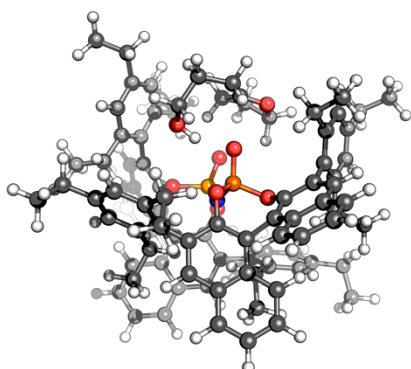
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C	-2.41707	2.47720	4.01693
C	-3.95744	-0.23324	1.81284
C	-5.14877	-0.67338	2.45169
C	-3.68096	-0.64881	0.49089
C	-6.12880	-1.35964	1.69425
C	-4.65963	-1.34882	-0.24076
C	-5.88620	-1.66270	0.35357
H	-6.64153	-2.17939	-0.22767
H	-0.53223	2.30566	5.04477
C	-2.77110	3.68000	4.64854
C	-4.00317	4.27896	4.38092
H	-2.09457	4.15713	5.34771
H	-4.26920	5.20812	4.86800
C	-4.88802	3.68804	3.47872
C	-4.55087	2.48982	2.84517
H	-5.83611	4.16367	3.26368
H	-5.25170	2.07223	2.13427
C	-7.33469	-1.75645	2.29433
C	-7.56215	-1.50750	3.64778
H	-8.09562	-2.27117	1.71947
H	-8.49126	-1.82035	4.10648
C	-6.58549	-0.87510	4.41541
C	-5.38505	-0.46743	3.82987
H	-6.75681	-0.70343	5.47032
H	-4.64423	-0.00732	4.46912
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O	1.07576	-1.07270	-2.04980
O	2.52753	0.02134	-0.21788
O	1.09790	1.39514	-1.95677
C	3.63994	0.49974	-0.87045
C	1.37220	2.56892	-1.29618
C	3.75068	1.87579	-1.16504

C	4.73925	-0.35124	-1.10721
C	0.43396	3.61653	-1.29849
C	2.65297	2.78997	-0.75582
C	4.88594	2.35723	-1.87108
C	5.90730	0.15773	-1.68554
C	0.69688	4.78605	-0.57231
C	2.89135	3.93466	0.04454
C	5.97943	1.48846	-2.09890
C	4.95629	3.67646	-2.37356
H	6.75394	-0.50114	-1.84191
C	1.89520	4.93600	0.13172
H	-0.02464	5.59355	-0.58143
C	4.10049	4.11289	0.74977
C	7.12930	1.95779	-2.75413
C	6.10238	4.12728	-3.03173
H	4.12609	4.36322	-2.28033
C	2.13067	6.09709	0.88498
C	4.31902	5.27037	1.50025
H	4.87404	3.35604	0.73747
C	7.18966	3.27384	-3.21275
H	7.97595	1.30282	-2.92311
H	6.14518	5.14175	-3.40682
C	3.33898	6.26130	1.56452
H	1.38034	6.87625	0.94875
H	5.24964	5.39683	2.03807
H	8.07588	3.62865	-3.72286
H	3.51362	7.15633	2.14741
C	-0.80084	3.55103	-2.11809
C	-0.72616	3.70124	-3.53074
C	-2.07238	3.48320	-1.49031
C	-1.91091	3.80137	-4.27729
C	-3.23450	3.60522	-2.26766
C	-3.16173	3.78150	-3.65319
H	-4.20608	3.56849	-1.78869
C	4.68959	-1.80171	-0.80910
C	4.86909	-2.26567	0.51820
C	4.62282	-2.74007	-1.87361
C	4.97819	-3.64310	0.76175
C	4.74465	-4.11070	-1.59493
C	4.92335	-4.56710	-0.28571
H	4.68840	-4.82699	-2.40626
C	-4.40698	-1.82974	-1.61976
C	-4.49645	-0.93741	-2.71780
C	-4.21134	-3.21627	-1.85994
C	-4.40850	-1.43775	-4.02611
C	-4.14271	-3.68425	-3.18117
C	-4.25235	-2.80666	-4.26473
H	-3.99416	-4.74140	-3.36842
C	0.46439	0.03135	4.03263
C	0.45339	-1.15223	4.82093
C	1.70520	0.61785	3.67058
C	1.67020	-1.71814	5.23104
C	2.90080	0.04105	4.12603
C	2.89116	-1.11671	4.91115
H	3.84674	0.50215	3.86765
H	5.11932	-3.99980	1.77559
H	1.66840	-2.61939	5.83285

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C	5.04925	-6.04153	-0.00064	H	-6.72445	0.30250	-1.63893
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C	6.47943	-6.40358	0.39028	H	-6.73508	0.51789	-3.43695
H	6.77541	-5.87682	1.32221	C	-4.05762	-4.22482	-0.73702
H	6.55129	-7.49766	0.56541	H	-3.87160	-3.73494	0.24102
H	7.18161	-6.12705	-0.42534	C	-5.28838	-5.12016	-0.61626
C	5.00258	-1.32477	1.69235	H	-5.14805	-5.83041	0.22555
H	4.40529	-0.40368	1.54873	H	-6.19554	-4.51383	-0.41798
C	6.46052	-0.95001	1.93238	H	-5.43900	-5.70506	-1.54808
H	7.06324	-1.86011	2.13870	C	-4.20767	-3.33561	-5.67599
H	6.87742	-0.42715	1.04614	H	-4.09061	-2.50369	-6.40430
H	6.52900	-0.27182	2.80889	C	-5.48444	-4.09985	-6.01456
C	4.39109	-2.32385	-3.31392	H	-5.43746	-4.45437	-7.06573
H	4.04915	-1.27127	-3.39397	H	-5.59966	-4.98205	-5.34959
C	5.65008	-2.50184	-4.15895	H	-6.36934	-3.43756	-5.90144
H	5.44590	-2.17425	-5.20005	H	-0.63785	-2.86612	5.58230
H	6.48262	-1.89095	-3.75471	H	4.22848	-2.78899	5.11616
H	5.95882	-3.56828	-4.18042	H	4.60153	-1.81522	2.60225
C	-4.42050	3.96787	-4.46363	H	3.58166	-2.94608	-3.74902
H	-4.20335	3.88923	-5.55124	H	4.76482	-6.64023	-0.89337
C	-5.04889	5.33190	-4.19350	H	-3.33161	-4.00739	-5.79803
H	-5.34783	5.41986	-3.12740	H	-3.17249	-4.86399	-0.93535
H	-4.32934	6.14155	-4.44085	H	-4.30205	1.10023	-3.38230
H	-5.95398	5.45532	-4.82476	H	-5.15202	3.17087	-4.21659
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C	1.15266	5.24216	-4.18822	H	2.53867	1.67717	1.99290
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H	1.41139	5.50485	-3.14329	C	0.01437	-4.28233	-1.63996
H	2.07598	5.31156	-4.80105	C	-0.80882	-3.39425	-3.53414
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H	-2.16074	5.45506	0.33451	H	-0.48827	-6.06012	-0.73015
H	-3.81392	4.73324	0.41927	H	-0.90915	-4.62291	0.19431
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H	5.05765	-1.20874	4.94711	C	1.44933	-4.09164	1.37994
C	4.30618	-1.59318	6.92423	H	1.03132	-6.17116	1.06352
H	5.28310	-2.00696	7.25186	H	2.02484	-5.44802	-0.19554
H	4.25204	-0.52569	7.22728	H	1.09041	-2.52235	-4.12130
H	3.49742	-2.16002	7.43188	H	1.01739	-4.29686	-4.32209
C	-0.83028	-1.80996	5.29234	H	2.34528	-4.30529	1.97170
H	-1.58358	-1.85522	4.48208	H	0.61022	-3.95980	2.08038
C	-1.41450	-1.08712	6.50267	H	0.81537	-2.57276	0.39207
H	-0.67093	-1.05642	7.32744	C	1.10428	-3.63108	-2.23267
H	-1.71202	-0.05207	6.24077	O	-1.07082	-4.23002	-2.36601
H	-2.31651	-1.62881	6.85742	H	2.09503	-3.93180	-1.92268
C	1.79753	1.85427	2.80063	H	1.04369	-2.36332	-1.86759
H	0.83698	2.08335	2.29456	O	1.68957	-2.90164	0.66817
C	2.22782	3.06908	3.61921				
H	3.29047	2.97191	3.92656				
H	2.11663	3.98704	3.00930				
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C	-4.75454	0.54058	-2.53763				

S-anti-ev(+)-intermediate



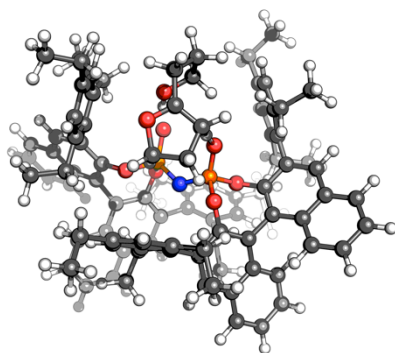
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C	-2.81559	0.59373	2.56131
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C	-3.85639	-0.20398	1.85506
C	-5.03873	-0.62409	2.52295
C	-3.65857	-0.55623	0.50013
C	-6.09305	-1.19638	1.77217
C	-4.72093	-1.12601	-0.23214
C	-5.93720	-1.40364	0.40131
H	-6.75711	-1.81203	-0.17751
H	-0.29843	2.06354	5.13247
C	-2.50655	3.51533	4.86172
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H	-1.80842	3.92946	5.57950
H	-3.95621	5.07029	5.19130
C	-4.63323	3.65752	3.71844
C	-4.33997	2.48902	3.01188
H	-5.56876	4.17288	3.54374
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C	-7.29057	-1.56656	2.40515
C	-7.43724	-1.40422	3.78280
H	-8.10800	-1.99376	1.83618
H	-8.35996	-1.69743	4.26664
C	-6.38942	-0.88298	4.54018
C	-5.19678	-0.50132	3.92212
H	-6.49941	-0.77785	5.61184
H	-4.39983	-0.12856	4.55111
N	0.00654	0.19597	-0.02746
P	1.12971	0.09276	-1.15820
O	1.03047	-0.95216	-2.22109
O	2.51517	-0.06165	-0.29651
O	1.20822	1.52772	-1.95190
C	3.66714	0.31811	-0.93929
C	1.60509	2.61238	-1.20955
C	3.91370	1.68491	-1.18092

C	4.66094	-0.63686	-1.23382
C	0.76077	3.73142	-1.10646
C	2.91920	2.68542	-0.70610
C	5.08179	2.07390	-1.88892
C	5.86145	-0.23228	-1.82793
C	1.14955	4.82805	-0.32735
C	3.28341	3.75604	0.14877
C	6.06851	1.10208	-2.18489
C	5.28772	3.40106	-2.32763
H	6.62942	-0.96965	-2.03035
C	2.38378	4.83465	0.32912
H	0.49497	5.68812	-0.25262
C	4.52097	3.78155	0.82634
C	7.24913	1.47539	-2.84694
C	6.46315	3.75604	-2.99281
H	4.54115	4.16901	-2.17756
C	2.74609	5.92378	1.13759
C	4.86349	4.86654	1.63627
H	5.22151	2.96047	0.74721
C	7.44495	2.79849	-3.24359
H	8.01504	0.74133	-3.06809
H	6.61097	4.77750	-3.31900
C	3.98184	5.93717	1.78659
H	2.07157	6.76108	1.27201
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H	8.35438	3.07938	-3.75889
H	4.25347	6.77615	2.41400
C	-0.51279	3.80729	-1.86300
C	-0.49595	4.07985	-3.25797
C	-1.75525	3.72948	-1.18261
C	-1.70723	4.29428	-3.93430
C	-2.94602	3.96057	-1.88874
C	-2.92891	4.26116	-3.25476
H	-3.89531	3.91521	-1.36763
C	4.45889	-2.08131	-0.96335
C	4.58143	-2.58594	0.35666
C	4.24650	-2.98587	-2.03847
C	4.47119	-3.96669	0.58384
C	4.14363	-4.36064	-1.77477
C	4.25433	-4.85606	-0.47253
H	3.97651	-5.04993	-2.59420
C	-4.58044	-1.48434	-1.66543
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C	-4.56098	-2.85128	-2.05760
C	-4.54734	-0.83871	-4.01804
C	-4.54056	-3.17779	-3.42200
C	-4.53900	-2.18246	-4.40336
H	-4.50850	-4.21836	-3.72352
C	0.61933	-0.16667	3.97391
C	0.58730	-1.37797	4.71795
C	1.87013	0.40911	3.63039
C	1.79381	-1.97669	5.11184
C	3.05526	-0.20430	4.06423
C	3.02494	-1.38573	4.81234
H	4.00958	0.24657	3.81828
H	4.56340	-4.35607	1.59120
H	1.77617	-2.89628	5.68505

H	-4.55925	-0.06843	-4.78040	H	-4.11768	1.25689	-1.42135
H	-1.69474	4.53031	-4.99196	C	-6.15174	1.40674	-2.13608
C	4.14170	-6.33503	-0.20539	H	-6.60856	0.84512	-1.29512
H	3.42682	-6.50979	0.62731	H	-6.20485	2.49118	-1.90391
C	5.49904	-6.93232	0.15381	H	-6.73070	1.21214	-3.06390
H	5.89456	-6.47213	1.08410	C	-4.52908	-3.99226	-1.05810
H	5.39182	-8.02507	0.31889	H	-4.28812	-3.64473	-0.03256
H	6.22201	-6.76644	-0.67338	C	-5.85385	-4.75138	-1.02938
C	4.87616	-1.69160	1.53895	H	-5.80010	-5.56029	-0.27071
H	4.32839	-0.73207	1.46454	H	-6.69022	-4.07416	-0.76341
C	6.37108	-1.42268	1.67252	H	-6.06153	-5.21152	-2.01845
H	6.92429	-2.37885	1.78989	C	-4.51179	-2.55997	-5.86267
H	6.75476	-0.88524	0.78141	H	-4.31049	-1.66871	-6.49623
H	6.55468	-0.79334	2.56866	C	-5.84043	-3.17252	-6.29713
C	4.10749	-2.52839	-3.47706	H	-5.80190	-3.41246	-7.38055
H	3.91837	-1.43781	-3.55282	H	-6.04162	-4.10948	-5.73574
C	5.34728	-2.87850	-4.29634	H	-6.66963	-2.45432	-6.12091
H	5.21838	-2.51373	-5.33707	H	-0.53698	-3.10695	5.38816
H	6.25046	-2.40145	-3.86498	H	4.32422	-3.09170	4.98587
H	5.49734	-3.97848	-4.32550	H	4.52393	-2.17909	2.47029
C	-4.21439	4.56816	-3.98244	H	3.23215	-3.03052	-3.93650
H	-4.04840	4.59108	-5.08155	H	3.74602	-6.86664	-1.09824
C	-4.77965	5.91824	-3.55068	H	-3.69027	-3.28655	-6.04306
H	-5.02940	5.90904	-2.46843	H	-3.72623	-4.70324	-1.34259
H	-4.04191	6.72473	-3.75007	H	-4.25883	1.60142	-3.14977
H	-5.70588	6.13349	-4.12396	H	-4.96357	3.77518	-3.77990
C	0.79203	4.21597	-4.04692	H	0.60316	4.01622	-5.12442
H	1.54250	3.46555	-3.72959	H	-2.60972	2.62470	0.45219
C	1.37765	5.61885	-3.91601	H	2.71476	1.50559	1.98439
H	0.64165	6.37631	-4.26045	O	-0.97758	-2.28643	-0.18233
H	1.65734	5.83358	-2.86503	C	-0.54840	-4.16812	-1.84683
H	2.29036	5.69909	-4.54320	C	-1.06395	-2.71302	-3.49365
C	-1.85173	3.42096	0.29574	C	-0.85244	-5.09874	-0.73057
H	-0.89786	3.02721	0.70370	H	-1.77861	-2.76823	-4.31032
C	-2.25185	4.66484	1.08589	H	-1.06274	-1.73925	-2.99862
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H	-1.60537	5.52632	0.82137	H	-1.34561	-5.95254	-1.21884
H	-3.31068	4.92969	0.88125	H	-1.60911	-4.59382	-0.12030
C	4.30606	-2.02281	5.29016	C	0.34037	-3.19795	-3.80261
H	5.18821	-1.52986	4.82651	C	0.80763	-4.53911	1.14137
C	4.44290	-1.91900	6.80670	H	-0.00919	-6.47091	0.66786
H	5.41022	-2.36298	7.12308	H	1.16268	-5.88078	-0.50549
H	4.42050	-0.85372	7.12159	H	0.97614	-2.35057	-4.05286
H	3.62144	-2.46834	7.31330	H	0.33859	-3.93830	-4.60810
C	-0.70774	-2.03170	5.16174	H	1.56483	-5.00076	1.78410
H	-1.46771	-2.01279	4.35661	H	-0.03177	-4.22656	1.77993
C	-1.26604	-1.36577	6.41607	H	0.67616	-2.80817	0.30391
H	-0.51667	-1.40047	7.23542	C	0.75057	-3.82311	-2.46251
H	-1.53932	-0.31043	6.21589	O	-1.53455	-3.66834	-2.46869
H	-2.17887	-1.90480	6.74623	H	1.40384	-4.69699	-2.50933
C	1.98386	1.67260	2.80324	H	1.22687	-3.06978	-1.81634
H	1.02486	1.94045	2.31361	O	1.39907	-3.42767	0.51935
C	2.44815	2.84887	3.65878				
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H	2.37024	3.78704	3.07544				
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S-anti-hc(-)



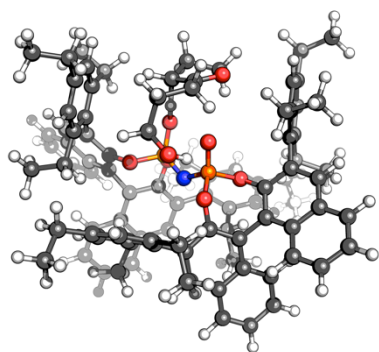
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C	-3.69672	-0.85075	-0.14003
C	-6.13390	-2.10934	0.47704
C	-4.43459	-1.49716	-1.14633
C	-5.66194	-2.09176	-0.83887
H	-6.22649	-2.58139	-1.62412
H	-1.42416	1.31766	5.26923
C	-3.78195	2.49058	4.90861
C	-5.03693	3.02223	4.60816
H	-3.24140	2.87022	5.76757
H	-5.45726	3.80048	5.23186
C	-5.74481	2.56239	3.49775
C	-5.21032	1.55683	2.68945
H	-6.71091	2.98859	3.26029
H	-5.77967	1.23864	1.82610
C	-7.33329	-2.77343	0.77986
C	-7.77994	-2.85302	2.09888
H	-7.91798	-3.24337	-0.00225
H	-8.70250	-3.37114	2.32681
C	-7.02873	-2.28522	3.12679
C	-5.83676	-1.61605	2.84103
H	-7.36822	-2.36851	4.15122
H	-5.27201	-1.21684	3.67193
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P	1.10625	0.37022	-1.05434
O	1.18441	-0.50840	-2.25413
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C	3.56621	0.89615	-0.62529
C	1.21305	2.91636	-0.73885
C	3.62398	2.30268	-0.67566
C	4.69907	0.13533	-0.96736

C	0.23207	3.90948	-0.56870
C	2.47732	3.08453	-0.13965
C	4.75462	2.93900	-1.25356
C	5.85091	0.77232	-1.44120
C	0.43174	4.93338	0.36563
C	2.64920	4.06458	0.86919
C	5.87998	2.15813	-1.61467
C	4.78873	4.32919	-1.50301
H	6.72147	0.17774	-1.69481
C	1.61184	4.99691	1.11209
H	-0.32659	5.69686	0.49105
C	3.82818	4.14096	1.64006
C	7.02053	2.77331	-2.15507
C	5.92725	4.92607	-2.04864
H	3.93618	4.96220	-1.29780
C	1.78321	6.00241	2.07680
C	3.97807	5.13606	2.60841
H	4.63050	3.42609	1.51054
C	7.04285	4.15223	-2.36567
H	7.89048	2.18602	-2.42459
H	5.94221	5.99296	-2.23076
C	2.96186	6.06779	2.82179
H	1.00223	6.73050	2.26129
H	4.88584	5.18458	3.19579
H	7.92268	4.62040	-2.78783
H	3.08527	6.83908	3.57094
C	-0.97981	3.95036	-1.42305
C	-0.88553	4.40582	-2.76665
C	-2.25520	3.65884	-0.87362
C	-2.05698	4.58467	-3.51875
C	-3.40550	3.85553	-1.65335
C	-3.31581	4.33720	-2.96331
H	-4.38130	3.63947	-1.23362
C	4.70308	-1.34255	-0.86853
C	4.91182	-1.97158	0.38484
C	4.64459	-2.13277	-2.04665
C	5.10467	-3.35991	0.43782
C	4.83045	-3.52116	-1.95624
C	5.08174	-4.13629	-0.72517
H	4.78221	-4.12527	-2.85465
C	-3.86558	-1.66226	-2.50446
C	-3.81568	-0.56416	-3.40054
C	-3.33485	-2.91782	-2.90361
C	-3.19946	-0.72127	-4.65206
C	-2.73970	-3.04299	-4.16769
C	-2.65864	-1.95225	-5.03901
H	-2.31302	-3.99371	-4.46630
C	-0.05196	-0.55444	3.93018
C	0.03145	-1.82096	4.56602
C	1.13234	0.19223	3.70266
C	1.28340	-2.31254	4.96449
C	2.36762	-0.32542	4.12246
C	2.44908	-1.56557	4.76481
H	3.27000	0.25247	3.96043
H	5.27748	-3.84155	1.39338
H	1.34957	-3.27704	5.45411
H	-3.15539	0.11698	-5.33746

H	-1.98934	4.95921	-4.53349	C	-5.95500	0.73411	-3.25539
C	5.29779	-5.62630	-0.64341	H	-6.41642	-0.03400	-2.60260
H	4.61170	-6.05885	0.11666	H	-6.39039	1.71953	-2.98959
C	6.74224	-5.95451	-0.27595	H	-6.20245	0.50794	-4.31440
H	6.99279	-5.55028	0.72768	C	-3.34975	-4.13774	-2.00162
H	6.87884	-7.05626	-0.25562	H	-3.55836	-3.88015	-0.94364
H	7.43672	-5.52362	-1.02860	C	-4.37975	-5.15970	-2.47355
C	4.97819	-1.19456	1.68020	H	-4.38217	-6.02958	-1.78354
H	4.31376	-0.30859	1.65954	H	-5.39498	-4.71147	-2.48289
C	6.40510	-0.75349	1.98530	H	-4.13128	-5.52003	-3.49428
H	7.07342	-1.63754	2.06222	C	-1.98387	-2.10433	-6.37831
H	6.78149	-0.07775	1.18918	H	-1.82994	-1.11232	-6.85637
H	6.42483	-0.20741	2.95192	C	-2.81583	-2.97099	-7.31962
C	4.36249	-1.53706	-3.41243	H	-2.31019	-3.03875	-8.30582
H	3.98527	-0.49595	-3.34184	H	-2.92814	-3.99730	-6.91031
C	5.60863	-1.54904	-4.29402	H	-3.82172	-2.52228	-7.46547
H	5.37123	-1.09055	-5.27699	H	-0.92661	-3.73086	4.91785
H	6.42553	-0.96625	-3.82068	H	3.94230	-3.11211	4.83147
H	5.95601	-2.58962	-4.46615	H	4.61276	-1.83184	2.51139
C	-4.56664	4.60376	-3.76236	H	3.56156	-2.12426	-3.91114
H	-4.31996	4.78727	-4.83082	H	5.06455	-6.11228	-1.61585
C	-5.31364	5.81988	-3.22214	H	-0.98116	-2.56302	-6.23721
H	-5.64230	5.64358	-2.17591	H	-2.34821	-4.61187	-2.00380
H	-4.65970	6.71750	-3.25477	H	-4.02691	1.56500	-3.72662
H	-6.21196	6.01119	-3.84607	H	-5.23216	3.71740	-3.72610
C	0.43588	4.77502	-3.41346	H	0.35281	4.70323	-4.52005
H	1.23900	4.06802	-3.12737	H	-3.10788	2.26526	0.51979
C	0.85072	6.19953	-3.05722	H	1.91951	1.58947	2.26901
H	0.06266	6.91842	-3.36742	O	-1.01376	-2.26782	-0.65677
H	1.02677	6.29904	-1.96739	C	1.18012	-4.76929	-0.27282
H	1.79276	6.45418	-3.58690	C	1.63004	-3.50429	1.52959
C	-2.43212	3.14492	0.53832	C	1.53191	-5.56967	-1.47612
H	-1.47548	2.79619	0.97724	H	1.61377	-2.46269	1.18678
C	-3.03120	4.21909	1.44302	H	2.32021	-3.61445	2.36456
H	-3.01216	3.87335	2.49499	C	0.67859	-5.24924	-2.71410
H	-2.44737	5.15968	1.37868	H	2.58215	-5.38421	-1.69248
H	-4.08406	4.42475	1.15613	H	1.41310	-6.62643	-1.20408
C	3.77799	-2.09352	5.24483	C	0.22940	-4.07568	1.72879
H	4.61054	-1.44866	4.88893	H	-0.31904	-5.68856	-2.61880
C	3.83751	-2.14179	6.76944	H	1.15928	-5.74772	-3.56076
H	4.84096	-2.49252	7.09035	H	0.23977	-4.93312	2.41170
H	3.66269	-1.12932	7.19226	H	-0.46124	-3.32267	2.10373
H	3.07588	-2.84317	7.17067	C	0.58178	-3.72925	-2.95070
C	-1.19512	-2.65230	4.88300	O	1.62202	-3.11785	-2.22763
H	-1.96638	-2.55669	4.09260	H	0.66023	-3.51268	-4.02454
C	-1.79181	-2.25468	6.22905	H	-0.38090	-3.34334	-2.60225
H	-1.04272	-2.39343	7.03762	H	1.48540	-2.14051	-2.23663
H	-2.11994	-1.19499	6.21379	O	2.17191	-4.29267	0.42640
H	-2.67337	-2.89336	6.44739	C	-0.07830	-4.49819	0.28813
C	1.11908	1.55081	3.03696	H	-0.46891	-3.34440	-0.26952
H	0.16582	1.74483	2.50542	H	-0.89607	-5.17673	0.05605
C	1.34656	2.65866	4.06163				
H	2.37993	2.60753	4.46509				
H	1.20188	3.64608	3.58211				
H	0.62323	2.57185	4.89862				
C	-4.44099	0.77308	-3.06695				
H	-4.20025	1.07552	-2.02849				

S-anti-hc(+)



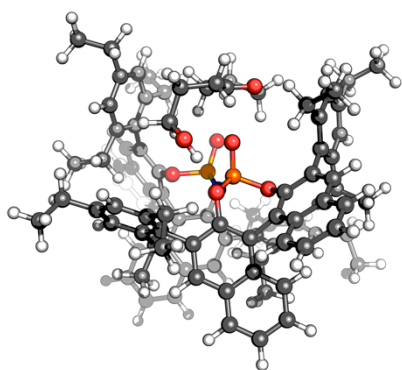
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C	-1.63642	-0.01793	2.67327
C	-0.78101	0.48740	3.66590
C	-2.93823	0.50271	2.54110
C	-1.15229	1.62634	4.39090
C	-3.28420	1.70168	3.21456
C	-2.37713	2.25671	4.15030
C	-3.94138	-0.29710	1.78536
C	-5.12877	-0.77419	2.40410
C	-3.67876	-0.62226	0.43626
C	-6.11839	-1.40428	1.61135
C	-4.66633	-1.26864	-0.33230
C	-5.88937	-1.61637	0.25087
H	-6.65250	-2.08906	-0.35685
H	-0.49018	2.00950	5.15789
C	-2.72252	3.41834	4.85910
C	-3.95047	4.04195	4.63180
H	-2.04182	3.84519	5.58614
H	-4.20959	4.93981	5.17774
C	-4.84009	3.51636	3.69456
C	-4.51247	2.35819	2.98610
H	-5.78509	4.01123	3.51176
H	-5.21732	1.99104	2.25167
C	-7.31993	-1.83735	2.19487
C	-7.53365	-1.67991	3.56426
H	-8.08790	-2.31013	1.59397
H	-8.45928	-2.02081	4.00983
C	-6.54785	-1.10298	4.36332
C	-5.35168	-0.65988	3.79504
H	-6.70867	-1.00230	5.42899
H	-4.60341	-0.24538	4.45650
N	-0.00414	0.15015	0.03142
P	1.11939	0.11156	-1.06508
O	1.08255	-0.94557	-2.16382
O	2.53147	-0.01267	-0.25335
O	1.14202	1.50540	-1.90777
C	3.65845	0.48153	-0.86938
C	1.43944	2.62801	-1.17331
C	3.80063	1.87001	-1.08599
C	4.74012	-0.37863	-1.15013

C	0.52188	3.69181	-1.10514
C	2.72553	2.78689	-0.62422
C	4.94752	2.36389	-1.76456
C	5.91953	0.13546	-1.70018
C	0.81460	4.81253	-0.31660
C	2.99245	3.87922	0.23841
C	6.02143	1.48467	-2.04030
C	5.04836	3.70697	-2.19351
H	6.75226	-0.53195	-1.89088
C	2.02041	4.89736	0.38523
H	0.10927	5.63332	-0.27318
C	4.20661	3.98896	0.94907
C	7.18232	1.96331	-2.66884
C	6.20504	4.16739	-2.82607
H	4.23385	4.40622	-2.06248
C	2.28597	6.00985	1.19945
C	4.45446	5.09765	1.76157
H	4.96167	3.21564	0.89270
C	7.27290	3.30087	-3.05423
H	8.01419	1.29970	-2.87376
H	6.27119	5.19976	-3.14465
C	3.49940	6.10743	1.88262
H	1.55465	6.80189	1.30903
H	5.38889	5.17182	2.30256
H	8.16743	3.66308	-3.54425
H	3.69706	6.96479	2.51287
C	-0.72499	3.69504	-1.90863
C	-0.66863	3.93966	-3.30849
C	-1.98805	3.60059	-1.26747
C	-1.86226	4.10732	-4.02825
C	-3.15957	3.78933	-2.01697
C	-3.10423	4.06093	-3.38787
H	-4.12459	3.73191	-1.52686
C	4.66019	-1.84149	-0.92621
C	4.81240	-2.37477	0.37851
C	4.58668	-2.72434	-2.03700
C	4.88865	-3.76465	0.55398
C	4.67359	-4.10955	-1.82527
C	4.82545	-4.63419	-0.53847
H	4.60945	-4.78351	-2.67150
C	-4.42686	-1.66008	-1.74177
C	-4.50515	-0.69489	-2.77747
C	-4.25287	-3.03046	-2.07508
C	-4.42411	-1.10751	-4.11656
C	-4.19126	-3.40929	-3.42489
C	-4.28724	-2.45930	-4.44683
H	-4.05746	-4.45341	-3.68305
C	0.49569	-0.19235	3.99409
C	0.48773	-1.41806	4.71483
C	1.73492	0.41771	3.66774
C	1.70569	-1.99727	5.10253
C	2.93162	-0.17624	4.09721
C	2.92454	-1.37218	4.82256
H	3.87638	0.30197	3.86679
H	5.00895	-4.17482	1.55012
H	1.70617	-2.92865	5.65662
H	-4.50510	-0.37205	-4.90857

H	-1.82156	4.32120	-5.08992	C	-6.23758	1.07508	-2.40863
C	4.90524	-6.12395	-0.32448	H	-6.70513	0.49401	-1.58669
H	4.18794	-6.42388	0.46998	H	-6.38446	2.15613	-2.20270
C	6.31649	-6.54648	0.07364	H	-6.73961	0.82311	-3.36698
H	6.60937	-6.07461	1.03546	C	-4.11245	-4.11516	-1.02332
H	6.35313	-7.64938	0.19644	H	-3.92005	-3.69586	-0.01420
H	7.04167	-6.25188	-0.71493	C	-5.35370	-5.00220	-0.96334
C	4.95659	-1.49612	1.59916	H	-5.22218	-5.76922	-0.17137
H	4.34572	-0.57693	1.51299	H	-6.25416	-4.40061	-0.72482
C	6.41435	-1.11854	1.83717	H	-5.51012	-5.52131	-1.93243
H	7.02969	-2.03217	1.98115	C	-4.24738	-2.89262	-5.89053
H	6.81260	-0.54048	0.97755	H	-4.12164	-2.01488	-6.56135
H	6.49000	-0.49110	2.75008	C	-5.53144	-3.61968	-6.27968
C	4.38270	-2.23266	-3.45772	H	-5.48767	-3.90230	-7.35257
H	4.07197	-1.16802	-3.49042	H	-5.65529	-4.54400	-5.67635
C	5.64550	-2.40625	-4.29810	H	-6.40992	-2.95814	-6.12131
H	5.46366	-2.01989	-5.32303	H	-0.59786	-3.18208	5.35844
H	6.49162	-1.84315	-3.85457	H	4.26786	-3.04650	4.96475
H	5.92185	-3.47923	-4.37124	H	4.57754	-2.03719	2.48971
C	-4.37162	4.32260	-4.16338	H	3.56055	-2.80926	-3.93041
H	-4.17144	4.31899	-5.25705	H	4.62087	-6.67000	-1.25036
C	-4.97539	5.67246	-3.78671	H	-3.37794	-3.56337	-6.05752
H	-5.25745	5.68797	-2.71252	H	-3.23596	-4.75083	-1.26554
H	-4.24742	6.48763	-3.98673	H	-4.30084	1.38041	-3.31200
H	-5.88767	5.85341	-4.39327	H	-5.11173	3.52074	-3.96249
C	0.64017	4.09801	-4.05954	H	0.48529	3.90393	-5.14349
H	1.38979	3.35374	-3.72744	H	-2.85998	2.49199	0.35632
C	1.20591	5.50706	-3.90623	H	2.56506	1.56257	2.04717
H	0.46528	6.25873	-4.25336	O	-1.00875	-2.31141	-0.20915
H	1.47021	5.71537	-2.85031	C	-0.05480	-4.14062	-1.90942
H	2.12606	5.60499	-4.51993	C	-0.85545	-3.12746	-3.74846
C	-2.12771	3.31405	0.21290	C	-0.15740	-5.01939	-0.71481
H	-1.17525	2.96422	0.66242	H	-1.44116	-3.48359	-4.59261
C	-2.60815	4.55130	0.96884	H	-1.18034	-2.13093	-3.43486
H	-2.50852	4.38388	2.05910	C	1.10402	-5.11916	0.14100
H	-2.00243	5.44075	0.70187	H	-0.43863	-6.00476	-1.11109
H	-3.67413	4.75725	0.73558	H	-1.00645	-4.66603	-0.12121
C	4.21707	-1.98751	5.29866	C	0.65750	-3.20680	-3.91574
H	5.09092	-1.45768	4.86107	C	1.33554	-3.90515	1.04275
C	4.33408	-1.92317	6.81919	H	1.00001	-5.99282	0.79256
H	5.31047	-2.34784	7.13422	H	1.98113	-5.29806	-0.49180
H	4.27684	-0.86853	7.16391	H	1.06292	-2.26456	-4.28789
H	3.52399	-2.51075	7.30054	H	0.95222	-4.02243	-4.58555
C	-0.79420	-2.10981	5.13875	H	1.45552	-2.98830	0.44757
H	-1.54527	-2.10443	4.32516	H	2.25848	-4.05746	1.61133
C	-1.38374	-1.46997	6.39236	H	-0.38762	-3.19955	1.59306
H	-0.64234	-1.49126	7.21940	C	1.05103	-3.48218	-2.46267
H	-1.68376	-0.42079	6.19806	O	-1.13766	-4.02012	-2.62839
H	-2.28487	-2.03655	6.70826	H	2.03188	-3.85109	-2.19556
C	1.82414	1.69759	2.86306	H	1.01229	-2.21513	-2.03301
H	0.86279	1.95043	2.36996	O	0.29433	-3.76607	1.98133
C	2.25277	2.86985	3.74245				
H	3.31450	2.75721	4.04762				
H	2.14403	3.81711	3.17878				
H	1.61980	2.93483	4.65078				
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S-anti-hc(+)-intermediate



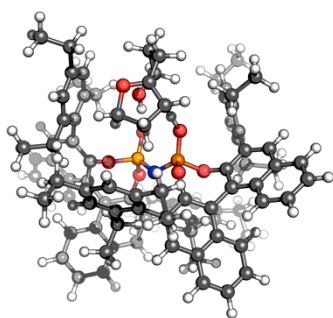
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C	-1.57550	-0.22411	2.57149
C	-0.71721	0.12785	3.62716
C	-2.86729	0.33326	2.51340
C	-1.06543	1.17214	4.49199
C	-3.18554	1.44938	3.32843
C	-2.27163	1.85900	4.32942
C	-3.89886	-0.35770	1.69246
C	-5.09154	-0.86403	2.27610
C	-3.67489	-0.52380	0.30938
C	-6.12568	-1.34149	1.43560
C	-4.70905	-1.01641	-0.51199
C	-5.93736	-1.37735	0.05309
H	-6.73743	-1.72329	-0.59032
H	-0.40014	1.43562	5.30559
C	-2.59285	2.93013	5.17833
C	-3.80073	3.61232	5.02303
H	-1.90748	3.24322	5.95702
H	-4.04050	4.44172	5.67565
C	-4.69492	3.23405	4.02128
C	-4.39352	2.16311	3.17703
H	-5.62422	3.77448	3.89609
H	-5.10177	1.90901	2.39919
C	-7.33254	-1.79659	1.99059
C	-7.50856	-1.81221	3.37432
H	-8.13411	-2.15340	1.35454
H	-8.43834	-2.17039	3.79708
C	-6.48088	-1.38577	4.21424
C	-5.27907	-0.92139	3.67561
H	-6.61369	-1.41891	5.28797
H	-4.49839	-0.62706	4.36374
N	0.00018	0.23840	-0.10339
P	1.13523	0.26099	-1.22372
O	1.04171	-0.63338	-2.41441
O	2.50186	-0.04844	-0.35986
O	1.26701	1.78310	-1.81343
C	3.67909	0.39931	-0.90611
C	1.65525	2.74905	-0.91949
C	3.94854	1.78329	-0.95864
C	4.67740	-0.52366	-1.27855

C	0.82056	3.85552	-0.68488
C	2.95657	2.73168	-0.38045
C	5.14445	2.24247	-1.57224
C	5.90438	-0.06202	-1.76833
C	1.20728	4.83731	0.23518
C	3.31578	3.67835	0.61231
C	6.13422	1.30321	-1.95032
C	5.37677	3.61118	-1.83506
H	6.67619	-0.77699	-2.02767
C	2.42832	4.74148	0.90906
H	0.56124	5.68959	0.40871
C	4.53731	3.59612	1.31424
C	7.34209	1.74119	-2.51673
C	6.57913	4.03157	-2.40758
H	4.63058	4.36347	-1.61828
C	2.78920	5.71463	1.85456
C	4.87822	4.56536	2.26022
H	5.22647	2.77842	1.14829
C	7.56267	3.10066	-2.73883
H	8.11044	1.03091	-2.79874
H	6.74673	5.08369	-2.59888
C	4.01037	5.62502	2.52470
H	2.12443	6.54021	2.07957
H	5.81782	4.49252	2.79240
H	8.49310	3.43215	-3.18148
H	4.28070	6.37419	3.25750
C	-0.44135	4.04088	-1.44207
C	-0.40251	4.49217	-2.78926
C	-1.69447	3.87907	-0.79650
C	-1.60298	4.79274	-3.45179
C	-2.87428	4.19764	-1.48698
C	-2.83556	4.67104	-2.80268
H	-3.83193	4.08578	-0.99171
C	4.45794	-1.98973	-1.19740
C	4.48551	-2.65071	0.05832
C	4.33516	-2.75915	-2.38663
C	4.37099	-4.04857	0.10856
C	4.24849	-4.15735	-2.29912
C	4.26480	-4.80561	-1.06090
H	4.15606	-4.74428	-3.20550
C	-4.51213	-1.22943	-1.96683
C	-4.46602	-0.12473	-2.85729
C	-4.45608	-2.55140	-2.48964
C	-4.33758	-0.35300	-4.23650
C	-4.34482	-2.74018	-3.87536
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H	-4.28688	-3.74560	-4.27604
C	0.52726	-0.63191	3.88875
C	0.46214	-1.91100	4.50407
C	1.79177	-0.04288	3.63269
C	1.65061	-2.57041	4.85139
C	2.95881	-0.71793	4.02116
C	2.89638	-1.97378	4.63442
H	3.92405	-0.25790	3.84466
H	4.39384	-4.55761	1.06532
H	1.60606	-3.54420	5.32504
H	-4.31161	0.48864	-4.91881

H	-1.57365	5.16396	-4.46957	C	-6.09879	1.66161	-2.20334
C	4.18132	-6.30844	-0.98340	H	-6.56824	1.01062	-1.43735
H	3.43385	-6.60351	-0.21605	H	-6.18613	2.71628	-1.86758
C	5.53662	-6.91262	-0.62849	H	-6.64351	1.54702	-3.16463
H	5.87274	-6.55760	0.36892	C	-4.48946	-3.78736	-1.60804
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H	6.29355	-6.63173	-1.39179	C	-5.81273	-4.53739	-1.74471
C	4.70456	-1.91067	1.35806	H	-5.81341	-5.41388	-1.06310
H	4.14734	-0.95486	1.37661	H	-6.66641	-3.88246	-1.47768
C	6.18647	-1.64774	1.60464	H	-5.94856	-4.90183	-2.78486
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H	6.60935	-1.00088	0.80928	H	-3.92841	-0.93262	-6.76350
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C	4.26949	-2.13119	-3.76539	H	-5.35961	-2.57251	-7.90855
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C	5.54845	-2.38625	-4.55991	H	-6.30510	-1.74049	-6.61569
H	5.47283	-1.89192	-5.55122	H	-0.72472	-3.67618	4.91584
H	6.43034	-1.97572	-4.02810	H	4.15982	-3.71475	4.64223
H	5.69742	-3.47475	-4.72132	H	4.31259	-2.51504	2.20133
C	-4.10958	5.06902	-3.50581	H	3.41709	-2.56891	-4.32448
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H	-5.60174	6.63966	-3.46972	H	-4.86004	4.25658	-3.41892
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H	1.64759	3.94952	-3.29758	H	-2.58002	2.58538	0.67511
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C	4.15859	-2.68326	5.05633	C	0.54385	-2.99643	-3.87425
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C	4.27816	-2.74032	6.57676	H	0.11697	-6.19776	0.56604
H	5.23197	-3.23571	6.85549	H	1.28139	-5.51987	-0.56420
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H	3.43903	-3.32115	7.01465	H	0.69916	-3.75583	-4.64628
C	-0.85137	-2.57225	4.87334	H	0.90953	-3.24626	0.53756
H	-1.63089	-2.38692	4.10872	H	1.52009	-4.49129	1.64363
C	-1.34658	-2.08951	6.23295	H	-0.80002	-3.13588	1.80078
H	-0.59102	-2.30869	7.01730	C	0.84384	-3.55228	-2.47593
H	-1.54619	-0.99868	6.21335	O	-1.42671	-3.64365	-2.78000
H	-2.29034	-2.61417	6.49148	H	1.55829	-4.37525	-2.43764
C	1.93768	1.30434	2.95751	H	1.17032	-2.73966	-1.81148
H	0.99396	1.63526	2.47669	O	-0.47229	-4.04431	1.86292
C	2.38469	2.36989	3.95532				
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H	1.72886	2.37280	4.84971				
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S-gau-ev(-)



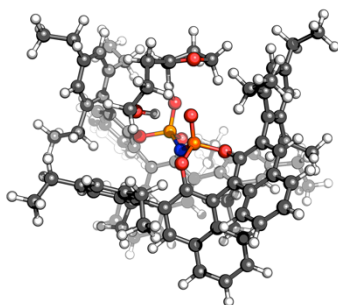
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C	-6.09423	-2.16105	0.41951
C	-4.36720	-1.54872	-1.17484
C	-5.58282	-2.17402	-0.88221
H	-6.10851	-2.70662	-1.66662
H	-1.56776	1.53212	5.20786
C	-3.93219	2.65629	4.74820
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C	-5.86302	2.64496	3.29209
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H	-7.83000	-3.36248	-0.07254
H	-8.68375	-3.43046	2.23465
C	-7.06752	-2.26811	3.04548
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O	2.45727	0.30584	-0.04472
O	1.04705	1.85866	-1.65227
C	3.57778	0.90839	-0.55706
C	1.23134	2.91396	-0.79219
C	3.64193	2.31362	-0.63993
C	4.70487	0.13329	-0.88460
C	0.23778	3.90325	-0.67977

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C	5.86906	0.75348	-1.34889
C	0.40838	4.96194	0.22106
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C	4.83484	4.31620	-1.48880
H	6.73360	0.14613	-1.59364
C	1.56867	5.06082	0.99426
H	-0.35816	5.72335	0.30081
C	3.77386	4.23767	1.61298
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C	5.98754	4.89529	-2.02371
H	3.98282	4.95883	-1.31473
C	1.70866	6.10159	1.92608
C	3.89221	5.26788	2.54846
H	4.58298	3.52348	1.53107
C	7.10407	4.10879	-2.30353
H	7.93845	2.13630	-2.31155
H	6.01273	5.95818	-2.22689
C	2.86611	6.20086	2.69996
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H	4.78317	5.34283	3.15834
H	7.99479	4.56318	-2.71787
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H	-2.07674	-4.04894	-4.37958
C	-0.14145	-0.37482	3.97682
C	-0.04916	-1.61501	4.66194
C	1.03791	0.37038	3.72042
C	1.20847	-2.08972	5.06447
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C	2.37084	-1.35048	4.82155
H	3.17884	0.44155	3.94857
H	5.24819	-3.90039	1.38593
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H	4.47914	-6.07648	0.08708	H	-6.39052	1.56119	-3.15663
C	6.59909	-6.02313	-0.36361	H	-6.14276	0.30450	-4.42829
H	6.88846	-5.64756	0.64066	C	-3.12618	-4.15398	-1.91839
H	6.70490	-7.12840	-0.36968	H	-3.36355	-3.87000	-0.87310
H	7.28458	-5.59580	-1.12645	C	-4.09506	-5.24522	-2.36344
C	5.01143	-1.25221	1.73120	H	-4.05721	-6.09017	-1.64405
H	4.40423	-0.32505	1.72188	H	-5.13263	-4.85219	-2.39512
C	6.46156	-0.90388	2.04617	H	-3.81823	-5.62597	-3.36933
H	7.07342	-1.82832	2.11824	C	-1.83595	-2.22047	-6.36236
H	6.88185	-0.24664	1.25602	H	-1.72420	-1.24076	-6.87619
H	6.51119	-0.36795	3.01735	C	-2.63291	-3.15416	-7.26955
C	4.27240	-1.47886	-3.34845	H	-2.12644	-3.23687	-8.25421
H	3.92158	-0.43101	-3.24926	H	-2.70260	-4.16870	-6.82300
C	5.50117	-1.49919	-4.25358	H	-3.65670	-2.75277	-7.42861
H	5.25597	-1.01491	-5.22213	H	-0.97978	-3.52018	5.10971
H	6.33868	-0.94377	-3.78260	H	3.86110	-2.89826	4.91595
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C	-4.50828	4.45493	-3.97804	H	3.44746	-2.03584	-3.84151
H	-4.24714	4.57342	-5.05225	H	4.88197	-6.10737	-1.65800
C	-5.24402	5.70937	-3.51614	H	-0.81489	-2.63189	-6.20774
H	-5.58256	5.59813	-2.46409	H	-2.09969	-4.57119	-1.89434
H	-4.57857	6.59556	-3.59550	H	-4.01157	1.45292	-3.82856
H	-6.13499	5.87481	-4.15777	H	-5.18722	3.58126	-3.89831
C	0.48776	4.64896	-3.55585	H	0.42242	4.53666	-4.66026
H	1.28732	3.95465	-3.23158	H	-3.11272	2.28460	0.41343
C	0.89468	6.08655	-3.24580	H	1.81496	1.73608	2.25236
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H	1.84355	6.32419	-3.77118	H	-0.49418	-3.36024	-0.00287
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C	3.79688	-1.85691	6.81818	C	1.91063	-3.75618	1.48612
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H	3.63430	-0.82880	7.20675	H	-0.35712	-6.09326	-1.37001
H	3.04043	-2.53957	7.25956	H	1.13082	-6.91322	-0.87504
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H	-1.20629	-2.04185	7.12376	H	1.17954	-6.04214	-3.25212
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C	1.01388	1.71044	3.01962	H	0.00325	-3.82469	-2.81640
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H	1.07719	3.81935	3.51206				
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C	-4.41612	0.66683	-3.15665				
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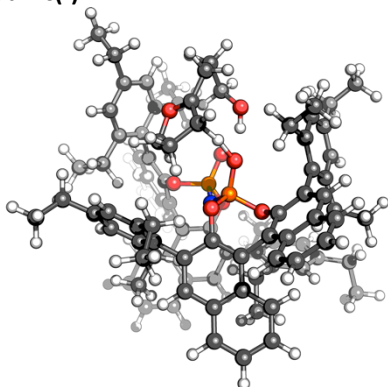
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C	-3.87454	3.78409	4.84389
H	-1.95115	3.53449	5.75542
H	-4.12277	4.65235	5.44042
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C	-4.46723	2.18913	3.12236
H	-5.72866	3.81264	3.75621
H	-5.18492	1.86142	2.38168
C	-7.30477	-1.93790	2.21922
C	-7.47617	-1.85296	3.60090
H	-8.09508	-2.37065	1.61710
H	-8.39160	-2.20952	4.05520
C	-6.46132	-1.32831	4.39959
C	-5.27818	-0.86538	3.81991
H	-6.58935	-1.28384	5.47350
H	-4.50625	-0.49365	4.47969
N	-0.02275	0.14936	-0.00486
P	1.12538	0.16266	-1.08625
O	1.10370	-0.85311	-2.22328
O	2.52748	0.03161	-0.27153
O	1.12667	1.59874	-1.86124
C	3.65239	0.57299	-0.85204
C	1.39751	2.68855	-1.06701
C	3.77269	1.97280	-0.99125
C	4.75487	-0.25115	-1.16509

C	0.46063	3.73215	-0.95186
C	2.67534	2.84269	-0.49564
C	4.92173	2.52474	-1.61943
C	5.93844	0.31704	-1.65061
C	0.72724	4.81538	-0.10326
C	2.91415	3.89210	0.42671
C	6.02072	1.68426	-1.91351
C	5.00196	3.88992	-1.97706
H	6.78776	-0.32269	-1.86129
C	1.92301	4.88343	0.61647
H	0.00883	5.62200	-0.02595
C	4.12044	3.98727	1.15341
C	7.18538	2.21921	-2.48730
C	6.16265	4.40712	-2.55614
H	4.16864	4.56359	-1.83062
C	2.16032	5.95615	1.49065
C	4.34177	5.05759	2.02293
H	4.88990	3.23132	1.06573
C	7.25516	3.57662	-2.80104
H	8.03626	1.58468	-2.70585
H	6.21293	5.45573	-2.81983
C	3.36644	6.04125	2.18821
H	1.41336	6.72788	1.63427
H	5.27044	5.12088	2.57511
H	8.15278	3.98265	-3.24927
H	3.54283	6.86835	2.86357
C	-0.78184	3.75869	-1.76172
C	-0.72144	4.06906	-3.14847
C	-2.04712	3.63443	-1.12944
C	-1.91326	4.26860	-3.86330
C	-3.21608	3.86020	-1.87219
C	-3.15698	4.19390	-3.22902
H	-4.18227	3.78306	-1.38729
C	4.68887	-1.72880	-1.06835
C	4.78869	-2.37141	0.19161
C	4.67703	-2.51385	-2.25367
C	4.85282	-3.77177	0.25209
C	4.75744	-3.91232	-2.15566
C	4.84518	-4.54487	-0.91217
H	4.74075	-4.51205	-3.05811
C	-4.53267	-1.57797	-1.78537
C	-4.62100	-0.56006	-2.76823
C	-4.40909	-2.93330	-2.19206
C	-4.58139	-0.90501	-4.12822
C	-4.41345	-3.24528	-3.55954
C	-4.49026	-2.24131	-4.52947
H	-4.32081	-4.27861	-3.87311
C	0.53465	-0.43760	3.93929
C	0.51527	-1.70169	4.59065
C	1.77909	0.18522	3.66003
C	1.72773	-2.30963	4.95043
C	2.96921	-0.43760	4.06525
C	2.95134	-1.67595	4.71512
H	3.91763	0.05006	3.87326
H	4.92881	-4.26586	1.21387
H	1.72023	-3.27199	5.44869
H	-4.65508	-0.12758	-4.87985

H	-1.86978	4.53179	-4.91370	C	-6.30430	1.22514	-2.27255
C	4.92486	-6.04737	-0.82258	H	-6.76647	0.61592	-1.46789
H	4.17624	-6.41639	-0.08839	H	-6.42249	2.29848	-2.01419
C	6.32055	-6.49835	-0.40111	H	-6.83216	1.02900	-3.23007
H	6.56853	-6.10978	0.60938	C	-4.22595	-4.06892	-1.20267
H	6.35943	-7.60762	-0.37171	H	-3.99279	-3.70061	-0.18236
H	7.07716	-6.13497	-1.12920	C	-5.46382	-4.96015	-1.13450
C	4.89351	-1.59947	1.48577	H	-5.29974	-5.76438	-0.38677
H	4.26487	-0.68907	1.46504	H	-6.35293	-4.37149	-0.82934
C	6.33893	-1.21516	1.78243	H	-5.66115	-5.43217	-2.11996
H	6.96981	-2.12600	1.86241	C	-4.45770	-2.60029	-5.99304
H	6.74150	-0.56025	0.98224	H	-4.32773	-1.69046	-6.61881
H	6.38599	-0.66399	2.74500	C	-5.74678	-3.29877	-6.41722
C	4.55276	-1.90219	-3.63890	H	-5.70732	-3.52297	-7.50396
H	4.26031	-0.83295	-3.59971	H	-5.87455	-4.25390	-5.86501
C	5.85484	-2.02867	-4.42689	H	-6.62126	-2.64212	-6.22081
H	5.73542	-1.54496	-5.41916	H	-0.58213	-3.49035	5.14038
H	6.68804	-1.53087	-3.89056	H	4.27948	-3.36734	4.76514
H	6.11313	-3.09674	-4.58633	H	4.51202	-2.22179	2.32094
C	-4.42237	4.49216	-3.99467	H	3.74690	-2.41726	-4.20275
H	-4.21909	4.54095	-5.08666	H	4.68413	-6.51295	-1.80318
C	-5.02753	5.82245	-3.55562	H	-3.58973	-3.26569	-6.19170
H	-5.31364	5.78626	-2.48300	H	-3.35626	-4.68600	-1.51248
H	-4.29882	6.64619	-3.71336	H	-4.37924	1.53372	-3.19983
H	-5.93756	6.03261	-4.15609	H	-5.16300	3.68146	-3.83438
C	0.58915	4.26884	-3.88663	H	0.43737	4.13262	-4.97980
H	1.33883	3.50884	-3.59309	H	-2.91736	2.44537	0.43838
C	1.15294	5.66847	-3.65766	H	2.62427	1.42140	2.11467
H	0.41113	6.43670	-3.96356	O	-0.99769	-2.28718	-0.40472
H	1.41768	5.82010	-2.59225	C	0.45272	-4.28601	-1.96357
H	2.07272	5.80067	-4.26544	C	-1.11123	-3.41988	-3.32054
C	-2.19157	3.27931	0.33590	C	0.94580	-5.21737	-0.90972
H	-1.23847	2.91648	0.77365	H	-1.83145	-3.89078	-3.98515
C	-2.68610	4.47642	1.14610	H	-1.53130	-2.55854	-2.79515
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H	-2.10448	5.38912	0.90574	H	2.03565	-5.16726	-0.88724
H	-3.75952	4.66802	0.93597	H	0.64650	-6.21599	-1.24927
C	4.23763	-2.32806	5.15714	C	0.23987	-3.10820	-3.95617
H	5.11642	-1.78312	4.74945	C	1.24297	-3.94908	1.24937
C	4.35292	-2.34863	6.67891	H	-0.65222	-4.56022	0.39832
H	5.32420	-2.80044	6.97112	H	0.31815	-5.89241	1.05145
H	4.30643	-1.31393	7.08092	H	0.28666	-2.07443	-4.30322
H	3.53561	-2.95283	7.12630	H	0.46257	-3.78193	-4.79152
C	-0.77269	-2.40792	4.97123	H	2.17792	-4.42847	1.56242
H	-1.51747	-2.36082	4.15348	H	0.72025	-3.60134	2.15116
C	-1.36988	-1.82807	6.25034	H	0.77153	-2.51087	0.07843
H	-0.63327	-1.88788	7.07977	C	1.14895	-3.35965	-2.75432
H	-1.67024	-0.77128	6.10436	O	-0.80524	-4.39961	-2.27944
H	-2.27240	-2.40933	6.53401	H	2.20636	-3.54564	-2.87732
C	1.88023	1.51081	2.93404	H	1.12741	-2.14021	-2.20931
H	0.92289	1.79833	2.45214	O	1.60927	-2.86813	0.42209
C	2.31168	2.62600	3.88388				
H	3.37892	2.50308	4.16490				
H	2.18514	3.60786	3.38684				
H	1.69362	2.62485	4.80453				
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H	-4.29936	1.15788	-1.47058				

S-gau-hc(-)



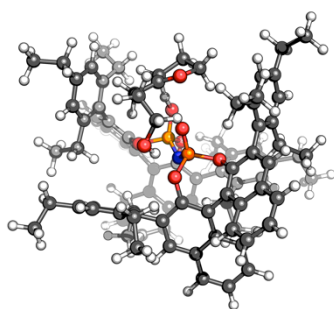
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C	-2.14646	-0.27494	2.48537
C	-1.50441	0.29874	3.59364
C	-3.48169	0.07084	2.18514
C	-2.12773	1.33105	4.30255
C	-4.08282	1.16813	2.85211
C	-3.39505	1.78922	3.92544
C	-4.22271	-0.76888	1.19883
C	-5.39854	-1.48613	1.54729
C	-3.67344	-0.92303	-0.09059
C	-6.07258	-2.24032	0.55256
C	-4.33283	-1.70443	-1.05656
C	-5.54173	-2.33031	-0.73798
H	-6.04828	-2.92175	-1.49219
H	-1.62236	1.77350	5.15313
C	-3.99109	2.85554	4.61720
C	-5.24865	3.32588	4.23599
H	-3.48028	3.33111	5.44609
H	-5.70002	4.15309	4.76828
C	-5.91968	2.74047	3.16232
C	-5.34456	1.67195	2.47112
H	-6.88826	3.11835	2.86162
H	-5.88568	1.25570	1.63166
C	-7.25401	-2.92893	0.87104
C	-7.75658	-2.90004	2.17193
H	-7.78099	-3.50138	0.11674
H	-8.66483	-3.43733	2.41260
C	-7.07902	-2.19815	3.16770
C	-5.90591	-1.50341	2.86553
H	-7.46108	-2.19653	4.18047
H	-5.39872	-0.99681	3.67464
N	-0.01187	0.10456	0.14704
P	1.12607	0.20746	-0.98482
O	1.21920	-0.84446	-2.03194
O	2.48523	0.25859	-0.05478
O	0.98459	1.65147	-1.74518
C	3.57422	0.90968	-0.58258
C	1.10967	2.77126	-0.95735
C	3.54178	2.30739	-0.76169
C	4.77919	0.21039	-0.79709

C	0.08056	3.73194	-0.92695
C	2.33621	3.05965	-0.32940
C	4.65044	2.96907	-1.35456
C	5.90805	0.88899	-1.27044
C	0.20043	4.85421	-0.09615
C	2.42359	4.14058	0.58244
C	5.84654	2.24783	-1.58212
C	4.59644	4.32688	-1.74268
H	6.83396	0.34453	-1.41623
C	1.34082	5.04460	0.68787
H	-0.58748	5.59721	-0.08544
C	3.56623	4.34921	1.38325
C	6.96760	2.89421	-2.12711
C	5.71619	4.95484	-2.29220
H	3.68982	4.90829	-1.64378
C	1.43105	6.15189	1.54636
C	3.63603	5.44536	2.24586
H	4.40173	3.66146	1.35817
C	6.90111	4.24343	-2.47540
H	7.89150	2.35293	-2.29391
H	5.66296	5.99664	-2.58106
C	2.57483	6.34785	2.32231
H	0.61439	6.85987	1.62338
H	4.51641	5.59540	2.85723
H	7.76642	4.73536	-2.90055
H	2.63598	7.19790	2.98939
C	-1.09615	3.64590	-1.82627
C	-0.95655	3.94824	-3.20941
C	-2.39214	3.42853	-1.28788
C	-2.10314	4.04729	-4.01330
C	-3.51561	3.54866	-2.12021
C	-3.38083	3.87758	-3.47245
H	-4.50643	3.38967	-1.71036
C	4.88796	-1.24950	-0.57199
C	5.01994	-1.76207	0.74406
C	4.99685	-2.13148	-1.68048
C	5.24998	-3.13411	0.93168
C	5.22094	-3.49785	-1.45463
C	5.34793	-4.00460	-0.15773
H	5.29185	-4.17465	-2.29783
C	-3.71122	-1.96069	-2.37816
C	-3.72178	-0.95847	-3.38106
C	-3.10114	-3.21523	-2.64916
C	-3.09957	-1.20687	-4.61473
C	-2.49646	-3.43232	-3.89621
C	-2.48920	-2.43742	-4.87844
H	-2.01379	-4.38149	-4.09923
C	-0.17608	-0.19152	4.03481
C	-0.07074	-1.40872	4.75884
C	0.99273	0.56838	3.77300
C	1.18618	-1.83428	5.21450
C	2.23189	0.12053	4.25694
C	2.33348	-1.06643	4.99015
H	3.12153	0.71062	4.07020
H	5.35974	-3.52601	1.93618
H	1.27014	-2.76035	5.77097
H	-3.10950	-0.44353	-5.38396

H	-2.00179	4.30472	-5.06115	C	-5.92541	0.23669	-3.40198
C	5.57336	-5.47874	0.06167	H	-6.36865	-0.48432	-2.68589
H	5.44711	-5.74049	1.13494	H	-6.41160	1.22232	-3.24725
C	6.97607	-5.89164	-0.37502	H	-6.13276	-0.10488	-4.43845
H	7.73897	-5.31639	0.19212	C	-3.04370	-4.33741	-1.63059
H	7.12424	-6.97343	-0.17356	H	-3.27594	-3.98712	-0.60423
H	7.11593	-5.71311	-1.46224	C	-4.00600	-5.46416	-1.99471
C	4.95452	-0.87618	1.96928	H	-3.95322	-6.26039	-1.22263
H	4.18569	-0.08716	1.85727	H	-5.04780	-5.08451	-2.04172
C	6.30703	-0.23906	2.26814	H	-3.73473	-5.90666	-2.97656
H	7.07696	-1.02529	2.41991	C	-1.82750	-2.69398	-6.20826
H	6.62073	0.42471	1.43676	H	-1.73337	-1.75077	-6.78948
H	6.23216	0.36888	3.19434	C	-2.62910	-3.69460	-7.03681
C	4.85752	-1.66126	-3.11652	H	-2.13707	-3.84043	-8.02147
H	4.44085	-0.63531	-3.18249	H	-2.68239	-4.67664	-6.52072
C	6.19720	-1.69842	-3.84832	H	-3.65911	-3.31399	-7.20673
H	6.06306	-1.32601	-4.88566	H	-0.96693	-3.31446	5.27065
H	6.94094	-1.05464	-3.33595	H	3.87291	-2.55317	5.20614
H	6.58786	-2.73682	-3.89584	H	4.64787	-1.47796	2.84909
C	-4.60448	4.06195	-4.33455	H	4.14235	-2.31917	-3.65244
H	-4.32516	4.10963	-5.40966	H	4.81790	-6.05978	-0.50961
C	-5.34368	5.34569	-3.96843	H	-0.80024	-3.08480	-6.04175
H	-5.70205	5.30388	-2.91793	H	-2.01163	-4.74483	-1.59185
H	-4.67345	6.22308	-4.09261	H	-4.02678	1.11507	-3.90266
H	-6.22210	5.47162	-4.63581	H	-5.28733	3.19638	-4.20980
C	0.38530	4.24669	-3.85207	H	0.33020	4.07468	-4.94933
H	1.17331	3.56223	-3.48327	H	-3.28714	2.18646	0.21758
C	0.80707	5.69481	-3.61945	H	1.77130	1.85137	2.23372
H	0.02962	6.38849	-4.00470	O	-0.99287	-2.32202	-0.40583
H	0.97027	5.89174	-2.54114	C	1.10241	-4.69068	-0.06442
H	1.75852	5.89379	-4.15616	C	1.80533	-3.07816	1.35810
C	-2.61975	3.07088	0.16579	C	1.21929	-5.66523	-1.17924
H	-1.67802	2.78437	0.67733	H	1.62280	-2.09343	0.91775
C	-3.26886	4.22492	0.92714	H	2.67603	-3.04167	2.00820
H	-3.28205	3.99500	2.01083	C	2.03303	-5.19175	-2.39452
H	-2.70158	5.16588	0.78087	H	1.67005	-6.56849	-0.74440
H	-4.31441	4.37587	0.58507	H	0.20094	-5.92013	-1.47654
C	3.66405	-1.51438	5.54178	C	0.56269	-3.71197	1.97983
H	4.48543	-0.86751	5.16434	H	1.76127	-5.84454	-3.22971
C	3.68062	-1.45414	7.06715	H	3.10360	-5.32244	-2.22013
H	4.68522	-1.74657	7.43889	H	0.82522	-4.40841	2.78356
H	3.46044	-0.42135	7.41259	H	-0.11594	-2.95324	2.36719
H	2.93106	-2.15186	7.49650	C	1.73377	-3.73065	-2.73563
C	-1.27800	-2.26147	5.09437	O	0.37138	-3.50249	-2.46785
H	-1.99507	-2.29561	4.24991	H	2.34138	-3.05951	-2.12197
C	-1.98124	-1.75132	6.34809	H	1.97489	-3.53763	-3.78941
H	-1.27874	-1.75031	7.20870	H	0.25636	-2.55294	-2.28227
H	-2.36799	-0.72384	6.19196	O	2.14453	-3.97276	0.23747
H	-2.83766	-2.41563	6.58889	C	-0.00846	-4.43382	0.76037
C	0.96027	1.86363	2.99161	H	-0.51469	-3.45946	0.09005
H	0.01177	1.99070	2.43119	H	-0.78062	-5.19317	0.84522
C	1.14906	3.06110	3.91863				
H	2.17820	3.07045	4.33575				
H	0.98721	3.99932	3.35349				
H	0.41758	3.02942	4.75247				
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S-gau-hc(+)



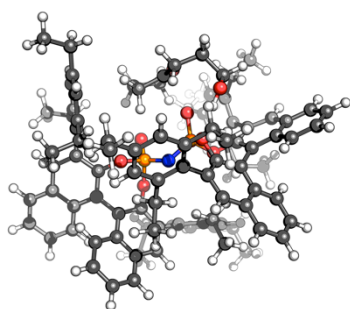
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C	-1.52138	-0.24582	2.59273
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C	-2.13937	1.84015	4.37689
C	-3.85855	-0.31682	1.75299
C	-5.04300	-0.81704	2.35725
C	-3.66785	-0.46037	0.36260
C	-6.10312	-1.26647	1.53490
C	-4.73189	-0.91939	-0.44207
C	-5.95010	-1.27648	0.14791
H	-6.77018	-1.60254	-0.48122
H	-0.26639	1.36163	5.32246
C	-2.42106	2.91233	5.23834
C	-3.61926	3.61768	5.11444
H	-1.71386	3.20600	6.00499
H	-3.82925	4.44659	5.77787
C	-4.54285	3.26210	4.13117
C	-4.27891	2.19304	3.27210
H	-5.46490	3.81981	4.03063
H	-5.00845	1.95775	2.50811
C	-7.30068	-1.71899	2.11183
C	-7.44204	-1.75844	3.49913
H	-8.12197	-2.05515	1.48988
H	-8.36476	-2.11452	3.93878
C	-6.38921	-1.35775	4.32040
C	-5.19634	-0.89635	3.75992
H	-6.49546	-1.40867	5.39640
H	-4.39558	-0.62204	4.43323
N	0.02145	0.22727	-0.08345
P	1.15693	0.25928	-1.16909
O	1.04834	-0.61166	-2.41801
O	2.54125	-0.09992	-0.37796
O	1.30479	1.75364	-1.79079
C	3.72018	0.39368	-0.89017
C	1.66992	2.72723	-0.89346
C	3.96820	1.78546	-0.90396
C	4.75122	-0.49732	-1.25726

C	0.82600	3.82944	-0.66789
C	2.95697	2.70987	-0.32411
C	5.16863	2.28073	-1.48216
C	5.98394	-0.00006	-1.69516
C	1.19048	4.80487	0.26891
C	3.29315	3.65070	0.68251
C	6.18977	1.37127	-1.84524
C	5.37618	3.65824	-1.72215
H	6.77624	-0.69385	-1.95145
C	2.39587	4.70732	0.96945
H	0.54104	5.65631	0.43242
C	4.50526	3.57356	1.40168
C	7.40373	1.84455	-2.36891
C	6.58476	4.11455	-2.25239
H	4.60612	4.39037	-1.52038
C	2.73513	5.67715	1.92636
C	4.82719	4.54206	2.35515
H	5.20178	2.76075	1.24258
C	7.59962	3.21160	-2.56520
H	8.19607	1.15598	-2.63810
H	6.73291	5.17281	-2.42502
C	3.94766	5.59377	2.61280
H	2.06203	6.49784	2.14444
H	5.75988	4.47365	2.89990
H	8.53501	3.57062	-2.97464
H	4.20224	6.34168	3.35251
C	-0.42030	4.02315	-1.44795
C	-0.35348	4.46602	-2.79735
C	-1.68521	3.89914	-0.81582
C	-1.53824	4.79158	-3.47630
C	-2.84698	4.25041	-1.52058
C	-2.78068	4.71045	-2.83997
H	-3.81266	4.17080	-1.03511
C	4.55833	-1.96795	-1.25088
C	4.55863	-2.68786	-0.02825
C	4.49832	-2.67977	-2.48007
C	4.46816	-4.08820	-0.04918
C	4.43191	-4.08238	-2.46280
C	4.41483	-4.78946	-1.25712
H	4.37661	-4.62529	-3.39904
C	-4.58724	-1.10424	-1.90653
C	-4.57628	0.01629	-2.77669
C	-4.59011	-2.41519	-2.45764
C	-4.54663	-0.18518	-4.16574
C	-4.59355	-2.57742	-3.85112
C	-4.56357	-1.47368	-4.70754
H	-4.58995	-3.57517	-4.27421
C	0.59188	-0.71583	3.87595
C	0.50599	-2.01495	4.44695
C	1.86654	-0.13794	3.64293
C	1.68436	-2.70058	4.77934
C	3.02213	-0.84124	4.01492
C	2.93919	-2.11393	4.58911
H	3.99459	-0.39037	3.85553
H	4.46511	-4.64188	0.88266
H	1.62553	-3.68880	5.22041
H	-4.54483	0.67055	-4.83092

H	-1.48799	5.15334	-4.49667	C	-6.12902	1.85416	-2.08543
C	4.33309	-6.29473	-1.25497	H	-6.62871	1.20210	-1.33873
H	3.53461	-6.62387	-0.55526	H	-6.17144	2.90289	-1.72315
C	5.66343	-6.91553	-0.83919	H	-6.67305	1.78901	-3.05175
H	5.92984	-6.61205	0.19545	C	-4.54315	-3.66583	-1.59947
H	5.58298	-8.02245	-0.87256	H	-4.31618	-3.43733	-0.53838
H	6.46934	-6.59608	-1.53411	C	-5.85577	-4.44365	-1.66343
C	4.72659	-2.00672	1.31087	H	-5.79266	-5.33032	-0.99804
H	4.16123	-1.05632	1.35291	H	-6.70292	-3.81122	-1.32837
C	6.19758	-1.74314	1.61611	H	-6.05269	-4.79547	-2.69792
H	6.76331	-2.69904	1.63121	C	-4.54095	-1.67683	-6.20092
H	6.64209	-1.06751	0.85713	H	-4.32148	-0.72110	-6.72498
H	6.28941	-1.25961	2.61109	C	-5.88048	-2.20798	-6.70445
C	4.46062	-1.98259	-3.82894	H	-5.84505	-2.31785	-7.80875
H	4.27485	-0.89336	-3.73281	H	-6.10054	-3.20122	-6.25881
C	5.75819	-2.19465	-4.60569	H	-6.69633	-1.50045	-6.44316
H	5.70653	-1.64591	-5.56955	H	-0.69026	-3.77986	4.84112
H	6.62637	-1.81446	-4.02980	H	4.17892	-3.87167	4.54976
H	5.91164	-3.27254	-4.82355	H	4.31193	-2.65095	2.11347
C	-4.03582	5.13376	-3.56260	H	3.61699	-2.38364	-4.42992
H	-3.83509	5.28058	-4.64628	H	4.06531	-6.67517	-2.26485
C	-4.58419	6.43810	-2.99157	H	-3.73250	-2.39273	-6.46467
H	-4.86763	6.30890	-1.92547	H	-3.72241	-4.32239	-1.95769
H	-3.82303	7.24318	-3.07423	H	-4.19070	2.12236	-2.99573
H	-5.48716	6.74209	-3.56180	H	-4.80893	4.34246	-3.47650
C	0.96127	4.67091	-3.52586	H	0.79984	4.63165	-4.62539
H	1.68016	3.85939	-3.29980	H	-2.61164	2.61612	0.64294
C	1.58283	6.02203	-3.18399	H	2.78015	1.15081	2.18347
H	0.87726	6.84351	-3.43173	O	-1.09178	-2.14810	-0.60144
H	1.84344	6.07687	-2.10805	C	0.15003	-3.94678	-2.11943
H	2.51262	6.16181	-3.77463	C	-1.35869	-3.21892	-3.60247
C	-1.83632	3.41030	0.60973	C	0.63030	-4.65272	-0.90116
H	-0.90302	2.94958	0.99472	H	-2.07113	-3.72252	-4.25271
C	-2.24549	4.55062	1.53954	H	-1.78546	-2.32219	-3.14448
H	-2.16456	4.21953	2.59323	C	-0.35637	-5.63165	-0.26488
H	-1.58333	5.42973	1.40423	H	0.89695	-3.87268	-0.17531
H	-3.29502	4.85418	1.34096	H	1.56365	-5.15230	-1.17839
C	4.18930	-2.85345	4.99529	C	0.00994	-2.93716	-4.21427
H	5.09541	-2.33417	4.61510	C	-1.43430	-4.93644	0.56329
C	4.29974	-2.95881	6.51387	H	-0.82508	-6.25740	-1.03312
H	5.24515	-3.47567	6.78209	H	0.20882	-6.29268	0.40040
H	4.30685	-1.94530	6.96902	H	0.05868	-1.92682	-4.62634
H	3.45036	-3.54124	6.92935	H	0.26160	-3.65588	-5.00262
C	-0.81830	-2.67710	4.77707	H	-2.11956	-5.69456	0.96253
H	-1.56675	-2.50828	3.97877	H	-1.99917	-4.24410	-0.06559
C	-1.36902	-2.18265	6.11128	H	-0.95171	-3.29858	1.52398
H	-0.63525	-2.37153	6.92367	C	0.88035	-3.11096	-2.97320
H	-1.59475	-1.09817	6.06806	O	-1.08678	-4.12261	-2.49047
H	-2.30874	-2.72483	6.34757	H	1.93550	-3.32383	-3.06556
C	2.03581	1.22446	3.00426	H	0.91519	-1.84998	-2.45838
H	1.09644	1.58797	2.53848	O	-0.84566	-4.25054	1.65191
C	2.51202	2.25357	4.02711				
H	3.56858	2.05941	4.30828				
H	2.44015	3.27008	3.59366				
H	1.88392	2.22502	4.94057				
C	-4.67411	1.43700	-2.26979				
H	-4.13187	1.57201	-1.31565				

S-gau-hc(+)-intermediate



E(RM062X) = -5019.79679362

P	-1.13018	-0.90002	-0.09291
O	-2.38559	0.07314	-0.46177
O	-1.46311	-1.54002	1.40442
C	-1.97116	-0.68044	2.34554
C	-1.27471	-0.49456	3.55128
C	-3.26340	-0.13662	2.18923
C	-1.79202	0.35357	4.53478
C	-3.74115	0.80209	3.13951
C	-2.99883	1.02897	4.32608
C	-4.11120	-0.61842	1.05840
C	-5.37122	-1.23564	1.27261
C	-3.62832	-0.47111	-0.25708
C	-6.19940	-1.52833	0.15982
C	-4.45673	-0.77258	-1.35795
C	-5.74975	-1.26074	-1.13685
H	-6.39087	-1.47046	-1.98483
H	-1.24826	0.48767	5.46290
C	-3.47966	1.92423	5.29474
C	-4.67080	2.61907	5.08023
H	-2.92742	2.09649	6.21097
H	-5.03173	3.31543	5.82600
C	-5.39077	2.42762	3.90107
C	-4.93356	1.52852	2.93533
H	-6.30652	2.97959	3.73327
H	-5.50892	1.42031	2.02534
C	-7.46519	-2.10283	0.35696
C	-7.90335	-2.41534	1.64411
H	-8.11036	-2.32192	-0.48572
H	-8.87763	-2.86391	1.78930
C	-7.08135	-2.16658	2.74248
C	-5.82338	-1.58742	2.56327
H	-7.41833	-2.42722	3.73753
H	-5.20731	-1.43448	3.43891
N	0.11958	0.04568	0.02874
P	1.25823	0.34250	-1.05720
O	1.20659	-0.31787	-2.39088
O	2.60580	-0.10000	-0.21842
O	1.34367	1.95532	-1.33606
C	3.79133	0.47672	-0.60032
C	1.68596	2.75399	-0.27206
C	4.00428	1.85387	-0.39035
C	4.85680	-0.33351	-1.04333

C	0.84570	3.81948	0.10297
C	2.96171	2.64549	0.31532
C	5.21109	2.45508	-0.83674
C	6.08893	0.24834	-1.36414
C	1.18497	4.62353	1.19846
C	3.26364	3.39314	1.48132
C	6.26384	1.63192	-1.30271
C	5.39516	3.85595	-0.84215
H	6.90928	-0.38401	-1.68249
C	2.36458	4.39740	1.91137
H	0.53716	5.44601	1.47786
C	4.44079	3.16895	2.22626
C	7.48134	2.20422	-1.70483
C	6.60807	4.41219	-1.25401
H	4.60308	4.53136	-0.54782
C	2.67368	5.18432	3.03238
C	4.72614	3.94556	3.35133
H	5.13607	2.38519	1.95442
C	7.65116	3.58869	-1.67572
H	8.29745	1.58138	-2.05184
H	6.73780	5.48679	-1.24974
C	3.84933	4.95507	3.74894
H	2.00032	5.96694	3.36128
H	5.63104	3.76397	3.91663
H	8.58961	4.02503	-1.99263
H	4.07781	5.55692	4.61894
C	-0.35105	4.18616	-0.69212
C	-0.19822	4.89120	-1.91717
C	-1.65101	3.99221	-0.15680
C	-1.33193	5.41138	-2.56057
C	-2.76005	4.53955	-0.81980
C	-2.60705	5.26384	-2.00665
H	-3.75334	4.39790	-0.40964
C	4.70988	-1.80039	-1.20979
C	4.68800	-2.65293	-0.07407
C	4.71288	-2.37180	-2.51228
C	4.66474	-4.04454	-0.25524
C	4.69331	-3.76803	-2.65386
C	4.67783	-4.60698	-1.53555
H	4.68249	-4.20325	-3.64623
C	-3.96259	-0.61069	-2.75184
C	-3.69936	0.68614	-3.26847
C	-3.72714	-1.74661	-3.57741
C	-3.10009	0.82103	-4.53102
C	-3.13465	-1.57151	-4.83743
C	-2.80351	-0.29979	-5.31102
H	-2.91807	-2.43740	-5.45257
C	-0.01984	-1.23511	3.81949
C	-0.07160	-2.57017	4.29728
C	1.23638	-0.59542	3.66955
C	1.12275	-3.24237	4.59840
C	2.41133	-1.29159	3.99231
C	2.36240	-2.60834	4.46207
H	3.36949	-0.79484	3.89242
H	4.64788	-4.69930	0.60831
H	1.08495	-4.26254	4.96258
H	-2.88373	1.80858	-4.92150

H	-1.21457	5.97106	-3.48120	C	-5.61157	2.17340	-2.60702
C	4.63607	-6.10423	-1.70440	H	-6.16386	1.33699	-2.13365
H	3.80171	-6.52162	-1.10000	H	-5.87296	3.10841	-2.06886
C	5.95258	-6.74414	-1.27264	H	-5.93236	2.26934	-3.66618
H	6.14370	-6.55767	-0.19460	C	-4.08668	-3.16145	-3.16757
H	5.90339	-7.84117	-1.43686	H	-4.33422	-3.24235	-2.09485
H	6.79343	-6.33209	-1.87070	C	-5.27591	-3.68315	-3.97088
C	4.74736	-2.12316	1.34316	H	-5.54387	-4.70136	-3.61792
H	4.13116	-1.21210	1.46288	H	-6.15557	-3.01895	-3.83918
C	6.18297	-1.82969	1.76549	H	-5.02325	-3.74110	-5.05082
H	6.80075	-2.74996	1.69141	C	-2.14577	-0.14235	-6.65816
H	6.62655	-1.03895	1.12644	H	-1.77094	0.89567	-6.79378
H	6.19421	-1.47740	2.81841	C	-3.12239	-0.45604	-7.78843
C	4.70880	-1.53154	-3.77642	H	-2.61995	-0.30166	-8.76650
H	4.47711	-0.46656	-3.57009	H	-3.46290	-1.51159	-7.73025
C	6.04608	-1.61495	-4.50939	H	-4.00421	0.21733	-7.73103
H	6.01562	-0.96610	-5.40989	H	-1.30011	-4.34409	4.21622
H	6.87425	-1.27266	-3.85643	H	3.66443	-4.31306	4.30201
H	6.24880	-2.65703	-4.83493	H	4.32141	-2.87201	2.04342
C	-3.80804	5.87595	-2.68331	H	3.91113	-1.89529	-4.45803
H	-3.54205	6.24831	-3.69659	H	4.44365	-6.37570	-2.76535
C	-4.36189	7.04246	-1.87005	H	-1.26844	-0.82191	-6.72314
H	-4.71085	6.69446	-0.87471	H	-3.21956	-3.82990	-3.34135
H	-3.58029	7.82017	-1.73338	H	-3.60388	2.82679	-2.98560
H	-5.22277	7.49364	-2.40688	H	-4.59845	5.10761	-2.81258
C	1.15809	5.17131	-2.53516	H	1.05411	5.31326	-3.63317
H	1.84743	4.31391	-2.40847	H	-2.69549	2.46256	0.93460
C	1.78804	6.42971	-1.94553	H	2.18064	0.91714	2.46715
H	1.11782	7.30262	-2.09680	O	-1.14056	-2.12050	-0.97034
H	1.98272	6.30252	-0.86158	C	-0.09061	-4.04780	-1.65172
H	2.75519	6.63184	-2.45212	C	-0.13698	-3.00195	-3.63718
C	-1.89573	3.21075	1.11617	C	-0.51066	-4.94140	-0.55119
H	-0.99900	2.63979	1.42925	H	-0.41181	-3.30986	-4.64386
C	-2.31946	4.13218	2.25750	H	-0.56448	-2.03613	-3.35790
H	-2.35315	3.56003	3.20512	C	-1.96810	-5.39989	-0.53321
H	-1.59605	4.96333	2.38221	H	-0.23811	-4.45059	0.39098
H	-3.32811	4.55359	2.06250	H	0.17395	-5.79982	-0.64130
C	3.63042	-3.33645	4.83148	C	1.33334	-3.08683	-3.27176
H	4.52434	-2.75523	4.51723	C	-2.88076	-4.40515	0.18279
C	3.71774	-3.56558	6.33805	H	-2.32817	-5.58192	-1.55130
H	4.67756	-4.06781	6.58177	H	-2.01271	-6.34957	0.00893
H	3.67767	-2.59454	6.87649	H	1.80739	-2.11981	-3.42374
H	2.88456	-4.21216	6.68578	H	1.83845	-3.87690	-3.83396
C	-1.37836	-3.29020	4.56121	H	-3.90150	-4.80431	0.20071
H	-2.22471	-2.84100	4.00476	H	-2.87472	-3.45254	-0.35152
C	-1.71713	-3.26765	6.04830	H	-2.03999	-3.34094	1.57314
H	-0.92482	-3.77862	6.63594	C	1.25750	-3.42248	-1.77522
H	-1.81781	-2.21925	6.40222	O	-0.76858	-3.98059	-2.72203
H	-2.67983	-3.79413	6.21843	H	2.00650	-4.12751	-1.41180
C	1.36196	0.83970	3.21255	H	1.29873	-2.51970	-1.15983
H	0.44270	1.19443	2.70587	O	-2.44696	-4.21776	1.51497
C	1.65869	1.75545	4.39668				
H	2.68214	1.56679	4.78446				
H	1.58670	2.81304	4.07891				
H	0.92354	1.59214	5.21187				
C	-4.10428	1.94619	-2.53302				
H	-3.78356	1.91636	-1.47476				

Energies of TS structures of the reaction of 2 with cat II

TS	dist C-O	$\Delta\Delta G$
R-anti-C ₄ -C(-)	2.59	13.7
R-anti-C ₄ -B(-)	2.53	16.0
R-anti-C ₄ -C(+)	2.68	14.6
R-anti-C ₄ -C(+)	2.66	11.4
R-anti-B _{2,5} -C(-)	3.53	7.2
R-anti-B _{2,5} -B(-)	3.52	2.4
R-anti-B _{2,5} -B(-) intermediate		-2.0
R-anti-B _{2,5} -B(-) 2 nd step		10.2
R-anti-B _{2,5} -C(+)	2.70	19.5
R-anti-B _{2,5} -C(+)	2.83	14.8
R-anti-B _{1,4} -C(-)	2.58	23.7
R-anti-B _{1,4} -B(-)	2.58	21.9
R-anti-B _{1,4} -C(+)	2.60	21.1
R-anti-B _{1,4} -C(+)	2.71	17.5
R-gau-C ₄ -C(-)	3.42	1.6
R-gau-C ₄ -C(-) intermediate		-2.7
R-gau-C ₄ -C(-) 2 nd step		4.1
R-gau-C ₄ -B(-)		0.0
R-gau-C ₄ -B(-) intermediate		-3.0
R-gau-C ₄ -B(-) 2 nd step		1.9
R-gau-C ₄ -C(+)	2.57	19.4
R-gau-C ₄ -C(+)	2.58	17.0
R-gau-B _{2,5} -C(-)	3.07	8.0
R-gau-B _{2,5} -B(-)	2.88	10.6
R-gau-B _{2,5} -C(+)	2.70	16.3
R-gau-B _{2,5} -C(+)	2.72	13.0
R-gau-B _{1,4} -C(-)	3.47	3.0
R-gau-B _{1,4} -C(-) intermediate		-0.6
R-gau-B _{1,4} -C(-) 2 nd step		13.7
R-gau-B _{1,4} -B(-)	3.27	1.7
R-gau-B _{1,4} -B(-) intermediate		-1.1
R-gau-B _{1,4} -B(-) 2 nd step		13.7
R-gau-B _{1,4} -C(+)	2.78	16.9
R-gau-B _{1,4} -C(+)	2.78	14.1

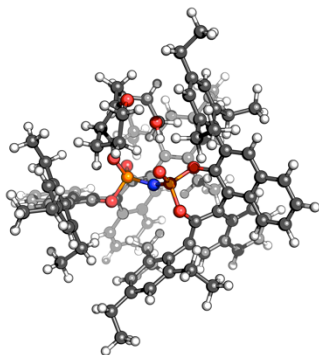
TS	Dist C-O	$\Delta\Delta G$
S-anti-C ₄ -C(-)	2.62	7.2
S-anti-C ₄ -B(-)	2.59	4.0
S-anti-C ₄ -C(+)*	3.31	18.7
S-anti-C ₄ -C(+)*	3.43	14.8
S-anti-B _{2,5} -C(-)	2.75	7.2
S-anti-B _{2,5} -B(-)	2.68	10.1
S-anti-B _{2,5} -C(+)	2.81	21.2
S-anti-B _{2,5} -C(+)	2.85	22.4
S-anti-B _{1,4} -C(-)	2.73	9.1
S-anti-B _{1,4} -B(-)	2.70	5.7
S-anti-B _{1,4} -C(+)*	3.80	12.5
S-anti-B _{1,4} -C(+)*	3.48	10.8
S-gau-C ₄ -C(-)	2.62	7.1
S-gau-C ₄ -B(-)	2.62	5.9
S-gau-C ₄ -C(+)	2.57	18.7
S-gau-C ₄ -C(+)	2.72	15.9
S-gau-B _{2,5} -C(-)	2.78	4.1
S-gau-B _{2,5} -B(-)	2.88	6.4
S-gau-B _{2,5} -C(+)*	3.42	16.2
S-gau-B _{2,5} -C(+)	2.72	11.4
S-gau-B _{1,4} -C(-)	2.90	8.8
S-gau-B _{1,4} -B(-)	2.89	6.6
S-gau-B _{1,4} -C(+)	3.00	15.1
S-gau-B _{1,4} -C(+)	2.84	12.4

*These TS structures correspond to the first step of an stepwise mechanism; however, since the high energy of them prevent that these stepwise paths contribute to the product distribution, none of the other points in the path have been calculated.

Cartesian coordinates of TS structures and intermediates for the reaction of 2 with cat I.

R-anti-C₄-C(-)

E(RM062X) = -5098.38438836



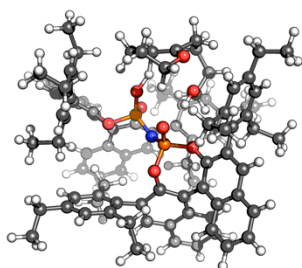
C	1.09513	2.82209	-1.10922
C	0.08789	3.80391	-1.06072
C	2.36492	3.12153	-0.57668
C	0.27390	4.95701	-0.28560
C	2.52915	4.24317	0.27304
C	1.46465	5.16316	0.41482
C	3.52510	2.32259	-1.04013
C	4.59470	2.91760	-1.76121
C	3.53446	0.93887	-0.78224
C	5.73933	2.14302	-2.06596
C	4.68691	0.18478	-1.08516
C	5.78387	0.79641	-1.70198
H	6.66563	0.20612	-1.92605
H	-0.50205	5.71190	-0.25644
C	1.62335	6.30323	1.21870
C	2.82285	6.52241	1.89833
H	0.81926	7.02191	1.32384
H	2.93811	7.39956	2.52176
C	3.87136	5.60959	1.78051
C	3.73046	4.47700	0.97551
H	4.79608	5.77850	2.31691
H	4.55777	3.78135	0.91936
C	6.82188	2.72166	-2.74776
C	6.76554	4.05511	-3.15382
H	7.70647	2.13912	-2.97693
H	7.60044	4.49456	-3.68422
C	5.62782	4.81750	-2.89313
C	4.54699	4.25712	-2.20916
H	5.58027	5.84613	-3.22679
H	3.67382	4.87588	-2.05355
C	-3.73330	-0.82457	0.36137
C	-1.80425	-0.07341	2.65655
C	-4.05955	-0.52268	1.70371
C	-4.65956	-1.52281	-0.44393
C	-1.00490	0.50907	3.65473

C	-3.14005	0.34422	2.49446
C	-5.23741	-1.07133	2.27967
C	-5.88826	-1.92207	0.09470
C	-1.48341	1.60964	4.37533
C	-3.59388	1.51106	3.16211
C	-6.17004	-1.73736	1.44895
C	-5.50778	-0.98771	3.66439
H	-6.60842	-2.42617	-0.54112
C	-2.75355	2.13399	4.11733
H	-0.86649	2.04810	5.15038
C	-4.86480	2.07072	2.90816
C	-7.36733	-2.23430	1.98892
C	-6.69798	-1.49537	4.18958
H	-4.80068	-0.54644	4.35341
C	-3.20672	3.25936	4.82411
C	-5.30019	3.19353	3.61538
H	-5.52148	1.65557	2.15507
C	-7.63034	-2.10656	3.35280
H	-8.09303	-2.73455	1.35845
H	-6.89595	-1.41753	5.25089
C	-4.47661	3.78223	4.57491
H	-2.57748	3.73645	5.56611
H	-6.27759	3.61235	3.41377
H	-8.55190	-2.49718	3.76473
H	-4.81899	4.65254	5.11957
C	0.33085	-0.04382	3.98792
C	0.43908	-1.24998	4.73142
C	1.50754	0.67315	3.64658
C	1.70575	-1.70182	5.13179
C	2.75710	0.19423	4.07017
C	2.86219	-0.97814	4.82545
H	3.65298	0.75059	3.82124
C	-4.35140	-1.88946	-1.85179
C	-4.34782	-0.89615	-2.86467
C	-4.12005	-3.25241	-2.19798
C	-4.03909	-1.25410	-4.18459
C	-3.85618	-3.57489	-3.54504
C	-3.79102	-2.58418	-4.52935
H	-3.67038	-4.59488	-3.84793
C	4.76080	-1.26863	-0.82646
C	5.11235	-1.74507	0.46047
C	4.61554	-2.18690	-1.89904
C	5.28604	-3.12233	0.66447
C	4.79870	-3.55791	-1.66110
C	5.12993	-4.03086	-0.38713
H	4.69443	-4.26060	-2.47823
C	-1.14128	3.70073	-1.88258
C	-1.08070	3.92893	-3.28531
C	-2.40408	3.53520	-1.25632
C	-2.27210	3.99839	-4.02369

C	-3.57468	3.64052	-2.02258	C	-3.12899	4.44737	0.96638
C	-3.51718	3.88257	-3.39879	H	-4.20611	4.56514	0.72362
H	-4.53901	3.53010	-1.54054	H	-3.02525	4.29598	2.05862
H	-4.02440	-0.49470	-4.95775	H	-2.59516	5.38111	0.69778
H	-2.23358	4.17798	-5.09180	C	5.32730	-0.81427	1.63202
H	5.54929	-3.49110	1.64917	H	4.66011	0.06963	1.57394
H	1.79218	-2.61599	5.70722	C	6.77914	-0.35662	1.71173
C	-3.45093	-2.95276	-5.95148	H	7.05903	0.21212	0.80093
H	-3.23868	-2.04275	-6.55415	H	6.91117	0.30285	2.59520
C	-4.59577	-3.71486	-6.61314	H	7.45365	-1.23294	1.81780
H	-5.52055	-3.09911	-6.60648	C	4.26547	-1.74303	-3.30640
H	-4.32886	-3.94442	-7.66620	H	3.89366	-0.69833	-3.33611
H	-4.78833	-4.67123	-6.08243	C	5.46601	-1.86261	-4.24109
C	-4.73820	0.53873	-2.58923	H	5.18216	-1.51141	-5.25548
H	-4.28675	0.90367	-1.64737	H	6.30763	-1.23957	-3.87378
C	-6.25446	0.69631	-2.52768	H	5.79956	-2.91925	-4.31516
H	-6.71011	0.39579	-3.49516	C	5.32353	-5.50536	-0.14662
H	-6.68408	0.07707	-1.71458	H	4.76811	-5.81040	0.76640
H	-6.51028	1.75744	-2.32777	C	6.80222	-5.84190	0.02040
C	-4.14840	-4.33147	-1.11557	H	6.91931	-6.93536	0.17360
H	-3.39403	-4.07886	-0.34028	H	7.36760	-5.54741	-0.88970
C	-3.89993	-5.76879	-1.58066	H	7.22531	-5.31415	0.90147
H	-3.93281	-6.44905	-0.70356	H	0.09492	3.95856	-5.10723
H	-4.69024	-6.08601	-2.29384	H	-4.73552	3.31386	-5.07818
H	-2.90324	-5.87004	-2.05485	H	-4.35397	1.19660	-3.39609
C	4.20702	-1.45933	5.31117	H	-5.14459	-4.33268	-0.63022
H	4.36769	-2.50670	4.97547	H	-2.53117	-3.57722	-5.96165
C	4.30777	-1.38588	6.83281	H	4.91734	-6.09800	-0.99537
H	4.13305	-0.34468	7.17898	H	3.44173	-2.37137	-3.69843
H	3.56568	-2.06025	7.30965	H	5.06659	-1.33892	2.57323
H	5.32339	-1.70095	7.15255	H	5.02543	-0.83974	4.88512
C	-0.77156	-2.05159	5.16821	H	-0.47949	-3.10384	5.37829
H	-1.53221	-2.10644	4.36526	H	2.22947	1.89499	2.03235
C	-1.39554	-1.46780	6.43226	H	-3.21379	2.37205	0.35960
H	-0.64587	-1.43653	7.25151	P	1.08182	0.25297	-1.03458
H	-1.77695	-0.44330	6.24758	O	2.46256	0.35984	-0.14190
H	-2.24659	-2.10452	6.75337	O	0.89962	1.66903	-1.83628
C	1.47375	1.95535	2.84231	N	-0.06451	0.13979	0.07409
H	0.49457	2.11250	2.34456	P	-1.17564	-0.93462	0.34362
C	1.78296	3.16309	3.72385	O	-1.07144	-2.36302	-0.16222
H	1.59732	4.09603	3.15650	O	-2.58242	-0.31722	-0.19790
H	1.13489	3.17201	4.62364	O	-1.33374	-1.15445	1.95523
H	2.84639	3.14726	4.04321	O	1.22254	-0.84678	-2.03130
C	-4.78369	4.00425	-4.20846	H	-0.41750	-3.27951	-0.71701
H	-5.66827	3.71333	-3.60234	C	-0.31415	-4.42377	-1.41984
C	-4.98996	5.43467	-4.69930	C	0.92761	-4.96367	-1.08839
H	-5.94591	5.50019	-5.26033	C	-0.59418	-3.97172	-2.84309
H	-5.03513	6.13331	-3.83657	H	-1.12608	-4.85334	-0.83390
H	-4.16378	5.74035	-5.37552	C	1.24040	-5.59132	0.23770
C	0.22434	4.16685	-4.02259	O	1.92248	-5.06612	-1.93054
H	1.01596	3.47334	-3.67914	C	0.72909	-3.64504	-3.52733
C	0.69811	5.60985	-3.87223	H	-1.13166	-4.74360	-3.40746
H	-0.08675	6.31128	-4.22726	H	-1.21916	-3.07475	-2.81614
H	0.94275	5.83945	-2.81615	C	0.77966	-4.86052	1.51174
H	1.61405	5.76363	-4.48077	H	2.31963	-5.75942	0.26507
C	-2.54436	3.24725	0.22379	H	0.76627	-6.58229	0.19038
H	-1.57552	2.97184	0.68980	C	1.67545	-4.80782	-3.33614

H	1.14933	-2.73355	-3.09179
H	0.58792	-3.47113	-4.59858
C	1.81059	-3.87145	2.07180
H	-0.17197	-4.34023	1.34241
H	0.58669	-5.62530	2.27096
H	2.66336	-4.64136	-3.76190
H	1.26460	-5.73596	-3.75160
C	1.84399	-2.56083	1.30877
H	2.80612	-4.33389	2.06070
H	1.56791	-3.65808	3.11755
O	2.06781	-2.87859	-0.05253
H	2.62372	-1.89571	1.69760
H	0.88771	-2.04961	1.44854
H	1.89964	-2.12348	-0.64155

R-anti-C₄-B(-)



E(RM062X) = -5098.38041751

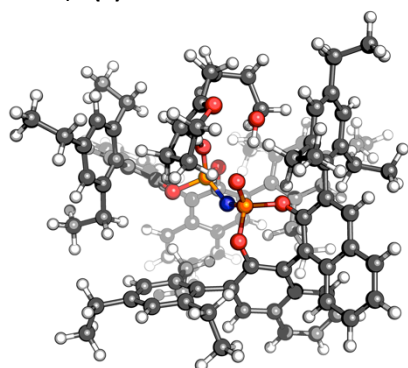
C	0.92638	2.85771	-0.94974
C	-0.10762	3.81067	-0.88560
C	2.18184	3.18571	-0.40004
C	0.02746	4.93305	-0.05585
C	2.29813	4.27310	0.50043
C	1.19967	5.14608	0.67271
C	3.37767	2.48166	-0.92031
C	4.40510	3.17842	-1.61251
C	3.46250	1.08722	-0.75375
C	5.58383	2.48672	-1.97948
C	4.64285	0.41538	-1.12788
C	5.69936	1.12221	-1.71219
H	6.60295	0.59200	-1.99380
H	-0.76971	5.66444	-0.01162
C	1.31028	6.25496	1.52672
C	2.49693	6.48926	2.22388
H	0.47948	6.93853	1.65569
H	2.57527	7.34191	2.88584
C	3.58074	5.62364	2.07248
C	3.48711	4.52261	1.21814
H	4.49578	5.80421	2.62149
H	4.34060	3.86196	1.13563
C	6.62729	3.16500	-2.62973
C	6.49825	4.51792	-2.94411
H	7.53771	2.64575	-2.90513
H	7.30365	5.03490	-3.44965
C	5.32534	5.20038	-2.62517

C	4.28255	4.53988	-1.97237
H	5.22075	6.24493	-2.88914
H	3.38029	5.10065	-1.77175
C	-3.71149	-0.98132	0.30068
C	-1.83146	-0.28283	2.66481
C	-4.06492	-0.71603	1.64486
C	-4.64582	-1.60949	-0.55430
C	-1.05460	0.28902	3.68843
C	-3.16704	0.13009	2.48325
C	-5.27350	-1.24977	2.16894
C	-5.91362	-1.95280	-0.06955
C	-1.56194	1.36021	4.43247
C	-3.64634	1.27391	3.17572
C	-6.21777	-1.82500	1.28604
C	-5.56886	-1.22626	3.55067
H	-6.63922	-2.39293	-0.74571
C	-2.83342	1.87540	4.16726
H	-0.96350	1.78631	5.22862
C	-4.91861	1.82922	2.91490
C	-7.44939	-2.28955	1.77511
C	-6.79275	-1.70264	4.02520
H	-4.85585	-0.85421	4.27410
C	-3.31434	2.97088	4.90221
C	-5.38478	2.91773	3.65528
H	-5.55373	1.43817	2.13136
C	-7.73539	-2.22146	3.13880
H	-8.18448	-2.71901	1.10462
H	-7.00969	-1.67103	5.08516
C	-4.58762	3.48324	4.65000
H	-2.70514	3.43095	5.67124
H	-6.36363	3.33082	3.44906
H	-8.68361	-2.58695	3.51134
H	-4.95221	4.32898	5.21840
C	0.29618	-0.23078	4.01255
C	0.44025	-1.44100	4.74170
C	1.45122	0.52415	3.67878
C	1.72073	-1.86342	5.12998
C	2.71786	0.06145	4.06688
C	2.85941	-1.12114	4.79876
H	3.59866	0.63625	3.80521
C	-4.30780	-1.94334	-1.96356
C	-4.20419	-0.91165	-2.93247
C	-4.10529	-3.29998	-2.35556
C	-3.79167	-1.22228	-4.23577
C	-3.69008	-3.56709	-3.67629
C	-3.52114	-2.53971	-4.60863
H	-3.46536	-4.57591	-3.99124
C	4.79132	-1.04732	-0.99093
C	5.30506	-1.59729	0.20893
C	4.61613	-1.87937	-2.12717
C	5.67516	-2.94973	0.24411
C	4.96285	-3.23674	-2.04710
C	5.51467	-3.77008	-0.87732
H	4.83151	-3.87350	-2.91408
C	-1.30077	3.72554	-1.76077
C	-1.18442	4.00566	-3.15116
C	-2.58683	3.53093	-1.19331

C	-2.34466	4.08709	-3.93613	H	-1.83101	2.91460	0.76636
C	-3.72585	3.65891	-2.00266	C	-3.42020	4.35458	1.02584
C	-3.61351	3.94265	-3.36776	H	-4.49838	4.43626	0.77303
H	-4.70790	3.52750	-1.56425	H	-3.32035	4.18891	2.11645
H	-3.70148	-0.43362	-4.97375	H	-2.92025	5.31290	0.77892
H	-2.26346	4.29981	-4.99569	C	5.50075	-0.76739	1.45826
H	6.09555	-3.36703	1.15195	H	4.83398	0.11918	1.46922
H	1.83496	-2.78223	5.69316	C	6.94821	-0.30614	1.58827
C	-3.05477	-2.85602	-6.00726	H	7.23174	0.32377	0.71875
H	-2.76304	-1.92712	-6.54434	H	7.06412	0.29457	2.51483
C	-4.15026	-3.55443	-6.80793	H	7.63032	-1.18105	1.64452
H	-5.05334	-2.90972	-6.86503	C	4.08509	-1.34906	-3.44511
H	-3.78825	-3.75113	-7.83903	H	3.61949	-0.34833	-3.33480
H	-4.42091	-4.52377	-6.33822	C	5.19069	-1.25654	-4.49276
C	-4.59598	0.51747	-2.63240	H	4.77206	-0.85058	-5.43768
H	-4.20978	0.84205	-1.64765	H	5.99844	-0.57985	-4.14409
C	-6.11135	0.69052	-2.67358	H	5.61815	-2.26028	-4.69979
H	-6.49643	0.44696	-3.68667	C	5.95586	-5.20977	-0.82852
H	-6.60518	0.03443	-1.92882	H	5.61050	-5.67745	0.11861
H	-6.37365	1.74177	-2.43616	C	7.47518	-5.31437	-0.92054
C	-4.24421	-4.44642	-1.35170	H	7.77635	-6.38286	-0.90136
H	-3.31338	-4.52860	-0.75349	H	7.83420	-4.86037	-1.86905
C	-4.59119	-5.80725	-1.96572	H	7.95385	-4.79601	-0.06250
H	-4.87066	-6.51695	-1.15830	H	0.06112	4.13332	-4.92282
H	-5.45228	-5.71080	-2.66112	H	-4.75819	3.39137	-5.10298
H	-3.72397	-6.24166	-2.50207	H	-4.14832	1.19912	-3.38532
C	4.22621	-1.60244	5.21648	H	-5.06161	-4.24219	-0.63851
H	4.37152	-2.64855	4.87018	H	-2.15455	-3.50627	-5.96032
C	4.39924	-1.53401	6.73146	H	5.50684	-5.78566	-1.66701
H	4.24571	-0.49314	7.08836	H	3.28666	-2.02020	-3.82030
H	3.67673	-2.20646	7.24023	H	5.22710	-1.37262	2.34824
H	5.42728	-1.85468	7.00201	H	5.02213	-0.98302	4.74930
C	-0.74671	-2.28276	5.16590	H	-0.42681	-3.33198	5.34892
H	-1.51027	-2.33608	4.36509	H	2.13088	1.83169	2.11479
C	-1.37796	-1.74426	6.44603	H	-3.44127	2.29745	0.34884
H	-0.62565	-1.71630	7.26292	P	1.04058	0.28263	-0.98988
H	-1.78265	-0.72427	6.28734	O	2.43983	0.41403	-0.12772
H	-2.21314	-2.40772	6.75445	O	0.77304	1.72517	-1.72009
C	1.37625	1.83548	2.92772	N	-0.05236	0.05778	0.15943
H	0.39130	1.98434	2.43898	P	-1.13579	-1.06451	0.34916
C	1.65239	3.01157	3.86185	O	-0.96509	-2.45469	-0.24033
H	1.40902	3.96179	3.34831	O	-2.54318	-0.47258	-0.22204
H	1.02869	2.94660	4.77647	O	-1.33726	-1.34202	1.94512
H	2.72332	3.02834	4.15531	O	1.19655	-0.76918	-2.03423
C	-4.84559	4.07131	-4.22808	H	-0.26165	-3.47395	-0.39772
H	-5.75411	3.77117	-3.66361	C	-0.03685	-4.75869	-0.80693
C	-5.03662	5.50682	-4.71093	C	1.34749	-4.94002	-0.83314
H	-5.96980	5.57600	-5.30867	C	-0.80476	-4.73735	-2.13248
H	-5.11789	6.19580	-3.84316	H	-0.52102	-5.26705	0.02654
H	-4.18590	5.82256	-5.35107	C	2.14285	-5.51541	0.29844
C	0.14627	4.28935	-3.82513	O	2.06906	-4.70417	-1.89323
H	0.93112	3.58617	-3.48678	C	0.13562	-4.84568	-3.32821
C	0.60043	5.72738	-3.58893	H	-1.51540	-5.56585	-2.14351
H	-0.17625	6.43878	-3.94203	H	-1.36401	-3.80192	-2.19547
H	0.80128	5.90991	-2.51479	C	1.82249	-4.98348	1.70533
H	1.53837	5.91633	-4.15247	H	3.19740	-5.35746	0.06833
C	-2.78436	3.18947	0.26911	H	1.95388	-6.59712	0.26665

C	1.40666	-4.08104	-3.01728
H	-0.32929	-4.43431	-4.22806
H	0.39725	-5.89030	-3.53381
C	2.55171	-3.68929	2.07825
H	0.74091	-4.84521	1.82982
H	2.11704	-5.75988	2.41928
H	1.20663	-3.03618	-2.74227
H	2.13860	-4.12494	-3.82242
C	2.06030	-2.46568	1.32525
H	3.62607	-3.81744	1.90541
H	2.42268	-3.52381	3.15019
O	2.26687	-2.72150	-0.04981
H	2.59856	-1.56299	1.63625
H	0.99510	-2.31055	1.54638
H	1.98283	-1.98617	-0.61789

R-anti-C₄-C(+)



E(RM062X) = -5098.37997671

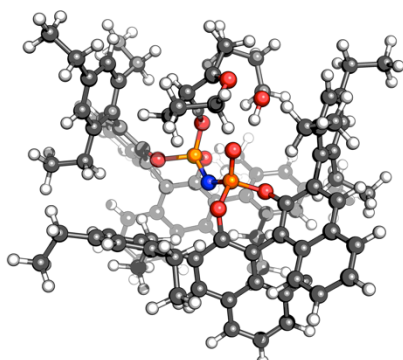
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C	0.52349	-1.68220	3.37145
C	2.73889	-1.50315	2.38672
C	0.79376	-3.01246	3.72122
C	2.97874	-2.87287	2.66055
C	1.98990	-3.62497	3.33733
C	3.83246	-0.57879	1.99125
C	4.98691	-0.41895	2.80544
C	3.70043	0.17554	0.80295
C	6.08243	0.32833	2.31404
C	4.79474	0.94232	0.34721
C	5.98819	0.96549	1.07752
H	6.83356	1.52719	0.69678
H	0.07591	-3.56427	4.31490
C	2.22853	-4.97055	3.65927
C	3.43410	-5.57625	3.30106
H	1.48306	-5.55314	4.18749
H	3.61158	-6.61472	3.54890
C	4.40763	-4.84787	2.61704
C	4.18449	-3.50781	2.29280
H	5.33592	-5.32486	2.33054
H	4.95208	-2.97950	1.74248
C	7.25384	0.45157	3.07864

C	7.33323	-0.13286	4.34267
H	8.10199	1.01323	2.70502
H	8.23575	-0.02877	4.93100
C	6.24344	-0.83274	4.85795
C	5.07647	-0.97153	4.10368
H	6.30070	-1.26637	5.84808
H	4.24585	-1.49756	4.55407
N	0.02293	-0.31367	-0.01022
P	-1.15371	0.15600	-0.98739
O	-2.53784	-0.03313	-0.12740
O	-1.21160	-0.90171	-2.23493
C	-3.67777	-0.21380	-0.87789
C	-1.54613	-2.19368	-1.90153
C	-3.88130	-1.43486	-1.55363
C	-4.68955	0.76879	-0.89732
C	-0.65346	-3.24507	-2.17453
C	-2.84299	-2.49025	-1.43837
C	-5.02841	-1.60810	-2.37398
C	-5.86618	0.54874	-1.62133
C	-0.97955	-4.55227	-1.78907
C	-3.14748	-3.79627	-0.98129
C	-6.03563	-0.61352	-2.37498
C	-5.18998	-2.73225	-3.21531
H	-6.63970	1.30919	-1.62222
C	-2.19724	-4.82962	-1.16062
H	-0.29124	-5.35980	-2.00609
C	-4.37676	-4.10133	-0.35894
C	-7.19389	-0.78259	-3.15060
C	-6.34390	-2.88386	-3.98707
H	-4.42555	-3.49236	-3.29898
C	-2.49583	-6.13759	-0.74712
C	-4.65869	-5.40626	0.05137
H	-5.11759	-3.33462	-0.17309
C	-7.34732	-1.91703	-3.94757
H	-7.97468	-0.03108	-3.15007
H	-6.45765	-3.75278	-4.62244
C	-3.72258	-6.42191	-0.14476
H	-1.78069	-6.93913	-0.88946
H	-5.60420	-5.62932	0.52843
H	-8.23965	-2.03958	-4.54776
H	-3.94614	-7.43130	0.17539
C	0.60314	-3.01703	-2.92844
C	0.55904	-2.79062	-4.33170
C	1.85982	-3.15673	-2.28304
C	1.75810	-2.73141	-5.05888
C	3.03716	-3.10655	-3.04546
C	2.99370	-2.91355	-4.43060
H	3.99680	-3.22816	-2.55692
C	-4.53217	2.07649	-0.22286
C	-4.83952	2.20858	1.15283
C	-4.24695	3.23618	-0.98962
C	-4.85861	3.48304	1.73957
C	-4.26512	4.49657	-0.37108
C	-4.57100	4.62705	0.98761
H	-4.02865	5.37997	-0.95263
C	4.71232	1.79893	-0.85887
C	4.80867	1.22818	-2.15296

C	4.71566	3.21425	-0.71738	H	-3.68535	0.19306	7.74564
C	4.90196	2.06654	-3.27474	C	0.60528	0.37760	5.53726
C	4.81290	4.02162	-1.86099	H	1.36020	0.61237	4.76277
C	4.91796	3.45787	-3.13594	C	1.17280	-0.63914	6.52408
H	4.79466	5.10038	-1.75839	H	0.42307	-0.87190	7.31010
C	-0.73138	-1.06073	3.86119	H	1.46288	-1.57547	6.00709
C	-0.69218	-0.11047	4.91927	H	2.07776	-0.21753	7.01005
C	-1.98776	-1.51412	3.37674	C	-2.11300	-2.49754	2.23035
C	-1.89546	0.35454	5.47234	H	-1.15384	-2.63409	1.68924
C	-3.16821	-1.04581	3.97348	C	-2.60872	-3.85834	2.71636
C	-3.12977	-0.12877	5.02846	H	-3.67937	-3.79936	3.00480
H	-4.12520	-1.41046	3.61937	H	-2.50097	-4.60501	1.90456
H	-5.09237	3.58499	2.79309	H	-2.02068	-4.20961	3.58780
H	-1.87262	1.07058	6.28553	C	4.88952	-0.26399	-2.37812
H	4.98590	1.62828	-4.26253	H	4.43796	-0.83939	-1.54827
H	1.72598	-2.58521	-6.13225	C	6.33770	-0.71105	-2.54712
C	-4.56415	5.98253	1.64600	H	6.92760	-0.45002	-1.64258
H	-3.94038	5.94440	2.56518	H	6.37365	-1.81190	-2.68734
C	-5.97928	6.42650	2.00544	H	6.79253	-0.22415	-3.43584
H	-6.43547	5.72577	2.73649	C	4.58080	3.90374	0.62948
H	-5.94640	7.43853	2.46102	H	4.26759	3.20113	1.42892
H	-6.61183	6.46723	1.09295	C	5.88396	4.58145	1.04732
C	-5.18685	1.01960	2.01612	H	5.75185	5.05454	2.04310
H	-4.68867	0.09668	1.65691	H	6.70729	3.84211	1.11577
C	-6.69393	0.79584	2.06371	H	6.16511	5.37075	0.31864
H	-7.20448	1.69237	2.47553	C	5.01863	4.34647	-4.34927
H	-7.08658	0.58516	1.04691	H	4.88869	3.75540	-5.28200
H	-6.91842	-0.07287	2.71784	C	6.37280	5.04816	-4.40567
C	-3.88417	3.16729	-2.45845	H	6.43042	5.67101	-5.32304
H	-3.63975	2.13462	-2.78207	H	6.50878	5.70800	-3.52266
C	-5.01097	3.70321	-3.33675	H	7.19238	4.29843	-4.43245
H	-4.71524	3.62858	-4.40435	H	0.43497	1.32976	6.08589
H	-5.93672	3.11053	-3.18350	H	-4.43558	1.44291	5.70270
H	-5.21657	4.76898	-3.10223	H	-4.81577	1.19691	3.04496
C	4.26584	-2.92049	-5.24234	H	-2.97105	3.77049	-2.63097
H	4.06989	-2.58471	-6.28399	H	-4.11478	6.74481	0.97270
C	4.87824	-4.31733	-5.29366	H	4.20610	5.10456	-4.32184
H	5.16362	-4.65676	-4.27539	H	3.78617	4.67737	0.57135
H	4.15457	-5.03777	-5.73146	H	4.30917	-0.52413	-3.28715
H	5.79013	-4.29967	-5.92696	H	4.99925	-2.21340	-4.80397
C	-0.74331	-2.67526	-5.10173	H	-0.57398	-2.14259	-6.06308
H	-1.48681	-2.06697	-4.55098	H	2.72971	-2.66175	-0.37688
C	-1.32913	-4.04857	-5.41748	H	-2.83471	-2.09822	1.48822
H	-0.59540	-4.65778	-5.98716	O	1.12320	2.08972	0.49074
H	-1.60541	-4.58489	-4.48779	O	-1.09283	1.53768	-1.54538
H	-2.24492	-3.92736	-6.03354	H	0.94912	2.86323	-0.50042
C	1.98568	-3.37530	-0.78947	C	1.21797	3.78501	-1.46399
H	1.03341	-3.17366	-0.25647	C	0.27710	4.79451	-1.26504
C	2.43432	-4.80196	-0.47945	C	1.33082	3.08578	-2.81080
H	2.31069	-5.00448	0.60257	H	2.14316	4.00042	-0.93732
H	1.82504	-5.54108	-1.03792	C	0.23978	5.71705	-0.08169
H	3.50294	-4.93791	-0.74912	O	-0.61710	5.12614	-2.16424
C	-4.40507	0.33192	5.69015	C	0.06042	3.28001	-3.64018
H	-5.29382	-0.02021	5.12240	H	2.18543	3.48973	-3.36429
C	-4.51162	-0.20056	7.11677	H	1.51631	2.01670	-2.66020
H	-5.47623	0.12217	7.56206	C	0.62328	5.17235	1.30625
H	-4.47435	-1.31098	7.11536	H	-0.76311	6.15269	-0.05970

H	0.92701	6.52876	-0.36725
C	-0.39193	4.71875	-3.53846
H	-0.72553	2.61927	-3.27399
H	0.24939	3.04753	-4.69352
C	-0.58600	4.76738	2.16137
H	1.30828	4.32217	1.22340
H	1.16705	5.96360	1.83249
H	-1.34355	4.90341	-4.03645
H	0.35834	5.41122	-3.94004
C	-1.23443	3.47153	1.69782
H	-1.32762	5.57704	2.13475
H	-0.27509	4.65237	3.20640
O	-1.49473	3.60496	0.31497
H	-0.55802	2.63483	1.89331
H	-2.16170	3.29388	2.25822
H	-1.45086	2.75886	-0.16499

R-anti-C₄-B(+)



E(RM062X) = -5098.38659718

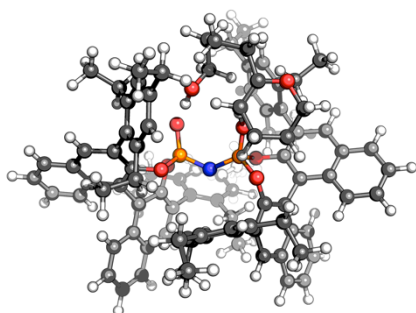
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C	1.34810	-1.18392	2.57053
C	0.39832	-1.99344	3.22194
C	2.63913	-1.68971	2.33758
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C	2.89347	-3.07585	2.48474
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C	4.83979	-0.62770	2.97759
C	3.66344	0.12672	0.96038
C	5.96162	0.14802	2.60670
C	4.79782	0.89356	0.60741
C	5.94469	0.86140	1.40936
H	6.81976	1.42660	1.10953
H	-0.04658	-3.96335	3.96784
C	2.14860	-5.27056	3.25113
C	3.37317	-5.82255	2.87101
H	1.39752	-5.91170	3.69716
H	3.56011	-6.87788	3.02153
C	4.35368	-5.01799	2.28988
C	4.11978	-3.65500	2.09443
H	5.29732	-5.45236	1.98620
H	4.89512	-3.06395	1.62441

C	7.08709	0.20871	3.44435
C	7.09380	-0.46979	4.66318
H	7.95610	0.79148	3.16220
H	7.96102	-0.41412	5.30841
C	5.97773	-1.20530	5.05910
C	4.85646	-1.28256	4.23033
H	5.97913	-1.71511	6.01394
H	4.00254	-1.84190	4.58805
N	0.01938	-0.26153	-0.06817
P	-1.16225	0.31568	-0.98206
O	-1.09753	1.74267	-1.41183
O	-2.54838	0.05620	-0.14837
O	-1.21916	-0.61653	-2.32679
C	-3.68841	-0.00582	-0.91838
C	-1.59421	-1.92490	-2.12875
C	-3.91473	-1.13484	-1.73357
C	-4.67942	0.99605	-0.82528
C	-0.71914	-2.96904	-2.47818
C	-2.90981	-2.22907	-1.72543
C	-5.05835	-1.18409	-2.57444
C	-5.85898	0.88167	-1.56987
C	-1.09390	-4.29887	-2.24624
C	-3.26157	-3.56682	-1.41657
C	-6.04577	-0.17708	-2.45947
C	-5.23734	-2.19732	-3.54327
H	-6.62416	1.64377	-1.47330
C	-2.33767	-4.60427	-1.68671
H	-0.41870	-5.09919	-2.52422
C	-4.51098	-3.89845	-0.84993
C	-7.20331	-0.22977	-3.25268
C	-6.38964	-2.23283	-4.33140
H	-4.48759	-2.95796	-3.71269
C	-2.68398	-5.93937	-1.42450
C	-4.83935	-5.23028	-0.58747
H	-5.23243	-3.13371	-0.59350
C	-7.37424	-1.25765	-4.18007
H	-7.96957	0.53145	-3.16450
H	-6.51700	-3.01773	-5.06581
C	-3.93089	-6.24814	-0.87839
H	-1.98926	-6.74296	-1.63840
H	-5.80019	-5.47330	-0.15264
H	-8.26557	-1.29003	-4.79325
H	-4.19083	-7.27857	-0.67353
C	0.57841	-2.70550	-3.14569
C	0.61125	-2.36076	-4.52434
C	1.79627	-2.94572	-2.45708
C	1.84503	-2.29641	-5.19053
C	3.00982	-2.88657	-3.15945
C	3.04059	-2.58517	-4.52543
H	3.93938	-3.08774	-2.63995
C	-4.50527	2.21312	0.00318
C	-4.73686	2.16416	1.40018
C	-4.27796	3.46923	-0.62128
C	-4.72362	3.35170	2.14799
C	-4.27514	4.63868	0.15539
C	-4.49799	4.58811	1.53443
H	-4.08500	5.59423	-0.31933

C	4.82919	1.76881	-0.58770	H	-5.72063	-0.85729	7.46085
C	5.03838	1.21200	-1.87515	H	-4.69327	-2.20585	6.84157
C	4.85401	3.18159	-0.42685	H	-3.93441	-0.79787	7.69254
C	5.24978	2.06205	-2.97265	C	0.39743	-0.18402	5.59968
C	5.05146	4.00140	-1.54892	H	1.16237	0.13925	4.86776
C	5.25433	3.45185	-2.81821	C	0.96553	-1.28427	6.49191
H	5.03603	5.07900	-1.43415	H	0.20711	-1.60434	7.23788
C	-0.87621	-1.44343	3.74205	H	1.27892	-2.16072	5.89035
C	-0.87779	-0.63058	4.90927	H	1.85554	-0.89920	7.03273
C	-2.11206	-1.86410	3.18266	C	-2.19240	-2.69254	1.91626
C	-2.10070	-0.27255	5.49768	H	-1.21942	-2.73880	1.38444
C	-3.31296	-1.50761	3.81437	C	-2.66629	-4.11476	2.20989
C	-3.31458	-0.72889	4.97586	H	-3.73921	-4.11441	2.49577
H	-4.25485	-1.84656	3.39918	H	-2.54175	-4.74235	1.30531
H	-4.89720	3.31547	3.21728	H	-2.07520	-4.57056	3.02923
H	-2.10885	0.33687	6.39389	C	5.07496	-0.27875	-2.12210
H	5.40742	1.63427	-3.95603	H	4.61069	-0.85900	-1.30249
H	1.86951	-2.06398	-6.24879	C	6.50641	-0.77134	-2.30665
C	-4.46271	5.84835	2.36049	H	7.10554	-0.55277	-1.39690
H	-3.77821	5.70581	3.22460	H	6.50214	-1.86902	-2.47472
C	-5.85550	6.21555	2.86437	H	6.97809	-0.28114	-3.18451
H	-6.25454	5.41889	3.52735	C	4.63239	3.85720	0.91434
H	-5.80329	7.16184	3.44286	H	4.23796	3.15367	1.67629
H	-6.54752	6.36006	2.00727	C	5.91651	4.49325	1.44188
C	-5.05708	0.87471	2.11740	H	5.71835	4.96248	2.42848
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H	-6.91613	0.46818	1.05606	H	5.38999	3.77088	-4.95699
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H	-5.38804	5.24794	-2.45809	H	-4.72423	0.94856	3.17195
C	4.34820	-2.59341	-5.27901	H	-3.11198	4.25414	-2.24425
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C	-1.23927	-3.44390	-5.83430	H	-2.90759	-2.21291	1.21643
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C	-4.61201	-0.37972	5.66150	H	2.59628	2.54480	-2.78279
H	-5.48083	-0.65801	5.02598	H	1.07120	1.74982	-2.42137
C	-4.74315	-1.10681	6.99696	C	0.82353	5.44916	1.11877

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H	-0.99393	4.46122	-4.15209
C	-1.04948	3.88169	1.81426
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R-anti-B_{2,5}-C(-)



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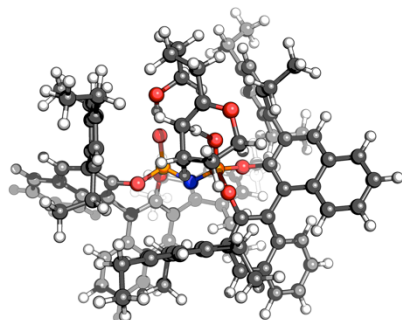
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H	-7.29347	-0.54697	4.52587
H	-5.03732	0.13629	3.89309
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C	4.25043	1.45153	-0.76314
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H	6.60416	-1.50811	-1.69965
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H	1.31808	5.79388	0.34530
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C	7.62814	0.87779	-2.25054
C	7.19374	3.25535	-2.22909
H	5.30117	3.88498	-1.48547
C	3.49510	5.61037	1.85824
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H	5.57357	2.37360	1.34359
C	8.04036	2.18452	-2.51299
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H	7.51072	4.26622	-2.45116
C	4.66880	5.39419	2.58182
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H	5.00271	6.12999	3.30186
C	0.17167	4.19593	-1.46955
C	0.29592	4.58313	-2.83116
C	-1.11106	4.17909	-0.86348
C	-0.84992	4.95796	-3.54936
C	-2.23421	4.56846	-1.60947
C	-2.10967	4.97228	-2.94269
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C	4.22550	-2.35586	-0.82512
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H	3.39249	-5.08539	-2.71176
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C	-3.22820	-1.15318	-4.96815
H	-3.33091	-3.23124	-4.42760

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C	1.06006	-2.21015	5.10226	H	0.85306	1.84656	2.41587
C	2.55079	-0.55314	4.17297	C	2.20183	2.57149	3.93542
C	2.36007	-1.74612	4.87825	H	3.20236	2.32434	4.34907
H	3.55744	-0.19159	3.99798	H	2.26765	3.54019	3.40330
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H	-3.24734	0.97772	-5.22490	H	-3.80851	2.09802	-1.85329
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C	3.14700	-6.53380	-0.42155	H	-6.25336	1.57127	-2.22792
H	2.28734	-6.62801	0.27693	H	-5.84297	3.26044	-2.68984
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H	4.07669	-1.16747	1.70031	H	-6.35364	-3.24565	-2.21275
C	5.97808	-2.16916	1.97132	H	-5.39944	-4.30286	-3.32766
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H	6.49811	-1.63000	1.15345	H	-1.81299	-0.79115	-6.54665
H	6.18693	-1.64336	2.92672	C	-3.77463	-1.12875	-7.40920
C	3.95452	-2.55528	-3.38027	H	-3.37496	-1.36287	-8.41832
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C	5.14621	-3.06287	-4.18794	H	-4.06437	-0.05684	-7.38485
H	5.13449	-2.59927	-5.19676	H	-1.43115	-3.09840	5.06367
H	6.09879	-2.79419	-3.68635	H	3.46599	-3.58093	5.07363
H	5.09628	-4.16574	-4.30734	H	3.99013	-2.69375	2.59612
C	-3.32001	5.41916	-3.72329	H	3.01573	-2.84296	-3.90123
H	-3.36627	4.86614	-4.68631	H	2.83007	-6.95893	-1.39865
C	-3.27615	6.91993	-3.99681	H	-2.39292	-2.48317	-6.46048
H	-3.22786	7.48278	-3.04010	H	-3.34575	-3.87623	-1.99666
H	-2.39381	7.17907	-4.61947	H	-3.65345	2.55594	-3.56065
H	-4.19379	7.22451	-4.54274	H	-4.25369	5.19287	-3.16448
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H	2.29889	3.82513	-3.24112	H	-2.16633	3.03390	0.61601
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H	2.55282	6.10189	-2.17838	P	-1.20374	-0.53730	0.09262
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H	3.67867	-1.40791	7.26741	O	1.59208	1.74549	-1.70029
H	2.70881	-2.93412	7.37772	C	-1.22021	-6.02926	-1.65653
C	-1.42966	-1.98678	5.04333	O	-2.63038	-5.48279	0.06554
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H	-4.12545	-4.91771	1.29741
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R-anti-B_{2,5}-B(-)



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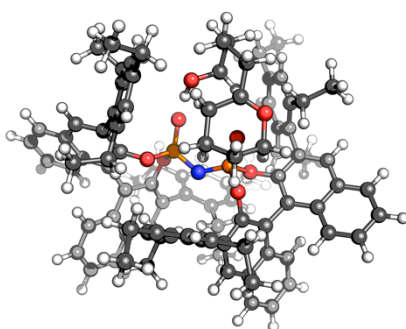
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C	-7.49628	-1.53572	1.24766

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C	4.70245	-0.63375	-0.97472
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C	3.49577	3.73408	0.63723
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C	5.63334	3.42267	-1.72968
H	6.68907	-1.03808	-1.68830
C	2.65304	4.85501	0.83770
H	0.84677	5.85361	0.22173
C	4.68538	3.63458	1.38936
C	7.50599	1.41694	-2.27564
C	6.86716	3.74771	-2.29741
H	4.92550	4.22403	-1.56743
C	3.03002	5.86529	1.73678
C	5.03946	4.63947	2.29223
H	5.33809	2.77633	1.29666
C	7.80411	2.74954	-2.56122
H	8.23928	0.65308	-2.50621
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C	4.21839	5.75458	2.46030
H	2.40037	6.73409	1.88796
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H	-3.19996	-3.55336	-4.37454	H	-1.08869	-1.32666	7.31055
C	0.11812	-0.18967	4.01351	H	-2.01520	-0.14221	6.30701
C	-0.00071	-1.37578	4.78525	H	-2.79057	-1.67861	6.82533
C	1.40604	0.32142	3.71109	C	1.60792	1.60630	2.93890
C	1.15933	-2.04532	5.20390	H	0.69209	1.91136	2.39497
C	2.54457	-0.35962	4.16773	C	2.02895	2.73795	3.87274
C	2.43003	-1.53758	4.91330	H	3.05144	2.55551	4.26588
H	3.52777	0.04180	3.95134	H	2.02695	3.69790	3.32143
H	4.01486	-4.51426	1.53505	H	1.32242	2.82815	4.72342
H	1.07414	-2.95397	5.78821	C	-4.36263	1.49464	-2.83317
H	-3.43028	0.64255	-5.20752	H	-3.97842	1.75311	-1.82695
H	-1.16040	5.05917	-4.69935	C	-5.87104	1.71639	-2.88251
C	3.59495	-6.31722	-0.43779	H	-6.39050	1.06579	-2.15019
H	2.74122	-6.46396	0.25901	H	-6.09878	2.77377	-2.63277
C	4.81890	-7.06568	0.08320	H	-6.25692	1.50029	-3.90152
H	5.09466	-6.70896	1.09804	C	-3.98354	-3.53415	-1.81801
H	4.59297	-8.15117	0.14171	H	-4.04358	-3.25069	-0.74781
H	5.67969	-6.91792	-0.60361	C	-5.20072	-4.38178	-2.17607
C	4.58684	-1.90054	1.71985	H	-5.27068	-5.24236	-1.47795
H	4.11302	-0.90084	1.68678	H	-6.13063	-3.78218	-2.09417
C	6.08227	-1.75181	1.97904	H	-5.11119	-4.77447	-3.21103
H	6.55961	-2.75190	2.05637	C	-2.76667	-1.72597	-6.33809
H	6.56757	-1.17734	1.16370	H	-1.92361	-1.03723	-6.56230
H	6.24008	-1.20751	2.93384	C	-3.88445	-1.51747	-7.35618
C	4.18585	-2.30064	-3.39717	H	-3.50273	-1.73296	-8.37630
H	4.12106	-1.19340	-3.39691	H	-4.73174	-2.20329	-7.14107
C	5.43554	-2.72176	-4.16599	H	-4.24713	-0.46803	-7.32998
H	5.41975	-2.26405	-5.17748	H	-1.26066	-3.00497	5.46324
H	6.35081	-2.38273	-3.63887	H	3.62120	-3.31742	5.11592
H	5.46981	-3.82579	-4.28032	H	4.13259	-2.42810	2.58410
C	-3.73076	5.06127	-3.85176	H	3.29095	-2.65990	-3.94822
H	-3.73499	4.47916	-4.79863	H	3.30566	-6.76043	-1.41534
C	-3.78598	6.55325	-4.16807	H	-2.38231	-2.76414	-6.44336
H	-3.78014	7.14502	-3.22777	H	-3.07542	-4.15893	-1.91841
H	-2.91995	6.85315	-4.79529	H	-3.88564	2.20477	-3.54003
H	-4.71923	6.78002	-4.72530	H	-4.65018	4.78873	-3.28982
C	1.26358	4.64784	-3.62691	H	1.13752	4.51074	-4.72321
H	1.98195	3.86761	-3.30632	H	-2.44154	2.87622	0.55737
C	1.86098	6.03020	-3.38205	H	2.39358	1.45315	2.17023
H	1.16259	6.81864	-3.73529	O	-1.24147	-2.02715	-0.46400
H	2.06945	6.18424	-2.30405	P	-1.18291	-0.64317	0.15880
H	2.81615	6.12530	-3.94011	H	-0.39123	-3.14931	-0.32388
C	-1.64924	3.65064	0.49468	O	-2.44902	0.23248	-0.36799
H	-0.73453	3.19704	0.92536	O	-1.46000	-0.95468	1.76116
C	-2.04972	4.85556	1.34183	N	0.06872	0.28595	0.01165
H	-2.03497	4.57895	2.41378	C	0.23656	-4.15139	0.08909
H	-1.33911	5.69431	1.19256	P	1.24039	0.28557	-1.07691
H	-3.07348	5.19361	1.07576	C	-0.77202	-5.06419	-0.27402
C	3.66268	-2.24764	5.41452	C	0.41047	-3.80722	1.57667
H	4.57986	-1.81106	4.96281	H	1.12512	-4.18768	-0.53127
C	3.78344	-2.14184	6.93234	O	1.17888	-0.62561	-2.25247
H	4.71916	-2.63823	7.26541	O	2.54496	0.00564	-0.12951
H	3.81768	-1.07500	7.24082	O	1.40903	1.78101	-1.71522
H	2.92480	-2.64005	7.42994	C	-0.75213	-6.04553	-1.40775
C	-1.34334	-1.92069	5.23319	O	-1.88255	-5.14992	0.40598
H	-2.10121	-1.83020	4.42785	C	-0.72192	-4.42317	2.39518
C	-1.83546	-1.21869	6.49515	H	0.42364	-2.72074	1.70633

H	1.37641	-4.18827	1.91787
H	1.16303	-2.24087	-2.46147
C	0.26171	-5.89065	-2.54347
H	-0.55233	-6.99124	-0.87914
H	-1.77273	-6.14097	-1.79399
C	-2.01469	-4.34256	1.60574
H	-0.84794	-3.90823	3.34569
H	-0.51641	-5.47785	2.61520
O	1.08830	-3.21074	-2.62480
C	-0.15776	-4.92734	-3.65558
H	0.40602	-6.88688	-2.97362
H	1.23154	-5.57320	-2.15369
H	-2.87122	-4.77361	2.12368
H	-2.22977	-3.31759	1.29018
C	-0.16265	-3.47590	-3.20240
H	0.55918	-5.02839	-4.47799
H	-1.14677	-5.20291	-4.04442
H	-0.35374	-2.81714	-4.06117
H	-0.96987	-3.28835	-2.47715

R-anti-B_{2,5}-B(-) intermediate



E(RM062X) = -5098.4094466

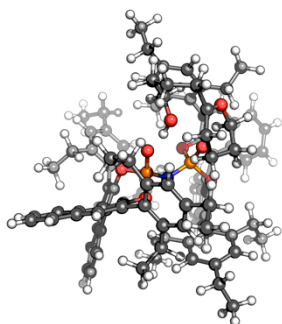
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C	-3.76164	1.70708	2.88415
C	-2.99621	2.27612	3.93217
C	-4.13869	-0.24440	1.29650
C	-5.36793	-0.82010	1.71333
C	-3.68654	-0.45578	-0.01929
C	-6.19312	-1.46312	0.75585
C	-4.50935	-1.10201	-0.95826
C	-5.76770	-1.57486	-0.57163
H	-6.40075	-2.06182	-1.30408
H	-1.21046	2.10751	5.12581
C	-3.47904	3.39706	4.62609
C	-4.69569	3.97725	4.26451
H	-2.90939	3.83187	5.43884
H	-5.05836	4.84743	4.79613
C	-5.43945	3.44544	3.21126
C	-4.98019	2.32044	2.52306
H	-6.37559	3.90742	2.92553
H	-5.57578	1.94646	1.70072

C	-7.42744	-2.00821	1.14364
C	-7.83704	-1.94506	2.47579
H	-8.06962	-2.49416	0.41851
H	-8.78717	-2.37203	2.76984
C	-7.01651	-1.34869	3.43243
C	-5.78917	-0.79558	3.06103
H	-7.33036	-1.31858	4.46791
H	-5.17228	-0.36621	3.83857
C	3.70321	0.55883	-0.62424
C	1.62586	2.84277	-0.92781
C	3.94594	1.93904	-0.77809
C	4.72740	-0.37048	-0.88606
C	0.76628	3.95224	-0.84451
C	2.90287	2.90641	-0.33301
C	5.16204	2.37348	-1.37049
C	5.96675	0.07418	-1.35851
C	1.09183	5.02609	-0.00811
C	3.19257	3.94629	0.58622
C	6.18359	1.42698	-1.63098
C	5.38326	3.72161	-1.73071
H	6.75516	-0.64669	-1.54255
C	2.27747	5.01762	0.73222
H	0.42367	5.87712	0.05184
C	4.36993	3.94662	1.36369
C	7.40770	1.84359	-2.17819
C	6.60296	4.11986	-2.28203
H	4.61571	4.47348	-1.60806
C	2.57183	6.07889	1.60299
C	4.64150	5.00088	2.23837
H	5.07659	3.12851	1.31245
C	7.61551	3.18582	-2.49635
H	8.19905	1.12887	-2.37139
H	6.76142	5.15691	-2.54862
C	3.74925	6.06710	2.35240
H	1.88599	6.91058	1.71268
H	5.54729	4.99045	2.83067
H	8.55895	3.50032	-2.92358
H	3.96678	6.88296	3.02946
C	-0.45670	4.03836	-1.67956
C	-0.35416	4.35918	-3.06019
C	-1.73931	3.89545	-1.09032
C	-1.52318	4.54385	-3.81441
C	-2.88688	4.09627	-1.87262
C	-2.78685	4.43435	-3.22591
H	-3.86606	3.99584	-1.41871
C	4.51165	-1.83038	-0.73424
C	4.53187	-2.43013	0.55175
C	4.40261	-2.65405	-1.88742
C	4.47781	-3.82821	0.66334
C	4.33948	-4.04820	-1.73708
C	4.39958	-4.64055	-0.47224
H	4.25424	-4.67641	-2.61605
C	-4.02334	-1.36677	-2.33361
C	-3.92149	-0.31001	-3.27510
C	-3.64504	-2.68197	-2.71465
C	-3.40201	-0.57112	-4.55266
C	-3.14941	-2.90979	-4.00717

C	-3.01414	-1.86267	-4.92327	C	-1.88416	-1.07464	6.62891
H	-2.85343	-3.91134	-4.29561	H	-1.13233	-1.19315	7.43814
C	-0.01218	-0.03033	4.04989	H	-2.06186	0.00543	6.45321
C	-0.08031	-1.17256	4.88920	H	-2.83744	-1.53850	6.95877
C	1.25190	0.51816	3.71779	C	1.39484	1.77936	2.89756
C	1.10663	-1.76722	5.34335	H	0.47867	1.99837	2.31456
C	2.41942	-0.09207	4.20088	C	1.70759	2.97066	3.79863
C	2.35525	-1.23145	5.00999	H	2.72594	2.87147	4.23061
H	3.38451	0.33668	3.95727	H	1.65959	3.90726	3.21136
H	4.51373	-4.29141	1.64265	H	0.96791	3.04418	4.62244
H	1.05844	-2.64485	5.97726	C	-4.39049	1.09542	-2.96497
H	-3.30813	0.23446	-5.27158	H	-4.05780	1.41496	-1.95802
H	-1.45046	4.80037	-4.86493	C	-5.90840	1.20771	-3.06713
C	4.38209	-6.14167	-0.33008	H	-6.40450	0.54670	-2.32796
H	3.64213	-6.43886	0.44338	H	-6.21776	2.25386	-2.86230
C	5.75971	-6.66878	0.05960	H	-6.24500	0.93063	-4.08887
H	6.07067	-6.25786	1.04354	C	-3.71991	-3.86339	-1.76743
H	5.72627	-7.77611	0.13394	H	-3.82825	-3.55124	-0.70892
H	6.51008	-6.38614	-0.70942	C	-4.87168	-4.79544	-2.13211
C	4.67080	-1.62014	1.82175	H	-4.91120	-5.63590	-1.40759
H	4.12568	-0.65943	1.75016	H	-5.83852	-4.25247	-2.09831
C	6.13615	-1.35170	2.14627	H	-4.72566	-5.21481	-3.15005
H	6.68333	-2.31008	2.27318	C	-2.44716	-2.11907	-6.29612
H	6.61386	-0.76205	1.33662	H	-1.63492	-1.38929	-6.50372
H	6.20645	-0.77374	3.09164	C	-3.52710	-2.00365	-7.36827
C	4.32935	-2.08646	-3.29292	H	-3.08760	-2.22680	-8.36321
H	4.13538	-0.99418	-3.29245	H	-4.34413	-2.72978	-7.16918
C	5.61340	-2.35889	-4.07275	H	-3.94761	-0.97600	-7.39135
H	5.53415	-1.90965	-5.08502	H	-1.28352	-2.84376	5.56525
H	6.48685	-1.91157	-3.55573	H	3.61021	-2.95549	5.28867
H	5.77811	-3.45125	-4.18532	H	4.21229	-2.17066	2.67037
C	-4.02778	4.67829	-4.04721	H	3.47785	-2.55084	-3.83454
H	-3.98389	4.07050	-4.97674	H	4.07532	-6.62336	-1.28408
C	-4.16887	6.15468	-4.40688	H	-2.00017	-3.13573	-6.35334
H	-4.21221	6.77169	-3.48391	H	-2.77307	-4.43478	-1.82278
H	-3.31370	6.48914	-5.03152	H	-3.94217	1.81309	-3.68304
H	-5.10622	6.30855	-4.98183	H	-4.93654	4.36622	-3.48858
C	0.97890	4.56991	-3.75105	H	0.87582	4.39203	-4.84389
H	1.73763	3.84393	-3.39788	H	-2.66932	2.71511	0.44356
C	1.49045	5.99213	-3.54292	H	2.21396	1.64969	2.16010
H	0.75075	6.72659	-3.92705	O	-1.10719	-2.15866	-0.35386
H	1.67699	6.19061	-2.46818	P	-1.17458	-0.75463	0.16235
H	2.44474	6.12704	-4.09421	H	1.13020	-3.65845	-0.57987
C	-1.92692	3.53588	0.36664	O	-2.47512	0.05405	-0.40693
H	-0.99242	3.15588	0.82437	O	-1.45530	-0.97732	1.79349
C	-2.41643	4.73919	1.16832	N	0.01600	0.26811	-0.00085
H	-2.39960	4.49897	2.24913	C	0.90389	-4.29927	0.30825
H	-1.75929	5.61700	1.00014	P	1.19925	0.31093	-1.06140
H	-3.45588	5.00138	0.87860	C	-0.29925	-5.03642	-0.08135
C	3.61743	-1.87087	5.53135	C	0.83602	-3.52119	1.62237
H	4.51337	-1.42698	5.04581	H	1.70743	-5.04497	0.28924
C	3.75069	-1.68239	7.04012	O	1.23907	-0.62467	-2.22594
H	4.70618	-2.12940	7.38670	O	2.51359	0.13114	-0.09479
H	3.75192	-0.60041	7.29267	O	1.29261	1.79398	-1.74716
H	2.91486	-2.18241	7.57352	C	-0.26840	-6.08971	-1.14431
C	-1.39928	-1.75824	5.35455	O	-1.40947	-4.96689	0.53344
H	-2.17689	-1.67954	4.56710	C	-0.26416	-4.09616	2.50886

H	0.63707	-2.46844	1.41830
H	1.80282	-3.58146	2.12812
H	1.35692	-2.16983	-2.29847
C	0.70103	-5.92049	-2.32074
H	0.02183	-6.98483	-0.56973
H	-1.29337	-6.26902	-1.48243
C	-1.56995	-4.15905	1.74973
H	-0.42028	-3.47253	3.38684
H	0.00511	-5.10156	2.86018
O	1.34734	-3.16601	-2.38530
C	0.19714	-4.96981	-3.40822
H	0.85843	-6.91542	-2.74857
H	1.67552	-5.56872	-1.96874
H	-2.35927	-4.68448	2.28741
H	-1.90011	-3.17953	1.40815
C	0.09955	-3.53405	-2.91938
H	0.89836	-5.00971	-4.24880
H	-0.78051	-5.30599	-3.77679
H	-0.17775	-2.86965	-3.74836
H	-0.68283	-3.41630	-2.15237

R-anti-B_{2,5}-B(-) 2nd step



E(RM062X) = -5098.39292629

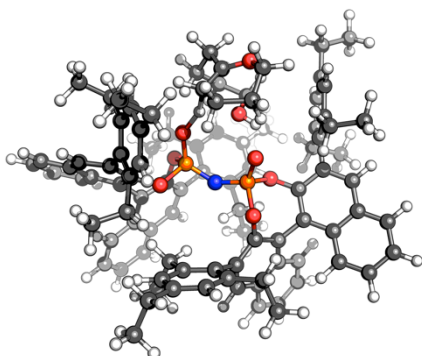
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C	4.10151	-2.37423	2.21841
C	3.45204	-3.48625	2.80952
C	4.14258	0.13538	1.78995
C	5.31157	0.57805	2.46431
C	3.62265	0.90221	0.72671
C	6.03796	1.67799	1.94415
C	4.34807	2.00236	0.22652
C	5.56607	2.35659	0.81721
H	6.13514	3.18220	0.40788
H	1.67208	-4.19074	3.79635
C	4.11578	-4.72005	2.90470
C	5.40307	-4.86786	2.38681
H	3.63385	-5.57314	3.36749
H	5.90634	-5.82368	2.45445
C	6.03569	-3.79081	1.76684
C	5.39360	-2.55386	1.67778
H	7.02681	-3.91530	1.35015

H	5.90811	-1.74923	1.16972
C	7.22510	2.09560	2.56698
C	7.68045	1.45113	3.71748
H	7.79494	2.92751	2.17000
H	8.59403	1.78012	4.19570
C	6.95121	0.39512	4.26239
C	5.77287	-0.03648	3.64953
H	7.29852	-0.08995	5.16558
H	5.22490	-0.84272	4.11800
C	-3.47202	-0.80526	-0.97124
C	-0.86691	-2.10533	-2.09235
C	-3.32467	-1.86516	-1.88237
C	-4.72847	-0.18458	-0.83491
C	0.20428	-2.92824	-2.49585
C	-2.10705	-2.70333	-1.80410
C	-4.34281	-2.12966	-2.83419
C	-5.77005	-0.51294	-1.71279
C	0.09868	-4.32126	-2.37007
C	-2.18911	-4.09992	-1.58706
C	-5.57694	-1.44621	-2.73293
C	-4.15953	-3.04567	-3.89360
H	-6.73353	-0.02872	-1.60165
C	-1.06820	-4.90928	-1.87840
H	0.92020	-4.95061	-2.68989
C	-3.36256	-4.71002	-1.09587
C	-6.60709	-1.71247	-3.64889
C	-5.18925	-3.29391	-4.80360
H	-3.21874	-3.55955	-4.03959
C	-1.14496	-6.30160	-1.71456
C	-3.41983	-6.09412	-0.91917
H	-4.23191	-4.12189	-0.83058
C	-6.41147	-2.63407	-4.67832
H	-7.55963	-1.20129	-3.57385
H	-5.03676	-3.99768	-5.61173
C	-2.31657	-6.88841	-1.23299
H	-0.29676	-6.93364	-1.94932
H	-4.32332	-6.55224	-0.53807
H	-7.20638	-2.83077	-5.38604
H	-2.36794	-7.96108	-1.09864
C	1.41586	-2.38619	-3.15645
C	1.35598	-1.96658	-4.51401
C	2.67809	-2.49339	-2.51618
C	2.54736	-1.69741	-5.20561
C	3.84905	-2.23891	-3.24619
C	3.79252	-1.86293	-4.59166
H	4.81252	-2.33154	-2.75868
C	-4.99528	0.82630	0.21286
C	-5.19325	0.42501	1.56007
C	-5.21664	2.17887	-0.15486
C	-5.61883	1.37051	2.50574
C	-5.67828	3.08791	0.80970
C	-5.88380	2.69226	2.13480
H	-5.87084	4.11575	0.52701
C	3.82181	2.82670	-0.89199
C	3.80149	2.31275	-2.21451
C	3.35610	4.14854	-0.65377
C	3.24147	3.07998	-3.24817

C	2.83678	4.90075	-1.71818	H	1.79134	-0.30183	5.12384
C	2.75589	4.36819	-3.00748	C	1.75098	-1.82398	6.66341
H	2.47574	5.90604	-1.53401	H	1.02931	-2.27848	7.37537
C	0.10236	-2.03059	3.75769	H	2.19457	-2.62313	6.03470
C	-0.08946	-1.40073	5.01553	H	2.56500	-1.33996	7.24292
C	-1.00160	-2.63550	3.10301	C	-0.87548	-3.30792	1.75242
C	-1.36506	-1.40032	5.59968	H	0.07070	-3.03939	1.24029
C	-2.26037	-2.63071	3.72390	C	-0.94668	-4.82632	1.89048
C	-2.44569	-2.03182	4.97472	H	-1.96241	-5.13997	2.21139
H	-3.09764	-3.11312	3.23355	H	-0.72183	-5.30050	0.91555
H	-5.77326	1.07041	3.53577	H	-0.20247	-5.18739	2.63000
H	-1.51208	-0.93090	6.56538	C	4.41842	0.97946	-2.57008
H	3.19904	2.68056	-4.25476	H	4.13369	0.19984	-1.83785
H	2.50838	-1.38938	-6.24395	C	5.93849	1.07708	-2.65698
C	-6.36435	3.68453	3.16253	H	6.37330	1.37889	-1.68307
H	-5.69904	3.64868	4.05221	H	6.35872	0.08778	-2.93232
C	-7.80093	3.38615	3.58340	H	6.23080	1.81669	-3.43254
H	-7.86988	2.38441	4.05817	C	3.37093	4.79181	0.71755
H	-8.13919	4.14766	4.31721	H	3.49599	4.04832	1.53102
H	-8.47415	3.41955	2.70008	C	4.46868	5.84764	0.82482
C	-5.01037	-1.00674	2.01751	H	4.47210	6.27574	1.84925
H	-4.11747	-1.46763	1.55311	H	5.46432	5.40297	0.62450
C	-6.24344	-1.85333	1.71895	H	4.28884	6.67006	0.10045
H	-7.14088	-1.40824	2.19899	C	2.14255	5.16983	-4.12735
H	-6.41374	-1.93173	0.62622	H	1.36531	4.55962	-4.63636
H	-6.09456	-2.87683	2.12311	C	3.19829	5.60449	-5.13954
C	-4.93739	2.69327	-1.55480	H	2.72136	6.22014	-5.93097
H	-4.40364	1.94729	-2.17839	H	3.98173	6.21261	-4.63888
C	-6.21882	3.10517	-2.27571	H	3.66992	4.72021	-5.61793
H	-5.97163	3.44251	-3.30429	H	0.66872	0.02837	6.45480
H	-6.92024	2.24842	-2.34376	H	-4.10549	-1.03903	5.91663
H	-6.71717	3.94282	-1.74434	H	-4.83062	-1.02999	3.11170
C	5.05985	-1.60923	-5.36854	H	-4.26160	3.56712	-1.48976
H	5.00912	-0.60564	-5.84344	H	-6.32238	4.72009	2.75974
C	5.27259	-2.67509	-6.44022	H	1.64078	6.07913	-3.73051
H	5.31939	-3.68291	-5.97477	H	2.39601	5.28777	0.89266
H	4.44858	-2.65317	-7.18436	H	4.03997	0.64104	-3.55619
H	6.22961	-2.48334	-6.96957	H	5.94316	-1.61368	-4.69413
C	0.05314	-1.86493	-5.28407	H	0.16711	-1.15666	-6.13374
H	-0.75772	-1.44809	-4.65645	H	3.45288	-2.11647	-0.55256
C	-0.37146	-3.21889	-5.84557	H	-1.69762	-2.95913	1.09247
H	0.42754	-3.63288	-6.49690	O	0.81002	2.18465	1.16940
H	-0.58526	-3.93686	-5.02877	P	1.09338	0.73343	0.97363
H	-1.29490	-3.09565	-6.44967	H	-3.59068	4.81512	0.46618
C	2.81632	-2.87215	-1.05734	O	2.46732	0.50094	0.10420
H	1.84057	-2.86072	-0.53007	O	1.40245	0.14997	2.47982
C	3.45049	-4.25296	-0.89783	N	0.02956	-0.21892	0.27914
H	3.37175	-4.57927	0.15735	C	-2.85548	5.02218	1.24037
H	2.93293	-5.00365	-1.52809	P	-1.07527	0.11859	-0.80103
H	4.52402	-4.22232	-1.17950	C	-1.74634	5.77467	0.59124
C	-3.79355	-2.07219	5.65117	C	-2.37991	3.77688	1.98412
H	-4.56506	-2.49121	4.96978	H	-3.30906	5.74386	1.94020
C	-3.75725	-2.93753	6.90848	O	-1.32312	1.52219	-1.27808
H	-4.77183	-2.98196	7.35742	O	-2.44520	-0.48907	-0.11519
H	-3.43551	-3.97014	6.65413	O	-0.76718	-0.73527	-2.17811
H	-3.05977	-2.51101	7.65987	C	-2.00234	6.84013	-0.43385
C	1.05212	-0.78126	5.79607	O	-0.57252	5.78858	1.06582

C	-1.17714	4.14760	2.84647
H	-2.09910	3.00175	1.26511
H	-3.18769	3.38818	2.60661
H	-1.41731	3.01004	-0.90675
C	-2.58081	6.35089	-1.77418
H	-2.72418	7.52401	0.03398
H	-1.06828	7.38945	-0.58553
C	-0.08611	4.74982	1.99527
H	-0.74233	3.25206	3.30022
H	-1.47638	4.83435	3.64862
O	-1.52316	4.01824	-0.86739
C	-1.57061	5.60905	-2.66004
H	-2.96101	7.22902	-2.30489
H	-3.44290	5.71237	-1.57416
H	0.67656	5.26818	2.57460
H	0.35733	3.99264	1.34457
C	-0.72185	4.62178	-1.85780
H	-2.12454	5.08162	-3.44310
H	-0.90894	6.32855	-3.15789
H	-0.27620	3.85856	-2.50302
H	0.09911	5.16132	-1.36252

R-anti-B_{2,5}-C(+)



E(RM062X) = -5098.37543730

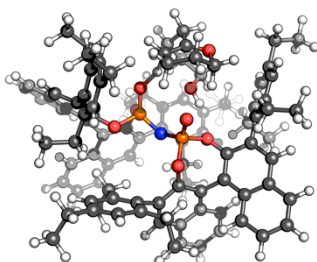
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C	-1.66736	-0.00694	2.64737
C	-0.78492	0.50065	3.61851
C	-2.97478	0.51985	2.55820
C	-1.14177	1.63533	4.35949
C	-3.30084	1.71887	3.24230
C	-2.36861	2.27048	4.15198
C	-4.00201	-0.26471	1.82400
C	-5.18447	-0.72832	2.46180
C	-3.76275	-0.58724	0.47310
C	-6.19693	-1.33746	1.68278
C	-4.75254	-1.26379	-0.27040
C	-5.98373	-1.56682	0.32285
H	-6.75621	-2.04174	-0.26982
H	-0.46550	2.01178	5.11667
C	-2.69195	3.43088	4.87349
C	-3.92821	4.05206	4.68989
H	-1.98922	3.85629	5.58016

H	-4.17142	4.94732	5.24733
C	-4.84774	3.52606	3.78277
C	-4.53797	2.37414	3.05640
H	-5.79981	4.01856	3.63306
H	-5.26472	2.01173	2.34144
C	-7.39786	-1.74899	2.28288
C	-7.58763	-1.59223	3.65593
H	-8.18229	-2.20814	1.69275
H	-8.51236	-1.91775	4.11465
C	-6.57804	-1.03875	4.44192
C	-5.38244	-0.61662	3.85661
H	-6.72004	-0.93990	5.51043
H	-4.61558	-0.21901	4.50715
N	-0.06233	0.08550	-0.03567
P	1.10170	0.17355	-1.11431
O	1.25956	-0.89285	-2.14592
O	2.49016	0.24805	-0.21330
O	0.94861	1.60412	-1.90672
C	3.56950	0.83755	-0.83382
C	1.14134	2.74586	-1.16382
C	3.56020	2.22263	-1.08956
C	4.73954	0.09630	-1.10387
C	0.14930	3.74399	-1.12976
C	2.40765	3.02543	-0.61799
C	4.63042	2.82046	-1.80723
C	5.84070	0.71563	-1.70611
C	0.34289	4.89084	-0.34604
C	2.58322	4.14601	0.23041
C	5.78523	2.05500	-2.09122
C	4.57460	4.15528	-2.26814
H	6.73804	0.13745	-1.89736
C	1.52892	5.07775	0.36836
H	-0.41785	5.66066	-0.32841
C	3.79034	4.37379	0.92528
C	6.87009	2.63732	-2.76615
C	5.65659	4.71911	-2.94748
H	3.69382	4.76670	-2.12668
C	1.69879	6.21725	1.17065
C	3.94525	5.51024	1.72233
H	4.61158	3.67098	0.86888
C	6.80459	3.96544	-3.18799
H	7.76342	2.06158	-2.97795
H	5.60223	5.74355	-3.29270
C	2.90321	6.43003	1.84365
H	0.90226	6.94466	1.27338
H	4.87446	5.67505	2.25217
H	7.64080	4.40750	-3.71413
H	3.02845	7.30927	2.46218
C	-1.06051	3.67090	-1.98546
C	-0.95236	3.87203	-3.39061
C	-2.34711	3.56258	-1.39386
C	-2.11921	3.96452	-4.16548
C	-3.49017	3.68564	-2.19837
C	-3.38500	3.89772	-3.57676
H	-4.47250	3.61660	-1.74610
C	4.85220	-1.34421	-0.79166
C	5.25321	-1.75520	0.50283

C	4.76149	-2.30310	-1.83356	H	-2.58455	5.49468	0.43633
C	5.55085	-3.10537	0.73979	H	-4.19218	4.68261	0.54075
C	5.03721	-3.65161	-1.55694	C	4.26164	-1.81584	5.31575
C	5.44745	-4.05561	-0.28129	H	5.12534	-1.22748	4.93814
H	4.95534	-4.38634	-2.34918	C	4.30326	-1.77938	6.84172
C	-4.48459	-1.78123	-1.63416	H	5.28855	-2.14990	7.19502
C	-4.44360	-0.90031	-2.74432	H	4.16450	-0.73829	7.20439
C	-4.35092	-3.18279	-1.84705	H	3.51038	-2.42609	7.27297
C	-4.22513	-1.41704	-4.03075	C	-0.73190	-2.12847	5.04215
C	-4.14202	-3.66390	-3.14846	H	-1.48092	-2.14300	4.22775
C	-4.08264	-2.79215	-4.24023	C	-1.34354	-1.51247	6.29755
H	-4.02909	-4.72903	-3.31440	H	-0.60177	-1.50861	7.12456
C	0.50737	-0.16350	3.91839	H	-1.68134	-0.47435	6.10559
C	0.53062	-1.39725	4.62569	H	-2.22379	-2.11128	6.61278
C	1.73099	0.49657	3.62668	C	1.79070	1.79548	2.84795
C	1.76179	-1.93751	5.02803	H	0.82546	2.03159	2.35388
C	2.93878	-0.05618	4.07831	C	2.18857	2.96442	3.74783
C	2.96117	-1.25969	4.79010	H	3.26531	2.89999	4.01135
H	3.86708	0.46889	3.88909	H	2.00924	3.92060	3.21748
H	5.86196	-3.41989	1.72943	H	1.59053	2.97240	4.68110
H	1.78522	-2.87326	5.57405	C	-4.72226	0.57889	-2.60691
H	-4.20834	-0.74640	-4.88193	H	-4.23562	0.99439	-1.70501
H	-2.04108	4.13717	-5.23251	C	-6.22252	0.85210	-2.54833
C	5.75954	-5.50280	0.00091	H	-6.68534	0.33056	-1.68589
H	5.19193	-5.83551	0.89689	H	-6.39955	1.94127	-2.42981
C	7.25411	-5.70746	0.23603	H	-6.71056	0.51068	-3.48590
H	7.59282	-5.13669	1.12664	C	-4.43966	-4.19986	-0.72009
H	7.45897	-6.78467	0.41045	H	-4.34720	-3.73040	0.27995
H	7.83155	-5.37467	-0.65295	C	-5.74528	-4.99016	-0.78321
C	5.41470	-0.77818	1.64365	H	-5.79645	-5.69045	0.07698
H	4.73946	0.09438	1.53298	H	-6.62091	-4.31200	-0.73819
C	6.85583	-0.29297	1.75476	H	-5.79631	-5.58241	-1.72123
H	7.54036	-1.15096	1.92589	C	-3.90116	-3.33634	-5.63413
H	7.15906	0.23827	0.82857	H	-3.64917	-2.51940	-6.34499
H	6.94501	0.40867	2.61076	C	-5.17260	-4.02712	-6.11980
C	4.40569	-1.92042	-3.25625	H	-5.02348	-4.39451	-7.15688
H	3.96021	-0.90619	-3.31779	H	-5.41900	-4.89374	-5.47013
C	5.62626	-1.98118	-4.17070	H	-6.02340	-3.31239	-6.11458
H	5.33228	-1.68715	-5.20018	H	-0.50423	-3.19544	5.25749
H	6.41423	-1.28559	-3.81639	H	4.38693	-2.86192	4.96199
H	6.03848	-3.01189	-4.20345	H	5.12964	-1.27685	2.59069
C	-4.62551	4.06574	-4.41882	H	3.64088	-2.61764	-3.64409
H	-4.37184	4.05003	-5.50121	H	5.44467	-6.14635	-0.84921
C	-5.32773	5.38441	-4.10754	H	-3.05766	-4.05885	-5.64842
H	-5.66952	5.40570	-3.05104	H	-3.60165	-4.92036	-0.79099
H	-4.63917	6.23753	-4.28777	H	-4.29491	1.12728	-3.47268
H	-6.21426	5.49732	-4.76645	H	-5.32325	3.22317	-4.23465
C	0.37873	4.06954	-4.09434	H	0.27114	3.86646	-5.18236
H	1.14018	3.35179	-3.73508	H	-3.24491	2.48627	0.24105
C	0.89421	5.49677	-3.93147	H	2.53898	1.69691	2.03416
H	0.14160	6.22238	-4.30696	O	-1.34472	-2.30439	-0.27903
H	1.11875	5.71965	-2.86961	H	-0.72178	-3.16202	-1.12987
H	1.83015	5.62059	-4.51602	C	-0.66770	-4.11737	-1.98115
C	-2.54266	3.33310	0.09104	C	0.39454	-4.90065	-1.49620
H	-1.59795	3.04379	0.59652	C	-0.60320	-3.52817	-3.38227
C	-3.11088	4.57818	0.77105	H	-1.62782	-4.51837	-1.66924
H	-2.98492	4.49422	1.86860	C	0.32622	-5.68481	-0.21480

O	1.51202	-5.07713	-2.14182
C	0.85201	-3.41137	-3.82457
H	-1.16560	-4.15872	-4.08138
H	-1.06852	-2.53794	-3.37724
C	-0.03571	-4.89999	1.06070
H	1.27318	-6.22211	-0.10075
H	-0.44825	-6.44099	-0.40056
C	1.56263	-4.71705	-3.55421
H	1.32232	-2.59200	-3.27663
H	0.92381	-3.18676	-4.89358
C	1.17340	-4.28385	1.77858
H	-0.75097	-4.11050	0.81915
H	-0.53628	-5.58865	1.74842
H	2.62622	-4.70287	-3.78566
H	1.09777	-5.55399	-4.08862
C	2.14856	-3.59387	0.83478
H	1.72310	-5.05735	2.33042
H	0.80017	-3.55947	2.50918
O	1.39158	-2.82993	-0.07333
H	2.83469	-2.96563	1.41484
H	2.73858	-4.35170	0.29561
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R-anti-B_{2,5}-B(+)



E(RM062X) = -5098.38362133

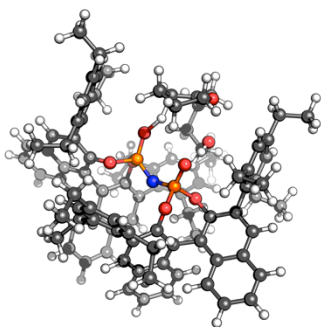
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C	-1.09220	-0.29786	3.62398
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C	-1.60161	0.62821	4.54174
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C	-6.14667	-2.11247	0.84854
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C	-5.81840	-2.00488	-0.50482
H	-6.49531	-2.39361	-1.25586
H	-1.01147	0.89877	5.40907
C	-3.35657	2.13282	5.27928
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H	-2.74729	2.45811	6.11425
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C	-5.43493	2.27382	4.05205
C	-4.96579	1.32979	3.13596
H	-6.41942	2.70529	3.92565
H	-5.60490	1.06698	2.30353
C	-7.33789	-2.74934	1.23180
C	-7.64053	-2.92092	2.58277
H	-8.02698	-3.12862	0.48635
H	-8.55704	-3.41850	2.87250
C	-6.75344	-2.47213	3.56022
C	-5.56917	-1.82909	3.19384
H	-6.98182	-2.62663	4.60693
H	-4.89679	-1.52116	3.98291
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P	1.03056	0.40345	-1.17246
O	1.17055	-0.37931	-2.43096
O	2.45858	0.31126	-0.30231
O	0.79669	1.97159	-1.59529
C	3.49439	1.14039	-0.67904
C	0.90474	2.90778	-0.59386
C	3.35306	2.54114	-0.59169
C	4.76519	0.60319	-0.99089
C	-0.13827	3.82726	-0.36276
C	2.14113	3.11089	0.04230
C	4.38361	3.39109	-1.07518
C	5.82681	1.45694	-1.32001
C	-0.01702	4.77470	0.66421
C	2.24079	4.01302	1.13107
C	5.63586	2.83372	-1.41527
C	4.19841	4.78358	-1.23240
H	6.80320	1.03675	-1.52971
C	1.14264	4.84771	1.43795
H	-0.81312	5.48956	0.82855
C	3.42036	4.12900	1.89783
C	6.68519	3.66214	-1.84485
C	5.24589	5.59546	-1.67235
H	3.24336	5.25222	-1.03666
C	1.24461	5.79266	2.47155
C	3.50788	5.07051	2.92581
H	4.27275	3.48698	1.71592
C	6.48870	5.03777	-1.96933
H	7.65308	3.24410	-2.09549
H	5.09167	6.66077	-1.78622
C	2.42459	5.90275	3.20952
H	0.41415	6.44834	2.70511
H	4.41706	5.15152	3.50730
H	7.29831	5.67132	-2.30792
H	2.49756	6.63138	4.00645
C	-1.32696	3.90686	-1.24689
C	-1.20387	4.44496	-2.55896
C	-2.61885	3.62446	-0.72842
C	-2.36049	4.68526	-3.31726
C	-3.75233	3.90332	-1.50697
C	-3.63242	4.44050	-2.79243
H	-4.73888	3.69514	-1.10959
C	5.03374	-0.85379	-1.00531

C	5.15428	-1.57099	0.21351	H	-3.36759	3.72223	2.64236
C	5.33598	-1.50647	-2.23260	H	-2.96560	5.05255	1.51040
C	5.50746	-2.92845	0.18421	H	-4.54321	4.19088	1.35740
C	5.70150	-2.86196	-2.21910	C	4.04559	-2.61880	5.03157
C	5.76929	-3.58067	-1.02304	H	4.88159	-1.94460	4.74498
H	5.91981	-3.36508	-3.15340	C	4.11666	-2.84749	6.53904
C	-4.18224	-1.58297	-2.32320	H	5.11921	-3.24207	6.80734
C	-4.13356	-0.43859	-3.15907	H	3.95443	-1.89086	7.08000
C	-3.86306	-2.85819	-2.86655	H	3.35181	-3.58511	6.86114
C	-3.69292	-0.56742	-4.48560	C	-0.93336	-3.09927	4.62852
C	-3.44771	-2.95271	-4.20305	H	-1.66376	-2.98286	3.80368
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H	-3.18757	-3.92093	-4.61506	H	-0.87938	-2.90739	6.79507
C	0.22607	-0.91931	3.89460	H	-1.96776	-1.72203	5.96843
C	0.29871	-2.24508	4.40010	H	-2.46490	-3.44379	6.12046
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C	2.64360	-0.72201	4.13253	C	1.68128	2.25764	4.33429
C	2.71787	-2.02737	4.62879	H	2.74498	2.21111	4.64982
H	3.54735	-0.13061	4.04891	H	1.45854	3.28160	3.97818
H	5.58361	-3.48527	1.11080	H	1.03476	2.05381	5.21214
H	1.60981	-3.79876	5.12047	C	-4.60900	0.91721	-2.69036
H	-3.64857	0.30721	-5.12401	H	-4.23379	1.13702	-1.67331
H	-2.27100	5.11160	-4.30958	C	-6.13264	1.00373	-2.70517
C	6.10841	-5.04926	-1.03175	H	-6.58033	0.23543	-2.04306
H	5.34420	-5.60803	-0.44905	H	-6.45282	2.00206	-2.34121
C	7.49148	-5.30046	-0.43784	H	-6.51354	0.86087	-3.73876
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H	7.72579	-6.38456	-0.48955	H	-3.99848	-3.95407	-0.96920
H	8.26222	-4.74177	-1.01078	C	-5.15128	-4.98273	-2.48209
C	4.96797	-0.91523	1.56458	H	-5.20739	-5.89313	-1.84891
H	4.09015	-0.24168	1.56606	H	-6.09354	-4.41066	-2.36277
C	6.21383	-0.14603	1.99219	H	-5.05258	-5.29763	-3.54260
H	7.09707	-0.82017	2.00284	C	-2.87595	-1.94032	-6.43821
H	6.40986	0.70359	1.30710	H	-2.66521	-0.93821	-6.87146
H	6.06377	0.25909	3.01528	C	-3.92459	-2.63150	-7.30551
C	5.25922	-0.80154	-3.57798	H	-3.56471	-2.68031	-8.35488
H	4.77036	0.19077	-3.50619	H	-4.10804	-3.66678	-6.94767
C	6.64266	-0.62522	-4.20164	H	-4.87787	-2.06117	-7.28222
H	6.55028	-0.06303	-5.15462	H	-0.65728	-4.17645	4.63743
H	7.31225	-0.05995	-3.52252	H	4.19686	-3.58263	4.49914
H	7.10100	-1.61210	-4.42156	H	4.76382	-1.68857	2.33306
C	-4.86476	4.75546	-3.60335	H	4.63330	-1.39284	-4.27652
H	-4.59266	5.00878	-4.65112	H	6.09163	-5.45073	-2.06845
C	-5.63150	5.93234	-3.00653	H	-1.92747	-2.51856	-6.46870
H	-5.99184	5.68725	-1.98503	H	-3.03442	-4.74418	-2.22207
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H	-6.51106	6.16358	-3.64347	H	-5.52546	3.86473	-3.64301
C	0.12854	4.85924	-3.15681	H	0.05582	4.89534	-4.26584
H	0.92248	4.12097	-2.93728	H	-3.49886	2.15830	0.57872
C	0.55619	6.23951	-2.66591	H	2.20186	1.35097	2.43641
H	-0.22310	6.99259	-2.90979	O	-1.20185	-2.34700	-0.75688
H	0.72923	6.23506	-1.57134	H	-0.33908	-3.08259	-1.57113
H	1.50327	6.53298	-3.16575	C	0.00073	-3.87617	-2.45970
C	-2.83106	3.04192	0.65413	C	1.16665	-4.45509	-1.91333
H	-1.88431	2.67643	1.10329	C	0.08252	-3.07676	-3.76003
C	-3.46541	4.06667	1.59402	H	-0.83416	-4.56694	-2.36356

C	1.09554	-5.52511	-0.86390
O	2.36112	-4.12647	-2.27088
C	1.46317	-3.24489	-4.37958
H	-0.68219	-3.43509	-4.45131
H	-0.10021	-2.01910	-3.55115
C	0.31184	-5.09594	0.39847
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H	0.58433	-6.37137	-1.33744
C	2.52167	-3.11225	-3.30713
H	1.65370	-2.47563	-5.13309
H	1.56033	-4.22513	-4.86392
C	1.19081	-4.49234	1.50115
H	-0.46015	-4.37040	0.12635
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C	2.22986	-3.50588	0.99393
H	1.71860	-5.28717	2.04402
H	0.53009	-3.98537	2.20843
O	1.60088	-2.56689	0.14611
H	2.70962	-3.01308	1.84664
H	3.01109	-4.04605	0.43732
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R-anti-B_{1,4}-C(-)



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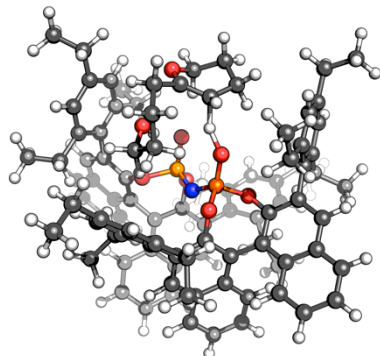
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C	4.70691	0.59789	-0.96837
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H	6.71974	1.00738	-1.59272
H	-1.10611	5.38937	0.09439
C	0.49192	5.67821	2.19910
C	1.47024	5.80277	3.18723
H	-0.40201	6.28744	2.26180
H	1.32580	6.49627	4.00547

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C	2.83526	4.15272	2.05814
H	3.40291	5.15653	3.87430
H	3.75893	3.59241	2.01692
C	6.71077	3.65837	-1.54705
C	6.55562	5.04413	-1.55478
H	7.66446	3.23519	-1.83996
H	7.38389	5.67949	-1.84075
C	5.32767	5.61110	-1.21953
C	4.25388	4.79831	-0.85111
H	5.20399	6.68600	-1.25180
H	3.31417	5.28450	-0.63443
C	-3.66964	-0.35451	0.49116
C	-1.39625	-0.15641	2.55728
C	-3.73849	0.17456	1.80518
C	-4.80260	-0.95463	-0.09064
C	-0.41051	0.08893	3.53037
C	-2.49732	0.71511	2.44057
C	-4.94689	0.03676	2.54638
C	-6.01624	-0.96976	0.60086
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C	-5.03471	0.36529	3.91941
H	-6.88267	-1.43155	0.13913
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C	-3.44214	2.95874	2.86207
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C	-6.24702	0.25774	4.60378
H	-4.17310	0.68959	4.48425
C	-1.24765	3.57671	4.48516
C	-3.34123	4.21719	3.46001
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C	0.50871	-0.99174	3.97485
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C	2.23393	-3.06820	4.81999
H	3.81519	-1.87474	3.99798
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C	4.53890	-1.37015	-2.51266	H	-2.94407	5.24737	-6.54637
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C	-1.09043	3.73018	-2.05590	H	1.01506	5.91172	-2.03916
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H	-6.07974	-5.63740	-4.28104	C	5.16136	-0.15898	-4.61560
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C	-6.37312	0.80507	-2.65058	H	5.57532	-1.08551	-5.06715
H	-6.98896	0.29491	-3.42162	C	5.46189	-5.04825	-2.08808
H	-6.77590	0.56719	-1.64516	H	5.10958	-5.66690	-1.23486
H	-6.44712	1.90139	-2.80721	C	6.93870	-5.33038	-2.34477
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C	-4.20958	-5.34162	0.10932	H	7.54328	-5.08465	-1.44585
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C	3.14685	-4.19268	5.23749	H	-5.35834	-3.63276	0.70572
H	2.74194	-5.15724	4.86170	H	-3.78518	-4.83867	-4.91571
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H	2.76832	1.53526	4.90294	O	-1.33549	-1.29286	1.78529
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R-anti-B_{1,4}-B(-)



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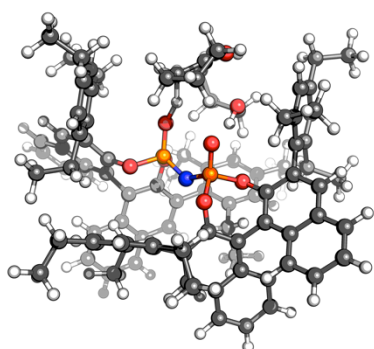
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C	2.68985	4.28230	1.92349
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H	3.62819	3.74523	1.90879
C	6.58163	3.79542	-1.66413
C	6.37665	5.17345	-1.72170
H	7.55027	3.39670	-1.94192
H	7.18172	5.82763	-2.03059
C	5.12872	5.70730	-1.40687
C	4.08477	4.87003	-1.00884
H	4.96619	6.77513	-1.47804
H	3.12820	5.32997	-0.81028
C	-3.66168	-0.40697	0.47608
C	-1.45206	-0.07963	2.59018
C	-3.78125	0.17175	1.76516
C	-4.76092	-1.05757	-0.11379
C	-0.48454	0.23224	3.56264
C	-2.56946	0.76143	2.41502
C	-5.00971	0.03827	2.47340
C	-5.99489	-1.07406	0.54004
C	-0.48554	1.50398	4.14896
C	-2.54547	2.06559	2.97140
C	-6.13052	-0.53706	1.82175
C	-5.14842	0.42235	3.82754
H	-6.83503	-1.57662	0.07247
C	-1.46943	2.44109	3.81528
H	0.26740	1.75320	4.88600
C	-3.57034	2.99951	2.72415
C	-7.36390	-0.63027	2.48672
C	-6.37995	0.31794	4.47724
H	-4.31217	0.78919	4.40443
C	-1.42435	3.73205	4.36415
C	-3.50917	4.28317	3.27173
H	-4.41488	2.74578	2.09832
C	-7.48808	-0.19246	3.80451
H	-8.22789	-1.05911	1.99266
H	-6.47301	0.62838	5.51003
C	-2.43641	4.65048	4.08357
H	-0.60656	4.03044	5.00952
H	-4.29683	4.99611	3.06548
H	-8.44010	-0.27173	4.31336
H	-2.39309	5.64699	4.50361
C	0.46747	-0.80158	4.04868
C	-0.02158	-1.93813	4.75740
C	1.86859	-0.65790	3.85163
C	0.88047	-2.92474	5.18635
C	2.73508	-1.67485	4.28474
C	2.25142	-2.80493	4.94681
H	3.79910	-1.58450	4.10004
C	-4.59269	-1.90289	-1.32486
C	-4.66789	-1.33990	-2.62329
C	-4.41664	-3.30593	-1.17199
C	-4.57887	-2.17335	-3.74669
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H	-4.24851	-5.18583	-2.24894

C	4.88603	-0.76404	-1.17730	H	-4.63720	4.29861	-7.27333
C	5.45103	-1.56360	-0.15223	H	-4.43456	5.20051	-5.72302
C	4.59141	-1.34428	-2.43914	H	-3.00164	4.87434	-6.78248
C	5.69968	-2.92364	-0.39768	C	0.76854	4.24452	-3.77204
C	4.84528	-2.70772	-2.64811	H	1.50966	3.59454	-3.27190
C	5.40122	-3.49909	-1.63802	C	0.98353	5.69592	-3.34940
H	4.62267	-3.15059	-3.61206	H	0.25440	6.35741	-3.86386
C	-1.18902	3.59679	-2.19749	H	0.87322	5.81403	-2.25336
C	-0.66012	3.78815	-3.51033	H	2.01053	6.01385	-3.62769
C	-2.58716	3.37338	-2.04380	C	-3.27754	3.30367	-0.69670
C	-1.49825	3.61605	-4.62357	H	-2.56092	3.20709	0.13895
C	-3.39304	3.23609	-3.18487	C	-4.15743	4.53714	-0.47874
C	-2.85557	3.32864	-4.46915	H	-4.96562	4.58023	-1.23866
H	-4.45519	3.06134	-3.06959	H	-4.63521	4.49724	0.51916
H	-4.64247	-1.74264	-4.73923	H	-3.55513	5.46635	-0.54505
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C	-4.36066	-4.44203	-4.82441	H	7.70093	-0.13738	0.56334
H	-4.23677	-3.83334	-5.74654	H	7.56031	-0.41111	2.34162
C	-5.61979	-5.29186	-4.97178	H	7.83649	-1.81215	1.24039
H	-6.51550	-4.63947	-5.05213	C	4.03467	-0.53821	-3.59575
H	-5.54542	-5.90907	-5.89178	H	3.54216	0.39493	-3.25426
H	-5.73814	-5.97117	-4.10115	C	5.13566	-0.17375	-4.58614
C	-4.86839	0.13816	-2.84707	H	4.70397	0.42063	-5.41883
H	-4.32909	0.71628	-2.07671	H	5.91841	0.43420	-4.08513
C	-6.34939	0.50205	-2.83058	H	5.59822	-1.09126	-5.00794
H	-6.89241	-0.06408	-3.61712	C	5.69146	-4.95612	-1.88692
H	-6.79720	0.27467	-1.84157	H	5.36172	-5.56025	-1.01447
H	-6.46906	1.58744	-3.02945	C	7.18122	-5.17911	-2.12681
C	-4.29674	-3.90327	0.22891	H	7.36864	-6.25515	-2.32649
H	-3.48548	-3.37410	0.77337	H	7.52043	-4.59001	-3.00585
C	-3.99202	-5.40020	0.30060	H	7.76849	-4.87620	-1.23389
H	-3.87019	-5.69975	1.36299	H	1.00698	4.17572	-4.85587
H	-4.83039	-5.98850	-0.12893	H	-3.26124	2.41084	-6.37127
H	-3.04833	-5.63281	-0.23497	H	-4.43628	0.44184	-3.82569
C	3.19523	-3.89467	5.38716	H	-5.24534	-3.72598	0.77830
H	2.81901	-4.87718	5.02839	H	-3.47204	-5.10449	-4.74575
C	3.33449	-3.92208	6.90682	H	5.12830	-5.32104	-2.77376
H	3.70893	-2.94308	7.27530	H	3.25226	-1.12879	-4.11989
H	2.35747	-4.14435	7.38586	H	5.44310	-1.68692	2.00118
H	4.05753	-4.71237	7.19919	H	4.20372	-3.74519	4.94329
C	-1.48791	-2.12066	5.11515	H	-1.67645	-3.16085	5.45993
H	-2.14135	-1.98203	4.23273	H	3.17294	0.17633	2.36585
C	-1.91811	-1.17960	6.23792	H	-3.91635	2.40007	-0.64467
H	-1.26254	-1.31424	7.12454	P	1.11289	0.23706	-1.05984
H	-1.87823	-0.12197	5.91106	O	2.46767	0.33540	-0.14329
H	-2.96419	-1.40875	6.53164	O	0.90094	1.68863	-1.77656
C	2.49122	0.53803	3.16123	N	0.00944	0.01403	0.06617
H	1.74167	1.18201	2.65889	P	-1.16665	-0.99701	0.27015
C	3.29556	1.38066	4.15109	O	-1.15877	-2.38987	-0.33943
H	3.79714	2.21090	3.61873	O	-2.51189	-0.25032	-0.25614
H	2.63117	1.80679	4.93046	O	-1.35403	-1.24854	1.87280
H	4.08345	0.77145	4.64151	O	1.26813	-0.79984	-2.11737
C	-3.73469	3.14081	-5.67964	H	-0.44359	-3.26254	-0.85685
H	-4.72345	2.72439	-5.38680	C	-0.23254	-4.46252	-1.49365
C	-3.96253	4.46311	-6.40697	C	1.13792	-4.72457	-1.55412

C	-1.00986	-4.22879	-2.79329
H	-0.73305	-5.04710	-0.72108
C	1.92040	-5.45135	-0.50177
O	1.87091	-4.40791	-2.58633
C	-0.08012	-4.26184	-4.00618
H	-1.76927	-5.00829	-2.89131
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C	1.47108	-5.25835	0.95739
H	2.95772	-5.14264	-0.62816
H	1.85951	-6.51978	-0.75345
C	1.24844	-3.63036	-3.63435
H	-0.51785	-3.72226	-4.85050
H	0.10097	-5.29416	-4.32866
C	1.22393	-3.81669	1.42578
H	0.56154	-5.84134	1.14604
H	2.25302	-5.71456	1.57630
H	1.13185	-2.60997	-3.25180
H	1.97361	-3.64239	-4.44791
C	2.27810	-2.80059	0.99506
H	1.17077	-3.82389	2.51904
H	0.24482	-3.47581	1.08621
O	2.45972	-2.82637	-0.40765
H	3.24408	-3.03988	1.46216
H	1.98572	-1.79805	1.32346
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R-anti-B_{1,4}-C(+)



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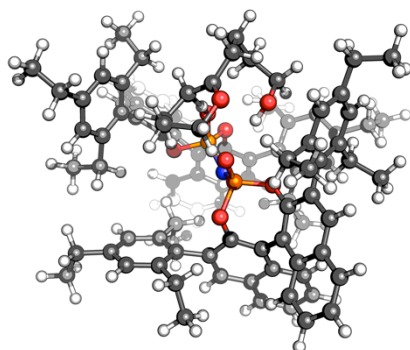
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C	-3.73913	-0.53419	0.54405
C	-6.18286	-1.13047	1.82422
C	-4.73904	-1.27126	-0.12507
C	-5.97042	-1.50416	0.49741
H	-6.74814	-2.02957	-0.04399

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C	-4.83213	3.93233	3.39452
C	-4.52149	2.71047	2.79357
H	-5.77935	4.41166	3.18391
H	-5.24189	2.27887	2.11121
C	-7.38619	-1.47048	2.46325
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H	-8.17148	-1.98820	1.92501
H	-8.50397	-1.43615	4.30044
C	-6.56727	-0.53307	4.53362
C	-5.36985	-0.18019	3.90776
H	-6.70999	-0.31910	5.58506
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N	-0.04110	0.21550	0.05981
P	1.11031	0.10226	-1.04711
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C	3.59770	0.71190	-0.85070
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C	0.25298	3.63971	-1.47716
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C	5.86299	0.42399	-1.69667
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C	5.86569	1.72937	-2.18859
C	4.73876	3.85041	-2.56283
H	6.73254	-0.20814	-1.84108
C	1.63790	5.09263	-0.09980
H	-0.29597	5.63077	-0.86847
C	3.87902	4.40999	0.55802
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C	5.84934	4.31254	-3.27219
H	3.88080	4.50448	-2.48856
C	1.81448	6.29952	0.59528
C	4.04033	5.61357	1.24804
H	4.68913	3.69262	0.58181
C	6.96988	3.49846	-3.43074
H	7.85084	1.58420	-3.04750
H	5.83845	5.30465	-3.70487
C	3.01193	6.55626	1.26538
H	1.02798	7.04453	0.61785
H	4.96364	5.81301	1.77630
H	7.82819	3.86172	-3.98105
H	3.14195	7.48719	1.80184
C	-0.95850	3.48916	-2.31987
C	-0.85198	3.55210	-3.73762
C	-2.24376	3.43275	-1.71886
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C	-3.38816	3.47403	-2.52989

C	-3.28491	3.55478	-3.92241	C	-2.43615	3.34434	-0.21879
H	-4.36987	3.44634	-2.07185	H	-1.49074	3.10220	0.30962
C	4.76989	-1.52005	-0.65620	C	-2.99922	4.64970	0.34139
C	5.13522	-1.87708	0.66392	H	-2.88051	4.66485	1.44281
C	4.62236	-2.53141	-1.64003	H	-2.46311	5.52783	-0.07171
C	5.35602	-3.22568	0.98012	H	-4.07826	4.74041	0.09519
C	4.82337	-3.87501	-1.28557	C	4.22890	-1.36438	5.47096
C	5.20108	-4.22700	0.01507	H	5.10013	-0.82665	5.03836
H	4.69434	-4.64917	-2.03288	C	4.28581	-1.20382	6.98832
C	-4.49541	-1.90533	-1.44334	H	5.26685	-1.56454	7.36298
C	-4.49686	-1.12647	-2.62824	H	4.17119	-0.13395	7.26538
C	-4.37969	-3.32084	-1.53702	H	3.48446	-1.79675	7.47740
C	-4.35646	-1.75891	-3.87337	C	-0.77191	-1.60863	5.25026
C	-4.25330	-3.91940	-2.79934	H	-1.51312	-1.70191	4.43398
C	-4.24616	-3.14966	-3.96679	C	-1.39071	-0.86426	6.43033
H	-4.15561	-4.99625	-2.87423	H	-0.65534	-0.77770	7.25850
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C	2.92912	0.31034	4.09823	C	2.22476	3.30683	3.50573
C	2.93447	-0.82764	4.91111	H	3.29693	3.24195	3.78723
H	3.86664	0.79467	3.85301	H	2.07463	4.21221	2.88466
H	5.63913	-3.49965	1.98999	H	1.61719	3.41650	4.42652
H	1.73575	-2.34740	5.83470	C	-4.73911	0.36516	-2.61109
H	-4.37324	-1.16551	-4.78013	H	-4.24502	0.84384	-1.74507
H	-1.94293	3.63704	-5.59533	C	-6.23215	0.67729	-2.57962
C	5.42000	-5.67168	0.38421	H	-6.70521	0.24043	-1.67609
H	4.82457	-5.91625	1.29041	H	-6.38311	1.77668	-2.55519
C	6.89675	-5.95385	0.64951	H	-6.72837	0.26893	-3.48565
H	7.26171	-5.35514	1.51092	C	-4.39186	-4.22986	-0.31978
H	7.03293	-7.02996	0.88673	H	-4.23634	-3.66902	0.62442
H	7.50195	-5.70809	-0.24930	C	-5.69492	-5.02102	-0.22317
C	5.32594	-0.84732	1.75202	H	-5.67978	-5.64830	0.69292
H	4.70716	0.05529	1.57368	H	-6.56799	-4.34055	-0.16885
C	6.78968	-0.43984	1.87437	H	-5.81173	-5.68827	-1.10313
H	7.41837	-1.32388	2.11351	C	-4.13406	-3.81838	-5.31325
H	7.14441	0.01698	0.92667	H	-3.93619	-3.06819	-6.10965
H	6.89920	0.30524	2.69039	C	-5.41805	-4.56683	-5.66144
C	4.24914	-2.21551	-3.07377	H	-5.32072	-5.02360	-6.66875
H	3.86297	-1.18185	-3.18895	H	-5.61156	-5.37542	-4.92493
C	5.43724	-2.40502	-4.01259	H	-6.28026	-3.86599	-5.67038
H	5.13183	-2.15688	-5.05082	H	-0.55581	-2.64951	5.57658
H	6.27321	-1.73629	-3.72030	H	4.33041	-2.43845	5.20390
H	5.78808	-3.45848	-3.99120	H	4.98635	-1.27333	2.71658
C	-4.52675	3.64276	-4.77470	H	3.42951	-2.88622	-3.39142
H	-4.27569	3.51615	-5.85040	H	5.07340	-6.34323	-0.43128
C	-5.22128	4.98982	-4.59682	H	-3.27946	-4.52842	-5.30812
H	-5.55851	5.12010	-3.54668	H	-3.55645	-4.95477	-0.38660
H	-4.52937	5.81657	-4.86543	H	-4.29437	0.82814	-3.51679
H	-6.10992	5.03968	-5.26069	H	-5.22906	2.82751	-4.50474
C	0.47938	3.67431	-4.45730	H	0.37006	3.36835	-5.52079
H	1.23635	2.98969	-4.02917	H	-3.13947	2.51660	0.01175
C	1.00269	5.10787	-4.43225	H	2.55146	1.88430	1.91373
H	0.25177	5.79900	-4.87090	O	-1.14138	-2.25313	0.00891
H	1.23422	5.42875	-3.39734	H	-0.61402	-3.09230	-0.76633
H	1.93610	5.17105	-5.03036	C	-0.60741	-4.17337	-1.58326

C	0.55522	-4.88211	-1.28084
C	-0.85151	-3.66249	-2.99297
H	-1.46517	-4.54042	-1.02577
C	0.81412	-5.59664	0.01359
O	1.51995	-5.08406	-2.14268
C	0.47877	-3.53002	-3.72792
H	-1.50848	-4.35196	-3.53701
H	-1.35416	-2.69068	-2.94808
C	0.12971	-5.08633	1.29225
H	1.90008	-5.64734	0.12904
H	0.47509	-6.62747	-0.17161
C	1.26212	-4.81135	-3.54386
H	1.03541	-2.68256	-3.32096
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C	0.66218	-3.78243	1.93838
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H	0.22113	-5.90468	2.01439
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H	0.71089	-5.67819	-3.92951
C	2.01080	-3.29617	1.41953
H	0.76269	-3.93653	3.02012
H	-0.07155	-2.99068	1.81005
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H	2.26717	-2.33931	1.89325
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R-anti-B_{1,4}-B(+)



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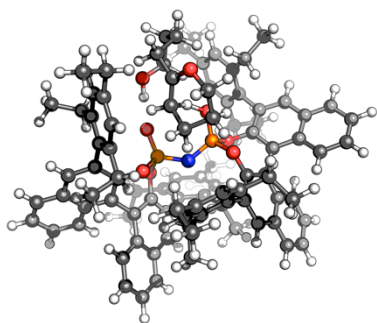
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C	5.96315	1.29418	0.91716

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C	2.50095	-4.57892	4.00675
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H	1.79014	-5.14841	4.59381
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H	5.60480	-4.90179	2.66220
H	5.10614	-2.63265	1.88975
C	7.28450	0.95839	2.91882
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C	6.35265	-0.23233	4.80242
C	5.17732	-0.46160	4.08393
H	6.44309	-0.59368	5.81872
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C	1.97526	-2.97676	-4.87340

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C	3.22046	-3.06951	-4.24471	C	2.25575	-3.30669	-0.57213
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C	4.86838	3.49882	-3.39699	C	1.31607	-0.08522	6.55134
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H	-3.99430	-1.25117	3.80957	H	-2.28563	-4.51213	2.30691
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H	1.93212	-2.91192	-5.95433	C	6.39908	-0.58941	-2.47414
C	-5.30706	5.76049	1.23222	H	6.91815	-0.26681	-1.54671
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H	-7.43054	5.83417	0.76158	C	5.62247	4.87460	0.74923
C	-5.08914	0.80033	1.91792	H	5.43905	5.39449	1.71296
H	-4.41839	-0.03091	1.62635	H	6.46689	4.16936	0.88603
C	-6.52652	0.29694	1.99081	H	5.90372	5.63367	-0.01085
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C	-4.49055	2.83628	-2.76303	H	6.35520	5.65733	-5.65495
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C	-5.77171	3.13303	-3.53945	H	7.14775	4.37317	-4.66476
H	-5.57140	3.04845	-4.62829	H	0.51215	1.81890	5.96894
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H	4.27605	-2.83138	-6.12338	H	-5.03308	6.54258	0.49093
C	5.13516	-4.47633	-5.03074	H	4.12553	5.04004	-4.69881
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H	6.04341	-4.47606	-5.66947	H	5.20446	-2.34265	-4.67625
C	-0.52658	-3.02267	-4.90060	H	-0.37781	-2.58183	-5.91060
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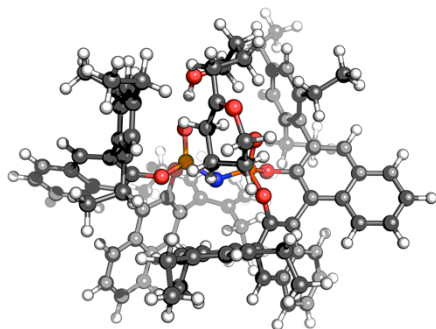
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C	-7.32777	-2.25059	1.73665
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C	0.40187	3.92984	-0.83512
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C	4.84628	2.71474	-1.62476
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C	6.06117	4.58613	-2.61475
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H	7.90718	1.75005	-2.83807
H	6.10834	5.63405	-2.88177
C	3.38472	6.25494	2.21351
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C	-2.10337	3.75011	-0.99160
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C	-3.25115	4.25009	-3.08510
H	-4.24333	3.77273	-1.23832
C	4.62523	-1.52790	-0.97196
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H	4.44178	-4.39443	-2.82889	C	4.26906	-1.65494	6.79674
C	-4.27260	-1.57613	-2.03190	H	5.26872	-2.03750	7.09205
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H	4.98924	-3.96585	1.39903	H	1.17721	2.98016	4.67172
H	1.63232	-2.76960	5.76803	C	-4.72118	0.88466	-2.60515
H	-4.01403	0.01599	-5.04924	H	-4.27495	1.18696	-1.63759
H	-1.99325	4.66337	-4.77387	C	-6.23936	1.01610	-2.53671
C	4.77439	-5.83544	-0.54608	H	-6.65936	0.34367	-1.76145
H	4.04878	-6.14794	0.23597	H	-6.51030	2.06047	-2.27631
C	6.17370	-6.31192	-0.16730	H	-6.69024	0.76575	-3.52063
H	6.47720	-5.89406	0.81583	C	-3.87136	-4.06542	-1.50586
H	6.18152	-7.41994	-0.09618	H	-3.83205	-3.74394	-0.44509
H	6.90749	-5.99974	-0.94094	C	-5.04336	-5.02582	-1.68938
C	4.98003	-1.28751	1.55965	H	-4.95855	-5.85707	-0.95812
H	4.33887	-0.38486	1.53802	H	-6.00665	-4.50246	-1.51967
C	6.43581	-0.87920	1.75451	H	-5.03862	-5.45644	-2.71292
H	7.08186	-1.78048	1.82047	C	-3.35441	-2.34955	-6.19216
H	6.78011	-0.24296	0.91344	H	-2.58653	-1.62259	-6.53460
H	6.53450	-0.30094	2.69726	C	-4.59526	-2.23973	-7.07340
C	4.27142	-1.81063	-3.50837	H	-4.32451	-2.46846	-8.12565
H	3.97828	-0.74075	-3.49216	H	-5.36797	-2.96482	-6.73922
C	5.51794	-1.96859	-4.37549	H	-5.01452	-1.21214	-7.03224
H	5.32728	-1.53633	-5.38028	H	-0.68385	-3.14055	5.43501
H	6.37969	-1.43828	-3.92114	H	4.17761	-2.84074	4.98208
H	5.77516	-3.04195	-4.49758	H	4.65632	-1.87375	2.44465
C	-4.53064	4.44210	-3.85996	H	3.43236	-2.35444	-3.98992
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C	-4.73843	5.90869	-4.22744	H	-2.92319	-3.36725	-6.31504
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H	1.87205	6.15400	-4.14315	H	0.17499	-2.96729	-0.38478
C	-2.22036	3.37668	0.46972	O	-2.53060	-0.17021	-0.24871
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C	-2.73739	4.55323	1.29408	N	-0.00709	0.16970	0.04231
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H	1.02763	-2.10229	-2.99820
C	-0.05504	-5.70412	-2.29883
H	1.90038	-4.73413	-2.36453
H	1.89852	-6.32350	-1.53936
C	0.77999	-5.26500	1.95630
H	-0.58689	-3.60054	1.82360
H	0.48301	-3.60615	3.22733
O	1.00688	-3.03132	-3.30904
C	-0.34623	-4.96409	-3.60538
H	-0.82414	-5.46180	-1.55768
H	-0.13045	-6.78236	-2.46783
H	1.74587	-5.51806	2.40579
H	0.01912	-5.94205	2.34619
C	-0.32878	-3.44505	-3.48991
H	0.39107	-5.25441	-4.36497
H	-1.32633	-5.28929	-3.97128
H	-0.74573	-3.00812	-4.40914
H	-0.95321	-3.11653	-2.64531

R-gau-C₄-C(-) intermediate



E(RM062X) = -5098.41082367

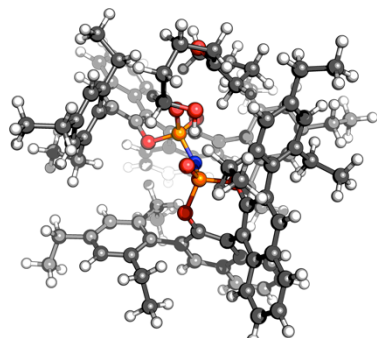
C	-1.88215	-0.35147	2.58960
C	-1.14946	0.15643	3.67782
C	-3.23711	0.01450	2.43233
C	-1.70330	1.14922	4.49289
C	-3.76959	1.07829	3.20560
C	-2.99104	1.63418	4.25015
C	-4.08621	-0.77986	1.50095
C	-5.23988	-1.47916	1.94449
C	-3.70246	-0.85925	0.14845
C	-6.07576	-2.11303	0.99142
C	-4.53553	-1.50180	-0.78673
C	-5.72905	-2.09606	-0.36253
H	-6.37209	-2.57591	-1.09116

H	-1.13019	1.53357	5.32864
C	-3.52016	2.65667	5.05387
C	-4.80206	3.15117	4.80914
H	-2.93872	3.07974	5.86448
H	-5.20195	3.94499	5.42662
C	-5.56379	2.63353	3.76174
C	-5.05555	1.60738	2.96239
H	-6.55145	3.03061	3.56619
H	-5.66811	1.24452	2.14763
C	-7.24058	-2.77726	1.40776
C	-7.56769	-2.84166	2.76244
H	-7.89130	-3.25734	0.68633
H	-8.46399	-3.35991	3.07801
C	-6.73220	-2.25533	3.71222
C	-5.57406	-1.58499	3.31279
H	-6.98011	-2.32421	4.76361
H	-4.94076	-1.16752	4.08360
C	3.54534	0.97788	-0.73262
C	1.12471	2.93465	-0.78701
C	3.55109	2.38583	-0.80634
C	4.70601	0.25814	-1.08532
C	0.13693	3.92237	-0.61718
C	2.40454	3.14181	-0.23653
C	4.64113	3.05457	-1.42602
C	5.82462	0.93513	-1.58360
C	0.35380	4.98144	0.27327
C	2.59590	4.15832	0.73284
C	5.79262	2.31524	-1.78744
C	4.61042	4.43826	-1.71210
H	6.71715	0.37405	-1.83600
C	1.55636	5.08716	0.97595
H	-0.40878	5.74123	0.39521
C	3.80019	4.27887	1.45810
C	6.89816	2.96535	-2.35906
C	5.71386	5.07039	-2.28911
H	3.73328	5.03849	-1.51197
C	1.74825	6.13250	1.89344
C	3.97153	5.31380	2.38009
H	4.60625	3.56816	1.32867
C	6.85802	4.33828	-2.60276
H	7.78867	2.40943	-2.62800
H	5.67916	6.13186	-2.49817
C	2.95163	6.24174	2.59233
H	0.96495	6.85850	2.07634
H	4.89869	5.39612	2.93232
H	7.71077	4.83337	-3.04907
H	3.09142	7.04401	3.30518
C	-1.10358	3.92476	-1.42904
C	-1.06107	4.33054	-2.79120
C	-2.35685	3.65984	-0.81884
C	-2.26057	4.47574	-3.50500
C	-3.53660	3.83461	-1.55817
C	-3.49711	4.25366	-2.89180
H	-4.49413	3.64419	-1.08741
C	4.77375	-1.21853	-0.98704
C	4.97196	-1.84423	0.27075
C	4.75662	-2.01033	-2.16743

C	5.13492	-3.23706	0.33168	H	-4.11956	4.47484	1.25819
C	4.92617	-3.40007	-2.06875	C	4.07737	-1.83921	5.25000
C	5.11582	-4.01753	-0.82835	H	4.89096	-1.22954	4.80049
H	4.89992	-4.00560	-2.96712	C	4.22431	-1.77938	6.76817
C	-4.13467	-1.63256	-2.20825	H	5.24211	-2.11743	7.05576
C	-4.21223	-0.51776	-3.08158	H	4.08116	-0.73747	7.12645
C	-3.70702	-2.88866	-2.71552	H	3.48199	-2.44187	7.26123
C	-3.82042	-0.66017	-4.42190	C	-0.90998	-2.40694	5.15775
C	-3.35009	-3.00102	-4.06773	H	-1.70587	-2.36803	4.38666
C	-3.39163	-1.89426	-4.91997	C	-1.46396	-1.92368	6.49404
H	-3.02824	-3.95900	-4.45660	H	-0.68640	-2.00284	7.28351
C	0.18875	-0.38160	4.01674	H	-1.80277	-0.87026	6.42074
C	0.30087	-1.59502	4.74368	H	-2.33151	-2.55250	6.78500
C	1.35931	0.35258	3.69986	C	1.31058	1.68041	2.97926
C	1.57037	-2.05989	5.12043	H	0.34109	1.84065	2.46484
C	2.61282	-0.13693	4.09778	C	1.55173	2.82894	3.95565
C	2.72570	-1.33502	4.81044	H	2.60570	2.82404	4.30562
H	3.50503	0.43300	3.86649	H	1.34719	3.79470	3.45617
H	5.27813	-3.72032	1.29116	H	0.87733	2.74808	4.83279
H	1.65951	-2.98886	5.67129	C	-4.74945	0.82193	-2.63132
H	-3.86575	0.19170	-5.09047	H	-4.35846	1.09175	-1.63086
H	-2.23511	4.79392	-4.54075	C	-6.27463	0.82915	-2.60948
C	5.27101	-5.51386	-0.73523	H	-6.66322	0.08129	-1.88904
H	4.55961	-5.91362	0.01954	H	-6.63602	1.83216	-2.30028
C	6.69655	-5.89689	-0.34883	H	-6.67340	0.60340	-3.62144
H	6.95165	-5.49458	0.65440	C	-3.58824	-4.12532	-1.84661
H	6.78815	-7.00301	-0.31837	H	-3.61924	-3.88541	-0.76431
H	7.41616	-5.50053	-1.09679	C	-4.68838	-5.13535	-2.16195
C	5.03970	-1.06045	1.56328	H	-4.58649	-6.01511	-1.49228
H	4.30458	-0.23230	1.56947	H	-5.68936	-4.68410	-2.00348
C	6.44019	-0.50859	1.80507	H	-4.60895	-5.48312	-3.21360
H	7.17934	-1.33728	1.83613	C	-2.97435	-2.02645	-6.36228
H	6.72455	0.20539	1.00536	H	-2.24621	-1.22483	-6.61248
H	6.46373	0.02571	2.77819	C	-4.17931	-1.93491	-7.29430
C	4.52813	-1.41867	-3.54517	H	-3.84624	-2.06523	-8.34545
H	4.14331	-0.37936	-3.49554	H	-4.91304	-2.73326	-7.05192
C	5.80787	-1.43350	-4.37757	H	-4.67185	-0.94387	-7.20097
H	5.60955	-0.97621	-5.36971	H	-0.63470	-3.47968	5.25757
H	6.60804	-0.85266	-3.87514	H	4.21257	-2.88598	4.90163
H	6.15932	-2.47512	-4.53466	H	4.76973	-1.71706	2.41644
C	-4.77392	4.45598	-3.66844	H	3.75348	-2.01064	-4.07558
H	-4.71720	3.89803	-4.62808	H	5.02763	-5.99591	-1.70713
C	-5.01953	5.93569	-3.94970	H	-2.46636	-3.00015	-6.53695
H	-5.07602	6.50293	-2.99605	H	-2.60516	-4.60275	-2.02750
H	-4.20580	6.35543	-4.57819	H	-4.41006	1.61679	-3.32658
H	-5.98082	6.05561	-4.49230	H	-5.64494	4.05801	-3.10421
C	0.23326	4.67949	-3.50114	H	0.10711	4.57210	-4.60074
H	1.04871	3.98334	-3.22437	H	-3.14800	2.30831	0.65087
C	0.65880	6.11524	-3.20815	H	2.09086	1.69606	2.19056
H	-0.14348	6.82279	-3.50784	O	-1.06692	-2.33808	-0.46576
H	0.88032	6.24979	-2.13046	P	-1.17636	-0.99031	0.18299
H	1.57722	6.35407	-3.78464	H	0.66838	-2.96104	-0.73645
C	-2.47859	3.19272	0.61564	O	-2.55285	-0.23392	-0.26429
H	-1.50438	2.86377	1.03182	O	-1.32815	-1.33052	1.79926
C	-3.05241	4.29307	1.50541	N	-0.03138	0.09613	0.04388
H	-2.98259	3.98770	2.56745	C	1.65181	-3.25200	-0.28067
H	-2.48551	5.23790	1.38097	P	1.06909	0.37419	-1.06938

C	1.70860	-4.68659	-0.53483
C	1.61017	-2.84857	1.18864
H	2.36064	-2.72500	-0.92120
O	1.18624	-0.49463	-2.27508
O	2.46570	0.32400	-0.18856
O	0.90479	1.89521	-1.65734
C	1.79933	-5.26546	-1.89158
O	1.53513	-5.56758	0.38123
C	0.67122	-3.82077	1.89335
H	1.26017	-1.81757	1.27046
H	2.60508	-2.88963	1.64539
H	1.34984	-1.92441	-3.04867
C	0.31666	-5.43309	-2.38181
H	2.32448	-4.58210	-2.55607
H	2.29624	-6.23592	-1.83132
C	1.24067	-5.21261	1.77475
H	-0.32521	-3.75568	1.44081
H	0.56634	-3.60114	2.95501
O	1.38389	-2.84675	-3.39039
C	0.04877	-4.78541	-3.74053
H	-0.36541	-4.98451	-1.64837
H	0.08890	-6.50219	-2.40486
H	2.19346	-5.32198	2.30055
H	0.55786	-5.99985	2.09435
C	0.06895	-3.26315	-3.68726
H	0.78936	-5.12951	-4.47362
H	-0.93299	-5.12097	-4.09143
H	-0.25883	-2.85903	-4.65615
H	-0.62771	-2.90507	-2.91393

R-gau-C₄-C(-) 2nd step



E(RM062X) = -5098.40471165

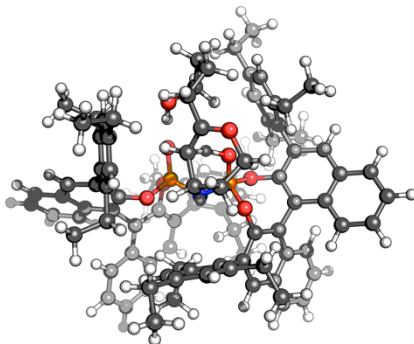
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C	-1.24232	0.32753	3.62768
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C	-1.77295	1.35463	4.41480
C	-3.79946	1.36800	3.05971
C	-3.02889	1.89694	4.12523
C	-4.14059	-0.48890	1.34999
C	-5.34380	-1.13261	1.74460
C	-3.69084	-0.61486	0.02030
C	-6.15036	-1.76010	0.76144
C	-4.49158	-1.25792	-0.94167
C	-5.72766	-1.79717	-0.57059

H	-6.34175	-2.28309	-1.32019
H	-1.20567	1.72447	5.26110
C	-3.53225	2.95556	4.89792
C	-4.77645	3.51344	4.60050
H	-2.95804	3.35936	5.72337
H	-5.15547	4.33558	5.19361
C	-5.52662	3.02258	3.53197
C	-5.04577	1.96005	2.76384
H	-6.48423	3.46839	3.29615
H	-5.64722	1.61783	1.93203
C	-7.36053	-2.37030	1.12811
C	-7.76319	-2.38832	2.46359
H	-7.98853	-2.84494	0.38332
H	-8.69446	-2.86506	2.74098
C	-6.95825	-1.81069	3.44441
C	-5.75511	-1.19408	3.09453
H	-7.26496	-1.84498	4.48191
H	-5.14895	-0.78348	3.89019
C	3.63829	0.81442	-0.65326
C	1.38782	2.93866	-0.82632
C	3.76663	2.21205	-0.77727
C	4.72062	-0.02097	-0.98903
C	0.45484	3.98148	-0.68323
C	2.67174	3.07789	-0.26278
C	4.91385	2.75939	-1.41123
C	5.89221	0.53173	-1.51675
C	0.72399	5.04223	0.19063
C	2.91197	4.09911	0.68958
C	5.98885	1.90429	-1.75696
C	5.01275	4.13195	-1.73143
H	6.72334	-0.11968	-1.76359
C	1.92422	5.09010	0.90541
H	0.00183	5.84300	0.29620
C	4.11068	4.15915	1.43088
C	7.14629	2.43204	-2.35133
C	6.16704	4.64133	-2.33009
H	4.19872	4.81790	-1.54070
C	2.16334	6.13366	1.81360
C	4.32824	5.19391	2.34319
H	4.87634	3.40194	1.32189
C	7.23407	3.79596	-2.63097
H	7.97843	1.78771	-2.60969
H	6.23198	5.69576	-2.56593
C	3.36070	6.18155	2.52946
H	1.42062	6.90553	1.97692
H	5.25073	5.22972	2.90810
H	8.12649	4.19645	-3.09436
H	3.53647	6.98314	3.23508
C	-0.78481	4.02576	-1.49634
C	-0.72378	4.40238	-2.86572
C	-2.04885	3.81550	-0.88694
C	-1.91504	4.57832	-3.58655
C	-3.21947	4.01170	-1.63547
C	-3.16082	4.40876	-2.97497
H	-4.18455	3.86005	-1.16592
C	4.65185	-1.49174	-0.82811
C	4.90517	-2.08073	0.43618

C	4.49628	-2.32326	-1.96843	H	-2.11199	5.43924	1.28579
C	5.03961	-3.47384	0.53625	H	-3.77880	4.74945	1.16131
C	4.61889	-3.71457	-1.83043	C	3.84836	-1.90284	5.32954
C	4.90484	-4.29420	-0.58944	H	4.70095	-1.32771	4.90767
H	4.48877	-4.34957	-2.69897	C	3.94830	-1.84510	6.85176
C	-4.00367	-1.45688	-2.32783	H	4.94215	-2.22216	7.17272
C	-3.96142	-0.36835	-3.23653	H	3.83490	-0.79744	7.20401
C	-3.58008	-2.74376	-2.75762	H	3.16493	-2.47654	7.32148
C	-3.45040	-0.56613	-4.52872	C	-1.15594	-2.22345	5.14587
C	-3.09460	-2.90877	-4.06407	H	-1.95253	-2.13594	4.37944
C	-3.01432	-1.82757	-4.94634	C	-1.67436	-1.70260	6.48226
H	-2.75825	-3.88681	-4.38824	H	-0.90158	-1.82944	7.27028
C	0.06223	-0.26843	4.00213	H	-1.94460	-0.62943	6.40610
C	0.10146	-1.48839	4.72693	H	-2.57984	-2.27372	6.77677
C	1.27390	0.40655	3.70478	C	1.30625	1.72903	2.97118
C	1.33891	-2.01542	5.12572	H	0.35351	1.93455	2.44419
C	2.49405	-0.14394	4.12697	C	1.59472	2.87646	3.93520
C	2.53364	-1.34369	4.84556	H	2.63097	2.80176	4.32754
H	3.41797	0.37923	3.90940	H	1.48431	3.84390	3.40806
H	5.23523	-3.92510	1.50216	H	0.88106	2.86270	4.78470
H	1.37152	-2.94541	5.68115	C	-4.49311	1.00194	-2.87739
H	-3.40271	0.26508	-5.22263	H	-4.17545	1.29861	-1.85865
H	-1.87466	4.87842	-4.62721	C	-6.01476	1.04723	-2.97745
C	5.00282	-5.79196	-0.44942	H	-6.47912	0.33162	-2.26910
H	4.31519	-6.13247	0.35504	H	-6.37358	2.06720	-2.72727
C	6.42917	-6.22487	-0.12272	H	-6.33810	0.79966	-4.01099
H	6.75312	-5.80300	0.85217	C	-3.59645	-3.95911	-1.84936
H	6.47501	-7.33245	-0.05899	H	-3.75228	-3.68898	-0.78638
H	7.12509	-5.88481	-0.91917	C	-4.68429	-4.94624	-2.26275
C	5.06802	-1.25856	1.69444	H	-4.68846	-5.80740	-1.56177
H	4.51548	-0.29999	1.63565	H	-5.68130	-4.45943	-2.23268
C	6.53863	-0.97249	1.97552	H	-4.49592	-5.32863	-3.28814
H	7.09988	-1.92268	2.10301	C	-2.45783	-2.01575	-6.33438
H	6.98458	-0.39172	1.14040	H	-1.68333	-1.24317	-6.53114
H	6.62840	-0.37864	2.90946	C	-3.55910	-1.91803	-7.38645
C	4.18589	-1.76719	-3.34439	H	-3.12594	-2.08913	-8.39439
H	3.86307	-0.70659	-3.30081	H	-4.33814	-2.68766	-7.19859
C	5.39366	-1.87370	-4.27186	H	-4.02752	-0.91114	-7.37049
H	5.13917	-1.44257	-5.26285	H	-0.94603	-3.31044	5.24810
H	6.25525	-1.31329	-3.85353	H	3.95149	-2.95517	4.98703
H	5.68471	-2.93584	-4.41460	H	4.63261	-1.81244	2.55155
C	-4.42712	4.64950	-3.75763	H	3.33851	-2.33314	-3.78760
H	-4.38940	4.07934	-4.71094	H	4.68823	-6.29723	-1.38859
C	-4.61642	6.13423	-4.05581	H	-1.96567	-3.00844	-6.42945
H	-4.65375	6.71380	-3.10860	H	-2.61218	-4.46892	-1.89612
H	-3.78606	6.51618	-4.68665	H	-4.07776	1.76405	-3.56910
H	-5.57133	6.28417	-4.60221	H	-5.31352	4.29171	-3.19083
C	0.58506	4.68687	-3.57682	H	0.46063	4.55502	-4.67396
H	1.37400	3.96997	-3.27604	H	-2.89537	2.52745	0.60623
C	1.05834	6.11403	-3.31744	H	2.09603	1.69710	2.19247
H	0.28494	6.84098	-3.64539	O	-1.02643	-2.16374	-0.47800
H	1.27204	6.26960	-2.24084	P	-1.16485	-0.81775	0.16085
H	1.99078	6.30467	-3.88931	H	0.89762	-2.89067	0.31362
C	-2.19220	3.38377	0.55572	O	-2.50500	-0.03337	-0.35095
H	-1.23292	3.02645	0.98017	O	-1.44051	-1.17083	1.76290
C	-2.72314	4.52379	1.42146	N	-0.00642	0.25662	0.09109
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P	1.14382	0.38805	-1.00193
C	0.62468	-4.82027	-0.38291
C	1.11011	-4.32221	1.93718
H	2.38977	-3.83441	0.18799
O	1.21032	-0.54836	-2.16468
O	2.50761	0.28209	-0.08662
O	1.11100	1.88687	-1.66484
C	1.23614	-5.68403	-1.43620
O	-0.56765	-5.14362	-0.08345
C	-0.38151	-4.18654	2.24620
H	1.69111	-3.68647	2.60828
H	1.46147	-5.35140	2.07913
H	1.26286	-2.15277	-2.05952
C	0.35988	-5.89815	-2.68715
H	2.20728	-5.27367	-1.70450
H	1.38806	-6.64684	-0.92298
C	-1.28683	-4.57413	1.06540
H	-0.59373	-3.13768	2.45844
H	-0.64538	-4.78170	3.12412
O	1.25804	-3.13840	-2.19756
C	0.50878	-4.78897	-3.73284
H	-0.68663	-5.99857	-2.38054
H	0.64775	-6.85459	-3.13422
H	-1.99542	-5.36686	1.30387
H	-1.78873	-3.69807	0.65665
C	0.27880	-3.38972	-3.18398
H	1.52060	-4.82600	-4.15605
H	-0.19561	-4.98178	-4.55023
H	0.35420	-2.65098	-3.99199
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R-gau-C₄-B(-)



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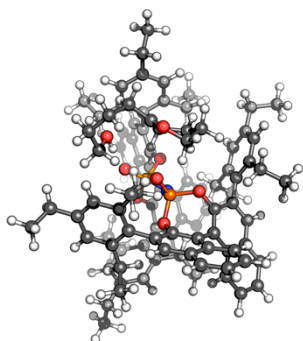
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H	6.45916	-2.19185	0.94583
H	1.04950	2.30603	-5.05952
C	3.32279	3.59426	-4.57995
C	4.54911	4.16641	-4.23821
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C	5.33452	3.59365	-3.23786
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H	5.53392	2.03053	-1.80070
C	7.42336	-1.94675	-1.51301
C	7.79340	-1.79362	-2.84916
H	8.08799	-2.47682	-0.84095
H	8.73603	-2.19484	-3.19843
C	6.94147	-1.14267	-3.74013
C	5.72325	-0.62312	-3.29713
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H	5.08110	-0.15207	-4.02839
C	-3.67223	0.63230	0.71619
C	-1.48500	2.79635	1.10391
C	-3.84281	2.01232	0.94960
C	-4.73745	-0.25652	0.95911
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C	-5.01932	2.47426	1.59897
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C	-3.02102	4.05155	-0.32110
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H	-6.75853	-0.46724	1.65930
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C	-4.21058	4.14931	-1.07337
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C	-7.39795	3.34567	2.83620
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C	-3.50969	6.29274	-1.95314
H	-1.59987	7.01454	-1.30136
H	-5.36375	5.32753	-2.45541
H	-8.31270	3.68305	3.30621
H	-3.70088	7.15500	-2.57868
C	0.64722	3.86619	1.90610
C	0.56141	4.08882	3.30750
C	1.92216	3.73808	1.29708
C	1.73973	4.18984	4.06313
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H	4.05286	3.76852	1.61381
C	-4.60393	-1.71306	0.72085

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C	-4.48782	-2.60496	1.82117	H	1.98462	5.60873	-0.65938
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C	-4.46127	-3.98864	1.58783	C	-3.80419	-1.57667	-5.51025
C	-4.55178	-4.50349	0.29037	H	-4.68292	-1.09851	-5.02556
H	-4.36259	-4.66877	2.42578	C	-3.92723	-1.37604	-7.01840
C	4.11375	-1.60785	2.07781	H	-4.90037	-1.78051	-7.36808
C	4.09277	-0.66784	3.13891	H	-3.88219	-0.29390	-7.26616
C	3.73450	-2.95325	2.32421	H	-3.11294	-1.90880	-7.55335
C	3.67354	-1.07629	4.41446	C	1.21319	-1.65022	-5.35059
C	3.35356	-3.33433	3.61910	H	1.97618	-1.65586	-4.54580
C	3.30884	-2.40397	4.66193	C	1.76065	-0.93301	-6.58065
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C	-0.10451	0.12257	-4.03183	H	2.01057	0.12078	-6.34545
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C	-1.34813	0.70349	-3.67581	C	-1.44668	1.94456	-2.81679
C	-1.29106	-1.56717	-5.32777	H	-0.50539	2.14684	-2.26680
C	-2.53866	0.13659	-4.15585	C	-1.79434	3.16303	-3.66781
C	-2.51818	-0.99101	-4.98330	H	-2.83134	3.08062	-4.05657
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H	-1.27797	-2.44028	-5.96949	C	4.54657	0.76324	2.95502
H	3.64526	-0.35986	5.22721	H	4.18778	1.17361	1.99043
H	1.68077	4.37073	5.13011	C	6.06627	0.87243	3.02832
C	-4.50288	-5.99095	0.05229	H	6.54358	0.27614	2.22426
H	-3.73374	-6.21669	-0.71788	H	6.36950	1.93266	2.90322
C	-5.85842	-6.52063	-0.40639	H	6.42905	0.51219	4.01455
H	-6.15165	-6.06062	-1.37375	C	3.68329	-4.00096	1.22760
H	-5.79974	-7.62093	-0.54323	H	3.75217	-3.55678	0.21392
H	-6.63511	-6.29766	0.35613	C	4.79884	-5.02980	1.38704
C	-4.85409	-1.34654	-1.80880	H	4.74666	-5.76423	0.55593
H	-4.25149	-0.42242	-1.71365	H	5.79082	-4.53265	1.35922
C	-6.31701	-0.98479	-2.03984	H	4.69165	-5.57736	2.34707
H	-6.92303	-1.90551	-2.17792	C	2.85633	-2.82218	6.03751
H	-6.71858	-0.40791	-1.18163	H	2.06925	-2.12438	6.39661
H	-6.40365	-0.36138	-2.95459	C	4.02244	-2.83102	7.02184
C	-4.36998	-2.12292	3.25498	H	3.66564	-3.17102	8.01680
H	-4.13474	-1.04044	3.31428	H	4.81483	-3.52643	6.67120
C	-5.65071	-2.39427	4.04040	H	4.45075	-1.81210	7.13042
H	-5.53863	-2.00988	5.07600	H	1.04462	-2.71566	-5.61991
H	-6.51493	-1.88535	3.56670	H	-3.84093	-2.66185	-5.27274
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C	4.24797	4.25559	4.28325	H	-3.52968	-2.64881	3.75445
H	4.20027	3.58017	5.16464	H	-4.21047	-6.52892	0.98037
C	4.41942	5.69785	4.75195	H	2.40855	-3.83980	6.01176
H	4.46590	6.38211	3.87783	H	2.70415	-4.51858	1.26207
H	3.57630	5.99927	5.40893	H	4.11060	1.40476	3.74922
H	5.36455	5.79114	5.32719	H	5.14632	3.97126	3.69422
C	-0.76123	4.28268	4.02401	H	-0.64866	4.05067	5.10570
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C	-1.25748	5.71972	3.89424	H	-2.23356	1.79640	-2.04846
H	-0.50024	6.42558	4.29731	O	1.08569	-2.15573	0.25211
H	-1.46428	5.97239	2.83494	P	1.17867	-0.72745	-0.26581
H	-2.19841	5.84006	4.47131	H	-0.10364	-2.86171	0.15542
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H	1.14564	3.15698	-0.66324	O	1.44486	-0.92850	-1.88140
C	2.61066	4.72543	-0.89987	N	-0.01479	0.26993	-0.05602

C	-1.12355	-3.49145	-0.29307
P	-1.16625	0.24971	1.05840
C	-0.59651	-4.76209	-0.00389
C	-1.14642	-3.02062	-1.75430
H	-1.94712	-3.19612	0.34652
O	-1.16130	-0.79287	2.11842
O	-2.51756	0.17508	0.13116
O	-1.18589	1.68120	1.84704
C	-1.04637	-5.68597	1.08405
O	0.38589	-5.26006	-0.71009
C	-0.33789	-3.97965	-2.62711
H	-0.75403	-2.00345	-1.82853
H	-2.18235	-2.98317	-2.09834
H	-1.26034	-2.40411	2.53665
C	0.03953	-6.09945	2.10054
H	-1.89818	-5.24326	1.59489
H	-1.37998	-6.57573	0.53261
C	0.85804	-4.49517	-1.84871
H	0.01592	-3.49391	-3.53546
H	-0.94982	-4.83832	-2.92836
O	-1.25085	-3.36876	2.71734
C	0.05651	-5.23951	3.36860
H	1.01637	-6.08601	1.60712
H	-0.14061	-7.14062	2.38583
H	1.46869	-5.20033	-2.41187
H	1.47255	-3.67529	-1.46450
C	0.04853	-3.73651	3.12398
H	-0.82697	-5.47022	3.97658
H	0.93402	-5.51530	3.96332
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R-gau-C₄-B(-) intermediate



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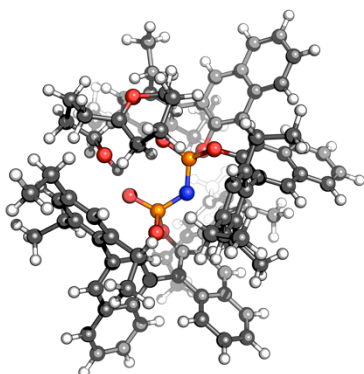
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C	3.53924	3.51161	4.53272
C	4.78551	4.03127	4.17967
H	2.95980	4.00957	5.30112
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C	5.54368	3.41655	3.18328
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H	6.50320	3.83149	2.90302
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C	7.36056	-2.26875	1.45353
C	7.75905	-2.12658	2.78277
H	7.98170	-2.84425	0.77724
H	8.68095	-2.58086	3.12224
C	6.96129	-1.41770	3.67978
C	5.76986	-0.82971	3.24966
H	7.26425	-1.32749	4.71502
H	5.16876	-0.31326	3.98511
C	-3.63357	0.74950	-0.69525
C	-1.33387	2.79459	-1.12225
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C	-0.38182	3.83054	-1.12039
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C	-7.16157	2.33063	-2.39583
C	-6.10337	4.48829	-2.64590
H	-4.09464	4.66304	-1.96718
C	-1.99144	6.28322	1.15538
C	-4.15302	5.44616	1.84614
H	-4.74932	3.55414	1.05893
C	-7.21358	3.66147	-2.81043
H	-8.02713	1.69736	-2.55132
H	-6.14062	5.51473	-2.98746
C	-3.16902	6.43416	1.88960
H	-1.23522	7.05750	1.20749
H	-5.05940	5.56221	2.42614
H	-8.11176	4.04872	-3.27393
H	-3.31605	7.31603	2.49954
C	0.83541	3.76217	-1.96475
C	0.73992	3.96485	-3.36883
C	2.11405	3.61510	-1.36668
C	1.91207	4.02274	-4.13847
C	3.26475	3.69156	-2.16621
C	3.17249	3.90893	-3.54443
H	4.24110	3.58845	-1.70696

C	-4.72932	-1.53091	-0.64816	C	2.86251	4.61873	0.80613
C	-4.86582	-2.02467	0.67470	H	2.84278	4.47624	1.90432
C	-4.70136	-2.44471	-1.73666	H	2.25931	5.51701	0.56380
C	-4.96968	-3.40815	0.88950	H	3.91294	4.79115	0.49003
C	-4.80287	-3.82194	-1.48503	C	-3.78782	-1.34381	5.55701
C	-4.93922	-4.30907	-0.18057	H	-4.64818	-0.83545	5.07026
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C	3.54619	-1.26029	-4.42098	C	1.22137	-1.62845	5.37756
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C	3.09756	-2.56728	-4.63749	C	1.79036	-0.92937	6.60810
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C	-1.27706	-1.44150	5.36475	H	-0.35257	2.18647	2.24061
C	-2.45884	0.29014	4.16603	C	-1.58662	3.27528	3.63755
C	-2.48115	-0.82202	5.01398	H	-2.62622	3.24635	4.02707
H	-3.38941	0.77748	3.89969	H	-1.46523	4.18266	3.01574
H	-5.06710	-3.78918	1.89943	H	-0.88059	3.34674	4.49036
H	-1.29664	-2.30328	6.02146	C	4.56431	0.54544	-3.01541
H	3.54076	-0.55640	-5.24510	H	4.25130	0.99389	-2.05204
H	1.84615	4.18785	-5.20761	C	6.08593	0.56040	-3.12097
C	-5.00491	-5.79241	0.07777	H	6.54320	-0.04560	-2.31251
H	-4.24810	-6.06747	0.84415	H	6.45470	1.60301	-3.02711
C	-6.39335	-6.20833	0.55469	H	6.40568	0.15692	-4.10534
H	-6.64097	-5.71388	1.51779	C	3.47907	-4.14058	-1.19439
H	-6.41945	-7.30793	0.70654	H	3.59931	-3.68993	-0.18842
H	-7.15715	-5.93560	-0.20466	C	4.53683	-5.22596	-1.37249
C	-4.93209	-1.10911	1.87669	H	4.47086	-5.94856	-0.53205
H	-4.26583	-0.23315	1.75336	H	5.55300	-4.77970	-1.37745
C	-6.35853	-0.63636	2.13318	H	4.37559	-5.77689	-2.32302
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H	-6.37759	0.00806	3.03721	C	3.73210	-3.07847	-7.00292
C	-4.54330	-1.99445	-3.17697	H	3.33367	-3.41218	-7.98411
H	-4.21169	-0.93828	-3.25039	H	4.48690	-3.81620	-6.65581
C	-5.84402	-2.16007	-3.95902	H	4.22072	-2.09038	-7.13855
H	-5.69806	-1.80312	-5.00021	H	1.01285	-2.68743	5.64485
H	-6.65820	-1.56760	-3.49414	H	-3.87252	-2.42989	5.33660
H	-6.14586	-3.22822	-3.99282	H	-4.56940	-1.64672	2.77732
C	4.41851	4.02158	-4.38630	H	-3.75486	-2.60098	-3.66954
H	4.34232	3.33531	-5.25726	H	-4.76297	-6.36397	-0.84482
C	4.62378	5.45168	-4.87789	H	2.08070	-3.96694	-5.94171
H	4.69968	6.14673	-4.01440	H	2.47406	-4.61076	-1.19848
H	3.78120	5.76684	-5.52910	H	4.15225	1.19740	-3.81355
H	5.56401	5.51064	-5.46555	H	5.31540	3.72057	-3.80312
C	-0.58403	4.18913	-4.07434	H	-0.49049	3.93703	-5.15335
H	-1.37330	3.52102	-3.67800	H	2.99402	2.53146	0.26368
C	-1.03378	5.64297	-3.96231	H	-2.09575	1.90783	2.03829
H	-0.25862	6.31856	-4.38281	O	1.12833	-2.20541	-0.24234
H	-1.22296	5.91797	-2.90531	P	1.21361	-0.79468	0.25609
H	-1.97582	5.78412	-4.53283	H	-0.74798	-2.77084	-0.31859
C	2.29498	3.37979	0.11727	O	2.54622	-0.05349	-0.32365
H	1.34584	3.09296	0.61403	O	1.46359	-0.96111	1.89249

N	0.01546	0.21877	0.05808
C	-1.42665	-3.39642	0.30927
P	-1.13884	0.23642	-1.04225
C	-0.84517	-4.70184	0.02110
C	-1.32444	-2.90569	1.76793
H	-2.39749	-3.30258	-0.15957
O	-1.20776	-0.82029	-2.09206
O	-2.50142	0.22951	-0.11489
O	-1.10245	1.65707	-1.85604
C	-1.36890	-5.67086	-0.98532
O	0.18769	-5.11343	0.64903
C	-0.44107	-3.83518	2.60050
H	-0.92283	-1.89001	1.77163
H	-2.32522	-2.85852	2.20242
H	-1.47246	-2.40178	-2.47156
C	-0.32347	-6.14857	-2.02048
H	-2.23776	-5.23983	-1.47829
H	-1.68705	-6.52677	-0.37232
C	0.72336	-4.33884	1.77515
H	-0.03896	-3.31989	3.47120
H	-1.01456	-4.69794	2.96281
O	-1.50265	-3.37452	-2.62662
C	-0.27679	-5.29127	-3.28970
H	0.66039	-6.18346	-1.54160
H	-0.57011	-7.17886	-2.29355
H	1.35100	-5.05922	2.29817
H	1.31057	-3.52825	1.33819
C	-0.21888	-3.78947	-3.04328
H	-1.17134	-5.48434	-3.89402
H	0.58694	-5.60726	-3.88426
H	0.07152	-3.27381	-3.96837
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R-gau-C₄-B(-) 2nd step



E(RM062X) = -5098.40542323

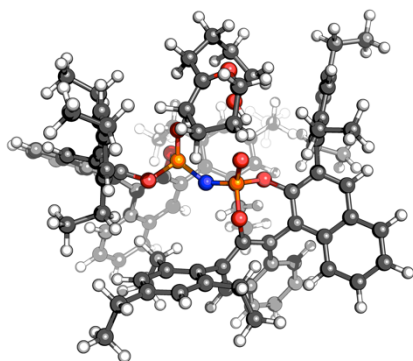
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C	-3.76388	1.20898	3.15898
C	-2.97434	1.68328	4.23573
C	-4.13155	-0.54337	1.34911
C	-5.33212	-1.20959	1.71121
C	-3.69541	-0.57806	0.01017

C	-6.14677	-1.77255	0.69615
C	-4.50027	-1.16370	-0.98455
C	-5.73388	-1.72530	-0.63894
H	-6.35502	-2.16042	-1.41312
H	-1.13233	1.45496	5.32892
C	-3.46044	2.70559	5.06630
C	-4.70655	3.28195	4.81610
H	-2.87100	3.06767	5.90033
H	-5.07220	4.07630	5.45380
C	-5.47576	2.84588	3.73749
C	-5.01199	1.81958	2.91177
H	-6.43484	3.30631	3.53857
H	-5.62831	1.52070	2.07423
C	-7.35503	-2.40352	1.03265
C	-7.74816	-2.50461	2.36734
H	-7.98900	-2.82994	0.26413
H	-8.67815	-2.99682	2.62103
C	-6.93584	-1.98950	3.37662
C	-5.73429	-1.35338	3.05742
H	-7.23583	-2.08730	4.41203
H	-5.12270	-0.99121	3.87232
C	3.63507	0.83761	-0.62621
C	1.41078	2.98170	-0.72631
C	3.78145	2.23550	-0.71136
C	4.69571	-0.00299	-1.01039
C	0.47698	4.01467	-0.52461
C	2.69876	3.09553	-0.16585
C	4.92674	2.78669	-1.34451
C	5.86306	0.54749	-1.55009
C	0.75507	5.03491	0.39411
C	2.94859	4.07341	0.82815
C	5.97904	1.92626	-1.74340
C	5.04444	4.16840	-1.61424
H	6.67658	-0.10901	-1.83861
C	1.96212	5.05176	1.09870
H	0.03331	5.82892	0.54415
C	4.15364	4.09995	1.56111
C	7.13299	2.45547	-2.34312
C	6.19528	4.67948	-2.21810
H	4.24793	4.86104	-1.37893
C	2.20800	6.05162	2.05308
C	4.37794	5.09057	2.51962
H	4.91924	3.34998	1.41002
C	7.23977	3.82720	-2.57391
H	7.94766	1.80679	-2.64291
H	6.27502	5.74082	-2.41523
C	3.41110	6.06696	2.76062
H	1.46580	6.81367	2.25928
H	5.30506	5.10071	3.07796
H	8.12941	4.22904	-3.04141
H	3.59191	6.83426	3.50218
C	-0.77452	4.09567	-1.31641
C	-0.73282	4.53538	-2.66766
C	-2.03075	3.87251	-0.69428
C	-1.93423	4.76310	-3.35634
C	-3.21145	4.12242	-1.41020
C	-3.17099	4.58456	-2.72937

H	-4.17014	3.96099	-0.93101	H	-1.19094	2.98511	1.11642
C	4.60554	-1.47564	-0.88820	C	-2.66739	4.46091	1.66081
C	4.87033	-2.10227	0.35531	H	-2.61391	4.10917	2.70990
C	4.40832	-2.27289	-2.04587	H	-2.04901	5.37711	1.57147
C	4.97715	-3.49966	0.41659	H	-3.72334	4.71019	1.42464
C	4.51557	-3.66857	-1.94851	C	3.94764	-2.04103	5.22859
C	4.81570	-4.28590	-0.72913	H	4.78552	-1.40919	4.86157
H	4.36440	-4.27735	-2.83231	C	4.01787	-2.08030	6.75299
C	-4.01644	-1.28129	-2.38200	H	5.01853	-2.44338	7.06883
C	-3.97120	-0.14092	-3.22420	H	3.86070	-1.06271	7.17044
C	-3.59125	-2.54013	-2.88706	H	3.24909	-2.76803	7.16422
C	-3.44983	-0.25993	-4.52203	C	-1.03180	-2.55468	4.88643
C	-3.09582	-2.62608	-4.19726	H	-1.77131	-2.50249	4.06220
C	-3.00835	-1.49334	-5.01145	C	-1.67925	-2.11100	6.19463
H	-2.75938	-3.58352	-4.57832	H	-0.94990	-2.18673	7.02919
C	0.12407	-0.45624	3.94637	H	-2.04264	-1.06648	6.12192
C	0.19944	-1.72855	4.57282	H	-2.54608	-2.76727	6.41978
C	1.31618	0.27843	3.71309	C	1.31559	1.63982	3.05195
C	1.44970	-2.23353	4.96192	H	0.35081	1.85875	2.55406
C	2.54946	-0.25761	4.11552	C	1.60624	2.74241	4.06662
C	2.62174	-1.49917	4.75550	H	2.65031	2.66432	4.43667
H	3.45783	0.30824	3.94429	H	1.47391	3.73292	3.58862
H	5.18777	-3.98044	1.36493	H	0.90849	2.67685	4.92672
H	1.51061	-3.19986	5.44871	C	-4.51037	1.20351	-2.78826
H	-3.39776	0.61158	-5.16423	H	-4.19486	1.44345	-1.75408
H	-1.90838	5.11189	-4.38218	C	-6.03208	1.24688	-2.88708
C	4.92571	-5.78683	-0.63749	H	-6.49343	0.49252	-2.21810
H	4.25811	-6.15725	0.17051	H	-6.39558	2.25061	-2.58349
C	6.36204	-6.21920	-0.35614	H	-6.35363	1.05316	-3.93260
H	6.70500	-5.82606	0.62424	C	-3.62039	-3.80943	-2.05742
H	6.41718	-7.32784	-0.32916	H	-3.74577	-3.60160	-0.97610
H	7.03768	-5.84866	-1.15651	C	-4.73725	-4.74400	-2.51325
C	5.08397	-1.31490	1.62819	H	-4.74861	-5.64873	-1.86963
H	4.49811	-0.37433	1.63043	H	-5.72301	-4.24090	-2.43486
C	6.55978	-0.99461	1.83551	H	-4.57403	-5.06191	-3.56474
H	7.15354	-1.93179	1.89096	C	-2.43911	-1.59673	-6.40332
H	6.94149	-0.36788	1.00272	H	-1.66156	-0.81513	-6.54468
H	6.68723	-0.43606	2.78667	C	-3.52986	-1.43203	-7.45796
C	4.06857	-1.67487	-3.39691	H	-3.08715	-1.54271	-8.47020
H	3.76778	-0.61002	-3.31633	H	-4.31240	-2.20945	-7.32483
C	5.24563	-1.77775	-4.36315	H	-3.99602	-0.42661	-7.38532
H	4.96959	-1.31449	-5.33371	H	-0.75715	-3.62746	4.98433
H	6.12962	-1.24473	-3.95571	H	4.09586	-3.06450	4.82118
H	5.51181	-2.84054	-4.54398	H	4.71878	-1.90677	2.49195
C	-4.44743	4.88246	-3.47514	H	3.19748	-2.21328	-3.82782
H	-4.43676	4.35830	-4.45519	H	4.59590	-6.26516	-1.58548
C	-4.61742	6.38251	-3.69874	H	-1.94760	-2.58269	-6.55485
H	-4.62761	6.91666	-2.72455	H	-2.65208	-4.34036	-2.15908
H	-3.79257	6.78099	-4.32658	H	-4.09922	2.00488	-3.43615
H	-5.57957	6.57341	-4.21903	H	-5.32908	4.51163	-2.90917
C	0.56673	4.83448	-3.38985	H	0.41919	4.75842	-4.48941
H	1.34909	4.09127	-3.14036	H	-2.86155	2.51229	0.74489
C	1.06863	6.23981	-3.07143	H	2.09048	1.65984	2.25818
H	0.29970	6.99369	-3.34445	O	-1.02591	-2.05643	-0.63676
H	1.31002	6.33847	-1.99402	P	-1.16906	-0.77046	0.11079
H	1.99056	6.44481	-3.65526	H	0.74284	-2.98617	0.39517
C	-2.15496	3.36727	0.72680	O	-2.51864	0.03818	-0.33134

O	-1.42552	-1.25116	1.68307
N	-0.02009	0.31804	0.11510
C	1.18992	-3.98396	0.49223
P	1.13759	0.44469	-0.97152
C	0.54890	-4.77613	-0.58344
C	0.84228	-4.56273	1.88539
H	2.25734	-3.89873	0.31507
O	1.18746	-0.48910	-2.13804
O	2.50288	0.30623	-0.06173
O	1.12682	1.95986	-1.60067
C	1.24182	-5.64918	-1.57639
O	-0.70505	-5.00297	-0.48031
C	-0.59883	-5.10573	1.92010
H	0.96902	-3.75324	2.60418
H	1.55133	-5.35075	2.15301
H	1.11919	-2.13605	-1.90946
C	0.49915	-5.82153	-2.91213
H	2.24657	-5.26698	-1.73618
H	1.31812	-6.61916	-1.05852
C	-1.39864	-4.57829	0.74069
H	-1.11467	-4.81398	2.83737
H	-0.60039	-6.20069	1.88236
O	1.15329	-3.11178	-2.10266
C	0.70246	-4.63928	-3.86386
H	-0.56757	-5.97461	-2.71647
H	0.86923	-6.73700	-3.38371
H	-2.37977	-5.04167	0.64879
H	-1.47858	-3.49203	0.70638
C	0.33605	-3.30126	-3.24300
H	1.75523	-4.59895	-4.17097
H	0.10325	-4.80057	-4.76710
H	0.50020	-2.48360	-3.95429
H	-0.71548	-3.27063	-2.93409

R-gau-C₄-C(+)



E(RM062X) = -5098.37493544

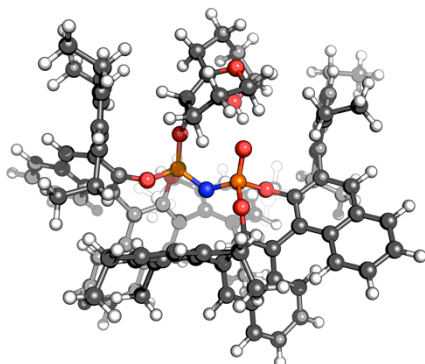
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C	0.69085	-1.52541	3.45286
C	2.88716	-1.24442	2.44770
C	1.03837	-2.82842	3.83409
C	3.20914	-2.58936	2.76232

C	2.26845	-3.37869	3.46487
C	3.92229	-0.27535	2.00391
C	5.08022	-0.02648	2.78970
C	3.73003	0.42589	0.79231
C	6.12759	0.75531	2.25029
C	4.77691	1.22996	0.28528
C	5.97972	1.34022	0.99342
H	6.78812	1.93137	0.57858
H	0.35428	-3.40610	4.44302
C	2.58830	-4.69660	3.82843
C	3.82984	-5.23785	3.49119
H	1.87937	-5.30660	4.37572
H	4.07059	-6.25470	3.77296
C	4.75793	-4.47337	2.78419
C	4.45181	-3.16198	2.41372
H	5.71430	-4.90133	2.51300
H	5.18575	-2.60797	1.84338
C	7.30436	0.96541	2.98730
C	7.43520	0.43318	4.27001
H	8.11652	1.55408	2.57712
H	8.34155	0.60370	4.83653
C	6.39116	-0.30019	4.83143
C	5.21967	-0.52468	4.10533
H	6.48752	-0.69343	5.83529
H	4.42435	-1.07465	4.58976
N	0.03602	-0.15506	0.07860
P	-1.11507	0.12834	-0.98504
O	-1.18781	1.46150	-1.65677
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O	-0.98462	-1.00588	-2.16712
C	-3.60183	-0.50938	-0.96549
C	-1.20984	-2.30833	-1.78480
C	-3.61664	-1.77258	-1.59171
C	-4.74907	0.31067	-1.04498
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C	-4.68312	-2.12448	-2.46150
C	-5.84823	-0.09463	-1.81193
C	-0.46032	-4.61131	-1.58471
C	-2.69618	-4.00870	-0.84646
C	-5.81410	-1.28054	-2.54424
C	-4.64703	-3.28579	-3.26663
H	-6.73025	0.53564	-1.85247
C	-1.66045	-4.96413	-0.96211
H	0.28815	-5.37091	-1.77124
C	-3.91703	-4.39400	-0.25273
C	-6.89804	-1.63009	-3.36568
C	-5.72776	-3.61718	-4.08654
H	-3.78305	-3.93590	-3.28508
C	-1.86197	-6.27710	-0.50766
C	-4.10334	-5.70284	0.19802
H	-4.72468	-3.68560	-0.12038
C	-6.85408	-2.79682	-4.12906
H	-7.77424	-0.99521	-3.42555
H	-5.68936	-4.51197	-4.69441
C	-3.07955	-6.64208	0.06966
H	-1.07970	-7.02092	-0.60218

H	-5.04262	-5.98790	0.65388	H	4.54610	-4.94449	-5.68214
H	-7.68980	-3.05884	-4.76499	H	6.15633	-4.15894	-5.90131
H	-3.22892	-7.65490	0.42070	C	-0.40716	-2.78739	-4.95924
C	0.99277	-3.01290	-2.80015	H	-1.16237	-2.17884	-4.42640
C	0.91202	-2.82191	-4.20832	C	-0.95151	-4.19224	-5.20370
C	2.26728	-3.09729	-2.18009	H	-0.20394	-4.80422	-5.75196
C	2.09397	-2.72921	-4.96030	H	-1.20333	-4.69305	-4.24795
C	3.42530	-3.02945	-2.96921	H	-1.87645	-4.12918	-5.81484
C	3.34731	-2.85764	-4.35492	C	2.43315	-3.27657	-0.68487
H	4.39808	-3.11320	-2.49958	H	1.48113	-3.11732	-0.13718
C	-4.86242	1.61035	-0.34518	C	2.97082	-4.66816	-0.35349
C	-5.29149	1.64669	1.00487	H	2.82501	-4.87740	0.72449
C	-4.82634	2.81392	-1.09667	H	2.43753	-5.45206	-0.92821
C	-5.70063	2.86402	1.57066	H	4.05479	-4.72782	-0.58718
C	-5.26192	4.01134	-0.50818	C	-4.35860	0.28265	5.68535
C	-5.70531	4.04295	0.81801	H	-5.22189	-0.14824	5.13354
H	-5.23701	4.92882	-1.08441	C	-4.44398	-0.18923	7.13482
C	4.62908	2.05019	-0.94213	H	-5.43074	0.09239	7.55900
C	4.67197	1.44626	-2.22423	H	-4.33755	-1.29404	7.18533
C	4.59443	3.46887	-0.84131	H	-3.64995	0.28393	7.75013
C	4.63620	2.25259	-3.37299	C	0.64602	0.56795	5.58594
C	4.58704	4.24467	-2.01137	H	1.40370	0.81179	4.81693
C	4.60124	3.64662	-3.27421	C	1.23917	-0.39670	6.60919
H	4.53387	5.32468	-1.93790	H	0.48898	-0.63449	7.39328
C	-0.59932	-0.96779	3.92751	H	1.56990	-1.33636	6.12331
C	-0.61913	0.00702	4.96319	H	2.12154	0.07307	7.09253
C	-1.82553	-1.50049	3.44725	C	-1.88825	-2.52278	2.33039
C	-1.85025	0.42618	5.49125	H	-0.91932	-2.62202	1.79868
C	-3.03396	-1.08196	4.02431	C	-2.30887	-3.89333	2.85843
C	-3.05411	-0.13168	5.05001	H	-3.38830	-3.89219	3.11894
H	-3.96573	-1.51351	3.67906	H	-2.13160	-4.66251	2.08107
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H	-1.87160	1.16445	6.28429	C	4.84762	-0.04226	-2.40825
H	4.67266	1.79081	-4.35283	H	4.29590	-0.61378	-1.63902
H	2.03644	-2.60426	-6.03528	C	6.32300	-0.42770	-2.36631
C	-6.14244	5.34090	1.44695	H	6.76948	-0.15740	-1.38687
H	-5.59864	5.48950	2.40495	H	6.42674	-1.52362	-2.50863
C	-7.64679	5.34861	1.70381	H	6.87823	0.09024	-3.17714
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H	-7.94437	6.32654	2.13736	H	4.24930	3.50455	1.32480
H	-8.19918	5.19867	0.75151	C	5.76172	4.95988	0.82069
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H	-4.68065	-0.38433	1.50710	H	6.63016	4.27185	0.86711
C	-6.79486	-0.15519	1.87922	H	5.95901	5.74206	0.05771
H	-7.50168	0.59760	2.28865	C	4.56965	4.50149	-4.51524
H	-7.11351	-0.43813	0.85384	H	4.38321	3.87893	-5.41739
H	-6.82671	-1.05911	2.52334	C	5.88901	5.24533	-4.70407
C	-4.31179	2.86351	-2.52010	H	5.84844	5.84203	-5.63955
H	-3.77386	1.93302	-2.79717	H	6.07439	5.93551	-3.85383
C	-5.44067	3.09667	-3.52081	H	6.72949	4.52253	-4.77905
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H	-5.94541	4.06583	-3.32364	H	-5.06872	0.65511	2.89239
C	4.60360	-2.82600	-5.18990	H	-3.57802	3.69191	-2.60638
H	4.37838	-2.49481	-6.22712	H	-5.89306	6.20127	0.78825
C	5.25536	-4.20423	-5.25392	H	3.73644	5.23337	-4.43999
H	5.56589	-4.53700	-4.24082	H	3.63873	4.91435	0.44161

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H	5.32379	-2.09777	-4.76252
H	-0.27301	-2.29513	-5.94731
H	3.14086	-2.51159	-0.30131
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O	1.14581	2.26110	0.52020
H	0.85873	2.96874	-0.58973
C	1.05134	3.85201	-1.53701
C	0.26911	4.88539	-1.00962
C	0.84245	3.37228	-2.96087
H	2.07265	3.93236	-1.18511
C	0.58002	5.48355	0.32958
O	-0.73041	5.43783	-1.64297
C	-0.55762	3.75545	-3.43753
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H	0.95394	2.28535	-3.00194
C	-0.57246	6.17510	1.06831
H	1.36947	6.22175	0.12329
H	1.02544	4.69220	0.94221
C	-0.86148	5.19136	-3.07125
H	-1.27990	3.08327	-2.97375
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C	-1.50646	5.22960	1.82707
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H	-0.17524	5.89283	-3.56007
C	-2.27594	4.27964	0.92621
H	-2.22435	5.82706	2.40164
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O	-1.34163	3.41113	0.33703
H	-3.00579	3.71934	1.52311
H	-2.80694	4.86844	0.16207
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R-gau-C₄-B(+)



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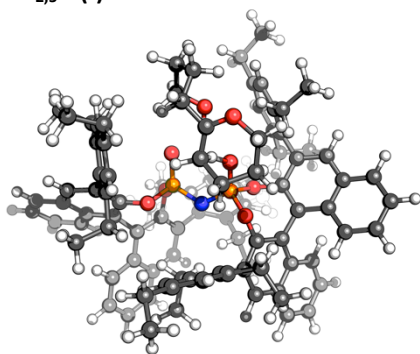
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C	0.58581	-2.15524	3.14995
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C	3.12121	-3.07582	2.33229
C	2.16741	-3.98118	2.85220
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C	3.70312	0.24320	0.97998
C	6.04458	0.28020	2.56525
C	4.78148	1.10091	0.65648
C	5.95284	1.07379	1.42343
H	6.78401	1.71291	1.14732
H	0.23323	-4.18724	3.76591
C	2.48216	-5.34454	2.96874
C	3.73090	-5.81544	2.55988
H	1.76306	-6.04504	3.37664
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C	4.67174	-4.93344	2.02814
C	4.37223	-3.57452	1.90841
H	5.63414	-5.30470	1.70059
H	5.11741	-2.92351	1.47025
C	7.19108	0.34374	3.37372
C	7.26822	-0.41016	4.54479
H	8.02145	0.98694	3.10688
H	8.15137	-0.35269	5.16787
C	6.20081	-1.22283	4.92345
C	5.05933	-1.30246	4.12295
H	6.25572	-1.79103	5.84311
H	4.24404	-1.92388	4.46793
N	0.01735	-0.15890	0.06675
P	-1.14637	0.35592	-0.89055
O	-1.21556	1.80680	-1.25583
O	-2.56449	-0.06927	-0.17246
O	-1.01713	-0.49903	-2.29012
C	-3.63876	-0.22976	-1.02180
C	-1.26459	-1.84999	-2.19082
C	-3.66480	-1.32346	-1.91081
C	-4.77520	0.60646	-0.92813
C	-0.29325	-2.78828	-2.59036
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C	-4.72500	-1.46046	-2.84501
C	-5.87209	0.39176	-1.77300
C	-0.54989	-4.15979	-2.44460
C	-2.79206	-3.68093	-1.64091
C	-5.84392	-0.60293	-2.74946
C	-4.69466	-2.41910	-3.88327
H	-6.74979	1.02107	-1.67573
C	-1.76875	-4.61097	-1.93278
H	0.19321	-4.87910	-2.76497
C	-4.02757	-4.15667	-1.15207
C	-6.92236	-0.74721	-3.63724
C	-5.76924	-2.54577	-4.76605
H	-3.83944	-3.06386	-4.03398
C	-1.99740	-5.98518	-1.75824
C	-4.24033	-5.52599	-0.97776
H	-4.82674	-3.47582	-0.88862
C	-6.88386	-1.71815	-4.63826
H	-7.78946	-0.10133	-3.56414
H	-5.73520	-3.28633	-5.55476

C	-3.22932	-6.43792	-1.28244	C	5.26119	-3.34431	-5.73217
H	-1.22429	-6.70810	-1.99022	H	5.50885	-3.87112	-4.78622
H	-5.19072	-5.88055	-0.60040	H	4.53025	-3.95042	-6.30906
H	-7.71474	-1.82101	-5.32422	H	6.19014	-3.24172	-6.33167
H	-3.39937	-7.49802	-1.14599	C	-0.32228	-1.69128	-5.37127
C	0.97258	-2.38196	-3.24761	H	-1.08198	-1.17807	-4.75141
C	0.96073	-1.92803	-4.59605	C	-0.89526	-2.99546	-5.91948
C	2.21528	-2.63353	-2.60786	H	-0.14257	-3.50948	-6.55451
C	2.17659	-1.76013	-5.27792	H	-1.20174	-3.67145	-5.09658
C	3.40788	-2.47988	-3.33046	H	-1.79087	-2.77494	-6.53766
C	3.39607	-2.06291	-4.66515	C	2.30930	-3.08271	-1.16376
H	4.35573	-2.69366	-2.85090	H	1.33843	-2.98989	-0.63399
C	-4.87974	1.72861	0.03441	C	2.79419	-4.52848	-1.06302
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C	-5.58874	2.53925	2.22292	H	3.88084	-4.58739	-1.28376
C	-5.29227	4.10482	0.41037	C	-4.50166	-0.90663	5.64936
C	-5.64105	3.85007	1.73994	H	-5.35450	-1.23171	5.01463
H	-5.30655	5.12396	0.04218	C	-4.58256	-1.66338	6.97268
C	4.71697	2.09706	-0.43972	H	-5.57552	-1.49043	7.43856
C	4.87613	1.69150	-1.78847	H	-4.45603	-2.75350	6.79933
C	4.69449	3.48455	-0.12813	H	-3.79896	-1.31062	7.67591
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C	4.80761	4.42741	-1.16246	H	1.25446	-0.10641	4.93635
C	4.94722	4.02521	-2.49365	C	1.09613	-1.63225	6.46794
H	4.75505	5.48498	-0.93155	H	0.34440	-2.02335	7.18631
C	-0.71409	-1.70033	3.69882	H	1.44478	-2.45926	5.81757
C	-0.75634	-0.95282	4.90820	H	1.96779	-1.24914	7.03919
C	-1.92775	-2.14707	3.11124	C	-1.96652	-2.90933	1.80124
C	-1.99688	-0.67431	5.50267	H	-0.99008	-2.88542	1.27435
C	-3.14504	-1.88305	3.75668	C	-2.37923	-4.36448	2.01556
C	-3.18723	-1.15960	4.95277	H	-3.45654	-4.42684	2.27708
H	-4.06715	-2.25425	3.32586	H	-2.20699	-4.94076	1.08505
H	-5.85659	2.34441	3.25507	H	-1.78439	-4.83261	2.82535
H	-2.03540	-0.11019	6.42720	C	5.01246	0.24142	-2.18427
H	5.10832	2.34898	-3.82818	H	4.42630	-0.42114	-1.52030
H	2.16988	-1.44118	-6.31365	C	6.47334	-0.19532	-2.16923
C	-6.03503	4.97997	2.65633	H	6.89987	-0.08625	-1.14997
H	-5.43433	4.92633	3.59000	H	6.54598	-1.26145	-2.47035
C	-7.52122	4.91842	2.99767	H	7.06570	0.41668	-2.88232
H	-7.75986	3.97875	3.53947	C	4.47091	4.00237	1.28127
H	-7.78867	5.77771	3.64799	H	4.15803	3.19796	1.97817
H	-8.13020	4.97126	2.06985	C	5.72229	4.67801	1.83755
C	-5.30619	0.07345	1.94649	H	5.52643	5.02258	2.87469
H	-4.55445	-0.59230	1.48036	H	6.57454	3.96864	1.85730
C	-6.69780	-0.52262	1.76493	H	5.99792	5.55965	1.22142
H	-7.45805	0.11293	2.26706	C	5.03200	5.05566	-3.59023
H	-6.94736	-0.60968	0.68725	H	4.93841	4.57625	-4.58908
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C	-4.46736	3.42823	-1.85420	H	6.40472	6.53796	-4.37331
H	-3.96089	2.58218	-2.36377	H	6.45564	6.36355	-2.58015
C	-5.64849	3.88435	-2.70797	H	7.20680	5.09835	-3.63718
H	-5.29084	4.13255	-3.72940	H	0.25611	0.34036	6.32446
H	-6.40855	3.08131	-2.78806	H	-4.61885	0.18312	5.83387
H	-6.12079	4.79008	-2.27287	H	-5.07033	0.10274	3.02866
C	4.68600	-1.96102	-5.44139	H	-3.72823	4.25476	-1.80221
H	4.52285	-1.43714	-6.40836	H	-5.82247	5.96331	2.18277

H	4.18982	5.77402	-3.48818
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H	4.60018	0.10176	-3.20408
H	5.42853	-1.36819	-4.86781
H	-0.13003	-1.01140	-6.22999
H	3.02076	-2.42325	-0.62396
H	-2.69724	-2.42467	1.12074
O	1.11909	2.11642	0.96606
H	1.00246	2.92008	-0.07946
C	1.24671	3.79331	-1.03693
C	0.36356	4.82393	-0.69154
C	1.20669	3.19967	-2.43950
H	2.22265	4.00960	-0.62006
C	0.63123	5.69154	0.50449
O	-0.67814	5.15452	-1.39789
C	0.36710	4.09941	-3.34700
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H	0.77307	2.19775	-2.41641
C	-0.55100	6.47805	1.08083
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H	1.08073	5.04482	1.26632
C	-0.93205	4.45030	-2.64871
H	0.12563	3.59862	-4.28918
H	0.91393	5.02051	-3.58699
C	-1.47234	5.67120	1.99888
H	-0.13727	7.31649	1.65131
H	-1.13328	6.91483	0.26105
H	-1.48499	3.54435	-2.39568
H	-1.55000	5.14590	-3.21755
C	-2.16426	4.51424	1.29983
H	-2.23419	6.34036	2.41612
H	-0.89646	5.26598	2.84063
O	-1.17929	3.57090	0.95763
H	-2.90417	4.06720	1.97575
H	-2.67678	4.89566	0.40461
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R-gau-B_{2,5}-C(-)



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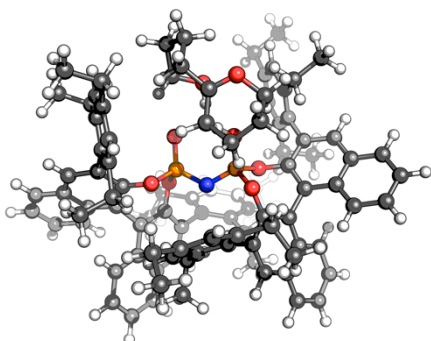
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H	-6.28479	-2.37517	-1.00562
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C	-5.47884	3.56155	3.10366
C	-5.00837	2.40002	2.48752
H	-6.42990	3.98295	2.80488
H	-5.61049	1.95470	1.70632
C	-7.29414	-2.17805	1.44084
C	-7.69594	-2.03096	2.76862
H	-7.91106	-2.76010	0.76631
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C	-6.90552	-1.31011	3.66267
C	-5.71745	-0.71632	3.23137
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P	1.19123	0.21183	-1.04817
O	1.16060	-0.92461	-2.00762
O	2.53969	0.17867	-0.10996
O	1.23543	1.59765	-1.92172
C	3.70122	0.63239	-0.68276
C	1.49295	2.74693	-1.21351
C	3.85494	2.00417	-0.96972
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C	2.75405	2.93957	-0.61531
C	5.04683	2.46363	-1.59056
C	6.01344	0.24601	-1.32520
C	0.82191	4.96498	-0.48295
C	2.97291	4.06759	0.21476
C	6.13804	1.57403	-1.73800
C	5.17892	3.78228	-2.08057
H	6.86023	-0.42489	-1.40802
C	1.99528	5.08939	0.26496
H	0.11064	5.78185	-0.50613
C	4.14151	4.20511	0.99367
C	7.34140	2.02236	-2.30597
C	6.37862	4.21189	-2.65185
H	4.35720	4.48462	-2.04298
C	2.21857	6.23832	1.04047
C	4.34304	5.34558	1.77412
H	4.89582	3.42934	1.01604
C	7.45971	3.33766	-2.75585

H	8.18636	1.35221	-2.41233	C	-4.22683	4.37706	-4.44392
H	6.46859	5.22625	-3.01877	H	-4.00293	4.31577	-5.53127
C	3.38851	6.36270	1.79145	C	-4.79199	5.76170	-4.14149
H	1.48392	7.03410	1.07420	H	-5.09042	5.83618	-3.07413
H	5.24271	5.44053	2.36820	H	-4.03436	6.54287	-4.36575
H	8.38769	3.67640	-3.19817	H	-5.68765	5.94333	-4.77211
H	3.55156	7.24598	2.39524	C	0.77641	4.11697	-4.18483
C	-0.65509	3.76680	-2.06940	H	1.52779	3.40922	-3.78410
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H	-4.06574	3.82398	-1.79544	H	-1.18995	3.09163	0.49978
C	4.69614	-1.68418	-0.50540	C	-2.63492	4.67840	0.73644
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C	4.71355	-3.49148	1.13310	H	-3.67246	4.91525	0.41967
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C	4.77980	-4.43955	0.10836	H	4.65933	-0.65605	5.23506
H	4.81324	-4.75481	-2.01441	C	3.82580	-0.97078	7.19242
C	-3.99129	-1.59960	-2.13648	H	4.80278	-1.31297	7.59407
C	-4.04512	-0.62420	-3.16478	H	3.70255	0.10801	7.42796
C	-3.53567	-2.91113	-2.43858	H	3.01894	-1.54914	7.69015
C	-3.65199	-0.96947	-4.46702	C	-1.18660	-1.63129	5.24294
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C	-3.21962	-2.26423	-4.76925	C	-1.86151	-0.98814	6.45023
H	-2.79775	-4.21896	-3.98678	H	-1.16414	-0.96868	7.31478
C	0.05798	0.27959	4.04737	H	-2.18223	0.04735	6.21707
C	0.07656	-0.88632	4.85899	H	-2.75932	-1.57809	6.73068
C	1.27787	0.93279	3.73527	C	1.33919	2.15410	2.84369
C	1.29903	-1.35868	5.35994	H	0.39724	2.30626	2.27899
C	2.48080	0.44043	4.26493	C	1.63214	3.41048	3.65897
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H	3.41066	0.94927	4.03878	H	1.53758	4.30436	3.01224
H	4.72888	-3.82479	2.16433	H	0.91039	3.51116	4.49570
H	1.31736	-2.24219	5.98735	C	-4.55276	0.77967	-2.92052
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C	6.33262	-6.38410	0.28132	H	-6.45341	0.48216	-3.93533
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H	4.07568	-0.26999	1.82831	H	-5.49532	-4.64286	-1.53402
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H	6.56909	-0.14492	1.43980	H	-2.71903	-1.72131	-6.80523
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C	4.72412	-2.27225	-3.01833	H	-3.64314	-3.74261	-7.86561
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H	6.88071	-1.96757	-3.16661	H	3.91088	-2.26930	5.45715
H	6.32357	-3.61903	-3.64166	H	4.31397	-1.64219	2.91872

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H	0.00174	-2.97182	0.14717
C	0.72785	-3.73559	0.81929
C	0.46093	-4.91294	0.08962
C	0.10493	-3.61868	2.20410
H	1.73450	-3.34525	0.67727
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C	0.63745	-5.91093	-2.28458
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H	0.37764	-5.37545	-4.34358
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R-gau-B_{2,5}-B(-)



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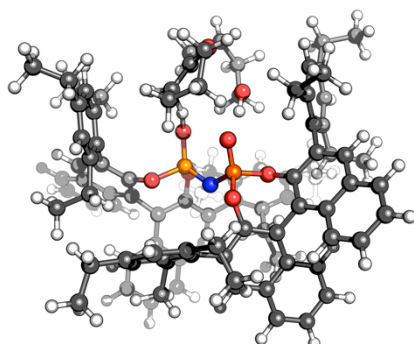
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C	-5.44685	-1.12088	3.47149
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H	4.82733	3.43059	1.07233

C	7.19649	3.83718	-2.78717	H	6.42519	-3.08335	-4.17168
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H	6.10335	5.68593	-2.86298	H	-4.32744	4.78524	-5.00352
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C	-0.85057	3.91205	-1.74338	H	1.27497	3.76823	-3.54750
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H	-4.24648	3.90579	-1.33380	H	-1.27309	2.97491	0.76086
C	4.78859	-1.48236	-0.84186	C	-2.72665	4.50656	1.21091
C	4.86069	-2.00161	0.47796	H	-2.65132	4.23349	2.28125
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C	5.13528	-4.25327	-0.41706	H	4.96527	-0.99362	4.98763
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C	5.35680	-5.72733	-0.19537	H	-6.61695	0.49721	-1.53906
H	5.14320	-6.00245	0.86052	H	-6.44143	2.23156	-1.98827
C	6.79666	-6.11557	-0.51845	H	-6.75862	1.00302	-3.27166
H	7.50120	-5.54408	0.12320	C	-3.86469	-4.00976	-1.77840
H	6.94135	-7.19968	-0.32728	H	-3.82190	-3.75608	-0.70148
H	7.02563	-5.91096	-1.58598	C	-5.02596	-4.97934	-1.99075
C	4.85144	-1.11337	1.70304	H	-4.91137	-5.84894	-1.30988
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C	6.24127	-0.56007	1.99992	H	-5.04163	-5.35270	-3.03618
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H	6.59846	0.07528	1.16396	H	-3.79814	-1.06727	-6.91206
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H	2.54745	-4.75528	-1.29636
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R-gau-B_{2,5}-C(+)



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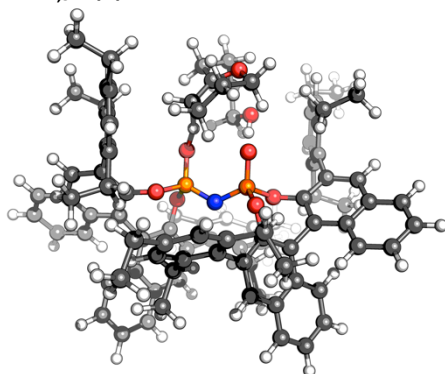
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H	-7.83689	-2.61732	-4.83336	H	6.18350	-4.38937	-5.62534
H	-3.55650	-7.58197	0.31698	C	-0.37730	-2.84628	-5.01719
C	0.91269	-3.09364	-2.79600	H	-1.14125	-2.22279	-4.51370
C	0.90424	-2.91396	-4.20704	C	-0.94205	-4.23699	-5.29258
C	2.15290	-3.17656	-2.11066	H	-0.18419	-4.86468	-5.80793
C	2.12279	-2.85233	-4.90145	H	-1.24978	-4.73406	-4.35126
C	3.35027	-3.13173	-2.84119	H	-1.83556	-4.15010	-5.94608
C	3.34280	-2.98933	-4.23261	C	2.24002	-3.32159	-0.60564
H	4.29798	-3.21396	-2.32207	H	1.26546	-3.12953	-0.11065
C	-4.70098	1.75113	-0.30029	C	2.72770	-4.71526	-0.21488
C	-5.07015	1.76243	1.06800	H	2.57997	-4.87017	0.87180
C	-4.57028	2.98157	-0.99660	H	2.16002	-5.50103	-0.75305
C	-5.32302	2.98494	1.70851	H	3.80767	-4.82642	-0.44807
C	-4.82568	4.18822	-0.32456	C	-4.44102	0.17613	5.67553
C	-5.22348	4.19530	1.01623	H	-5.29596	-0.26492	5.11839
H	-4.72279	5.12744	-0.85525	C	-4.51655	-0.31197	7.12013
C	4.65242	2.01282	-0.92380	H	-5.50784	-0.05265	7.54790
C	4.73568	1.36523	-2.18307	H	-4.38982	-1.41507	7.15934
C	4.60434	3.43363	-0.87102	H	-3.73062	0.16939	7.73953
C	4.74865	2.13347	-3.35777	C	0.55507	0.57425	5.56807
C	4.62772	4.16929	-2.06588	H	1.30618	0.83232	4.79720
C	4.70775	3.52993	-3.30624	C	1.17020	-0.37338	6.59418
H	4.57015	5.25095	-2.03055	H	0.42591	-0.62538	7.37942
C	-0.65893	-0.98517	3.90818	H	1.52219	-1.30681	6.11133
C	-0.69819	-0.01543	4.94797	H	2.04192	0.11791	7.07547
C	-1.87417	-1.53283	3.41734	C	-1.91655	-2.52914	2.27523
C	-1.93711	0.37426	5.47960	H	-0.94171	-2.60561	1.75056
C	-3.09037	-1.14505	3.99964	C	-2.32734	-3.91743	2.76177
C	-3.12898	-0.20647	5.03593	H	-3.39733	-3.92357	3.05826
H	-4.01437	-1.58704	3.64656	H	-2.18240	-4.65456	1.94722
H	-5.62267	2.99371	2.75028	H	-1.71096	-4.23359	3.62724
H	-1.97334	1.10719	6.27708	C	4.90111	-0.13160	-2.31350
H	4.82733	1.63967	-4.31938	H	4.32381	-0.67538	-1.54271
H	2.11968	-2.74240	-5.97961	C	6.37016	-0.53125	-2.22064
C	-5.55023	5.49210	1.71189	H	6.79477	-0.23217	-1.23980
H	-5.02174	5.53604	2.68844	H	6.46339	-1.63283	-2.32240
C	-7.05300	5.62465	1.94324	H	6.95192	-0.04797	-3.03425
H	-7.41969	4.81064	2.60421	C	4.47768	4.20331	0.43267
H	-7.26959	6.59858	2.43047	H	4.22449	3.54221	1.28656
H	-7.59589	5.58243	0.97475	C	5.75891	4.96699	0.76084
C	-5.26241	0.49189	1.86152	H	5.63773	5.49311	1.73106
H	-4.57925	-0.30924	1.51643	H	6.62013	4.27334	0.84188
C	-6.70411	0.00224	1.78542	H	5.97523	5.72280	-0.02330
H	-7.39636	0.77965	2.17325	C	4.74566	4.34337	-4.57459
H	-6.97795	-0.24290	0.73853	H	4.60029	3.69232	-5.46411
H	-6.81585	-0.91345	2.40353	C	6.08013	5.07017	-4.71950
C	-4.12751	3.05065	-2.44354	H	6.09376	5.63564	-5.67491
H	-3.71488	2.08353	-2.79833	H	6.22832	5.78647	-3.88365
C	-5.27499	3.46334	-3.36171	H	6.91653	4.33868	-4.72710

H	0.31510	1.53014	6.08314
H	-4.55794	1.28106	5.64751
H	-5.00847	0.68430	2.92250
H	-3.30780	3.79332	-2.53339
H	-5.20657	6.35989	1.10758
H	3.91644	5.08346	-4.56644
H	3.64311	4.93228	0.35222
H	4.49760	-0.46573	-3.29163
H	5.35924	-2.29253	-4.55150
H	-0.18643	-2.35252	-5.99516
H	2.94518	-2.56188	-0.20699
H	-2.65014	-2.18207	1.51791
O	1.00911	2.20303	0.48543
H	0.83260	2.90981	-0.55818
C	1.05802	3.84154	-1.52674
C	0.17414	4.85897	-1.16756
C	1.05180	3.27270	-2.93269
H	2.01865	3.96948	-1.03765
C	0.25814	5.56470	0.15728
O	-0.73694	5.34614	-1.96886
C	-0.29136	3.56020	-3.60110
H	1.86317	3.71536	-3.52294
H	1.21943	2.19205	-2.89437
C	-1.08793	5.99085	0.77386
H	0.86607	6.45731	-0.04900
H	0.84184	4.93855	0.84182
C	-0.67582	5.00655	-3.37760
H	-1.05139	2.90058	-3.18001
H	-0.23776	3.37739	-4.67946
C	-1.63714	5.02784	1.83531
H	-0.97172	6.97997	1.22778
H	-1.82064	6.09190	-0.02997
H	-1.67012	5.24388	-3.75633
H	0.05055	5.69520	-3.82603
C	-1.59862	3.56571	1.38630
H	-2.66286	5.33336	2.05978
H	-1.06876	5.12491	2.76857
O	-1.81447	3.54726	-0.01026
H	-0.62535	3.12669	1.62530
H	-2.36516	2.98311	1.91585
H	-1.60270	2.68439	-0.41098

R-gau-B_{2,5}-B(+)



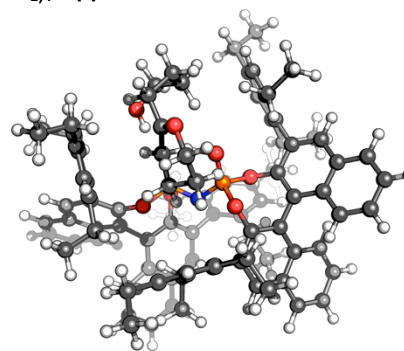
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C	1.47218	-1.04156	2.62378
C	0.56567	-1.87221	3.30770
C	2.77947	-1.49952	2.37981
C	0.90571	-3.20608	3.57063
C	3.09511	-2.86930	2.56717
C	2.14178	-3.72103	3.17289
C	3.82621	-0.49013	2.07955
C	4.95348	-0.33391	2.93181
C	3.68791	0.33159	0.93673
C	6.03050	0.48007	2.51272
C	4.77352	1.14613	0.54263
C	5.94503	1.17510	1.30794
H	6.78156	1.78030	0.97718
H	0.21036	-3.83743	4.11001
C	2.45457	-5.06847	3.41321
C	3.69989	-5.57814	3.04225
H	1.73633	-5.72660	3.88780
H	3.93469	-6.61837	3.22710
C	4.63929	-4.75126	2.42586
C	4.34237	-3.40798	2.18390
H	5.59894	-5.15378	2.12859
H	5.08640	-2.80119	1.68455
C	7.17765	0.60280	3.31339
C	7.24942	-0.05029	4.54378
H	8.01276	1.21503	2.99369
H	8.13306	0.05307	5.16025
C	6.17610	-0.82016	4.98909
C	5.03395	-0.95879	4.19756
H	6.22690	-1.30889	5.95356
H	4.21412	-1.54225	4.59408
N	0.04226	-0.24735	0.01234
P	-1.10827	0.22048	-0.99496
O	-1.09626	1.62779	-1.49223
O	-2.51785	-0.07970	-0.21130
O	-1.03870	-0.75791	-2.30484
C	-3.61723	-0.27055	-1.01830
C	-1.33171	-2.08083	-2.07639
C	-3.70999	-1.44060	-1.80074
C	-4.70848	0.62674	-0.98020
C	-0.38685	-3.07670	-2.38070
C	-2.63273	-2.45619	-1.69437
C	-4.79993	-1.61312	-2.69338
C	-5.83256	0.39025	-1.78120
C	-0.67683	-4.41852	-2.09742
C	-2.90366	-3.79940	-1.33668
C	-5.87493	-0.69482	-2.65759
C	-4.84079	-2.66577	-3.63536
H	-6.67705	1.06757	-1.72559
C	-1.90658	-4.78238	-1.54091
H	0.05028	-5.18398	-2.33868
C	-4.14436	-4.18965	-0.78970
C	-6.98066	-0.86987	-3.50531
C	-5.94187	-2.82211	-4.47976

H	-4.02097	-3.36334	-3.74095	H	-3.90702	2.43706	-2.62847
C	-2.16936	-6.12493	-1.22597	C	-5.53435	3.82420	-2.94375
C	-4.38997	-5.52803	-0.47504	H	-5.24669	3.97576	-4.00540
H	-4.92216	-3.46447	-0.58826	H	-6.34676	3.07107	-2.90452
C	-7.01274	-1.93221	-4.40911	H	-5.91286	4.78768	-2.54184
H	-7.81440	-0.17821	-3.47708	C	4.63388	-2.49592	-5.23001
H	-5.96238	-3.63466	-5.19460	H	4.48246	-2.05950	-6.24134
C	-3.40699	-6.49330	-0.69557	C	5.21711	-3.89689	-5.39041
H	-1.41758	-6.88815	-1.38857	H	5.45104	-4.33824	-4.39834
H	-5.34428	-5.81673	-0.05406	H	4.49668	-4.55371	-5.92343
H	-7.86432	-2.05866	-5.06507	H	6.15489	-3.84338	-5.98251
H	-3.60276	-7.52903	-0.45015	C	-0.37772	-2.25905	-5.25591
C	0.89052	-2.75584	-3.06367	H	-1.13672	-1.67803	-4.69751
C	0.89586	-2.42774	-4.44793	C	-0.96022	-3.60579	-5.67521
C	2.12471	-2.92547	-2.38256	H	-0.20660	-4.19006	-6.24493
C	2.12077	-2.31090	-5.12409	H	-1.28494	-4.19047	-4.79172
C	3.32822	-2.82102	-3.09672	H	-1.84574	-3.43919	-6.32409
C	3.33346	-2.53610	-4.46595	C	2.19910	-3.22783	-0.90026
H	4.27078	-2.97136	-2.58346	H	1.22184	-3.08207	-0.39494
C	-4.72697	1.83040	-0.11268	C	2.67655	-4.65763	-0.65276
C	-5.02011	1.70470	1.26898	H	2.51388	-4.92594	0.40950
C	-4.65301	3.12675	-0.69135	H	2.11389	-5.37964	-1.27829
C	-5.22222	2.85711	2.04417	H	3.75919	-4.74885	-0.88222
C	-4.86575	4.25833	0.11249	C	-4.50083	-0.35703	5.69847
C	-5.16485	4.13055	1.47159	H	-5.35873	-0.73140	5.09852
H	-4.80459	5.24634	-0.32879	C	-4.58502	-0.98342	7.08795
C	4.71391	2.03536	-0.64084	H	-5.57437	-0.75599	7.53777
C	4.89761	1.50619	-1.94313	H	-4.47057	-2.08636	7.01886
C	4.66809	3.44486	-0.45991	H	-3.79514	-0.57374	7.75226
C	5.02816	2.37911	-3.03455	C	0.49811	0.01327	5.62599
C	4.78829	4.28822	-1.57541	H	1.25246	0.33852	4.88430
C	4.97597	3.76574	-2.85877	C	1.10374	-1.03537	6.55480
H	4.72233	5.36200	-1.44455	H	0.35706	-1.35439	7.31295
C	-0.72848	-1.36150	3.81838	H	1.44567	-1.92130	5.98327
C	-0.75978	-0.50223	4.95149	H	1.98065	-0.60193	7.08023
C	-1.94741	-1.85128	3.27870	C	-1.99726	-2.72255	2.03859
C	-1.99533	-0.16091	5.52262	H	-1.02271	-2.75153	1.50851
C	-3.15952	-1.52157	3.90330	C	-2.41917	-4.15084	2.37727
C	-3.19115	-0.68838	5.02639	H	-3.49154	-4.18062	2.66353
H	-4.08660	-1.92202	3.51092	H	-2.27134	-4.80144	1.49258
H	-5.45942	2.76221	3.09765	H	-1.81160	-4.55792	3.21038
H	-2.02594	0.48985	6.38869	C	5.02482	0.02357	-2.20336
H	5.17933	1.97314	-4.02812	H	4.46001	-0.57579	-1.46433
H	2.12778	-2.08976	-6.18501	C	6.48596	-0.41172	-2.18587
C	-5.44174	5.35077	2.31186	H	6.93933	-0.20143	-1.19414
H	-4.84169	5.30383	3.24618	H	6.55112	-1.50293	-2.38045
C	-6.92478	5.44958	2.65989	H	7.05809	0.12474	-2.97247
H	-7.24416	4.57373	3.26370	C	4.44955	4.08832	0.89836
H	-7.10764	6.37125	3.25138	H	4.12958	3.35095	1.66306
H	-7.53445	5.49587	1.73201	C	5.70867	4.79720	1.39220
C	-5.20330	0.36214	1.93582	H	5.51800	5.23403	2.39499
H	-4.50418	-0.39155	1.52449	H	6.55386	4.08404	1.47403
C	-6.63784	-0.13681	1.79978	H	5.99209	5.61787	0.69998
H	-7.34441	0.59723	2.24257	C	5.08179	4.69080	-4.04375
H	-6.89816	-0.29778	0.73381	H	5.01831	4.11996	-4.99582
H	-6.74516	-1.10225	2.33774	C	6.40055	5.45839	-4.02668
C	-4.31814	3.35078	-2.15111	H	6.46251	6.10951	-4.92391

H	6.46937	6.09813	-3.12143
H	7.25642	4.75006	-4.04108
H	0.26598	0.91661	6.23158
H	-4.60631	0.74653	5.77892
H	-4.96692	0.45468	3.01387
H	-3.53085	4.12931	-2.21926
H	-5.14426	6.27591	1.77146
H	4.23177	5.40709	-4.03062
H	3.62879	4.83345	0.82730
H	4.58217	-0.21144	-3.19286
H	5.36647	-1.85192	-4.70102
H	-0.17157	-1.67165	-6.17739
H	2.90555	-2.51846	-0.41965
H	-2.72684	-2.29230	1.32104
O	1.00014	2.14879	0.73604
H	0.91539	2.89336	-0.28647
C	1.17698	3.78665	-1.28001
C	0.22151	4.79136	-1.10380
C	1.30167	3.08485	-2.62690
H	2.09618	4.05715	-0.77003
C	0.29248	5.76119	0.04455
O	-0.73500	5.03707	-1.95016
C	0.50959	3.85289	-3.68426
H	2.34931	3.02820	-2.91840
H	0.91968	2.06400	-2.55797
C	-1.05345	6.20092	0.64674
H	0.81429	6.63641	-0.36723
H	0.95619	5.33525	0.80573
C	-0.85703	4.19599	-3.12640
H	0.37654	3.25548	-4.59095
H	1.03327	4.77597	-3.96347
C	-1.51230	5.37073	1.85278
H	-0.97345	7.24853	0.95375
H	-1.81519	6.14928	-0.13453
H	-1.38148	3.28990	-2.81569
H	-1.46621	4.78683	-3.81086
C	-1.43628	3.86833	1.59229
H	-2.53957	5.66424	2.08957
H	-0.90318	5.60733	2.73447
O	-1.83937	3.65548	0.25640
H	-0.41409	3.50808	1.74651
H	-2.08506	3.32657	2.29571
H	-1.57760	2.78546	-0.09124

R-gau-B_{1,4}-C(-)



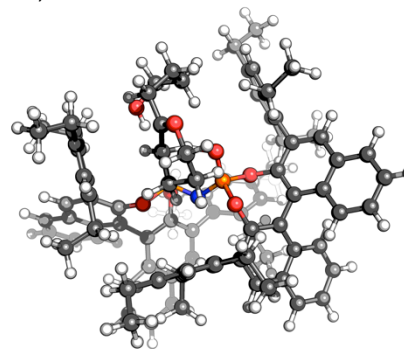
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C	-2.89421	1.90867	4.16486
C	-4.07964	-0.56277	1.50760
C	-5.25794	-1.19256	1.99141
C	-3.70287	-0.73303	0.15914
C	-6.12725	-1.83456	1.07536
C	-4.57531	-1.37721	-0.73737
C	-5.79075	-1.89618	-0.27874
H	-6.46021	-2.38089	-0.98025
H	-1.04858	1.75510	5.26427
C	-3.38389	2.97724	4.93274
C	-4.64401	3.51504	4.66627
H	-2.78914	3.40103	5.73324
H	-5.01365	4.34344	5.25656
C	-5.42294	2.99505	3.63253
C	-4.95380	1.92453	2.86815
H	-6.39327	3.42489	3.42027
H	-5.57739	1.55957	2.06262
C	-7.31620	-2.42791	1.52897
C	-7.63507	-2.41531	2.88692
H	-7.99246	-2.91262	0.83462
H	-8.55015	-2.87928	3.23169
C	-6.76725	-1.82292	3.80314
C	-5.58485	-1.22226	3.36568
H	-7.00877	-1.83316	4.85822
H	-4.92745	-0.79999	4.11323
C	3.60540	0.82997	-0.74924
C	1.27106	2.89149	-0.88111
C	3.67231	2.23732	-0.83323
C	4.75376	0.06106	-1.03675
C	0.31851	3.91764	-0.74572
C	2.54509	3.05179	-0.30342
C	4.81424	2.85308	-1.41322
C	5.92692	0.69146	-1.46747
C	0.55965	4.98309	0.13034
C	2.75671	4.07759	0.65277
C	5.95597	2.06720	-1.69761
C	4.84738	4.23037	-1.72850

H	6.81239	0.09641	-1.65540	H	4.10460	-0.41735	1.59725
C	1.75122	5.05290	0.85629	C	6.20615	-0.80271	1.94925
H	-0.17564	5.77295	0.22545	H	6.89812	-1.66886	2.01964
C	3.94910	4.16295	1.40276	H	6.57363	-0.10370	1.17081
C	7.11294	2.66652	-2.22102	H	6.20225	-0.27043	2.92363
C	6.00114	4.81158	-2.25871	C	4.86336	-1.60853	-3.51613
H	3.98219	4.86397	-1.58717	H	4.58430	-0.53547	-3.52045
C	1.96732	6.10767	1.75750	C	6.24558	-1.76692	-4.14630
C	4.14508	5.20984	2.30613	H	6.25562	-1.28083	-5.14454
H	4.72667	3.41617	1.30710	H	7.02376	-1.29258	-3.51497
C	7.13402	4.03421	-2.49492	H	6.49284	-2.84164	-4.27695
H	7.99618	2.07461	-2.43062	C	-4.54089	4.45484	-3.88260
H	6.01485	5.86868	-2.49103	H	-4.47900	3.86535	-4.82285
C	3.16058	6.18319	2.47788	C	-4.75878	5.92843	-4.21452
H	1.21099	6.86849	1.90988	H	-4.81978	6.52685	-3.28038
H	5.06328	5.26534	2.87638	H	-3.92964	6.31512	-4.84405
H	8.02613	4.48989	-2.90479	H	-5.71023	6.04577	-4.77474
H	3.31912	6.99391	3.17712	C	0.46672	4.61034	-3.64325
C	-0.91308	3.94021	-1.57110	H	1.26300	3.90251	-3.34090
C	-0.84388	4.30358	-2.94390	C	0.91892	6.04244	-3.37311
C	-2.17943	3.71689	-0.97156	H	0.13583	6.76046	-3.69769
C	-2.03019	4.44372	-3.68058	H	1.12898	6.19419	-2.29540
C	-3.34519	3.88429	-1.73446	H	1.84963	6.25031	-3.94180
C	-3.27917	4.25774	-3.08046	C	-2.33056	3.30579	0.47692
H	-4.31251	3.72586	-1.27189	H	-1.37047	2.96833	0.91884
C	4.74708	-1.41952	-0.94138	C	-2.88764	4.45352	1.31615
C	4.75982	-2.05769	0.32681	H	-2.82834	4.19290	2.39055
C	4.81752	-2.21082	-2.12217	H	-2.30265	5.38171	1.15496
C	4.78954	-3.45923	0.39469	H	-3.94985	4.64451	1.05486
C	4.83826	-3.60995	-2.01387	C	3.95607	-1.95012	5.33258
C	4.81857	-4.23812	-0.76513	H	4.80979	-1.39906	4.88210
H	4.86791	-4.21402	-2.91317	C	4.09208	-1.87991	6.85119
C	-4.20097	-1.59411	-2.15410	H	5.08317	-2.27893	7.15353
C	-4.26231	-0.52620	-3.08567	H	4.01283	-0.82634	7.19489
C	-3.85249	-2.89559	-2.60289	H	3.30369	-2.48678	7.34443
C	-3.94811	-0.76512	-4.43248	C	-1.05422	-2.22312	5.18044
C	-3.59430	-3.10718	-3.96533	H	-1.82206	-2.18043	4.38168
C	-3.62156	-2.04948	-4.87881	C	-1.62431	-1.65809	6.47754
H	-3.36194	-4.10559	-4.31499	H	-0.87284	-1.73376	7.29223
C	0.17802	-0.27781	4.03313	H	-1.91766	-0.59671	6.35028
C	0.20835	-1.49014	4.77096	H	-2.52508	-2.23771	6.76979
C	1.39331	0.38445	3.72712	C	1.43298	1.69790	2.97900
C	1.44319	-2.02520	5.16844	H	0.48051	1.90624	2.44969
C	2.60950	-0.16981	4.15431	C	1.73197	2.85014	3.93463
C	2.64244	-1.36891	4.87363	H	2.78032	2.79059	4.29620
H	3.53654	0.34638	3.93407	H	1.58955	3.81548	3.41303
H	4.79219	-3.95194	1.36003	H	1.04540	2.82738	4.80578
H	1.47132	-2.95374	5.72647	C	-4.70502	0.86466	-2.69017
H	-3.98120	0.04973	-5.14643	H	-4.27894	1.15584	-1.71036
H	-1.98433	4.72886	-4.72519	C	-6.22606	0.96766	-2.64164
C	4.81868	-5.74204	-0.66517	H	-6.64446	0.27305	-1.88517
H	3.99943	-6.06800	0.01185	H	-6.51932	2.00208	-2.36581
C	6.15410	-6.25930	-0.13863	H	-6.65829	0.72807	-3.63654
H	6.34409	-5.87888	0.88733	C	-3.71250	-4.07540	-1.65872
H	6.13473	-7.36894	-0.10483	H	-3.69016	-3.76205	-0.59495
H	6.98054	-5.93783	-0.80798	C	-4.84290	-5.08329	-1.85007
C	4.79477	-1.28150	1.62599	H	-4.72368	-5.91519	-1.12438

H	-5.82737	-4.60180	-1.67726
H	-4.82004	-5.50687	-2.87619
C	-3.29395	-2.28724	-6.33075
H	-2.53509	-1.54728	-6.66547
C	-4.54130	-2.17331	-7.20252
H	-4.27523	-2.38225	-8.26009
H	-5.30594	-2.91018	-6.87572
H	-4.96884	-1.15007	-7.14210
H	-0.83755	-3.30239	5.33722
H	4.02914	-3.00776	4.99870
H	4.44700	-1.92409	2.46155
H	4.12627	-2.11844	-4.16942
H	4.62885	-6.20217	-1.65941
H	-2.85433	-3.29862	-6.47405
H	-2.74323	-4.58146	-1.84656
H	-4.32854	1.60419	-3.42697
H	-5.42645	4.08927	-3.31931
H	0.35314	4.48394	-4.74220
H	-3.02219	2.43993	0.53527
H	2.22074	1.65033	2.19823
O	-1.04321	-2.26900	-0.40439
P	-1.16195	-0.88326	0.20875
H	0.20224	-2.93327	-0.45015
O	-2.53487	-0.17586	-0.30207
O	-1.35338	-1.19601	1.81466
N	-0.01149	0.17571	0.03662
P	1.09715	0.34006	-1.10516
O	1.09703	-0.58187	-2.27393
O	2.48558	0.22160	-0.23342
O	1.02437	1.84530	-1.73491
C	1.43769	-5.32628	-1.81543
H	1.68483	-1.98002	-2.92396
C	0.19582	-5.35759	-2.73530
H	2.22667	-4.75361	-2.30042
H	1.76610	-6.35474	-1.63697
O	1.91769	-2.86170	-3.28904
C	-0.23545	-4.00734	-3.30847
H	-0.63410	-5.83154	-2.19841
H	0.45050	-6.02582	-3.56703
C	0.85318	-3.29446	-4.10442
H	-1.07111	-4.20118	-3.98786
H	-0.60192	-3.33128	-2.52625
H	1.27236	-3.97804	-4.85668
H	0.41058	-2.44437	-4.64037
C	1.17432	-4.73751	-0.46845
C	1.33492	-3.37944	-0.12567
O	0.71881	-5.63238	0.36696
C	1.35182	-3.02440	1.35730
H	1.98365	-2.83169	-0.80897
C	0.55491	-5.33784	1.78125
C	0.29494	-3.87448	2.05688
H	1.14676	-1.95778	1.48303
H	2.33732	-3.21247	1.79661
H	1.47850	-5.68400	2.25673
H	-0.26800	-5.98124	2.09426
H	-0.70094	-3.58696	1.70815
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R-gau-B_{1,4}-C(-) intermediate



E(RM062X) = -5098.40879573

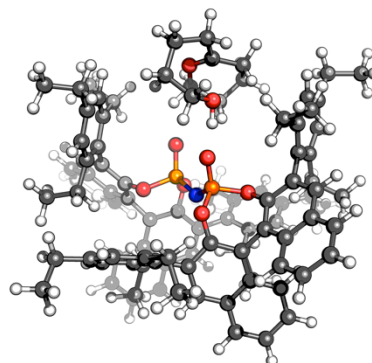
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C	-3.79451	1.15542	3.15629
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C	-4.11154	-0.72186	1.47296
C	-5.26087	-1.42271	1.92603
C	-3.71889	-0.82633	0.12471
C	-6.08317	-2.08845	0.98322
C	-4.53558	-1.50616	-0.79807
C	-5.72546	-2.10305	-0.36751
H	-6.35509	-2.61288	-1.08776
H	-1.16973	1.60072	5.29932
C	-3.54445	2.74987	4.99022
C	-4.82287	3.24848	4.73517
H	-2.96466	3.17698	5.79989
H	-5.22119	4.05045	5.34305
C	-5.58388	2.72309	3.69093
C	-5.07750	1.68675	2.90361
H	-6.56919	3.12238	3.48819
H	-5.68875	1.31724	2.09076
C	-7.24269	-2.75690	1.40755
C	-7.57738	-2.79460	2.76129
H	-7.88274	-3.26169	0.69348
H	-8.46928	-3.31646	3.08328
C	-6.75424	-2.17777	3.70239
C	-5.60158	-1.50297	3.29465
H	-7.00719	-2.22667	4.75370
H	-4.97756	-1.06274	4.06016
C	3.55297	0.96888	-0.71509
C	1.11788	2.91836	-0.82996
C	3.54460	2.37946	-0.77682
C	4.75013	0.27199	-0.99421
C	0.11939	3.89987	-0.68588
C	2.37710	3.12548	-0.23682
C	4.65501	3.06674	-1.33759
C	5.88979	0.97467	-1.40303
C	0.30746	4.96081	0.20910
C	2.53614	4.14357	0.73758
C	5.84234	2.35159	-1.61844

C	4.61299	4.44803	-1.63444	C	4.84615	-1.08069	1.66152
H	6.81154	0.43478	-1.58337	H	4.09708	-0.26739	1.62409
C	1.48809	5.07082	0.94712	C	6.21356	-0.50575	2.01515
H	-0.46007	5.71879	0.30746	H	6.96388	-1.32116	2.09335
C	3.71884	4.27032	1.49714	H	6.54475	0.22359	1.24825
C	6.96919	3.02266	-2.12015	H	6.15336	0.01716	2.99277
C	5.73744	5.10123	-2.14344	C	4.98701	-1.37177	-3.48144
H	3.71149	5.02934	-1.49483	H	4.62637	-0.32318	-3.48085
C	1.65169	6.12136	1.86425	C	6.37864	-1.41986	-4.10907
C	3.86303	5.31205	2.41614	H	6.35254	-0.93114	-5.10573
H	4.52905	3.55976	1.39627	H	7.11628	-0.88818	-3.47487
C	6.91538	4.39288	-2.37620	H	6.70940	-2.47149	-4.24277
H	7.88720	2.48487	-2.32618	C	-4.72982	4.35542	-3.84899
H	5.69337	6.16048	-2.36173	H	-4.64754	3.78338	-4.79841
C	2.83577	6.23902	2.59410	C	-4.98165	5.82848	-4.15822
H	0.86196	6.84650	2.02109	H	-5.06380	6.40962	-3.21484
H	4.77426	5.39969	2.99349	H	-4.15786	6.24571	-4.77517
H	7.78466	4.90410	-2.76929	H	-5.93178	5.93176	-4.72341
H	2.95412	7.04619	3.30530	C	0.27006	4.62982	-3.57581
C	-1.10457	3.88993	-1.52269	H	1.08346	3.93815	-3.28276
C	-1.03584	4.27558	-2.88976	C	0.68302	6.06827	-3.27761
C	-2.36962	3.63050	-0.93376	H	-0.11816	6.77108	-3.59111
C	-2.22080	4.39820	-3.63175	H	0.88659	6.20549	-2.19676
C	-3.53411	3.78307	-1.70155	H	1.60928	6.31152	-3.83952
C	-3.46861	4.17620	-3.04184	C	-2.52101	3.19390	0.50789
H	-4.50047	3.59665	-1.24751	H	-1.55521	2.87772	0.95331
C	4.84003	-1.20613	-0.90669	C	-3.12086	4.30960	1.36101
C	4.89113	-1.84880	0.35835	H	-3.06678	4.03041	2.43131
C	4.98358	-1.98290	-2.09076	H	-2.56222	5.25741	1.22388
C	5.02982	-3.24435	0.41974	H	-4.18524	4.47434	1.09093
C	5.11586	-3.37644	-1.98926	C	3.96449	-1.89391	5.32596
C	5.13355	-4.01163	-0.74394	H	4.79888	-1.29381	4.90271
H	5.20071	-3.97108	-2.89130	C	4.07440	-1.85322	6.84779
C	-4.12069	-1.68252	-2.20963	H	5.07822	-2.21336	7.15684
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C	-3.85696	-0.80360	-4.46803	C	-1.02672	-2.37737	5.10958
C	-3.36710	-3.12536	-4.02401	H	-1.79513	-2.33807	4.31132
C	-3.43645	-2.05714	-4.92275	C	-1.61965	-1.87609	6.42251
H	-3.06443	-4.10144	-4.38188	H	-0.86767	-1.95097	7.23680
C	0.13186	-0.35442	4.02147	H	-1.95063	-0.82216	6.32824
C	0.20710	-1.58354	4.72771	H	-2.49949	-2.49704	6.69278
C	1.32127	0.36357	3.74078	C	1.31278	1.69293	3.02058
C	1.45986	-2.07718	5.12255	H	0.35574	1.87443	2.48942
C	2.55574	-0.14893	4.16766	C	1.56106	2.83609	4.00143
C	2.63262	-1.36205	4.85956	H	2.61031	2.81314	4.36450
H	3.46195	0.41147	3.97010	H	1.37882	3.80545	3.50015
H	5.05712	-3.74110	1.38262	H	0.87463	2.76605	4.87010
H	1.52198	-3.01731	5.65798	C	-4.76122	0.74775	-2.72479
H	-3.92250	0.01856	-5.17126	H	-4.37521	1.05061	-1.73203
H	-2.17572	4.69977	-4.67179	C	-6.28636	0.75477	-2.70911
C	5.24621	-5.51181	-0.65250	H	-6.67660	0.02944	-1.96657
H	4.44489	-5.90330	0.01111	H	-6.64947	1.76688	-2.43330
C	6.60992	-5.93004	-0.11080	H	-6.68126	0.49661	-3.71481
H	6.75707	-5.54312	0.91975	C	-3.51043	-4.14392	-1.74123
H	6.67425	-7.03816	-0.08352	H	-3.54064	-3.85135	-0.67187
H	7.41835	-5.54252	-0.76704	C	-4.58007	-5.20440	-1.98928

H	-4.44198	-6.04353	-1.27541
H	-5.59337	-4.77736	-1.84135
H	-4.50142	-5.60545	-3.02168
C	-3.05894	-2.25141	-6.36901
H	-2.34165	-1.45924	-6.67459
C	-4.28981	-2.20462	-7.27005
H	-3.98564	-2.37998	-8.32341
H	-5.01307	-2.99379	-6.97242
H	-4.78386	-1.21197	-7.20647
H	-0.76832	-3.45211	5.23067
H	4.09095	-2.93892	4.96914
H	4.52796	-1.75252	2.48551
H	4.29262	-1.93451	-4.13846
H	5.10482	-5.97843	-1.65178
H	-2.55171	-3.23022	-6.51484
H	-2.51012	-4.59665	-1.90540
H	-4.41725	1.51908	-3.44426
H	-5.60956	3.95847	-3.29765
H	0.16564	4.52071	-4.67752
H	-3.18815	2.30825	0.54752
H	2.10599	1.69189	2.24394
O	-1.08005	-2.29610	-0.47498
P	-1.19420	-0.94555	0.16407
H	0.67672	-2.91466	-0.75827
O	-2.57213	-0.19881	-0.29412
O	-1.35919	-1.27633	1.78164
N	-0.04526	0.13849	0.02475
P	1.06091	0.36599	-1.09682
O	1.13348	-0.53236	-2.28678
O	2.46139	0.29025	-0.22328
O	0.93283	1.87899	-1.70771
C	1.85589	-5.28641	-1.91075
H	1.81536	-1.87015	-2.90004
C	0.57425	-5.36254	-2.79014
H	2.59293	-4.66113	-2.41277
H	2.23140	-6.30159	-1.75452
O	2.09454	-2.74323	-3.26708
C	0.03119	-4.03276	-3.31542
H	-0.20244	-5.90300	-2.23658
H	0.84926	-5.99350	-3.64351
C	1.05535	-3.21399	-4.09475
H	-0.79274	-4.28045	-3.99206
H	-0.39115	-3.41040	-2.51630
H	1.50995	-3.83465	-4.88087
H	0.54757	-2.37446	-4.58616
C	1.56207	-4.71748	-0.57218
C	1.60704	-3.29562	-0.26031
O	1.19337	-5.60425	0.27718
C	1.49990	-2.94421	1.21960
H	2.40230	-2.81506	-0.83220
C	0.83468	-5.28305	1.66541
C	0.43069	-3.84050	1.83543
H	1.23670	-1.88785	1.31639
H	2.45832	-3.09029	1.73083
H	1.72510	-5.54539	2.24400
H	0.03722	-5.99183	1.88838
H	-0.53054	-3.64406	1.35036

H	0.31040	-3.65758	2.90368
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R-gau-B_{1,4}-C(-) 2nd step



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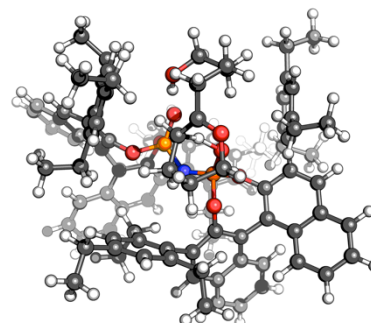
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C	-3.12209	-3.95221	-2.46170
C	-4.12973	-0.32741	-1.80633
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C	-3.70952	0.59081	-0.82215
C	-6.11940	1.04097	-2.20766
C	-4.52510	1.69332	-0.49188
C	-5.74231	1.87974	-1.15650
H	-6.38380	2.70381	-0.86925
H	-1.29466	-4.57969	-3.41182
C	-3.67971	-5.24073	-2.45010
C	-4.96124	-5.44792	-1.93763
H	-3.12240	-6.08781	-2.83225
H	-5.38393	-6.44419	-1.92601
C	-5.69336	-4.37548	-1.42840
C	-5.15466	-3.08703	-1.44065
H	-6.68051	-4.54345	-1.01769
H	-5.74313	-2.28392	-1.01704
C	-7.30357	1.29705	-2.91746
C	-7.65995	0.49684	-4.00313
H	-7.94617	2.12476	-2.64112
H	-8.57075	0.70263	-4.55050
C	-6.83433	-0.55537	-4.39658
C	-5.65834	-0.82753	-3.69426
H	-7.10421	-1.16108	-5.25209
H	-5.03403	-1.63600	-4.04934
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C	0.99536	-1.93339	2.24467
C	3.43643	-1.65262	1.91241
C	4.74978	0.05802	0.78292
C	-0.04186	-2.74963	2.73491
C	2.23235	-2.51983	1.92402
C	4.50899	-1.87984	2.81496
C	5.84939	-0.26946	1.58649
C	0.08378	-4.14464	2.68060

C	2.33316	-3.92675	1.78633	H	7.95065	4.54459	-4.36644
C	5.72968	-1.19331	2.62419	H	8.33839	3.78129	-2.77751
C	4.39621	-2.76744	3.90897	C	4.90212	-0.67213	-2.10710
H	6.80184	0.21611	1.40893	H	4.09126	-1.19225	-1.56396
C	1.24221	-4.73845	2.17462	C	6.19420	-1.47181	-1.98084
H	-0.71236	-4.76823	3.06811	H	7.00626	-0.98507	-2.56194
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C	6.81915	-1.44037	3.47498	H	6.03590	-2.49581	-2.38002
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C	1.34419	-6.13671	2.09819	C	6.34087	3.25616	2.25099
C	3.58319	-5.93691	1.20505	H	6.15157	3.58585	3.29422
H	4.34334	-3.95898	0.94749	H	6.99999	2.36569	2.27906
C	6.69468	-2.34112	4.53311	H	6.86256	4.07644	1.71466
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H	0.52048	-6.76894	2.40782	H	-5.14349	-3.03952	6.39014
H	4.48183	-6.40123	0.82010	H	-4.19857	-1.94910	7.48568
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C	-1.23666	-2.17819	3.40100	H	0.99509	-1.15623	4.78043
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O	0.45796	5.58480	-1.01567
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H	3.16385	3.79184	-3.09912
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H	1.65546	3.09582	0.94502
C	0.82146	6.89703	1.41470
H	2.88298	6.42344	0.84144
H	2.14571	7.69745	-0.11972
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H	-0.13823	5.81646	3.00490

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R-gau-B_{1,4}-B(-)



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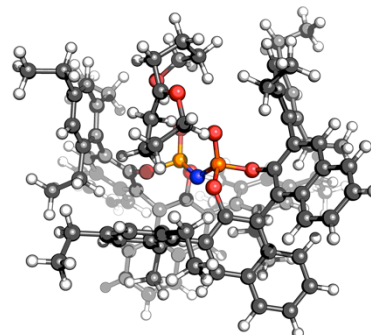
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C	-7.40289	-2.04480	1.55191
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C	3.38602	6.19469	2.21788	C	-4.47711	5.82029	-4.58657
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R-gau-B_{1,4}-B(-) intermediate



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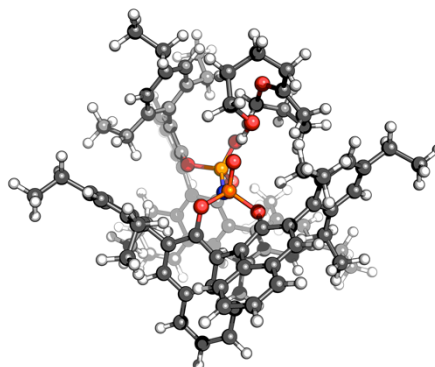
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C	-6.16338	-1.71724	1.06585
C	-4.56523	-1.35243	-0.72817
C	-5.78673	-1.85949	-0.27196
H	-6.42410	-2.40648	-0.95756
H	-1.09687	2.03237	5.15219
C	-3.40632	3.27805	4.74269
C	-4.65621	3.82226	4.44321
H	-2.80748	3.73270	5.52296
H	-5.01389	4.68625	4.98811
C	-5.44048	3.26188	3.43499
C	-4.98637	2.14589	2.72884
H	-6.40296	3.69581	3.19685
H	-5.61361	1.74992	1.94103
C	-7.35639	-2.29985	1.52265
C	-7.70914	-2.21658	2.86969
H	-8.00868	-2.83216	0.84035
H	-8.62699	-2.67286	3.21734
C	-6.87085	-1.56439	3.77271
C	-5.68447	-0.97418	3.33180
H	-7.13830	-1.52018	4.82064
H	-5.05096	-0.50359	4.07088
C	3.62921	0.76534	-0.71961
C	1.28805	2.80251	-1.01403
C	3.68748	2.16641	-0.88582
C	4.79038	-0.00688	-0.94839
C	0.32973	3.83168	-0.95643
C	2.54863	3.00159	-0.42076
C	4.83052	2.75821	-1.48870

C	5.96144	0.60864	-1.40571	C	6.38265	-6.22735	0.32089
C	0.55261	4.94768	-0.13967	H	6.56257	-5.78489	1.32348
C	2.74026	4.08205	0.47728	H	6.38866	-7.33342	0.41799
C	5.98147	1.96811	-1.71528	H	7.20248	-5.92582	-0.36565
C	4.85576	4.11539	-1.88307	C	4.86902	-1.18314	1.78793
H	6.85437	0.01201	-1.55016	H	4.15978	-0.33830	1.69741
C	1.72906	5.06367	0.60452	C	6.26508	-0.65319	2.09644
H	-0.18363	5.74144	-0.10766	H	6.97601	-1.49698	2.22530
C	3.91991	4.21705	1.24006	H	6.62474	0.00673	1.28094
C	7.13932	2.54636	-2.26017	H	6.23731	-0.06461	3.03756
C	6.01054	4.67553	-2.43341	C	4.88447	-1.81557	-3.32407
H	3.98391	4.74850	-1.78845	H	4.56529	-0.75513	-3.38251
C	1.92612	6.17086	1.44525	C	6.25642	-1.95849	-3.97940
C	4.09740	5.31675	2.08249	H	6.22162	-1.53889	-5.00681
H	4.70162	3.46943	1.20112	H	7.02801	-1.41130	-3.40104
C	7.15240	3.89608	-2.61214	H	6.54631	-3.02835	-4.04699
H	8.02972	1.95120	-2.42567	C	-4.46314	4.20622	-4.21653
H	6.01802	5.71755	-2.72625	H	-4.39015	3.55808	-5.11650
C	3.10675	6.29420	2.17982	C	-4.65839	5.65794	-4.64483
H	1.16515	6.93655	1.53870	H	-4.73059	6.31479	-3.75164
H	5.00587	5.41020	2.66327	H	-3.81313	5.99587	-5.28096
H	8.04532	4.33529	-3.03793	H	-5.59762	5.74895	-5.23002
H	3.25083	7.14584	2.83195	C	0.53926	4.33590	-3.89005
C	-0.88524	3.80688	-1.80611	H	1.32417	3.64088	-3.53388
C	-0.78642	4.07967	-3.19826	C	0.99888	5.77793	-3.69498
C	-2.16587	3.64060	-1.21708	H	0.22667	6.48189	-4.07213
C	-1.95714	4.18144	-3.96556	H	1.19417	5.98965	-2.62468
C	-3.31480	3.76699	-2.01265	H	1.93977	5.94622	-4.26002
C	-3.21910	4.04805	-3.37902	C	-2.35071	3.33396	0.25371
H	-4.29258	3.65066	-1.55965	H	-1.40362	3.01901	0.73839
C	4.80957	-1.47837	-0.76415	C	-2.91559	4.54028	1.00076
C	4.86712	-2.03763	0.53919	H	-2.88314	4.35167	2.09162
C	4.89433	-2.33572	-1.89668	H	-2.31975	5.45141	0.79101
C	4.95997	-3.43043	0.69090	H	-3.96999	4.72114	0.70320
C	4.97391	-3.72425	-1.70631	C	3.84545	-1.71033	5.48173
C	5.00155	-4.27677	-0.42197	H	4.71181	-1.18337	5.02642
H	5.00678	-4.37943	-2.56894	C	3.94788	-1.56857	6.99807
C	-4.12488	-1.69257	-2.10045	H	4.93087	-1.95458	7.34100
C	-4.16271	-0.71914	-3.13052	H	3.86412	-0.49975	7.28972
C	-3.72989	-3.02228	-2.40674	H	3.14712	-2.14991	7.50196
C	-3.78301	-1.07674	-4.43342	C	-1.16407	-1.94955	5.26143
C	-3.40292	-3.35488	-3.72908	H	-1.92119	-1.94055	4.45141
C	-3.41087	-2.38956	-4.74024	C	-1.74416	-1.31225	6.52008
H	-3.13392	-4.37591	-3.96928	H	-1.00322	-1.35191	7.34689
C	0.10388	-0.07732	4.03410	H	-2.02593	-0.25646	6.33410
C	0.11162	-1.25206	4.83097	H	-2.65384	-1.86773	6.83102
C	1.33027	0.55729	3.71337	C	1.39407	1.83251	2.90325
C	1.33531	-1.77836	5.27236	H	0.44996	2.02633	2.35368
C	2.53458	0.01389	4.18581	C	1.69814	3.02661	3.80461
C	2.54507	-1.14683	4.96606	H	2.74369	2.97490	4.17533
H	3.46953	0.51112	3.95587	H	1.56799	3.96712	3.23642
H	4.98874	-3.86275	1.68430	H	1.00660	3.05237	4.67160
H	1.34601	-2.67768	5.87687	C	-4.64841	0.69165	-2.88688
H	-3.79966	-0.33386	-5.22244	H	-4.27777	1.07773	-1.91730
H	-1.88885	4.39762	-5.02539	C	-6.17160	0.76400	-2.92129
C	5.03649	-5.77177	-0.23461	H	-6.61429	0.12933	-2.12676
H	4.22282	-6.07570	0.45927	H	-6.49756	1.81163	-2.75357

H	-6.54899	0.42747	-3.91041
C	-3.61036	-4.10553	-1.34998
H	-3.64918	-3.69502	-0.32044
C	-4.70755	-5.15618	-1.49821
H	-4.60570	-5.91353	-0.69267
H	-5.70936	-4.68597	-1.41720
H	-4.62555	-5.67259	-2.47768
C	-3.01496	-2.75627	-6.14761
H	-2.25521	-2.03486	-6.51876
C	-4.22430	-2.75251	-7.07843
H	-3.90810	-3.05480	-8.09896
H	-4.98971	-3.47143	-6.71546
H	-4.67202	-1.73768	-7.13435
H	-0.96125	-3.02134	5.47708
H	3.92128	-2.78277	5.19986
H	4.52422	-1.78239	2.65600
H	4.15095	-2.38991	-3.92670
H	4.85817	-6.29372	-1.20010
H	-2.55182	-3.76688	-6.17515
H	-2.62088	-4.60027	-1.44298
H	-4.24775	1.36982	-3.66879
H	-5.36300	3.88582	-3.64849
H	0.44431	4.14753	-4.98186
H	-3.05356	2.48214	0.35771
H	2.18952	1.73725	2.13493
O	-1.15595	-2.24272	-0.34211
P	-1.21889	-0.85376	0.21495
H	0.80613	-2.71574	-0.53487
O	-2.55940	-0.07979	-0.30254
O	-1.42773	-1.08299	1.85031
N	-0.01541	0.16012	0.03404
C	1.44428	-3.39153	0.08089
P	1.12114	0.24419	-1.08035
C	0.82904	-4.66300	-0.28556
C	1.34056	-2.97883	1.56174
H	2.42635	-3.31734	-0.37366
O	1.16464	-0.75600	-2.18863
O	2.50495	0.17887	-0.18390
O	1.06828	1.70690	-1.81232
C	1.27774	-5.51377	-1.42387
O	-0.18043	-5.12551	0.34135
C	0.51311	-3.98690	2.35880
H	0.89676	-1.98375	1.62900
H	2.34398	-2.91082	1.98564
H	1.79676	-2.21384	-2.57445
C	0.22588	-5.58871	-2.55467
H	2.22139	-5.12720	-1.80205
H	1.42140	-6.51945	-1.00897
C	-0.67654	-4.45568	1.54990
H	0.13919	-3.54610	3.28171
H	1.11967	-4.85965	2.63302
O	2.02199	-3.14166	-2.82150
C	-0.09804	-4.24876	-3.21773
H	-0.68671	-6.04161	-2.15346
H	0.62494	-6.28204	-3.30417
H	-1.26118	-5.23158	2.04267
H	-1.30253	-3.63040	1.20458

C	1.11616	-3.55169	-3.82014
H	-0.81456	-4.44383	-4.02222
H	-0.57579	-3.56171	-2.50458
H	1.64604	-4.23880	-4.49624
H	0.78565	-2.69013	-4.41351

R-gau-B_{1,4}-B(-) 2nd step



E(RM062X) = -1694.56123066

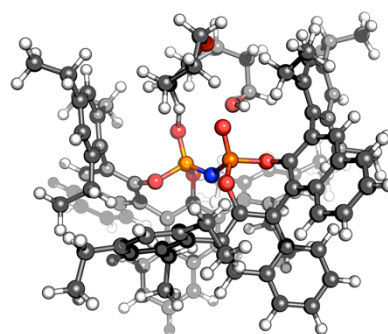
C	-2.24931	-1.85681	-1.99666
C	-1.67851	-3.11145	-2.26564
C	-3.57937	-1.77847	-1.52922
C	-2.35551	-4.28034	-1.90138
C	-4.23434	-2.95821	-1.08835
C	-3.61109	-4.21476	-1.28990
C	-4.28410	-0.46541	-1.59742
C	-5.48700	-0.29693	-2.33469
C	-3.71759	0.64087	-0.93107
C	-6.19901	0.92332	-2.23068
C	-4.41944	1.86293	-0.86786
C	-5.67591	1.97372	-1.47349
H	-6.22648	2.90274	-1.38868
H	-1.90654	-5.24371	-2.11178
C	-4.26628	-5.39452	-0.90224
C	-5.52358	-5.33566	-0.29929
H	-3.80469	-6.36160	-1.06299
H	-6.02219	-6.24815	0.00087
C	-6.13337	-4.10234	-0.07094
C	-5.49572	-2.92069	-0.45474
H	-7.10113	-4.06063	0.41186
H	-5.98868	-1.98237	-0.23778
C	-7.41674	1.08923	-2.90965
C	-7.91659	0.06757	-3.71716
H	-7.97404	2.01507	-2.82781
H	-8.85239	0.20366	-4.24370
C	-7.20180	-1.12039	-3.86380
C	-5.99400	-1.30316	-3.18688
H	-7.58274	-1.90218	-4.50819
H	-5.45863	-2.22851	-3.34993
C	3.47674	-0.58267	0.92211
C	0.86250	-1.30172	2.49609
C	3.30385	-1.36673	2.08368
C	4.78420	-0.18011	0.56090
C	-0.21077	-1.85359	3.22415

C	2.02005	-2.07478	2.30477	C	6.41915	2.64559	-4.24329
C	4.37349	-1.50920	3.00850	H	5.64705	2.55042	-5.03714
C	5.86583	-0.47349	1.40164	C	7.74541	2.08055	-4.74360
C	-0.21270	-3.22080	3.53595	H	7.63488	1.01064	-5.02037
C	1.98540	-3.47333	2.53675	H	8.07549	2.64568	-5.64050
C	5.66773	-1.08233	2.63869	H	8.52401	2.17667	-3.95658
C	4.18849	-2.06930	4.29330	C	4.64455	-1.52486	-2.10716
H	6.86796	-0.19770	1.09609	H	3.80266	-1.79954	-1.44579
C	0.85301	-4.04117	3.16294	C	5.82752	-2.44811	-1.83421
H	-1.03100	-3.63707	4.10991	H	6.66410	-2.21578	-2.52723
C	3.06439	-4.31394	2.18825	H	6.17797	-2.33652	-0.78737
C	6.75141	-1.27224	3.51143	H	5.51889	-3.50305	-1.99076
C	5.27191	-2.24214	5.15718	C	5.59591	2.69443	0.70233
H	3.20862	-2.36070	4.64695	H	5.01008	2.19754	1.50288
C	0.82922	-5.41243	3.46443	C	7.01727	2.94164	1.20390
C	3.02425	-5.67840	2.48405	H	6.97713	3.50081	2.16247
H	3.93496	-3.92469	1.67596	H	7.54838	1.98510	1.37845
C	6.55173	-1.85371	4.76376	H	7.59141	3.54613	0.47080
H	7.75023	-0.96039	3.22946	C	-4.58493	0.94551	5.81245
H	5.11737	-2.67690	6.13634	H	-4.37949	2.03473	5.89439
C	1.91283	-6.22516	3.12626	C	-4.78740	0.35421	7.20503
H	-0.02669	-5.85490	3.96017	H	-4.99046	-0.73579	7.13290
H	3.85690	-6.31414	2.21229	H	-3.88807	0.51819	7.83559
H	7.38901	-1.99229	5.43553	H	-5.65442	0.84566	7.69452
H	1.88766	-7.28254	3.35575	C	0.32828	0.00510	5.50079
C	-1.30071	-1.01421	3.77618	H	1.10674	0.10314	4.72048
C	-1.05204	-0.17058	4.89464	C	0.67747	-1.14808	6.43779
C	-2.63302	-1.18938	3.31750	H	-0.08542	-1.23576	7.24052
C	-2.12797	0.47519	5.52299	H	0.73519	-2.10606	5.88366
C	-3.68579	-0.55252	3.99167	H	1.66627	-0.95839	6.90600
C	-3.44295	0.27100	5.09520	C	-2.97328	-2.05203	2.11965
H	-4.70342	-0.69707	3.64829	H	-2.07034	-2.34280	1.54354
C	5.07681	0.57550	-0.68195	C	-3.72172	-3.31553	2.54235
C	5.03697	-0.07164	-1.94609	H	-3.75442	-4.03017	1.69672
C	5.57877	1.90482	-0.59493	H	-3.21603	-3.81501	3.39287
C	5.45789	0.62283	-3.09127	H	-4.76248	-3.06700	2.83895
C	6.02624	2.55147	-1.75646	C	3.39358	-3.72633	-5.04173
C	5.95920	1.92453	-3.00288	H	4.22597	-3.88692	-4.32275
H	6.40180	3.56600	-1.69113	C	3.33403	-4.93148	-5.97642
C	-3.82435	3.06757	-0.23482	H	4.32069	-5.06952	-6.46666
C	-3.72300	3.15981	1.17719	H	3.09059	-5.85067	-5.40175
C	-3.40198	4.16484	-1.03723	H	2.56790	-4.77874	-6.76562
C	-3.14922	4.30050	1.75829	C	-1.50096	-2.62407	-5.20145
C	-2.83627	5.29282	-0.42008	H	-2.15424	-1.89821	-4.67805
C	-2.70853	5.36720	0.97052	C	-2.30450	-3.86676	-5.57258
H	-2.50295	6.12417	-1.03029	H	-1.66459	-4.58656	-6.12623
C	-0.37362	-3.21553	-2.96319	H	-2.70874	-4.36070	-4.66605
C	-0.29014	-2.98346	-4.36250	H	-3.15696	-3.57639	-6.22206
C	0.79134	-3.59242	-2.24791	C	0.78097	-3.84273	-0.75660
C	0.94406	-3.13363	-5.01404	H	-0.12699	-3.43244	-0.26799
C	2.00422	-3.75306	-2.93479	C	0.87209	-5.33755	-0.46044
C	2.08679	-3.53381	-4.31349	H	1.88476	-5.71992	-0.70844
H	2.88886	-4.05870	-2.38865	H	0.67588	-5.51758	0.61366
H	5.42705	0.13508	-4.05875	H	0.11778	-5.90266	-1.04554
H	1.01276	-2.96127	-6.08175	C	-4.28954	2.10235	2.09616
H	-3.06886	4.37346	2.83681	H	-4.05862	1.08641	1.72407
H	-1.94590	1.11545	6.37828	C	-5.79836	2.26144	2.25584

H	-6.31226	2.16019	1.27852
H	-6.18544	1.47412	2.93513
H	-6.03439	3.25565	2.69151
C	-3.54444	4.18125	-2.54997
H	-3.74566	3.17314	-2.96476
C	-4.65447	5.13321	-2.99072
H	-4.76487	5.08884	-4.09461
H	-5.62176	4.85233	-2.52706
H	-4.40749	6.17738	-2.70415
C	-2.12770	6.59573	1.62280
H	-1.35343	6.29248	2.35996
C	-3.20979	7.40694	2.32993
H	-2.75872	8.31872	2.77501
H	-3.99394	7.71458	1.60552
H	-3.67586	6.81175	3.14371
H	-1.18226	-2.12259	-6.14138
H	3.63010	-2.81100	-5.62610
H	4.28734	-1.70480	-3.14267
H	5.11476	3.67964	0.53134
H	6.55168	3.73087	-4.04035
H	-1.63474	7.24648	0.86784
H	-2.59672	4.51721	-3.01753
H	-3.82346	2.18457	3.10028
H	-5.53204	0.82832	5.24329
H	0.37207	0.94992	6.08551
H	-3.61062	-1.46815	1.42312
H	1.64476	-3.31910	-0.29575
O	-0.97279	1.64189	-1.95847
P	-1.20621	0.37026	-1.21800
H	3.38312	3.35237	-1.22823
O	-2.53202	0.48758	-0.25543
O	-1.57752	-0.72488	-2.38350
N	-0.08825	-0.26053	-0.27226
C	3.09504	3.90152	-2.13265
P	1.07284	0.39411	0.57872
C	2.33615	5.03310	-1.54571
C	2.34374	2.96478	-3.10405
H	4.01488	4.32159	-2.55128
O	1.29444	1.88162	0.53642
O	2.43019	-0.38174	0.04878
O	0.87013	0.03457	2.17118
C	3.03376	6.20850	-0.95813
O	1.07812	5.06872	-1.54764
C	0.89128	3.39807	-3.28959
H	2.35362	1.95493	-2.68430
H	2.87108	2.93010	-4.06053
H	2.08526	3.25369	0.84624
C	2.19308	7.01748	0.04336
H	3.94902	5.81773	-0.50256
H	3.35067	6.84456	-1.79794
C	0.35487	3.83042	-1.94671
H	0.27307	2.56796	-3.63254
H	0.80373	4.22898	-4.00151
O	2.59135	4.10528	0.75471
C	1.44659	6.20420	1.11467
H	1.46587	7.62287	-0.50773
H	2.87986	7.72062	0.52707

H	-0.68284	4.12445	-1.93800
H	0.54643	3.11064	-1.14620
C	2.25205	5.06587	1.73508
H	1.13361	6.89544	1.90543
H	0.53624	5.77531	0.68737
H	3.18377	5.45291	2.17288
H	1.67329	4.60344	2.54274

R-gau-B_{1,4}-C(+)



E(RM062X) = -5098.3754069

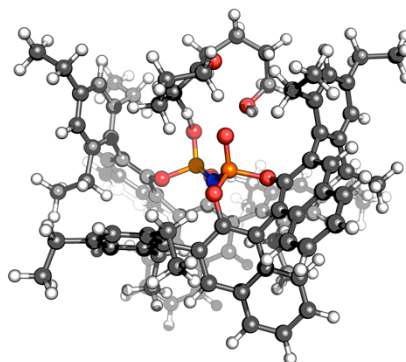
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C	-1.64325	0.24680	2.74674
C	-0.76414	0.89555	3.63181
C	-2.96622	0.71570	2.61486
C	-1.14623	2.10092	4.23509
C	-3.32656	1.97388	3.16149
C	-2.40050	2.66224	3.98083
C	-3.97073	-0.18818	1.99556
C	-5.11839	-0.62347	2.71180
C	-3.74470	-0.65329	0.68222
C	-6.11991	-1.35749	2.03369
C	-4.73647	-1.42250	0.03549
C	-5.93303	-1.71845	0.69919
H	-6.70272	-2.27920	0.18158
H	-0.46941	2.58961	4.92506
C	-2.75646	3.88651	4.56892
C	-4.01850	4.43668	4.33946
H	-2.05924	4.41681	5.20677
H	-4.28681	5.38162	4.79383
C	-4.93141	3.77562	3.51778
C	-4.59035	2.55764	2.92548
H	-5.90379	4.21267	3.33120
H	-5.31442	2.08659	2.27388
C	-7.28666	-1.75061	2.70900
C	-7.45179	-1.44992	4.06106
H	-8.06358	-2.30428	2.19495
H	-8.35004	-1.76116	4.57852
C	-6.45125	-0.76838	4.75216
C	-5.29005	-0.36354	4.09047
H	-6.57324	-0.55625	5.80656
H	-4.52781	0.13720	4.67153

N	-0.06586	0.09491	0.07004	C	0.61219	-0.83196	4.84047
P	1.04914	0.03598	-1.06444	C	1.75087	0.94487	3.58609
O	1.15150	-1.14993	-1.96518	C	1.86284	-1.30201	5.26906
O	2.47990	0.22531	-0.24718	C	2.97948	0.47208	4.07166
O	0.83811	1.35203	-2.03042	C	3.04316	-0.63980	4.91825
C	3.52382	0.74369	-0.98173	H	3.89068	0.98932	3.80010
C	1.05160	2.57893	-1.44735	H	6.24227	-2.67339	2.30588
C	3.47074	2.07676	-1.43241	H	1.91730	-2.16604	5.92084
C	4.70775	0.00113	-1.18029	H	-4.55458	-1.22003	-4.62877
C	0.05184	3.56907	-1.48342	H	-2.32091	3.52643	-5.50068
C	2.33777	2.92647	-1.00201	C	6.28681	-5.09335	1.08638
C	4.48329	2.57985	-2.29073	H	5.79796	-5.25997	2.07063
C	5.74331	0.52853	-1.96133	C	7.80318	-5.11656	1.25586
C	0.26953	4.79957	-0.84608	H	8.12901	-4.33134	1.97054
C	2.54310	4.13745	-0.29842	H	8.11744	-6.10544	1.65115
C	5.62938	1.79115	-2.54350	H	8.30099	-4.95032	0.27652
C	4.37704	3.84040	-2.92037	C	5.58394	-0.15902	1.64373
H	6.64732	-0.05215	-2.10975	H	4.80704	0.59882	1.41578
C	1.48637	5.07313	-0.21549	C	6.96839	0.46238	1.49225
H	-0.49814	5.56214	-0.87960	H	7.75370	-0.27418	1.76609
C	3.77879	4.44670	0.30824	H	7.13364	0.80136	0.44926
C	6.65621	2.28161	-3.36605	H	7.05507	1.34070	2.16595
C	5.40168	4.31253	-3.74339	C	4.34509	-2.50172	-2.75025
H	3.50014	4.46172	-2.79858	H	3.78558	-1.57267	-2.98499
C	1.68158	6.29590	0.44597	C	5.45862	-2.67925	-3.77852
C	3.95772	5.66439	0.96863	H	5.02251	-2.67340	-4.79962
H	4.60391	3.74618	0.28942	H	6.19255	-1.85062	-3.70316
C	6.54115	3.53873	-3.96013	H	5.98256	-3.64629	-3.62557
H	7.54417	1.68979	-3.55476	C	-4.86628	3.54342	-4.56639
H	5.30952	5.28104	-4.21785	H	-4.66385	3.40871	-5.65132
C	2.91312	6.58716	1.03566	C	-5.54815	4.89394	-4.36683
H	0.88311	7.02604	0.50500	H	-5.83720	5.03254	-3.30345
H	4.90828	5.89128	1.43371	H	-4.86667	5.71660	-4.67215
H	7.33335	3.91020	-4.59725	H	-6.46571	4.94214	-4.99024
H	3.05743	7.52970	1.54765	C	0.14818	3.57013	-4.47132
C	-1.19310	3.39389	-2.27076	H	0.93103	2.90204	-4.06464
C	-1.14934	3.44850	-3.69242	C	0.65564	5.00934	-4.49533
C	-2.45078	3.34254	-1.61381	H	-0.11823	5.68273	-4.92151
C	-2.35029	3.46259	-4.41921	H	0.91909	5.35489	-3.47607
C	-3.62970	3.38330	-2.37380	H	1.56670	5.06966	-5.12727
C	-3.58792	3.45718	-3.76976	C	-2.57706	3.25879	-0.10664
H	-4.59039	3.35887	-1.87302	H	-1.60753	3.02680	0.38121
C	4.93582	-1.31818	-0.55087	C	-3.12721	4.56090	0.47378
C	5.43498	-1.38651	0.77445	H	-2.96949	4.57632	1.57017
C	4.88630	-2.49603	-1.33791	H	-2.61133	5.44206	0.04205
C	5.86275	-2.61887	1.29197	H	-4.21500	4.64558	0.26719
C	5.33763	-3.70955	-0.79694	C	4.36738	-1.11727	5.46219
C	5.82481	-3.77892	0.51197	H	5.20965	-0.55953	5.00154
H	5.30079	-4.60893	-1.40060	C	4.45063	-0.92046	6.97418
C	-4.52219	-2.02288	-1.30376	H	5.45276	-1.23495	7.33444
C	-4.59756	-1.22390	-2.47278	H	4.30087	0.15027	7.23041
C	-4.37099	-3.43182	-1.42967	H	3.68390	-1.53239	7.49422
C	-4.48803	-1.82909	-3.73479	C	-0.62621	-1.52577	5.37713
C	-4.28853	-4.00491	-2.70843	H	-1.39499	-1.65162	4.59102
C	-4.34536	-3.21430	-3.85957	C	-1.21828	-0.76950	6.56321
H	-4.15725	-5.07614	-2.80812	H	-0.45737	-0.65473	7.36446
C	0.54845	0.30543	3.98887	H	-1.57769	0.23265	6.25490

H	-2.08080	-1.33742	6.97110
C	1.76662	2.13159	2.64260
H	0.78521	2.28620	2.14821
C	2.16266	3.41475	3.37025
H	3.23730	3.38684	3.64814
H	1.99138	4.28605	2.70754
H	1.55598	3.55454	4.28763
C	-4.87962	0.25925	-2.41682
H	-4.34715	0.73718	-1.57335
C	-6.37620	0.52969	-2.29455
H	-6.78419	0.07210	-1.37004
H	-6.55495	1.62421	-2.24950
H	-6.91342	0.11641	-3.17460
C	-4.25078	-4.35562	-0.22907
H	-4.08409	-3.79763	0.71480
C	-5.48913	-5.23530	-0.07164
H	-5.37809	-5.87237	0.83097
H	-6.40002	-4.61393	0.04565
H	-5.61313	-5.89696	-0.95469
C	-4.25901	-3.85506	-5.22141
H	-4.10104	-3.08595	-6.00863
C	-5.53500	-4.62684	-5.54582
H	-5.45581	-5.06464	-6.56313
H	-5.68858	-5.45169	-4.81797
H	-6.41256	-3.94596	-5.51854
H	-0.37395	-2.55435	5.71619
H	4.50225	-2.19273	5.21642
H	5.44301	-0.44420	2.70401
H	3.62652	-3.33877	-2.84825
H	5.99271	-5.93685	0.42417
H	-3.38956	-4.54630	-5.25437
H	-3.36475	-5.01349	-0.35332
H	-4.50277	0.74774	-3.33952
H	-5.55825	2.73222	-4.25936
H	-0.00421	3.24233	-5.52294
H	-3.26269	2.42578	0.15561
H	2.49629	1.93920	1.82836
O	-1.20078	-2.35986	0.10659
H	-0.72379	-2.91325	-1.06410
C	-0.77343	-3.74442	-2.04260
C	0.16824	-4.66879	-1.56814
C	-0.65402	-3.15195	-3.43372
H	-1.77008	-4.01586	-1.70968
C	0.01219	-5.30821	-0.22250
O	1.21995	-5.03687	-2.24627
C	0.76618	-3.33558	-3.96474
H	-1.37155	-3.63510	-4.10688
H	-0.89309	-2.08603	-3.39379
C	1.25013	-5.99774	0.36159
H	-0.78923	-6.05234	-0.33790
H	-0.37632	-4.53170	0.44494
C	1.23751	-4.74389	-3.67504
H	1.41905	-2.60667	-3.48195
H	0.80677	-3.17112	-5.04637
C	2.49280	-5.11389	0.52301
H	0.95223	-6.38316	1.34383
H	1.50854	-6.86910	-0.25006

H	2.26734	-4.93268	-3.97632
H	0.58885	-5.49465	-4.14167
C	2.19419	-3.72682	1.08621
H	2.96748	-4.99123	-0.45491
H	3.20979	-5.63213	1.17090
O	1.48513	-2.94161	0.15233
H	1.54758	-3.80484	1.97049
H	3.11301	-3.22591	1.40903
H	2.05244	-2.47022	-0.47278

R-gau-B_{1,4}-B(+)



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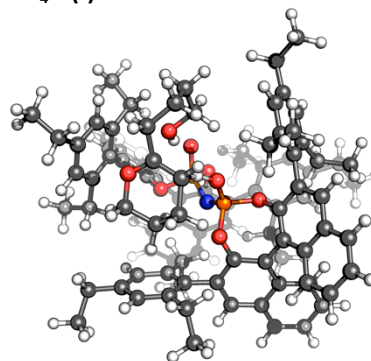
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C	0.64957	-2.10610	3.15232
C	2.86570	-1.61534	2.28601
C	1.01590	-3.44990	3.30960
C	3.20852	-2.98881	2.36664
C	2.26675	-3.90578	2.88792
C	3.89237	-0.56980	2.05332
C	5.01395	-0.43314	2.91475
C	3.72490	0.31457	0.96693
C	6.05382	0.45657	2.55977
C	4.76558	1.21404	0.64168
C	5.93407	1.24029	1.41278
H	6.73798	1.91361	1.13690
H	0.32917	-4.13733	3.78787
C	2.60452	-5.26215	3.02059
C	3.86428	-5.71508	2.62553
H	1.89463	-5.97122	3.42980
H	4.11847	-6.76217	2.72723
C	4.79344	-4.82199	2.09191
C	4.47124	-3.46973	1.95684
H	5.76459	-5.17948	1.77501
H	5.20840	-2.81031	1.51780
C	7.19493	0.56910	3.37042
C	7.29677	-0.17193	4.54786
H	8.00143	1.24073	3.10047
H	8.17555	-0.07670	5.17250
C	6.25896	-1.02012	4.93112
C	5.12288	-1.14818	4.12917
H	6.33247	-1.57809	5.85572

H	4.33010	-1.79602	4.47777	C	-0.66142	-1.66946	3.68941
N	0.04446	-0.06190	0.04709	C	-0.72422	-0.91409	4.89298
P	-1.12123	0.38192	-0.93663	C	-1.86301	-2.14451	3.09965
O	-1.25313	1.80969	-1.36561	C	-1.97255	-0.65854	5.48128
O	-2.52727	-0.07877	-0.20839	C	-3.08777	-1.90501	3.74053
O	-0.94795	-0.51109	-2.31020	C	-3.14984	-1.17584	4.93238
C	-3.59521	-0.26983	-1.05838	H	-3.99935	-2.30210	3.31071
C	-1.17851	-1.86260	-2.19070	H	-5.93232	2.13688	3.24241
C	-3.59010	-1.36416	-1.94586	H	-2.02631	-0.08919	6.40182
C	-4.75188	0.53776	-0.96963	H	5.08814	2.48413	-3.83436
C	-0.19183	-2.79211	-2.57292	H	2.27244	-1.43979	-6.29434
C	-2.46824	-2.32809	-1.87664	C	-6.10039	4.79147	2.73029
C	-4.63598	-1.52042	-2.89273	H	-5.50998	4.70864	3.66840
C	-5.83056	0.31037	-1.83417	C	-7.59018	4.71621	3.05267
C	-0.43261	-4.16527	-2.41774	H	-7.83281	3.75954	3.56194
C	-2.69030	-3.70741	-1.64533	H	-7.86684	5.55402	3.72676
C	-5.76992	-0.68056	-2.81354	H	-8.18878	4.79717	2.12013
C	-4.57658	-2.48103	-3.92763	C	-5.34441	-0.08794	1.87060
H	-6.72199	0.92116	-1.74505	H	-4.56722	-0.72782	1.40905
C	-1.65209	-4.62718	-1.91707	C	-6.72110	-0.69698	1.62791
H	0.32250	-4.87788	-2.72461	H	-7.50576	-0.08500	2.12174
C	-3.92567	-4.19443	-1.16735	H	-6.93557	-0.75919	0.54133
C	-6.83314	-0.84284	-3.71635	H	-6.75094	-1.72272	2.05207
C	-5.63653	-2.62559	-4.82524	C	-4.49997	3.38796	-1.81736
H	-3.70967	-3.11337	-4.06391	H	-3.98932	2.56147	-2.35358
C	-1.86629	-6.00271	-1.73480	C	-5.68887	3.85719	-2.65280
C	-4.12366	-5.56483	-0.98433	H	-5.33890	4.13300	-3.66982
H	-4.73627	-3.52144	-0.91904	H	-6.44404	3.05095	-2.74771
C	-6.76521	-1.81451	-4.71517	H	-6.16444	4.74866	-2.19249
H	-7.71171	-0.21132	-3.65574	C	4.79183	-1.90172	-5.40039
H	-5.58026	-3.36726	-5.61162	H	4.62560	-1.38784	-6.37221
C	-3.09822	-6.46673	-1.27008	C	5.39279	-3.27685	-5.67721
H	-1.08179	-6.71793	-1.95196	H	5.64300	-3.79244	-4.72575
H	-5.07409	-5.92806	-0.61541	H	4.67636	-3.89965	-6.25452
H	-7.58473	-1.93148	-5.41245	H	6.32390	-3.16247	-6.27122
H	-3.25706	-7.52774	-1.12739	C	-0.22062	-1.72953	-5.36717
C	1.07217	-2.37460	-3.22747	H	-0.99579	-1.22695	-4.75798
C	1.06107	-1.93354	-4.58033	C	-0.76242	-3.04973	-5.90851
C	2.31518	-2.59759	-2.57755	H	0.00495	-3.55253	-6.53488
C	2.27816	-1.74840	-5.25547	H	-1.05947	-3.72559	-5.08206
C	3.50983	-2.42479	-3.29278	H	-1.65865	-2.85306	-6.53382
C	3.49905	-2.02059	-4.63139	C	2.40823	-3.03605	-1.13025
H	4.45861	-2.61447	-2.80470	H	1.43342	-2.95381	-0.60593
C	-4.89919	1.63099	0.01982	C	2.91412	-4.47366	-1.01777
C	-5.27053	1.32951	1.35461	H	2.74502	-4.84884	0.01075
C	-4.91953	2.98170	-0.41916	H	2.37743	-5.14379	-1.71873
C	-5.64903	2.36622	2.22154	H	4.00122	-4.51875	-1.23963
C	-5.32558	3.99142	0.46726	C	-4.47085	-0.95300	5.62706
C	-5.69302	3.69274	1.78241	H	-5.31426	-1.31069	4.99762
H	-5.34478	5.02125	0.13048	C	-4.52981	-1.69693	6.95895
C	4.65390	2.20542	-0.45391	H	-5.52801	-1.54915	7.42230
C	4.85270	1.81112	-1.80036	H	-4.37000	-2.78460	6.79805
C	4.54462	3.58790	-0.14107	H	-3.75815	-1.31264	7.65882
C	4.92892	2.78733	-2.80601	C	0.51439	-0.43160	5.62478
C	4.63121	4.53813	-1.17099	H	1.27091	-0.03107	4.92341
C	4.82253	4.14750	-2.49945	C	1.13058	-1.54233	6.47085
H	4.52023	5.59096	-0.93910	H	0.38186	-1.93857	7.18955

H	1.49727	-2.37031	5.83169
H	1.99213	-1.13744	7.04240
C	-1.88039	-2.91184	1.79213
H	-0.90190	-2.87044	1.27004
C	-2.26540	-4.37418	2.00914
H	-3.34156	-4.45695	2.26965
H	-2.08141	-4.94895	1.08004
H	-1.66219	-4.82901	2.82030
C	5.05618	0.36884	-2.19618
H	4.50093	-0.31962	-1.53135
C	6.53545	-0.00050	-2.17983
H	6.95668	0.13287	-1.16119
H	6.65630	-1.06378	-2.47567
H	7.09909	0.63453	-2.89607
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H	3.99459	3.26501	1.95619
C	5.48499	4.82078	1.84382
H	5.25846	5.15037	2.87960
H	6.37016	4.15313	1.87239
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H	4.83358	4.70378	-4.59354
C	6.16318	6.00473	-3.50681
H	6.19106	6.73787	-4.34022
H	6.20945	6.56102	-2.54666
H	7.04931	5.33946	-3.58815
H	0.25584	0.41323	6.30007
H	-4.61943	0.13494	5.79913
H	-5.14545	-0.08970	2.96020
H	-3.76845	4.21867	-1.74494
H	-5.88492	5.79009	2.29132
H	3.99878	5.85786	-3.50801
H	3.40977	4.78399	1.25150
H	4.65047	0.21017	-3.21601
H	5.52038	-1.29195	-4.82687
H	-0.03569	-1.05301	-6.23016
H	3.10806	-2.36344	-0.59175
H	-2.61686	-2.44339	1.10641
O	1.22678	2.17832	0.96117
H	0.98397	2.95169	-0.11866
C	1.09916	3.85012	-1.04850
C	0.06494	4.71583	-0.66390
C	1.13447	3.32072	-2.47370
H	2.03315	4.21358	-0.63223
C	0.14989	5.45329	0.64013
O	-0.99101	4.95034	-1.38041
C	0.28078	4.22818	-3.36012
H	2.16157	3.29799	-2.83845
H	0.74116	2.30260	-2.50788
C	-1.11109	6.17552	1.12230
H	0.96080	6.18554	0.52494
H	0.49732	4.71681	1.37372
C	-1.08714	4.40296	-2.73265
H	0.14188	3.79857	-4.35671
H	0.76368	5.20648	-3.48123
C	-2.35605	5.29987	1.30541
H	-0.85272	6.63659	2.08311

H	-1.34635	6.99748	0.43706
H	-1.59143	3.44136	-2.63675
H	-1.70918	5.12885	-3.25810
C	-2.07222	3.94800	1.95361
H	-2.81158	5.12220	0.32748
H	-3.08946	5.85055	1.90647
O	-1.35388	3.09249	1.09699
H	-1.43934	4.07877	2.84127
H	-2.99996	3.47616	2.29677
H	-1.86035	2.80189	0.32169

S-anti-C₄-C(-)



E(RM062X) = -5098.39020660

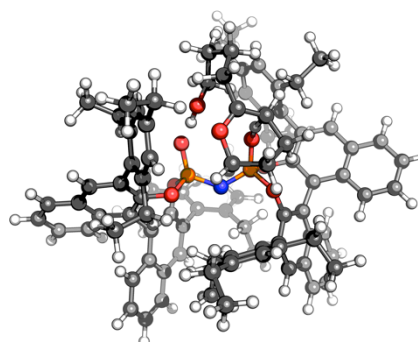
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C	-2.07208	-0.14440	2.52963
C	-1.42276	0.49142	3.60465
C	-3.41210	0.18455	2.22825
C	-2.05594	1.53643	4.28497
C	-4.01556	1.30515	2.85582
C	-3.33090	1.96485	3.90611
C	-4.16461	-0.68698	1.28090
C	-5.36126	-1.35288	1.65665
C	-3.65160	-0.86457	-0.01932
C	-6.10579	-2.05083	0.67240
C	-4.39825	-1.56189	-0.98579
C	-5.63121	-2.12550	-0.64054
H	-6.20396	-2.65349	-1.39395
H	-1.54795	2.01758	5.11300
C	-3.93383	3.04615	4.56856
C	-5.19284	3.49955	4.17289
H	-3.42496	3.54970	5.38197
H	-5.64855	4.33992	4.68029
C	-5.85807	2.88206	3.11414
C	-5.27779	1.79540	2.45652
H	-6.82692	3.24799	2.79972
H	-5.81601	1.35552	1.62749
C	-7.31025	-2.68375	1.01857
C	-7.76805	-2.65256	2.33608
H	-7.89160	-3.21236	0.27227
H	-8.69472	-3.14669	2.59806
C	-7.02511	-2.00059	3.31948
C	-5.82853	-1.36065	2.98930

H	-7.37531	-1.99434	4.34365	H	-2.42833	-4.22253	-4.27390
H	-5.27061	-0.88834	3.78638	C	-0.07969	0.05805	4.05640
N	0.00794	0.12517	0.15077	C	0.04899	-1.04339	4.94019
P	1.13742	0.31698	-0.96587	C	1.07428	0.79701	3.68993
O	1.27275	-0.67395	-2.06933	C	1.31830	-1.39551	5.42553
O	2.48257	0.38584	-0.03393	C	2.33067	0.40843	4.17928
O	0.95855	1.76629	-1.70888	C	2.45936	-0.67816	5.05035
C	3.57958	0.93012	-0.64896	H	3.21100	0.97379	3.89596
C	1.19841	2.89931	-0.96958	H	5.46079	-3.48047	1.91087
C	3.61988	2.31437	-0.89609	H	1.41920	-2.23856	6.09899
C	4.70308	0.13147	-0.92994	H	-3.13687	-0.11082	-5.24404
C	0.22600	3.91474	-0.92441	H	-1.97250	4.58617	-4.97867
C	2.47965	3.15200	-0.43607	C	5.34992	-5.53513	0.13824
C	4.72382	2.87151	-1.59406	H	5.39648	-5.73498	1.23103
C	5.83019	0.70170	-1.53133	C	6.65696	-6.00231	-0.49557
C	0.44336	5.05434	-0.14014	H	7.50975	-5.41438	-0.09370
C	2.67244	4.25918	0.42663	H	6.82151	-7.07472	-0.25953
C	5.84163	2.05245	-1.88934	H	6.61940	-5.88610	-1.59951
C	4.73718	4.21574	-2.02818	C	5.12601	-0.82438	1.85634
H	6.69449	0.08041	-1.73795	H	4.44704	0.04504	1.75150
C	1.63871	5.21600	0.56583	C	6.56060	-0.33442	2.01768
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C	3.86862	4.43768	1.15262	H	6.88227	0.23117	1.11862
C	6.95609	2.59323	-2.55023	H	6.62529	0.33691	2.89975
C	5.84977	4.73752	-2.69156	C	4.27544	-1.85919	-3.11026
H	3.88769	4.86784	-1.87726	H	3.90890	-0.81387	-3.17146
C	1.82827	6.34029	1.38499	C	5.48989	-2.00647	-4.02311
C	4.03645	5.55151	1.97818	H	5.22157	-1.68474	-5.05134
H	4.67045	3.71248	1.09973	H	6.32665	-1.37361	-3.66186
C	6.95913	3.93157	-2.94426	H	5.82387	-3.06487	-4.06165
H	7.82022	1.97788	-2.77152	C	-4.55743	4.37732	-4.17676
H	5.84924	5.77038	-3.01534	H	-4.30612	4.46290	-5.25642
C	3.02201	6.50268	2.08985	C	-5.28785	5.64700	-3.74866
H	1.04954	7.08660	1.48839	H	-5.62343	5.56790	-2.69286
H	4.95696	5.67753	2.53333	H	-4.62016	6.52850	-3.85624
H	7.81876	4.34167	-3.45841	H	-6.18070	5.79636	-4.39161
H	3.15936	7.36601	2.72793	C	0.44909	4.43926	-3.84854
C	-0.98292	3.86637	-1.78285	H	1.24026	3.76454	-3.46706
C	-0.88023	4.18057	-3.16568	C	0.88623	5.89152	-3.68214
C	-2.26354	3.65806	-1.20912	H	0.11396	6.57536	-4.09442
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C	-3.41058	3.81239	-2.00306	H	1.83735	6.05700	-4.23065
C	-3.31190	4.16382	-3.35343	C	-2.44776	3.27495	0.24227
H	-4.39033	3.66044	-1.56490	H	-1.49549	2.95215	0.70655
C	4.72067	-1.31964	-0.63191	C	-3.02259	4.43653	1.04886
C	5.00037	-1.77159	0.68288	H	-3.01197	4.18264	2.12658
C	4.60306	-2.26426	-1.68609	H	-2.41559	5.35360	0.90494
C	5.21113	-3.13939	0.91278	H	-4.07021	4.64099	0.74270
C	4.78549	-3.62902	-1.41302	C	3.81282	-1.07217	5.58586
C	5.11221	-4.06972	-0.12632	H	4.61949	-0.50187	5.07614
H	4.68359	-4.35393	-2.21228	C	3.91543	-0.80253	7.08476
C	-3.85360	-1.78356	-2.34694	H	4.93442	-1.06439	7.43970
C	-3.78836	-0.71489	-3.27794	H	3.73126	0.27292	7.29436
C	-3.37886	-3.06760	-2.72289	H	3.17962	-1.41660	7.64564
C	-3.19774	-0.92727	-4.53405	C	-1.14421	-1.85583	5.39933
C	-2.81361	-3.24903	-3.99390	H	-1.92327	-1.91222	4.61186
C	-2.70570	-2.18588	-4.89485	C	-1.74534	-1.27128	6.67312

H	-0.98760	-1.25857	7.48542
H	-2.10706	-0.23756	6.49565
H	-2.60463	-1.89478	6.99803
C	1.00195	2.03036	2.81908
H	0.04958	2.08286	2.25701
C	1.14929	3.29452	3.66143
H	2.18381	3.37705	4.05691
H	0.93281	4.18515	3.04059
H	0.43419	3.28606	4.50986
C	-4.37093	0.64935	-2.97839
H	-4.08536	0.98948	-1.96371
C	-5.89111	0.64453	-3.11277
H	-6.35049	-0.07995	-2.41095
H	-6.28902	1.65317	-2.87615
H	-6.18198	0.37982	-4.15161
C	-3.41486	-4.25977	-1.78818
H	-3.59241	-3.96882	-0.73314
C	-4.47967	-5.26659	-2.21381
H	-4.49424	-6.11525	-1.49802
H	-5.48276	-4.79250	-2.22221
H	-4.25704	-5.66409	-3.22667
C	-2.05347	-2.39736	-6.23722
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C	-2.92515	-3.26153	-7.14423
H	-2.43467	-3.37255	-8.13415
H	-3.06529	-4.27218	-6.70559
H	-3.91775	-2.78426	-7.29031
H	-0.83586	-2.90530	5.59927
H	3.98938	-2.15128	5.38649
H	4.81684	-1.34285	2.78856
H	3.45510	-2.50082	-3.49700
H	4.50726	-6.13227	-0.26867
H	-1.06480	-2.88539	-6.09462
H	-2.42841	-4.75884	-1.80314
H	-3.96335	1.40129	-3.68601
H	-5.23556	3.50642	-4.06559
H	0.36721	4.22065	-4.93577
H	-3.13689	2.40668	0.30414
H	1.81273	1.99469	2.06309
O	-0.98231	-2.34326	-0.28834
C	1.06811	-5.01853	0.13048
C	2.02263	-4.16631	2.16516
C	1.44763	-5.89955	-1.02271
C	0.73118	-3.42639	2.41824
H	2.88983	-3.52007	2.28623
H	2.12915	-5.03098	2.82913
C	0.49999	-6.02421	-2.21843
H	2.43582	-5.57632	-1.35599
H	1.57357	-6.88376	-0.54488
C	-0.45571	-4.27347	1.97657
H	0.73872	-2.46672	1.89209
H	0.67888	-3.22026	3.48671
C	0.70940	-4.95711	-3.29523
H	-0.54185	-6.03341	-1.88456
H	0.67282	-7.00813	-2.66779
H	-0.55627	-5.15332	2.62530
H	-1.37657	-3.69000	2.05856

C	0.52790	-3.53557	-2.79786
H	1.72483	-5.05471	-3.70054
H	0.01073	-5.14188	-4.11952
O	1.48917	-3.28177	-1.79215
H	0.64864	-2.82430	-3.62449
H	-0.48196	-3.39209	-2.38930
H	1.53043	-2.30281	-1.72127
O	2.12981	-4.69237	0.82040
C	-0.23454	-4.68294	0.52677
H	-0.45339	-3.48168	-0.01973
H	-1.00759	-5.28937	0.06082

RSanti-C₄-B(-)



E(RM062X) = -5098.39663607

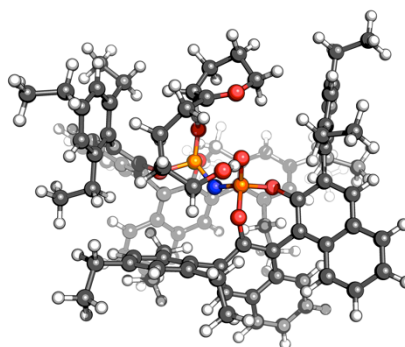
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C	-1.19819	0.22936	3.64601
C	-3.26533	0.13950	2.35906
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C	-3.78183	1.22275	3.11583
C	-3.00967	1.75970	4.17537
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C	-5.30171	-1.28314	1.79965
C	-3.68654	-0.71380	0.05581
C	-6.12772	-1.88533	0.81744
C	-4.51055	-1.32426	-0.90737
C	-5.73658	-1.87807	-0.52457
H	-6.37218	-2.33239	-1.27559
H	-1.16992	1.61866	5.28623
C	-3.52470	2.80222	4.96232
C	-4.78269	3.33812	4.68341
H	-2.94883	3.21119	5.78406
H	-5.17067	4.14840	5.28695
C	-5.53478	2.84147	3.61906
C	-5.04222	1.79405	2.83772
H	-6.50298	3.27104	3.39669
H	-5.64626	1.44799	2.00946
C	-7.32890	-2.50767	1.19311
C	-7.70337	-2.56156	2.53591
H	-7.97222	-2.96273	0.44919
H	-8.62808	-3.04702	2.82009
C	-6.87958	-2.00685	3.51447

C	-5.68517	-1.37847	3.15566	C	-3.19303	-1.73785	-4.98669
H	-7.16520	-2.06741	4.55677	H	-2.87590	-3.80830	-4.50470
H	-5.06375	-0.98422	3.94808	C	0.12356	-0.33570	4.00453
N	-0.00459	0.18897	0.07829	C	0.19841	-1.54116	4.74895
P	1.12382	0.40754	-1.03473	C	1.31571	0.36274	3.68452
O	1.17865	-0.48415	-2.22620	C	1.45293	-2.03299	5.14174
O	2.48286	0.30951	-0.12517	C	2.55418	-0.16113	4.08592
O	1.03239	1.92677	-1.63338	C	2.63018	-1.35046	4.81796
C	3.60152	0.86185	-0.69331	H	3.46370	0.37613	3.84351
C	1.32398	2.96334	-0.78030	H	5.19154	-3.94620	1.28598
C	3.71540	2.26196	-0.78930	H	1.51364	-2.95357	5.71032
C	4.67801	0.04027	-1.07322	H	-3.62176	0.35659	-5.17686
C	0.38842	3.99863	-0.60671	H	-1.96937	4.95570	-4.51893
C	2.61897	3.10550	-0.23966	C	4.96233	-5.74440	-0.72663
C	4.84846	2.83158	-1.42928	H	4.30544	-6.13111	0.08236
C	5.83546	0.61152	-1.61189	C	6.40715	-6.15374	-0.45433
C	0.66241	5.04573	0.28131	H	6.74802	-5.75979	0.52644
C	2.86617	4.11217	0.72692	H	6.48142	-7.26139	-0.43357
C	5.92160	1.99102	-1.81618	H	7.07261	-5.76751	-1.25587
C	4.93447	4.21210	-1.71696	C	5.05899	-1.28310	1.56429
H	6.66281	-0.02978	-1.89500	H	4.45558	-0.35382	1.56912
C	1.87415	5.09125	0.97637	C	6.52792	-0.93616	1.77755
H	-0.06454	5.83853	0.41217	H	7.13911	-1.86241	1.82822
C	4.07559	4.16835	1.45107	H	6.89997	-0.29658	0.95010
C	7.06553	2.54019	-2.41717	H	6.64233	-0.38183	2.73283
C	6.07577	4.74289	-2.32185	C	4.09575	-1.62683	-3.47423
H	4.12031	4.88849	-1.49545	H	3.78628	-0.56452	-3.39309
C	2.11957	6.12038	1.89927	C	5.28629	-1.71777	-4.42504
C	4.29902	5.18779	2.37909	H	5.02008	-1.25267	-5.39745
H	4.84509	3.41910	1.31708	H	6.16118	-1.18038	-4.00410
C	7.14171	3.91137	-2.66257	H	5.56220	-2.77807	-4.60599
H	7.89606	1.90724	-2.70688	C	-4.51495	4.66360	-3.64889
H	6.13135	5.80335	-2.53158	H	-4.47023	4.10943	-4.61135
C	3.32711	6.16435	2.59794	C	-4.72893	6.14957	-3.92318
H	1.37345	6.88306	2.08831	H	-4.77285	6.71354	-2.96692
H	5.22946	5.22022	2.93103	H	-3.90672	6.55473	-4.55022
H	8.02396	4.32854	-3.13068	H	-5.68761	6.29254	-4.46481
H	3.50737	6.95404	3.31577	C	0.49681	4.77565	-3.48143
C	-0.85654	4.05203	-1.41075	H	1.29505	4.06109	-3.19985
C	-0.80579	4.46049	-2.77139	C	0.95543	6.20200	-3.19292
C	-2.11456	3.80716	-0.80248	H	0.17239	6.92725	-3.50108
C	-2.00184	4.63361	-3.48458	H	1.17297	6.33647	-2.11434
C	-3.29075	4.00328	-1.54245	H	1.88287	6.41558	-3.76485
C	-3.24277	4.43037	-2.87340	C	-2.24510	3.33848	0.62984
H	-4.25171	3.82596	-1.07348	H	-1.27907	2.98286	1.04015
C	4.60731	-1.43467	-0.95869	C	-2.78248	4.45265	1.52441
C	4.86368	-2.06549	0.28469	H	-2.72744	4.13821	2.58470
C	4.42215	-2.22856	-2.12123	H	-2.17992	5.37650	1.40704
C	4.97949	-3.46246	0.33946	H	-3.84143	4.67438	1.27436
C	4.52828	-3.62485	-2.02748	C	3.96602	-1.89087	5.26278
C	4.82755	-4.24490	-0.80975	H	4.79759	-1.31513	4.80147
H	4.38413	-4.23113	-2.91414	C	4.11877	-1.81194	6.77952
C	-4.06330	-1.46480	-2.31413	H	5.12598	-2.17786	7.07024
C	-4.07084	-0.34578	-3.18578	H	4.00984	-0.76052	7.12168
C	-3.64080	-2.72926	-2.80423	H	3.35700	-2.44261	7.28453
C	-3.62293	-0.49611	-4.50773	C	-1.03796	-2.30987	5.17224
C	-3.20908	-2.84557	-4.13439	H	-1.82326	-2.27192	4.38987

C	-1.59342	-1.77780	6.48941
H	-0.82512	-1.85265	7.28832
H	-1.90875	-0.72012	6.38570
H	-2.47725	-2.37945	6.78878
C	1.30702	1.68814	2.95715
H	0.34441	1.87103	2.43989
C	1.57459	2.83609	3.92688
H	2.62180	2.79579	4.29450
H	1.41485	3.80396	3.41426
H	0.88263	2.78771	4.79283
C	-4.58978	1.00806	-2.75421
H	-4.23493	1.26566	-1.73693
C	-6.11384	1.05592	-2.79746
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H	-4.63718	-2.57517	-7.17071
H	-4.37880	-0.78805	-7.31628
H	-0.79345	-3.38582	5.30799
H	4.06634	-2.94691	4.93092
H	4.70258	-1.88526	2.42609
H	3.23414	-2.16913	-3.91981
H	4.63697	-6.22283	-1.67599
H	-2.21383	-2.85677	-6.56219
H	-2.63916	-4.49126	-2.09257
H	-4.19890	1.79609	-3.43056
H	-5.39411	4.28214	-3.08617
H	0.36925	4.66664	-4.58071
H	-2.93772	2.47213	0.66490
H	2.09036	1.68074	2.17180
O	-1.06957	-2.21119	-0.52371
C	0.86526	-4.86775	-0.33142
C	1.62823	-3.60572	1.49419
C	1.25954	-5.74480	-1.48069
C	0.65260	-4.37716	2.36263
H	1.22876	-2.63429	1.17651
H	2.60055	-3.45972	1.96104
C	0.29611	-5.84794	-2.67146
H	2.24294	-5.41849	-1.81990
H	1.37732	-6.73695	-1.01885
C	-0.68279	-4.48033	1.63160
H	0.54121	-3.89107	3.32883
H	1.07990	-5.37066	2.54365
C	0.46545	-4.74569	-3.72097
H	-0.74183	-5.88337	-2.32457
H	0.47921	-6.81442	-3.15303
H	-1.25134	-5.33915	2.00085

H	-1.27954	-3.58295	1.81769
C	0.28037	-3.33907	-3.18040
H	1.47144	-4.81683	-4.15399
H	-0.25273	-4.91804	-4.53135
O	1.26082	-3.11250	-2.19112
H	0.37889	-2.60623	-3.99169
H	-0.72213	-3.21406	-2.74696
H	1.31221	-2.13654	-2.07569
O	1.89526	-4.38768	0.31022
C	-0.44406	-4.65022	0.12313
H	-0.65009	-3.39526	-0.29534
H	-1.18921	-5.24253	-0.39894

S-anti-C₄-C(+)



E(RM062X) = -5098.38139576

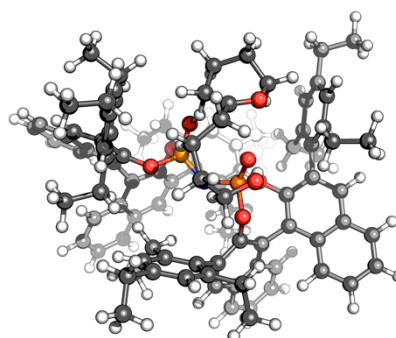
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C	-0.76790	0.37551	3.67284
C	-2.94033	0.37526	2.58322
C	-1.14539	1.49893	4.41933
C	-3.29828	1.55421	3.28732
C	-2.38365	2.11163	4.21218
C	-3.94407	-0.42929	1.84054
C	-5.11048	-0.92925	2.48155
C	-3.70949	-0.72522	0.47976
C	-6.12090	-1.53938	1.70190
C	-4.71942	-1.35629	-0.27460
C	-5.92841	-1.71558	0.33191
H	-6.70545	-2.17971	-0.26530
H	-0.48004	1.87862	5.18489
C	-2.73820	3.25009	4.95344
C	-3.98956	3.84243	4.77765
H	-2.04925	3.67876	5.67168
H	-4.25726	4.72013	5.35158
C	-4.89273	3.31017	3.85759
C	-4.55128	2.18075	3.10990
H	-5.85679	3.78078	3.71464
H	-5.26648	1.81253	2.38629
C	-7.30525	-1.98977	2.30722
C	-7.48033	-1.86901	3.68581
H	-8.08951	-2.44758	1.71583
H	-8.39282	-2.22274	4.14818

C	-6.47240	-1.31246	4.47159	C	-4.38688	-3.50645	-3.36724
C	-5.29325	-0.85286	3.88121	C	-4.50117	-2.56085	-4.39033
H	-6.60285	-1.24017	5.54371	H	-4.29505	-4.55471	-3.62455
H	-4.52638	-0.45471	4.53152	C	0.52049	-0.28599	3.98619
N	-0.02790	0.10497	0.06948	C	0.53652	-1.50758	4.71221
P	1.05265	0.19923	-1.07087	C	1.74689	0.35113	3.66385
O	1.06203	-0.82149	-2.19669	C	1.76700	-2.07469	5.07896
O	2.50927	0.16359	-0.31452	C	2.95595	-0.23006	4.07324
O	0.91543	1.62409	-1.85501	C	2.97468	-1.43816	4.77707
C	3.56281	0.83312	-0.90029	H	3.88952	0.27191	3.85001
C	1.10611	2.74448	-1.08144	H	6.00112	-3.56233	1.31374
C	3.52679	2.23821	-1.05068	H	1.78628	-3.01066	5.62474
C	4.76199	0.14656	-1.19567	H	-4.72567	-0.47438	-4.85510
C	0.11085	3.73700	-1.00570	H	-2.12113	4.28626	-5.06853
C	2.36919	2.99840	-0.52080	C	6.40543	-5.36811	-0.66441
C	4.59299	2.90911	-1.70953	H	5.83868	-5.91017	0.12323
C	5.86702	0.84450	-1.69733	C	7.89076	-5.35980	-0.31185
C	0.30374	4.85206	-0.17709	H	8.05690	-4.87344	0.67280
C	2.54200	4.08280	0.37492	H	8.26564	-6.40343	-0.25626
C	5.78091	2.20155	-1.99867	H	8.46706	-4.81560	-1.09049
C	4.50533	4.26606	-2.09714	C	5.16373	-1.03094	1.51410
H	6.79195	0.31107	-1.88749	H	4.45592	-0.18605	1.41373
C	1.48836	5.00979	0.54660	C	6.52988	-0.48461	1.91354
H	-0.45801	5.61960	-0.12817	H	7.24343	-1.31655	2.09348
C	3.74863	4.28359	1.07909	H	6.92821	0.17529	1.11384
C	6.86846	2.85871	-2.59638	H	6.43325	0.10773	2.84776
C	5.58952	4.90546	-2.70183	C	4.65878	-1.65328	-3.56552
H	3.59847	4.83795	-1.95525	H	4.09711	-0.69652	-3.53210
C	1.65834	6.11830	1.39126	C	5.89578	-1.47292	-4.44311
C	3.90468	5.39072	1.91628	H	5.58752	-1.10809	-5.44538
H	4.56842	3.58142	0.99855	H	6.58922	-0.73118	-3.99867
C	6.77180	4.20683	-2.94117	H	6.42982	-2.43807	-4.57047
H	7.78797	2.32608	-2.80902	C	-4.69743	4.19642	-4.22615
H	5.51065	5.94609	-2.98896	H	-4.46074	4.19962	-5.31250
C	2.86306	6.30598	2.07124	C	-5.36792	5.52122	-3.87393
H	0.86210	6.84175	1.52079	H	-5.68828	5.52645	-2.81048
H	4.83356	5.53490	2.45264	H	-4.66662	6.36483	-4.04997
H	7.61029	4.70714	-3.40815	H	-6.26465	5.66493	-4.51274
H	2.98845	7.16153	2.72211	C	0.31152	4.16772	-3.95922
C	-1.10617	3.69085	-1.85306	H	1.07460	3.43539	-3.63408
C	-1.01266	3.94570	-3.25039	C	0.83114	5.58708	-3.74720
C	-2.38660	3.56110	-1.25276	H	0.07713	6.32749	-4.08953
C	-2.18784	4.07151	-4.00839	H	1.06404	5.77002	-2.67949
C	-3.53785	3.72138	-2.03826	H	1.76285	5.73110	-4.33386
C	-3.44732	3.98706	-3.40806	C	-2.56679	3.27354	0.22356
H	-4.51544	3.64088	-1.57769	H	-1.61627	2.96924	0.70880
C	4.91794	-1.31609	-1.02524	C	-3.13254	4.49034	0.95551
C	5.25075	-1.84710	0.24617	H	-2.98065	4.37368	2.04654
C	5.02239	-2.14390	-2.17594	H	-2.62369	5.42315	0.63890
C	5.72995	-3.16169	0.34363	H	-4.21975	4.59012	0.75255
C	5.48177	-3.46323	-2.03929	C	4.28257	-2.05090	5.21148
C	5.87147	-3.96430	-0.79308	H	5.14192	-1.50640	4.76345
H	5.55953	-4.09473	-2.91637	C	4.43456	-2.01243	6.72991
C	-4.51724	-1.74589	-1.68809	H	5.42214	-2.43246	7.01466
C	-4.64869	-0.78789	-2.72389	H	4.37490	-0.96472	7.09485
C	-4.36446	-3.11799	-2.01942	H	3.64185	-2.61661	7.21953
C	-4.61798	-1.20649	-4.06312	C	-0.73257	-2.21736	5.14636

H	-1.48767	-2.22442	4.33604
C	-1.32461	-1.58585	6.40276
H	-0.57660	-1.59072	7.22401
H	-1.64750	-0.54375	6.20871
H	-2.21193	-2.16946	6.72678
C	1.80783	1.66135	2.90729
H	0.84040	1.91127	2.42470
C	2.21142	2.80647	3.83438
H	3.29507	2.74761	4.06986
H	2.00350	3.77645	3.34213
H	1.63596	2.77519	4.78186
C	-4.89674	0.67423	-2.44107
H	-4.39964	0.99602	-1.50582
C	-6.39053	0.96724	-2.34582
H	-6.85039	0.37889	-1.52441
H	-6.54598	2.04621	-2.13582
H	-6.89401	0.71516	-3.30340
C	-4.14729	-4.19005	-0.96627
H	-3.91907	-3.75704	0.02949
C	-5.36155	-5.10626	-0.83611
H	-5.17416	-5.85726	-0.04005
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H	-5.55005	-5.64430	-1.78878
C	-4.49407	-3.00278	-5.83113
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H	-5.87814	-4.66974	-5.57588
H	-6.66140	-3.09361	-6.00414
H	-0.51923	-3.28604	5.36758
H	4.33343	-3.10301	4.85666
H	4.76992	-1.67284	2.32916
H	3.98880	-2.39147	-4.05279
H	6.27231	-5.92902	-1.61506
H	-3.61897	-3.66426	-6.01096
H	-3.26252	-4.80183	-1.24001
H	-4.45721	1.28641	-3.25542
H	-5.40963	3.36392	-4.04789
H	0.19277	4.00618	-5.05301
H	-3.26287	2.41703	0.34675
H	2.54971	1.57615	2.08538
O	-1.01428	-2.34555	-0.30940
C	0.79959	-4.31953	-1.86434
C	-1.14636	-4.12721	-3.16367
C	1.48755	-5.10433	-0.79564
C	-0.25895	-4.00535	-4.38685
H	-1.97489	-4.81249	-3.32464
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C	2.44330	-4.31256	0.12131
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C	0.90290	-3.07100	-4.06930
H	-0.85604	-3.63290	-5.22403
H	0.10096	-5.00618	-4.65520
C	2.08293	-4.41441	1.60434
H	3.44844	-4.71309	-0.01188
H	2.47491	-3.25452	-0.16869

H	0.58322	-2.02907	-4.16341
H	1.72131	-3.22519	-4.77778
C	0.76856	-3.73915	1.97379
H	2.88522	-3.94822	2.19081
H	2.03956	-5.47067	1.90108
O	-0.33795	-4.37780	1.37078
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H	0.81063	-2.67945	1.68523
H	-0.76310	-3.73835	0.76791
C	1.41286	-3.31685	-2.63730
O	-0.41187	-4.73025	-2.07874
H	2.49171	-3.33359	-2.50129
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S-anti-C₄-B(+)



E(RM062X) = -5098.38139576

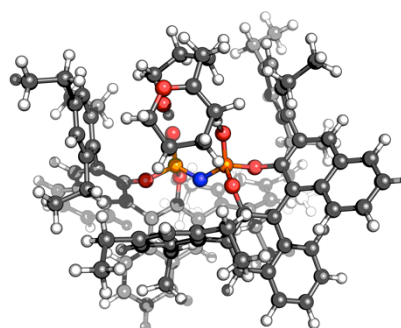
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C	-0.76790	0.37551	3.67284
C	-2.94033	0.37526	2.58322
C	-1.14539	1.49893	4.41933
C	-3.29828	1.55421	3.28732
C	-2.38365	2.11163	4.21218
C	-3.94407	-0.42929	1.84054
C	-5.11048	-0.92925	2.48155
C	-3.70949	-0.72522	0.47976
C	-6.12090	-1.53938	1.70190
C	-4.71942	-1.35629	-0.27460
C	-5.92841	-1.71558	0.33191
H	-6.70545	-2.17971	-0.26530
H	-0.48004	1.87862	5.18489
C	-2.73820	3.25009	4.95344
C	-3.98956	3.84243	4.77765
H	-2.04925	3.67876	5.67168
H	-4.25726	4.72013	5.35158
C	-4.89273	3.31017	3.85759
C	-4.55128	2.18075	3.10990
H	-5.85679	3.78078	3.71464
H	-5.26648	1.81253	2.38629
C	-7.30525	-1.98977	2.30722
C	-7.48033	-1.86901	3.68581
H	-8.08951	-2.44758	1.71583

H	-8.39282	-2.22274	4.14818	C	-4.61798	-1.20649	-4.06312
C	-6.47240	-1.31246	4.47159	C	-4.38688	-3.50645	-3.36724
C	-5.29325	-0.85286	3.88121	C	-4.50117	-2.56085	-4.39033
H	-6.60285	-1.24017	5.54371	H	-4.29505	-4.55471	-3.62455
H	-4.52638	-0.45471	4.53152	C	0.52049	-0.28599	3.98619
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P	1.05265	0.19923	-1.07087	C	1.74689	0.35113	3.66385
O	1.06203	-0.82149	-2.19669	C	1.76700	-2.07469	5.07896
O	2.50927	0.16359	-0.31452	C	2.95595	-0.23006	4.07324
O	0.91543	1.62409	-1.85501	C	2.97468	-1.43816	4.77707
C	3.56281	0.83312	-0.90029	H	3.88952	0.27191	3.85001
C	1.10611	2.74448	-1.08144	H	6.00112	-3.56233	1.31374
C	3.52679	2.23821	-1.05068	H	1.78628	-3.01066	5.62474
C	4.76199	0.14656	-1.19567	H	-4.72567	-0.47438	-4.85510
C	0.11085	3.73700	-1.00570	H	-2.12113	4.28626	-5.06853
C	2.36919	2.99840	-0.52080	C	6.40543	-5.36811	-0.66441
C	4.59299	2.90911	-1.70953	H	5.83868	-5.91017	0.12323
C	5.86702	0.84450	-1.69733	C	7.89076	-5.35980	-0.31185
C	0.30374	4.85206	-0.17709	H	8.05690	-4.87344	0.67280
C	2.54200	4.08280	0.37492	H	8.26564	-6.40343	-0.25626
C	5.78091	2.20155	-1.99867	H	8.46706	-4.81560	-1.09049
C	4.50533	4.26606	-2.09714	C	5.16373	-1.03094	1.51410
H	6.79195	0.31107	-1.88749	H	4.45592	-0.18605	1.41373
C	1.48836	5.00979	0.54660	C	6.52988	-0.48461	1.91354
H	-0.45801	5.61960	-0.12817	H	7.24343	-1.31655	2.09348
C	3.74863	4.28359	1.07909	H	6.92821	0.17529	1.11384
C	6.86846	2.85871	-2.59638	H	6.43325	0.10773	2.84776
C	5.58952	4.90546	-2.70183	C	4.65878	-1.65328	-3.56552
H	3.59847	4.83795	-1.95525	H	4.09711	-0.69652	-3.53210
C	1.65834	6.11830	1.39126	C	5.89578	-1.47292	-4.44311
C	3.90468	5.39072	1.91628	H	5.58752	-1.10809	-5.44538
H	4.56842	3.58142	0.99855	H	6.58922	-0.73118	-3.99867
C	6.77180	4.20683	-2.94117	H	6.42982	-2.43807	-4.57047
H	7.78797	2.32608	-2.80902	C	-4.69743	4.19642	-4.22615
H	5.51065	5.94609	-2.98896	H	-4.46074	4.19962	-5.31250
C	2.86306	6.30598	2.07124	C	-5.36792	5.52122	-3.87393
H	0.86210	6.84175	1.52079	H	-5.68828	5.52645	-2.81048
H	4.83356	5.53490	2.45264	H	-4.66662	6.36483	-4.04997
H	7.61029	4.70714	-3.40815	H	-6.26465	5.66493	-4.51274
H	2.98845	7.16153	2.72211	C	0.31152	4.16772	-3.95922
C	-1.10617	3.69085	-1.85306	H	1.07460	3.43539	-3.63408
C	-1.01266	3.94570	-3.25039	C	0.83114	5.58708	-3.74720
C	-2.38660	3.56110	-1.25276	H	0.07713	6.32749	-4.08953
C	-2.18784	4.07151	-4.00839	H	1.06404	5.77002	-2.67949
C	-3.53785	3.72138	-2.03826	H	1.76285	5.73110	-4.33386
C	-3.44732	3.98706	-3.40806	C	-2.56679	3.27354	0.22356
H	-4.51544	3.64088	-1.57769	H	-1.61627	2.96924	0.70880
C	4.91794	-1.31609	-1.02524	C	-3.13254	4.49034	0.95551
C	5.25075	-1.84710	0.24617	H	-2.98065	4.37368	2.04654
C	5.02239	-2.14390	-2.17594	H	-2.62369	5.42315	0.63890
C	5.72995	-3.16169	0.34363	H	-4.21975	4.59012	0.75255
C	5.48177	-3.46323	-2.03929	C	4.28257	-2.05090	5.21148
C	5.87147	-3.96430	-0.79308	H	5.14192	-1.50640	4.76345
H	5.55953	-4.09473	-2.91637	C	4.43456	-2.01243	6.72991
C	-4.51724	-1.74589	-1.68809	H	5.42214	-2.43246	7.01466
C	-4.64869	-0.78789	-2.72389	H	4.37490	-0.96472	7.09485
C	-4.36446	-3.11799	-2.01942	H	3.64185	-2.61661	7.21953

C	-0.73257	-2.21736	5.14636
H	-1.48767	-2.22442	4.33604
C	-1.32461	-1.58585	6.40276
H	-0.57660	-1.59072	7.22401
H	-1.64750	-0.54375	6.20871
H	-2.21193	-2.16946	6.72678
C	1.80783	1.66135	2.90729
H	0.84040	1.91127	2.42470
C	2.21142	2.80647	3.83438
H	3.29507	2.74761	4.06986
H	2.00350	3.77645	3.34213
H	1.63596	2.77519	4.78186
C	-4.89674	0.67423	-2.44107
H	-4.39964	0.99602	-1.50582
C	-6.39053	0.96724	-2.34582
H	-6.85039	0.37889	-1.52441
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C	-4.14729	-4.19005	-0.96627
H	-3.91907	-3.75704	0.02949
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H	-5.17416	-5.85726	-0.04005
H	-6.26422	-4.52211	-0.56362
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H	-5.87814	-4.66974	-5.57588
H	-6.66140	-3.09361	-6.00414
H	-0.51923	-3.28604	5.36758
H	4.33343	-3.10301	4.85666
H	4.76992	-1.67284	2.32916
H	3.98880	-2.39147	-4.05279
H	6.27231	-5.92902	-1.61506
H	-3.61897	-3.66426	-6.01096
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H	-4.45721	1.28641	-3.25542
H	-5.40963	3.36392	-4.04789
H	0.19277	4.00618	-5.05301
H	-3.26287	2.41703	0.34675
H	2.54971	1.57615	2.08538
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C	0.79959	-4.31953	-1.86434
C	-1.14636	-4.12721	-3.16367
C	1.48755	-5.10433	-0.79564
C	-0.25895	-4.00535	-4.38685
H	-1.97489	-4.81249	-3.32464
H	-1.49836	-3.15675	-2.79710
C	2.44330	-4.31256	0.12131
H	2.05234	-5.86562	-1.35402
H	0.72103	-5.61652	-0.21368
C	0.90290	-3.07100	-4.06930
H	-0.85604	-3.63290	-5.22403
H	0.10096	-5.00618	-4.65520
C	2.08293	-4.41441	1.60434
H	3.44844	-4.71309	-0.01188

H	2.47491	-3.25452	-0.16869
H	0.58322	-2.02907	-4.16341
H	1.72131	-3.22519	-4.77778
C	0.76856	-3.73915	1.97379
H	2.88522	-3.94822	2.19081
H	2.03956	-5.47067	1.90108
O	-0.33795	-4.37780	1.37078
H	0.64311	-3.78202	3.06152
H	0.81063	-2.67945	1.68523
H	-0.76310	-3.73835	0.76791
C	1.41286	-3.31685	-2.63730
O	-0.41187	-4.73025	-2.07874
H	2.49171	-3.33359	-2.50129
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S-anti-B_{2,5}-C(-)



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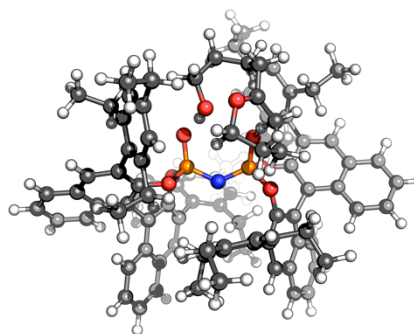
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C	-1.12622	0.04981	3.63103
C	-3.20525	0.07918	2.36499
C	-1.63050	1.04002	4.48132
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C	-2.88369	1.61233	4.24445
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C	-5.29423	-1.26989	1.83127
C	-3.69149	-0.74021	0.05984
C	-6.16917	-1.81537	0.86002
C	-4.55413	-1.32544	-0.88796
C	-5.80494	-1.80874	-0.48803
H	-6.47406	-2.22882	-1.22939
H	-1.04643	1.35510	5.33786
C	-3.36107	2.63187	5.08343
C	-4.61609	3.19912	4.85742
H	-2.76253	2.99155	5.91201
H	-4.97736	3.98732	5.50516
C	-5.40085	2.76045	3.79106
C	-4.94052	1.74480	2.95024
H	-6.36681	3.21390	3.61034
H	-5.56631	1.44819	2.11896
C	-7.38732	-2.39264	1.25299

C	-7.72926	-2.46251	2.60355	C	-4.01871	-0.44212	-3.18526
H	-8.06760	-2.80402	0.51652	C	-3.82526	-2.84903	-2.75324
H	-8.66650	-2.91467	2.90127	C	-3.54894	-0.65672	-4.49010
C	-6.85538	-1.97062	3.57195	C	-3.38730	-3.02953	-4.07416
C	-5.64446	-1.38587	3.19519	C	-3.22814	-1.94198	-4.93782
H	-7.11472	-2.04657	4.62010	H	-3.16992	-4.02786	-4.43261
H	-4.98430	-1.04305	3.98003	C	0.18086	-0.57161	3.94748
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P	1.13877	0.39422	-1.06378	C	1.38689	0.13267	3.70160
O	1.22961	-0.50720	-2.24887	C	1.46885	-2.37755	4.95875
O	2.51345	0.34353	-0.16670	C	2.61025	-0.43444	4.08980
O	0.97701	1.92188	-1.63880	C	2.65892	-1.68197	4.72077
C	3.59283	1.04193	-0.65322	H	3.52980	0.11108	3.91341
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C	4.78317	0.36520	-0.98800	H	-3.45130	0.17949	-5.17264
C	0.13427	3.92074	-0.58474	H	-1.96549	4.98594	-4.61022
C	2.38708	3.15456	-0.11304	C	5.69143	-5.36045	-1.15380
C	4.67508	3.17055	-1.19663	H	4.99381	-5.89186	-0.47131
C	5.91703	1.08888	-1.37498	C	7.13154	-5.66077	-0.74795
C	0.28996	4.94480	0.35966	H	7.31819	-5.33959	0.29872
C	2.51546	4.13471	0.90280	H	7.31722	-6.75313	-0.81950
C	5.86381	2.47525	-1.51983	H	7.83836	-5.13447	-1.42463
C	4.62240	4.56318	-1.43176	C	5.00957	-1.19097	1.54601
H	6.83350	0.55815	-1.60715	H	4.41034	-0.26037	1.54456
C	1.44919	5.03428	1.13288	C	6.41644	-0.86824	2.03613
H	-0.48153	5.69751	0.46358	H	7.01779	-1.79765	2.12650
C	3.68658	4.25297	1.68168	H	6.91850	-0.17283	1.33032
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C	5.73839	5.24475	-1.92183	C	4.74752	-1.06792	-3.59266
H	3.71924	5.13254	-1.25888	H	4.32518	-0.05090	-3.45875
C	1.57852	6.04610	2.09772	C	6.05457	-0.95756	-4.37488
C	3.79877	5.25815	2.64485	H	5.87423	-0.40513	-5.32103
H	4.51208	3.56332	1.56170	H	6.81785	-0.40861	-3.78660
C	6.91794	4.55430	-2.19687	H	6.44616	-1.96560	-4.62673
H	7.90003	2.65129	-2.24267	C	-4.56733	4.73839	-3.88627
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C	2.75002	6.15525	2.84899	C	-5.30812	5.96349	-3.35745
H	0.77366	6.75043	2.27162	H	-5.67511	5.78347	-2.32479
H	4.70094	5.33949	3.23713	H	-4.63626	6.84836	-3.35899
H	7.78031	5.08747	-2.57576	H	-6.18150	6.17876	-4.00843
H	2.84286	6.93368	3.59515	C	0.42903	4.73304	-3.44371
C	-1.05161	3.96356	-1.47396	H	1.19764	3.98662	-3.16587
C	-0.91530	4.40795	-2.81867	C	0.90232	6.13181	-3.05816
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C	-3.34303	4.44174	-3.05630	C	-2.57055	3.23408	0.46920
H	-4.46626	3.81507	-1.33588	H	-1.63140	2.87079	0.93603
C	4.86559	-1.11179	-1.01797	C	-3.17455	4.32508	1.35181
C	5.04845	-1.84313	0.18247	H	-3.12217	4.01634	2.41438
C	4.94890	-1.78334	-2.26757	H	-2.61946	5.27856	1.24479
C	5.32894	-3.21568	0.11832	H	-4.23807	4.49557	1.08174
C	5.21870	-3.16041	-2.29299	C	3.97952	-2.27470	5.14346
C	5.41190	-3.87967	-1.10990	H	4.82638	-1.67860	4.74027
H	5.27624	-3.67512	-3.24490	C	4.10704	-2.31436	6.66391
C	-4.12025	-1.53743	-2.29002	H	5.10302	-2.71880	6.94208

H	4.00914	-1.29028	7.08365
H	3.32616	-2.96817	7.10649
C	-1.02211	-2.61686	4.94073
H	-1.82221	-2.47087	4.18797
C	-1.54174	-2.21260	6.31638
H	-0.76852	-2.40294	7.09102
H	-1.81461	-1.13702	6.32952
H	-2.44558	-2.80892	6.56177
C	1.40839	1.50346	3.06166
H	0.45368	1.74007	2.54770
C	1.69102	2.58109	4.10560
H	2.74382	2.51567	4.45295
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H	1.01453	2.47350	4.97794
C	-4.46149	0.95202	-2.80226
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C	-5.98144	1.08123	-2.85087
H	-6.46382	0.36076	-2.16008
H	-6.27862	2.10526	-2.54320
H	-6.34766	0.89705	-3.88326
C	-3.95552	-4.08008	-1.87344
H	-4.03461	-3.82608	-0.79745
C	-5.16003	-4.92704	-2.27654
H	-5.24907	-5.79508	-1.58990
H	-6.09475	-4.33297	-2.21908
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H	-4.21567	-0.89828	-7.32222
H	-0.80364	-3.70721	4.94699
H	4.07135	-3.30347	4.73278
H	4.51550	-1.87682	2.26594
H	4.01083	-1.62323	-4.20893
H	5.52204	-5.76249	-2.17654
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H	-5.24797	3.86237	-3.87817
H	0.35634	4.68687	-4.55241
H	-3.26088	2.36505	0.44303
H	2.19820	1.53132	2.28221
O	-1.05475	-2.23735	-0.61645
C	0.22732	-5.30222	-0.56205
C	2.11517	-4.94537	0.88039
C	-0.19854	-5.81422	-1.90450
C	1.30579	-3.85246	1.54409
H	3.06598	-4.57939	0.50516
H	2.28454	-5.79535	1.54866
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H	0.56380	-6.50830	-2.27218
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C	-0.13808	-4.32075	1.70800
H	1.33954	-2.94597	0.93031
H	1.77874	-3.63064	2.50352

C	0.78072	-4.20291	-3.69197
H	-0.90122	-3.82225	-2.42377
H	-1.18127	-5.06132	-3.65367
H	-0.18773	-5.19497	2.37056
H	-0.74749	-3.52807	2.14319
C	1.95874	-3.86096	-2.78288
H	1.10735	-4.96444	-4.41339
H	0.49366	-3.31533	-4.26736
O	1.57298	-3.15361	-1.62715
H	2.44454	-4.78170	-2.43676
H	2.69471	-3.30225	-3.36710
H	1.36963	-2.22008	-1.86424
O	1.47924	-5.50665	-0.30200
C	-0.65449	-4.63939	0.31494
H	-0.75614	-3.48318	-0.22465
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S-anti- B_{2,5}-B(-)



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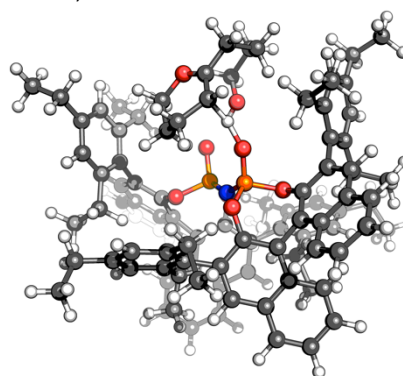
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C	-1.17248	0.11846	3.60681
C	-3.23780	0.15101	2.31750
C	-1.67456	1.12798	4.43570
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C	-3.70174	-0.70214	0.01954
C	-6.19943	-1.74153	0.80155
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C	-5.81377	-1.76579	-0.54057
H	-6.47375	-2.19659	-1.28383
H	-1.09640	1.44988	5.29356
C	-3.39693	2.74308	4.99836
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C	-5.42336	2.87063	3.68501
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H	-6.38361	3.32971	3.48878
H	-5.58399	1.53702	2.02936

C	-7.42869	-2.30032	1.18643	C	-4.08771	-1.55604	-2.31452
C	-7.79132	-2.34271	2.53272	C	-3.94043	-0.48342	-3.23099
H	-8.10160	-2.71905	0.44734	C	-3.78763	-2.88153	-2.73399
H	-8.73710	-2.78084	2.82433	C	-3.41702	-0.73346	-4.50879
C	-6.92707	-1.84215	3.50530	C	-3.29345	-3.09696	-4.02948
C	-5.70519	-1.27542	3.13654	C	-3.08592	-2.03150	-4.91031
H	-7.20247	-1.89738	4.55064	H	-3.06804	-4.10518	-4.35378
H	-5.05334	-0.92548	3.92513	C	0.12569	-0.51280	3.94360
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P	1.13931	0.42011	-1.05347	C	1.34085	0.18321	3.71811
O	1.23131	-0.48414	-2.23704	C	1.38933	-2.34786	4.93328
O	2.49858	0.34853	-0.13493	C	2.55551	-0.40093	4.10881
O	1.02670	1.94661	-1.64028	C	2.58722	-1.65907	4.71892
C	3.59846	1.02374	-0.60655	H	3.48193	0.13767	3.94743
C	1.18706	2.97034	-0.73565	H	5.22388	-3.89924	1.00210
C	3.61006	2.43317	-0.60998	H	1.41726	-3.32091	5.40955
C	4.77365	0.31879	-0.93579	H	-3.28254	0.08510	-5.20621
C	0.18931	3.95452	-0.60649	H	-1.83071	4.98054	-4.68404
C	2.42485	3.16256	-0.09046	C	5.38804	-5.44623	-1.22005
C	4.73837	3.12831	-1.12376	H	4.63303	-5.95192	-0.58130
C	5.93057	1.01663	-1.30079	C	6.79025	-5.84494	-0.76886
C	0.33839	4.97931	0.33763	H	6.95348	-5.56701	0.29389
C	2.54580	4.14588	0.92355	H	6.91341	-6.94396	-0.86798
C	5.91482	2.40539	-1.43267	H	7.55372	-5.34277	-1.40080
C	4.72336	4.52265	-1.35457	C	4.90371	-1.30073	1.56279
H	6.83516	0.46430	-1.52872	H	4.25778	-0.40237	1.59359
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H	-0.42807	5.73908	0.42672	H	6.95761	-1.82504	2.05125
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C	7.05723	3.07923	-1.89360	H	6.27110	-0.46480	3.01905
C	5.86367	5.17894	-1.82261	C	4.75170	-1.05424	-3.57498
H	3.83156	5.11335	-1.19538	H	4.37638	-0.02073	-3.42884
C	1.60903	6.07299	2.09376	C	6.08058	-0.99308	-4.32507
C	3.80994	5.26223	2.68412	H	5.95058	-0.41121	-5.26173
H	4.52266	3.55376	1.62243	H	6.85661	-0.49721	-3.70709
C	7.03052	4.46127	-2.08121	H	6.42658	-2.01391	-4.59167
H	7.96589	2.53493	-2.12263	C	-4.44575	4.70653	-4.02089
H	5.84032	6.24810	-1.98985	H	-4.14365	4.88948	-5.07512
C	2.76820	6.17233	2.86524	C	-5.21494	5.92656	-3.52168
H	0.80927	6.78711	2.25040	H	-5.60536	5.75083	-2.49693
H	4.70204	5.33575	3.29247	H	-4.55449	6.81995	-3.51446
H	7.91174	4.97492	-2.44331	H	-6.07441	6.12493	-4.19609
H	2.85658	6.95298	3.60961	C	0.53864	4.76354	-3.45901
C	-0.98030	3.99945	-1.51710	H	1.30578	4.02377	-3.15959
C	-0.81709	4.43255	-2.86233	C	0.99351	6.16749	-3.07035
C	-2.28627	3.76125	-1.01456	H	0.23652	6.91760	-3.38394
C	-1.95092	4.62971	-3.66573	H	1.15237	6.24432	-1.97636
C	-3.39689	3.98616	-1.84254	H	1.95413	6.39859	-3.57703
C	-3.23855	4.43305	-3.15860	C	-2.53667	3.28026	0.39950
H	-4.39518	3.81171	-1.45826	H	-1.60717	2.92328	0.88983
C	4.80839	-1.15999	-0.99907	C	-3.15685	4.38441	1.25378
C	4.92137	-1.92778	0.18723	H	-3.12606	4.09133	2.32150
C	4.88658	-1.80671	-2.26222	H	-2.59802	5.33552	1.14390
C	5.11813	-3.31366	0.09655	H	-4.21438	4.55213	0.95951
C	5.08147	-3.19533	-2.31435	C	3.89799	-2.27026	5.14601
C	5.19527	-3.95282	-1.14494	H	4.75411	-1.67472	4.76209
H	5.13521	-3.69021	-3.27696	C	4.00864	-2.33648	6.66684

H	4.99829	-2.75360	6.94877
H	3.91428	-1.31889	7.10276
H	3.21795	-2.99137	7.08995
C	-1.10349	-2.57108	4.88092
H	-1.85140	-2.48093	4.06803
C	-1.71668	-2.11162	6.19987
H	-0.98439	-2.23256	7.02647
H	-2.02768	-1.04902	6.14094
H	-2.61288	-2.72680	6.42596
C	1.38291	1.55763	3.08714
H	0.43444	1.81019	2.56941
C	1.67508	2.62554	4.13839
H	2.72650	2.54673	4.48707
H	1.51800	3.63113	3.70286
H	0.99619	2.51967	5.00908
C	-4.38753	0.92347	-2.90011
H	-4.05409	1.21835	-1.88723
C	-5.90475	1.05693	-2.99853
H	-6.41127	0.35468	-2.30619
H	-6.20716	2.08882	-2.72417
H	-6.23979	0.84952	-4.03707
C	-3.97351	-4.09163	-1.83441
H	-4.08547	-3.81358	-0.76746
C	-5.18033	-4.92167	-2.26477
H	-5.31372	-5.77288	-1.56442
H	-6.10353	-4.30724	-2.25512
H	-5.02745	-5.32806	-3.28692
C	-2.51733	-2.27808	-6.28426
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H	-3.14068	-2.30313	-8.35916
H	-4.43097	-2.77867	-7.19022
H	-3.95283	-1.03977	-7.36268
H	-0.87264	-3.65580	4.96246
H	3.98547	-3.29293	4.71936
H	4.47132	-2.01706	2.29300
H	4.00324	-1.55996	-4.21931
H	5.23573	-5.81064	-2.25942
H	-2.11635	-3.31228	-6.36373
H	-3.07584	-4.73761	-1.87973
H	-3.92722	1.64790	-3.60485
H	-5.11499	3.82194	-4.02165
H	0.49137	4.71133	-4.56880
H	-3.22684	2.41111	0.37171
H	2.17663	1.57895	2.31155
O	-1.03896	-2.20600	-0.60812
C	0.40298	-5.24088	-0.44893
C	2.13288	-4.69635	1.04675
C	0.01810	-5.84929	-1.76108
C	1.17123	-4.93791	2.19226
H	2.21831	-3.63739	0.77864
H	3.11633	-5.12761	1.22235
C	-0.44412	-4.79282	-2.79576
H	0.86212	-6.43384	-2.13968
H	-0.81011	-6.53655	-1.55857
C	-0.17967	-4.31759	1.84895
H	1.59093	-4.50651	3.10369

H	1.08127	-6.01941	2.35052
C	0.67821	-4.20954	-3.65124
H	-0.93442	-3.96706	-2.27366
H	-1.18165	-5.26797	-3.44740
H	-0.96395	-4.72675	2.49121
H	-0.15397	-3.23987	2.02818
C	1.88880	-3.78133	-2.82529
H	1.00920	-4.93837	-4.40362
H	0.27555	-3.34504	-4.19122
O	1.53170	-3.11059	-1.64002
H	2.46359	-4.66638	-2.52283
H	2.53841	-3.16331	-3.45130
H	1.31282	-2.17288	-1.84896
O	1.65470	-5.36781	-0.14549
C	-0.53355	-4.57778	0.37983
H	-0.62357	-3.45058	-0.15719
H	-1.55014	-4.92239	0.18369

S-anti- B_{2,5}-C(+)



E(RM062X) = -5098.37133991

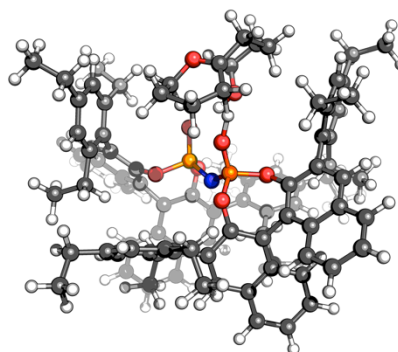
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C	0.44686	-1.91142	3.25345
C	2.67906	-1.64079	2.33678
C	0.72893	-3.25791	3.52358
C	2.93493	-3.02145	2.53392
C	1.94254	-3.82821	3.13546
C	3.77436	-0.69219	2.02215
C	4.90219	-0.55799	2.87402
C	3.67377	0.09152	0.85592
C	6.00794	0.20811	2.43974
C	4.78060	0.86735	0.44541
C	5.95083	0.87496	1.21584
H	6.80777	1.44482	0.87552
H	0.00725	-3.85567	4.06628
C	2.19533	-5.18692	3.38393
C	3.42092	-5.75115	3.02625
H	1.44581	-5.81160	3.85522
H	3.60970	-6.79957	3.21730
C	4.40002	-4.96792	2.41514
C	4.16196	-3.61486	2.16427
H	5.34431	-5.41188	2.12776

H	4.93566	-3.04397	1.66775	H	-5.04408	5.37781	-0.60079
C	7.15268	0.31498	3.24600	C	4.74296	1.74711	-0.74727
C	7.19447	-0.30791	4.49378	C	4.85956	1.19749	-2.04894
H	8.00869	0.89267	2.91765	C	4.79264	3.15830	-0.58013
H	8.07607	-0.21598	5.11492	C	5.01009	2.05160	-3.15283
C	6.09454	-1.03321	4.94986	C	4.99081	3.97835	-1.70145
C	4.95411	-1.15591	4.15341	C	5.09198	3.43658	-2.98511
H	6.12321	-1.49910	5.92648	H	5.04633	5.05294	-1.57648
H	4.11334	-1.70500	4.55565	C	-0.82423	-1.34836	3.76882
N	-0.03877	0.10212	-0.02749	C	-0.81947	-0.50211	4.91200
P	-1.19027	0.38764	-1.08168	C	-2.06273	-1.79431	3.23655
O	-1.29044	1.73117	-1.73161	C	-2.03932	-0.12979	5.49863
O	-2.58079	0.09159	-0.25563	C	-3.25905	-1.42902	3.87057
O	-1.07010	-0.70850	-2.29407	C	-3.25542	-0.60891	5.00255
C	-3.69227	-0.13362	-1.03727	H	-4.20145	-1.79593	3.48164
C	-1.40681	-2.01395	-2.01813	O	1.49287	2.16310	0.80398
C	-3.78272	-1.32049	-1.79120	H	-0.04514	2.79892	-1.78198
C	-4.80181	0.74167	-0.99346	O	0.59672	3.54617	-1.77730
C	-0.50858	-3.05143	-2.33646	C	0.19229	4.49512	-2.73498
C	-2.72276	-2.34685	-1.63880	H	0.02832	4.02409	-3.71359
C	-4.88218	-1.52435	-2.66688	H	-0.75524	4.96875	-2.43934
C	-5.94294	0.46143	-1.75610	C	1.29909	5.55107	-2.84369
C	-0.84837	-4.38153	-2.05335	H	2.01681	5.23746	-3.61039
C	-3.04033	-3.68076	-1.27658	H	0.87663	6.50763	-3.17587
C	-5.97887	-0.63417	-2.61762	C	2.09982	5.72314	-1.55198
C	-4.91576	-2.58725	-3.59771	H	2.94767	6.38508	-1.75478
H	-6.79949	1.12322	-1.69504	H	2.48438	4.74124	-1.27835
C	-2.08475	-4.70019	-1.48960	C	1.37177	6.30796	-0.32352
H	-0.15881	-5.17537	-2.31191	C	0.43460	5.36079	0.36589
C	-4.29497	-4.02794	-0.72957	H	2.12321	6.62125	0.40637
C	-7.09914	-0.84751	-3.43692	C	-1.82181	4.51261	0.29340
C	-6.03163	-2.78248	-4.41439	C	-0.37483	3.98196	2.26945
H	-4.07909	-3.26281	-3.71493	C	-1.40870	3.44271	1.28618
C	-2.40022	-6.03488	-1.18861	H	-2.57873	5.18454	0.70093
C	-4.59450	-5.35881	-0.42989	H	-2.16280	4.05816	-0.63823
H	-5.04278	-3.27494	-0.51713	H	-0.00934	3.17390	2.90910
C	-7.12442	-1.92101	-4.32753	H	-0.81261	4.75368	2.91639
H	-7.94999	-0.17756	-3.39630	H	-0.98805	2.59522	0.74176
H	-6.04713	-3.60343	-5.11965	H	-2.30843	3.08566	1.79405
C	-3.65151	-6.36009	-0.66249	H	-5.40285	3.08150	2.99679
H	-1.68014	-6.82584	-1.36195	H	-2.04273	0.50599	6.37633
H	-5.55935	-5.61359	-0.01098	H	5.11042	1.62981	-4.14626
H	-7.98791	-2.07778	-4.96103	H	1.93702	-2.22649	-6.22250
H	-3.88868	-7.39004	-0.42950	C	-5.46753	5.63096	2.06215
C	0.76209	-2.79587	-3.05774	H	-5.40125	5.43480	3.15464
C	0.74278	-2.48276	-4.44572	C	-6.83298	6.24247	1.76238
C	2.00416	-3.04640	-2.41699	H	-7.63963	5.52132	2.01463
C	1.95061	-2.44134	-5.16033	H	-6.97122	7.15899	2.37380
C	3.18714	-3.02461	-3.17091	H	-6.91054	6.51925	0.68962
C	3.16759	-2.73720	-4.53936	C	-5.12527	0.62879	1.96303
H	4.13358	-3.23664	-2.68791	H	-4.42220	-0.12237	1.55573
C	-4.81359	1.98782	-0.19092	C	-6.54424	0.07128	1.93478
C	-5.03267	1.93411	1.20934	H	-7.25292	0.80057	2.38192
C	-4.81992	3.24786	-0.84905	H	-6.85641	-0.15177	0.89378
C	-5.23367	3.12350	1.92700	H	-6.58402	-0.86921	2.52365
C	-5.05479	4.41432	-0.10481	C	-4.53728	3.39522	-2.33312
C	-5.25632	4.36094	1.27799	H	-4.15594	2.45417	-2.78026

C	-5.78054	3.83716	-3.10263
H	-5.54075	3.90650	-4.18447
H	-6.60380	3.10595	-2.97104
H	-6.12268	4.83466	-2.75518
C	4.44587	-2.76457	-5.34064
H	4.28745	-2.32356	-6.34890
C	4.95486	-4.19275	-5.51195
H	5.19621	-4.64211	-4.52531
H	4.18795	-4.81490	-6.02102
H	5.87650	-4.18646	-6.13117
C	-0.54403	-2.26892	-5.22147
H	-1.27424	-1.67168	-4.64307
C	-1.17460	-3.59570	-5.63502
H	-0.45565	-4.19239	-6.23593
H	-1.48292	-4.18185	-4.74639
H	-2.07705	-3.40007	-6.25168
C	2.10688	-3.35617	-0.93741
H	1.15545	-3.15599	-0.40201
C	2.51199	-4.81087	-0.70404
H	2.34835	-5.07744	0.35847
H	1.90654	-5.49988	-1.32650
H	3.58563	-4.95634	-0.94724
C	-4.54907	-0.24792	5.68880
H	-5.42169	-0.54930	5.06908
C	-4.66458	-0.93933	7.04464
H	-5.63932	-0.68281	7.51040
H	-4.61016	-2.04194	6.91848
H	-3.85132	-0.60791	7.72438
C	0.45941	-0.04062	5.58503
H	1.22517	0.25461	4.84248
C	1.02292	-1.11644	6.50947
H	0.26466	-1.40855	7.26700
H	1.32844	-2.01315	5.93412
H	1.91703	-0.72097	7.03574
C	-2.15004	-2.66983	2.00345
H	-1.18115	-2.73338	1.46589
C	-2.61573	-4.08134	2.35861
H	-3.69861	-4.08073	2.60419
H	-2.44727	-4.75726	1.49761
H	-2.05167	-4.48327	3.22407
C	4.91928	-0.29060	-2.29434
H	4.29143	-0.84886	-1.57550
C	6.35367	-0.80257	-2.21595
H	6.77644	-0.61993	-1.20579
H	6.36993	-1.89499	-2.41319
H	6.98579	-0.29490	-2.97530
C	4.61048	3.82864	0.77046
H	4.25781	3.11805	1.54596
C	5.89866	4.49014	1.25645
H	5.72724	4.94125	2.25646
H	6.71545	3.74545	1.34225
H	6.21349	5.29522	0.55979
C	5.29440	4.34140	-4.17337
H	5.14343	3.78320	-5.12301
C	6.70124	4.93361	-4.17792
H	6.83384	5.56988	-5.07813
H	6.86470	5.56067	-3.27584

H	7.45929	4.12153	-4.20150
H	0.26488	0.86995	6.19296
H	-4.60266	0.85390	5.82424
H	-4.83063	0.79169	3.01959
H	-3.73761	4.15275	-2.47974
H	-4.66844	6.36081	1.80889
H	4.54521	5.16180	-4.14788
H	3.82412	4.60634	0.68846
H	4.50901	-0.51122	-3.30035
H	5.22434	-2.15620	-4.83479
H	-0.34146	-1.68033	-6.14297
H	2.86661	-2.68974	-0.47782
H	-2.87052	-2.21784	1.29016
O	-0.76501	5.41521	-0.12509
H	1.15802	3.39076	0.90713
H	1.68369	4.84478	1.96755
C	0.77920	4.53787	1.44602
H	0.78797	7.18815	-0.61597

S-anti- B_{2,5}-B(+)



E(RM062X) = -5098.36909968

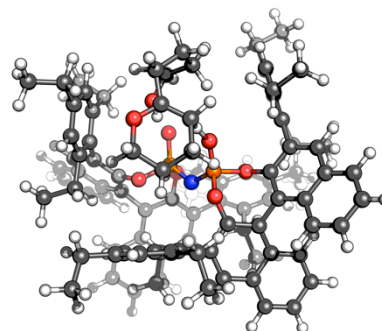
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C	1.49368	-3.86894	3.16341
C	3.50316	-0.79833	2.20889
C	4.57740	-0.79122	3.13802
C	3.55633	0.02691	1.06144
C	5.79515	-0.17355	2.78056
C	4.79817	0.60915	0.70481
C	5.90842	0.46365	1.54732
H	6.86458	0.87309	1.24454
H	-0.46244	-3.81038	4.05064
C	1.68072	-5.23799	3.41284
C	2.88872	-5.85425	3.08126
H	0.89356	-5.83039	3.86401
H	3.02661	-6.91064	3.27188
C	3.91521	-5.11282	2.49548
C	3.74421	-3.74890	2.24800

H	4.84534	-5.59719	2.22796	C	-4.65335	4.82513	1.21017
H	4.55382	-3.20793	1.77523	H	-4.30500	5.78952	-0.67480
C	6.89098	-0.21059	3.65802	C	5.00364	1.37099	-0.55334
C	6.77371	-0.82912	4.90313	C	5.07799	0.69254	-1.79849
H	7.83400	0.24845	3.38529	C	5.35954	2.74772	-0.49345
H	7.61885	-0.84893	5.57902	C	5.45465	1.39720	-2.95305
C	5.56455	-1.40993	5.28326	C	5.78388	3.40419	-1.65908
C	4.47206	-1.39107	4.41370	C	5.81698	2.74455	-2.88928
H	5.47196	-1.87519	6.25619	H	6.05269	4.45298	-1.61556
H	3.54497	-1.83225	4.75526	C	-1.15298	-1.25493	3.76864
N	-0.05755	-0.16939	-0.10349	C	-1.11190	-0.41379	4.91516
P	-1.17249	0.36002	-1.12039	C	-2.40851	-1.62373	3.21789
O	-1.04995	1.72668	-1.71360	C	-2.31434	0.03510	5.48315
O	-2.59355	0.23948	-0.30211	C	-3.58891	-1.18400	3.83465
O	-1.22951	-0.69485	-2.37039	C	-3.55044	-0.36330	4.96600
C	-3.72570	0.15130	-1.08109	H	-4.54687	-1.48438	3.42685
C	-1.68806	-1.96022	-2.09089	O	0.95774	2.11194	0.76274
C	-3.96954	-1.01781	-1.83191	H	0.42362	2.51172	-1.86094
C	-4.70980	1.16369	-1.03892	O	1.20745	3.09584	-1.97129
C	-0.88339	-3.07736	-2.37866	C	0.97870	3.94280	-3.07348
C	-3.02782	-2.15827	-1.70580	H	0.72793	3.36526	-3.97339
C	-5.09233	-1.08214	-2.69941	H	0.13454	4.61807	-2.87178
C	-5.87767	1.03490	-1.80098	C	2.25563	4.75006	-3.31052
C	-1.34725	-4.36638	-2.08486	H	2.94700	4.15867	-3.92221
C	-3.47349	-3.45292	-1.33721	H	2.02240	5.66000	-3.87760
C	-6.06176	-0.05378	-2.65308	C	2.99768	5.08957	-2.01741
C	-5.26926	-2.13600	-3.62434	H	3.93234	5.59666	-2.27516
H	-6.63607	1.80791	-1.74659	H	3.23668	4.14827	-1.52341
C	-2.61631	-4.56095	-1.53452	C	2.27054	5.98709	-0.99502
H	-0.72422	-5.22254	-2.31359	C	1.24838	5.28368	-0.15282
C	-4.75618	-3.67388	-0.79063	H	3.01458	6.41562	-0.31750
C	-7.20240	-0.12135	-3.46928	C	-0.98264	4.60799	0.01621
C	-6.40360	-2.18617	-4.43729	C	0.39025	4.56176	2.10982
H	-4.52998	-2.91693	-3.74068	C	-0.97602	4.91295	1.50393
C	-3.05723	-5.85608	-1.21921	H	-1.88670	4.92966	-0.48473
C	-5.18023	-4.96707	-0.47680	H	-0.78556	3.55413	-0.20894
H	-5.43021	-2.85155	-0.58904	H	0.36386	3.56581	2.55780
C	-7.37219	-1.18698	-4.35341	H	0.64052	5.27612	2.90032
H	-7.95639	0.65614	-3.43183	H	-1.77685	4.34785	1.98731
H	-6.52953	-3.00146	-5.13805	H	-1.19660	5.97813	1.63547
C	-4.33519	-6.05544	-0.69445	H	-4.98044	3.59089	2.93699
H	-2.41360	-6.71319	-1.37816	H	-2.29101	0.67212	6.35966
H	-6.16568	-5.12491	-0.05812	H	5.50852	0.87696	-3.90260
H	-8.25020	-1.23115	-4.98478	H	1.79116	-2.48441	-6.15583
H	-4.66879	-7.05550	-0.44970	C	-4.69262	6.11859	1.98293
C	0.43162	-2.93642	-3.04763	H	-4.65220	5.92485	3.07705
C	0.49792	-2.64711	-4.43831	C	-5.96506	6.90352	1.67664
C	1.62334	-3.23964	-2.34007	H	-6.86039	6.29806	1.93411
C	1.73984	-2.68488	-5.09203	H	-5.98062	7.83561	2.27981
C	2.84108	-3.29888	-3.03312	H	-6.00571	7.17875	0.60139
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H	3.74780	-3.55380	-2.49845	H	-4.47403	0.27171	1.51827
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H	5.63806	-4.62363	-5.81445
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H	-1.44886	-1.70924	-4.73306
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H	-0.72935	-4.30002	-6.26098
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H	-2.29324	-3.40457	-6.35709
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C	1.93075	-4.98499	-0.56607
H	1.72863	-5.20572	0.49971
H	1.28597	-5.64547	-1.18065
H	2.99524	-5.21540	-0.78233
C	-4.82881	0.09603	5.62118
H	-5.70719	-0.14579	4.98387
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C	6.20546	-1.53638	-1.89732
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H	6.85487	-1.20201	-2.73416
C	5.24849	3.56920	0.77732
H	4.70554	3.02710	1.57893
C	6.61634	4.00031	1.30442
H	6.48369	4.57743	2.24369
H	7.25368	3.12053	1.52160
H	7.13448	4.64885	0.56724
C	6.23503	3.48550	-4.13353
H	6.01969	2.88186	-5.04207
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H	8.01217	4.32254	-5.04854

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H	0.03432	0.88298	6.22185
H	-4.80492	1.20010	5.74711
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H	-3.13856	4.37154	-2.52441
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H	-0.45387	-1.79983	-6.19201
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S-anti-B_{1,4}-C(-)



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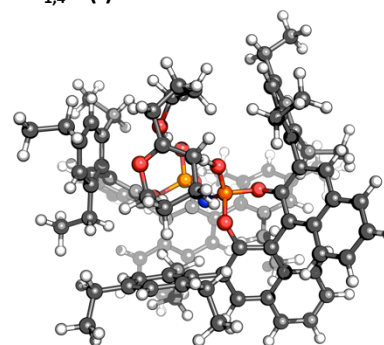
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C	-6.16747	-1.76950	0.84273
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H	-1.14625	1.63746	5.28496
C	-3.48090	2.85525	4.94767
C	-4.72990	3.40847	4.66224
H	-2.90409	3.25564	5.77297
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C	-5.48276	2.92272	3.59344

C	-5.00017	1.86903	2.81435	C	4.55780	-3.62753	-2.16043
H	-6.44376	3.36556	3.36591	C	4.73253	-4.31277	-0.95439
H	-5.60399	1.53202	1.98218	H	4.46575	-4.18776	-3.08349
C	-7.38508	-2.35076	1.23124	C	-4.12315	-1.43007	-2.31129
C	-7.74409	-2.39728	2.57855	C	-4.04036	-0.30214	-3.16877
H	-8.05299	-2.78051	0.49394	C	-3.81751	-2.72053	-2.82363
H	-8.68118	-2.85200	2.87285	C	-3.58494	-0.46731	-4.48621
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C	-5.67890	-1.28615	3.17611	C	-3.25831	-1.73294	-4.98273
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O	1.20666	-0.52501	-2.21475	C	1.43679	-2.01727	5.18063
O	2.50037	0.26937	-0.11600	C	2.56261	-0.17829	4.09326
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C	3.63336	0.81441	-0.66478	H	3.47893	0.34490	3.84552
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C	3.76167	2.21459	-0.75201	H	1.48497	-2.92917	5.76429
C	4.71408	-0.01365	-1.02422	H	-3.50175	0.39304	-5.14013
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C	5.01550	4.15707	-1.65111	C	4.90413	-1.47161	1.56878
H	6.72788	-0.09060	-1.77185	H	4.30304	-0.54178	1.59275
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C	4.10147	4.12384	1.48728	H	6.77249	-0.46592	1.07743
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H	4.19615	4.83669	-1.46082	H	4.02672	-0.48298	-3.43531
C	2.16457	6.10539	1.88355	C	5.55449	-1.65456	-4.40781
C	4.32265	5.14883	2.40965	H	5.37950	-1.13350	-5.37251
H	4.86280	3.36289	1.37438	H	6.41990	-1.17935	-3.90193
C	7.25194	3.84594	-2.52144	H	5.79645	-2.71707	-4.62132
H	7.99973	1.83900	-2.53465	C	-4.43204	4.75040	-3.68263
H	6.24323	5.74122	-2.43319	H	-4.40549	4.18806	-4.64101
C	3.36050	6.14035	2.60236	C	-4.60192	6.24038	-3.96639
H	1.42529	6.87925	2.05302	H	-4.62591	6.81183	-3.01379
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H	8.15033	4.25826	-2.96239	H	-5.55763	6.40866	-4.50608
H	3.53893	6.93433	3.31588	C	0.58054	4.73538	-3.51237
C	-0.79150	4.04363	-1.44351	H	1.36637	4.01175	-3.21964
C	-0.72957	4.44924	-2.80437	C	1.06059	6.15720	-3.23677
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C	4.61293	-1.49154	-0.98257	C	-2.71775	4.47848	1.49228
C	4.76060	-2.18758	0.24408	H	-2.66751	4.16017	2.55164
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C	3.95233	-1.91494	5.28492
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H	4.04781	-0.72971	7.10704
H	3.35365	-2.38841	7.32887
C	-1.05679	-2.26290	5.20966
H	-1.85492	-2.19540	4.44231
C	-1.57858	-1.73555	6.54221
H	-0.80251	-1.84550	7.32951
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H	-2.47626	-2.31482	6.84446
C	1.33821	1.67524	2.94735
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H	2.64816	2.78622	4.28637
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H	0.90702	2.78368	4.77670
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H	-6.47448	0.47824	-2.06304
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H	-6.38631	1.01916	-3.78708
C	-3.90721	-3.98133	-1.98443
H	-3.95881	-3.76399	-0.89826
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H	-4.27534	-0.60937	-7.31879
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H	4.02562	-2.98246	4.98409
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H	-2.35782	-2.90884	-6.56393
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H	1.69273	-5.60546	2.32979
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H	-1.60494	-3.73533	1.76189
C	1.04030	-3.40320	-3.34092
H	-0.75589	-4.19480	-4.23311
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H	1.46179	-2.17904	-1.91632
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S-anti- B_{1,4}-B(-)



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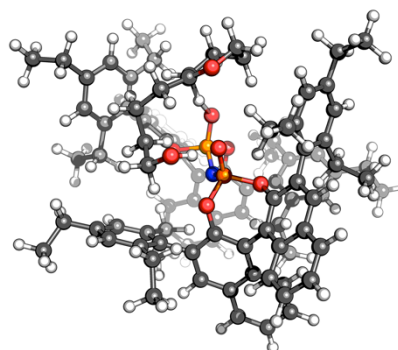
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C	-7.39900	-2.32973	1.14614	C	-4.12364	-1.33281	-2.36466
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H	-8.06895	-2.73491	0.39689	C	-3.80699	-2.61288	-2.89674
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C	-6.89890	-1.92726	3.47619	C	-3.36149	-2.71647	-4.22306
C	-5.68661	-1.33196	3.12092	C	-3.21450	-1.58228	-5.02653
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O	1.18696	-0.42344	-2.28175	C	1.37193	-2.29163	5.05310
O	2.49040	0.25819	-0.14471	C	2.55748	-0.42005	4.09166
O	1.10521	1.97206	-1.60678	C	2.57836	-1.64173	4.77251
C	3.63317	0.81470	-0.66125	H	3.48961	0.09383	3.88800
C	1.39794	2.96619	-0.70501	H	4.88125	-4.13789	1.13347
C	3.77409	2.21599	-0.69556	H	1.39005	-3.23481	5.58649
C	4.71261	-0.00841	-1.03509	H	-3.46160	0.54584	-5.14717
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C	2.68377	3.05871	-0.13354	C	4.73542	-5.81625	-0.98522
C	4.93472	2.79117	-1.27894	H	3.99619	-6.20394	-0.25130
C	5.89924	0.56658	-1.50290	C	6.12893	-6.32224	-0.62365
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C	2.93365	4.02285	0.87518	H	6.14009	-7.43210	-0.65411
C	6.01027	1.95030	-1.65598	H	6.87665	-5.93865	-1.35040
C	5.04733	4.17929	-1.51722	C	4.87231	-1.48781	1.54515
H	6.72888	-0.07511	-1.77735	H	4.25820	-0.56712	1.57985
C	1.95829	5.01337	1.14325	C	6.32816	-1.14228	1.83722
H	0.04520	5.82045	0.57648	H	6.94656	-2.06499	1.85214
C	4.13090	4.02698	1.62182	H	6.72638	-0.44718	1.06938
C	7.18139	2.50367	-2.19792	H	6.39962	-0.64993	2.82987
C	6.21522	4.71472	-2.06455	C	4.33291	-1.52568	-3.57023
H	4.23370	4.85841	-1.30191	H	4.06912	-0.45369	-3.46190
C	2.20891	6.00362	2.10647	C	5.59332	-1.63794	-4.42422
C	4.36003	5.00864	2.58835	H	5.43699	-1.10706	-5.38678
H	4.88636	3.26595	1.47525	H	6.45875	-1.17839	-3.90401
C	7.28252	3.88095	-2.39530	H	5.82366	-2.70190	-4.64326
H	8.01367	1.86955	-2.48000	C	-4.39933	4.88089	-3.53361
H	6.29054	5.78060	-2.23739	H	-4.36885	4.35115	-4.51023
C	3.40532	5.99779	2.82536	C	-4.57382	6.37894	-3.76782
H	1.47568	6.77497	2.31021	H	-4.60145	6.91817	-2.79677
H	5.28129	5.00159	3.15635	H	-3.74209	6.77880	-4.38555
H	8.18541	4.30150	-2.81892	H	-5.52912	6.56188	-4.30338
H	3.58984	6.75801	3.57327	C	0.61301	4.88066	-3.35113
C	-0.76132	4.11238	-1.31097	H	1.39707	4.14262	-3.09137
C	-0.69778	4.56541	-2.65673	C	1.09604	6.28761	-3.01174
C	-2.02605	3.87471	-0.71383	H	0.32741	7.03716	-3.29724
C	-1.88780	4.78775	-3.36639	H	1.31141	6.38048	-1.92827
C	-3.19559	4.12297	-1.44854	H	2.02945	6.50409	-3.57274
C	-3.13461	4.59293	-2.76439	C	-2.17067	3.36092	0.70190
H	-4.16146	3.95174	-0.98743	H	-1.21345	2.97171	1.10400
C	4.61035	-1.48656	-1.00947	C	-2.69013	4.45498	1.63149
C	4.73358	-2.19272	0.21423	H	-2.63668	4.10810	2.68156
C	4.50992	-2.21032	-2.22783	H	-2.07563	5.37384	1.54090

H	-3.74648	4.69885	1.39132
C	3.88643	-2.25046	5.21123
H	4.74532	-1.69455	4.77650
C	4.02568	-2.22769	6.73104
H	5.01336	-2.64523	7.01917
H	3.95734	-1.18430	7.10668
H	3.23232	-2.84153	7.20734
C	-1.12925	-2.45706	5.06997
H	-1.90773	-2.36548	4.28515
C	-1.66752	-1.93527	6.39856
H	-0.90606	-2.06176	7.19753
H	-1.93914	-0.86361	6.32168
H	-2.57642	-2.50736	6.68034
C	1.39757	1.51357	3.01032
H	0.44982	1.75168	2.48667
C	1.69462	2.61566	4.02379
H	2.73422	2.52241	4.40314
H	1.57910	3.60631	3.54409
H	0.98940	2.56379	4.87863
C	-4.48311	1.18173	-2.74244
H	-4.12188	1.40352	-1.71985
C	-6.00333	1.30290	-2.78892
H	-6.48042	0.56342	-2.11448
H	-6.30590	2.31845	-2.45970
H	-6.36865	1.14053	-3.82534
C	-3.91105	-3.89080	-2.08499
H	-3.97120	-3.69541	-0.99513
C	-5.11547	-4.72497	-2.51396
H	-5.18171	-5.63360	-1.87925
H	-6.05478	-4.14642	-2.40253
H	-5.01046	-5.04271	-3.57294
C	-2.69844	-1.70867	-6.43712
H	-1.87189	-0.98263	-6.59569
C	-3.80725	-1.45401	-7.45438
H	-3.40564	-1.58375	-8.48138
H	-4.63884	-2.17526	-7.30370
H	-4.19773	-0.41889	-7.35700
H	-0.93383	-3.54534	5.18289
H	3.94774	-3.29815	4.84519
H	4.49230	-2.14205	2.35750
H	3.48768	-1.99542	-4.11480
H	4.46009	-6.22688	-1.98112
H	-2.28358	-2.72510	-6.61422
H	-2.99853	-4.50017	-2.23616
H	-4.05385	1.96458	-3.40196
H	-5.28884	4.50942	-2.98113
H	0.48781	4.81184	-4.45392
H	-2.88058	2.50804	0.70529
H	2.19162	1.50419	2.23535
O	-1.08599	-2.15451	-0.64013
C	0.67347	-4.89863	-0.46554
C	1.44942	-3.80649	1.45934
C	1.03557	-5.65401	-1.70254
C	0.40943	-4.57871	2.24885
H	1.10923	-2.79693	1.19789
H	2.41686	-3.74705	1.95476
C	0.03240	-5.59074	-2.86275

H	2.01693	-5.29927	-2.01872
H	1.14691	-6.69923	-1.37653
C	-0.91063	-4.55391	1.48218
H	0.30289	-4.15202	3.24364
H	0.77431	-5.60550	2.37098
C	-0.25165	-4.18159	-3.39693
H	-0.90455	-6.08703	-2.58335
H	0.46501	-6.19639	-3.66795
H	-1.54207	-5.39391	1.78578
H	-1.45303	-3.63015	1.70376
C	1.00467	-3.33403	-3.52719
H	-0.74888	-4.27235	-4.36925
H	-0.91902	-3.62861	-2.72870
O	1.50231	-3.03358	-2.23929
H	1.77552	-3.87766	-4.09759
H	0.77958	-2.40753	-4.06815
H	1.41714	-2.05919	-2.12703
O	1.70549	-4.51734	0.22711
C	-0.63977	-4.64666	-0.02723
H	-0.75413	-3.41118	-0.39976
H	-1.39248	-5.16810	-0.61302

S-anti- B_{1,4}-C(+)



E(RM062X) = -5098.38411377

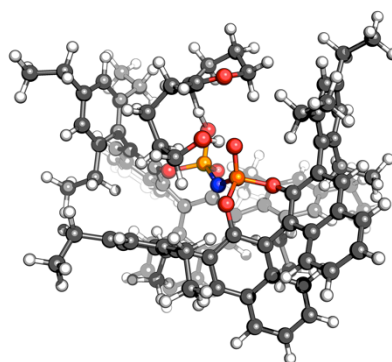
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C	-0.91005	0.88747	3.64030
C	-3.04632	0.68225	2.49620
C	-1.33666	2.08966	4.21737
C	-3.45419	1.93300	3.02633
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C	-4.00076	-0.23090	1.81408
C	-5.17428	-0.70224	2.46172
C	-3.69786	-0.66942	0.50857
C	-6.11334	-1.46342	1.72481
C	-4.63354	-1.44386	-0.20325
C	-5.84553	-1.80243	0.39727
H	-6.56671	-2.38356	-0.16674
H	-0.70225	2.58870	4.93994
C	-2.98622	3.85342	4.46122
C	-4.24141	4.38635	4.16378
H	-2.33143	4.39327	5.13503

H	-4.54619	5.32789	4.60187	C	5.07330	-2.44103	-1.74506
C	-5.10015	3.71248	3.29536	C	5.55748	-3.12830	0.93459
C	-4.71169	2.49889	2.72348	C	5.45612	-3.74608	-1.39748
H	-6.06695	4.13632	3.05667	C	5.71850	-4.09026	-0.06771
H	-5.39371	2.01755	2.03504	H	5.55486	-4.49728	-2.17220
C	-7.30172	-1.89842	2.33326	C	-4.34587	-1.96884	-1.55756
C	-7.55111	-1.61038	3.67523	C	-4.48750	-1.13636	-2.69571
H	-8.03167	-2.47202	1.77424	C	-4.08753	-3.35338	-1.73283
H	-8.46656	-1.95224	4.14062	C	-4.37645	-1.69246	-3.97964
C	-6.61346	-0.90006	4.42334	C	-4.04394	-3.88564	-3.02893
C	-5.43074	-0.45487	3.82918	C	-4.17370	-3.06482	-4.15285
H	-6.80123	-0.69667	5.46978	H	-3.90319	-4.95034	-3.16459
H	-4.71903	0.06794	4.45329	C	0.38162	0.30539	4.07532
N	-0.00788	0.10590	0.11120	C	0.40030	-0.78518	4.98583
P	1.06593	0.04920	-1.03773	C	1.60595	0.88764	3.65831
O	1.06276	-1.10865	-2.01931	C	1.63128	-1.28890	5.43349
O	2.51895	0.10364	-0.27497	C	2.81684	0.37829	4.15086
O	0.94082	1.36025	-2.00334	C	2.83818	-0.70631	5.03375
C	3.58222	0.68874	-0.92829	H	3.74957	0.83957	3.84943
C	1.13300	2.57111	-1.38239	H	5.74760	-3.40084	1.96639
C	3.55258	2.06164	-1.26365	H	1.65136	-2.13087	6.11536
C	4.78534	-0.03197	-1.10495	H	-4.49114	-1.05701	-4.85018
C	0.14253	3.56931	-1.44639	H	-2.04195	3.61256	-5.57048
C	2.39334	2.89018	-0.84939	C	6.13725	-5.49280	0.29064
C	4.63103	2.63705	-1.98917	H	5.48806	-5.87620	1.10740
C	5.89946	0.59110	-1.67992	C	7.59750	-5.53307	0.73294
C	0.33467	4.78289	-0.77082	H	7.74694	-4.91928	1.64644
C	2.56377	4.08188	-0.10147	H	7.88814	-6.58022	0.96049
C	5.82109	1.89557	-2.16304	H	8.25428	-5.14971	-0.07719
C	4.55398	3.93096	-2.55393	C	5.08308	-0.81844	1.75510
H	6.82667	0.03796	-1.77865	H	4.37043	-0.00192	1.53212
C	1.51477	5.02955	-0.06491	C	6.45046	-0.21763	2.06039
H	-0.42363	5.55331	-0.83021	H	7.16701	-1.01511	2.35108
C	3.76275	4.36504	0.58710	H	6.84178	0.32173	1.17201
C	6.91965	2.46650	-2.82583	H	6.35964	0.50201	2.90111
C	5.64938	4.48320	-3.22098	C	4.80301	-2.14463	-3.20874
H	3.64701	4.51791	-2.50258	H	4.28015	-1.17549	-3.34676
C	1.68451	6.23944	0.62686	C	6.08931	-2.13749	-4.03205
C	3.91740	5.57132	1.27412	H	5.84835	-1.90735	-5.09120
H	4.57755	3.65288	0.61030	H	6.79263	-1.36707	-3.65750
C	6.83267	3.75727	-3.34762	H	6.58453	-3.13051	-3.99315
H	7.84075	1.90954	-2.95138	C	-4.62819	3.62359	-4.75398
H	5.57852	5.47696	-3.64414	H	-4.37952	3.48412	-5.82867
C	2.88254	6.50700	1.29177	C	-5.29711	4.98455	-4.58515
H	0.89250	6.97858	0.65035	H	-5.62740	5.12963	-3.53471
H	4.84054	5.77834	1.79971	H	-4.59113	5.79611	-4.86338
H	7.67985	4.19041	-3.86353	H	-6.18718	5.04519	-5.24620
H	3.00728	7.44005	1.82580	C	0.37740	3.63052	-4.42626
C	-1.06543	3.41894	-2.29444	H	1.13704	2.94883	-3.99858
C	-0.95547	3.49920	-3.71128	C	0.89253	5.06691	-4.39401
C	-2.35274	3.36377	-1.69740	H	0.14230	5.75442	-4.83949
C	-2.12142	3.53052	-4.49276	H	1.11083	5.38774	-3.35616
C	-3.49478	3.42490	-2.51034	H	1.83181	5.13622	-4.98216
C	-3.38788	3.51984	-3.90140	C	-2.54999	3.25514	-0.19928
H	-4.47815	3.39809	-2.05558	H	-1.60540	3.01121	0.32980
C	4.93054	-1.45800	-0.72776	C	-3.12266	4.54966	0.37626
C	5.16762	-1.81662	0.62377	H	-3.01808	4.54569	1.47900

H	-2.58318	5.43561	-0.01509
H	-4.19892	4.64283	0.11913
C	4.14798	-1.24621	5.55182
H	5.00584	-0.77062	5.02884
C	4.30195	-0.98758	7.04831
H	5.29140	-1.35901	7.38881
H	4.23944	0.10172	7.25765
H	3.51230	-1.51715	7.62195
C	-0.86816	-1.43123	5.50877
H	-1.62654	-1.53603	4.70756
C	-1.45283	-0.64097	6.67522
H	-0.70656	-0.55603	7.49371
H	-1.75666	0.37472	6.35165
H	-2.35018	-1.16590	7.06510
C	1.66237	2.06779	2.71260
H	0.69956	2.22720	2.18445
C	2.03340	3.34424	3.46424
H	3.10617	3.32504	3.75077
H	1.85082	4.22446	2.81819
H	1.41746	3.45945	4.37948
C	-4.81731	0.33241	-2.58269
H	-4.35811	0.78174	-1.68125
C	-6.32524	0.55649	-2.54901
H	-6.77517	0.04575	-1.67223
H	-6.53736	1.64350	-2.47093
H	-6.79266	0.16847	-3.47902
C	-3.82426	-4.28728	-0.56685
H	-3.65188	-3.73331	0.37904
C	-4.97709	-5.26621	-0.35723
H	-4.75753	-5.91406	0.51732
H	-5.92218	-4.71903	-0.16189
H	-5.10925	-5.91402	-1.24913
C	-4.09079	-3.65816	-5.53580
H	-4.00445	-2.85770	-6.30262
C	-5.32698	-4.49696	-5.84889
H	-5.25333	-4.89576	-6.88248
H	-5.40778	-5.35303	-5.14595
H	-6.24317	-3.87294	-5.77281
H	-0.65632	-2.46466	5.86051
H	4.20110	-2.33861	5.35375
H	4.69679	-1.32656	2.66281
H	4.12877	-2.92407	-3.62017
H	6.01364	-6.17486	-0.57870
H	-3.18031	-4.29106	-5.61366
H	-2.89170	-4.85926	-0.76331
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H	-5.34615	2.82369	-4.47659
H	0.27264	3.32752	-5.49107
H	-3.24969	2.42055	0.01696
H	2.41949	1.87082	1.92426
O	-1.05129	-2.35958	0.05579
C	0.79292	-4.57073	-1.46345
C	-0.61128	-4.97026	-3.35252
C	1.15390	-5.16501	-0.14169
C	-0.22269	-3.60792	-3.87793
H	-0.07464	-5.76752	-3.87881
H	-1.67317	-5.18220	-3.40273

C	2.18139	-4.43543	0.72180
H	1.55045	-6.15351	-0.42568
H	0.23159	-5.34829	0.41536
C	1.27696	-3.43222	-3.65723
H	-0.77306	-2.82696	-3.34039
H	-0.48999	-3.54800	-4.93716
C	1.66447	-3.19067	1.44087
H	2.55142	-5.15210	1.46515
H	3.04111	-4.16838	0.10376
H	1.59592	-2.43225	-3.95660
H	1.83625	-4.16375	-4.25414
C	0.63152	-3.48712	2.52981
H	1.24593	-2.48562	0.71572
H	2.50867	-2.67914	1.91955
O	-0.52411	-4.16745	2.07839
H	1.08356	-4.12899	3.29673
H	0.34474	-2.54244	2.99907
H	-0.95269	-3.58650	1.42127
C	1.54490	-3.61085	-2.16639
O	-0.28103	-5.12751	-1.94904
H	2.57690	-3.57453	-1.82896
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S-anti- B_{1,4}-B(+)



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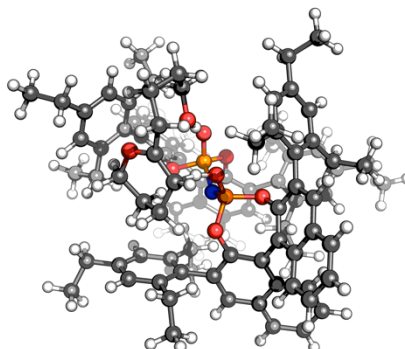
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C	-0.81020	0.35254	3.68084
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C	-3.71445	-0.71508	0.44359
C	-6.11283	-1.60794	1.63264
C	-4.70289	-1.35563	-0.33130
C	-5.90625	-1.75625	0.26092
H	-6.66860	-2.22674	-0.35008
H	-0.54916	1.84072	5.21255
C	-2.81659	3.19769	4.97177
C	-4.06988	3.78345	4.78671

H	-2.13845	3.62493	5.70100	C	5.20926	-1.89520	0.30096
H	-4.34992	4.65450	5.36482	C	5.08978	-2.18002	-2.13026
C	-4.95916	3.25330	3.85195	C	5.62175	-3.23142	0.41910
C	-4.60255	2.13175	3.09981	C	5.48439	-3.51845	-1.97457
H	-5.92480	3.71855	3.70218	C	5.76927	-4.04358	-0.71010
H	-5.30769	1.76387	2.36611	H	5.57728	-4.15231	-2.84855
C	-7.29102	-2.09508	2.22122	C	-4.48767	-1.70416	-1.75426
C	-7.47985	-1.99950	3.60005	C	-4.63417	-0.72158	-2.76478
H	-8.05972	-2.56160	1.61640	C	-4.31588	-3.06462	-2.12274
H	-8.38751	-2.38131	4.04939	C	-4.60379	-1.10482	-4.11470
C	-6.49186	-1.43103	4.40259	C	-4.34606	-3.41886	-3.47979
C	-5.31895	-0.93536	3.82924	C	-4.47450	-2.44870	-4.47767
H	-6.63290	-1.37750	5.47446	H	-4.23827	-4.45886	-3.76453
H	-4.56722	-0.52825	4.49159	C	0.47592	-0.30741	4.00535
N	-0.02123	0.09255	0.04834	C	0.48592	-1.52183	4.74273
P	1.06861	0.19174	-1.08107	C	1.70454	0.32395	3.68296
O	1.07280	-0.81808	-2.21944	C	1.71272	-2.09515	5.11052
O	2.52185	0.12772	-0.31862	C	2.91053	-0.25779	4.10084
O	0.94831	1.62522	-1.85012	C	2.92355	-1.46351	4.80953
C	3.58909	0.79844	-0.88003	H	3.84602	0.24181	3.88043
C	1.14364	2.73403	-1.06130	H	5.82971	-3.64361	1.39986
C	3.56013	2.20477	-1.02404	H	1.72615	-3.02777	5.66220
C	4.79485	0.11113	-1.15411	H	-4.71999	-0.35331	-4.88706
C	0.15422	3.73193	-0.97319	H	-2.08422	4.36175	-5.01977
C	2.40647	2.97030	-0.49284	C	6.19776	-5.48032	-0.55736
C	4.63588	2.87484	-1.66759	H	5.55954	-5.97813	0.20455
C	5.90779	0.80941	-1.63833	C	7.66320	-5.57497	-0.14118
C	0.35494	4.83699	-0.13331	H	7.82091	-5.09589	0.84834
C	2.58587	4.04417	0.41452	H	7.96024	-6.64231	-0.06715
C	5.82650	2.16630	-1.94174	H	8.30917	-5.07740	-0.89605
C	4.55556	4.23317	-2.05199	C	5.12156	-1.06943	1.56213
H	6.83590	0.27663	-1.81269	H	4.40755	-0.23059	1.45598
C	1.54021	4.97899	0.59220	C	6.48722	-0.51541	1.95203
H	-0.40144	5.60940	-0.07679	H	7.20503	-1.34450	2.12882
C	3.79142	4.22633	1.12578	H	6.87871	0.14458	1.14922
C	6.92265	2.82316	-2.52403	H	6.39359	0.07829	2.88564
C	5.64838	4.87232	-2.64118	C	4.80899	-1.67844	-3.53485
H	3.64782	4.80613	-1.91933	H	4.28262	-0.70145	-3.53066
C	1.71820	6.07863	1.44683	C	6.08972	-1.54970	-4.35687
C	3.95514	5.32414	1.97365	H	5.84103	-1.17218	-5.37100
H	4.60460	3.51686	1.04231	H	6.79343	-0.83781	-3.88086
C	6.83238	4.17218	-2.86735	H	6.58786	-2.53639	-4.46278
H	7.84423	2.28978	-2.72549	C	-4.65930	4.27286	-4.17240
H	5.57496	5.91390	-2.92635	H	-4.42542	4.29247	-5.25920
C	2.92240	6.24873	2.13233	C	-5.32050	5.59569	-3.79639
H	0.92829	6.80819	1.58074	H	-5.63787	5.58512	-2.73207
H	4.88330	5.45416	2.51488	H	-4.61455	6.43777	-3.96056
H	7.67755	4.67229	-3.32238	H	-6.21819	5.75526	-4.43011
H	3.05385	7.09721	2.79121	C	0.35021	4.21008	-3.91822
C	-1.06494	3.70366	-1.81802	H	1.11256	3.47319	-3.60149
C	-0.97355	3.98225	-3.21078	C	0.87172	5.62630	-3.69015
C	-2.34465	3.57224	-1.21626	H	0.11843	6.37164	-4.02330
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C	-3.49693	3.75311	-1.99595	H	1.80327	5.77611	-4.27560
C	-3.40828	4.04185	-3.36126	C	-2.52291	3.25913	0.25531
H	-4.47397	3.67009	-1.53458	H	-1.57300	2.94059	0.73265
C	4.94733	-1.35301	-0.98275	C	-3.08056	4.46451	1.01154

H	-2.94650	4.31601	2.10106
H	-2.55278	5.39694	0.72676
H	-4.16327	4.58645	0.79700
C	4.22845	-2.07709	5.25222
H	5.09085	-1.53631	4.80556
C	4.37493	-2.03212	6.77097
H	5.36038	-2.45357	7.06109
H	4.31703	-0.98258	7.13086
H	3.57887	-2.63194	7.26046
C	-0.78749	-2.21581	5.18761
H	-1.56246	-2.18482	4.39622
C	-1.33584	-1.59877	6.47056
H	-0.57467	-1.65130	7.27802
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H	-2.23776	-2.15933	6.79486
C	1.77011	1.63152	2.92303
H	0.80663	1.87755	2.43045
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H	1.96604	3.74765	3.35131
H	1.56566	2.75481	4.78780
C	-4.89355	0.73043	-2.44444
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C	-6.38906	1.00998	-2.34078
H	-6.84279	0.40014	-1.53162
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H	-6.89215	0.77521	-3.30294
C	-4.06393	-4.15902	-1.10132
H	-3.83534	-3.74688	-0.09673
C	-5.25533	-5.10665	-0.98335
H	-5.04081	-5.87561	-0.21162
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H	-6.62414	-2.97881	-6.10867
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H	4.27869	-3.13085	4.90239
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H	-3.22440	2.40542	0.36437
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C	0.84470	-4.27491	-1.90248
C	-0.97760	-3.79666	-3.28697
C	1.38728	-5.14384	-0.81085
C	-0.03761	-3.75910	-4.47724
H	-1.88697	-4.34178	-3.51537

H	-1.20109	-2.80473	-2.87781
C	2.28532	-4.43096	0.20680
H	1.98356	-5.90467	-1.33744
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C	1.26810	-3.06844	-4.08831
H	-0.53221	-3.24372	-5.30506
H	0.14642	-4.79168	-4.79592
C	1.58470	-3.39830	1.08782
H	2.74725	-5.20153	0.83546
H	3.09599	-3.93714	-0.33132
H	1.20477	-1.99283	-4.27185
H	2.08702	-3.46159	-4.69747
C	0.47466	-3.96580	1.97217
H	1.17478	-2.59689	0.46334
H	2.33408	-2.92909	1.73847
O	-0.60450	-4.53233	1.25405
H	0.87932	-4.76602	2.60506
H	0.10901	-3.16836	2.62502
H	-0.98166	-3.82663	0.69490
C	1.58500	-3.30504	-2.59956
O	-0.38188	-4.55879	-2.21687
H	2.63871	-3.34789	-2.34320
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S-gau-C₄-C(-)



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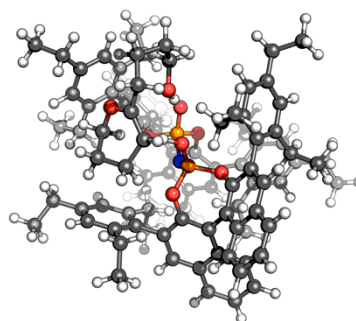
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C	-3.58611	-0.16096	2.13010
C	-2.47214	1.14246	4.36222
C	-4.32030	0.85510	2.79409
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C	-5.32561	-1.82083	1.27209
C	-3.55668	-1.02036	-0.20896
C	-5.88755	-2.53833	0.18409
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C	-5.29279	-2.47393	-1.08085
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H	-4.06619	2.96574	5.48775	C	5.31072	-1.46133	0.61837
H	-6.30161	3.62410	4.69395	C	4.89639	-1.70365	-1.78676
C	-6.29900	2.25956	3.03265	C	5.67157	-2.81589	0.67433
C	-5.59368	1.26813	2.34743	C	5.22083	-3.06517	-1.68695
H	-7.27497	2.56783	2.68067	C	5.61319	-3.62496	-0.46649
H	-6.04438	0.84244	1.46079	H	5.18156	-3.68926	-2.57187
C	-7.02875	-3.33223	0.38006	C	-3.45089	-1.76906	-2.60155
C	-7.60185	-3.44024	1.64739	C	-3.51730	-0.64945	-3.46826
H	-7.47106	-3.87791	-0.44513	C	-2.70830	-2.91214	-2.99590
H	-8.47902	-4.05739	1.79297	C	-2.79928	-0.66329	-4.67450
C	-7.03645	-2.76857	2.73050	C	-2.00357	-2.89415	-4.20964
C	-5.90428	-1.97091	2.55132	C	-2.03882	-1.77589	-5.04725
H	-7.47414	-2.87014	3.71525	H	-1.41991	-3.75906	-4.50129
H	-5.48298	-1.48859	3.42260	C	-0.35928	-0.15483	4.13461
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P	1.16199	0.34714	-0.83977	C	0.74479	0.68552	3.84255
O	1.32545	-0.65431	-1.92944	C	1.13129	-1.64603	5.35805
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C	3.54892	1.20171	-0.45503	H	2.86911	0.96855	4.05907
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C	4.77240	0.57219	-0.74860	H	-2.83595	0.19573	-5.33440
C	-0.09520	3.83159	-0.69847	H	-2.14038	4.59566	-4.81498
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H	6.78514	0.82169	-1.46158	H	4.62251	0.18555	1.87074
C	1.10308	5.16674	0.94581	C	6.74223	-0.11422	2.16945
H	-0.84800	5.64577	0.18367	H	7.46951	-0.94909	2.25908
C	3.36271	4.56769	1.61804	H	7.05972	0.56183	1.34790
C	6.77690	3.40826	-2.04839	H	6.74008	0.45925	3.12025
C	5.42044	5.40765	-2.08997	C	4.51497	-1.15226	-3.14827
H	3.42425	5.23566	-1.37536	H	4.03936	-0.15264	-3.07570
C	1.14102	6.25677	1.83000	C	5.73150	-1.04813	-4.06405
C	3.37963	5.64291	2.50923	H	5.42371	-0.62333	-5.04263
H	4.23250	3.92501	1.57109	H	6.49862	-0.38318	-3.61554
C	6.63128	4.76424	-2.34185	H	6.17530	-2.05088	-4.23935
H	7.71880	2.92044	-2.27023	C	-4.74903	4.30593	-4.11962
H	5.30510	6.45505	-2.33764	H	-4.46315	4.42328	-5.18763
C	2.27474	6.48871	2.61055	C	-5.50090	5.55836	-3.67864
H	0.29054	6.92138	1.92529	H	-5.86505	5.44809	-2.63511
H	4.25352	5.82192	3.12213	H	-4.83719	6.44702	-3.74348
H	7.45462	5.31429	-2.77899	H	-6.37639	5.71887	-4.34243
H	2.29520	7.32375	3.29877	C	0.23874	4.45916	-3.59909
C	-1.25415	3.74006	-1.62066	H	1.03135	3.77394	-3.24204
C	-1.10651	4.12465	-2.98253	C	0.63922	5.90455	-3.31736
C	-2.55292	3.48047	-1.10828	H	-0.13991	6.60041	-3.69518
C	-2.24845	4.27557	-3.78521	H	0.78183	6.07115	-2.23099
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C	-3.52946	4.07704	-3.26229	C	-2.78667	3.00976	0.31103
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C	-3.46308	4.08866	1.15433
H	-3.48774	3.77048	2.21509
H	-2.90679	5.04547	1.09432
H	-4.50615	4.25315	0.81117
C	3.60655	-1.19847	5.52822
H	4.37293	-0.54265	5.06064
C	3.72497	-1.06671	7.04409
H	4.76178	-1.31087	7.35763
H	3.49417	-0.02613	7.35770
H	3.02949	-1.76621	7.55416
C	-1.29536	-2.26160	5.26691
H	-2.05433	-2.31112	4.45973
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H	-1.22151	-1.81564	7.39473
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H	-2.77897	-2.52569	6.82232
C	0.59610	1.97852	3.07432
H	-0.35462	2.01778	2.50822
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H	-0.07353	3.05383	4.84794
C	-4.36348	0.56141	-3.14952
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C	-5.83744	0.30500	-3.44788
H	-6.23158	-0.51993	-2.82141
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H	-5.97170	0.04544	-4.51964
C	-2.60869	-4.15554	-2.13965
H	-2.95859	-3.98797	-1.10123
C	-3.40227	-5.31079	-2.74119
H	-3.31722	-6.20030	-2.08201
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H	-3.00607	-5.57722	-3.74385
C	-1.26510	-1.76646	-6.34076
H	-0.66228	-0.83489	-6.40567
C	-2.20190	-1.85619	-7.54230
H	-1.60471	-1.87686	-8.47813
H	-2.80862	-2.78535	-7.48686
H	-2.88015	-0.97737	-7.57637
H	-0.91506	-3.29878	5.39424
H	3.83310	-2.24337	5.22435
H	5.03147	-1.29914	2.75135
H	3.76165	-1.81379	-3.62253
H	5.64350	-5.62325	-1.30328
H	-0.55635	-2.62244	-6.38119
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H	-5.42561	3.42795	-4.05354
H	0.19764	4.31837	-4.70141
H	-3.43483	2.10930	0.28898
H	1.41036	2.05491	2.32486
O	-0.84575	-2.33445	-0.33884
C	0.79626	-5.18873	0.06143
C	2.40407	-4.10170	1.48373
C	0.65011	-6.24148	-0.99315
C	1.28205	-3.23782	2.01582

H	3.21783	-3.49289	1.10728
H	2.78375	-4.79400	2.24158
C	1.65882	-6.25961	-2.15132
H	0.76016	-7.17399	-0.41687
H	-0.37763	-6.23962	-1.36053
C	0.00239	-4.05872	2.13677
H	1.12243	-2.38219	1.35221
H	1.61147	-2.84142	2.97730
C	1.32687	-5.33265	-3.32617
H	1.69197	-7.29027	-2.51970
H	2.66029	-6.03286	-1.76667
H	0.12491	-4.85369	2.88437
H	-0.82404	-3.42183	2.45188
H	1.89661	-5.65951	-4.20402
H	0.26329	-5.42509	-3.57961
O	2.03733	-4.94303	0.35842
C	-0.29034	-4.63422	0.75804
H	-0.51875	-3.52782	0.08818
H	-1.22066	-5.18323	0.61692
C	1.65959	-3.87606	-3.05631
H	2.74382	-3.79129	-2.89527
H	1.39658	-3.25608	-3.92311
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RSgau-C₄-B(-)



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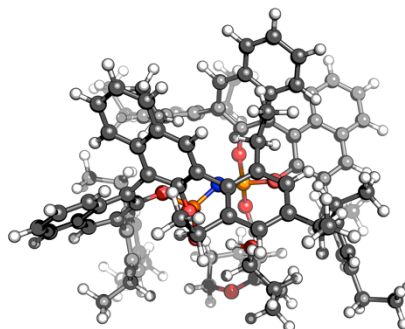
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C	-4.24909	-1.62901	-1.07650
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H	-3.61362	3.25726	5.53927	C	5.13063	-1.64643	0.50731
H	-5.85469	4.00296	4.84439	C	4.77738	-1.82632	-1.91266
C	-6.00046	2.60520	3.21720	C	5.39175	-3.02324	0.55218
C	-5.37721	1.56809	2.51993	C	5.00429	-3.20840	-1.82483
H	-6.97838	2.95111	2.90838	C	5.31784	-3.81040	-0.60206
H	-5.89161	1.14461	1.66747	H	4.95128	-3.81615	-2.72038
C	-7.13647	-3.00868	0.79727	C	-3.65868	-1.75276	-2.43180
C	-7.64217	-3.04228	2.09699	C	-3.74531	-0.67755	-3.35137
H	-7.65228	-3.55774	0.01828	C	-3.00490	-2.95074	-2.82060
H	-8.54067	-3.60580	2.31298	C	-3.15709	-0.80152	-4.62008
C	-6.98195	-2.36629	3.12206	C	-2.42587	-3.04142	-4.09571
C	-5.82215	-1.63704	2.85171	C	-2.49947	-1.97647	-4.99775
H	-7.36739	-2.41123	4.13254	H	-1.91549	-3.95195	-4.38684
H	-5.32740	-1.15050	3.68093	C	-0.14264	-0.08971	4.09254
N	0.03208	0.20156	0.23121	C	0.02814	-1.29662	4.81975
P	1.15700	0.36318	-0.90274	C	0.98983	0.70825	3.78852
O	1.27661	-0.66398	-1.97452	C	1.31285	-1.67296	5.23995
O	2.51564	0.46099	0.01485	C	2.26303	0.29315	4.20889
O	0.96281	1.81845	-1.64147	C	2.43030	-0.88615	4.94187
C	3.57600	1.12959	-0.54291	H	3.12775	0.90242	3.97204
C	1.07893	2.93628	-0.84654	H	5.63157	-3.49147	1.49999
C	3.52699	2.52897	-0.68643	H	1.44593	-2.58891	5.80377
C	4.76347	0.43837	-0.84052	H	-3.21894	0.01891	-5.32567
C	0.03328	3.87933	-0.79841	H	-2.08531	4.58396	-4.88943
C	2.30967	3.24973	-0.23341	C	5.55317	-5.29687	-0.52041
C	4.61885	3.21467	-1.28503	H	4.91481	-5.72921	0.28029
C	5.87814	1.13175	-1.32268	C	7.01930	-5.60716	-0.23142
C	0.13991	4.99586	0.04188	H	7.32055	-5.19254	0.75388
C	2.38343	4.32189	0.69021	H	7.16899	-6.70711	-0.21082
C	5.81031	2.50411	-1.57073	H	7.66640	-5.17452	-1.02422
C	4.55150	4.58391	-1.62834	C	5.18796	-0.86490	1.80143
H	6.79010	0.58698	-1.54101	H	4.53485	0.03029	1.76939
C	1.28358	5.20177	0.81621	C	6.61511	-0.43392	2.11842
H	-0.66205	5.72368	0.06698	H	7.27389	-1.32281	2.21743
C	3.52820	4.54412	1.48428	H	7.00633	0.22549	1.31512
C	6.91499	3.17196	-2.12303	H	6.62834	0.12696	3.07667
C	5.65579	5.23347	-2.18406	C	4.47009	-1.23318	-3.27543
H	3.64649	5.15915	-1.48950	H	4.06191	-0.20434	-3.20089
C	1.35889	6.30117	1.68629	C	5.71409	-1.20257	-4.15936
C	3.58272	5.63059	2.36022	H	5.46167	-0.74529	-5.13912
H	4.37742	3.87424	1.44344	H	6.51393	-0.59848	-3.68302
C	6.83724	4.53245	-2.42125	H	6.09184	-2.23147	-4.33780
H	7.83432	2.63886	-2.33512	C	-4.68223	4.32469	-4.14152
H	5.59289	6.28421	-2.43639	H	-4.41562	4.41388	-5.21722
C	2.50435	6.51051	2.45602	C	-5.41058	5.59606	-3.71563
H	0.52863	6.99132	1.77857	H	-5.75585	5.51413	-2.66311
H	4.46481	5.79104	2.96647	H	-4.73784	6.47482	-3.81366
H	7.69019	5.04120	-2.85158	H	-6.29674	5.75197	-4.36626
H	2.55368	7.35348	3.13302	C	0.31422	4.46622	-3.71098
C	-1.14615	3.79259	-1.69412	H	1.11198	3.78883	-3.34988
C	-1.02121	4.14748	-3.06591	C	0.71915	5.91727	-3.46717
C	-2.43616	3.55185	-1.15203	H	-0.06482	6.60511	-3.84970
C	-2.17644	4.28484	-3.85173	H	0.87621	6.10767	-2.38658
C	-3.56891	3.71426	-1.96426	H	1.66991	6.13075	-3.99949
C	-3.44873	4.10116	-3.30253	C	-2.64626	3.12625	0.28556

H	-1.69619	2.82603	0.77215
C	-3.29460	4.23962	1.10584
H	-3.29344	3.96110	2.17780
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H	-4.34512	4.39833	0.78317
C	3.80100	-1.31120	5.40494
H	4.58628	-0.66429	4.95692
C	3.92356	-1.22581	6.92402
H	4.95376	-1.50575	7.22928
H	3.71994	-0.18903	7.26754
H	3.21075	-1.92135	7.41523
C	-1.13728	-2.18999	5.19319
H	-1.88611	-2.23856	4.37715
C	-1.80700	-1.71061	6.47664
H	-1.07413	-1.70093	7.31144
H	-2.22335	-0.69104	6.34484
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C	0.88263	2.01180	3.02991
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H	0.33564	3.12129	4.82463
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H	-6.39192	-0.33526	-2.54360
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H	-6.20722	0.16654	-4.27192
C	-2.87247	-4.14247	-1.89882
H	-3.10360	-3.88937	-0.84441
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H	-3.66478	-6.13917	-1.63073
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H	-3.50570	-5.63711	-3.35419
C	-1.87919	-2.09192	-6.36657
H	-1.24388	-1.20139	-6.56298
C	-2.95154	-2.20610	-7.44683
H	-2.46817	-2.32128	-8.43975
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H	-5.36861	3.45778	-4.04268
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H	-3.30452	2.23303	0.30403
H	1.67329	2.04595	2.25259
O	-0.84192	-2.27569	-0.29680
C	0.69061	-5.17525	-0.00185
C	2.11738	-3.92650	1.37537
C	0.56609	-6.22789	-1.05665

C	1.26634	-4.34337	2.55867
H	1.86316	-2.92898	0.99704
H	3.17797	-3.98774	1.59709
C	1.55051	-6.20646	-2.23485
H	0.71022	-7.15898	-0.48538
H	-0.46735	-6.25270	-1.40809
C	-0.20708	-4.23818	2.17950
H	1.51017	-3.71313	3.41486
H	1.53496	-5.37364	2.82209
C	1.13453	-5.31152	-3.40905
H	1.63332	-7.23791	-2.59274
H	2.54560	-5.91685	-1.87717
H	-0.81215	-4.88399	2.82250
H	-0.55972	-3.21469	2.32189
H	1.67673	-5.62833	-4.30743
H	0.06432	-5.44543	-3.61300
O	1.91736	-4.86457	0.29175
C	-0.40685	-4.65154	0.71256
H	-0.56429	-3.51606	0.11867
H	-1.33517	-5.17449	0.49001
C	1.42191	-3.84151	-3.16501
H	2.50728	-3.70880	-3.06137
H	1.08753	-3.23575	-4.01735
O	0.75817	-3.46189	-1.98611
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S-gau-C₄-C(+)



E(RM062X) = -5098.37797379

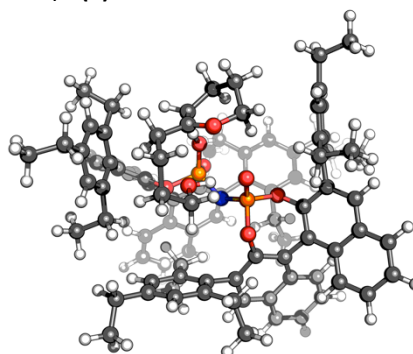
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C	-3.78024	-0.75884	0.42476
C	-6.22072	-1.54699	1.60116
C	-4.72264	-1.50664	-0.31037
C	-5.95581	-1.83623	0.26272
H	-6.68514	-2.38253	-0.32451

H	-0.76104	2.16378	5.07997	C	-3.51670	3.50582	-3.85824
C	-3.02621	3.48979	4.69469	H	-4.67480	3.25312	-2.06788
C	-4.27841	4.05303	4.44477	C	5.02204	-1.11210	-0.83217
H	-2.36821	3.96693	5.41135	C	5.22431	-1.64423	0.46682
H	-4.57733	4.95631	4.96065	C	5.31563	-1.91910	-1.96903
C	-5.14356	3.45691	3.52753	C	5.71288	-2.95147	0.61277
C	-4.76169	2.29439	2.85410	C	5.78532	-3.22938	-1.78429
H	-6.10901	3.90353	3.32804	C	6.00213	-3.74412	-0.50200
H	-5.44711	1.87664	2.12855	H	5.99038	-3.84969	-2.64871
C	-7.42002	-1.98297	2.18708	C	-4.39685	-2.08721	-1.63329
C	-7.65822	-1.76813	3.54440	C	-4.43380	-1.28614	-2.80136
H	-8.16496	-2.50617	1.59905	C	-4.16852	-3.48595	-1.74869
H	-8.58107	-2.11295	3.99269	C	-4.22776	-1.88068	-4.05569
C	-6.69790	-1.13250	4.32968	C	-3.97886	-4.04889	-3.01984
C	-5.50477	-0.68568	3.75774	C	-4.01448	-3.25794	-4.17297
H	-6.87576	-0.98960	5.38778	H	-3.79821	-5.11341	-3.11305
H	-4.77554	-0.22609	4.41044	C	0.32002	-0.03784	4.01438
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P	1.06506	0.14389	-1.03793	C	1.54126	0.61522	3.70447
O	1.18080	-0.94063	-2.10127	C	1.57459	-1.76556	5.19462
O	2.48654	0.24202	-0.23478	C	2.75025	0.07589	4.16722
O	0.87918	1.50877	-1.92105	C	2.77574	-1.10940	4.90861
C	3.52129	0.95251	-0.81048	H	3.67824	0.59191	3.95373
C	0.95716	2.68331	-1.20893	H	5.87361	-3.35498	1.60598
C	3.39980	2.34427	-1.03082	H	1.59963	-2.68352	5.76997
C	4.78280	0.34027	-1.01367	H	-4.27124	-1.27087	-4.95063
C	-0.09714	3.61701	-1.24836	H	-2.11002	3.74965	-5.45983
C	2.16922	3.04864	-0.59898	C	6.49549	-5.15615	-0.31704
C	4.45310	3.05871	-1.66454	H	5.82088	-5.69427	0.38377
C	5.87048	1.10337	-1.45683	C	7.92093	-5.17479	0.22758
C	-0.01399	4.79016	-0.48326	H	7.96394	-4.69610	1.22883
C	2.22819	4.19280	0.23528	H	8.26740	-6.22521	0.32461
C	5.70712	2.43324	-1.83403	H	8.60317	-4.63737	-0.46531
C	4.28990	4.38099	-2.13864	C	5.01446	-0.82881	1.72091
H	6.84308	0.63547	-1.55685	H	4.30473	0.00423	1.56187
C	1.11548	5.06211	0.29219	C	6.33487	-0.25704	2.22634
H	-0.81717	5.51411	-0.52591	H	7.04127	-1.07640	2.47803
C	3.38250	4.51280	0.98223	H	6.79106	0.39671	1.45269
C	6.78122	3.14100	-2.39762	H	6.15403	0.34815	3.13924
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H	3.33451	4.88550	-2.09066	H	4.58220	-0.46443	-3.43757
C	1.17469	6.22957	1.06992	C	6.49213	-1.23178	-4.09482
C	3.43024	5.67965	1.74834	H	6.32389	-0.84165	-5.12065
H	4.24524	3.85919	0.98890	H	7.12820	-0.50957	-3.54586
C	6.60712	4.45602	-2.82904	H	7.03015	-2.19986	-4.17346
H	7.75016	2.67132	-2.52004	C	-4.72391	3.58243	-4.75983
H	5.22375	6.08350	-3.06499	H	-4.42091	3.53435	-5.82846
C	2.32924	6.53532	1.79272	C	-5.49687	4.87935	-4.53571
H	0.33192	6.90939	1.11143	H	-5.88683	4.92809	-3.49692
H	4.32034	5.91575	2.31693	H	-4.83909	5.75519	-4.72191
H	7.43539	4.99451	-3.27115	H	-6.35686	4.92494	-5.23655
H	2.37006	7.43703	2.38985	C	0.25258	3.86051	-4.21074
C	-1.26013	3.45077	-2.15584	H	1.03568	3.19824	-3.79635
C	-1.09659	3.60709	-3.56166	C	0.67815	5.31944	-4.06830
C	-2.56821	3.30924	-1.61911	H	-0.09429	5.98917	-4.50280
C	-2.22921	3.61158	-4.39156	H	0.83529	5.58593	-3.00431
C	-3.67630	3.34580	-2.47864	H	1.63393	5.48051	-4.61008

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H	-3.36823	4.40364	1.54973
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H	-4.57253	4.40455	0.20503
C	4.08416	-1.67889	5.39667
H	4.94324	-1.13367	4.94970
C	4.19769	-1.58179	6.91560
H	5.18540	-1.97233	7.23932
H	4.11048	-0.52259	7.23954
H	3.40383	-2.18228	7.40783
C	-0.92094	-1.96256	5.19965
H	-1.65556	-2.01404	4.37284
C	-1.55772	-1.29964	6.41770
H	-0.83174	-1.26161	7.25773
H	-1.89350	-0.27073	6.17861
H	-2.44258	-1.88828	6.73919
C	1.59620	1.89727	2.90067
H	0.63892	2.10562	2.37961
C	1.94560	3.08564	3.79497
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H	1.70900	4.03115	3.26900
H	1.35936	3.06466	4.73613
C	-4.77402	0.18455	-2.75439
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C	-3.82580	-3.88926	-5.52893
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H	4.55568	-2.15207	-3.98135
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H	-0.47083	-5.61436	-3.16618
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C	2.35935	-5.47844	0.56834
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H	-0.72079	-2.62325	-2.55220
H	-1.22028	-3.46139	-4.03523
C	2.36576	-4.52671	1.76873
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H	1.01545	-2.26022	-4.26627
H	1.14657	-4.00124	-4.57114
C	1.28450	-3.46212	1.68644
H	3.34521	-4.03684	1.83770
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O	1.40948	-2.76772	0.46108
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S-gau-C₄-B(+)



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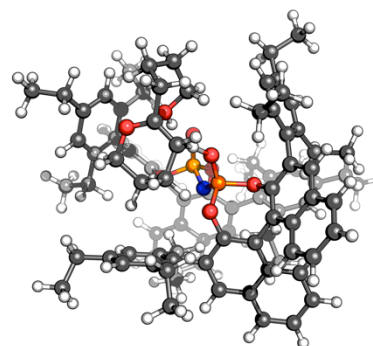
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C	-3.75585	-0.80748	0.46172
C	-6.15907	-1.68181	1.65196
C	-4.67668	-1.58301	-0.27048
C	-5.88948	-1.96634	0.31289

H	-6.60116	-2.54025	-0.26966	C	-3.75087	3.33734	-2.40402
H	-0.81660	2.28709	5.05176	C	-3.64101	3.49259	-3.78920
C	-3.13293	3.52304	4.66141	H	-4.73398	3.24279	-1.95784
C	-4.40401	4.03984	4.40577	C	5.01875	-1.08735	-0.80968
H	-2.48783	4.03637	5.36464	C	5.21790	-1.52748	0.52459
H	-4.73042	4.94316	4.90461	C	5.33920	-1.96480	-1.88602
C	-5.25190	3.39855	3.50284	C	5.73045	-2.81171	0.76311
C	-4.83533	2.23508	2.85211	C	5.84613	-3.24464	-1.60857
H	-6.23180	3.80989	3.29792	C	6.05937	-3.66651	-0.29241
H	-5.50936	1.78046	2.13812	H	6.08097	-3.91525	-2.42661
C	-7.33803	-2.16052	2.24582	C	-4.35130	-2.11521	-1.61377
C	-7.58191	-1.94097	3.60150	C	-4.44728	-1.28559	-2.75816
H	-8.06293	-2.71874	1.66504	C	-4.06217	-3.49761	-1.77215
H	-8.48909	-2.31800	4.05579	C	-4.25299	-1.83860	-4.03295
C	-6.64743	-1.25696	4.37733	C	-3.87612	-4.01843	-3.06251
C	-5.47477	-0.76799	3.79773	C	-3.98634	-3.20196	-4.19351
H	-6.82940	-1.10888	5.43403	H	-3.65622	-5.07205	-3.18897
H	-4.76430	-0.27018	4.44315	C	0.33277	0.10323	4.01699
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O	1.09977	-0.94382	-2.10511	C	1.66005	-1.55501	5.21658
O	2.46664	0.26484	-0.29415	C	2.75719	0.31410	4.15300
O	0.81514	1.50704	-1.96352	C	2.83207	-0.85260	4.92027
C	3.49316	0.96044	-0.90013	H	3.66355	0.86074	3.92328
C	0.91927	2.69455	-1.27859	H	5.89274	-3.14310	1.78249
C	3.36537	2.34467	-1.16084	H	1.72361	-2.45926	5.81047
C	4.75671	0.34698	-1.08917	H	-4.35386	-1.20943	-4.90971
C	-0.13283	3.63067	-1.30484	H	-2.29223	3.72351	-5.44221
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C	4.40568	3.03979	-1.83484	H	5.96691	-5.55160	0.73786
C	5.83260	1.09655	-1.58210	C	8.03984	-4.95669	0.52433
C	-0.02281	4.81965	-0.56878	H	8.06741	-4.40163	1.48599
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H	6.80826	0.63312	-1.66962	H	4.23292	0.14601	1.52020
C	1.13066	5.10317	0.16612	C	6.29176	0.04586	2.14578
H	-0.82537	5.54508	-0.60233	H	7.05036	-0.71495	2.42772
C	3.41021	4.55091	0.81153	H	6.68904	0.67181	1.31881
C	6.72016	3.10215	-2.61082	H	6.10091	0.69853	3.02330
C	5.29226	5.02027	-2.95481	C	5.16050	-1.57381	-3.34351
H	3.27734	4.85297	-2.29031	H	4.57044	-0.64066	-3.45411
C	1.21739	6.28621	0.91725	C	6.50147	-1.40292	-4.05685
C	3.48365	5.73110	1.55482	H	6.32330	-1.09764	-5.10938
H	4.26818	3.89095	0.81045	H	7.11663	-0.62297	-3.56668
C	6.53618	4.40332	-3.07882	H	7.06740	-2.35813	-4.06192
H	7.68804	2.63062	-2.73449	C	-4.87997	3.56619	-4.64685
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C	2.39111	6.59728	1.60617	C	-5.63577	4.87063	-4.40972
H	0.38025	6.97244	0.96629	H	-5.98435	4.93486	-3.35714
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H	7.35571	4.92916	-3.55141	H	-6.52212	4.91275	-5.07715
H	2.45260	7.51016	2.18424	C	0.11476	3.83066	-4.27929
C	-1.32525	3.44781	-2.16906	H	0.91073	3.17607	-3.87684
C	-1.21182	3.59185	-3.58071	C	0.54538	5.29159	-4.18032
C	-2.61225	3.30484	-1.58496	H	-0.24024	5.95326	-4.60336
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C	-2.81452	3.13674	-0.09290
H	-1.86267	2.92268	0.43604
C	-3.45763	4.38058	0.52031
H	-3.32962	4.36332	1.62073
H	-2.98718	5.30829	0.13696
H	-4.54267	4.40775	0.28557
C	4.16188	-1.35071	5.42860
H	4.99850	-0.77936	4.97141
C	4.26211	-1.20874	6.94505
H	5.26353	-1.54799	7.28404
H	4.12793	-0.14601	7.24021
H	3.49146	-1.82918	7.44937
C	-0.82604	-1.84252	5.25036
H	-1.56957	-1.93387	4.43514
C	-1.46908	-1.17947	6.46524
H	-0.73427	-1.10267	7.29490
H	-1.84154	-0.16639	6.21297
H	-2.32994	-1.79092	6.80855
C	1.52912	2.04806	2.83360
H	0.55927	2.20734	2.31847
C	1.85048	3.27907	3.67876
H	2.92783	3.29181	3.94760
H	1.61373	4.19671	3.10565
H	1.24713	3.29245	4.60914
C	-4.83716	0.17037	-2.66336
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C	-6.35374	0.33275	-2.63426
H	-6.78811	-0.19585	-1.76087
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H	-6.80095	-0.07303	-3.56657
C	-3.95572	-4.44813	-0.59156
H	-3.89518	-3.91198	0.37719
C	-5.13520	-5.41670	-0.54429
H	-5.04033	-6.07242	0.34668
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H	-3.76028	-2.99312	-6.33844
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H	-5.17392	-5.49748	-5.21557
H	-6.00372	-4.02484	-5.86727
H	-0.55584	-2.88460	5.52890
H	4.29164	-2.41693	5.14270
H	4.60176	-1.23903	2.56075
H	4.59193	-2.36676	-3.87136
H	6.61305	-5.66203	-0.92896
H	-2.94683	-4.42262	-5.63541
H	-3.01991	-5.03391	-0.66523
H	-4.43340	0.72303	-3.53726
H	-5.54618	2.70775	-4.42161
H	0.03293	3.56942	-5.35709
H	-3.47250	2.26135	0.08962
H	2.29019	1.94399	2.03138
O	-1.04322	-2.37314	-0.09786
C	1.65477	-4.36074	-1.58211

C	-0.59707	-4.77843	-2.13078
C	2.86614	-4.76407	-0.80122
C	-0.20081	-4.63811	-3.58690
H	-1.23089	-5.64586	-1.95339
H	-1.05231	-3.86733	-1.72731
C	2.65462	-5.58589	0.47644
H	3.37656	-3.82850	-0.57205
H	3.49098	-5.31940	-1.51522
C	0.70800	-3.42450	-3.74097
H	-1.10417	-4.53581	-4.19009
H	0.30924	-5.55547	-3.90599
C	2.48376	-4.74464	1.74479
H	1.79339	-6.25156	0.35033
H	3.52897	-6.23269	0.60181
H	0.11223	-2.50649	-3.74549
H	1.24813	-3.46715	-4.69091
C	1.26885	-3.83385	1.70429
H	3.37634	-4.12381	1.89478
H	2.40802	-5.41188	2.61149
O	1.42916	-2.92691	0.63297
H	0.35589	-4.43207	1.55861
H	1.16478	-3.29321	2.65571
H	0.52536	-2.69056	0.32334
C	1.71491	-3.37607	-2.58417
O	0.58063	-5.04254	-1.32582
H	2.74471	-3.15585	-2.84994
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S-gau-B_{2,5}-C(-)



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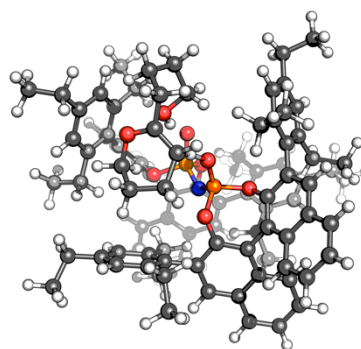
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C	-4.13237	0.96425	2.90732
C	-3.48419	1.51664	4.04052
C	-4.20167	-0.83851	1.10770
C	-5.39964	-1.55880	1.35889
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C	-6.08529	-2.16639	0.27580
C	-4.30821	-1.50276	-1.24261
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H	-6.06996	-2.57790	-1.83958
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C	-4.12084	2.51236	4.79854	C	4.80265	-3.33037	-1.79761
C	-5.37704	2.98829	4.42096	C	5.14184	-3.92555	-0.57849
H	-3.64022	2.93304	5.67387	H	4.69175	-3.94822	-2.68102
H	-5.85870	3.76303	5.00331	C	-3.67200	-1.61472	-2.57918
C	-6.00583	2.47942	3.28503	C	-3.55146	-0.47452	-3.41440
C	-5.39182	1.47815	2.52979	C	-3.13712	-2.85712	-3.01434
H	-6.97234	2.86415	2.98625	C	-2.83536	-0.57106	-4.61800
H	-5.90182	1.12398	1.64390	C	-2.44056	-2.92114	-4.23088
C	-7.29162	-2.84857	0.50080	C	-2.27108	-1.78399	-5.02566
C	-7.80825	-2.95740	1.79212	H	-2.01512	-3.86477	-4.55283
H	-7.82799	-3.30914	-0.32052	C	-0.19055	-0.32898	4.04706
H	-8.73578	-3.48939	1.96005	C	-0.03694	-1.52876	4.78771
C	-7.12188	-2.39870	2.86947	C	0.94682	0.47598	3.77975
C	-5.92440	-1.71101	2.66110	C	1.23627	-1.89748	5.24998
H	-7.51681	-2.50247	3.87192	C	2.21023	0.06223	4.22847
H	-5.41139	-1.31537	3.52697	C	2.36113	-1.11413	4.96935
C	3.56366	1.07709	-0.48961	H	3.07869	0.67480	4.01486
C	1.13283	2.99524	-0.66211	H	5.51583	-3.59240	1.51077
C	3.56839	2.47933	-0.59775	H	1.35499	-2.81117	5.82064
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C	0.12693	3.97169	-0.53623	H	-2.06914	4.86152	-4.55590
C	2.39611	3.23389	-0.08090	C	5.35595	-5.41540	-0.48861
C	4.66190	3.13296	-1.22558	H	4.72909	-5.83205	0.32895
C	5.81893	0.99492	-1.38694	C	6.82273	-5.74710	-0.22880
C	0.29740	5.03647	0.35800	H	7.15205	-5.33014	0.74639
C	2.53975	4.25603	0.88920	H	6.95481	-6.84925	-0.20266
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C	4.64398	4.51488	-1.51871	C	5.17870	-0.94652	1.78825
H	6.69443	0.41724	-1.66241	H	4.49348	-0.07501	1.79595
C	1.47458	5.16336	1.10034	C	6.61236	-0.47034	1.99390
H	-0.48115	5.78405	0.45249	H	7.30388	-1.33868	2.03800
C	3.71775	4.39820	1.65196	H	6.92162	0.20212	1.16683
C	6.90436	3.00930	-2.19101	H	6.68287	0.08943	2.95024
C	5.74648	5.12942	-2.11627	C	4.25251	-1.36829	-3.25274
H	3.77817	5.12749	-1.30784	H	3.88216	-0.32531	-3.17811
C	1.61502	6.20737	2.02843	C	5.44707	-1.39399	-4.20227
C	3.83679	5.43034	2.58521	H	5.15536	-0.94912	-5.17683
H	4.54306	3.70625	1.54357	H	6.28858	-0.80478	-3.78200
C	6.87651	4.38109	-2.44336	H	5.78418	-2.43726	-4.37859
H	7.78391	2.44104	-2.47004	C	-4.64606	4.54411	-3.79175
H	5.72191	6.19000	-2.33127	H	-4.56293	3.97616	-4.74352
C	2.79115	6.33538	2.76912	C	-4.85352	6.02560	-4.09463
H	0.81160	6.91657	2.18855	H	-4.93274	6.60297	-3.14866
H	4.74367	5.52886	3.16769	H	-4.01087	6.42448	-4.69801
H	7.72805	4.86294	-2.90623	H	-5.79278	6.15820	-4.67178
H	2.89063	7.13585	3.49073	C	0.35284	4.70952	-3.41836
C	-1.07641	3.96529	-1.40450	H	1.14628	4.00055	-3.11150
C	-0.97361	4.37651	-2.76197	C	0.78674	6.13872	-3.10600
C	-2.35674	3.69940	-0.85283	H	0.00563	6.85784	-3.43285
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C	-3.50301	3.88829	-1.63975	H	1.72878	6.36620	-3.64798
C	-3.40444	4.32497	-2.96435	C	-2.54189	3.20296	0.56360
H	-4.48033	3.69137	-1.21452	H	-1.58521	2.87399	1.01215
C	4.74410	-1.13579	-0.73624	C	-3.16089	4.27865	1.45276
C	5.04676	-1.74327	0.50827	H	-3.15192	3.93971	2.50738
C	4.61359	-1.94329	-1.89700	H	-2.58315	5.22310	1.38858
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H	3.09575	-2.12130	7.46610
C	-1.20837	-2.42647	5.12594
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C	-1.83008	-2.03015	6.46072
H	-1.07728	-2.10707	7.27406
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H	-2.67578	-2.71093	6.69315
C	0.85114	1.79556	3.04883
H	-0.10113	1.88975	2.49360
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H	0.24460	2.85535	4.85515
C	-4.20946	0.84401	-3.07337
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C	-5.70865	0.80084	-3.35380
H	-6.20547	0.02596	-2.73579
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H	-5.89092	0.58328	-4.42781
C	-3.26084	-4.13215	-2.20506
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C	-4.29780	-5.07309	-2.81162
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H	-3.99453	-5.37639	-3.83616
C	-1.48621	-1.86150	-6.31016
H	-0.72993	-1.04718	-6.33199
C	-2.40352	-1.74276	-7.52410
H	-1.80275	-1.83319	-8.45354
H	-3.16338	-2.55331	-7.51117
H	-2.91781	-0.75841	-7.53141
H	-0.87104	-3.48444	5.18518
H	3.91980	-2.58543	5.14094
H	4.88213	-1.57671	2.65400
H	3.42388	-1.96193	-3.69487
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O	1.80072	-5.24449	0.29257
C	0.94410	-3.65189	1.98829
H	-1.21528	-3.61288	2.06027
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C	1.72185	-5.77671	-2.51665
H	-0.39044	-5.99302	-1.97556
H	0.68958	-7.11851	-1.16303
C	2.02970	-4.62214	1.58343
H	1.00378	-2.73952	1.38417
H	1.12916	-3.37756	3.02636
C	1.36864	-4.66489	-3.50850
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H	1.95859	-6.69445	-3.06319
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H	2.27065	-4.40895	-4.07521
O	1.64381	-3.13387	-1.69384
H	-0.20368	-3.59443	-2.47602
H	0.79833	-2.57076	-3.49618
H	1.61140	-2.15824	-1.61004

S-gau- B_{2,5}-B(-)



E(RM062X) = -5098.39480610

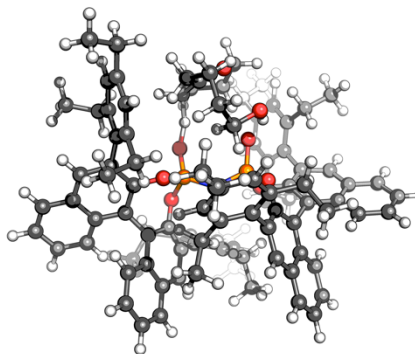
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H	-6.31862	-2.40136	-1.34823

H	-1.25255	1.59814	5.29363	C	5.08964	-3.34938	0.32289
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C	-4.87184	3.29738	4.66111	C	4.92648	-4.11528	-0.83600
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H	-5.27265	4.10018	5.26626	C	-3.99506	-1.52035	-2.34897
C	-5.60858	2.80278	3.58497	C	-3.99760	-0.40909	-3.23054
C	-5.09919	1.76556	2.80078	C	-3.53770	-2.78165	-2.81731
H	-6.57762	3.22654	3.35528	C	-3.50909	-0.56192	-4.53769
H	-5.69085	1.42086	1.96302	C	-3.05712	-2.89866	-4.13042
C	-7.32268	-2.56344	1.10196	C	-3.03960	-1.79839	-4.99227
C	-7.72207	-2.61209	2.43771	H	-2.69739	-3.85842	-4.48335
H	-7.94651	-3.03131	0.34945	C	0.08153	-0.32208	3.98872
H	-8.64671	-3.10564	2.70783	C	0.18241	-1.56160	4.67283
C	-6.92245	-2.04289	3.42778	C	1.25904	0.41727	3.70685
C	-5.72836	-1.40394	3.08720	C	1.44423	-2.03039	5.06925
H	-7.22649	-2.10050	4.46503	C	2.50673	-0.08968	4.10252
H	-5.12592	-0.99986	3.88909	C	2.60563	-1.30178	4.79328
C	3.58606	0.96222	-0.63435	H	3.40516	0.47694	3.88666
C	1.26502	3.00374	-0.75958	H	5.33684	-3.84340	1.25553
C	3.67086	2.36518	-0.71856	H	1.52332	-2.96995	5.60368
C	4.68206	0.16753	-1.01552	H	-3.50734	0.28432	-5.21497
C	0.29944	4.01436	-0.60559	H	-1.97966	4.91134	-4.57835
C	2.54300	3.17873	-0.18963	C	5.09339	-5.61284	-0.78283
C	4.80040	2.96503	-1.33733	H	4.46027	-6.02770	0.03094
C	5.83486	0.76784	-1.53157	C	6.55120	-5.99707	-0.54477
C	0.52606	5.06512	0.29194	H	6.90232	-5.61463	0.43694
C	2.74271	4.18834	0.78460	H	6.64849	-7.10313	-0.54641
C	5.89637	2.15117	-1.71722	H	7.19363	-5.58224	-1.35081
C	4.86105	4.34974	-1.61160	C	5.11518	-1.19599	1.59325
H	6.67688	0.14591	-1.81520	H	4.55839	-0.23780	1.59152
C	1.71964	5.13934	1.01538	C	6.58995	-0.91694	1.85926
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C	3.93479	4.27487	1.53395	H	7.01736	-0.29531	1.04420
C	7.03720	2.73025	-2.29563	H	6.69593	-0.36767	2.81844
C	5.99977	4.91049	-2.19387	C	4.09996	-1.46451	-3.43880
H	4.02958	5.00682	-1.39680	H	3.76914	-0.41086	-3.33327
C	1.91772	6.17209	1.94558	C	5.28140	-1.50944	-4.40394
C	4.11119	5.29729	2.46884	H	4.99361	-1.03246	-5.36436
H	4.72688	3.54711	1.41389	H	6.14769	-0.95906	-3.98133
C	7.08823	4.10515	-2.52604	H	5.58027	-2.55929	-4.60792
H	7.88493	2.11777	-2.57951	C	-4.53983	4.58505	-3.76672
H	6.03588	5.97389	-2.39268	H	-4.46471	4.02155	-4.72185
C	3.10884	6.24669	2.66951	C	-4.76824	6.06483	-4.06208
H	1.14763	6.91407	2.12030	H	-4.84200	6.63827	-3.11335
H	5.02864	5.35318	3.04027	H	-3.93771	6.47502	-4.67471
H	7.96840	4.54550	-2.97650	H	-5.71612	6.18830	-4.62704
H	3.25263	7.03887	3.39278	C	0.46394	4.77787	-3.48261
C	-0.92618	4.04150	-1.43979	H	1.26297	4.06849	-3.19085
C	-0.84972	4.44477	-2.80104	C	0.90355	6.20653	-3.17601
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C	-3.28295	4.37779	-2.95942	C	-2.35163	3.31360	0.57104
H	-4.32478	3.76921	-1.17990	H	-1.38979	2.97558	1.00639
C	4.63801	-1.30919	-0.92699	C	-2.93202	4.41870	1.45004
C	4.93098	-1.95629	0.29889	H	-2.89901	4.10583	2.51186
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H	-3.98803	4.62090	1.17255
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C	4.07414	-1.79120	6.76307
H	5.08599	-2.14012	7.05857
H	3.93061	-0.75600	7.14011
H	3.32161	-2.45973	7.23200
C	-1.03429	-2.38610	5.04188
H	-1.81428	-2.33176	4.25626
C	-1.61933	-1.93319	6.37555
H	-0.85972	-2.02833	7.18057
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H	-2.49205	-2.56950	6.63291
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H	0.25950	1.94118	2.50061
C	1.48102	2.88994	4.00488
H	2.52825	2.85352	4.37281
H	1.31211	3.86646	3.51139
H	0.78868	2.81593	4.86873
C	-4.55582	0.93766	-2.82708
H	-4.23512	1.21172	-1.80285
C	-6.07874	0.95417	-2.91336
H	-6.52198	0.20992	-2.22131
H	-6.45550	1.95956	-2.63186
H	-6.40617	0.72881	-3.95068
C	-3.53001	-4.02398	-1.95033
H	-3.61435	-3.78348	-0.87081
C	-4.65403	-4.98011	-2.33960
H	-4.63028	-5.86909	-1.67467
H	-5.64186	-4.48698	-2.23529
H	-4.52810	-5.32146	-3.38897
C	-2.53187	-1.94348	-6.40393
H	-1.80276	-1.13343	-6.62219
C	-3.68060	-1.88522	-7.40762
H	-3.28401	-2.02447	-8.43536
H	-4.41486	-2.69242	-7.19744
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H	-0.75821	-3.46018	5.12299
H	4.08500	-2.86052	4.87540
H	4.69832	-1.79275	2.43136
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H	0.35977	4.67611	-4.58505
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P	1.12019	0.44523	-0.99549
O	1.20582	-0.47200	-2.16709
O	2.47679	0.38171	-0.07476
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P	-1.14910	-0.85525	0.17601

O	-1.00420	-2.19848	-0.50928
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C	-0.63060	-4.65644	0.32653
C	0.50125	-5.19612	-0.32510
C	-0.56314	-4.40808	1.84179
H	-1.55651	-5.10445	-0.02794
C	0.42318	-6.06053	-1.54589
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C	0.86129	-4.61432	2.35268
H	-0.89770	-3.39082	2.05494
H	-1.24923	-5.09302	2.34857
C	1.45965	-5.76681	-2.64220
H	-0.59823	-6.02604	-1.93536
H	0.57648	-7.07714	-1.15492
C	1.84572	-4.17337	1.28715
H	1.04400	-4.05309	3.26889
H	1.05514	-5.67056	2.57310
C	1.00675	-4.69220	-3.63487
H	2.38554	-5.44480	-2.16314
H	1.67271	-6.69660	-3.17801
H	2.87992	-4.29694	1.59751
H	1.67330	-3.14683	0.94081
C	0.51819	-3.43268	-2.93317
H	0.20430	-5.08007	-4.27645
H	1.85501	-4.44658	-4.28336
O	1.41991	-3.10844	-1.89811
H	-0.48596	-3.59118	-2.51214
H	0.42885	-2.60180	-3.64288
H	1.40854	-2.12737	-1.83800

S-gau- B_{2,5}-C(+)



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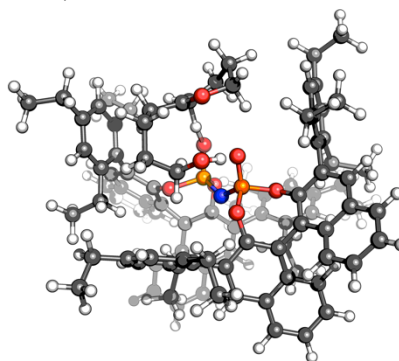
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H	-6.59967	-2.39315	-0.79803	C	-3.75493	3.74312	-1.82985
H	-0.82162	1.35561	5.34190	C	-3.63179	4.14075	-3.16479
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H	-2.49217	3.02457	5.94786	C	5.33621	-1.54110	0.17855
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C	-5.24671	2.72903	3.98924	C	5.87472	-2.83714	0.19459
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H	-6.22486	3.17219	3.85437	C	6.13664	-3.52488	-0.99452
H	-5.49836	1.37796	2.35964	H	6.02037	-3.45837	-3.14011
C	-7.34907	-2.48409	1.74045	C	-4.33331	-1.76229	-2.02560
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C	-6.66394	-2.00202	4.00662	C	-3.87203	-3.38279	-3.78679
C	-5.48320	-1.42523	3.53407	C	-3.89565	-2.36741	-4.74812
H	-6.85145	-2.05195	5.07151	H	-3.67229	-4.40195	-4.09675
H	-4.77242	-1.06262	4.26393	C	0.32580	-0.62136	3.96124
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O	1.09487	-0.60063	-2.28160	C	1.64411	-2.45163	4.88982
O	2.48771	0.27817	-0.31321	C	2.75629	-0.47124	4.07014
O	0.78926	1.79206	-1.70228	C	2.82457	-1.73788	4.65888
C	3.49658	1.08772	-0.79688	H	3.66798	0.08861	3.90054
C	0.90266	2.84132	-0.82010	H	6.09424	-3.31450	1.14276
C	3.34934	2.49380	-0.80780	H	1.70172	-3.43420	5.34310
C	4.76342	0.53753	-1.11020	H	-4.18475	-0.26700	-5.09704
C	-0.14236	3.77545	-0.67796	H	-2.26631	4.64487	-4.74168
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C	4.36637	3.31148	-1.37196	H	6.09486	-5.54540	-0.25952
C	5.81662	1.37365	-1.50157	C	8.15565	-4.91358	-0.49109
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C	5.61787	2.73899	-1.68601	H	8.77108	-4.29214	-1.17625
C	4.16931	4.68698	-1.63411	C	5.14118	-0.84281	1.50446
H	6.79288	0.94472	-1.69683	H	4.37786	-0.04411	1.44603
C	1.13644	4.95996	1.02210	C	6.44916	-0.24018	2.00450
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C	3.42246	4.30275	1.53209	H	6.82680	0.51275	1.28047
C	6.65759	3.53989	-2.18580	H	6.27745	0.26001	2.98086
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H	3.21300	5.16338	-1.46670	H	4.43138	-0.09094	-3.57546
C	1.23486	5.99280	1.96810	C	6.33642	-0.70354	-4.38990
C	3.50747	5.33387	2.47046	H	6.09434	-0.24996	-5.37402
H	4.27921	3.65388	1.40269	H	6.96064	0.01222	-3.81905
C	6.45080	4.90120	-2.40917	H	6.91977	-1.63160	-4.56667
H	7.62542	3.11019	-2.41620	C	-4.86223	4.37630	-4.00543
H	5.04324	6.52346	-2.33576	H	-4.58840	4.51509	-5.07403
C	2.41734	6.17740	2.68701	C	-5.62070	5.61511	-3.53731
H	0.40046	6.66085	2.14594	H	-5.98300	5.48183	-2.49595
H	4.41929	5.47479	3.03618	H	-4.96253	6.50891	-3.58533
H	7.25280	5.51301	-2.80158	H	-6.49847	5.78373	-4.19608
H	2.48792	6.97468	3.41550	C	0.13078	4.51225	-3.56343

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C	0.56513	5.93170	-3.20839
H	-0.20973	6.66135	-3.52647
H	0.73599	6.03379	-2.11826
H	1.51472	6.17017	-3.73222
C	-2.83968	3.11287	0.41187
H	-1.89447	2.79590	0.89943
C	-3.47364	4.23468	1.23445
H	-3.34636	4.02375	2.31464
H	-2.99603	5.21183	1.01970
H	-4.55827	4.31087	1.00875
C	4.15655	-2.33183	5.04352
H	4.99297	-1.70997	4.65731
C	4.30157	-2.43086	6.55978
H	5.30582	-2.83254	6.81083
H	4.19507	-1.42588	7.02148
H	3.53452	-3.11241	6.98422
C	-0.84681	-2.71130	4.90638
H	-1.59682	-2.65764	4.09278
C	-1.47082	-2.24533	6.21834
H	-0.72999	-2.31785	7.04300
H	-1.82572	-1.19833	6.13778
H	-2.34062	-2.89017	6.46418
C	1.53160	1.46769	3.07299
H	0.56105	1.71223	2.59381
C	1.85863	2.54110	4.10902
H	2.93673	2.50600	4.37307
H	1.62228	3.54142	3.69750
H	1.25737	2.40162	5.03050
C	-4.76058	0.68260	-2.65369
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H	-4.95443	-4.44683	-6.26801
H	-5.76774	-2.88520	-6.69442
H	-0.58874	-3.78809	5.00871
H	4.25530	-3.34202	4.59051
H	4.76652	-1.57487	2.24868
H	4.45429	-1.73274	-4.25286
H	6.65093	-5.39769	-1.95505
H	-2.72586	-3.29254	-6.29911
H	-3.06250	-4.81793	-1.61927
H	-4.35678	1.37795	-3.41905
H	-5.53000	3.49162	-3.95094
H	0.05821	4.44188	-4.67083

H	-3.50820	2.22657	0.43088
H	2.29085	1.49367	2.26269
O	-1.07650	-2.36891	-0.54163
C	1.74241	-4.06985	-1.92841
C	-0.21593	-5.04611	-2.87051
C	2.90926	-4.29787	-1.01847
C	-0.52924	-3.70172	-3.48964
H	0.16709	-5.75560	-3.61251
H	-1.05615	-5.50067	-2.35264
C	2.70518	-5.09853	0.27288
H	3.32952	-3.31185	-0.80649
H	3.62716	-4.81705	-1.67000
C	0.75692	-3.06848	-4.01124
H	-0.99084	-3.05147	-2.73801
H	-1.23293	-3.86846	-4.30826
C	2.39794	-4.19126	1.46393
H	1.88853	-5.81298	0.14042
H	3.61695	-5.67032	0.46951
H	0.56443	-2.05385	-4.36947
H	1.16104	-3.64971	-4.85049
C	1.14534	-3.37581	1.21648
H	3.24022	-3.51326	1.65139
H	2.25838	-4.79822	2.36542
O	0.06458	-4.26490	1.05073
H	0.96491	-2.67717	2.03923
H	1.27570	-2.75312	0.31473
H	-0.61470	-3.77656	0.55330
C	1.74331	-3.01118	-2.85718
O	0.81815	-4.96900	-1.84993
H	2.75766	-2.68868	-3.07966
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S-gau- B_{2,5}-B(+)



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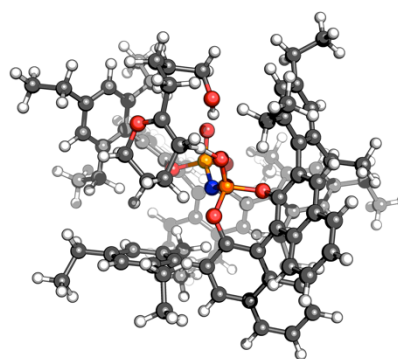
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C	-0.93709	0.32530	3.65782
C	-3.07241	0.29686	2.49458
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C	-2.61598	2.00324	4.18601

C	-4.03256	-0.50609	1.69221	H	7.57026	4.96170	-3.13932
C	-5.21387	-1.04547	2.26984	H	2.79604	7.17118	2.90744
C	-3.73859	-0.75887	0.33611	C	-1.15835	3.74321	-1.81939
C	-6.18039	-1.65012	1.43157	C	-1.03882	4.04353	-3.20531
C	-4.69187	-1.41003	-0.47418	C	-2.44819	3.56279	-1.25413
C	-5.92511	-1.79190	0.06717	C	-2.19822	4.15880	-3.98844
H	-6.66481	-2.25809	-0.57287	C	-3.58453	3.71060	-2.06375
H	-0.73911	1.79504	5.21586	C	-3.46886	4.01752	-3.42332
C	-3.02440	3.11391	4.94162	H	-4.56975	3.58518	-1.63033
C	-4.28196	3.68232	4.73383	C	4.94614	-1.18222	-0.99604
H	-2.37226	3.54013	5.69478	C	5.19087	-1.75887	0.27667
H	-4.59116	4.53888	5.31867	C	5.13051	-1.97066	-2.16621
C	-5.13771	3.15400	3.76751	C	5.63160	-3.08849	0.36212
C	-4.74309	2.05154	3.00630	C	5.55714	-3.30241	-2.04232
H	-6.10642	3.60653	3.59973	C	5.82768	-3.85958	-0.78789
H	-5.42228	1.68715	2.24697	H	5.68646	-3.90623	-2.93269
C	-7.37941	-2.13889	1.97485	C	-4.38305	-1.81349	-1.86666
C	-7.61157	-2.06287	3.34827	C	-4.36343	-0.85205	-2.90817
H	-8.12938	-2.59498	1.33931	C	-4.19229	-3.18791	-2.17889
H	-8.53427	-2.44787	3.76287	C	-4.11302	-1.26369	-4.22622
C	-6.64667	-1.51226	4.19041	C	-3.94915	-3.56412	-3.50901
C	-5.45404	-1.01358	3.66218	C	-3.91420	-2.61311	-4.53437
H	-6.82090	-1.47535	5.25808	H	-3.79197	-4.60913	-3.74938
H	-4.72124	-0.62106	4.35396	C	0.36165	-0.30519	3.99261
N	-0.04856	0.09413	0.02205	C	0.39625	-1.53349	4.70696
P	1.04509	0.26104	-1.09610	C	1.57700	0.36137	3.69038
O	1.10557	-0.71680	-2.25657	C	1.63447	-2.07581	5.08585
O	2.48747	0.22978	-0.30803	C	2.79419	-0.19786	4.10632
O	0.88968	1.70953	-1.83159	C	2.83154	-1.41098	4.80103
C	3.54170	0.93626	-0.84820	H	3.71927	0.32452	3.89426
C	1.04909	2.80956	-1.02303	H	5.82649	-3.52690	1.33417
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C	4.76565	0.28332	-1.12489	H	-4.11350	-0.53125	-5.02506
C	0.03860	3.78646	-0.94431	H	-2.11158	4.40602	-5.04004
C	2.29788	3.06881	-0.43324	C	6.28805	-5.28980	-0.66922
C	4.54763	3.05399	-1.57514	H	5.64537	-5.82672	0.06106
C	5.86994	1.02002	-1.57037	C	7.74407	-5.36354	-0.21868
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C	5.76035	2.38140	-1.84354	H	8.39669	-4.82855	-0.94133
C	4.43881	4.41720	-1.93454	C	5.05843	-0.97577	1.56221
H	6.81361	0.51421	-1.74064	H	4.34684	-0.13439	1.46316
C	1.36729	5.04423	0.66062	C	6.40878	-0.43056	2.01326
H	-0.57533	5.64038	-0.03732	H	7.12241	-1.26283	2.19177
C	3.62582	4.33620	1.22391	H	6.82510	0.25156	1.24187
C	6.84934	3.07786	-2.39237	H	6.28246	0.13773	2.95873
C	5.52488	5.09587	-2.49118	C	4.88417	-1.42817	-3.56344
H	3.51424	4.96389	-1.80758	H	4.34527	-0.45832	-3.54310
C	1.50619	6.13795	1.52996	C	6.18783	-1.25491	-4.34091
C	3.75044	5.42772	2.08646	H	5.96600	-0.83942	-5.34638
H	4.45624	3.64633	1.14591	H	6.87072	-0.55705	-3.81658
C	6.73046	4.43102	-2.70965	H	6.69879	-2.23207	-4.47108
H	7.78748	2.57216	-2.58878	C	-4.70383	4.20338	-4.26981
H	5.42950	6.14077	-2.75711	H	-4.43644	4.27145	-5.34685
C	2.69464	6.32720	2.23756	C	-5.45446	5.47324	-3.87847
H	0.69812	6.84844	1.65793	H	-5.81056	5.40947	-2.82844
H	4.66639	5.57262	2.64444	H	-4.79315	6.35919	-3.98858

H	-6.33581	5.60249	-4.54133
C	0.29521	4.32491	-3.87292
H	1.07453	3.61273	-3.54092
C	0.75846	5.75651	-3.61716
H	-0.01090	6.47768	-3.96648
H	0.95333	5.92429	-2.53931
H	1.70104	5.94519	-4.17294
C	-2.65465	3.23188	0.20951
H	-1.70928	2.93103	0.70695
C	-3.25741	4.41823	0.96099
H	-3.14032	4.26737	2.05217
H	-2.74814	5.36543	0.69151
H	-4.33840	4.51373	0.72535
C	4.14851	-2.00126	5.23887
H	4.99957	-1.43844	4.79781
C	4.29239	-1.96750	6.75803
H	5.28580	-2.37169	7.04555
H	4.21307	-0.92268	7.12752
H	3.50771	-2.58757	7.24063
C	-0.86118	-2.28591	5.09620
H	-1.60341	-2.28167	4.27368
C	-1.48597	-1.70674	6.36181
H	-0.75316	-1.72846	7.19645
H	-1.81977	-0.66284	6.19632
H	-2.37019	-2.31369	6.64914
C	1.61675	1.67953	2.94726
H	0.65352	1.90594	2.44491
C	1.96418	2.82545	3.89536
H	3.03949	2.78590	4.16993
H	1.75540	3.79450	3.40218
H	1.35433	2.77602	4.82034
C	-4.69418	0.60224	-2.66487
H	-4.23700	0.96270	-1.72420
C	-6.20360	0.82165	-2.61682
H	-6.66333	0.22466	-1.80300
H	-6.41934	1.89330	-2.42520
H	-6.66347	0.53265	-3.58578
C	-4.24754	-4.28324	-1.12655
H	-4.20079	-3.88200	-0.09427
C	-5.50638	-5.13553	-1.27204
H	-5.53380	-5.89654	-0.46390
H	-6.41738	-4.50789	-1.19697
H	-5.50952	-5.66198	-2.24977
C	-3.69787	-3.04391	-5.96341
H	-3.51715	-2.16260	-6.61675
C	-4.91095	-3.80054	-6.49845
H	-4.73939	-4.07439	-7.56071
H	-5.07870	-4.73217	-5.91747
H	-5.81865	-3.16262	-6.43756
H	-0.62573	-3.35629	5.28442
H	4.22125	-3.05029	4.87873
H	4.64683	-1.63811	2.35189
H	4.23588	-2.13212	-4.12549
H	6.19274	-5.81632	-1.64381
H	-2.79862	-3.69130	-6.02912
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H	-4.27030	1.22775	-3.47840

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H	0.21114	4.18234	-4.97255
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H	2.37960	1.62380	2.14203
O	-1.07750	-2.34511	-0.37484
C	1.37513	-4.19396	-1.67809
C	-0.81937	-4.72669	-2.33974
C	2.55978	-4.53035	-0.82286
C	-0.35831	-4.53940	-3.77122
H	-1.40158	-5.63583	-2.19760
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C	2.33019	-5.28671	0.49152
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H	3.20920	-5.11268	-1.49079
C	0.46802	-3.26172	-3.85446
H	-1.23483	-4.49522	-4.42025
H	0.23417	-5.41099	-4.07595
C	2.21343	-4.34252	1.68879
H	1.41858	-5.88611	0.42194
H	3.16622	-5.97562	0.64368
H	-0.18867	-2.38657	-3.81113
H	1.01502	-3.21008	-4.79960
C	1.04158	-3.39402	1.52613
H	3.13786	-3.76356	1.81009
H	2.07138	-4.92743	2.60449
O	-0.14133	-4.15763	1.46443
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H	1.16441	-2.79542	0.60801
H	-0.76354	-3.65975	0.90764
C	1.46216	-3.21462	-2.68858
O	0.32573	-4.91354	-1.46865
H	2.50325	-3.03481	-2.94760
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S-gau-B_{1,4}-C(-)



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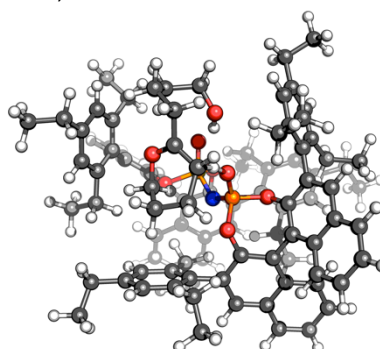
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C	-1.59097	0.00638	3.66477
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C	-2.30273	0.92721	4.43976

C	-4.21612	0.73661	2.94055	H	0.25141	6.81326	2.09241
C	-3.59484	1.31717	4.07469	H	4.23918	5.68765	3.17830
C	-4.19504	-1.05809	1.13391	H	7.30370	5.46264	-2.74635
C	-5.34421	-1.85422	1.38346	H	2.28182	7.17869	3.43856
C	-3.62408	-1.04979	-0.15414	C	-1.35311	3.73904	-1.51895
C	-5.98240	-2.51133	0.30060	C	-1.23424	4.16807	-2.87020
C	-4.25248	-1.72784	-1.21573	C	-2.64045	3.46389	-0.98641
C	-5.44342	-2.42461	-0.98684	C	-2.39266	4.34425	-3.64291
H	-5.92872	-2.93243	-1.81208	C	-3.77660	3.66790	-1.78430
H	-1.84092	1.34567	5.32680	C	-3.66226	4.12788	-3.09993
C	-4.27686	2.28254	4.83240	H	-4.76066	3.46312	-1.37871
C	-5.55542	2.69683	4.45696	C	5.00112	-0.83766	-0.63431
H	-3.81615	2.72527	5.70756	C	5.28442	-1.38332	0.64336
H	-6.07311	3.44735	5.04012	C	5.12544	-1.65407	-1.78905
C	-6.16167	2.15641	3.32324	C	5.70508	-2.71818	0.74577
C	-5.50075	1.18659	2.56648	C	5.52306	-2.99268	-1.64681
H	-7.14684	2.49266	3.02698	C	5.81080	-3.53003	-0.38835
H	-5.99486	0.80672	1.68219	H	5.60625	-3.62069	-2.52581
C	-7.13982	-3.27405	0.52391	C	-3.61627	-1.79329	-2.55461
C	-7.65307	-3.41291	1.81363	C	-3.60814	-0.65550	-3.40007
H	-7.63991	-3.77366	-0.29748	C	-2.98780	-2.99004	-2.99050
H	-8.54254	-4.00671	1.98029	C	-2.90455	-0.69978	-4.61394
C	-7.01114	-2.80401	2.89112	C	-2.31303	-3.00704	-4.22081
C	-5.86266	-2.03682	2.68436	C	-2.24914	-1.86509	-5.02431
H	-7.40211	-2.93063	3.89248	H	-1.81822	-3.91531	-4.54489
H	-5.38186	-1.60368	3.55066	C	-0.22161	-0.37889	4.08098
N	0.00672	0.05539	0.22377	C	-0.00979	-1.57569	4.81218
P	1.10555	0.33530	-0.91417	C	0.87420	0.48190	3.81839
O	1.25772	-0.62136	-2.04584	C	1.27742	-1.87902	5.28300
O	2.48122	0.43200	-0.01194	C	2.15336	0.13642	4.28038
O	0.81780	1.81639	-1.56734	C	2.35974	-1.03105	5.02241
C	3.50476	1.19611	-0.52017	H	2.98947	0.79560	4.07688
C	0.89732	2.89640	-0.71791	H	5.92463	-3.13775	1.72079
C	3.35827	2.59269	-0.62305	H	1.44030	-2.78853	5.84934
C	4.76056	0.61377	-0.78582	H	-2.87332	0.17580	-5.25185
C	-0.17635	3.80464	-0.61887	H	-2.30601	4.69693	-4.66402
C	2.12111	3.22408	-0.10465	C	6.20058	-4.97906	-0.24787
C	4.39158	3.37244	-1.20801	H	5.55604	-5.46211	0.51831
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C	-0.09597	4.88460	0.27175	H	7.84901	-4.65198	1.14252
C	2.17295	4.25429	0.86613	H	7.93199	-6.19590	0.21663
C	5.63554	2.76547	-1.49953	H	8.31901	-4.63722	-0.60710
C	4.21501	4.73815	-1.52544	C	5.17239	-0.57071	1.91499
H	6.78027	0.94552	-1.44704	H	4.37728	0.19743	1.83968
C	1.04867	5.09195	1.04360	C	6.49705	0.10273	2.25467
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C	6.68289	3.52750	-2.04166	H	6.38970	0.67468	3.20035
C	5.26208	5.48218	-2.07320	C	4.83066	-1.13653	-3.18536
H	3.26711	5.23640	-1.37351	H	4.31306	-0.15556	-3.16804
C	1.10129	6.15425	1.96026	C	6.10704	-1.00207	-4.01220
C	3.35403	5.52576	2.57690	H	5.85735	-0.59829	-5.01592
H	4.19148	3.83907	1.57093	H	6.81896	-0.30823	-3.51957
C	6.49511	4.88110	-2.32269	H	6.59433	-1.99121	-4.14322
H	7.64283	3.07356	-2.25798	C	-4.89829	4.37901	-3.92667
H	5.11468	6.52824	-2.30919	H	-4.63145	4.55275	-4.99192
C	2.24964	6.36524	2.72541	C	-5.66329	5.59647	-3.41530

H	-6.01373	5.42938	-2.37468
H	-5.01360	6.49732	-3.44327
H	-6.54893	5.77631	-4.06042
C	0.09713	4.52612	-3.50352
H	0.89951	3.83422	-3.18360
C	0.49809	5.96400	-3.18650
H	-0.28945	6.66783	-3.53056
H	0.65839	6.09921	-2.09821
H	1.44645	6.20768	-3.71009
C	-2.84300	2.94982	0.42356
H	-1.88845	2.63068	0.88876
C	-3.50237	4.00153	1.31356
H	-3.50562	3.65033	2.36425
H	-2.94787	4.96024	1.27248
H	-4.55218	4.17590	0.99684
C	3.73500	-1.37697	5.53498
H	4.49784	-0.68736	5.11277
C	3.79880	-1.28048	7.05695
H	4.83170	-1.50109	7.39952
H	3.52568	-0.25561	7.38793
H	3.10893	-2.01330	7.52613
C	-1.13381	-2.53853	5.13074
H	-1.89516	-2.55385	4.32465
C	-1.80028	-2.17954	6.45450
H	-1.05787	-2.21166	7.28032
H	-2.24600	-1.16449	6.40354
H	-2.60778	-2.90938	6.67350
C	0.71495	1.79106	3.07930
H	-0.23887	1.83840	2.51687
C	0.77381	2.96715	4.05014
H	1.79994	3.07985	4.45969
H	0.49526	3.90045	3.52443
H	0.06071	2.81969	4.88762
C	-4.37190	0.60249	-3.05566
H	-4.20352	0.88810	-1.99869
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H	-6.28383	-0.39460	-2.70427
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C	-1.47657	-1.88536	-6.31850
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H	-1.81886	-1.88467	-8.45791
H	-3.11212	-2.70091	-7.49915
H	-2.99914	-0.89279	-7.52450
H	-0.73810	-3.57567	5.19679
H	4.00139	-2.40699	5.21338
H	4.87771	-1.23355	2.75618
H	4.14099	-1.83364	-3.70180
H	6.04149	-5.52395	-1.20405
H	-0.85599	-2.80526	-6.39154

H	-1.95996	-4.68033	-2.15400
H	-4.01066	1.44757	-3.67711
H	-5.55820	3.48744	-3.89424
H	0.03410	4.41805	-4.60850
H	-3.49178	2.05019	0.38839
H	1.52636	1.88708	2.32874
O	-0.92938	-2.34935	-0.49647
C	1.04890	-4.98359	-0.44355
C	2.40726	-4.00849	1.28593
C	1.08475	-5.76502	-1.71744
C	1.16184	-3.37436	1.85875
H	3.18634	-3.26880	1.13747
H	2.78658	-4.82188	1.91192
C	2.31964	-5.56285	-2.60338
H	1.03216	-6.81829	-1.40038
H	0.16480	-5.54900	-2.26089
C	-0.02979	-4.31586	1.72393
H	0.96268	-2.42623	1.35081
H	1.37368	-3.14195	2.90276
C	2.57198	-4.12529	-3.06601
H	2.18282	-6.20669	-3.48071
H	3.20686	-5.93316	-2.07787
H	0.09862	-5.19555	2.36761
H	-0.94195	-3.79973	2.03152
H	2.89482	-3.51466	-2.21780
H	3.38812	-4.14335	-3.79812
O	2.21936	-4.60102	-0.03055
C	-0.14101	-4.71355	0.25971
H	-0.45388	-3.59674	-0.26385
H	-0.96931	-5.35766	-0.03206
C	1.35070	-3.43218	-3.65740
H	1.64310	-2.47661	-4.10778
H	0.89902	-4.05250	-4.44595
O	0.37963	-3.22609	-2.65433
H	0.45380	-2.31036	-2.32352

S-gau- B_{1,4}-B(-)



E(RM062X) = -5098.39344639

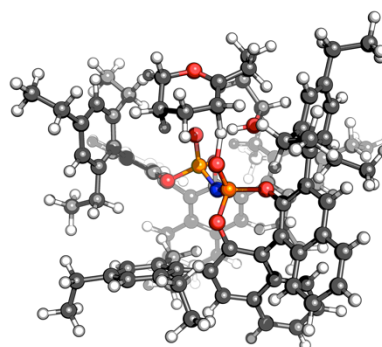
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C	-2.10645	-0.44238	2.52879
C	-1.48172	0.08828	3.66941
C	-3.45503	-0.12574	2.25336

C	-2.14337	1.04371	4.44747	C	2.51531	6.28714	2.70016
C	-4.09325	0.90479	2.98999	H	0.54101	6.81585	2.05499
C	-3.42778	1.47674	4.10328	H	4.47068	5.52640	3.16887
C	-4.17328	-0.91681	1.21216	H	7.62201	5.16298	-2.62746
C	-5.33469	-1.67798	1.50858	H	2.57659	7.09955	3.41258
C	-3.64038	-0.94334	-0.09222	C	-1.18639	3.78802	-1.53711
C	-6.02221	-2.33388	0.45603	C	-1.07342	4.20586	-2.89213
C	-4.32134	-1.61606	-1.12519	C	-2.47344	3.54678	-0.98748
C	-5.52203	-2.27809	-0.84848	C	-2.23650	4.40276	-3.65302
H	-6.05037	-2.77787	-1.65179	C	-3.61378	3.77177	-1.77353
H	-1.65073	1.45135	5.32275	C	-3.50439	4.21888	-3.09396
C	-4.05999	2.47358	4.86337	H	-4.59760	3.59506	-1.35434
C	-5.33194	2.92650	4.51042	C	4.95051	-1.05098	-0.70707
H	-3.56557	2.91041	5.72295	C	5.08776	-1.68102	0.55639
H	-5.81104	3.70111	5.09505	C	5.09660	-1.81937	-1.89339
C	-5.98150	2.39268	3.39762	C	5.36018	-3.05683	0.61493
C	-5.37064	1.39186	2.63914	C	5.36483	-3.19384	-1.79545
H	-6.96148	2.75800	3.11909	C	5.49609	-3.81685	-0.55064
H	-5.89698	1.01675	1.77147	H	5.46573	-3.78330	-2.69894
C	-7.19222	-3.06166	0.72572	C	-3.74666	-1.69939	-2.49135
C	-7.66983	-3.16724	2.03219	C	-3.75782	-0.56587	-3.34328
H	-7.73016	-3.55957	-0.07245	C	-3.18488	-2.91742	-2.96050
H	-8.56930	-3.73422	2.23466	C	-3.14809	-0.64166	-4.60548
C	-6.98003	-2.55929	3.08021	C	-2.60502	-2.96417	-4.23768
C	-5.81860	-1.82633	2.82710	C	-2.56681	-1.83124	-5.05467
H	-7.34396	-2.65989	4.09464	H	-2.16321	-3.88945	-4.58923
H	-5.30099	-1.39282	3.67173	C	-0.12593	-0.35723	4.06994
N	0.01979	0.09363	0.18017	C	0.04287	-1.57534	4.77729
P	1.13152	0.31423	-0.96137	C	1.00266	0.46070	3.80947
O	1.22876	-0.65409	-2.08820	C	1.32139	-1.94189	5.22568
O	2.50542	0.33983	-0.05593	C	2.26977	0.05661	4.25736
O	0.92452	1.80702	-1.61090	C	2.43439	-1.13268	4.97452
C	3.56915	1.05988	-0.54532	H	3.13038	0.68539	4.06020
C	1.04389	2.87785	-0.75496	H	5.46398	-3.54328	1.57793
C	3.49132	2.46393	-0.63493	H	1.45216	-2.86713	5.77467
C	4.79885	0.41871	-0.79989	H	-3.13565	0.22809	-5.25194
C	0.00312	3.82303	-0.65219	H	-2.15381	4.74728	-4.67724
C	2.27660	3.15195	-0.13150	C	5.76607	-5.29740	-0.46116
C	4.57403	3.19823	-1.18953	H	5.01593	-5.76961	0.20967
C	5.90575	1.16536	-1.22111	C	7.17185	-5.57209	0.06580
C	0.12380	4.89959	0.23730	H	7.28809	-5.17760	1.09733
C	2.36336	4.17879	0.84154	H	7.35303	-6.66733	0.08580
C	5.79572	2.53626	-1.45408	H	7.92854	-5.09826	-0.59542
C	4.46964	4.57294	-1.50049	C	4.98353	-0.91769	1.85983
H	6.84916	0.66275	-1.40143	H	4.18870	-0.14810	1.81437
C	1.27323	5.06216	1.01229	C	6.31121	-0.26373	2.22658
H	-0.67162	5.63227	0.30000	H	7.10700	-1.03374	2.31498
C	3.51419	4.35478	1.63888	H	6.60681	0.48140	1.45991
C	6.89219	3.25311	-1.95951	H	6.21008	0.25716	3.20191
C	5.56514	5.27194	-2.01173	C	4.95286	-1.21457	-3.27963
H	3.54161	5.11332	-1.37126	H	4.53190	-0.18909	-3.25046
C	1.36395	6.12244	1.92835	C	6.29094	-1.17346	-4.01436
C	3.58406	5.40139	2.56089	H	6.15400	-0.69421	-5.00652
H	4.35620	3.67852	1.56513	H	7.03519	-0.58605	-3.43840
C	6.77568	4.61635	-2.23198	H	6.68243	-2.20047	-4.17225
H	7.83530	2.75640	-2.15490	C	-4.74442	4.49653	-3.90645
H	5.47308	6.32555	-2.24209	H	-4.48769	4.64930	-4.97734

C	-5.46505	5.74237	-3.39928
H	-5.80412	5.59842	-2.35147
H	-4.78947	6.62302	-3.44838
H	-6.35479	5.94059	-4.03327
C	0.25858	4.53055	-3.54155
H	1.04818	3.82163	-3.22679
C	0.69586	5.95992	-3.23423
H	-0.08006	6.68038	-3.57019
H	0.87338	6.09432	-2.14845
H	1.64247	6.18079	-3.77092
C	-2.67178	3.05028	0.42964
H	-1.72034	2.71002	0.88669
C	-3.29239	4.12715	1.31741
H	-3.29028	3.78674	2.37159
H	-2.71459	5.07113	1.25897
H	-4.34164	4.32481	1.01275
C	3.79697	-1.54235	5.47381
H	4.58525	-0.87917	5.05621
C	3.87283	-1.47079	6.99657
H	4.89717	-1.74007	7.32988
H	3.64517	-0.44022	7.34380
H	3.15487	-2.18051	7.45916
C	-1.11879	-2.49248	5.09921
H	-1.86836	-2.49689	4.28223
C	-1.78910	-2.08837	6.40813
H	-1.05669	-2.12590	7.24259
H	-2.20565	-1.06284	6.33434
H	-2.61956	-2.79051	6.63184
C	0.89392	1.78093	3.08120
H	-0.06389	1.87671	2.53131
C	1.02116	2.94667	4.05803
H	2.05633	3.00743	4.45562
H	0.78200	3.89554	3.54086
H	0.31210	2.82858	4.90346
C	-4.44678	0.72259	-2.95601
H	-4.20710	1.00154	-1.91138
C	-5.95904	0.61784	-3.12969
H	-6.37890	-0.17903	-2.48375
H	-6.43301	1.58029	-2.84490
H	-6.20802	0.39719	-4.18954
C	-3.14948	-4.18069	-2.12493
H	-3.33786	-3.98156	-1.05030
C	-4.16133	-5.20684	-2.62700
H	-4.12396	-6.10973	-1.98188
H	-5.18897	-4.79047	-2.59436
H	-3.92495	-5.50881	-3.66932
C	-1.90168	-1.88754	-6.40603
H	-1.19056	-1.03906	-6.50449
C	-2.93208	-1.82679	-7.52998
H	-2.41649	-1.90038	-8.51054
H	-3.64777	-2.67180	-7.44003
H	-3.49124	-0.86781	-7.49692
H	-0.76244	-3.54183	5.19132
H	4.01864	-2.57796	5.13648
H	4.69251	-1.60829	2.67948
H	4.23650	-1.81443	-3.87534
H	5.66691	-5.77700	-1.45931

H	-1.31393	-2.82512	-6.51622
H	-2.13641	-4.62611	-2.18634
H	-4.08346	1.55133	-3.59738
H	-5.43113	3.62612	-3.85355
H	0.18094	4.41995	-4.64534
H	-3.34451	2.16795	0.41114
H	1.69911	1.84316	2.32050
O	-0.96623	-2.29768	-0.48842
C	0.86232	-4.80096	-0.48769
C	1.77575	-3.36408	1.13634
C	1.05089	-5.61787	-1.72429
C	1.06933	-4.20010	2.18493
H	1.22941	-2.45004	0.88500
H	2.79140	-3.10598	1.41657
C	2.27233	-5.30270	-2.59084
H	1.11183	-6.65812	-1.37032
H	0.12315	-5.53661	-2.29576
C	-0.35238	-4.50428	1.71953
H	1.07206	-3.66384	3.13288
H	1.64181	-5.12453	2.32774
C	2.34782	-3.88459	-3.16469
H	2.25622	-6.02384	-3.41728
H	3.18152	-5.51087	-2.01769
H	-0.73474	-5.39605	2.22456
H	-1.01361	-3.66975	1.96864
H	2.62044	-3.17051	-2.38169
H	3.13856	-3.87523	-3.92356
O	1.90993	-4.14298	-0.08363
C	-0.35993	-4.73724	0.20438
H	-0.66975	-3.56422	-0.24428
H	-1.10732	-5.42793	-0.17839
C	1.04567	-3.37952	-3.76882
H	1.22583	-2.44378	-4.31122
H	0.63358	-4.10863	-4.48095
O	0.08048	-3.18818	-2.75788
H	0.20554	-2.30151	-2.37231

S-gau- B_{1,4}-C(+)



E(RM062X) = -5098.3821295

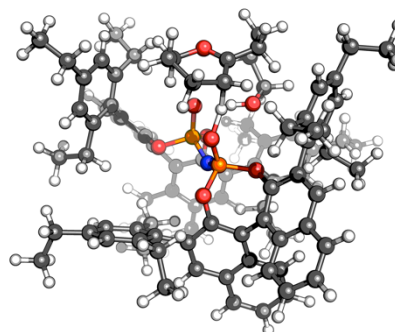
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C	-1.67173	0.20333	2.66295
C	-0.82532	0.80690	3.60937

C	-2.98437	0.68807	2.50117	H	5.72432	5.53508	-3.47337
C	-1.21508	1.99858	4.23444	C	2.87448	6.51968	1.40471
C	-3.35174	1.93341	3.07245	H	0.89118	6.99730	0.74772
C	-2.45002	2.58566	3.94652	H	4.82792	5.78676	1.92402
C	-3.98142	-0.19759	1.84624	H	7.81765	4.22796	-3.64319
C	-5.15080	-0.62795	2.53116	H	2.98941	7.44241	1.95846
C	-3.73682	-0.64321	0.52936	C	-1.04189	3.47554	-2.25604
C	-6.15355	-1.32584	1.81751	C	-0.95049	3.57473	-3.67271
C	-4.73537	-1.36483	-0.15486	C	-2.32153	3.40517	-1.64366
C	-5.94948	-1.65565	0.47777	C	-2.12678	3.61340	-4.43856
H	-6.71859	-2.19021	-0.06817	C	-3.47411	3.47227	-2.44074
H	-0.56152	2.45499	4.96751	C	-3.38559	3.59043	-3.83112
C	-2.81460	3.79583	4.55795	H	-4.45113	3.43697	-1.97317
C	-4.06187	4.36667	4.29980	C	4.87382	-1.46238	-0.78227
H	-2.13619	4.29834	5.23724	C	4.97976	-1.92725	0.55402
H	-4.33704	5.30049	4.77270	C	5.06585	-2.37880	-1.85580
C	-4.95156	3.73983	3.42733	C	5.25743	-3.28080	0.79795
C	-4.60129	2.53648	2.81082	C	5.33889	-3.72673	-1.57293
H	-5.91255	4.19248	3.22007	C	5.45245	-4.17913	-0.25489
H	-5.30600	2.09226	2.12020	H	5.47190	-4.42708	-2.38901
C	-7.34003	-1.71223	2.46156	C	-4.50459	-1.92958	-1.50379
C	-7.52493	-1.44037	3.81712	C	-4.57626	-1.10248	-2.65261
H	-8.11779	-2.23771	1.91992	C	-4.34705	-3.33317	-1.65883
H	-8.43875	-1.74584	4.31024	C	-4.47892	-1.67934	-3.92814
C	-6.52475	-0.79515	4.54270	C	-4.28697	-3.87890	-2.95029
C	-5.34357	-0.39779	3.91249	C	-4.34968	-3.06276	-4.08389
H	-6.66261	-0.60569	5.59947	H	-4.18043	-4.94980	-3.07607
H	-4.58261	0.07289	4.51980	C	0.45874	0.18113	4.00482
N	-0.06670	0.17943	0.01504	C	0.46520	-0.97550	4.83198
P	1.08501	0.10695	-1.06379	C	1.68853	0.79739	3.65600
O	1.11907	-1.04405	-2.05487	C	1.68927	-1.49258	5.28322
O	2.50282	0.16835	-0.25773	C	2.88932	0.27398	4.15715
O	0.99159	1.43246	-2.01934	C	2.89810	-0.86466	4.96895
C	3.58844	0.73419	-0.89139	H	3.82484	0.76298	3.91419
C	1.17202	2.63268	-1.37281	H	5.34564	-3.63565	1.81841
C	3.58809	2.11181	-1.20477	H	1.70173	-2.37488	5.91237
C	4.78063	-0.00846	-1.06601	H	-4.54523	-1.04904	-4.80737
C	0.17449	3.62513	-1.41965	H	-2.06157	3.71228	-5.51579
C	2.42433	2.94475	-0.81413	C	5.75961	-5.62616	0.03395
C	4.69410	2.68430	-1.88871	H	5.01972	-6.02423	0.76172
C	5.92485	0.61598	-1.57872	C	7.16983	-5.78566	0.59616
C	0.35789	4.82786	-0.72209	H	7.26973	-5.24642	1.56202
C	2.58159	4.12196	-0.04080	H	7.38142	-6.86168	0.77009
C	5.88044	1.93163	-2.03503	H	7.91702	-5.38795	-0.12371
C	4.64892	3.98654	-2.43703	C	4.90525	-0.99918	1.74326
H	6.84604	0.05171	-1.66266	H	4.19209	-0.17219	1.57144
C	1.52957	5.06552	0.00060	C	6.27763	-0.42267	2.07483
H	-0.40395	5.59534	-0.77156	H	6.99076	-1.24019	2.31371
C	3.76986	4.39440	0.67085	H	6.66912	0.16672	1.21964
C	7.00621	2.49924	-2.65342	H	6.19699	0.24726	2.95626
C	5.77102	4.53526	-3.06131	C	4.98479	-1.96272	-3.31628
H	3.74675	4.58250	-2.40583	H	4.56003	-0.94543	-3.43834
C	1.68603	6.26142	0.71936	C	6.35244	-2.01498	-3.99606
C	3.91243	5.58780	1.38217	H	6.25640	-1.66989	-5.04701
H	4.58595	3.68385	0.69370	H	7.07901	-1.35909	-3.47653
C	6.95002	3.79790	-3.15975	H	6.74585	-3.05326	-4.00399
H	7.92394	1.93270	-2.75931	C	-4.63703	3.71112	-4.66505

H	-4.40159	3.60149	-5.74610
C	-5.30979	5.06424	-4.45187
H	-5.62869	5.17990	-3.39424
H	-4.61053	5.88625	-4.71611
H	-6.20782	5.13880	-5.10060
C	0.37269	3.71943	-4.40244
H	1.13729	3.03000	-3.99661
C	0.88871	5.15492	-4.35076
H	0.13017	5.85145	-4.76723
H	1.12793	5.45420	-3.31104
H	1.81620	5.23623	-4.95582
C	-2.49970	3.27754	-0.14464
H	-1.54801	3.02920	0.36937
C	-3.06865	4.56340	0.45440
H	-2.93260	4.55492	1.55381
H	-2.55019	5.45756	0.05365
H	-4.15253	4.64703	0.22777
C	4.19696	-1.41405	5.50328
H	5.06475	-0.91161	5.02387
C	4.30257	-1.21259	7.01252
H	5.28193	-1.59445	7.37011
H	4.22981	-0.13210	7.26096
H	3.49610	-1.76490	7.53960
C	-0.80817	-1.65345	5.30155
H	-1.54876	-1.73608	4.48270
C	-1.42617	-0.91702	6.48683
H	-0.69441	-0.84732	7.31981
H	-1.74639	0.10354	6.19626
H	-2.31876	-1.47276	6.84361
C	1.76153	2.01831	2.76234
H	0.80322	2.20987	2.23667
C	2.14568	3.26114	3.56286
H	3.22124	3.22615	3.83681
H	1.96087	4.16809	2.95445
H	1.54112	3.34188	4.48892
C	-4.83349	0.38329	-2.56003
H	-4.32270	0.82622	-1.68409
C	-6.32792	0.67824	-2.47925
H	-6.77225	0.20413	-1.57974
H	-6.48799	1.77472	-2.41232
H	-6.84397	0.29754	-3.38624
C	-4.23286	-4.27691	-0.47258
H	-4.08135	-3.73474	0.48290
C	-5.46764	-5.16553	-0.34023
H	-5.36269	-5.81374	0.55517
H	-6.38241	-4.54909	-0.22409
H	-5.57901	-5.81642	-1.23278
C	-4.28141	-3.67393	-5.45996
H	-4.12589	-2.88870	-6.23166
C	-5.56665	-4.42850	-5.78845
H	-5.50206	-4.84236	-6.81671
H	-5.71873	-5.26916	-5.07866
H	-6.43870	-3.74197	-5.73530
H	-0.59345	-2.69755	5.61827
H	4.26681	-2.49733	5.26438
H	4.52649	-1.55689	2.62470
H	4.30285	-2.64625	-3.86304

H	5.67699	-6.23829	-0.89052
H	-3.41645	-4.36962	-5.51604
H	-3.33989	-4.92264	-0.59085
H	-4.41446	0.89053	-3.45381
H	-5.34769	2.90091	-4.40018
H	0.25396	3.43589	-5.47113
H	-3.19430	2.43825	0.06968
H	2.51896	1.84601	1.96871
O	-1.01794	-2.30676	-0.07050
C	1.15770	-4.52029	-1.60433
C	-0.91208	-4.85547	-2.74144
C	2.08823	-5.06778	-0.56989
C	-0.73955	-3.48384	-3.35532
H	-0.70129	-5.65151	-3.46410
H	-1.89256	-5.02207	-2.31284
C	1.45483	-5.66238	0.69181
H	2.77369	-4.26221	-0.31711
H	2.65779	-5.84861	-1.09748
C	0.72070	-3.31610	-3.76612
H	-1.01335	-2.71581	-2.62186
H	-1.41148	-3.40324	-4.21449
C	0.66569	-4.66596	1.54783
H	0.81144	-6.50474	0.41675
H	2.27918	-6.07573	1.28579
H	0.89914	-2.31045	-4.15188
H	0.98747	-4.03638	-4.55059
C	1.41860	-3.36806	1.83448
H	0.40337	-5.15122	2.49585
H	-0.27689	-4.39901	1.05380
O	1.59036	-2.60243	0.65658
H	0.87391	-2.78698	2.59004
H	2.42269	-3.57404	2.22921
H	0.68902	-2.48328	0.29139
C	1.55313	-3.52043	-2.51020
O	-0.00562	-5.09473	-1.62787
H	2.63367	-3.47077	-2.59113
H	1.34931	-2.36430	-1.95495

S-gau- B_{1,4}-B(+)



E(RM062X) = -5098.38475

P	-1.17677	-0.90544	0.48810
O	-2.58804	-0.31896	-0.09918
O	-1.29635	-0.87131	2.12226

C	-1.71591	0.31672	2.67186	C	6.83268	3.79370	-3.32334
C	-0.89167	0.99208	3.58778	H	7.87118	1.99113	-2.81272
C	-3.03588	0.76347	2.46838	H	5.54648	5.46409	-3.74101
C	-1.31060	2.21074	4.13715	C	2.73783	6.61057	1.08945
C	-3.43506	2.03151	2.96343	H	0.74866	7.02528	0.40764
C	-2.55533	2.75308	3.80536	H	4.70080	5.93317	1.64721
C	-4.00550	-0.17929	1.85259	H	7.68831	4.22868	-3.82342
C	-5.17302	-0.59830	2.54744	H	2.84015	7.56345	1.59223
C	-3.73422	-0.69182	0.56534	C	-1.12373	3.32614	-2.41879
C	-6.14887	-1.36150	1.86390	C	-1.01999	3.34800	-3.83814
C	-4.70840	-1.47151	-0.08993	C	-2.40803	3.27222	-1.81488
C	-5.92056	-1.76066	0.54697	C	-2.18932	3.32733	-4.61524
H	-6.67111	-2.34154	0.02280	C	-3.55369	3.28044	-2.62454
H	-0.67259	2.72378	4.84613	C	-3.45340	3.32107	-4.01852
C	-2.95127	3.98871	4.34183	H	-4.53463	3.25786	-2.16446
C	-4.20812	4.51608	4.04095	C	4.93226	-1.40288	-0.67785
H	-2.29003	4.54479	4.99583	C	5.03699	-1.78471	0.68514
H	-4.50746	5.46975	4.45605	C	5.19646	-2.36729	-1.69343
C	-5.07620	3.82020	3.19956	C	5.39351	-3.10195	1.01084
C	-4.69462	2.59103	2.65699	C	5.54407	-3.67755	-1.32824
H	-6.04461	4.23905	2.95842	C	5.66714	-4.04342	0.01525
H	-5.38327	2.09218	1.98781	H	5.74107	-4.41266	-2.09961
C	-7.33409	-1.73931	2.51539	C	-4.45953	-2.08440	-1.41457
C	-7.54366	-1.39359	3.85041	C	-4.56560	-1.30942	-2.59651
H	-8.09198	-2.31398	1.99603	C	-4.26215	-3.48768	-1.51258
H	-8.45653	-1.69209	4.34954	C	-4.46806	-1.93743	-3.84773
C	-6.56920	-0.68247	4.54885	C	-4.20468	-4.08696	-2.78023
C	-5.38963	-0.29326	3.91063	C	-4.30326	-3.32232	-3.94647
H	-6.72585	-0.43498	5.59092	H	-4.06873	-5.15894	-2.86121
H	-4.64865	0.23101	4.49840	C	0.39992	0.41364	4.02749
N	-0.06279	0.14570	0.05088	C	0.42006	-0.69325	4.91965
P	1.06293	0.04737	-1.05375	C	1.62180	1.02282	3.64197
O	1.08407	-1.13607	-2.00488	C	1.65013	-1.16925	5.39862
O	2.49143	0.15598	-0.27256	C	2.82891	0.54321	4.17070
O	0.93120	1.32675	-2.06416	C	2.85147	-0.54673	5.04660
C	3.56119	0.73248	-0.92353	H	3.75799	1.02949	3.90002
C	1.09260	2.55885	-1.47742	H	5.49351	-3.38954	2.05129
C	3.51884	2.09432	-1.29981	H	1.67285	-2.01183	6.07982
C	4.78289	0.02750	-1.04614	H	-4.56237	-1.34701	-4.75177
C	0.08299	3.53426	-1.58083	H	-2.11529	3.36617	-5.69573
C	2.33909	2.91707	-0.93616	C	6.10227	-5.43603	0.39248
C	4.60795	2.66778	-2.00945	H	5.40487	-5.85137	1.15187
C	5.91038	0.66842	-1.57550	C	7.52496	-5.42944	0.94816
C	0.24704	4.77377	-0.94569	H	7.58019	-4.82214	1.87662
C	2.47817	4.13473	-0.22437	H	7.83747	-6.46776	1.18711
C	5.82195	1.95316	-2.10593	H	8.22865	-5.01069	0.19669
C	4.51987	3.93588	-2.62796	C	4.89394	-0.79676	1.81924
H	6.85486	0.13903	-1.61231	H	4.15280	-0.01040	1.58754
C	1.41332	5.06467	-0.23372	C	6.23304	-0.14529	2.14892
H	-0.52434	5.52757	-1.03819	H	6.97323	-0.91720	2.44925
C	3.66221	4.46107	0.47143	H	6.62057	0.41204	1.27064
C	6.93213	2.52787	-2.74550	H	6.10388	0.56831	2.98926
C	5.62637	4.49086	-3.27413	C	5.12615	-2.04039	-3.17723
H	3.59595	4.49845	-2.63484	H	4.64696	-1.05798	-3.36585
C	1.55316	6.29954	0.41951	C	6.50887	-2.05378	-3.82859
C	3.78830	5.69292	1.11718	H	6.41470	-1.78093	-4.90071
H	4.48767	3.76361	0.53226	H	7.18618	-1.32554	-3.34069

H	6.96220	-3.06530	-3.76463	H	4.51554	-1.32147	2.72126
C	-4.69836	3.37559	-4.86876	H	4.49803	-2.79314	-3.69659
H	-4.45179	3.20216	-5.93894	H	6.07197	-6.11060	-0.49077
C	-5.38738	4.73156	-4.74503	H	-3.35979	-4.66594	-5.33695
H	-5.71645	4.90858	-3.69908	H	-3.18318	-5.00007	-0.40907
H	-4.69467	5.54346	-5.05401	H	-4.43858	0.65180	-3.47380
H	-6.28047	4.75586	-5.40431	H	-5.40264	2.57512	-4.56014
C	0.30800	3.46979	-4.56370	H	0.20225	3.12860	-5.61680
H	1.07719	2.81218	-4.11622	H	-3.28375	2.38673	-0.05943
C	0.80700	4.91196	-4.58431	H	2.44242	1.98697	1.90053
H	0.04588	5.57538	-5.04744	O	-0.99614	-2.34785	0.11387
H	1.02944	5.27046	-3.55973	C	1.29339	-4.52209	-1.43757
H	1.74116	4.97120	-5.18163	C	-0.88603	-4.40275	-2.30098
C	-2.59873	3.22311	-0.31288	C	2.23584	-5.13843	-0.45463
H	-1.64879	3.01607	0.22223	C	-0.29302	-4.40534	-3.69757
C	-3.19022	4.53172	0.21018	H	-1.72912	-5.08221	-2.21878
H	-3.06191	4.58626	1.30912	H	-1.14974	-3.40397	-1.93507
H	-2.68159	5.40977	-0.23632	C	1.61581	-5.71746	0.82083
H	-4.27348	4.58682	-0.02784	H	2.97021	-4.36913	-0.21939
C	4.15653	-1.04696	5.61273	H	2.75946	-5.93250	-1.00784
H	5.01840	-0.56751	5.10030	C	0.94902	-3.51688	-3.74153
C	4.26099	-0.74695	7.10567	H	-1.05347	-4.05624	-4.40133
H	5.24391	-1.09579	7.48645	H	-0.04496	-5.43923	-3.96601
H	4.17846	0.34672	7.28347	C	0.84326	-4.71416	1.68722
H	3.45965	-1.27094	7.66834	H	0.96084	-6.55544	0.55901
C	-0.84593	-1.35130	5.43523	H	2.44472	-6.13754	1.40358
H	-1.59124	-1.48480	4.62725	H	0.67000	-2.47691	-3.93126
C	-1.46133	-0.55086	6.57988	H	1.61159	-3.83443	-4.55217
H	-0.72635	-0.43213	7.40445	C	1.57106	-3.38688	1.88926
H	-1.78543	0.45099	6.23363	H	0.64404	-5.17621	2.66167
H	-2.35082	-1.08783	6.97144	H	-0.12967	-4.48924	1.23398
C	1.67932	2.19193	2.68105	O	1.64196	-2.65948	0.67685
H	0.72026	2.33836	2.14240	H	1.06069	-2.79537	2.66186
C	2.03960	3.48317	3.41297	H	2.60417	-3.55117	2.22379
H	3.11480	3.48181	3.69059	H	0.71165	-2.52752	0.39417
H	1.84050	4.35210	2.75581	C	1.70463	-3.59194	-2.40768
H	1.43078	3.60376	4.33199	O	0.07003	-4.94207	-1.35315
C	-4.85606	0.17248	-2.56429	H	2.78586	-3.53830	-2.45586
H	-4.36378	0.66130	-1.70203	H	1.41885	-2.42009	-1.91741
C	-6.35709	0.43756	-2.50892				
H	-6.79904	-0.00909	-1.59417				
H	-6.54110	1.53221	-2.48917				
H	-6.85632	0.00874	-3.40377				
C	-4.09113	-4.37377	-0.29051				
H	-3.93000	-3.78396	0.63503				
C	-5.29690	-5.28784	-0.08538				
H	-5.14675	-5.89820	0.82995				
H	-6.22356	-4.69078	0.03745				
H	-5.41891	-5.97492	-0.94894				
C	-4.24129	-3.99060	-5.29591				
H	-4.11920	-3.23589	-6.10324				
C	-5.51179	-4.79115	-5.56917				
H	-5.45364	-5.24719	-6.57980				
H	-5.63013	-5.60411	-4.82165				
H	-6.40063	-4.12551	-5.52981				
H	-0.62239	-2.37392	5.81039				
H	4.23761	-2.14261	5.44431				