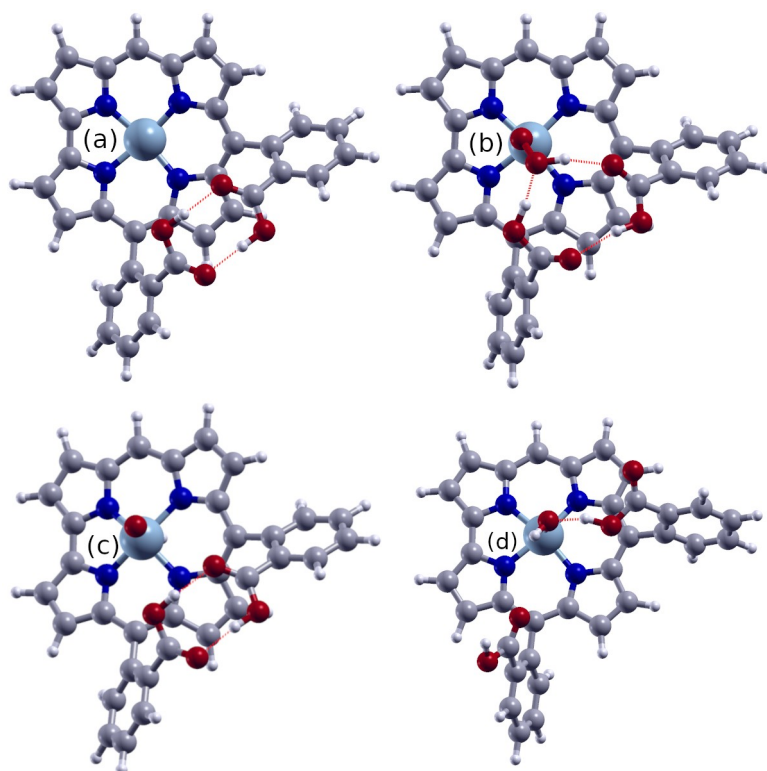


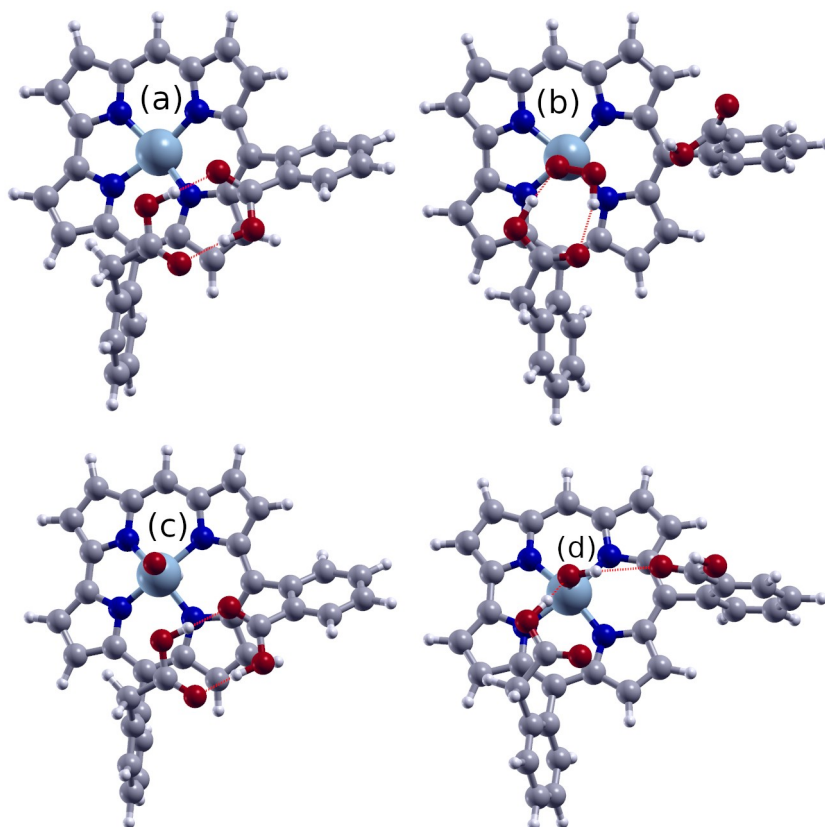
*Electronic Supplementary Information for*

Tuning of ORR activity through the stabilization of the adsorbates by hydrogen bonding with substituent groups

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**Figure S1:** Most stable conformers of the H-Mn-N-C without and with the OOH, O and OH adsorbates with the substituents  $R1=C_6H_4-COOH$  and  $R2=C_6H_4-COOH$ .



**Figure S2:** Most stable conformers of the H-Mn-N-C without and with the OOH, O and OH adsorbates with the substituents  $R1=C_6H_4-COOH$ ,  $R2=C_6H_4-CH_2-COOH$ .

**Table S1:** Relative energies of various H-Mn-N-C intermediates obtained from various level of theory with substituent R1=C<sub>6</sub>H<sub>4</sub>-COOH.

Complex	PBE/PW		PBE-D3/PW	
		E <sub>diff</sub> (eV)		E <sub>diff</sub> (eV)
*	-673.6347417731 Ry		-673.7091885374 Ry	
*OOH (no HB)	-739.1513230656 Ry	0.1552	-739.2337173423 Ry	0.1426
*OOH donating HB	-739.1570277716 Ry	0.0000	-739.2411543897 Ry	0.0415
*OOH cyclic	-739.1537149347 Ry	0.0450	-739.2442018291 Ry	0.0000
*OOH accepting HB	-739.1519010118 Ry	0.070	-739.2378243620 Ry	0.0868
*O (no HB)	-705.7897997368 Ry	0.0000	-705.8687325570 Ry	0.0000
*O accepting HB	-705.7510999004 Ry	0.5265	-705.8326758431 Ry	0.4906
*OH (no HB)	-707.0509118266 Ry	0.0324	-707.1310018532 Ry	0.0995
*OH accepting HB	-707.0532900904 Ry	0.0000	-707.1383171889 Ry	0.0000
*OH donating HB	-707.0509013481 Ry	0.0325	-707.1316387491 Ry	0.0909

Complex	M06L-D3/6-311++g**		M06L/6-311++g**	
		E <sub>diff</sub> (eV)		E <sub>diff</sub> (eV)
*	-1474.1345619 a.u		-1474.1296233 a.u	
*OOH (no HB)	-1625.0989289 a.u	0.1249	-1625.0933564 a.u	0.1169
*OOH donating HB	-1625.1023416 a.u	0.0321	-1625.0965538 a.u	0.0299
*OOH cyclic	-1625.1035194 a.u	0.0000	-1625.0976518 a.u	0.0000
*OOH accepting HB	-1625.1034636 a.u	0.0015	-1625.0976213 a.u	0.0008
*O (no HB)	-1549.2924138 a.u	0.0000	-1549.2872388 a.u	0.0000
*O accepting HB	-1549.2848378 a.u	0.2062	-1549.279598 a.u	0.2079
*OH (no HB)	-1549.9526499 a.u	0.0601	-1549.947219 a.u	0.0569
*OH accepting HB	-1549.954859 a.u	0.0000	-1549.9493086 a.u	0.0000
*OH donating HB	-1549.9521477 a.u	0.0738	-1549.9467833 a.u	0.0687

Complex	PBE(gas)/6-311++g**		PBE(solvent water)/6-311++g**	
		E <sub>diff</sub> (eV)		E <sub>diff</sub> (eV)
*	-1472.6389344 a.u		-1472.6934949 a.u	
*OOH (no HB)	-1623.4763892 a.u	0.0867	-1623.5348316 a.u	0.0417
*OOH donating HB	-1623.4795751 a.u	0.0000	-1623.5363637 a.u	0.0000
*OOH cyclic	-1623.4784644 a.u	0.0302	-1623.53231 a.u	0.1103
*OOH accepting HB	-1623.4780987 a.u	0.0402	-1623.5334812 a.u	0.0784
*O (no HB)	-1547.7485052 a.u	0.0000	-1547.8021768 a.u	0.0000
*O accepting HB	-1547.7335548 a.u	0.4068	didn't converge	
*OH (no HB)	-1548.3882007 a.u	0.0630	-1548.444474 a.u	
*OH accepting HB	-1548.3905158 a.u	0.0000	didn't converge	
*OH donating HB	-1548.3879341 a.u	0.0702	-1548.4452147 a.u	

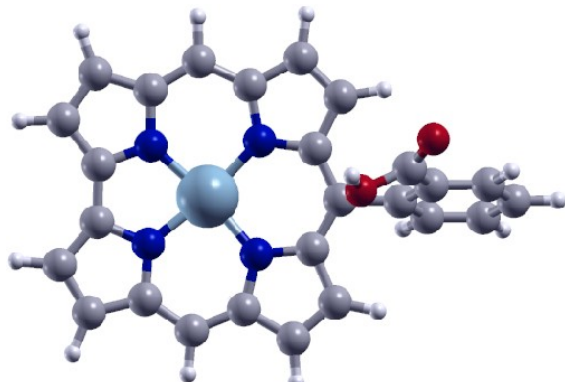
Complex	X3LYP/6-311++g**		M06-D3/6-311++g**	
		E <sub>diff</sub> (eV)		E <sub>diff</sub> (eV)
*	-1473.5933709 a.u		-1473.278319 a.u	
*OOH (no HB)	-1624.5161057 a.u	0.1554	-1624.1826302 a.u	0.2469
*OOH donating HB	-1624.5197524 a.u	0.0562	-1624.1878047 a.u	0.1061
*OOH cyclic	-1624.5190948 a.u	0.0741	-1624.1917033 a.u	0.0000

*OOH accepting HB	-1624.5218184 a.u	0.0000	-1624.1913139 a.u	0.0106
*O (no HB) *O accepting HB	-1548.7117827 a.u didn't converge	0.0000	-1548.3796348 a.u -1548.3872844 a.u	0.2082 0.0000
*OH (no HB) *OH accepting HB *OH donating HB	-1549.3899651 a.u -1549.392779 a.u -1549.3893084 a.u	0.0766 0.0000 0.0944	didn't converge -1549.072723 a.u -1549.0664339 a.u	 0.0000 0.1711

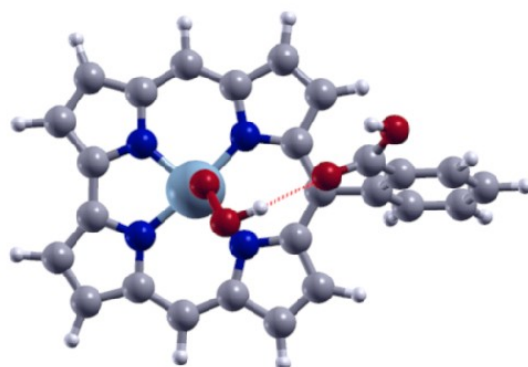
**Table S2:**  $E_{ads}$  of various H-Mn-N-C intermediates obtained from various level of theory with substituent  $R1=C_6H_4-COOH$ . Energies are in eV.

$E_{ads}$	PBE	PBE-D3	X3LYP	M06L	M06L-D3	M06-D3
OOH	4.3066	4.1334	4.5957	4.2623	4.237	4.5356
O	2.4734	2.4241	3.7245	3.0423	3.0358	3.7667
OH	1.1350	0.9910	1.1604	0.9677	0.9511	1.0414
$V_{onset}$ (in V)	0.61	0.78	0.32	0.66	0.68	0.38

**Table S3:** Structures, energies, and coordinates of the complexes with the substituent R1=C<sub>6</sub>H<sub>4</sub>-COOH. With out adsorbates (\*), with adsorbates \*OOH, \*O and \*OH complexes.

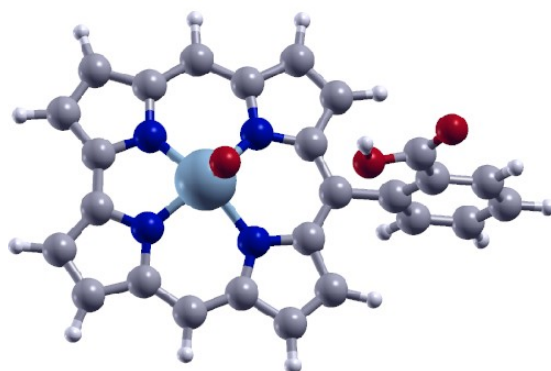
Gaussian data				QE data			
							
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C	5.189456	1.593353	0.397199	C	5.181661755	1.591171550	0.393598269
H	6.261626	1.457121	0.520985	H	6.256289541	1.458719935	0.516041966
C	4.492434	2.803385	0.420783	C	4.485372251	2.797399930	0.418202830
H	4.916534	3.795651	0.563514	H	4.912272107	3.790607749	0.560518183
C	3.100009	2.517569	0.230417	C	3.095760223	2.511778455	0.229088960
C	1.957405	3.333230	0.193420	C	1.955163315	3.324656635	0.191652944
C	0.650047	2.847992	0.038673	C	0.650907389	2.841346015	0.037196503
C	-0.561634	3.615248	0.039176	C	-0.558281554	3.606713056	0.035683841
H	-0.607644	4.696682	0.154900	H	-0.607448214	4.690032242	0.149035251
C	-1.620644	2.744387	-0.107236	C	-1.614462017	2.737972374	-0.110768713
H	-2.679161	2.991627	-0.130576	H	-2.673642161	2.989022193	-0.136104055
C	-1.085750	1.414372	-0.211743	C	-1.083277278	1.409524984	-0.213708437
C	-1.803780	0.208144	-0.355791	C	-1.801621236	0.206038721	-0.354686625
C	-1.215913	-1.074001	-0.420023	C	-1.212421047	-1.072843272	-0.414251401
C	-1.882785	-2.336669	-0.584519	C	-1.875211750	-2.335324937	-0.571247708
C	-0.920964	-3.325095	-0.584708	C	-0.915359640	-3.320642388	-0.570312708
C	0.360143	-2.701054	-0.426645	C	0.363148677	-2.696979547	-0.418264859
C	1.608531	-3.338177	-0.361188	C	1.609203135	-3.330847000	-0.355091618
C	2.828463	-2.663102	-0.193380	C	2.826759405	-2.657176149	-0.191807945
C	4.181746	-3.119157	-0.061212	C	4.177945375	-3.111308466	-0.063384217
H	4.499074	-4.160137	-0.083311	H	4.498976600	-4.153115742	-0.087252977
C	5.000756	-2.000390	0.106666	C	4.995046869	-1.995312784	0.101871234
H	6.079995	-1.998200	0.243248	H	6.076555897	-1.995969984	0.234859077
C	4.158266	-0.854884	0.078661	C	4.154967017	-0.852120839	0.076013333
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N	0.301825	1.497828	-0.111437	N	0.302362024	1.493335520	-0.113403177
N	0.152998	-1.317244	-0.324115	N	0.154872304	-1.314917883	-0.322102462
N	2.853762	-1.287636	-0.102663	N	2.852423775	-1.284280147	-0.103779757
Mn	1.500319	0.030218	-0.307357	Mn	1.499438880	0.029386862	-0.304941634
H	1.618678	-4.427089	-0.437398	H	1.619981953	-4.421552582	-0.429353113
H	-1.078238	-4.397750	-0.682695	H	-1.075714426	-4.394985008	-0.664145359
H	-2.957349	-2.466061	-0.690210	H	-2.951125779	-2.469275949	-0.673474865
H	1.648880	0.141062	-1.834905	H	1.645002173	0.136277680	-1.828661974
C	-3.292341	0.296163	-0.483404	C	-3.288826372	0.292166300	-0.484411674

C	-4.196483	-0.141547	0.517565	C	-4.195868359	-0.138315092	0.513044816
C	-3.824888	0.788337	-1.689937	C	-3.820787203	0.775332506	-1.691180082
C	-5.583187	-0.104166	0.273631	C	-5.578625256	-0.102418722	0.264438273
C	-5.203655	0.847409	-1.911283	C	-5.194968499	0.832921830	-1.917024463
H	-3.131144	1.111464	-2.469730	H	-3.127296142	1.096584649	-2.473544543
C	-6.089032	0.393340	-0.926420	C	-6.081232361	0.385532629	-0.935984297
H	-6.250381	-0.468345	1.057477	H	-6.249897487	-0.462859492	1.048476729
H	-5.584517	1.234992	-2.859386	H	-5.574084910	1.215908408	-2.869439598
H	-7.167918	0.425689	-1.093564	H	-7.161212421	0.416283883	-1.107348442
C	-3.799918	-0.658512	1.865785	C	-3.804307934	-0.644998108	1.863615378
O	-4.493115	-1.405978	2.537899	O	-4.495273858	-1.394070440	2.535345141
O	-2.605712	-0.180938	2.311510	O	-2.616833905	-0.157476889	2.313476362
H	-2.469037	-0.596200	3.187317	H	-2.486335717	-0.572772861	3.200177988
H	2.080236	4.412000	0.306569	H	2.078507529	4.405156267	0.303924392



E= -1623.4795751 a.u (*OOH)				E= -739.1570277716 Ry (*OOH)			
C	-4.182264	-0.542935	0.059466	C	4.178643043	0.540216446	0.057801197
C	-5.157481	-1.590202	0.112343	C	5.150004815	1.586874589	0.111435078
H	-6.235021	-1.458987	0.182164	H	6.229556210	1.458633926	0.181419683
C	-4.464474	-2.794972	0.052607	C	4.456995831	2.787875443	0.052322414
H	-4.893028	-3.795375	0.062830	H	4.885651193	3.789747721	0.062791066
C	-3.058822	-2.492209	-0.043840	C	3.054373951	2.485068963	-0.043981838
C	-1.923263	-3.300618	-0.183650	C	1.921855639	3.290562182	-0.183824799
C	-0.602750	-2.816868	-0.347127	C	0.603809937	2.809088848	-0.347265290
C	0.603058	-3.597499	-0.437332	C	-0.598951273	3.588759724	-0.436726127
H	0.644340	-4.684796	-0.411748	H	-0.640114693	4.677463539	-0.410799293
C	1.661991	-2.720014	-0.540334	C	-1.655656796	2.714748706	-0.540134694
H	2.718570	-2.966791	-0.610842	H	-2.713008834	2.965051731	-0.610809810
C	1.116833	-1.384543	-0.529075	C	-1.114042145	1.380806207	-0.529116319
C	1.825677	-0.153827	-0.582411	C	-1.823069936	0.153420691	-0.581433771
C	1.246759	1.141841	-0.612668	C	-1.242792066	-1.138417844	-0.611976543
C	1.920298	2.405174	-0.789210	C	-1.912714715	-2.400167821	-0.788633118
C	0.956424	3.392124	-0.788334	C	-0.951061285	-3.384185642	-0.787805936
C	-0.321634	2.755221	-0.606463	C	0.324030068	-2.749097978	-0.606644536
C	-1.588628	3.376266	-0.513424	C	1.588076583	-3.367928036	-0.513387263
C	-2.796154	2.697150	-0.299301	C	2.792507882	-2.691059056	-0.301466321
C	-4.162944	3.141224	-0.251217	C	4.155858209	-3.134268937	-0.251460561
H	-4.491924	4.173872	-0.351276	H	4.485274405	-4.168286558	-0.351193218
C	-4.972554	2.021073	-0.074923	C	4.964992323	-2.017206332	-0.076199045
H	-6.058093	2.004845	-0.007195	H	6.052228715	-2.003862993	-0.007475766
C	-4.109911	0.885256	-0.008190	C	4.106695883	-0.882551558	-0.012373027
N	-2.943076	-1.120600	-0.013843	N	2.940936485	1.115541993	-0.013420700

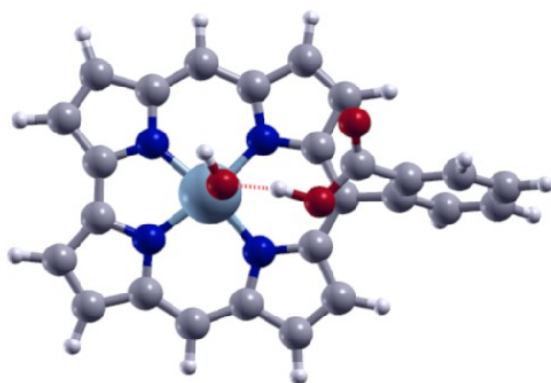
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N	-2.812023	1.327970	-0.122477	N	2.809626211	-1.323143262	-0.127416048
Mn	-1.419399	0.031803	-0.110560	Mn	1.421524277	-0.034469284	-0.106541515
H	-1.618716	4.462161	-0.625364	H	1.618032905	-4.455491391	-0.624355247
H	1.107440	4.463788	-0.904318	H	-1.103425032	-4.457146403	-0.903510606
H	2.992699	2.532899	-0.917860	H	-2.986320985	-2.531170517	-0.917656351
H	-2.054192	-4.384702	-0.170585	H	2.053294186	4.376082191	-0.170320064
H	-1.570480	-0.074912	-1.667941	H	1.555147122	0.081774105	-1.660809674
O	-0.851008	0.075220	1.746765	O	0.843012714	-0.070583461	1.732624261
O	-0.214897	-0.994796	2.411423	O	0.214044612	0.998768428	2.416059261
H	0.718600	-0.676342	2.438380	H	-0.725123161	0.670370585	2.445588255
C	3.316571	-0.227933	-0.650886	C	-3.312326604	0.226757946	-0.649827156
C	3.923448	-0.619503	-1.856413	C	-3.919698431	0.618050391	-1.852040852
C	4.151397	0.130863	0.438743	C	-4.147765231	-0.131258350	0.436321392
C	5.314836	-0.652999	-1.993596	C	-5.307851560	0.652241021	-1.989284202
H	3.281655	-0.882527	-2.700340	H	-3.279271338	0.883436769	-2.699000203
C	5.552063	0.114363	0.284425	C	-5.545413555	-0.112800199	0.281601679
C	6.132978	-0.280641	-0.921113	C	-6.125342303	0.281281272	-0.920496310
H	5.758407	-0.959932	-2.943883	H	-5.751673472	0.960850960	-2.941233520
H	6.179436	0.398877	1.130124	H	-6.175263352	-0.396844490	1.128285459
H	7.220278	-0.298386	-1.022230	H	-7.214913275	0.298760077	-1.021333468
C	3.577423	0.459184	1.776062	C	-3.579396632	-0.459634114	1.773819159
O	2.496083	0.095628	2.214567	O	-2.500896522	-0.093985974	2.215740505
O	4.427038	1.214480	2.531498	O	-4.428985313	-1.216333493	2.524901798
H	3.974386	1.339548	3.389971	H	-3.969070036	-1.338669990	3.390307492



E= -1547.7485052 a.u (*O)				E= -705.7897997368 Ry (*O)			
C	4.189558	0.576075	-0.033358	C	4.176325412	0.640710163	0.003247654
C	5.160175	1.619830	-0.062694	C	5.113575368	1.709285988	-0.055276340
H	6.236578	1.490897	-0.150643	C	6.197827803	1.610718135	-0.097247455
C	4.464130	2.821310	0.030328	C	4.380394655	2.888418184	-0.057906396
H	4.886629	3.824330	0.030090	H	4.773184644	3.904562219	-0.102363102
C	3.063404	2.514014	0.099227	C	2.990611922	2.543841017	-0.012582532
C	1.931451	3.329277	0.089890	C	1.840539918	3.325698543	-0.087456291
C	0.615225	2.835812	-0.011618	C	0.539407417	2.800503491	-0.160435942
C	-0.584662	3.620049	-0.129226	C	-0.680284799	3.543079781	-0.314089447
H	-0.619915	4.707651	-0.107220	H	-0.745621971	4.629801279	-0.356125565
C	-1.636224	2.746304	-0.281673	C	-1.706823073	2.637445869	-0.405145228
H	-2.690026	2.988692	-0.391560	H	-2.768218595	2.848395451	-0.524398033
C	-1.092518	1.412062	-0.265678	C	-1.128390471	1.323029203	-0.315529176
C	-1.815118	0.206255	-0.400325	C	-1.807722998	0.090783429	-0.394413359

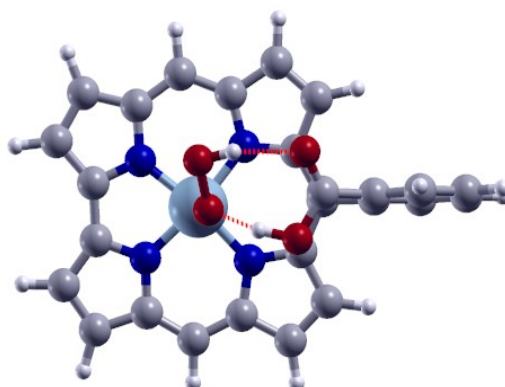


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C	-0.964700	-3.323124	-0.690450	C	-0.842054904	-3.405446863	-0.593802957
C	0.307023	-2.696853	-0.436166	C	0.408893184	-2.737810161	-0.368411122
C	1.569570	-3.322515	-0.435910	C	1.682272646	-3.330706611	-0.329430990
C	2.780762	-2.637814	-0.317877	C	2.867941177	-2.613586055	-0.192261222
C	4.141118	-3.081141	-0.443128	C	4.239966925	-3.019933783	-0.261943659
H	4.451438	-4.112624	-0.598856	H	4.584671607	-4.047819275	-0.377324289
C	4.965164	-1.964291	-0.348417	C	5.028135962	-1.879956306	-0.178453108
H	6.050299	-1.941976	-0.418387	H	6.115865312	-1.829756628	-0.216728504
C	4.113245	-0.837668	-0.149171	C	4.142459188	-0.774763948	-0.044790109
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N	0.277513	1.497703	-0.082627	N	0.233981229	1.457161922	-0.149124244
N	0.104742	-1.341400	-0.276973	N	0.167356685	-1.386700556	-0.246895855
N	2.809240	-1.270982	-0.109173	N	2.850947159	-1.243843807	-0.024475062
Mn	1.446634	-0.017891	0.330791	Mn	1.448913243	-0.014636488	0.334821483
H	1.594952	-4.402201	-0.597907	H	1.739111581	-4.414192235	-0.464055889
H	-1.109794	-4.387343	-0.866340	H	-0.957130390	-4.479620810	-0.733164967
H	-2.985009	-2.439003	-0.878603	H	-2.891372016	-2.595983169	-0.772030160
H	1.306156	0.023699	-1.297703	H	1.950444793	4.412165404	-0.141053799
O	0.996602	-0.202140	1.845616	H	1.328445852	0.055997761	-1.299548501
C	-3.297257	0.298276	-0.585515	O	0.975051935	-0.046047863	1.853465486
C	-4.230574	-0.105627	0.402032	C	-3.292146163	0.131112586	-0.586766720
C	-3.787359	0.745159	-1.826504	C	-3.767471122	0.331209093	-1.892447804
C	-5.607821	-0.076507	0.115139	C	-4.237946761	-0.051400342	0.449804915
C	-5.159088	0.791927	-2.092371	C	-5.131696288	0.355673125	-2.177386111
H	-3.070092	1.040720	-2.595815	H	-3.038541614	0.461750955	-2.698034017
C	-6.074767	0.375134	-1.118933	C	-5.610002833	-0.035733029	0.147268828
H	-6.298828	-0.411635	0.891402	C	-6.060058457	0.170550231	-1.151659929
H	-5.510212	1.142573	-3.065909	H	-5.467780205	0.514085396	-3.207049058
H	-7.147725	0.400907	-1.321508	H	-6.313373946	-0.189351580	0.970823743
C	-3.860677	-0.576656	1.775883	H	-7.132663765	0.186049721	-1.364822340
O	-4.565252	-1.301608	2.459583	C	-3.906822009	-0.271249644	1.893616459
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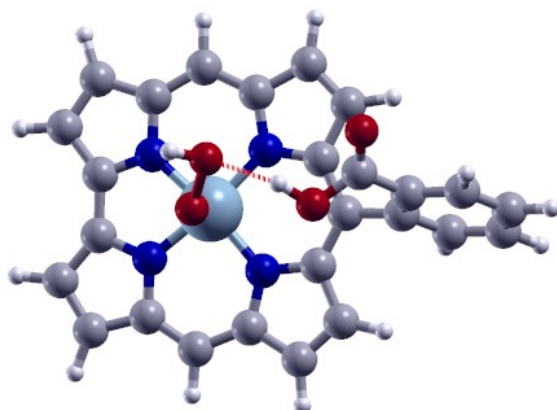
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H	6.044942	1.507361	0.586698	H	6.036184428	1.505753644	0.586831156
C	4.296022	2.850148	0.300671	C	4.286005043	2.843745508	0.302971539

H	4.724603	3.849344	0.348151	H	4.712405796	3.845305654	0.354092028
C	2.905735	2.549583	0.080857	C	2.898629053	2.543658377	0.082713197
C	1.786665	3.358356	-0.171355	C	1.782855100	3.348510293	-0.167654075
C	0.483629	2.882309	-0.442673	C	0.483505646	2.872427999	-0.440428017
C	-0.711195	3.659399	-0.618859	C	-0.707873926	3.647917169	-0.616038517
H	-0.752686	4.746877	-0.614782	H	-0.746914934	4.736840820	-0.609425321
C	-1.767646	2.780203	-0.757117	C	-1.762272357	2.771961843	-0.757102307
H	-2.820353	3.022103	-0.879631	H	-2.815606505	3.016626329	-0.882720570
C	-1.228199	1.450086	-0.705982	C	-1.226349659	1.443655612	-0.707225579
C	-1.936213	0.214033	-0.749262	C	-1.933790071	0.212766609	-0.746386225
C	-1.340515	-1.074401	-0.849783	C	-1.337978826	-1.069776217	-0.845734166
C	-2.004329	-2.336825	-1.058328	C	-1.997291354	-2.331446395	-1.051061450
C	-1.032083	-3.314637	-1.073408	C	-1.026848320	-3.305795948	-1.065736896
C	0.234567	-2.672687	-0.837641	C	0.236829539	-2.665397753	-0.832931830
C	1.494371	-3.295190	-0.651583	C	1.493684679	-3.287087014	-0.649635540
C	2.673250	-2.631063	-0.283030	C	2.669444761	-2.625520334	-0.286698156
C	4.035268	-3.076518	-0.137816	C	4.028679917	-3.068870413	-0.142047750
H	4.376964	-4.103374	-0.253258	H	4.369464445	-4.097733575	-0.255957289
C	4.819492	-1.963788	0.153196	C	4.811210370	-1.958745480	0.146256953
H	5.895740	-1.944499	0.308127	H	5.888977095	-1.939797505	0.302887323
C	3.940928	-0.834498	0.193995	C	3.935912298	-0.831413749	0.185317109
N	2.782799	1.179966	0.104131	N	2.778190742	1.175616158	0.102648210
N	0.133028	1.541884	-0.520738	N	0.133050181	1.536169866	-0.520387373
N	0.010218	-1.314976	-0.735242	N	0.012327032	-1.311198928	-0.730917194
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Mn	1.261105	0.034024	-0.136514	Mn	1.260081554	0.032231386	-0.138410719
H	1.536745	-4.376416	-0.800700	H	1.534607091	-4.370355012	-0.797530436
H	-1.173021	-4.384996	-1.209511	H	-1.166438935	-4.378138620	-1.199263497
H	-3.076561	-2.464279	-1.184382	H	-3.070786491	-2.461513542	-1.177324599
H	1.679988	0.080508	-1.647397	H	1.672852204	0.088332979	-1.646771264
O	0.655335	-0.137416	1.736757	O	0.646349855	-0.119994075	1.743721132
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C	-3.808013	-0.146921	0.845594	C	-3.802967227	-0.145925416	0.841928513
C	-4.374410	0.549230	-1.421266	C	-4.367302638	0.550198220	-1.419036576
C	-5.172053	-0.224669	1.152218	C	-5.163752493	-0.222350147	1.147441283
C	-5.735442	0.499194	-1.091953	C	-5.724729355	0.500135407	-1.090883034
H	-4.061338	0.816998	-2.433692	H	-4.054999765	0.820610799	-2.433016409
C	-6.133568	0.110775	0.192558	C	-6.122553034	0.111590615	0.190074119
H	-5.468714	-0.544675	2.153862	H	-5.459852963	-0.545569088	2.150476733
H	-6.484743	0.751180	-1.846226	H	-6.473982560	0.754233050	-1.846567221
H	-7.195333	0.064476	0.445946	H	-7.185435520	0.065347025	0.444138400
C	-2.754465	-0.513663	1.872499	C	-2.754415022	-0.515400160	1.871486433
O	-2.799352	-1.551675	2.517155	O	-2.809652176	-1.558597678	2.507904662
O	-1.800721	0.419219	1.936138	O	-1.801364918	0.411397183	1.952489890
H	-0.821283	0.074863	2.070420	H	-0.800170249	0.068071437	2.060761788
H	1.021169	-0.917140	2.187532	H	0.999485231	-0.917046853	2.192000467
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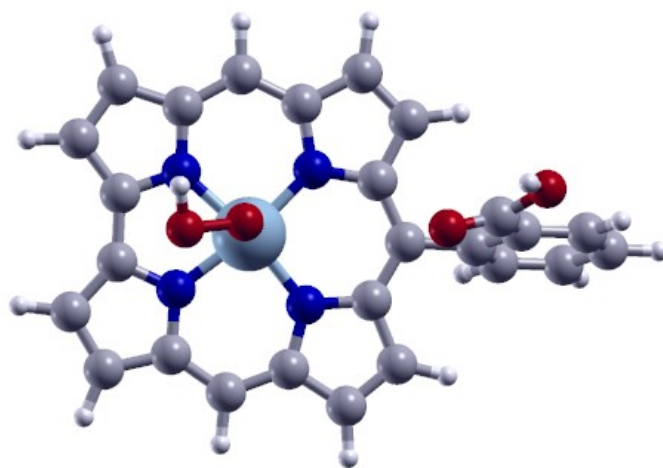
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C 4.918249 1.751769 0.357890	C 4.907678370 1.752596254 0.354570662
H 5.988497 1.635414 0.512302	H 5.979419917 1.635516592 0.508600936
C 4.210187 2.948676 0.273583	C 4.199006541 2.945774943 0.271337192
H 4.619024 3.954589 0.347254	H 4.603291485 3.955123747 0.346245762
C 2.825680 2.628124 0.052425	C 2.818202130 2.623827261 0.051145698
C 1.690126 3.423582 -0.164317	C 1.685106022 3.415914433 -0.165330906
C 0.396070 2.928320 -0.440628	C 0.394856711 2.920815376 -0.441814522
C -0.812483 3.685465 -0.610608	C -0.810955153 3.675201824 -0.611515675
H -0.874722 4.771696 -0.584077	H -0.869347585 4.763356438 -0.584759912
C -1.849525 2.789988 -0.784282	C -1.845039050 2.781752712 -0.785477346
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C -1.286949 1.468496 -0.758058	C -1.284317879 1.462696934 -0.756924325
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C -1.998848 -2.322898 -1.170411	C -1.990356719 -2.321491367 -1.166931783
C -1.013390 -3.285821 -1.168098	C -1.004942311 -3.280323266 -1.165406288
C 0.243419 -2.623172 -0.929237	C 0.247580943 -2.616583953 -0.928424733
C 1.511914 -3.230998 -0.745576	C 1.513796364 -3.221724441 -0.746326943
C 2.685962 -2.547752 -0.406621	C 2.684292657 -2.539616889 -0.407762015
C 4.051837 -2.977648 -0.247352	C 4.047532146 -2.967527629 -0.251269591
H 4.404414 -4.002317 -0.348372	H 4.397659604 -3.994912466 -0.352267587
C 4.822101 -1.855512 0.041901	C 4.815736827 -1.847709058 0.037253792
H 5.895488 -1.825823 0.214298	H 5.890873603 -1.815314268 0.208503145
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H 1.562539 -4.314272 -0.874838	H 1.564484454 -4.306872959 -0.873526664
H -1.136796 -4.359317 -1.297057	H -1.122722899 -4.356273780 -1.290298140
H -3.068592 -2.468005 -1.299602	H -3.061479948 -2.468908676 -1.294346982
H 1.584594 0.186879 -1.766783	H 1.570047109 0.184818723 -1.764620614
O 0.539488 -0.137287 1.634729	O 0.529168287 -0.123452416 1.642955293
C -3.436217 0.216107 -0.523832	C -3.428369162 0.213504568 -0.520218972
C -3.767760 -0.105573 0.819556	C -3.761409493 -0.105875007 0.819728746
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C -5.106524 -0.205829 1.210412	C -5.098074495 -0.199290351 1.206177940

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H	-4.212780	0.682810	-2.481683	H	-4.197129272	0.674414549	-2.479605891
C	-6.124887	0.046215	0.282333	C	-6.111036745	0.050262899	0.277745550
H	-5.349256	-0.472111	2.241755	H	-5.342395799	-0.464638017	2.239048740
H	-6.601441	0.566410	-1.763173	H	-6.584153640	0.562158326	-1.769061992
H	-7.170129	-0.019706	0.592934	H	-7.158288548	-0.014596508	0.586946191
C	-2.608830	-0.378969	1.747162	C	-2.606949771	-0.384650856	1.749052975
O	-2.315236	-1.507290	2.140351	O	-2.325014752	-1.519589017	2.134057577
O	-1.884567	0.715015	1.990533	O	-1.874256172	0.696055483	2.000905288
H	-0.897310	0.439725	2.081228	H	-0.866775698	0.412947874	2.059709987
O	0.586645	-1.480960	2.146450	O	0.550752922	-1.470507286	2.163317315
H	-0.378057	-1.673630	2.286483	H	-0.429313297	-1.647064338	2.295835985
H	1.803949	4.508986	-0.120751	H	1.797302045	4.503048228	-0.120418202



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C	5.082011	1.624547	0.292583	C	-5.073749319	-1.621171609	0.291783000
H	6.155270	1.470333	0.377437	H	-6.149050844	-1.470267737	0.377390458
C	4.406971	2.843275	0.317707	C	-4.400332069	-2.836647519	0.316671033
H	4.849569	3.831604	0.426666	H	-4.846388345	-3.825278962	0.425921558
C	3.002874	2.573062	0.158053	C	-2.999272404	-2.567623912	0.156938663
C	1.878245	3.406402	0.062279	C	-1.876829536	-3.398086230	0.061430045
C	0.554952	2.961315	-0.163878	C	-0.556544497	-2.955767665	-0.164144176
C	-0.639575	3.761570	-0.185992	C	0.635293300	-3.754070019	-0.186934481
H	-0.666233	4.843164	-0.067747	H	0.664527700	-4.837218784	-0.069595570
C	-1.711971	2.910844	-0.354388	C	1.705392368	-2.906043699	-0.355764361
H	-2.765145	3.176456	-0.393647	H	2.758660797	-3.176399395	-0.395295501
C	-1.189471	1.574029	-0.471858	C	1.187875651	-1.570434868	-0.472590019
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C	-1.056607	-3.144737	-1.226064	C	1.051706703	3.137578993	-1.224803197
C	0.217052	-2.542967	-0.944807	C	-0.219008600	2.536361336	-0.944724872
C	1.471294	-3.195883	-0.860326	C	-1.470902423	3.186626900	-0.860162149
C	2.686896	-2.569911	-0.549488	C	-2.683754035	2.563179776	-0.550147224
C	4.046766	-3.047995	-0.484067	C	-4.041141970	3.040863431	-0.484893701
H	4.361591	-4.076935	-0.647530	H	-4.358873494	4.070772433	-0.648495238
C	4.864042	-1.961710	-0.190423	C	-4.856608179	1.958396788	-0.191247585
H	5.945975	-1.967773	-0.079587	H	-5.940230404	1.967870398	-0.081059210
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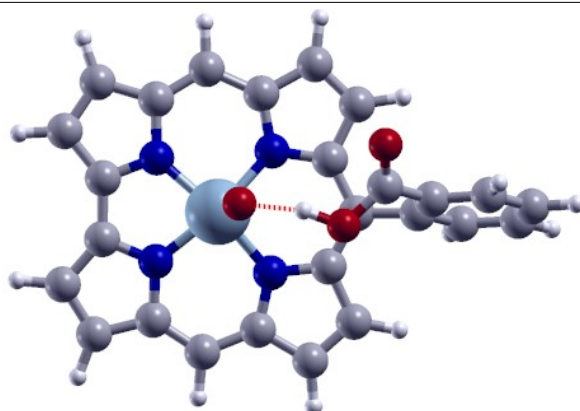
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N	0.010610	-1.192085	-0.729422	N	-0.010663399	1.187911487	-0.729987765
N	2.723079	-1.225425	-0.273908	N	-2.721393936	1.221662414	-0.274658789
Mn	1.324215	0.099103	-0.176339	Mn	-1.321840413	-0.102049384	-0.176132638
H	1.479440	-4.269259	-1.062968	H	-1.479438981	4.261642961	-1.063134469
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H	-3.085091	-2.256910	-1.305618	H	3.079308415	2.256999762	-1.305131329
H	2.023177	4.483621	0.170379	H	-2.022677093	-4.476861312	0.169280817
H	1.632884	0.228074	-1.716143	H	-1.634934230	-0.224689772	-1.715091438
O	1.028920	-0.148429	1.738787	O	-1.032985054	0.151463047	1.735314812
O	0.404475	-1.385044	2.178540	O	-0.400536653	1.386813736	2.179097242
H	1.043623	-1.677302	2.856847	H	-1.046094879	1.676956496	2.865152653
C	-3.399573	0.409234	-0.515204	C	3.396653630	-0.408024195	-0.514707167
C	-4.193179	1.011407	-1.506594	C	4.191507025	-1.008285664	-1.501365074
C	-4.039607	-0.210123	0.589978	C	4.037998065	0.210198057	0.586197162
C	-5.588981	1.005457	-1.409972	C	5.583215447	-1.003047052	-1.406145187
H	-3.704436	1.465017	-2.372299	H	3.705596946	-1.464918372	-2.368304652
C	-5.440816	-0.235089	0.661566	C	5.435886972	0.232588999	0.657267021
C	-6.215179	0.379683	-0.325184	C	6.208926797	-0.379704375	-0.325650786
H	-6.187776	1.477345	-2.192757	H	6.182758589	-1.475955467	-2.189701937
H	-5.908295	-0.740660	1.509502	H	5.905436827	0.738610834	1.505524032
H	-7.304954	0.366358	-0.251525	H	7.300351058	-0.366704949	-0.252416123
C	-3.263372	-0.889148	1.686937	C	3.266271166	0.885834058	1.684153926
O	-3.614666	-1.930348	2.216745	O	3.617772266	1.927487631	2.211077690
O	-2.148725	-0.198871	2.008249	O	2.155137995	0.194617635	2.012221393
H	-1.501364	-0.774227	2.483951	H	1.501490143	0.778536361	2.486687645



E=	-1623.4763892	a.u (*OOH)		E=	-739.1513230656	Ry (*OOH)	
C	4.097720	0.645284	-0.172773	C	4.093906240	0.644172260	-0.174616263
C	5.063322	1.697788	-0.084838	C	5.056655970	1.695229133	-0.085592707
H	6.144362	1.578687	-0.084926	H	6.139898347	1.578626484	-0.085015514
C	4.352162	2.892328	-0.003283	C	4.347140666	2.887238962	-0.003966564
H	4.767557	3.895441	0.073294	H	4.765247512	3.891346188	0.072989784
C	2.948493	2.571422	-0.041439	C	2.946009822	2.567665122	-0.042659003
C	1.785698	3.356829	-0.009541	C	1.784227436	3.350583836	-0.010499085
C	0.468193	2.857293	-0.089921	C	0.469946933	2.853517259	-0.091446211
C	-0.747072	3.623634	-0.114902	C	-0.743797707	3.616801854	-0.115132252
H	-0.796121	4.709322	-0.054413	H	-0.795247714	4.704361348	-0.054562648

C	-1.802090	2.743330	-0.228041	C	-1.796474579	2.739129736	-0.228072616
H	-2.861351	2.984258	-0.271186	H	-2.856726364	2.983908597	-0.270824478
C	-1.255045	1.412770	-0.276563	C	-1.254453239	1.409640988	-0.278163818
C	-1.958340	0.190973	-0.404415	C	-1.957870128	0.190991286	-0.405346799
C	-1.358489	-1.092176	-0.494051	C	-1.357392957	-1.089422477	-0.495096169
C	-2.009219	-2.356718	-0.711575	C	-2.003594087	-2.353409688	-0.710904120
C	-1.027676	-3.325921	-0.761193	C	-1.023793268	-3.319607833	-0.760379030
C	0.241558	-2.677428	-0.585985	C	0.243135151	-2.672430272	-0.586317397
C	1.515620	-3.287449	-0.611609	C	1.514946752	-3.280088664	-0.611136128
C	2.740257	-2.607333	-0.515515	C	2.737782950	-2.602051634	-0.515873942
C	4.115375	-3.047409	-0.514220	C	4.111053193	-3.041591538	-0.514402298
H	4.447242	-4.080333	-0.602594	H	4.445190013	-4.076016023	-0.602066130
C	4.920401	-1.920655	-0.380751	C	4.914190602	-1.917984825	-0.381036113
H	6.007209	-1.892599	-0.347561	H	6.002977176	-1.892436523	-0.347698968
C	4.041173	-0.788325	-0.302663	C	4.037142560	-0.786437011	-0.303887499
N	2.853695	1.206999	-0.143108	N	2.851752636	1.206091218	-0.144076595
N	0.124288	1.510810	-0.174795	N	0.124613857	1.507497798	-0.176026595
N	0.002347	-1.316856	-0.412378	N	0.001854978	-1.313108846	-0.412858246
N	2.761663	-1.242603	-0.397557	N	2.760539743	-1.240351156	-0.398211387
Mn	1.331770	0.033617	-0.122014	Mn	1.326664335	0.036806324	-0.119022625
H	1.535013	-4.373201	-0.730352	H	1.534650881	-4.367818579	-0.729833393
H	-1.162242	-4.394423	-0.919409	H	-1.160805918	-4.389857284	-0.918515300
H	-3.081650	-2.498636	-0.822804	H	-3.077331682	-2.499030659	-0.822296941
H	1.895054	4.441011	0.065649	H	1.894061399	4.436555589	0.065243462
H	1.499137	0.131147	-1.673454	H	1.504100158	0.127101590	-1.668135140
O	1.486494	-0.330161	1.778312	O	1.489187061	-0.332899765	1.769530302
C	-3.444474	0.263291	-0.565762	C	-3.442708904	0.262676209	-0.564858460
C	-3.955845	0.687071	-1.804813	C	-3.956271330	0.684771093	-1.800197175
C	-4.360310	-0.115433	0.448099	C	-4.358442285	-0.114005666	0.446453818
C	-5.332494	0.734511	-2.046221	C	-5.329306147	0.732791587	-2.041704564
H	-3.251089	0.969554	-2.590294	H	-3.253033431	0.968916644	-2.588445041
C	-5.744651	-0.078373	0.190436	C	-5.739317656	-0.076288876	0.187816146
C	-6.231302	0.346994	-1.046295	C	-6.226154278	0.346704307	-1.045166639
H	-5.700613	1.067393	-3.019732	H	-5.698295916	1.066404991	-3.016491605
H	-6.434188	-0.374766	0.981792	H	-6.431593717	-0.373198074	0.978691771
H	-7.307909	0.377497	-1.227928	H	-7.304420610	0.377177041	-1.227022224
C	-3.869837	-0.492026	1.807169	C	-3.873326985	-0.491955975	1.804957602
O	-2.760724	-0.266710	2.254184	O	-2.765282866	-0.267007458	2.253626147
O	-4.835058	-1.124057	2.550204	O	-4.837702050	-1.124036190	2.545625005
H	-4.416983	-1.294842	3.417707	H	-4.411949753	-1.293925100	3.419790474
O	2.757029	-0.213532	2.408958	O	2.756684342	-0.209166284	2.414178918
H	2.887680	-1.124366	2.742159	H	2.887472857	-1.129658042	2.745743251





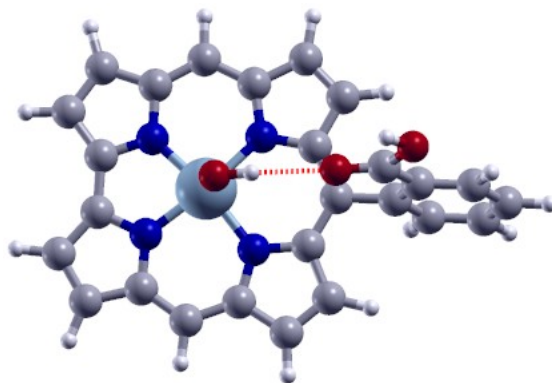
E= -1547.7335548 a.u (\*OOH)

C	4.063299	0.574834	0.214744
C	5.041932	1.610924	0.285437
H	6.117116	1.469194	0.367460
C	4.359843	2.823504	0.223322
H	4.796249	3.820191	0.241080
C	2.958493	2.536964	0.105165
C	1.844932	3.361761	-0.067301
C	0.527009	2.902099	-0.286653
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H	-0.683322	4.783217	-0.496415
C	-1.717887	2.827695	-0.632878
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C	-1.188477	1.491490	-0.563910
C	-1.899423	0.265483	-0.667298
C	-1.311163	-1.017342	-0.802984
C	-1.984405	-2.267511	-1.061800
C	-1.026713	-3.254728	-1.065107
C	0.242889	-2.632413	-0.782371
C	1.493084	-3.278006	-0.615168
C	2.685346	-2.636439	-0.277684
C	4.052667	-3.093770	-0.238900
H	4.377446	-4.119066	-0.404110
C	4.859735	-1.989415	-0.003162
H	5.945015	-1.973754	0.066584
C	3.988723	-0.854746	0.116627
N	2.822755	1.155709	0.129714
N	0.169570	1.568753	-0.344653
N	0.038749	-1.277134	-0.667705
N	2.704371	-1.280596	-0.017933
Mn	1.290557	0.032710	0.094088
H	1.516358	-4.356644	-0.786167
H	-1.172026	-4.319293	-1.236951
H	-3.052875	-2.376304	-1.228964
H	1.477045	0.055735	-1.505664
O	0.577912	-0.323429	1.596482
C	-3.382626	0.287290	-0.479201
C	-3.893548	-0.180380	0.759613
C	-4.274377	0.688800	-1.484396
C	-5.278062	-0.256294	0.956135

E= -705.7510999004 Ry (\*OOH)

C	4.060809906	0.574950490	0.211987473
C	5.033355984	1.609511648	0.282976567
H	6.110642481	1.471102837	0.364085184
C	4.349685696	2.818292260	0.221412276
H	4.784054637	3.817330828	0.238425197
C	2.952512117	2.531328621	0.104353672
C	1.842876340	3.354814092	-0.071406735
C	0.531307939	2.893160900	-0.292723803
C	-0.651936614	3.681191771	-0.486807067
H	-0.679740082	4.770382413	-0.504236891
C	-1.707942400	2.814443495	-0.638523040
H	-2.754413594	3.066009974	-0.801246713
C	-1.181325847	1.480647380	-0.566570528
C	-1.894812956	0.260378001	-0.666284934
C	-1.306310821	-1.019874932	-0.793172370
C	-1.975487498	-2.268376814	-1.054213940
C	-1.019960679	-3.252108031	-1.058928034
C	0.246725045	-2.631307153	-0.777664484
C	1.493838323	-3.271293607	-0.614722593
C	2.682506147	-2.625496946	-0.283540166
C	4.045278975	-3.079949923	-0.242264236
H	4.369411525	-4.107343896	-0.404997705
C	4.852733431	-1.978269439	-0.005989543
H	5.939607877	-1.966722678	0.064785207
C	3.988218232	-0.846464160	0.109965885
N	2.818447014	1.153295196	0.132114253
N	0.175084278	1.562323085	-0.348526999
N	0.039361785	-1.280214239	-0.659021625
N	2.702147839	-1.272302710	-0.024398684
Mn	1.295527152	0.029302709	0.100547925
H	1.520168973	-4.351207452	-0.783837472
H	-1.164569952	-4.317752656	-1.233782066
H	-3.044953929	-2.379443658	-1.223930300
H	1.455087219	0.053777304	-1.495320671
O	0.558967000	-0.309613062	1.584502395
C	-3.376413071	0.284381570	-0.481013594
C	-3.890667284	-0.174774827	0.756102714
C	-4.267850302	0.677286791	-1.485719916
C	-5.271743660	-0.249196799	0.952283068

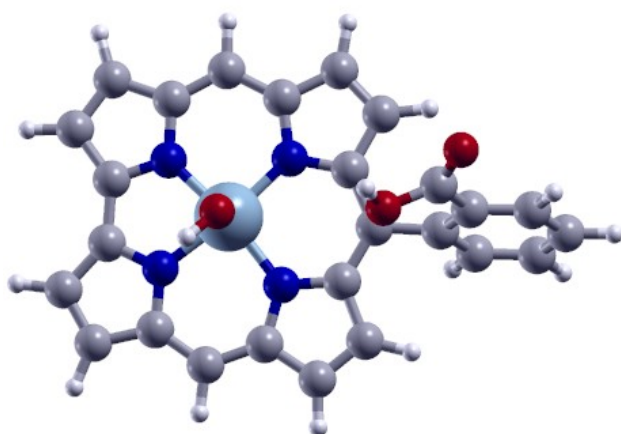
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H	-3.882080	1.022134	-2.448501	H	-3.877638196	1.006952924	-2.454054958
C	-6.158556	0.165738	-0.045483	C	-6.149776753	0.164132703	-0.049388518
H	-5.652848	-0.643704	1.906397	H	-5.646715170	-0.632029185	1.906423483
H	-6.342453	0.957769	-2.052613	H	-6.332992629	0.941578491	-2.059413041
H	-7.237118	0.120755	0.122340	H	-7.230006008	0.119591721	0.118930873
C	-2.932891	-0.650253	1.829578	C	-2.939524814	-0.638056856	1.832185859
O	-3.071793	-1.700000	2.433648	O	-3.080611047	-1.687783603	2.435048543
O	-1.928904	0.231482	1.982764	O	-1.939643702	0.243904862	2.000914866
H	-1.003583	-0.167960	2.128428	H	-1.009606298	-0.168186370	2.125188156
H	1.999761	4.443073	-0.063828	H	1.996589291	4.437374688	-0.067689567



E= -1548.3879341 Ry (*OH)				E= -707.0509013481 Ry (*OH)			
C	4.178156	0.622488	0.116560	C	4.159925740	0.636875661	0.139231043
C	5.135560	1.686048	0.171238	C	5.105626067	1.704610245	0.200177353
H	6.216522	1.573181	0.215689	H	6.188063634	1.598690658	0.263948791
C	4.420195	2.879552	0.150054	C	4.385922905	2.891145390	0.156852242
H	4.831072	3.887144	0.170156	H	4.791435321	3.902779229	0.173977618
C	3.019491	2.552270	0.075012	C	2.991750178	2.558247149	0.062786970
C	1.868279	3.342078	-0.036156	C	1.843306753	3.340667463	-0.072863669
C	0.549962	2.845072	-0.193440	C	0.532461264	2.838322718	-0.244781056
C	-0.665264	3.612051	-0.299174	C	-0.684832086	3.594747896	-0.359086985
H	-0.720489	4.698774	-0.275202	H	-0.746468571	4.682695584	-0.340922163
C	-1.710405	2.721892	-0.427314	C	-1.721289739	2.699494942	-0.483737972
H	-2.768005	2.954557	-0.525170	H	-2.780872248	2.927581473	-0.586981341
C	-1.146714	1.393420	-0.415429	C	-1.151983005	1.376459512	-0.463102419
C	-1.832306	0.154185	-0.518020	C	-1.829535126	0.134896875	-0.554363673
C	-1.233541	-1.134297	-0.573526	C	-1.224000649	-1.147019820	-0.612351030
C	-1.885827	-2.403232	-0.787463	C	-1.867390737	-2.420275135	-0.809685024
C	-0.906558	-3.374762	-0.774644	C	-0.885284866	-3.383520602	-0.788765157
C	0.355454	-2.717937	-0.549208	C	0.371094460	-2.718872710	-0.572222327
C	1.635402	-3.320915	-0.461506	C	1.650672683	-3.311651026	-0.460900957
C	2.837784	-2.634219	-0.251256	C	2.841336091	-2.618493975	-0.234084679
C	4.212182	-3.065742	-0.224547	C	4.214199445	-3.041679217	-0.182033408
H	4.551423	-4.094106	-0.333436	H	4.559572472	-4.070717024	-0.281401919
C	5.008939	-1.937592	-0.056505	C	5.001479325	-1.912604267	-0.005282136
H	6.094951	-1.906734	-0.003533	H	6.087912148	-1.877655491	0.067135157
C	4.127836	-0.811202	0.027434	C	4.118451047	-0.791083219	0.058247022
N	2.929954	1.176512	0.077121	N	2.908692717	1.182263849	0.078206919
N	0.218082	1.510698	-0.271927	N	0.209518719	1.505776884	-0.318581628
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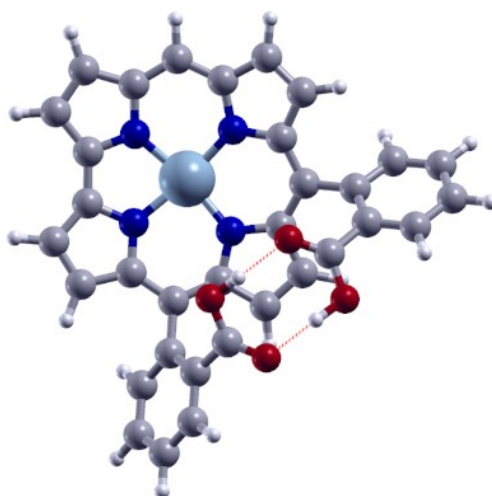
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Mn	1.419011	0.006007	0.023870	Mn	1.413091370	0.009643873	0.007913017
H	1.677384	-4.405246	-0.587025	H	1.701387709	-4.398699739	-0.574760354
H	-1.035571	-4.446555	-0.913248	H	-1.008457071	-4.459320461	-0.911640722
H	-2.952981	-2.543184	-0.943616	H	-2.935521202	-2.570189939	-0.959328121
H	1.985100	4.427976	-0.016087	H	1.956243190	4.428883565	-0.057131567
H	1.539472	0.086547	-1.559944	H	1.509221043	0.072964325	-1.571448831
O	0.966741	-0.094507	1.838266	O	0.863703915	-0.109564373	1.785329614
C	-3.324475	0.205684	-0.596159	C	-3.320991617	0.176230041	-0.596979813
C	-3.931477	0.540749	-1.817577	C	-3.961995705	0.476939504	-1.805490434
C	-4.153489	-0.100025	0.513785	C	-4.118005585	-0.096860254	0.541512072
C	-5.323678	0.569511	-1.951028	C	-5.353385634	0.502083874	-1.900928040
H	-3.291864	0.768824	-2.673258	H	-3.345757948	0.685199429	-2.685108616
C	-5.554178	-0.077997	0.365415	C	-5.518823200	-0.077359264	0.430563139
C	-6.138139	0.256361	-0.857131	C	-6.135365618	0.220093659	-0.780422744
H	-5.770431	0.831293	-2.913264	H	-5.825425420	0.738610914	-2.859214717
H	-6.178885	-0.315688	1.227138	H	-6.121232319	-0.290622457	1.316505672
H	-7.225786	0.274241	-0.954866	H	-7.226853044	0.234698297	-0.848438267
C	-3.553048	-0.394923	1.848571	C	-3.488185839	-0.360554541	1.866757186
O	-2.390129	-0.216893	2.172006	O	-2.306044544	-0.236936736	2.144067839
O	-4.471816	-0.890626	2.733529	O	-4.395249101	-0.757689073	2.807764282
H	-3.979997	-1.024166	3.568401	H	-3.866114658	-0.880243828	3.632687715
H	0.015169	-0.130862	2.049657	H	-0.104836251	-0.169236857	1.952342786



E= -1548.3882007 a.u (*OH)				E= -707.0509118266 Ry (*OH)			
C	4.181219	0.566695	0.044409	C	4.174543355	0.565029559	0.043812254
C	5.163904	1.611216	0.089915	C	5.155150052	1.607871368	0.089518514
H	6.243110	1.476444	0.087614	H	6.236233577	1.475195755	0.087564383
C	4.471222	2.816844	0.122584	C	4.463879003	2.809918794	0.121865044
H	4.901104	3.816284	0.152936	H	4.896102138	3.810144839	0.152721614
C	3.060705	2.514670	0.091668	C	3.055851000	2.507733189	0.091308147
C	1.914429	3.321298	0.030716	C	1.911955105	3.311615292	0.030712621
C	0.585540	2.848797	-0.098318	C	0.585717116	2.840728542	-0.098675094
C	-0.613676	3.642727	-0.164998	C	-0.610277549	3.633424448	-0.164820604
H	-0.644062	4.729752	-0.119554	H	-0.641754447	4.722180930	-0.119683484
C	-1.680909	2.778912	-0.288790	C	-1.675939677	2.773081846	-0.288345211
H	-2.735106	3.035446	-0.355416	H	-2.731066834	3.032533572	-0.355588679
C	-1.149000	1.438640	-0.311729	C	-1.148300303	1.434925057	-0.312219715
C	-1.864747	0.217458	-0.431272	C	-1.864309861	0.217097188	-0.431416732

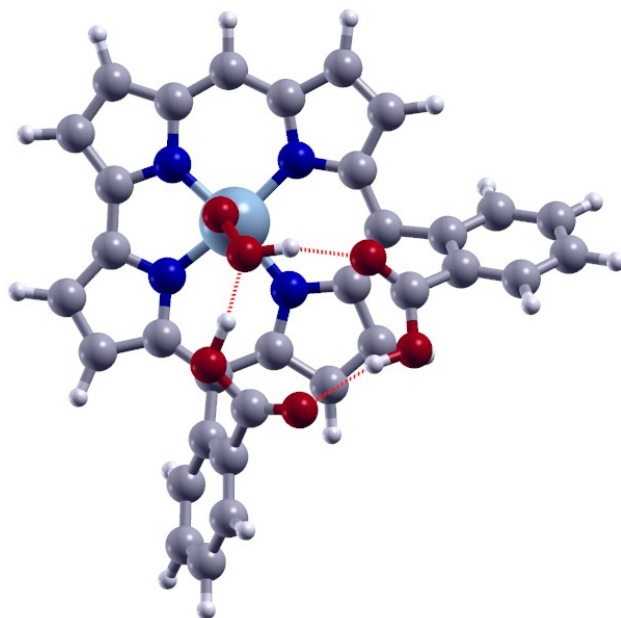
C	-1.283228	-1.076601	-0.494831	C	-1.281754532	-1.072894369	-0.494840613
C	-1.951457	-2.329807	-0.730047	C	-1.945503036	-2.324585034	-0.727821290
C	-0.987809	-3.317560	-0.746279	C	-0.983673957	-3.309247019	-0.744279651
C	0.286335	-2.692418	-0.525025	C	0.287773331	-2.686519267	-0.524909900
C	1.552503	-3.322279	-0.493441	C	1.550820820	-3.314100321	-0.492450197
C	2.779079	-2.662603	-0.331760	C	2.775257949	-2.656853224	-0.331144500
C	4.146824	-3.118614	-0.345609	C	4.140066173	-3.111264542	-0.345240809
H	4.465485	-4.152508	-0.463560	H	4.461345912	-4.146005110	-0.463121549
C	4.965531	-2.004669	-0.193913	C	4.956785986	-1.999934832	-0.193768888
H	6.052748	-1.990121	-0.168384	H	6.045616644	-1.987630027	-0.168371922
C	4.102153	-0.865269	-0.082832	C	4.095930948	-0.863135564	-0.082804993
N	2.947634	1.145700	0.066243	N	2.944311515	1.142336578	0.065555653
N	0.219981	1.518430	-0.188954	N	0.218115066	1.513358571	-0.189023097
N	0.070827	-1.330423	-0.367310	N	0.071173904	-1.326026505	-0.367591870
N	2.812159	-1.300252	-0.161701	N	2.808283674	-1.297837916	-0.161123484
Mn	1.393812	-0.008741	0.030161	Mn	1.388790693	-0.011662969	0.026844591
H	1.562985	-4.405825	-0.631832	H	1.562423332	-4.399247765	-0.631336965
H	-1.138220	-4.383472	-0.906622	H	-1.135686163	-4.376496801	-0.905147704
H	-3.021505	-2.451396	-0.879485	H	-3.016913459	-2.448662659	-0.876896800
H	1.638311	0.175032	-1.527214	H	1.644386871	0.180764551	-1.526886105
O	1.289645	-0.063702	1.914500	O	1.289763458	-0.062652464	1.908825088
C	-3.353478	0.296772	-0.543455	C	-3.350601575	0.295488708	-0.542821765
C	-4.228095	-0.141172	0.482980	C	-4.224349742	-0.140446606	0.480202367
C	-3.913205	0.769423	-1.744714	C	-3.911562534	0.766421026	-1.739888504
C	-5.618472	-0.122316	0.271199	C	-5.611306868	-0.120702898	0.268914399
C	-5.297899	0.805697	-1.935134	C	-5.292293067	0.803330835	-1.929816708
H	-3.241560	1.091696	-2.543906	H	-3.240701068	1.091373205	-2.540703391
C	-6.155326	0.353566	-0.925140	C	-6.147931080	0.353012903	-0.923560229
H	-6.263646	-0.483446	1.074823	H	-6.258858110	-0.481887623	1.072930010
H	-5.704874	1.175936	-2.879208	H	-5.700139678	1.174777526	-2.875040749
H	-7.237782	0.371354	-1.069760	H	-7.232277644	0.371202856	-1.068642070
C	-3.774736	-0.635423	1.823954	C	-3.771820803	-0.633344813	1.818291674
O	-4.421232	-1.399285	2.522192	O	-4.417638197	-1.397721121	2.514837383
O	-2.581683	-0.111989	2.203588	O	-2.579711862	-0.109814292	2.198890403
H	-2.341909	-0.527356	3.056750	H	-2.344664548	-0.530215498	3.060691952
H	2.046125	4.405305	0.064280	H	2.044852768	4.397211396	0.063930528
H	1.901007	0.537097	2.373491	H	1.904667201	0.542074710	2.374376647

**Table S4:** Structures, energies, and coordinates of the complexes with the substituent R1=C<sub>6</sub>H<sub>4</sub>-COOH, R2=C<sub>6</sub>H<sub>4</sub>-COOH.



E= -1891.8992024 a.u (*)	E= -823.2992479309 Ry (*)
C -2.681684 2.932608 0.070681	C -2.667039169 2.931769771 0.076638811
C -4.036934 2.584111 0.314863	C -4.019334234 2.587730796 0.319309353
H -4.819701 3.257753 0.656610	H -4.802148623 3.263644006 0.661441937
C -4.155751 1.213115 0.087253	C -4.142138242 1.220831199 0.090387490
H -5.051965 0.610827 0.215674	H -5.042809880 0.622026178 0.216133256
C -2.875855 0.718022 -0.334119	C -2.866595967 0.722569375 -0.329589830
C -2.421972 -0.581637 -0.654316	C -2.417822766 -0.574867001 -0.651506133
C -1.077722 -0.838684 -1.015330	C -1.077082024 -0.830970097 -1.012026243
C -0.536029 -2.069763 -1.506782	C -0.537864253 -2.058288308 -1.503430354
H -1.123167 -2.929789 -1.820323	H -1.125878845 -2.918577051 -1.819632802
C 0.840904 -1.960698 -1.498732	C 0.835231026 -1.952557267 -1.493615796
H 1.559597 -2.715676 -1.807864	H 1.552373480 -2.710831341 -1.803432785
C 1.171853 -0.662843 -0.988324	C 1.169339575 -0.659883126 -0.983136426
C 2.445192 -0.195290 -0.586557	C 2.441655363 -0.198896114 -0.582297095
C 2.712529 1.140844 -0.211310	C 2.710482015 1.134547120 -0.211342806
C 3.964578 1.709651 0.210220	C 3.959702936 1.703173312 0.207686471
C 3.764708 3.054348 0.435771	C 3.761147735 3.044557211 0.429931733
C 2.378692 3.342453 0.210559	C 2.379339910 3.333273735 0.205791467
C 1.731784 4.564203 0.449991	C 1.737083342 4.553569449 0.441977835
C 0.338576 4.734280 0.417278	C 0.348128566 4.725662568 0.411412836
C -0.514716 5.831329 0.772111	C -0.501122708 5.821771008 0.764540041
H -0.174758 6.822107 1.067933	H -0.158570576 6.814678869 1.055232274
C -1.837588 5.391777 0.692442	C -1.821594342 5.384819603 0.689483335
H -2.730887 5.970291 0.917644	H -2.713722539 5.968771036 0.913505791
C -1.803386 4.031037 0.278788	C -1.790152595 4.026496181 0.280231666
N -2.007522 1.791639 -0.342602	N -1.996929236 1.791297492 -0.335880576
N -0.013009 0.035237 -0.776636	N -0.012141739 0.039080300 -0.773750251
N 1.751561 2.152405 -0.188101	N 1.752454414 2.145463371 -0.190241078
N -0.478320 3.668352 0.107044	N -0.468727613 3.662889932 0.105669681
Mn -0.113501 1.915291 -0.524224	Mn -0.108260049 1.913204014 -0.520742027
H 2.355704 5.408543 0.748997	H 2.363587752 5.398199448 0.739690453
H 4.501212 3.784271 0.766937	H 4.499298316 3.776017780 0.759052106
H 4.891847 1.156365 0.331585	H 4.889809925 1.150982869 0.328675729

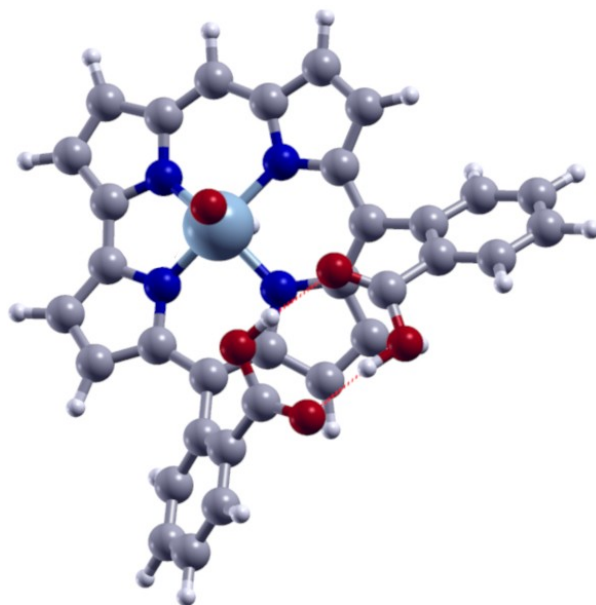
H	-0.098690	2.285209	-2.018909	H	-0.098926750	2.283695363	-2.010995774
C	3.520638	-1.215936	-0.434058	C	3.511944064	-1.221612115	-0.428798364
C	4.737752	-1.084558	-1.128906	C	4.730441429	-1.090377328	-1.115925292
C	3.338599	-2.366515	0.383831	C	3.325623728	-2.373718753	0.382023432
C	5.756075	-2.034248	-1.006421	C	5.744131869	-2.040494805	-0.995132414
H	4.866696	-0.229444	-1.796317	H	4.868042831	-0.230985845	-1.779692885
C	4.358085	-3.330017	0.477342	C	4.342070287	-3.336437087	0.474710141
C	5.569720	-3.159313	-0.195637	C	5.553661918	-3.166556411	-0.192182436
H	6.688713	-1.903442	-1.560637	H	6.680235998	-1.908681888	-1.547048798
H	4.191170	-4.215142	1.094070	H	4.173254159	-4.225343422	1.089226139
H	6.357952	-3.909183	-0.099068	H	6.340912607	-3.920505886	-0.096881082
C	2.068117	-2.604396	1.152080	C	2.055272569	-2.613021583	1.148622876
O	1.454994	-1.736459	1.777439	O	1.446122984	-1.743740585	1.777383359
O	1.671161	-3.883633	1.082664	O	1.651819735	-3.886136077	1.075761636
H	0.728352	-3.945831	1.422407	H	0.692462468	-3.938286857	1.405537298
C	-3.318910	-1.747738	-0.443399	C	-3.316220175	-1.737244715	-0.443043638
C	-2.956329	-2.813013	0.431065	C	-2.958385793	-2.804326309	0.427137456
C	-4.549337	-1.835904	-1.122065	C	-4.545926856	-1.819133098	-1.118308633
C	-3.806096	-3.923858	0.570257	C	-3.813516871	-3.907161187	0.566443395
C	-5.400984	-2.930348	-0.948127	C	-5.401236721	-2.906691744	-0.944939159
H	-4.817387	-1.039997	-1.820781	H	-4.815807716	-1.019450776	-1.815469127
C	-5.029176	-3.980298	-0.099946	C	-5.035241068	-3.956998374	-0.100062723
H	-3.490407	-4.739424	1.224229	H	-3.502853719	-4.727107615	1.220723805
H	-6.347457	-2.972305	-1.492704	H	-6.350529834	-2.942270552	-1.488818686
H	-5.685392	-4.843260	0.032483	H	-5.697753007	-4.817341964	0.033877406
C	-1.669126	-2.857819	1.204749	C	-1.670212302	-2.860702135	1.196875165
O	-1.032443	-3.910480	1.337406	O	-1.038542309	-3.918586118	1.315661150
O	-1.289824	-1.698346	1.744353	O	-1.281489604	-1.712248889	1.745536290
H	-0.321233	-1.765638	1.999312	H	-0.298247877	-1.788578562	1.987185398



E= -2042.7393047 a.u (*OOH)	E= -888.8174716015 Ry (*OOH)						
C	-2.648982	2.861004	-0.224901	C	-2.630677474	2.866946493	-0.216724895
C	-4.053861	2.585219	-0.187600	C	-4.033496517	2.597634595	-0.180293304
H	-4.845111	3.310440	-0.011835	H	-4.821638725	3.328653743	-0.003180901

C	-4.204188	1.218534	-0.393717	C	-4.189662143	1.235113055	-0.386779038
H	-5.136521	0.658722	-0.409669	H	-5.125893625	0.678432549	-0.403454335
C	-2.891323	0.657005	-0.587695	C	-2.881864972	0.668059313	-0.579265577
C	-2.437985	-0.660659	-0.795894	C	-2.434648307	-0.647680038	-0.786873488
C	-1.059817	-0.987917	-1.006122	C	-1.061013430	-0.980688019	-0.997646761
C	-0.537868	-2.248720	-1.447190	C	-0.544900123	-2.240018664	-1.440684708
H	-1.138217	-3.109756	-1.729523	H	-1.150164700	-3.099534439	-1.723533720
C	0.840089	-2.156237	-1.444935	C	0.829938629	-2.153495851	-1.437984591
H	1.548909	-2.929742	-1.728129	H	1.537228851	-2.930441132	-1.722342555
C	1.184005	-0.839884	-0.985393	C	1.179711126	-0.842134476	-0.976727339
C	2.487769	-0.331923	-0.706683	C	2.482706563	-0.340137819	-0.701951999
C	2.790196	1.025839	-0.426910	C	2.790552907	1.013871111	-0.428372014
C	4.076572	1.624310	-0.170689	C	4.077210115	1.609225351	-0.178553234
C	3.870543	2.970202	0.045237	C	3.876043030	2.952838485	0.035612364
C	2.455336	3.217331	-0.039942	C	2.464218656	3.202617973	-0.045450777
C	1.790601	4.448470	0.177341	C	1.806201914	4.434601463	0.169084790
C	0.399453	4.628447	0.163930	C	0.420392453	4.618769913	0.159886211
C	-0.442838	5.781116	0.350994	C	-0.415422398	5.773547024	0.342524663
H	-0.091816	6.794496	0.536472	H	-0.057662031	6.787297584	0.523717651
C	-1.768026	5.363799	0.247022	C	-1.739245657	5.362582949	0.242706347
H	-2.656877	5.983732	0.338856	H	-2.627750262	5.986156284	0.333949781
C	-1.743991	3.956175	-0.005080	C	-1.722201721	3.956478376	-0.002479741
N	-1.990781	1.691456	-0.482425	N	-1.978681047	1.697365309	-0.470184119
N	0.011709	-0.145122	-0.762769	N	0.011615083	-0.145783796	-0.753776339
N	1.831700	2.018149	-0.333545	N	1.838040692	2.008150800	-0.331405208
N	-0.435677	3.557026	-0.046108	N	-0.419315207	3.550956117	-0.040492911
Mn	-0.073527	1.698005	-0.259071	Mn	-0.065648581	1.693301949	-0.243843629
H	2.421147	5.316482	0.382066	H	2.442163837	5.301864159	0.368671957
H	4.622209	3.726949	0.261803	H	4.629482275	3.711115497	0.249296633
H	5.023734	1.091742	-0.151806	H	5.024728844	1.073672946	-0.162852718
H	-0.072145	1.995811	-1.808604	H	-0.055853289	1.979797082	-1.792015045
O	-0.106056	1.484114	1.709227	O	-0.091465746	1.457324573	1.712210609
O	-0.109358	0.225161	2.402568	O	-0.119565716	0.200119203	2.426744812
H	0.776403	-0.186158	2.234620	H	0.750490052	-0.250302636	2.221171626
C	3.566293	-1.355629	-0.610588	C	3.554564619	-1.364897422	-0.606507681
C	4.683023	-1.343820	-1.462847	C	4.672381654	-1.352966683	-1.451822897
C	3.436401	-2.420862	0.321019	C	3.420657193	-2.430246888	0.319494109
C	5.650133	-2.353317	-1.394445	C	5.635179008	-2.361064856	-1.385318800
C	4.393028	-3.444525	0.363590	C	4.374338299	-3.451562065	0.360492687
C	5.505682	-3.405395	-0.483428	C	5.486403344	-3.413219218	-0.481180283
C	2.295695	-2.404988	1.298195	C	2.279577691	-2.416404304	1.293123629
O	2.021488	-1.419503	1.976496	O	2.009050859	-1.430324093	1.971493781
O	1.621755	-3.563285	1.350387	O	1.603357931	-3.570841406	1.342214967
H	0.762709	-3.417401	1.828052	H	0.730812444	-3.420163561	1.814376357
C	-3.359823	-1.822810	-0.647665	C	-3.361226669	-1.800708221	-0.647387070
C	-3.135105	-2.730404	0.423871	C	-3.146275158	-2.713862824	0.416317163
C	-4.391383	-2.092429	-1.559529	C	-4.391309699	-2.054273458	-1.560196158
C	-3.907208	-3.892516	0.534107	C	-3.930376750	-3.864418959	0.516551291
C	-5.181982	-3.240646	-1.420927	C	-5.190069107	-3.193010142	-1.433393149
C	-4.935654	-4.144269	-0.381289	C	-4.955785451	-4.101786051	-0.400691114
C	-2.070669	-2.413412	1.444909	C	-2.078584893	-2.415564916	1.438210851
O	-1.176571	-3.198015	1.764549	O	-1.192035391	-3.214983732	1.741409491
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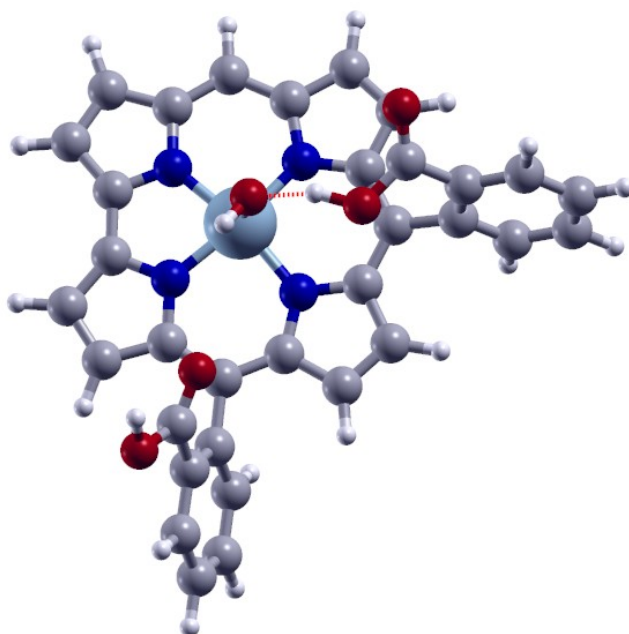
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H	-5.981163	-3.437117	-2.139592	H	-5.989463675	-3.377885875	-2.157524026
H	-5.545587	-5.044904	-0.280839	H	-5.573797288	-4.999784297	-0.308313586
H	-3.707568	-4.586607	1.353814	H	-3.738773570	-4.566586732	1.333093374
H	4.268494	-4.262801	1.076062	H	4.246631635	-4.272909177	1.070876739
H	6.254872	-4.198693	-0.434769	H	6.235788879	-4.208506310	-0.432207039
H	6.509184	-2.326080	-2.068962	H	6.497868252	-2.331777638	-2.057761071
H	4.771033	-0.548751	-2.206953	H	4.766326631	-0.552965359	-2.192078909



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C	-4.196971	1.312207	-0.155626	C	-4.261462922	1.070095476	-0.217574320
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C	-2.891975	0.739621	-0.339725	C	-2.927314046	0.570313340	-0.378545911
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H	-1.178714	-2.854066	-1.909294	H	-1.000808421	-2.914992161	-1.911759951
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C	2.437483	-0.239075	-0.571839	C	2.439879105	-0.095208012	-0.559551402
C	2.755499	1.096504	-0.218395	C	2.673898562	1.241830671	-0.163651876
C	4.048282	1.682067	0.052169	C	3.920989718	1.885289408	0.164734296
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C	0.401242	4.706914	0.192983	C	0.120635982	4.697199069	0.270912119
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H	4.990595	1.143286	0.093586	H	4.890616658	1.394622030	0.212226124
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C	4.690997	-1.151957	-1.218430	C	4.734726025	-0.860951759	-1.229315901
C	3.296786	-2.476921	0.265227	C	3.438385345	-2.279694892	0.246105414
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C	4.296511	-3.464128	0.286240	C	4.491432659	-3.204473500	0.243081646
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H	6.605285	-1.997413	-1.748447	H	6.688233186	-1.582523349	-1.790568338
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O	-1.081478	-3.984962	1.249084	O	-0.811394571	-4.037883089	1.217353307
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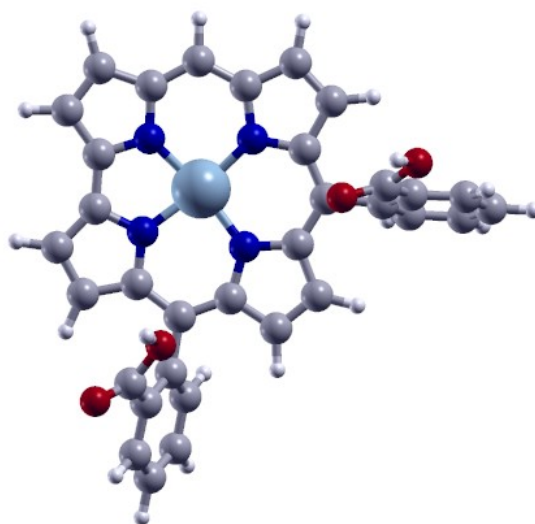
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C	-3.867510	1.646617	-0.215209
H	-4.888824	1.281220	-0.299105
C	-2.683550	0.837203	-0.296321
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C	-1.230998	-1.149425	-0.754532
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H	-1.706032	-3.336415	-0.962068
C	0.415351	-2.704654	-0.973204
H	0.975726	-3.631574	-1.064572
C	0.997836	-1.395433	-0.866242
C	2.380584	-1.064333	-0.783092
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C	2.586139	3.831260	-0.433261
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H	1.167515	6.474952	-0.083221
C	-0.727850	5.324944	0.057543
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C	-1.230431527	-1.146240635	-0.757195263
C	-0.951850613	-2.545232620	-0.921402292
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H	3.356264498	4.596585198	-0.470155199



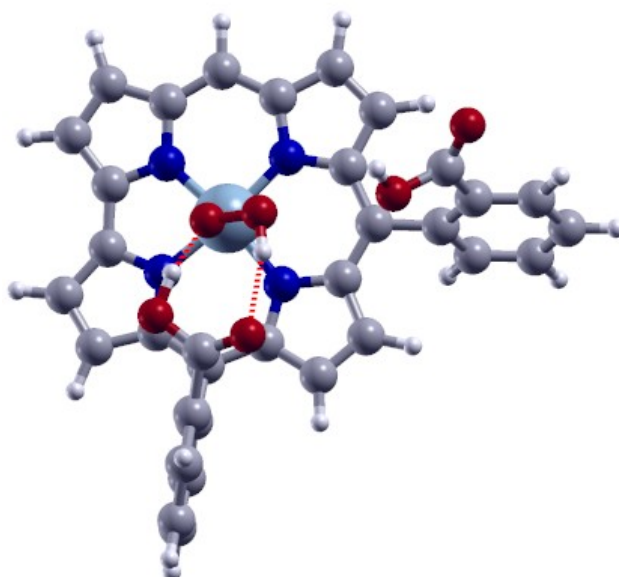
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H	0.079964	1.646258	-1.773808	H	0.065149726	1.640366972	-1.778725370
O	0.630439	0.945847	1.655265	O	0.646873858	0.934850441	1.653937011
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C	3.829018	-3.059161	-1.434357	C	3.822538296	-3.052397324	-1.430165700
C	4.812774	-3.182735	1.187023	C	4.804521134	-3.176795797	1.183076144
C	4.777488	-4.029199	-1.084460	C	4.769503815	-4.018765252	-1.082448359
H	3.469385	-2.985727	-2.463975	H	3.462583926	-2.980339468	-2.461440219
C	5.270118	-4.089555	0.224571	C	5.261277889	-4.079764175	0.222640293
H	5.198991	-3.207357	2.208788	H	5.191449285	-3.198780034	2.206492883
H	5.141348	-4.728887	-1.840801	H	5.132360701	-4.719759207	-1.840333936
H	6.015414	-4.841461	0.494799	H	6.007119009	-4.832855114	0.493711932
C	3.338202	-1.243302	1.896192	C	3.334434663	-1.243394331	1.896562357
O	4.093529	-0.620059	2.627088	O	4.098313707	-0.620593166	2.619609841
O	2.005066	-1.165762	1.868819	O	2.003993993	-1.168894893	1.887970726
H	1.555013	-0.224464	1.991482	H	1.536865892	-0.212045596	1.976448981
H	-0.195904	0.790620	2.146310	H	-0.187755809	0.769051826	2.144463798
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C	-4.537310	-1.701338	0.478077	C	-4.532023490	-1.697731067	0.475763973
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C	-5.714159	-2.453186	0.299037	C	-5.705392996	-2.448289667	0.295695364
C	-5.260422	-2.647922	-2.066312	C	-5.252907539	-2.642641435	-2.062454536
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C	-6.075201	-2.926515	-0.963439	C	-6.066090780	-2.920114562	-0.963122426
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O	-5.147529	-1.374462	2.752594	O	-5.148674248	-1.371722120	2.746830566
H	-4.756629	-1.130643	3.615445	H	-4.749259494	-1.127582824	3.616214613



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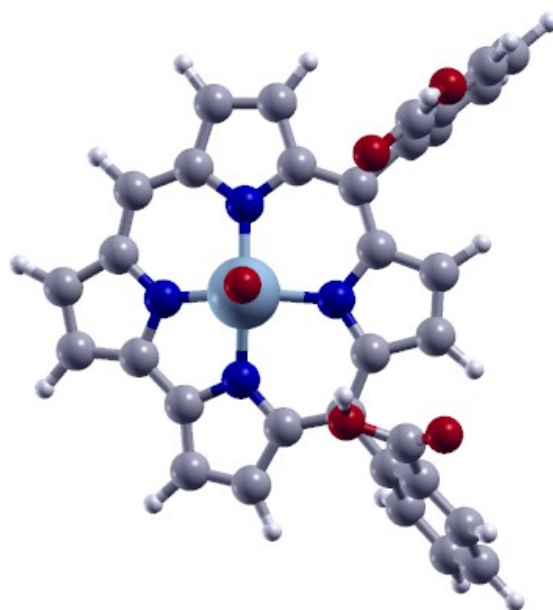
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H	5.069466	0.651918	-0.408082
H	-0.008892	1.655155	-2.011163
C	3.571028	-1.696510	-0.490931
C	3.838794	-2.310340	-1.726886
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H	5.070432	-3.684432	-2.850586
H	6.086220	-3.170230	1.312259
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H	-6.238279	-3.094415	1.185811
H	-4.921776	-3.875331	-2.856935
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H	-3.172651	-0.790051	3.213881



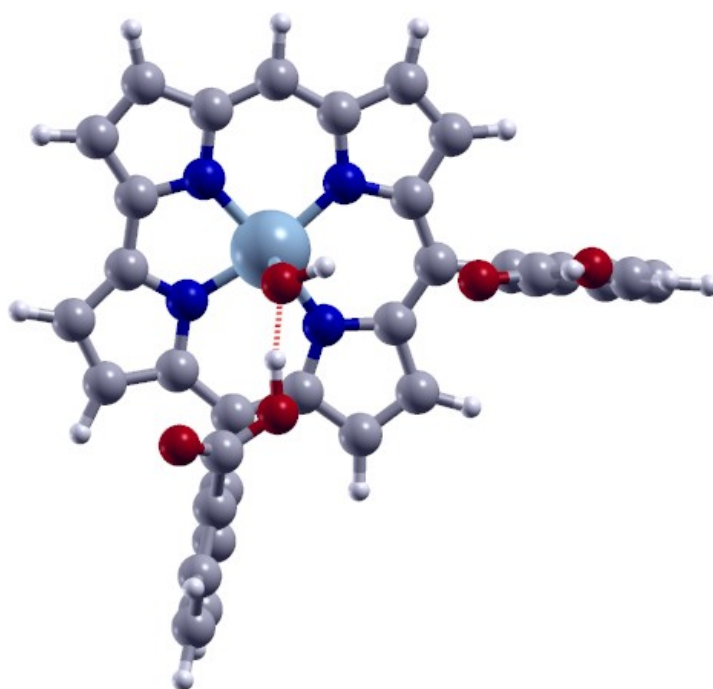
E= -2042.7324623 a.u (*OOH)			
C	-2.892843	2.525518	-0.646515
C	-4.281074	2.208144	-0.775150
H	-5.106113	2.916183	-0.747241
C	-4.369219	0.825544	-0.911677
H	-5.276946	0.234063	-1.007830
C	-3.031912	0.296427	-0.895306
C	-2.535253	-1.024952	-0.880521
C	-1.142999	-1.344797	-0.910706
C	-0.565040	-2.656369	-1.022168
H	-1.132092	-3.579528	-1.114197
C	0.805870	-2.514747	-0.981698
H	1.551053	-3.304685	-1.026332
C	1.092016	-1.113212	-0.818058
C	2.362322	-0.504015	-0.621945
C	2.578415	0.872791	-0.343469
C	3.838915	1.555426	-0.215073
C	3.568741	2.885906	0.032186
C	2.143235	3.049712	0.039712
C	1.428620	4.262327	0.173571
C	0.038902	4.391483	0.046156
C	-0.844109	5.527012	0.069870
H	-0.540231	6.557608	0.242810
C	-2.135642	5.067664	-0.178410
H	-3.042413	5.665406	-0.235457

C	-2.047658	3.651615	-0.354253
N	-2.177968	1.363740	-0.755345
N	-0.107290	-0.433347	-0.796030
N	1.567705	1.803142	-0.171044
N	-0.738920	3.282953	-0.199523
Mn	-0.304613	1.422462	-0.317356
H	2.019170	5.163662	0.351339
H	4.288199	3.689150	0.178657
H	4.817694	1.091685	-0.307719
H	-0.144758	1.681479	-1.849761
O	-0.768427	0.919848	1.599476
C	-3.463478	-2.133100	-0.491339
C	-3.461386	-2.487478	0.884771
C	-4.283799	-2.839084	-1.379508
C	-4.252843	-3.546909	1.338449
C	-5.094327	-3.883726	-0.912809
H	-4.276125	-2.575499	-2.440052
C	-5.075551	-4.238701	0.440075
H	-4.231844	-3.821956	2.395531
H	-5.733903	-4.427006	-1.612397
H	-5.702212	-5.058047	0.799741
C	-2.540358	-1.693865	1.781116
O	-1.486771	-2.148834	2.227425
O	-2.939759	-0.431991	1.930848
H	-2.105549	0.177899	1.998511
O	0.269715	0.146303	2.236234
H	-0.177990	-0.734585	2.346945
C	3.568970	-1.370021	-0.784649
C	4.492037	-1.639652	0.257535
C	3.842552	-1.885490	-2.066738
C	5.660397	-2.373524	-0.012789
C	4.993850	-2.636716	-2.318506
H	3.145141	-1.665663	-2.878375
C	5.911301	-2.877941	-1.289129
H	6.359349	-2.546637	0.808198
H	5.179891	-3.020673	-3.324392
H	6.817644	-3.456737	-1.479981
C	4.307468	-1.194750	1.676858
O	5.226813	-0.921395	2.430978
O	3.003818	-1.167945	2.045198
H	2.962820	-0.794103	2.948899



E=	-855.4409843835 Ry (*O)		
C	-2.814327114	2.804841390	-0.158466892
C	-4.191193122	2.454614943	-0.119362329
H	-5.029013787	3.143596613	-0.014505888
C	-4.261462922	1.070095476	-0.217574320
H	-5.166554928	0.465518974	-0.197404502
C	-2.927314046	0.570313340	-0.378545911
C	-2.404600602	-0.713077137	-0.618192613
C	-1.034623591	-0.887442746	-0.954742516
C	-0.447922795	-2.055575694	-1.536715408
H	-1.000808421	-2.914992161	-1.911759951
C	0.914408178	-1.867540032	-1.554046362
H	1.668286776	-2.553401092	-1.935077723
C	1.178782237	-0.589834684	-0.965209738
C	2.439879105	-0.095208012	-0.559551402
C	2.673898562	1.241830671	-0.163651876
C	3.920989718	1.885289408	0.164734296
C	3.648368407	3.210967513	0.396581113
C	2.230829543	3.394979142	0.251752301
C	1.506753284	4.592306905	0.394699176
C	0.120635982	4.697199069	0.270912119
C	-0.765996543	5.822414041	0.337881794
H	-0.454063628	6.856799989	0.481449988
C	-2.063389113	5.354743496	0.178185455
H	-2.976194020	5.948802646	0.173854329
C	-1.978189679	3.940320240	0.019418724
N	-2.076124096	1.655540383	-0.311852468
N	-0.032513874	0.016017195	-0.680186470
N	1.672348187	2.179218302	-0.070552285
N	-0.661143037	3.578651154	0.081123928
Mn	-0.239548607	1.728583500	0.166855659
H	2.076405017	5.500056856	0.612043240
H	4.355130099	3.999268635	0.654248375

H	4.890616658	1.394622030	0.212226124
H	0.112614043	2.108995585	-1.393921923
C	3.553140255	-1.077309186	-0.501551501
C	4.734726025	-0.860951759	-1.229315901
C	3.438385345	-2.279694892	0.246105414
C	5.782987182	-1.779283155	-1.208014536
H	4.811397214	0.037815387	-1.847568481
C	4.491432659	-3.204473500	0.243081646
C	5.665434873	-2.953226050	-0.463568782
H	6.688233186	-1.582523349	-1.790568338
H	4.381414800	-4.130899493	0.812640313
H	6.482527424	-3.680263054	-0.444175049
C	2.203891293	-2.606839253	1.038263923
O	1.577597784	-1.785639899	1.711072042
O	1.854463545	-3.892392957	0.926230396
H	0.902970817	-3.997294566	1.270440744
C	-3.228440091	-1.930024077	-0.438357975
C	-2.799305526	-2.991972646	0.407793299
C	-4.453034431	-2.077074815	-1.113150927
C	-3.597788468	-4.135232219	0.546594095
C	-5.245488283	-3.211111116	-0.946869825
H	-4.764198316	-1.292928821	-1.809620227
C	-4.822108049	-4.242741135	-0.107192356
H	-3.238625575	-4.942858565	1.190679682
H	-6.190898131	-3.296225310	-1.491634557
H	-5.440148422	-5.134706767	0.030458973
C	-1.491826285	-3.005760896	1.149949625
O	-0.811394571	-4.037883089	1.217353307
O	-1.148419753	-1.857984694	1.721989417
H	-0.157967067	-1.884104493	1.948120128
O	0.047214694	1.415378433	1.695774406

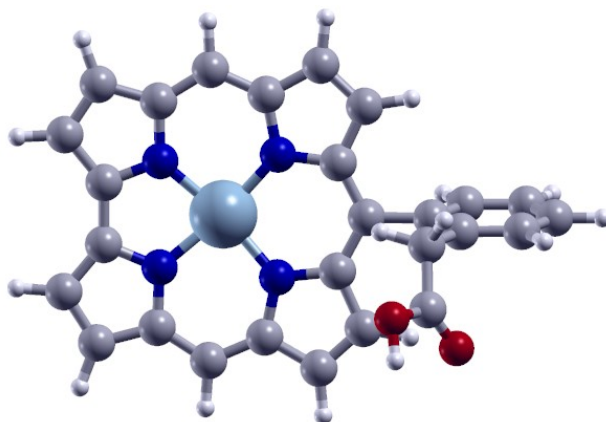


E=	-1967.6451345	a.u (*OH)	
C	-2.851543	2.437366	-0.578989
C	-4.231264	2.070842	-0.638440
H	-5.079199	2.747262	-0.562177
C	-4.276492	0.686311	-0.772269
H	-5.166093	0.063283	-0.829846
C	-2.920720	0.203771	-0.823809
C	-2.387424	-1.101440	-0.866990
C	-0.988101	-1.382573	-0.979611
C	-0.372557	-2.675763	-1.103233
H	-0.912145	-3.613573	-1.209475
C	0.992739	-2.494889	-1.039764
H	1.762232	-3.261294	-1.089849
C	1.233442	-1.087411	-0.851815
C	2.472697	-0.449862	-0.599486
C	2.663188	0.936874	-0.338129
C	3.908429	1.640874	-0.199113
C	3.608779	2.971124	0.027238
C	2.179725	3.102512	0.023263
C	1.430267	4.297055	0.158305
C	0.037145	4.387442	0.044883
C	-0.880510	5.498055	0.107255
H	-0.602990	6.534885	0.287331
C	-2.161788	5.002798	-0.110239
H	-3.088823	5.570913	-0.131554
C	-2.032794	3.589516	-0.307641
N	-2.101236	1.303121	-0.727894
N	0.009340	-0.442252	-0.850494
N	1.636254	1.843358	-0.182375
N	-0.713645	3.262369	-0.199592
Mn	-0.241384	1.401919	-0.317264
H	1.995829	5.213873	0.339003
H	4.895659	1.191217	-0.275270
H	-0.044959	1.718079	-1.838823
O	-0.538164	0.924704	1.581072
C	3.698702	-1.304560	-0.642555
C	4.406420	-1.698053	0.522526
C	4.183327	-1.716100	-1.895536
C	5.578056	-2.469957	0.398194
C	5.344559	-2.487752	-2.006375
H	3.639546	-1.409619	-2.792003
C	6.046662	-2.863588	-0.856015
H	6.109493	-2.768079	1.302557
H	5.701341	-2.790853	-2.993667
H	6.954673	-3.465388	-0.934431
C	3.886983	-1.348260	1.878488
O	4.779363	-1.654552	2.871203
O	2.797884	-0.860125	2.126101
H	0.294780	0.841724	2.077995
C	-3.316760	-2.216528	-0.517481
C	-3.721754	-2.314346	0.840028
C	-3.836906	-3.113531	-1.461549
C	-4.654150	-3.290536	1.213266

C	-4.744373	-4.105774	-1.068203
H	-3.542376	-3.019708	-2.509997
C	-5.153557	-4.192870	0.267739
H	-4.977566	-3.335180	2.255944
H	-5.142112	-4.801661	-1.810853
H	-5.867481	-4.961855	0.572459
C	-3.177155	-1.332798	1.862931
O	-1.849954	-1.229978	1.767038
O	-3.904342	-0.733872	2.641773
H	4.330107	-1.412272	3.705478
H	-1.407568	-0.285022	1.904440
H	4.309352	3.791994	0.168075

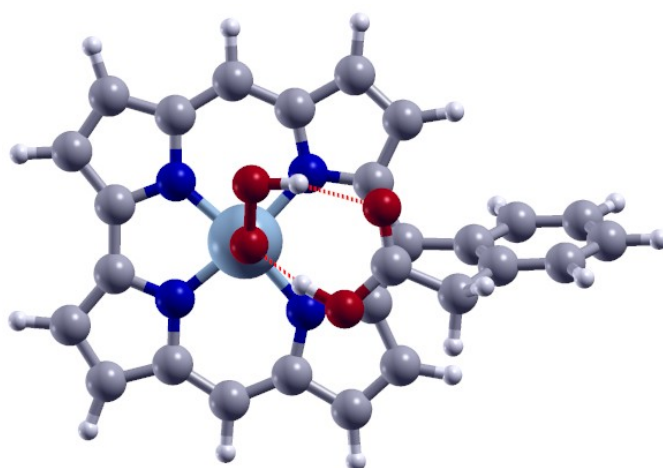


**Table S5:** Structures, energies, and coordinates of the complexes with the substituent R1=C<sub>6</sub>H<sub>4</sub>-CH<sub>2</sub>-COOH.



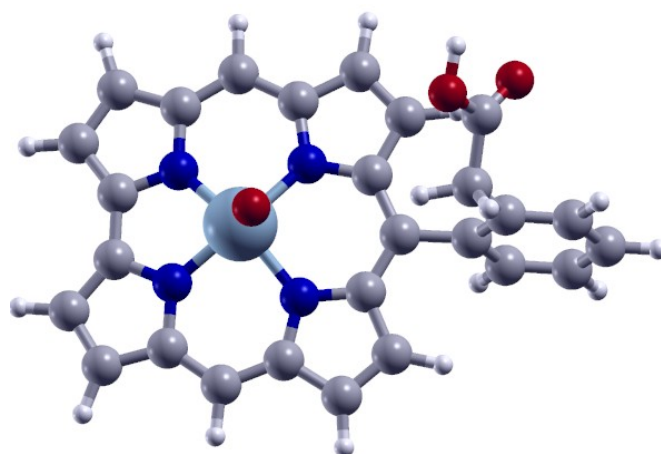
E= -1511.9082186 a.u (*)	E= -687.5009845858 Ry (*)
C -4.236832 -1.008568 0.046911	C -4.232564110 -1.006068105 0.046753793
C -5.004431 -2.204015 -0.020289	C -4.997105351 -2.199526386 -0.020294164
H -6.074764 -2.288355 0.154941	H -6.069197302 -2.287290029 0.153981974
C -4.125430 -3.241421 -0.339494	C -4.119969968 -3.233897885 -0.338547983
H -4.378183 -4.292775 -0.464392	H -4.375766299 -4.286466002 -0.463998331
C -2.810060 -2.684881 -0.469864	C -2.807217863 -2.678701276 -0.468809165
C -1.558169 -3.256131 -0.751798	C -1.557979530 -3.247909620 -0.750489482
C -0.355787 -2.534233 -0.790877	C -0.358097140 -2.528856069 -0.789550705
C 0.957117 -3.052790 -1.047059	C 0.951823450 -3.046402998 -1.045020700
H 1.178730 -4.098168 -1.254786	H 1.176506462 -4.092833812 -1.253439108
C 1.855293 -2.009186 -0.971305	C 1.847859751 -2.005628254 -0.970007917
H 2.934274 -2.054704 -1.100016	H 2.928218277 -2.055111084 -1.099418390
C 1.114360 -0.815666 -0.665174	C 1.111192692 -0.812617922 -0.665052385
C 1.624862 0.489529 -0.493963	C 1.622935083 0.489282261 -0.493787802
C 0.837560 1.621894 -0.189452	C 0.835289592 1.618411522 -0.190126584
C 1.291964 2.969531 0.020234	C 1.285795328 2.964270189 0.020135519
C 0.188814 3.747438 0.303892	C 0.185329703 3.739794802 0.303316210
C -0.970674 2.903238 0.281784	C -0.971591667 2.897406103 0.280948435
C -2.297552 3.280884 0.538567	C -2.295422366 3.272981182 0.536841462
C -3.384023 2.390983 0.530405	C -3.379829492 2.385607509 0.529180172
C -4.781689 2.561137 0.804024	C -4.774667732 2.555181924 0.802347671
H -5.259662 3.501662 1.071954	H -5.255899537 3.496361463 1.070076836
C -5.402591 1.317087 0.673231	C -5.394480952 1.314640350 0.671869063
H -6.457567 1.097163 0.821843	H -6.451965824 1.097792958 0.820787353
C -4.393600 0.378872 0.319853	C -4.388918756 0.377604759 0.318961929
N -2.917154 -1.331840 -0.228475	N -2.915141569 -1.328027856 -0.229873781
N -0.233806 -1.157474 -0.553243	N -0.235166813 -1.153580276 -0.555375019
N -0.546499 1.600771 -0.018225	N -0.546941228 1.597644417 -0.021069632
N -3.187220 1.057256 0.241684	N -3.184496765 1.054755152 0.239050960
Mn -1.658747 0.087337 -0.337222	Mn -1.657561325 0.087243832 -0.336238196
H 0.171529 4.814145 0.520581	H 0.170646627 4.808471312 0.519493664
H 2.329707 3.288644 -0.041609	H 2.323914630 3.287777415 -0.040995715
H -1.878213 0.354410 -1.836448	H -1.877083251 0.353604345 -1.831201352
C 3.101243 0.696429 -0.663358	C 3.098119273 0.695625681 -0.661445375
C 4.018036 0.417478 0.375263	C 4.015576343 0.417278675 0.373219711

C	3.581858	1.192485	-1.889858	C	3.581866046	1.190122254	-1.883839946
C	5.388322	0.635499	0.151740	C	5.382319452	0.636068848	0.149131038
C	4.947257	1.403618	-2.098017	C	4.943340842	1.401205690	-2.092438920
C	5.855632	1.122227	-1.070847	C	5.849814983	1.121063969	-1.069182546
C	3.555271	-0.095303	1.717996	C	3.557897951	-0.095832638	1.713264059
C	3.866654	-1.562086	1.971763	C	3.866516180	-1.559853946	1.971851426
O	4.525322	-2.302808	1.269789	O	4.525508733	-2.302055524	1.272153957
O	3.306878	-1.968393	3.151062	O	3.304831761	-1.963073105	3.149680292
H	3.547980	-2.911336	3.251712	H	3.551483022	-2.914190741	3.249603682
H	-2.483006	4.331554	0.769544	H	-2.481589133	4.325145487	0.768437657
H	-1.503637	-4.329328	-0.943998	H	-1.503742088	-4.322862808	-0.942507044
H	2.864812	1.407720	-2.686077	H	2.867155700	1.406952585	-2.683304795
H	5.300255	1.785846	-3.058848	H	5.297189143	1.783984776	-3.054420179
H	6.925957	1.281880	-1.221437	H	6.921628915	1.281126514	-1.220294271
H	6.098915	0.415343	0.953346	H	6.094816274	0.415779063	0.950745512
H	4.034360	0.471265	2.536269	H	4.036647822	0.471369251	2.533272737
H	2.471913	0.045938	1.853123	H	2.473751026	0.046034050	1.851004374



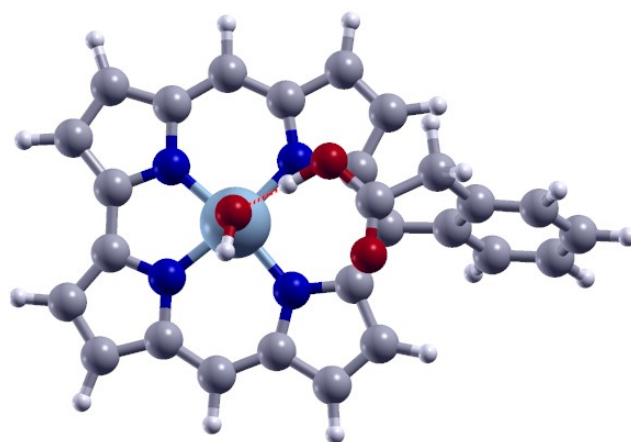
E= -1662.7591218 a.u (*OOH)				E= -753.0416636130 Ry (*OOH)			
C	4.059925	0.775844	-0.114077	C	-4.053980028	-0.775376690	-0.118678844
C	4.967227	1.879639	-0.110106	C	-4.957234558	-1.878051672	-0.112792547
H	6.050070	1.818490	-0.029194	H	-6.041828727	-1.817463165	-0.030365427
C	4.201669	3.036807	-0.234597	C	-4.191640022	-3.031339725	-0.237335122
H	4.568931	4.060595	-0.272230	H	-4.555391385	-4.058107755	-0.274013619
C	2.819826	2.645230	-0.319786	C	-2.813323938	-2.639231739	-0.323840105
C	1.634935	3.373302	-0.501151	C	-1.630791854	-3.363624797	-0.505522938
C	0.345654	2.804087	-0.620659	C	-0.345437147	-2.794322698	-0.626826103
C	-0.898699	3.496578	-0.812610	C	0.896339445	-3.484572371	-0.816118199
H	-1.001110	4.576149	-0.905246	H	0.996672269	-4.565832508	-0.906039210
C	-1.903442	2.551490	-0.859229	C	1.898975962	-2.542212688	-0.861609607
H	-2.967698	2.720888	-1.006549	H	2.965053998	-2.712950777	-1.006395151
C	-1.291353	1.259415	-0.702415	C	1.289114008	-1.252260389	-0.706014522
C	-1.936847	-0.005532	-0.688843	C	1.933664106	0.009396113	-0.689050373
C	-1.271984	-1.263244	-0.684286	C	1.268317309	1.262979179	-0.683327036
C	-1.865097	-2.576285	-0.709123	C	1.857092456	2.574859036	-0.704886533
C	-0.839189	-3.494737	-0.641726	C	0.831541984	3.488620171	-0.636148665
C	0.396160	-2.763336	-0.552065	C	-0.399673795	2.757217736	-0.548742879
C	1.697811	-3.305280	-0.406789	C	-1.698448393	3.296591012	-0.403215243
C	2.871496	-2.554967	-0.259771	C	-2.868868000	2.547886283	-0.257013717

C	4.260972	-2.920786	-0.152591	C	-4.255448506	2.911789897	-0.150396657
H	4.645819	-3.938785	-0.152690	H	-4.638332628	3.932217502	-0.148539730
C	5.004736	-1.748170	-0.058151	C	-4.997540001	1.741770590	-0.058067457
H	6.085278	-1.664923	0.032789	H	-6.079781730	1.657753300	0.033070689
C	4.075140	-0.660330	-0.101475	C	-4.070309040	0.656454675	-0.103137210
N	2.785361	1.271536	-0.222784	N	-2.780880974	-1.267969434	-0.228244944
N	0.073287	1.446136	-0.560917	N	-0.073344059	-1.439480199	-0.567925711
N	0.096360	-1.415827	-0.597344	N	-0.097569147	1.413393901	-0.596112628
N	2.816656	-1.182636	-0.210474	N	-2.813944413	1.177946902	-0.208877845
Mn	1.337602	0.027175	-0.265025	Mn	-1.336628791	-0.026988832	-0.266140697
H	1.777965	-4.394546	-0.410767	H	-1.779106634	4.387317875	-0.405056184
H	-0.922216	-4.579831	-0.633581	H	0.909988763	4.575161540	-0.622895657
H	-2.931799	-2.778189	-0.753399	H	2.924713450	2.780577068	-0.747907692
H	1.531373	-0.008397	-1.818552	H	-1.524324165	0.014337911	-1.818672754
O	0.936499	-0.030934	1.704880	O	-0.933404296	0.013596705	1.709598202
O	0.835926	-1.325502	2.313913	O	-0.811484594	1.307827500	2.329224409
C	-3.431340	-0.029894	-0.635262	C	3.424738707	0.034914008	-0.634168522
C	-4.147192	0.322208	0.539339	C	4.139228224	-0.322799502	0.536079379
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H	-3.573854	-0.725585	-2.669825	H	3.565540089	0.741933865	-2.664334577
C	-6.243516	-0.204451	-0.620386	C	6.230727164	0.203914942	-0.618676115
H	-6.108487	0.464935	1.424083	H	6.096525935	-0.476921217	1.422167827
H	-6.061328	-0.868010	-2.677318	H	6.050153383	0.880956010	-2.670940863
H	-7.333737	-0.272865	-0.598805	H	7.322964825	0.270399101	-0.596324467
C	-3.508215	0.862780	1.813684	C	3.504779224	-0.863740573	1.808851135
H	-4.188014	0.646564	2.654077	H	4.191212877	-0.646275738	2.645670850
H	-3.413163	1.958327	1.746385	H	3.415061559	-1.961727708	1.739278859
C	-2.144710	0.293757	2.183072	C	2.144175968	-0.295627175	2.185551271
O	-1.938127	-0.913757	2.326905	O	1.945807135	0.913694209	2.331608231
O	-1.213370	1.232637	2.332421	O	1.209468170	-1.225364384	2.332198495
H	-0.289415	0.776506	2.240963	H	0.273769100	-0.759094221	2.224799870
H	-0.153790	-1.392284	2.435508	H	0.190363451	1.352825552	2.449623182
H	1.701335	4.461433	-0.566780	H	-1.695714646	-4.453573214	-0.568686588



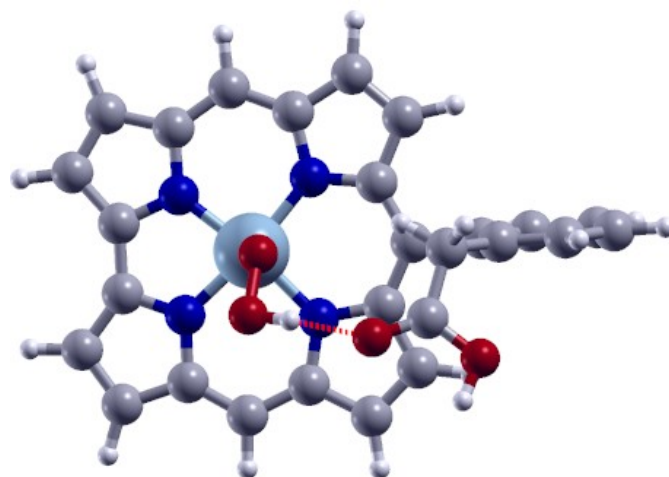
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C 5.421741 1.332194 0.238577	C -5.422307416 -1.314020882 0.233665044

H	6.488801	1.130484	0.178112	H	-6.490680125	-1.110970418	0.168641119
C	4.811629	2.565828	0.443916	C	-4.818872986	-2.546310173	0.442326749
H	5.305855	3.525989	0.579536	H	-5.320650783	-3.504816450	0.577101262
C	3.390178	2.363775	0.423868	C	-3.399673359	-2.351078305	0.426428281
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C	0.978769	2.897966	0.275961	C	-0.995821660	-2.893618808	0.283759292
C	-0.153197	3.785039	0.205190	C	0.130892033	-3.782146303	0.220157967
H	-0.106579	4.863407	0.345428	H	0.082542586	-4.861725491	0.364000729
C	-1.259264	3.020853	-0.086512	C	1.238283238	-3.024932708	-0.068106513
H	-2.284787	3.355525	-0.220119	H	2.263637419	-3.368151071	-0.193873958
C	-0.816709	1.652712	-0.201764	C	0.805813458	-1.657496718	-0.190213385
C	-1.615782	0.528876	-0.515619	C	1.612170017	-0.541468070	-0.503018809
C	-1.128258	-0.786584	-0.688968	C	1.130437255	0.773268075	-0.680992481
C	-1.890456	-1.938958	-1.104277	C	1.892433494	1.920315567	-1.101832436
C	-1.016025	-2.997435	-1.183132	C	1.024198407	2.979107385	-1.183975952
C	0.290082	-2.509455	-0.821386	C	-0.280905489	2.499035877	-0.820537510
C	1.497225	-3.235970	-0.845350	C	-1.483769977	3.225186650	-0.849779224
C	2.748875	-2.670549	-0.595843	C	-2.735553159	2.666204459	-0.603060844
C	4.076928	-3.200425	-0.725603	C	-4.058236376	3.200208692	-0.736357893
H	4.317947	-4.227162	-0.994427	H	-4.296673466	4.228750259	-1.008177082
C	4.975640	-2.168889	-0.471202	C	-4.960505223	2.176929662	-0.481505921
H	6.061486	-2.222627	-0.502922	H	-6.047599781	2.238835815	-0.516591266
C	4.201191	-1.010778	-0.169116	C	-4.195505037	1.017626975	-0.176149542
N	3.166039	1.009398	0.251899	N	-3.170798276	-1.000455918	0.252704794
N	0.543937	1.610312	0.038572	N	-0.554205066	-1.610426204	0.046030231
N	0.189005	-1.168630	-0.513401	N	-0.181891937	1.162192740	-0.506047370
N	2.866137	-1.343626	-0.222022	N	-2.861390191	1.343332044	-0.227903772
Mn	1.584072	-0.042502	0.301764	Mn	-1.584723979	0.042473262	0.305169280
H	1.446145	-4.287392	-1.135703	H	-1.429279516	4.277078046	-1.143897220
H	-1.236512	-4.021075	-1.480074	H	1.251137312	4.001343757	-1.487230191
H	-2.959237	-1.941024	-1.303525	H	2.962099256	1.921160916	-1.305317470
H	1.516244	0.283675	-1.296050	H	-1.513571181	-0.263783464	-1.300143465
O	1.032065	-0.264495	1.777703	O	-1.034614168	0.287979675	1.778716567
C	-3.079885	0.764072	-0.731761	C	3.073723605	-0.783467977	-0.716476722
C	-4.035773	0.445933	0.258677	C	4.034725133	-0.446918335	0.259288722
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C	-5.393425	0.695135	-0.005907	C	5.387479822	-0.702264220	-0.006794513
C	-4.859810	1.561901	-2.199220	C	4.846318714	-1.609445577	-2.171864933
H	-2.757170	1.567328	-2.709245	H	2.747570167	-1.626694735	-2.674635482
C	-5.808813	1.245248	-1.220127	C	5.797670069	-1.274322379	-1.207634140
H	-6.136191	0.448093	0.757719	H	6.135682493	-0.439803568	0.747983254
H	-5.172027	1.992057	-3.153803	H	5.154727089	-2.058984115	-3.120257455
H	-6.870753	1.426418	-1.402072	H	6.860116105	-1.459150571	-1.391610624
H	2.542224	4.324716	0.619545	H	-2.561844909	-4.314407877	0.625496175
C	-3.633891	-0.134778	1.593991	C	3.643651543	0.158688144	1.582254340
H	-2.547888	-0.062624	1.763936	H	2.557114080	0.095370215	1.758247312
H	-4.098899	0.432201	2.419617	H	4.106995736	-0.398145135	2.417889816
C	-4.030933	-1.590398	1.785370	C	4.049604343	1.611483549	1.756269973
O	-4.635234	-2.292791	0.999361	O	4.684646167	2.290115824	0.973898201
O	-3.618419	-2.036787	3.008206	O	3.608567067	2.087241369	2.956268771
H	-3.892216	-2.974710	3.059067	H	3.901093843	3.029667716	2.993264300



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C	4.093603	0.717230	0.026313	C	4.089488460	0.715502937	0.022907754
C	5.024540	1.804411	0.071352	C	5.016694021	1.801272362	0.069793697
H	6.106761	1.719732	0.136904	H	6.100582848	1.719786128	0.136687084
C	4.279045	2.978246	0.005458	C	4.272324197	2.972076371	0.004875054
H	4.663322	3.996468	0.009873	H	4.659446015	3.990825052	0.009606116
C	2.888545	2.612077	-0.085837	C	2.884742939	2.607444255	-0.086644838
C	1.712564	3.363472	-0.233699	C	1.711318217	3.355307162	-0.232993321
C	0.411753	2.824321	-0.383673	C	0.413640012	2.818122312	-0.383273093
C	-0.825953	3.552321	-0.474624	C	-0.821618808	3.544033438	-0.474565433
H	-0.913136	4.636895	-0.455983	H	-0.911248345	4.630080016	-0.455915707
C	-1.847530	2.631327	-0.557797	C	-1.840766868	2.626000574	-0.558574432
H	-2.914708	2.828462	-0.606100	H	-2.908700167	2.827777437	-0.607128768
C	-1.249112	1.320602	-0.545176	C	-1.246986486	1.316176726	-0.546798163
C	-1.908343	0.058503	-0.609310	C	-1.906455616	0.058440410	-0.609480282
C	-1.256198	-1.202873	-0.671990	C	-1.253814480	-1.198215213	-0.672302868
C	-1.861404	-2.488719	-0.893945	C	-1.854576623	-2.483494675	-0.893068560
C	-0.852211	-3.429912	-0.882063	C	-0.847426474	-3.421499799	-0.880816949
C	0.386397	-2.739493	-0.648536	C	0.388204275	-2.731759880	-0.648175935
C	1.679417	-3.307716	-0.544232	C	1.678845580	-3.299035977	-0.543661535
C	2.860338	-2.585583	-0.324370	C	2.855679807	-2.579847447	-0.324484865
C	4.245855	-2.973769	-0.257975	C	4.239365810	-2.967262987	-0.258310728
H	4.618755	-3.992948	-0.338970	H	4.614848904	-3.987232278	-0.338721892
C	5.003402	-1.818833	-0.087241	C	4.995445713	-1.816171198	-0.088265034
H	6.085908	-1.752515	-0.006721	H	6.079549766	-1.752695726	-0.007066848
C	4.085066	-0.721329	-0.043568	C	4.079944064	-0.719255397	-0.045505609
N	2.834460	1.238764	-0.046751	N	2.831770650	1.235119363	-0.048917591
N	0.115374	1.474235	-0.436168	N	0.116417759	1.470418341	-0.435133132
N	0.106292	-1.389340	-0.531819	N	0.107257382	-1.384993455	-0.532616070
N	2.819876	-1.218906	-0.171318	N	2.817054123	-1.214618075	-0.171222072
Mn	1.351365	0.014256	-0.126753	Mn	1.350965062	0.017039886	-0.127951454
H	-0.947903	-4.504657	-1.024097	H	-0.945474837	-4.497629330	-1.022816303
H	-2.923723	-2.655293	-1.056341	H	-2.917685145	-2.655037792	-1.055248375
H	1.601564	0.122948	-1.675537	H	1.598714019	0.120184612	-1.676977330
O	1.035834	-0.002799	1.805514	O	1.033545580	-0.014966309	1.810979762
C	-3.402788	0.067118	-0.586935	C	-3.398903286	0.067052433	-0.585799838
C	-4.132149	-0.365334	0.552655	C	-4.128563623	-0.365058140	0.550491608
C	-4.093961	0.549324	-1.715143	C	-4.092323162	0.547603032	-1.709520060
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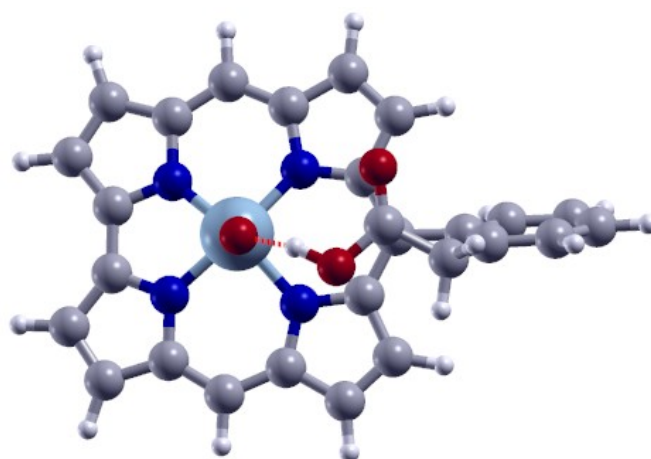
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C	-3.488425	-0.943919	1.803375	C	-3.488056920	-0.940736064	1.799918891
C	-2.194830	-0.254950	2.254897	C	-2.195333191	-0.256503967	2.254807076
O	-2.124467	0.949573	2.464090	O	-2.127558714	0.947879408	2.463540330
O	-1.183987	-1.118586	2.376201	O	-1.185910184	-1.117183066	2.380220392
H	-0.273748	-0.614531	2.310813	H	-0.266311754	-0.606149521	2.306877543
H	1.750091	-4.391692	-0.658352	H	1.749918077	-4.384448853	-0.658145434
H	1.794376	4.452779	-0.237591	H	1.793431077	4.446134217	-0.237814287
H	1.125786	0.874889	2.214935	H	1.117557780	0.873695044	2.218546544
H	-3.515600	0.873894	-2.583927	H	-3.516517392	0.873699147	-2.581264565
H	-6.004654	0.971305	-2.634033	H	-6.000206920	0.969696013	-2.630193396
H	-7.305420	0.236355	-0.619599	H	-7.300550333	0.235717788	-0.618512114
H	-6.106212	-0.590002	1.386356	H	-6.101536662	-0.589707431	1.384310636
H	-4.210910	-0.861123	2.631372	H	-4.213225654	-0.857661762	2.627426985
H	-3.280556	-2.016188	1.658278	H	-3.283529677	-2.015120161	1.655390611



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C	-4.087199	-3.038337	-0.700968
H	-4.373809	-4.061198	-0.938313
C	-2.740397	-2.525744	-0.719603
C	-1.513084	-3.108517	-1.060897
C	-0.275958	-2.418238	-1.111065
C	1.020188	-2.969110	-1.420471
H	1.206853	-4.007730	-1.687785
C	1.943086	-1.949441	-1.317191
H	3.015943	-2.003913	-1.488511
C	1.223855	-0.753553	-0.945588
C	1.756412	0.536998	-0.699704
C	1.003355	1.696804	-0.379677
C	1.494616	3.039126	-0.199838
C	0.409061	3.846969	0.074583
C	-0.764901	3.017056	0.082993
C	-2.097373	3.412486	0.336282
C	-3.198668	2.543228	0.349628



C	-4.609386	2.763405	0.524371
H	-5.076491	3.728604	0.710831
C	-5.254172	1.534929	0.398584
H	-6.323363	1.348619	0.471294
C	-4.245340	0.554820	0.150723
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N	-3.025684	1.191275	0.143553
Mn	-1.468939	0.143197	-0.176992
H	-2.272482	4.473673	0.525358
H	0.413319	4.920066	0.256959
H	2.536659	3.337871	-0.287539
H	-1.498257	-4.169463	-1.319367
H	-1.677612	0.387773	-1.711948
O	-0.779257	-0.253349	1.607874
O	-0.753949	-1.605008	2.016527
H	0.207291	-1.728040	2.224806
C	3.248285	0.669235	-0.697900
C	3.933808	1.074354	-1.855627
C	3.978800	0.390127	0.481825
C	5.326915	1.199929	-1.858469
H	3.358575	1.289686	-2.759523
C	5.376362	0.525220	0.465184
C	6.050197	0.924082	-0.692874
H	5.844456	1.515353	-2.767568
H	5.942943	0.312466	1.376051
H	7.138208	1.023588	-0.682865
C	3.262970	-0.031068	1.753480
H	2.275188	0.441724	1.840550
H	3.858509	0.287753	2.627617
C	3.046009	-1.524082	1.930322
O	2.029937	-2.047964	2.363727
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H	3.899755	-3.190738	1.779202



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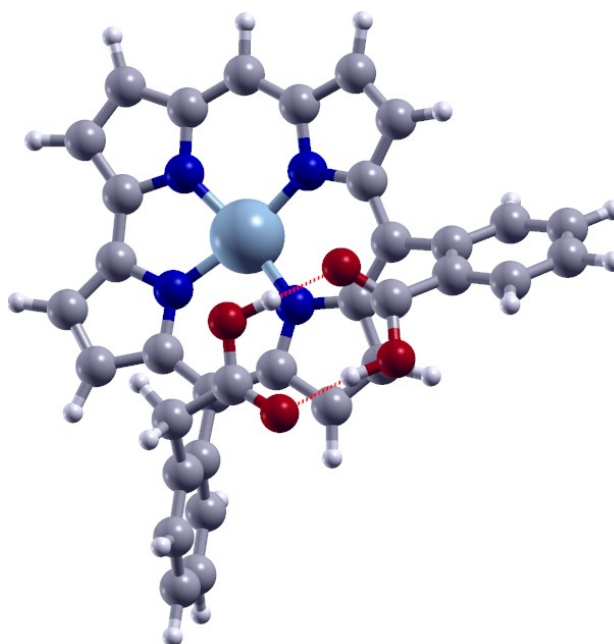
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H	-6.123879	-1.728290	-0.255132	H	-6.117551876	-1.726548700	-0.247922475
C	-4.274109	-2.950560	-0.365456	C	-4.265075276	-2.939736877	-0.364687894
H	-4.638470	-3.965439	-0.511600	H	-4.631664590	-3.956051213	-0.506816801
C	-2.885243	-2.561845	-0.314226	C	-2.879466389	-2.551731212	-0.318721270
C	-1.701586	-3.271665	-0.526702	C	-1.698703370	-3.261780738	-0.530656896
C	-0.410058	-2.697378	-0.623147	C	-0.410733078	-2.691009599	-0.626644653
C	0.827454	-3.387654	-0.892335	C	0.823880564	-3.380167997	-0.896718335
H	0.915336	-4.459527	-1.058878	H	0.913257590	-4.453432938	-1.064442518
C	1.832991	-2.449261	-0.912480	C	1.827289021	-2.444843678	-0.917136149
H	2.892029	-2.609089	-1.099699	H	2.887268830	-2.608727213	-1.104880015
C	1.228168	-1.166150	-0.652689	C	1.226482356	-1.162976568	-0.655496131
C	1.877919	0.089108	-0.555880	C	1.876831771	0.089502605	-0.558923279
C	1.220766	1.340786	-0.422586	C	1.216578411	1.336160134	-0.425950849
C	1.819904	2.650682	-0.456228	C	1.812079009	2.644304969	-0.453776256
C	0.803774	3.571477	-0.345342	C	0.799122449	3.563674669	-0.341351223
C	-0.431633	2.843921	-0.223665	C	-0.434730574	2.840526764	-0.225442869
C	-1.733583	3.383909	-0.115373	C	-1.731326887	3.379769973	-0.113788933
C	-2.905946	2.629445	-0.052336	C	-2.900746934	2.626151622	-0.049657478
C	-4.294539	2.993987	-0.047727	C	-4.285765726	2.988709039	-0.040902994
H	-4.675000	4.013383	-0.060865	H	-4.668348272	4.008805723	-0.050287975
C	-5.045316	1.821373	-0.043079	C	-5.036590830	1.819298140	-0.037658078
H	-6.129856	1.739887	-0.044765	H	-6.122936251	1.741407590	-0.036927524
C	-4.123501	0.731145	-0.036617	C	-4.119970756	0.730909627	-0.037089546
N	-2.856081	-1.197075	-0.120639	N	-2.853291354	-1.189965209	-0.126652632
N	-0.131918	-1.354126	-0.504806	N	-0.129306419	-1.351103749	-0.506594127
N	-0.145609	1.493090	-0.260144	N	-0.148972568	1.490667383	-0.265478316
N	-2.850293	1.243358	-0.028356	N	-2.846143888	1.242836969	-0.028234080
Mn	-1.384135	0.046119	0.092226	Mn	-1.385923401	0.050370521	0.090269280
H	-1.819438	4.472760	-0.118870	H	-1.816722026	4.470167530	-0.112246001
H	0.889014	4.656319	-0.343518	H	0.888323089	4.649884456	-0.335164471
H	2.884083	2.845229	-0.553027	H	2.877348407	2.843069255	-0.548451765
H	-1.447946	-0.042005	-1.518238	H	-1.445766981	-0.049709870	-1.513195481
O	-0.960046	-0.350009	1.686168	O	-0.959293026	-0.358577814	1.672413563
C	3.373381	0.103149	-0.616677	C	3.370881085	0.104664161	-0.615028671
C	4.176996	-0.348401	0.463061	C	4.171271314	-0.350433857	0.462250140
C	3.987766	0.604802	-1.780601	C	3.992201638	0.610068987	-1.769803584
C	5.574126	-0.258427	0.324450	C	5.565821322	-0.257231375	0.330283309
C	5.377914	0.663322	-1.901345	C	5.379073001	0.671985929	-1.884095339
H	3.352749	0.942760	-2.603470	H	3.362351970	0.952495082	-2.597058750
C	6.175842	0.232211	-0.837050	C	6.171468511	0.239281978	-0.821860217
H	6.202621	-0.582484	1.158876	H	6.193212063	-0.584848483	1.166579128
H	5.831578	1.047397	-2.817862	H	5.837130059	1.062210583	-2.798266932
H	7.265116	0.282528	-0.906354	H	7.263156229	0.292891379	-0.886271225
C	3.626849	-0.957482	1.744183	C	3.618955908	-0.966470678	1.734876625
H	4.387818	-0.843021	2.532732	H	4.380934316	-0.863663587	2.525809729
H	3.460949	-2.037723	1.603476	H	3.450325186	-2.046222605	1.583628315
C	2.330795	-0.325061	2.260688	C	2.326806150	-0.338014711	2.257790587
O	2.225516	0.866833	2.505772	O	2.223574268	0.851867841	2.510877464
O	1.354675	-1.234496	2.385516	O	1.351258878	-1.246295905	2.381040111
H	0.432649	-0.788539	2.339813	H	0.423823374	-0.796800034	2.327793624
H	-1.767732	-4.352481	-0.671482	H	-1.766692753	-4.344021138	-0.674518910

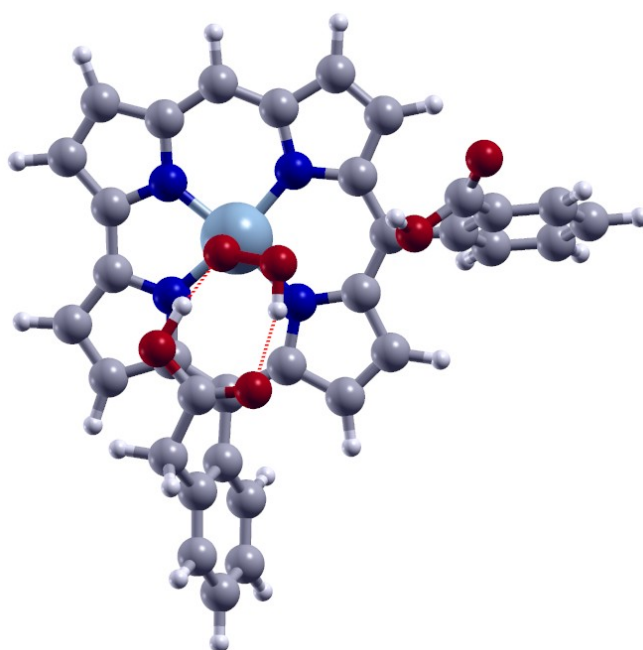


**Table S6:** Structures, energies, and coordinates of the complexes with the substituent R1=C<sub>6</sub>H<sub>4</sub>-COOH, R2=C<sub>6</sub>H<sub>4</sub>-CH<sub>2</sub>-COOH.



E= -1931.1750247 a.u (*)				E= -837.1782756734 Ry (*)			
C	-2.311234	3.188096	0.026852	C	-2.317923014	3.172856023	0.017617628
C	-3.716481	3.013292	0.150617	C	-3.718545419	2.994476248	0.140628601
H	-4.436345	3.784182	0.417029	H	-4.440078430	3.765863170	0.406730570
C	-3.989212	1.668737	-0.110548	C	-3.986321638	1.651812921	-0.117685188
H	-4.964026	1.185179	-0.100981	H	-4.961261548	1.165137736	-0.107785184
C	-2.748179	1.014989	-0.410290	C	-2.746115104	1.002543706	-0.415297944
C	-2.441935	-0.326373	-0.722143	C	-2.435984630	-0.335075112	-0.724143148
C	-1.123257	-0.761001	-0.976687	C	-1.118883708	-0.761398299	-0.978542119
C	-0.717312	-2.076329	-1.375868	C	-0.707871359	-2.071206021	-1.377037301
H	-1.398426	-2.890100	-1.612375	H	-1.386614502	-2.888872237	-1.611989384
C	0.660499	-2.113317	-1.378962	C	0.666698826	-2.102334160	-1.379788928
H	1.290579	-2.961485	-1.633977	H	1.301435569	-2.949131659	-1.632566525
C	1.136879	-0.825647	-0.956658	C	1.137278782	-0.816611268	-0.957715935
C	2.468879	-0.467264	-0.641314	C	2.464487638	-0.455993992	-0.642222963
C	2.881450	0.843550	-0.311993	C	2.870659504	0.852708989	-0.312822425
C	4.203575	1.294925	0.028733	C	4.186740720	1.308887502	0.031995965
C	4.141219	2.652697	0.257684	C	4.117028035	2.662136117	0.265934193
C	2.777136	3.067796	0.106586	C	2.755289784	3.070264679	0.113166386
C	2.259090	4.348081	0.354242	C	2.234486069	4.344527279	0.361095867
C	0.888993	4.656322	0.354787	C	0.867188435	4.647374552	0.356158053
C	0.160157	5.847167	0.683438	C	0.134996253	5.831454839	0.685544029
H	0.605757	6.802982	0.952939	H	0.579033311	6.788312013	0.959687811
C	-1.203065	5.551998	0.612731	C	-1.223850867	5.532734731	0.608851904
H	-2.027799	6.230635	0.819311	H	-2.053421049	6.207964114	0.814705545
C	-1.317670	4.185131	0.235757	C	-1.332041248	4.170370196	0.228218568
N	-1.754081	1.967791	-0.325136	N	-1.757524757	1.956997594	-0.333798316
N	0.034573	0.003642	-0.771767	N	0.033767590	0.007276033	-0.778305875
N	2.021937	1.939372	-0.245308	N	2.008046079	1.942317332	-0.245681928

N	-0.039434	3.675685	0.079815	N	-0.054364341	3.667600055	0.072260440
Mn	0.135086	1.884603	-0.528844	Mn	0.127892269	1.882035123	-0.533097681
H	2.972097	5.132667	0.614481	H	2.945041571	5.130478566	0.630178616
H	4.959636	3.312231	0.540801	H	4.930115258	3.327849799	0.554353933
H	5.081164	0.657557	0.097358	H	5.069592279	0.676149536	0.097213075
H	0.151926	2.240899	-2.026018	H	0.149263292	2.239710115	-2.025031125
C	-3.514523	-1.369436	-0.685067	C	-3.500717521	-1.380523079	-0.682136813
C	-3.789509	-2.068896	0.518278	C	-3.768439472	-2.078068328	0.519773778
C	-4.227925	-1.692639	-1.850949	C	-4.216996690	-1.706984439	-1.840742774
C	-4.756453	-3.086566	0.499451	C	-4.732626717	-3.093113625	0.507651781
C	-5.193547	-2.705516	-1.849403	C	-5.177538689	-2.719121648	-1.833519803
H	-4.008767	-1.142486	-2.769593	H	-4.003544284	-1.158137784	-2.763081809
C	-5.452452	-3.410010	-0.670184	C	-5.430901060	-3.419214270	-0.654928847
H	-4.967385	-3.633243	1.422821	H	-4.940708432	-3.635484779	1.435954234
H	-5.736615	-2.943788	-2.767046	H	-5.721935833	-2.961096513	-2.750595553
H	-6.198924	-4.207739	-0.656196	H	-6.176529117	-4.218768487	-0.635752731
C	-3.112501	-1.700994	1.828944	C	-3.088467325	-1.712190120	1.824851492
H	-3.638613	-2.213646	2.651418	H	-3.621080347	-2.219318591	2.648928441
H	-3.187772	-0.619176	2.011440	H	-3.161036042	-0.628247459	2.006115822
C	-1.644550	-2.096499	1.956437	C	-1.623390036	-2.114443014	1.955792952
O	-1.230483	-3.242328	1.752879	O	-1.217840631	-3.261461679	1.736063733
O	-0.875363	-1.084075	2.349376	O	-0.847853438	-1.119000220	2.363873154
H	0.095901	-1.368744	2.327328	H	0.136641381	-1.411047277	2.327009859
C	3.455144	-1.581726	-0.530577	C	3.452003310	-1.564212749	-0.530176979
C	4.607999	-1.618911	-1.334963	C	4.604055124	-1.593633585	-1.329810781
C	3.225889	-2.665498	0.360151	C	3.227695034	-2.646286578	0.359029955
C	5.516127	-2.679703	-1.254384	C	5.516362222	-2.645250006	-1.248901133
H	4.772917	-0.810575	-2.051235	H	4.767245002	-0.781636202	-2.044586426
C	4.123379	-3.743997	0.410813	C	4.131232178	-3.715153014	0.410340122
C	5.275839	-3.745195	-0.379313	C	5.281609860	-3.709411629	-0.376733056
H	6.403536	-2.682538	-1.891972	H	6.405066476	-2.640819158	-1.886704256
H	3.915166	-4.576866	1.085775	H	3.929300944	-4.550906923	1.086298942
H	5.977187	-4.580402	-0.319912	H	5.989259132	-4.540609235	-0.316301643
C	2.020381	-2.672002	1.252944	C	2.022607707	-2.660397364	1.251994285
O	1.679291	-1.695261	1.928296	O	1.687027973	-1.685320374	1.934357597
O	1.355202	-3.829718	1.235398	O	1.352911934	-3.810099652	1.230837231
H	0.434531	-3.676602	1.624006	H	0.414249712	-3.649681436	1.612105014



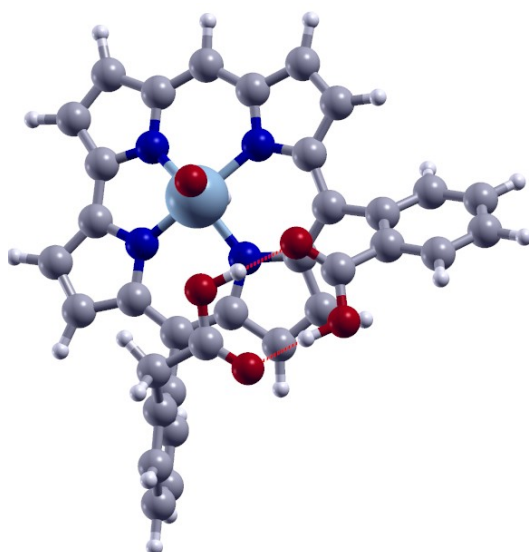
E= -2082.0139568 a.u (\*OOH)

C	-2.639389	2.611448	-0.680048
C	-4.040515	2.359827	-0.819827
H	-4.823928	3.111612	-0.882085
C	-4.201494	0.978025	-0.858208
H	-5.135337	0.430266	-0.966394
C	-2.896386	0.379535	-0.748207
C	-2.476431	-0.966603	-0.702424
C	-1.101034	-1.358059	-0.711012
C	-0.585122	-2.698998	-0.719337
H	-1.192881	-3.599675	-0.720433
C	0.791618	-2.620158	-0.698596
H	1.498060	-3.446057	-0.682442
C	1.146335	-1.227586	-0.656268
C	2.452109	-0.674812	-0.563330
C	2.755006	0.708686	-0.443792
C	4.054089	1.329085	-0.422252
C	3.861922	2.691442	-0.314621
C	2.447188	2.933600	-0.283775
C	1.798052	4.188939	-0.245293
C	0.410312	4.378225	-0.319156
C	-0.412777	5.556540	-0.380973
H	-0.049945	6.581496	-0.333521
C	-1.736788	5.145045	-0.520635
H	-2.614249	5.782382	-0.602068
C	-1.728438	3.715926	-0.541846
N	-1.990614	1.408969	-0.657005
N	-0.022260	-0.489032	-0.666173
N	1.802892	1.705928	-0.349468
N	-0.433403	3.295298	-0.405793
Mn	-0.091059	1.411068	-0.363934
H	2.438505	5.071766	-0.188330

E= -902.6933247200 Ry (\*OOH)

C	-2.634697673	2.606231954	-0.684369353
C	-4.031975767	2.354948377	-0.821408982
H	-4.815115631	3.109335141	-0.880331823
C	-4.193575477	0.976570546	-0.859380177
H	-5.129549040	0.429351645	-0.966304619
C	-2.892233033	0.377410756	-0.752857304
C	-2.473201480	-0.964628106	-0.703993725
C	-1.099859379	-1.353809141	-0.716987886
C	-0.583405015	-2.691014972	-0.725355991
H	-1.191010662	-3.593559924	-0.725767821
C	0.789590323	-2.612150882	-0.704198759
H	1.497404980	-3.438830396	-0.685393350
C	1.145357372	-1.223359106	-0.661104586
C	2.447925163	-0.674776724	-0.565336959
C	2.747890391	0.705430996	-0.443347712
C	4.043083261	1.327078385	-0.423135347
C	3.849321776	2.686272188	-0.317387054
C	2.438180295	2.925671694	-0.287645094
C	1.791235083	4.179104426	-0.248185778
C	0.408947359	4.367399967	-0.322995365
C	-0.412828906	5.543405935	-0.382625318
H	-0.046004892	6.568340277	-0.334737495
C	-1.733309161	5.133937067	-0.521601736
H	-2.611817817	5.772899385	-0.600866065
C	-1.725997120	3.707321513	-0.544373422
N	-1.986873706	1.406374684	-0.663945989
N	-0.023573788	-0.486817407	-0.668733266
N	1.797359660	1.700717632	-0.347933386
N	-0.435045624	3.286718540	-0.408808356
Mn	-0.096239146	1.405922924	-0.363665842
H	2.433741571	5.062919440	-0.189336700

H	4.626849	3.464401	-0.273189	H	4.611910814	3.463747940	-0.275461407
H	5.003358	0.803353	-0.486794	H	4.994947101	0.802247852	-0.484854426
H	-0.022759	1.528458	-1.925692	H	-0.005585356	1.529552861	-1.918944262
O	-0.383618	1.256342	1.636290	O	-0.393535865	1.267848577	1.645759942
O	0.450381	0.269131	2.271654	O	0.426223892	0.264438302	2.290899144
C	-3.505880	-2.038592	-0.566888	C	-3.498863999	-2.034732776	-0.565984382
C	-4.243025	-2.211920	0.634695	C	-4.235020253	-2.206436203	0.632736713
C	-3.721776	-2.918339	-1.645412	C	-3.716890087	-2.912189035	-1.641352627
C	-5.160289	-3.276371	0.699503	C	-5.151061574	-3.267109766	0.698282065
C	-4.653304	-3.955630	-1.564103	C	-4.646649410	-3.945429353	-1.559221029
H	-3.149336	-2.766942	-2.564000	H	-3.143605970	-2.762228045	-2.561753931
C	-5.373932	-4.137725	-0.379643	C	-5.365239398	-4.125750244	-0.377486029
H	-5.719012	-3.430841	1.627158	H	-5.710221214	-3.418402141	1.628367239
H	-4.810764	-4.618062	-2.418376	H	-4.803643468	-4.608753371	-2.414689777
H	-6.097770	-4.951365	-0.291499	H	-6.090317510	-4.939647980	-0.287703017
C	-4.148713	-1.294003	1.848451	C	-4.140176852	-1.294181956	1.845813247
H	-4.466126	-1.868164	2.734664	H	-4.461307300	-1.873454101	2.729611525
H	-4.854156	-0.455189	1.738920	H	-4.849899113	-0.456071341	1.737997359
C	-2.774167	-0.715913	2.162457	C	-2.766595769	-0.718263727	2.165642637
O	-1.769411	-1.420996	2.294805	O	-1.767709680	-1.433831511	2.298202854
O	-2.777541	0.607561	2.279427	O	-2.756282209	0.599629041	2.282159732
H	-1.800142	0.946306	2.158440	H	-1.758997074	0.942153268	2.140947925
H	-0.198484	-0.485041	2.372127	H	-0.245673427	-0.484586064	2.386905909
C	3.607999	-1.618271	-0.660850	C	3.602090194	-1.615458117	-0.662266032
C	3.845114	-2.255173	-1.893971	C	3.839950024	-2.252390311	-1.891601173
C	4.522965	-1.843126	0.398469	C	4.516275185	-1.838630084	0.394198068
C	4.955033	-3.084085	-2.081403	C	4.948054487	-3.077393390	-2.077377912
H	3.153984	-2.071172	-2.719837	H	3.148092685	-2.069995877	-2.719747726
C	5.650774	-2.655958	0.191398	C	5.640781821	-2.650159809	0.189173025
C	5.866211	-3.281609	-1.037118	C	5.856585199	-3.274212668	-1.035494938
H	5.114648	-3.563466	-3.050221	H	5.107185165	-3.558023942	-3.047051990
H	6.346462	-2.791869	1.022201	H	6.334760995	-2.784473668	1.024273793
H	6.740555	-3.920498	-1.179588	H	6.732197991	-3.914118580	-1.175649324
C	4.363121	-1.259301	1.770094	C	4.360271267	-1.258196071	1.765387782
O	5.294316	-0.944037	2.492414	O	5.294304032	-0.941714953	2.483202964
O	3.061596	-1.156166	2.128179	O	3.062918610	-1.159284588	2.134271769
H	3.016542	-0.675756	2.979747	H	3.030808149	-0.684839985	3.000355548



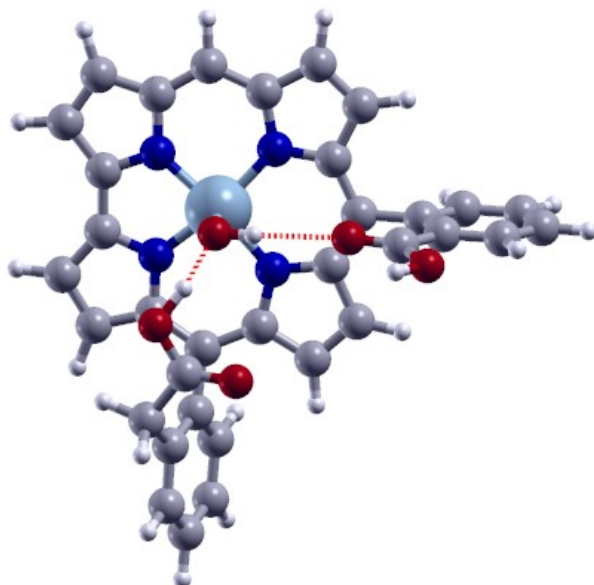
E= -2006.2812957 a.u (\*O)

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H	-4.325924	4.052401	-0.159108
C	-3.967112	1.864028	-0.323061
H	-4.964136	1.438096	-0.413650
C	-2.742226	1.116076	-0.365897
C	-2.479134	-0.238770	-0.619135
C	-1.159141	-0.708061	-0.848012
C	-0.805747	-1.994972	-1.376544
H	-1.516467	-2.756251	-1.687674
C	0.568202	-2.060100	-1.418182
H	1.175485	-2.887507	-1.774934
C	1.075825	-0.823272	-0.888808
C	2.433249	-0.533353	-0.595555
C	2.915081	0.760112	-0.278061
C	4.279745	1.189726	-0.079106
C	4.255052	2.552601	0.108431
C	2.877679	2.971994	0.063979
C	2.385668	4.286601	0.192336
C	1.031274	4.632088	0.147995
C	0.363770	5.904568	0.183551
H	0.859168	6.870340	0.263224
C	-1.004799	5.671843	0.090058
H	-1.796934	6.417091	0.078948
C	-1.179868	4.256552	0.006437
N	-1.700902	2.013162	-0.211407
N	0.003110	0.003746	-0.596652
N	2.092085	1.859393	-0.156376
N	0.053615	3.661556	0.053796
Mn	0.138398	1.762658	0.190535
H	3.120567	5.085382	0.314260
H	5.103612	3.216214	0.264494
H	5.151714	0.541735	-0.082631
H	0.446726	2.012841	-1.403538
C	-3.581269	-1.246252	-0.673076

E= -869.3270816045 Ry (\*O)

C	-2.151458938	3.279051834	0.013494234
C	-3.571771414	3.213825085	-0.016136272
H	-4.253531762	4.057879831	0.078967419
C	-3.915164795	1.878395064	-0.193617554
H	-4.919670889	1.463837008	-0.274417328
C	-2.701423479	1.126419262	-0.306178650
C	-2.457878499	-0.214131757	-0.631619577
C	-1.146512378	-0.683414996	-0.885332486
C	-0.802111965	-1.959956221	-1.435027876
H	-1.517300887	-2.703315704	-1.782173218
C	0.567669109	-2.049313773	-1.444865378
H	1.171218681	-2.881592662	-1.801674974
C	1.085012974	-0.835886916	-0.883371782
C	2.439079491	-0.580314201	-0.556656900
C	2.940052201	0.702805909	-0.243136416
C	4.305837354	1.115891882	-0.046242999
C	4.298936325	2.477407313	0.125161048
C	2.931012993	2.913717268	0.080447089
C	2.456342289	4.228721258	0.219153869
C	1.108061179	4.585062595	0.211026794
C	0.457749927	5.860400880	0.280391790
H	0.969610541	6.820644275	0.344645285
C	-0.912615969	5.643976162	0.237674837
H	-1.696832975	6.399528940	0.262077948
C	-1.106807259	4.234261057	0.146102369
N	-1.652404861	2.007845002	-0.137997682
N	0.022740411	0.003025639	-0.601672283
N	2.133647198	1.810848996	-0.131211892
N	0.118991433	3.628848819	0.143041451
Mn	0.187346452	1.729593765	0.234692183
H	3.198623854	5.023664200	0.334321484
H	5.157339208	3.132690159	0.269942348
H	5.170510875	0.456580611	-0.045599403
H	0.472790217	2.045409359	-1.359300117
C	-3.569181533	-1.208595311	-0.706178130

C	-3.845801	-2.079809	0.444799	C	-3.893427312	-2.001205910	0.421388469
C	-4.329976	-1.405919	-1.851104	C	-4.262424904	-1.404439177	-1.908474899
C	-4.836881	-3.066825	0.323579	C	-4.893091734	-2.973156138	0.292193615
C	-5.319187	-2.390575	-1.948705	C	-5.258875300	-2.375544336	-2.015406024
H	-4.115180	-0.755242	-2.702611	H	-4.000938811	-0.790436622	-2.776433355
C	-5.565634	-3.230730	-0.859167	C	-5.571054246	-3.166914644	-0.911189995
H	-5.043958	-3.714384	1.180083	H	-5.145750661	-3.590542544	1.160817697
H	-5.888395	-2.502553	-2.874498	H	-5.785170969	-2.516509185	-2.964025309
H	-6.329709	-4.008982	-0.923929	H	-6.347483939	-3.934462797	-0.982178243
C	-3.154387	-1.873812	1.783039	C	-3.226759062	-1.788076496	1.766032984
H	-3.704799	-2.442451	2.551051	H	-3.797494881	-2.340096852	2.533125461
H	-3.188681	-0.813313	2.072177	H	-3.244517527	-0.722721047	2.044748278
C	-1.700701	-2.332334	1.881314	C	-1.785028618	-2.271203531	1.873690886
O	-1.318709	-3.461189	1.555176	O	-1.436450035	-3.412482777	1.542664800
O	-0.915984	-1.391642	2.393866	O	-0.977855714	-1.356080357	2.377272732
H	0.051764	-1.676651	2.340307	H	0.002340502	-1.664118873	2.313604473
C	3.379353	-1.684857	-0.606150	C	3.347484881	-1.756017228	-0.515974490
C	4.509629	-1.683441	-1.444841	C	4.512765818	-1.804943230	-1.297054048
C	3.131360	-2.844065	0.179996	C	3.027464170	-2.891418740	0.273578095
C	5.382164	-2.774963	-1.490683	C	5.347827952	-2.921712441	-1.286395338
H	4.681169	-0.820962	-2.092520	H	4.745705270	-0.958409796	-1.949161640
C	3.997038	-3.946254	0.106826	C	3.853989372	-4.020317304	0.252370641
C	5.130376	-3.908290	-0.709653	C	5.020377324	-4.033481472	-0.509371173
H	6.250279	-2.745987	-2.153522	H	6.249905250	-2.929695153	-1.905325966
H	3.777050	-4.832534	0.705526	H	3.573842900	-4.891168072	0.851671623
H	5.805747	-4.765893	-0.745972	H	5.666279593	-4.916228581	-0.504364709
C	1.941878	-2.910089	1.093525	C	1.806872178	-2.905398758	1.143878024
O	1.634469	-1.994910	1.861223	O	1.525746415	-1.968776512	1.900556843
O	1.254374	-4.050092	0.977974	O	1.073812292	-4.004913841	1.014253049
H	0.339667	-3.915739	1.387213	H	0.129550162	-3.826264988	1.390059434
O	0.435082	1.443445	1.715483	O	0.498758525	1.372691770	1.748826857



didn't observe this isomer

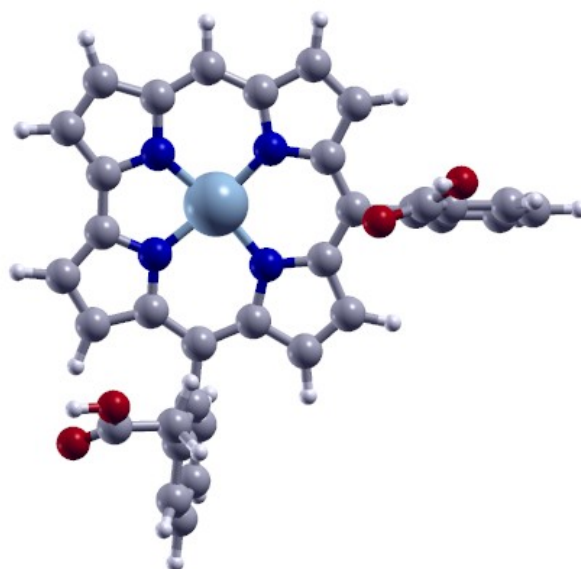
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	H	-4.843926333	3.140673118	-0.358845638
	C	-4.174045554	1.037003717	-0.585973793
	H	-5.103476778	0.481541483	-0.706004331
	C	-2.857464253	0.462622504	-0.605741579
	C	-2.416459264	-0.865615937	-0.746214701
	C	-1.035953948	-1.219929512	-0.865720411
	C	-0.492975372	-2.542752890	-1.012891436
	H	-1.082983294	-3.454048356	-1.085972780
	C	0.875771574	-2.436959869	-1.001994291
	H	1.597775787	-3.247940921	-1.085345936
	C	1.201752970	-1.046673916	-0.834675520
	C	2.486232411	-0.476488086	-0.681894173
	C	2.778862775	0.902974435	-0.521566713
	C	4.068312052	1.532628602	-0.456865995
	C	3.859747611	2.883427025	-0.283505054
	C	2.443351572	3.101991727	-0.229215077
	C	1.769199209	4.332730414	-0.063904252
	C	0.381366958	4.487898437	-0.028488550
	C	-0.466885628	5.645770883	0.049265994
	H	-0.123144254	6.676437649	0.136646054
	C	-1.784414820	5.213412248	-0.023503644
	H	-2.677455940	5.836362599	-0.000939152
	C	-1.749398477	3.790182631	-0.142578080
	N	-1.970248480	1.499889003	-0.442265650
	N	0.017906487	-0.339695969	-0.775646022
	N	1.821276978	1.878093637	-0.373520763
	N	-0.446166636	3.393563949	-0.123678392
	Mn	-0.071649259	1.519545517	-0.251845386
	H	2.391216976	5.228077818	0.023887631
	H	4.616995197	3.662924783	-0.199383631
	H	5.025135761	1.019080827	-0.538741099
	H	-0.046451745	1.771188408	-1.805270429
	O	-0.011474197	1.045306281	1.648982024
	C	-3.419927796	-1.965729727	-0.689249466
	C	-4.077484968	-2.292319812	0.524258104
	C	-3.694455082	-2.710589902	-1.847722198
	C	-4.982514562	-3.364350958	0.512672461
	C	-4.611793376	-3.759682329	-1.836241996
	H	-3.179197693	-2.447138953	-2.776670946
	C	-5.258080986	-4.089628420	-0.645632704
	H	-5.481058437	-3.639214774	1.448418264
	H	-4.816659521	-4.319438822	-2.753829991
	H	-5.973188977	-4.917949235	-0.614925310
	C	-3.866610228	-1.533439090	1.820639881
	H	-4.250396204	-2.152420729	2.649750766
	H	-4.453863589	-0.600171964	1.813470729
	C	-2.406922022	-1.185062909	2.144392034
	O	-1.520203763	-2.029366252	2.152480895
	O	-2.244390813	0.110613631	2.400599663
	H	-1.243172434	0.414340828	2.229790451
	C	3.645980167	-1.419618180	-0.672166425
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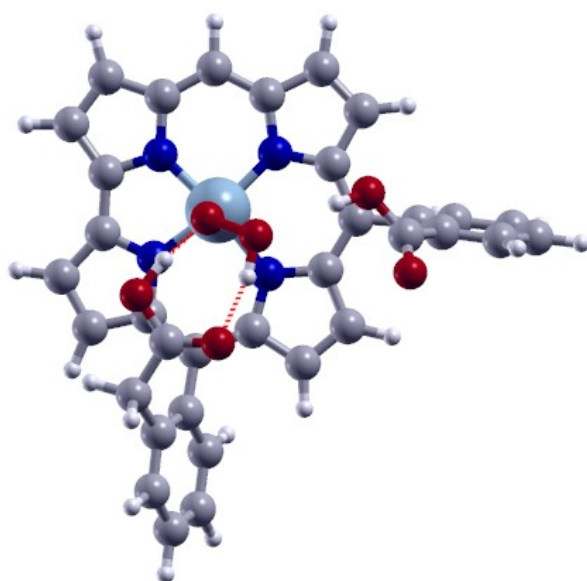


	C	5.358801455	-2.623984524	-1.919578194
	H	3.903816041	-1.293658673	-2.805320769
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	C	5.829937347	-3.203976216	-0.741708671
	H	5.833229050	-2.859979676	-2.877245698
	H	5.567882755	-3.356203829	1.394410878
	H	6.677281724	-3.895615769	-0.764335986
	C	3.478676835	-1.706066284	1.829618733
	O	2.615569981	-0.866045483	2.022243162
	O	3.960739342	-2.477925175	2.846182055
	H	3.452154338	-2.193566874	3.643364169
	H	0.766785557	0.486336867	1.875264270



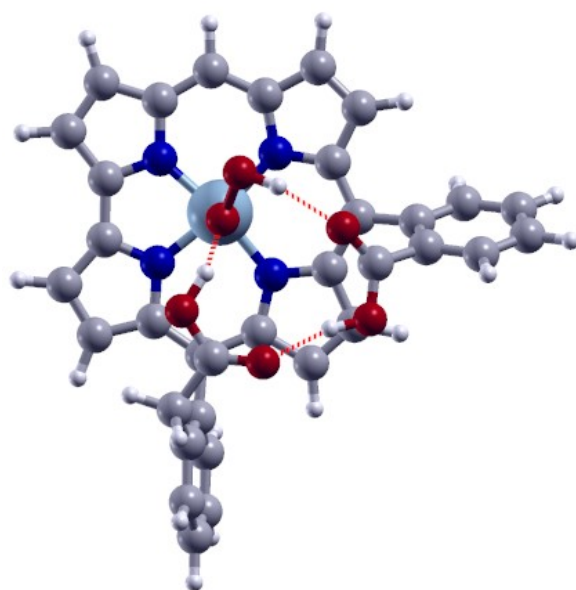
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C	-3.709859	2.572819	-0.435634	C	-3.699828511	2.569705202	-0.435194175
H	-4.475792	3.344139	-0.391732	H	-4.468254847	3.340846204	-0.391165704
C	-3.918698	1.196736	-0.548774	C	-3.908621880	1.197305820	-0.548315305
H	-4.877135	0.684550	-0.602467	H	-4.870122427	0.687401460	-0.602472027
C	-2.635204	0.555076	-0.560976	C	-2.629041140	0.554986386	-0.561553511
C	-2.262838	-0.805401	-0.642433	C	-2.259916761	-0.803715350	-0.641854587
C	-0.913554	-1.225414	-0.616095	C	-0.912775855	-1.220908906	-0.616619417
C	-0.435879	-2.578600	-0.632964	C	-0.434446746	-2.570163649	-0.632224192
H	-1.074841	-3.457052	-0.686000	H	-1.071023728	-3.451920273	-0.685314070
C	0.940387	-2.548293	-0.551153	C	0.938405763	-2.539645696	-0.550696361
H	1.616364	-3.399553	-0.523310	H	1.612682614	-3.393913398	-0.523018876
C	1.348469	-1.173561	-0.487504	C	1.347460530	-1.168539958	-0.488770199
C	2.664928	-0.676954	-0.376127	C	2.662421451	-0.675386133	-0.376692051
C	3.008279	0.688949	-0.293838	C	3.003172497	0.688057933	-0.295459575
C	4.324962	1.259558	-0.209359	C	4.315910252	1.260017459	-0.209475517
C	4.186803	2.630015	-0.140894	C	4.177051291	2.626987961	-0.141299913

C	2.787002	2.939556	-0.184935	C	2.780634436	2.935198468	-0.186366273
C	2.199104	4.212067	-0.124529	C	2.194086702	4.203870015	-0.125579867
C	0.813442	4.438917	-0.157948	C	0.812065047	4.430453175	-0.158821666
C	0.020216	5.630852	-0.071842	C	0.020371722	5.619333497	-0.071952895
H	0.412512	6.640478	0.036043	H	0.412267955	6.631033158	0.035147694
C	-1.324869	5.261217	-0.142419	C	-1.321397432	5.250917934	-0.142426785
H	-2.185856	5.924706	-0.098613	H	-2.181847506	5.918018892	-0.099038193
C	-1.364874	3.845288	-0.271419	C	-1.361695375	3.838407001	-0.272287062
N	-1.681785	1.546471	-0.454929	N	-1.677086659	1.544371566	-0.458703410
N	0.202925	-0.380083	-0.519842	N	0.202971327	-0.377072140	-0.522798072
N	2.083901	1.730060	-0.276908	N	2.080160199	1.727159244	-0.280588927
N	-0.060075	3.379188	-0.275397	N	-0.059337616	3.373301720	-0.277941463
Mn	0.212547	1.522384	-0.570379	Mn	0.213168265	1.520244204	-0.570141926
H	2.868798	5.069644	-0.036780	H	2.864515593	5.062793793	-0.036262631
H	4.981140	3.370301	-0.063069	H	4.973047794	3.367430326	-0.063326325
H	5.252137	0.690993	-0.205366	H	5.246445634	0.694256319	-0.204953548
H	0.266882	1.641225	-2.103823	H	0.267012095	1.639834682	-2.098939920
C	3.784385	-1.670616	-0.390405	C	3.781274825	-1.667666317	-0.388826467
C	4.134234	-2.266715	-1.614415	C	4.132776316	-2.263744105	-1.609136764
C	4.539942	-2.006753	0.761899	C	4.537248461	-2.004894396	0.759916202
C	5.198240	-3.169291	-1.709259	C	5.194062543	-3.164251254	-1.704603402
H	3.560665	-1.999308	-2.505011	H	3.560290178	-1.998534307	-2.503396321
C	5.623017	-2.901469	0.653151	C	5.616921990	-2.898553942	0.649987213
C	5.948989	-3.485528	-0.571583	C	5.943319801	-3.481189489	-0.570824615
H	5.445731	-3.616868	-2.674966	H	5.441498826	-3.612682453	-2.671939927
H	6.196409	-3.144302	1.548667	H	6.192192810	-3.143371640	1.546093172
H	6.785420	-4.184940	-0.637079	H	6.781610422	-4.181484856	-0.636030892
C	4.163345	-1.474677	2.106319	C	4.166402259	-1.476354105	2.104639850
O	3.073158	-1.040548	2.430157	O	3.076664137	-1.044424191	2.431578519
O	5.203972	-1.549753	2.998657	O	5.207252292	-1.550564366	2.993805032
H	4.840799	-1.212910	3.841964	H	4.834297405	-1.210354555	3.842055319
C	-3.334396	-1.842489	-0.772419	C	-3.331348686	-1.838945828	-0.770065873
C	-4.110455	-2.257803	0.333526	C	-4.108257279	-2.254361556	0.331988411
C	-3.573924	-2.417223	-2.035442	C	-3.572859715	-2.414047843	-2.029418648
C	-5.109143	-3.227263	0.138652	C	-5.103793465	-3.222455308	0.136931787
C	-4.570596	-3.379679	-2.213334	C	-4.566967923	-3.374252991	-2.207337211
H	-2.967723	-2.090196	-2.883908	H	-2.967191728	-2.089313430	-2.881617202
C	-5.344067	-3.785502	-1.119446	C	-5.339020477	-3.779998381	-1.117193869
H	-5.712362	-3.546954	0.993013	H	-5.708049089	-3.543381332	0.992474727
H	-4.743892	-3.809468	-3.202865	H	-4.739988021	-3.804887403	-3.198475453
H	-6.127956	-4.536068	-1.245711	H	-6.124079512	-4.532270469	-1.243763372
C	-3.871158	-1.706538	1.719038	C	-3.873422209	-1.706527923	1.715299083
H	-3.795190	-2.526987	2.454582	H	-3.798185495	-2.529784266	2.450636866
H	-2.913505	-1.166463	1.779584	H	-2.913858371	-1.166508789	1.777857395
C	-4.959358	-0.772910	2.224128	C	-4.958611330	-0.774782456	2.223661660
O	-5.998590	-0.487230	1.663378	O	-5.999429523	-0.489788691	1.666818505
O	-4.624779	-0.276234	3.452926	O	-4.619732613	-0.278840826	3.449857626
H	-5.360477	0.313986	3.713097	H	-5.365601944	0.313141588	3.710801928



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C	-2.616454	2.623251	-0.536064	C	-2.626337449	2.615652975	-0.536386510
C	-4.003897	2.339832	-0.723561	C	-4.011313091	2.326761516	-0.716525029
H	-4.810281	3.069288	-0.744652	H	-4.819745606	3.056186610	-0.737896580
C	-4.119075	0.960089	-0.872262	C	-4.121919985	0.949625022	-0.856964374
H	-5.031878	0.394192	-1.046218	H	-5.035401996	0.378984837	-1.021930330
C	-2.799110	0.396001	-0.783113	C	-2.801540313	0.390188793	-0.768350054
C	-2.339061	-0.937364	-0.828822	C	-2.336370119	-0.937608942	-0.811948229
C	-0.951236	-1.284060	-0.859971	C	-0.949004744	-1.277284492	-0.840526602
C	-0.385838	-2.602712	-0.950845	C	-0.380531760	-2.591956844	-0.921507536
H	-0.959354	-3.522923	-1.019141	H	-0.952825980	-3.515302216	-0.982876455
C	0.986511	-2.477254	-0.913116	C	0.988314391	-2.462620225	-0.883707053
H	1.722518	-3.276145	-0.956679	H	1.727626636	-3.260952760	-0.918858477
C	1.291831	-1.078387	-0.776324	C	1.289718835	-1.064976327	-0.756139929
C	2.576730	-0.485189	-0.667838	C	2.569609476	-0.468472837	-0.646730250
C	2.837372	0.903336	-0.527765	C	2.821433032	0.915603614	-0.504262867
C	4.116917	1.557250	-0.483475	C	4.094738002	1.576084106	-0.454221274
C	3.884674	2.905663	-0.304168	C	3.856762342	2.920757272	-0.280358267
C	2.462399	3.096986	-0.228890	C	2.437210970	3.108476804	-0.216795774
C	1.771434	4.322778	-0.083069	C	1.745808727	4.329943566	-0.082663531
C	0.377392	4.461622	-0.093066	C	0.355323117	4.464431008	-0.102752066
C	-0.483213	5.615171	-0.091905	C	-0.508629236	5.610678061	-0.102191430
H	-0.150587	6.648224	-0.010247	H	-0.178315117	6.646143246	-0.019269153
C	-1.795004	5.169081	-0.233974	C	-1.815912829	5.159565607	-0.244567416
H	-2.692555	5.781141	-0.283488	H	-2.718415746	5.767642309	-0.291778166
C	-1.741769	3.742988	-0.315064	C	-1.757860514	3.737529752	-0.326800334
N	-1.927000	1.443199	-0.591282	N	-1.936313694	1.440760279	-0.586443334
N	0.094112	-0.381330	-0.750484	N	0.092691625	-0.374468154	-0.737648247
N	1.857439	1.857744	-0.358133	N	1.836960792	1.867735815	-0.341897775
N	-0.434858	3.354907	-0.200909	N	-0.450669229	3.355314731	-0.213963185
Mn	-0.034605	1.480642	-0.303474	Mn	-0.043335002	1.488878125	-0.303506414
H	2.380738	5.225046	0.003146	H	2.354604828	5.234933828	0.003518062
H	4.624086	3.700475	-0.227316	H	4.591850440	3.721556973	-0.200342213
H	5.076705	1.054271	-0.569491	H	5.058960819	1.076806414	-0.533222729

H	0.036206	1.725213	-1.841219	H	0.004825689	1.708175185	-1.845959307
O	-0.239016	1.133635	1.704164	O	-0.298340515	1.122755451	1.702180134
O	0.489908	0.025915	2.293251	O	0.448518610	0.022335442	2.280049651
C	-3.343383	-2.036765	-0.756549	C	-3.331508810	-2.041469371	-0.753552370
C	-4.115352	-2.252126	0.417343	C	-4.108889394	-2.277426228	0.408268028
C	-3.508726	-2.893249	-1.862229	C	-3.485508000	-2.882570893	-1.868064416
C	-5.014362	-3.332978	0.427472	C	-5.000279743	-3.359746054	0.396226729
C	-4.423988	-3.947684	-1.834931	C	-4.391979508	-3.939087103	-1.862591388
H	-2.913094	-2.708384	-2.759668	H	-2.882617058	-2.683109101	-2.759421587
C	-5.178296	-4.170847	-0.678925	C	-5.151910508	-4.180927455	-0.718857402
H	-5.597501	-3.521428	1.333478	H	-5.589691378	-3.561142071	1.297372016
H	-4.543031	-4.591543	-2.709333	H	-4.500168895	-4.572618125	-2.747778789
H	-5.889483	-4.998962	-0.633543	H	-5.860814463	-5.013542494	-0.689124318
C	-4.063065	-1.365531	1.656637	C	-4.069444037	-1.416273179	1.661419464
H	-4.424811	-1.956303	2.514624	H	-4.428397820	-2.029688230	2.506374751
H	-4.747832	-0.510620	1.543219	H	-4.769171463	-0.569987340	1.562305927
C	-2.689399	-0.828023	2.035572	C	-2.706631621	-0.865925180	2.054338541
O	-1.701113	-1.563590	2.129969	O	-1.715766208	-1.597937788	2.160547795
O	-2.667738	0.482375	2.246216	O	-2.690461719	0.440883208	2.260150821
H	-1.681415	0.818489	2.170196	H	-1.692297875	0.788614833	2.157890396
H	-0.212086	-0.692196	2.310117	H	-0.268651554	-0.696540690	2.320268428
C	3.751530	-1.416645	-0.645796	C	3.747770036	-1.390658772	-0.650988013
C	4.481595	-1.673090	-1.817569	C	4.450120665	-1.628243312	-1.840041733
C	4.099955	-2.104008	0.542335	C	4.131403396	-2.090701847	0.514266597
C	5.543155	-2.585736	-1.812379	C	5.511721381	-2.533475232	-1.876924214
H	4.202706	-1.159036	-2.740730	H	4.145814552	-1.101444813	-2.749861257
C	5.140615	-3.044231	0.529617	C	5.173456099	-3.023520822	0.459841982
C	5.871264	-3.275099	-0.638884	C	5.871815429	-3.237061451	-0.726113127
H	6.105086	-2.767473	-2.731657	H	6.050757915	-2.698360951	-2.814978106
H	5.370677	-3.584618	1.450692	H	5.426441647	-3.575911655	1.369737878
H	6.692399	-3.995536	-0.635789	H	6.695083289	-3.956877986	-0.754113655
C	3.312868	-1.883725	1.804605	C	3.402897011	-1.903005282	1.811887666
O	2.866679	-2.785474	2.491895	O	3.023992286	-2.820715389	2.516145200
O	3.155975	-0.565227	2.052139	O	3.223050955	-0.592511532	2.090000823
H	2.332438	-0.406021	2.576968	H	2.475932985	-0.490860242	2.734453378



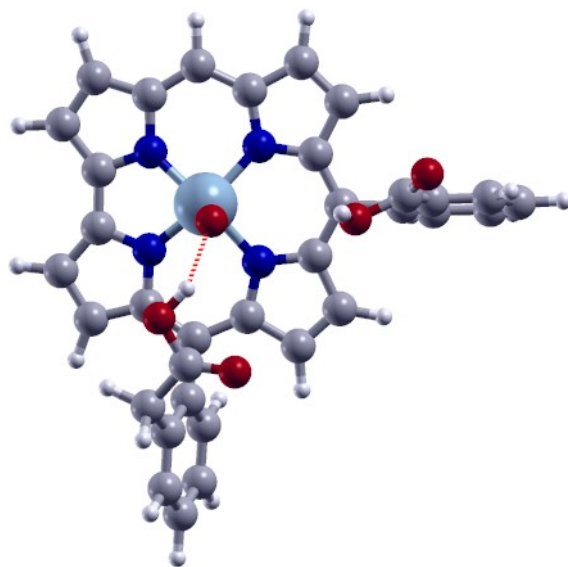
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C	-2.180011	3.058375	-0.225542
C	-3.606506	2.982213	-0.181273
H	-4.288282	3.813177	-0.015855
C	-3.947471	1.647582	-0.386437
H	-4.949992	1.226238	-0.424098
C	-2.728708	0.903868	-0.569913
C	-2.484377	-0.463081	-0.814820
C	-1.180242	-0.990455	-1.063716
C	-0.842227	-2.360044	-1.351357
H	-1.561483	-3.161277	-1.497791
C	0.530606	-2.457102	-1.364619
H	1.126953	-3.350167	-1.532030
C	1.061326	-1.149550	-1.077142
C	2.422399	-0.801968	-0.861863
C	2.923851	0.517281	-0.688078
C	4.291240	0.935666	-0.528811
C	4.287364	2.305870	-0.359754
C	2.919578	2.744875	-0.377520
C	2.439797	4.058724	-0.155294
C	1.087633	4.419409	-0.077149
C	0.416567	5.677913	0.130029
H	0.908294	6.639190	0.266189
C	-0.953972	5.435993	0.123036
H	-1.747668	6.167628	0.255071
C	-1.127699	4.030267	-0.088249
N	-1.691562	1.800642	-0.463672
N	-0.003005	-0.276537	-0.945728
N	2.120123	1.636281	-0.597273
N	0.109093	3.461707	-0.197540
Mn	0.208452	1.566062	-0.433570
H	3.191789	4.839155	-0.019442
H	5.148052	2.955485	-0.212740
H	5.153273	0.273645	-0.539676

E= -902.6903764706 Ry (\*OOH)

C	-2.175972850	3.065852818	-0.200356985
C	-3.598081912	2.990600313	-0.152516297
H	-4.277766279	3.823148884	0.024060193
C	-3.941611201	1.661722678	-0.369469775
H	-4.946826083	1.242830758	-0.409105636
C	-2.728641164	0.917502123	-0.562321364
C	-2.490021479	-0.444410174	-0.817009804
C	-1.188733634	-0.970861937	-1.063188988
C	-0.850747238	-2.336503860	-1.351561648
H	-1.571554911	-3.136590626	-1.507723936
C	0.518376085	-2.436297714	-1.351326802
H	1.114294754	-3.331780628	-1.516816110
C	1.050174180	-1.134436173	-1.055538437
C	2.409382996	-0.791253304	-0.842747963
C	2.912166418	0.524916880	-0.676658762
C	4.277061951	0.942379076	-0.512537013
C	4.274259802	2.310146031	-0.353979807
C	2.910332078	2.750087146	-0.382608962
C	2.433433650	4.061910580	-0.160641402
C	1.086285540	4.420774788	-0.072928139
C	0.418307876	5.675611064	0.143981291
H	0.913974385	6.636912295	0.277552400
C	-0.948849699	5.434762543	0.151175799
H	-1.742297492	6.167015781	0.294136198
C	-1.126003097	4.033054124	-0.062986072
N	-1.689602336	1.810986274	-0.448694437
N	-0.013338491	-0.262481291	-0.932714532
N	2.114077036	1.644890910	-0.600423678
N	0.106611424	3.464985888	-0.184192927
Mn	0.202615080	1.575652245	-0.427627911
H	3.187834528	4.842978772	-0.026394519
H	5.133831756	2.962561951	-0.202703777
H	5.139947716	0.278876137	-0.511596295

H	0.164911	1.881625	-1.965945	H	0.182822917	1.888169377	-1.961118774
O	0.238017	1.040675	1.485304	O	0.295609055	1.035447396	1.488400800
C	-3.609859	-1.445200	-0.752438	C	-3.613651179	-1.423849201	-0.757061677
C	-4.106395	-1.928703	0.486672	C	-4.098863732	-1.917376677	0.479039245
C	-4.140480	-1.942188	-1.957114	C	-4.157074179	-1.907970546	-1.956786408
C	-5.113082	-2.910998	0.453936	C	-5.104164095	-2.895380539	0.449253111
C	-5.154924	-2.903189	-1.963119	C	-5.168932817	-2.866124052	-1.960222459
H	-3.742658	-1.558873	-2.900237	H	-3.768468435	-1.516957847	-2.902739079
C	-5.638612	-3.394819	-0.747227	C	-5.639832972	-3.366831210	-0.747488567
H	-5.492366	-3.303486	1.401719	H	-5.474792827	-3.293585081	1.400324875
H	-5.556892	-3.268769	-2.910825	H	-5.579222679	-3.224366650	-2.908935815
H	-6.421617	-4.156663	-0.730398	H	-6.423293256	-4.129989897	-0.728963299
C	-3.674914	-1.404775	1.851240	C	-3.653820606	-1.408653299	1.840615645
H	-4.011426	-2.126156	2.612660	H	-4.008651271	-2.125946211	2.600036614
H	-4.185297	-0.449876	2.053859	H	-4.143364315	-0.441578024	2.047130266
C	-2.175981	-1.186238	2.078308	C	-2.151005095	-1.227952069	2.067575986
O	-1.363168	-2.113769	2.036522	O	-1.361922550	-2.174011996	2.025613714
O	-1.900827	0.079229	2.345486	O	-1.844165014	0.029794053	2.334149902
H	-0.908280	0.354958	2.176116	H	-0.843634907	0.289954528	2.167151035
C	3.358940	-1.945041	-0.638232	C	3.344672812	-1.933961127	-0.637204974
C	4.372029	-2.288725	-1.546363	C	4.364741141	-2.249456099	-1.543126684
C	3.193616	-2.724013	0.534555	C	3.174489861	-2.745501672	0.509258312
C	5.205322	-3.386989	-1.301829	C	5.196937007	-3.348401506	-1.323650718
H	4.488158	-1.700679	-2.460137	H	4.486814629	-1.634423930	-2.440360667
C	4.020111	-3.830759	0.766082	C	3.999427053	-3.854522215	0.714342245
C	5.028534	-4.158118	-0.147868	C	5.013527721	-4.151841897	-0.197493266
H	5.986404	-3.645935	-2.020451	H	5.983810219	-3.584227066	-2.046283243
H	3.878967	-4.429490	1.668890	H	3.851917762	-4.478795606	1.601395293
H	5.674285	-5.018538	0.041952	H	5.660783008	-5.016909902	-0.026840788
C	2.157334	-2.292557	1.545396	C	2.137420458	-2.350382688	1.529756578
O	2.276350	-1.264120	2.201498	O	2.236945805	-1.328426828	2.199327680
O	1.119757	-3.128923	1.618962	O	1.120279754	-3.209279070	1.608791956
H	0.333242	-2.674374	2.043548	H	0.320866299	-2.760796182	2.037543928
O	1.349916	1.404439	2.325322	O	1.434280642	1.357589993	2.308398650
H	1.792727	0.525586	2.412461	H	1.849608399	0.453466389	2.385446681

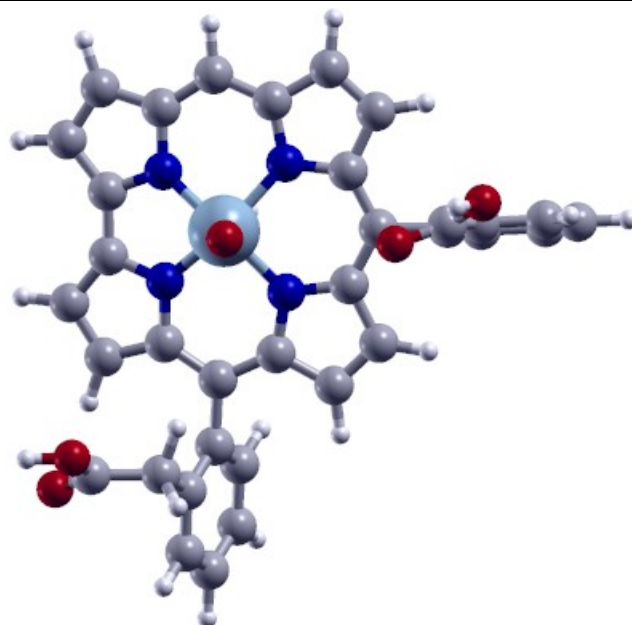




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C	-3.930587570	2.564485512	-0.584440111
H	-4.691589087	3.341406843	-0.653469192
C	-4.126120184	1.191204337	-0.633553814
H	-5.073923026	0.666349028	-0.751030704
C	-2.843617310	0.559273220	-0.530652514
C	-2.481259537	-0.794962479	-0.583225217
C	-1.127297123	-1.213030110	-0.638612685
C	-0.651415049	-2.557951005	-0.820506487
H	-1.289193448	-3.433747827	-0.918591333
C	0.717522700	-2.513636237	-0.838612154
H	1.406829128	-3.348048948	-0.952993048
C	1.103911623	-1.141089318	-0.657258299
C	2.411961203	-0.627057483	-0.582946011
C	2.736990554	0.740672842	-0.473257492
C	4.054325498	1.309096983	-0.512988806
C	3.917625560	2.671479554	-0.398612150
C	2.519485737	2.957284354	-0.284781146
C	1.931093548	4.230828940	-0.206163368
C	0.557215020	4.439575504	-0.198612341
C	-0.230483155	5.633604918	-0.257332785
H	0.167894143	6.648007104	-0.251258912
C	-1.564841304	5.258914998	-0.342935344
H	-2.428231664	5.919164235	-0.412824584
C	-1.597932418	3.837644101	-0.328366749
N	-1.904873699	1.559315740	-0.394496554
N	-0.036660401	-0.378734858	-0.533087463
N	1.820430829	1.765720557	-0.319666155
N	-0.312445029	3.366561135	-0.206346693
Mn	-0.060150190	1.507387152	0.068860733
H	2.597950785	5.096769571	-0.202854731
H	4.703509738	3.426535742	-0.408138316
H	4.977048279	0.741785017	-0.624832078
H	0.019067157	1.383890219	-1.553013081
O	-0.000920674	1.037085599	1.603103461
C	-3.549864952	-1.834541346	-0.601865429
C	-4.274481064	-2.169688906	0.566866625
C	-3.824603899	-2.509190583	-1.801367656
C	-5.236977347	-3.185292284	0.483607967
C	-4.800592388	-3.502204672	-1.866875901
H	-3.260654606	-2.235360710	-2.698924510
C	-5.507412484	-3.844801957	-0.714786149
H	-5.789640370	-3.462262648	1.388138234
H	-5.005649113	-4.006687322	-2.816150356
H	-6.271464608	-4.627314573	-0.745942511
C	-4.085872038	-1.452766365	1.888753676
H	-4.595987855	-2.032433892	2.677808109
H	-4.561649344	-0.458522160	1.855103140
C	-2.637928008	-1.285985329	2.334477696
O	-1.823563105	-2.187131610	2.388695683
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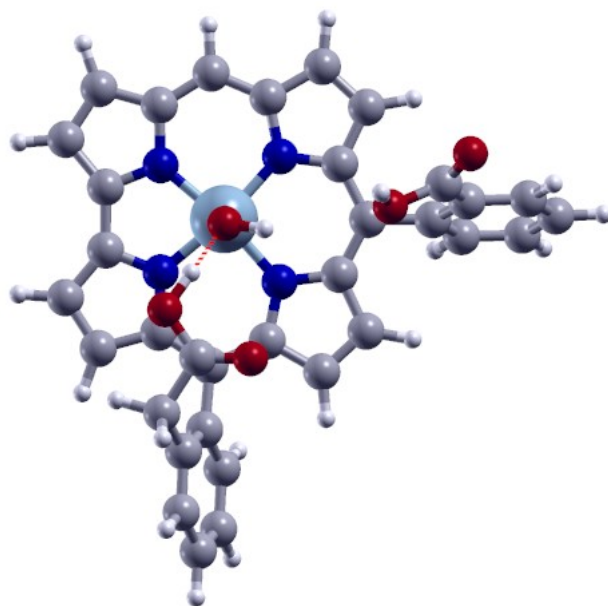


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	C	4.954986387	-2.970111827	-2.126866218
	H	3.267240365	-1.806219725	-2.808295752
	C	5.444836889	-2.825704372	0.226474030
	C	5.747818132	-3.328191696	-1.034699412
	H	5.182609552	-3.355762119	-3.126052458
	H	6.050742429	-3.087423386	1.099471514
	H	6.601967646	-3.999032003	-1.166090834
	C	4.108571640	-1.540164255	1.834882378
	O	4.974300431	-1.522695640	2.694190334
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	H	2.775469609	-0.933782824	3.030168984



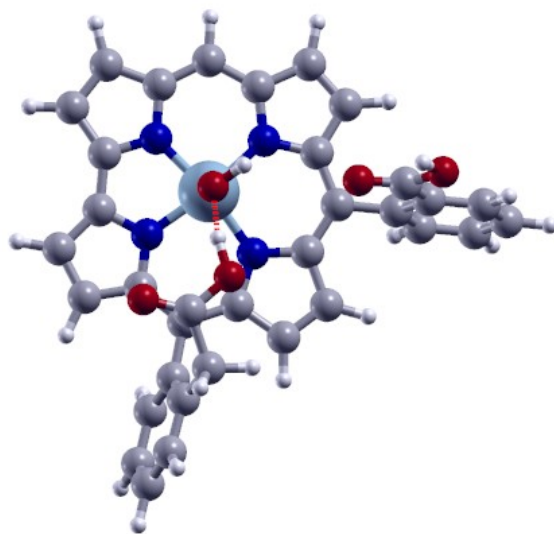
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C	-3.704569	2.449322	-0.853371	C	-3.696997542	2.434458125	-0.864309020
H	-4.457349	3.211585	-1.041455	H	-4.453287695	3.194088685	-1.057111223
C	-3.899216	1.071677	-0.822791	C	-3.888977239	1.059897330	-0.828225258
H	-4.835127	0.537026	-0.969700	H	-4.826674395	0.525264568	-0.973152908
C	-2.626494	0.455799	-0.568664	C	-2.619543176	0.446653977	-0.569848983
C	-2.243915	-0.895269	-0.555661	C	-2.239234166	-0.902105323	-0.547807823
C	-0.881051	-1.288764	-0.472494	C	-0.878061251	-1.290766553	-0.463542150
C	-0.380648	-2.635834	-0.546016	C	-0.373360488	-2.632528817	-0.532915604
H	-1.001449	-3.524271	-0.630095	H	-0.990216221	-3.526017257	-0.613820751
C	0.992916	-2.570298	-0.501600	C	0.996258302	-2.563493436	-0.490445822
H	1.696132	-3.398796	-0.529021	H	1.700259150	-3.393456419	-0.515392128
C	1.355841	-1.183095	-0.393242	C	1.357731488	-1.179331972	-0.386267318
C	2.669298	-0.668307	-0.321591	C	2.668795327	-0.664846553	-0.315773624
C	3.002589	0.703597	-0.256889	C	2.996992248	0.705475545	-0.251930616
C	4.322326	1.284943	-0.304522	C	4.311227272	1.291424138	-0.297050758
C	4.165629	2.651056	-0.264235	C	4.151298658	2.653381513	-0.256464125
C	2.751673	2.921222	-0.205312	C	2.740495156	2.920433504	-0.200878109

C	2.133116	4.185793	-0.263831	C	2.120595765	4.179990433	-0.261798770
C	0.753038	4.377308	-0.360515	C	0.744148604	4.367402763	-0.364355455
C	-0.032126	5.561705	-0.573492	C	-0.041251940	5.546703641	-0.581916316
H	0.364893	6.573198	-0.635219	H	0.353848171	6.560365927	-0.643552134
C	-1.362212	5.175073	-0.700282	C	-1.367112184	5.158451927	-0.713167991
H	-2.218408	5.819899	-0.884924	H	-2.223274395	5.804357127	-0.902916458
C	-1.396189	3.756078	-0.549636	C	-1.399209011	3.742933591	-0.561313979
N	-1.695394	1.466485	-0.409851	N	-1.692079703	1.457891155	-0.416311709
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N	2.076077	1.718837	-0.184749	N	2.070605942	1.717832172	-0.180496321
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Mn	0.129678	1.467956	0.109780	Mn	0.128714978	1.463920671	0.111839551
H	2.784006	5.062095	-0.297662	H	2.770151302	5.059121486	-0.294916701
H	4.942969	3.412073	-0.300473	H	4.928852850	3.416648157	-0.289856137
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H	0.481395	1.432987	-1.492332	H	0.484765409	1.422470990	-1.493155853
C	3.802222	-1.638744	-0.454441	C	3.802894809	-1.630713650	-0.452619739
C	4.077821	-2.163134	-1.729199	C	4.075035448	-2.153636354	-1.725465817
C	4.643205	-2.009803	0.624167	C	4.650556223	-2.000503976	0.617592457
C	5.155413	-3.028805	-1.941950	C	5.150898617	-3.014303694	-1.944418725
H	3.437283	-1.869377	-2.563975	H	3.430062865	-1.862723072	-2.560076019
C	5.735335	-2.869597	0.397278	C	5.740713640	-2.855840838	0.383968642
C	5.990290	-3.381214	-0.875818	C	5.990562726	-3.365121129	-0.886803439
H	5.345850	-3.420459	-2.944123	H	5.336530409	-3.405579622	-2.949470451
H	6.372779	-3.142178	1.239336	H	6.385350495	-3.128527650	1.222782631
H	6.836301	-4.053581	-1.034501	H	6.839201267	-4.036081060	-1.050097423
C	4.338706	-1.547617	2.010782	C	4.357707364	-1.543569453	2.005970641
O	3.270472	-1.111884	2.396929	O	3.288563000	-1.121370039	2.403677710
O	5.412527	-1.689531	2.852676	O	5.439854545	-1.671466843	2.836195087
H	5.093175	-1.387289	3.726363	H	5.114821886	-1.369001981	3.718069371
C	-3.290491	-1.948572	-0.725411	C	-3.284213034	-1.954769174	-0.713718935
C	-4.174547	-2.293818	0.322077	C	-4.175925283	-2.291396726	0.326370279
C	-3.398664	-2.607927	-1.965554	C	-3.386632213	-2.623982152	-1.945547087
C	-5.145635	-3.283235	0.091538	C	-5.143035911	-3.280545463	0.097447074
C	-4.372283	-3.586027	-2.178991	C	-4.356742350	-3.600742672	-2.157781973
H	-2.711240	-2.332400	-2.769135	H	-2.693369788	-2.357406880	-2.749477226
C	-5.251580	-3.925061	-1.143779	C	-5.241469033	-3.930856611	-1.129606844
H	-5.830998	-3.551393	0.900421	H	-5.834705055	-3.542904255	0.905294704
H	-4.445462	-4.079819	-3.150896	H	-4.422975102	-4.102648043	-3.127903129
H	-6.017688	-4.688537	-1.298157	H	-6.008175213	-4.696508576	-1.283361786
C	-4.082568	-1.650621	1.685673	C	-4.097277372	-1.642446995	1.683708221
H	-4.098875	-2.420417	2.477322	H	-4.123942937	-2.409238547	2.480398099
H	-3.132698	-1.110219	1.820522	H	-3.145297741	-1.104084552	1.825673444
C	-5.211711	-0.681564	1.999476	C	-5.222552297	-0.668761494	1.985658777
O	-6.172258	-0.427058	1.300150	O	-6.171897830	-0.405830523	1.274533805
O	-5.019555	-0.111516	3.225476	O	-5.043237841	-0.104019073	3.214284834
H	-5.771263	0.500320	3.359306	H	-5.802592267	0.515651473	3.335845200
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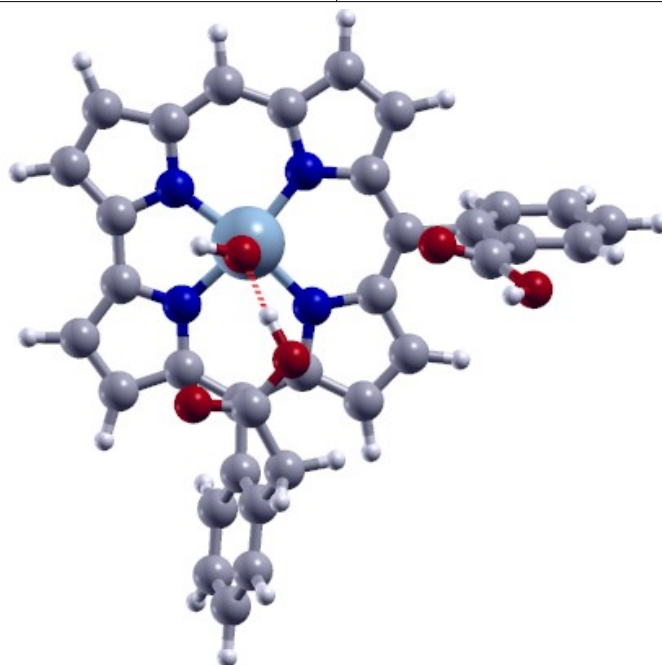
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C	-4.205260	1.006516	-0.731359
H	-5.137581	0.456262	-0.839040
C	-2.896184	0.412077	-0.662190
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C	-1.093435	-1.319873	-0.707141
C	-0.574706	-2.660895	-0.756760
H	-1.182281	-3.561339	-0.774813
C	0.800127	-2.580025	-0.741461
H	1.508203	-3.404570	-0.753284
C	1.152060	-1.186039	-0.666417
C	2.451457	-0.628117	-0.561861
C	2.757089	0.756472	-0.435304
C	4.056625	1.376052	-0.418484
C	3.862399	2.737851	-0.298219
C	2.446171	2.973782	-0.247219
C	1.790098	4.227057	-0.172804
C	0.401955	4.412035	-0.205308
C	-0.425521	5.591054	-0.233444
H	-0.063125	6.616064	-0.183720
C	-1.749986	5.178756	-0.348364
H	-2.630729	5.814282	-0.403590
C	-1.737899	3.747768	-0.386733
N	-1.993488	1.444191	-0.557276
N	-0.020938	-0.450785	-0.652061
N	1.807257	1.748351	-0.322395
N	-0.443363	3.329284	-0.281828
Mn	-0.101319	1.440930	-0.270849
H	2.427942	5.112041	-0.117773
H	4.625205	3.513071	-0.259611
H	5.005000	0.850555	-0.499114

H	-0.010963	1.608490	-1.827131
O	-0.189106	1.155324	1.676967
C	3.607585	-1.572057	-0.634049
C	4.463206	-1.850915	0.461895
C	3.893944	-2.167978	-1.876672
C	5.582551	-2.684244	0.275839
C	4.997472	-3.009237	-2.043472
H	3.243251	-1.943475	-2.724975
C	5.849985	-3.265137	-0.963231
H	6.228818	-2.869361	1.136119
H	5.195735	-3.454936	-3.021180
H	6.718349	-3.916145	-1.085321
C	4.271056	-1.342350	1.858128
O	5.166596	-1.276325	2.683982
O	2.985576	-1.001425	2.152068
H	2.998784	-0.708634	3.086573
H	0.424063	0.452543	1.956395
C	-3.498759	-2.008074	-0.551229
C	-4.215467	-2.211279	0.658557
C	-3.735116	-2.850910	-1.653808
C	-5.138594	-3.271091	0.704102
C	-4.673288	-3.883876	-1.588729
H	-3.176680	-2.675282	-2.576867
C	-5.375916	-4.096595	-0.398535
H	-5.681001	-3.451718	1.636565
H	-4.849401	-4.519035	-2.459936
H	-6.104084	-4.907883	-0.324160
C	-4.064817	-1.332979	1.891816
H	-4.686332	-0.429124	1.790436
H	-4.447503	-1.893266	2.760467
C	-2.631039	-0.900199	2.226990
O	-1.709459	-1.701177	2.338654
O	-2.521773	0.420328	2.371159
H	-1.521107	0.710808	2.232668



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H	-4.863412	3.168896	-0.299983	H	-4.848351524	3.174989224	-0.271619465
C	-4.223874	1.051869	-0.499472	C	-4.213816677	1.058704012	-0.486387744
H	-5.158084	0.497673	-0.541689	H	-5.151410074	0.506637802	-0.523588863
C	-2.909433	0.463399	-0.547466	C	-2.904115861	0.468206436	-0.546281939
C	-2.479060	-0.875582	-0.645435	C	-2.479028697	-0.868897028	-0.649242876
C	-1.101029	-1.248606	-0.737926	C	-1.104604911	-1.242901328	-0.750997895
C	-0.579236	-2.575631	-0.930382	C	-0.585209555	-2.567944155	-0.937696584
H	-1.187411	-3.467756	-1.061792	H	-1.195352344	-3.461858437	-1.060566000
C	0.796772	-2.488717	-0.924798	C	0.787449891	-2.483969561	-0.933763846
H	1.509401	-3.301455	-1.041864	H	1.498852820	-3.300713324	-1.045084336
C	1.140989	-1.103082	-0.734275	C	1.135720498	-1.101724394	-0.751015398
C	2.437807	-0.539657	-0.628983	C	2.432078087	-0.543942653	-0.641727915
C	2.741258	0.842447	-0.476472	C	2.737524541	0.835016767	-0.491860107
C	4.036373	1.466721	-0.492430	C	4.030897776	1.456836359	-0.497575473
C	3.842772	2.825584	-0.332545	C	3.839418517	2.812197689	-0.335938858
C	2.429469	3.054553	-0.220646	C	2.429587274	3.043722602	-0.232579902
C	1.768767	4.301171	-0.090756	C	1.773232658	4.287563224	-0.094091488
C	0.378746	4.475695	-0.069149	C	0.387263391	4.463763049	-0.066564771
C	-0.461069	5.646613	-0.005389	C	-0.448280884	5.632735201	0.010604797
H	-0.106346	6.672611	0.071928	H	-0.089603536	6.658416564	0.095941685
C	-1.784213	5.224038	-0.071840	C	-1.769714409	5.214192371	-0.051344525
H	-2.673329	5.849943	-0.052553	H	-2.658834575	5.842366274	-0.020302420
C	-1.759737	3.794364	-0.174536	C	-1.749183043	3.788739525	-0.165893779
N	-2.006216	1.493757	-0.428124	N	-1.999850292	1.494913853	-0.429330891
N	-0.033825	-0.381601	-0.636829	N	-0.036488751	-0.379703832	-0.657554126
N	1.792474	1.825995	-0.297965	N	1.792319769	1.819266376	-0.318402133
N	-0.458231	3.389340	-0.159106	N	-0.450991305	3.381659327	-0.160074276
Mn	-0.110661	1.500144	-0.199425	Mn	-0.107344264	1.496708307	-0.217007991
H	2.402649	5.188709	-0.030195	H	2.410009093	5.174698837	-0.027228077
H	4.603719	3.603254	-0.306588	H	4.601813509	3.590226879	-0.298940954
H	4.982335	0.945751	-0.620529	H	4.979080835	0.934751094	-0.617885635
H	-0.060191	1.708462	-1.754975	H	-0.058800775	1.711811309	-1.770864586
O	-0.132972	1.194250	1.735223	O	-0.114482933	1.172440192	1.721492529
C	3.597381	-1.477078	-0.754229	C	3.587446900	-1.483738126	-0.753632663
C	3.955826	-1.925198	-2.036801	C	3.952175469	-1.940311057	-2.027670745
C	4.356536	-1.922957	0.358084	C	4.338324572	-1.924029197	0.362919255
C	5.042653	-2.784516	-2.227872	C	5.034117044	-2.802078152	-2.207331496
H	3.371159	-1.580329	-2.892686	H	3.372729317	-1.599175186	-2.890794627
C	5.450029	-2.787271	0.153158	C	5.427656411	-2.790716384	0.168601717
C	5.794348	-3.215623	-1.129382	C	5.777063319	-3.227371070	-1.105620660
H	5.301849	-3.114022	-3.236928	H	5.296443620	-3.138764843	-3.214882747
H	6.021845	-3.125186	1.017961	H	5.995509117	-3.125657442	1.039185155
H	6.644524	-3.886577	-1.270258	H	6.627107510	-3.902935487	-1.237428816
C	3.980710	-1.512250	1.743741	C	3.960579227	-1.506302154	1.743820437
O	3.013761	-0.839374	2.055696	O	2.994162745	-0.829777166	2.049389419
O	4.856671	-1.988520	2.683310	O	4.829894797	-1.977910197	2.688728539
H	4.506525	-1.677390	3.541810	H	4.467488068	-1.654340264	3.548097803

C	-3.517876	-1.947184	-0.604434	C	-3.519216471	-1.935020110	-0.600532681
C	-3.704282	-2.756543	0.547810	C	-3.702152229	-2.741971832	0.549905431
C	-4.363588	-2.111379	-1.717631	C	-4.370607743	-2.098505643	-1.705298400
C	-4.745514	-3.701216	0.525212	C	-4.744201039	-3.680707976	0.533842908
C	-5.379948	-3.070380	-1.721304	C	-5.387421322	-3.051238762	-1.702487905
H	-4.205035	-1.476820	-2.593341	H	-4.217021605	-1.464125609	-2.583932386
C	-5.571943	-3.868691	-0.589763	C	-5.575138157	-3.846117556	-0.572647872
H	-4.912332	-4.315462	1.414742	H	-4.905614002	-4.295031437	1.426331248
H	-6.018967	-3.187091	-2.599704	H	-6.032452254	-3.165923378	-2.578563541
H	-6.369272	-4.615610	-0.568945	H	-6.374661115	-4.592506403	-0.546444687
C	-2.828699	-2.673284	1.787878	C	-2.824259831	-2.665453148	1.783882540
H	-3.367582	-3.150160	2.622315	H	-3.367471911	-3.137581152	2.620395454
H	-1.897671	-3.241347	1.631235	H	-1.901181866	-3.248726917	1.624578659
C	-2.460874	-1.249076	2.233708	C	-2.437552512	-1.248665637	2.230719278
O	-3.300460	-0.394393	2.475597	O	-3.271591053	-0.389643292	2.477743061
O	-1.136677	-1.090235	2.307202	O	-1.115266368	-1.098202983	2.300025275
H	-0.839197	-0.095939	2.244944	H	-0.803767622	-0.094263010	2.219389104
H	0.763732	1.190865	2.113879	H	0.799279093	1.131033189	2.078778913



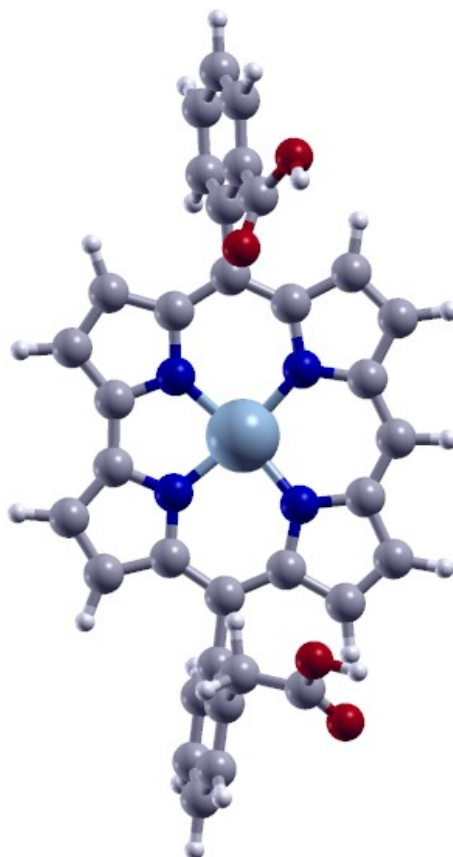
E= -2006.9208212 a.u (*OH)			
C	-2.791799	2.592037	-0.414497
C	-4.177251	2.238509	-0.506151
H	-5.019158	2.925073	-0.457125
C	-4.232072	0.856816	-0.636986
H	-5.124718	0.239728	-0.700105
C	-2.877389	0.361745	-0.648593
C	-2.347047	-0.945045	-0.716285
C	-0.944571	-1.221511	-0.756100
C	-0.330245	-2.494182	-1.006592
H	-0.872852	-3.414232	-1.211889
C	1.038523	-2.315695	-0.968281
H	1.805469	-3.068957	-1.131995
C	1.285515	-0.929842	-0.678514

C	2.542285	-0.286588	-0.523820
C	2.737221	1.099101	-0.284502
C	3.984693	1.805379	-0.154148
C	3.685915	3.134884	0.061272
C	2.254104	3.266311	0.064899
C	1.507811	4.461552	0.199421
C	0.109793	4.554813	0.121985
C	-0.802423	5.669894	0.145363
H	-0.519785	6.712627	0.277345
C	-2.089079	5.171483	-0.042107
H	-3.012749	5.743877	-0.085323
C	-1.968838	3.750779	-0.179678
N	-2.052260	1.450811	-0.521953
N	0.064562	-0.291670	-0.566516
N	1.710513	2.007082	-0.132314
N	-0.648504	3.424252	-0.061796
Mn	-0.164088	1.562360	-0.137196
H	2.079031	5.381400	0.343821
H	4.386169	3.956142	0.201411
H	4.970153	1.350051	-0.213278
H	-0.101776	1.856057	-1.679957
O	-0.421567	1.279745	1.778051
C	3.761906	-1.133394	-0.713829
C	4.431417	-1.072957	-1.947571
C	4.239596	-2.029804	0.273804
C	5.544778	-1.879376	-2.207118
H	4.057509	-0.390107	-2.713987
C	5.349941	-2.849367	-0.002577
C	6.003674	-2.773544	-1.233742
H	6.047581	-1.812658	-3.174911
H	5.701346	-3.536099	0.768719
H	6.869689	-3.409000	-1.431657
C	3.608766	-2.054098	1.627254
O	2.917195	-1.171684	2.099308
O	3.914487	-3.193366	2.324072
H	3.471187	-3.090650	3.190206
C	-3.303146	-2.089840	-0.708163
C	-3.424296	-2.948806	0.417370
C	-4.139960	-2.280093	-1.824534
C	-4.392908	-3.966387	0.365341
C	-5.081125	-3.312083	-1.858555
H	-4.031397	-1.608426	-2.679864
C	-5.208646	-4.158993	-0.753530
H	-4.511025	-4.619580	1.234686
H	-5.712061	-3.448367	-2.739948
H	-5.947641	-4.963908	-0.756171
C	-2.555732	-2.840713	1.660571
H	-3.055948	-3.385251	2.477756
H	-1.584241	-3.330880	1.488085
C	-2.295881	-1.410050	2.155305
O	-3.197970	-0.615737	2.387008
O	-0.991352	-1.160874	2.285612
H	-0.806422	-0.137148	2.253270



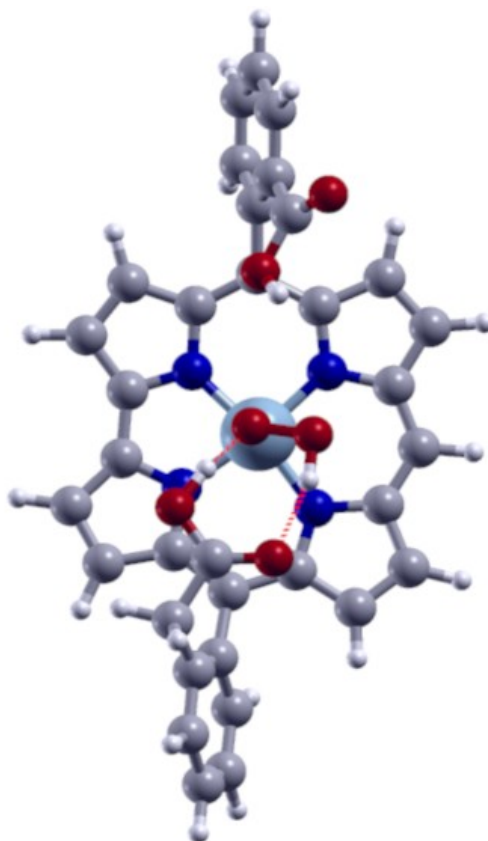
H	-1.013872	1.927711	2.196167	
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**Table S7:** Structures, energies, and coordinates of the complexes with the substituent R2=C<sub>6</sub>H<sub>4</sub>-CH<sub>2</sub>-COOH, R3=C<sub>6</sub>H<sub>4</sub>-COOH.



E= -1931.1633634 Ry (*)				E= -837.1555270225 Ry (*)			
C	-0.454880	2.765811	0.435541	C	-0.450957146	2.757135074	0.438508891
C	-1.511127	3.654677	0.771406	C	-1.504417318	3.644076008	0.773495404
H	-1.399252	4.660052	1.171630	H	-1.395088763	4.651800284	1.172946291
C	-2.710434	2.989150	0.506577	C	-2.701037171	2.981017799	0.509059151
H	-3.717229	3.374222	0.653307	H	-3.708101197	3.369793269	0.656758440
C	-2.392486	1.684481	0.002106	C	-2.386276486	1.678914588	0.005421811
C	-3.213919	0.600367	-0.385475	C	-3.208761078	0.598436538	-0.381251392
C	-2.678933	-0.636223	-0.808751	C	-2.672662450	-0.633841743	-0.804079161
C	-3.410191	-1.800180	-1.228935	C	-3.398774658	-1.796775322	-1.224780933
H	-4.495115	-1.869792	-1.267490	H	-4.484758301	-1.871493469	-1.264606517
C	-2.497655	-2.785716	-1.542922	C	-2.486643969	-2.778056887	-1.538273094
H	-2.710385	-3.794509	-1.892176	H	-2.700024084	-3.787786748	-1.888631912
C	-1.181979	-2.253476	-1.330410	C	-1.174692114	-2.245220425	-1.326340565
C	0.046699	-2.899939	-1.524988	C	0.051566944	-2.887928566	-1.521578453
C	1.320081	-2.357384	-1.299088	C	1.321947007	-2.347574245	-1.296628063
C	2.590850	-2.995504	-1.486120	C	2.589494733	-2.984681970	-1.484181116
C	3.572511	-2.088751	-1.143507	C	3.569714884	-2.081849845	-1.140824287
C	2.930744	-0.872746	-0.727170	C	2.932132679	-0.867992756	-0.723278402
C	3.551406	0.311776	-0.272808	C	3.552942589	0.312158984	-0.268193109
C	2.817536	1.465604	0.082439	C	2.816759472	1.461846633	0.086442090
C	3.227748	2.734549	0.610041	C	3.222480773	2.728421178	0.614252849
H	4.255779	3.028470	0.810020	H	4.250832716	3.026389833	0.815716508

C	2.081893	3.499825	0.836484	C	2.078541799	3.490292596	0.839982027
H	2.042083	4.507053	1.245467	H	2.040613334	4.499480883	1.248683599
C	0.966473	2.706370	0.456029	C	0.966657165	2.698108288	0.459484472
N	-1.016918	1.585039	-0.026090	N	-1.013180695	1.579444781	-0.023687297
N	-1.311262	-0.942341	-0.876260	N	-1.306625391	-0.937162095	-0.873170535
N	1.547645	-1.063583	-0.834059	N	1.550979232	-1.057110319	-0.831855561
N	1.441919	1.485620	0.001952	N	1.443443024	1.480661942	0.005024638
Mn	0.167134	0.236886	-0.643605	Mn	0.170359133	0.235430131	-0.637641791
H	4.648603	-2.244693	-1.174391	H	4.646533617	-2.241922842	-1.173263583
H	2.727419	-4.015176	-1.841639	H	2.727410076	-4.004742197	-1.842255729
H	0.204549	0.730904	-2.100576	H	0.208496182	0.731270181	-2.089228069
C	-4.698286	0.787969	-0.357359	C	-4.691021156	0.788382300	-0.357681757
C	-5.507345	0.234429	0.661403	C	-5.508400306	0.234627523	0.650556384
C	-5.300384	1.560979	-1.369148	C	-5.286050776	1.566178495	-1.366118380
C	-6.894565	0.457142	0.625449	C	-6.891070689	0.464677131	0.608366721
C	-6.680841	1.772927	-1.391348	C	-6.661847690	1.784209022	-1.394800123
H	-4.666201	1.988333	-2.149818	H	-4.647624660	1.996674050	-2.144289682
C	-7.482915	1.214976	-0.388938	C	-7.470374404	1.227655058	-0.402026047
H	-7.521871	0.025595	1.410409	H	-7.525846986	0.031974820	1.389230242
H	-7.128487	2.369904	-2.189548	H	-7.103073638	2.387684541	-2.194035324
H	-8.564204	1.371555	-0.395895	H	-8.552804175	1.389890757	-0.413599030
C	-4.913657	-0.558278	1.801659	C	-4.930412180	-0.564803373	1.789000414
H	-5.270332	-0.167917	2.771367	H	-5.281161815	-0.167070784	2.759900801
H	-3.816959	-0.463757	1.831046	H	-3.830584994	-0.485873616	1.818335539
C	-5.245815	-2.041479	1.783446	C	-5.279941422	-2.041691461	1.775196187
O	-5.954658	-2.624611	0.987554	O	-5.974852957	-2.623066829	0.966675750
O	-4.633650	-2.676702	2.827823	O	-4.700724086	-2.674333179	2.837840311
H	-4.883475	-3.619631	2.751938	H	-4.964947564	-3.622267987	2.757245989
H	0.008296	-3.930416	-1.884411	H	0.013469688	-3.919921323	-1.881748495
C	5.040911	0.366809	-0.203620	C	5.040576393	0.367672275	-0.199229311
C	5.724434	1.171126	-1.132868	C	5.723046423	1.177036887	-1.120560064
C	5.805025	-0.380856	0.728852	C	5.807557812	-0.384018260	0.723702944
C	7.121258	1.233456	-1.155034	C	7.116323829	1.241397413	-1.144389926
H	5.138488	1.738838	-1.859408	H	5.137695149	1.752408312	-1.844377787
C	7.211776	-0.330171	0.683582	C	7.210785875	-0.330431148	0.676246060
C	7.869239	0.474960	-0.247871	C	7.865534846	0.479559457	-0.246974640
H	7.624036	1.866407	-1.890343	H	7.618092186	1.882101838	-1.876249583
H	7.782480	-0.917086	1.404528	H	7.785462277	-0.922943473	1.392304762
H	8.960767	0.511865	-0.263129	H	8.958965516	0.516982594	-0.263370362
C	5.138356	-1.154086	1.819790	C	5.149906666	-1.166490579	1.810203137
O	5.943623	-2.152872	2.307403	O	5.951476864	-2.175599055	2.276617633
H	5.432456	-2.560917	3.034667	H	5.434121810	-2.587489858	3.009589170
O	4.031103	-0.940834	2.277855	O	4.049510626	-0.950819106	2.282415863



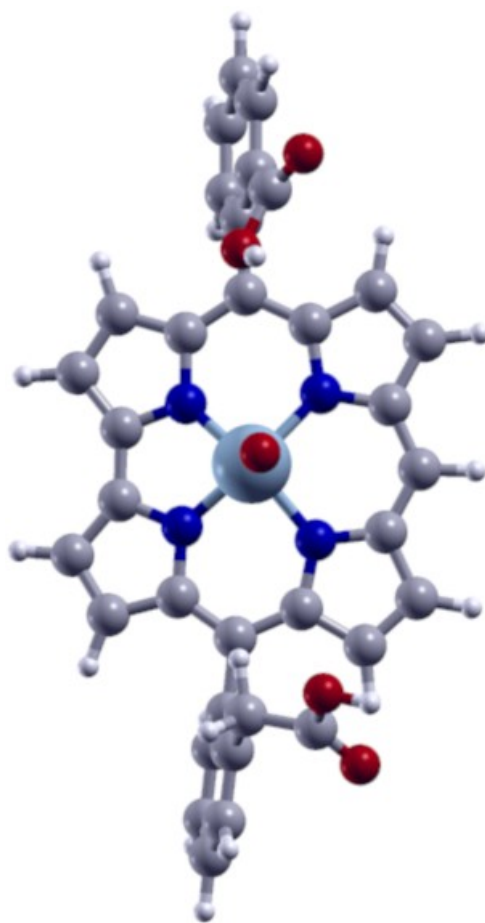
E= -2082.0157276 Ry (\*OOH)

C	0.809815	-2.617900	-0.614357
C	1.928316	-3.508186	-0.582150
H	1.882643	-4.594144	-0.543907
C	3.075028	-2.719259	-0.606020
H	4.106982	-3.064094	-0.600850
C	2.662044	-1.341298	-0.659325
C	3.398042	-0.137468	-0.665724
C	2.788209	1.145643	-0.826567
C	3.446329	2.423322	-0.912243
H	4.522240	2.571879	-0.878212
C	2.469404	3.390932	-1.023459
H	2.609578	4.467035	-1.105011
C	1.196039	2.725151	-0.981028
C	-0.085557	3.309976	-0.997479
C	-1.330065	2.657837	-0.896876
C	-2.640522	3.244406	-0.934302
C	-3.557630	2.221663	-0.794590
C	-2.823015	0.990359	-0.664901
C	-3.353761	-0.326279	-0.518127
C	-2.550697	-1.488036	-0.514362
C	-2.877467	-2.885291	-0.413062
H	-3.881834	-3.291258	-0.317525
C	-1.686070	-3.607550	-0.452235
H	-1.575966	-4.688075	-0.395895
C	-0.626976	-2.657851	-0.564795

E= -902.6950094757 Ry (\*OOH)

C	0.789199522	-2.490046963	-1.056614530
C	1.893811339	-3.392881465	-1.036944763
H	1.837037671	-4.478021078	-1.109049443
C	3.042079556	-2.625434144	-0.894591047
H	4.069429377	-2.985068468	-0.846529262
C	2.646332697	-1.246335052	-0.832764863
C	3.387509554	-0.066015322	-0.635715641
C	2.800009574	1.234089517	-0.709599542
C	3.466716193	2.504259750	-0.639557591
H	4.539076415	2.640031942	-0.515760009
C	2.508974515	3.487725625	-0.742737112
H	2.664318702	4.566501031	-0.722890932
C	1.233166765	2.840330049	-0.840022070
C	-0.037897377	3.438039165	-0.870309416
C	-1.289769182	2.798084222	-0.845210063
C	-2.592058292	3.395656291	-0.796310954
C	-3.514257938	2.375523352	-0.701369729
C	-2.791802896	1.134160936	-0.707442265
C	-3.326315650	-0.183965841	-0.648713587
C	-2.548211750	-1.343342080	-0.831017292
C	-2.889175297	-2.737629766	-0.845389002
H	-3.896921710	-3.140304621	-0.748680999
C	-1.712421505	-3.462717021	-0.994114987
H	-1.615179992	-4.546842225	-1.034110527
C	-0.646341262	-2.518963591	-1.054891278

N	1.285721	-1.337726	-0.676730	N	1.277841712	-1.219513135	-0.960160635
N	1.425152	1.368354	-0.871804	N	1.446847870	1.476711877	-0.824310671
N	-1.475867	1.292979	-0.730253	N	-1.448285156	1.429815855	-0.798328449
N	-1.179637	-1.403924	-0.599595	N	-1.185155939	-1.265276720	-0.976763382
Mn	0.010119	0.089925	-0.588209	Mn	0.014696897	0.201391910	-0.759548880
H	-4.641540	2.307849	-0.788598	H	-4.597908306	2.471513008	-0.646104800
H	-2.847656	4.305709	-1.056249	H	-2.791142580	4.466699671	-0.822066138
H	-0.016311	-0.008437	-2.153267	H	0.027315263	0.287537504	-2.324538852
O	0.165246	0.176715	1.430975	O	-0.001743790	-0.003832640	1.270682798
O	0.273636	1.509956	1.964754	O	0.097436484	1.246328593	1.998604227
C	4.868478	-0.181076	-0.413780	C	4.824886784	-0.160132429	-0.254184564
C	5.390928	-0.474601	0.873607	C	5.228166534	-0.619417738	1.025664457
C	5.751492	0.121081	-1.468407	C	5.801378000	0.267660308	-1.169540141
C	6.786919	-0.439262	1.043704	C	6.598105998	-0.603199767	1.329999837
C	7.135281	0.130401	-1.279385	C	7.156998480	0.253062086	-0.850741273
H	5.331497	0.341211	-2.453110	H	5.476988966	0.613141983	-2.156046136
C	7.655120	-0.147379	-0.011330	C	7.556732569	-0.177373146	0.413566159
H	7.199317	-0.645406	2.035687	H	6.917582173	-0.931500258	2.325138072
H	7.800411	0.357584	-2.115670	H	7.896446358	0.585460520	-1.585192558
H	8.734053	-0.132255	0.160140	H	8.614991847	-0.175238131	0.692036911
C	4.549324	-0.880117	2.078673	C	4.289063799	-1.168525030	2.087782756
H	5.119736	-0.634205	2.989607	H	4.781003137	-1.052731120	3.069562954
H	4.399856	-1.971522	2.077454	H	4.137750930	-2.250365994	1.933494501
C	3.182706	-0.219369	2.219692	C	2.921177132	-0.512638606	2.201797777
O	3.028595	1.005295	2.228620	O	2.786278043	0.709628836	2.333846964
O	2.190909	-1.095865	2.338501	O	1.917878906	-1.371057187	2.149071932
H	1.300758	-0.607933	2.104369	H	1.035851075	-0.830626147	1.880093763
H	1.255483	1.556659	2.144085	H	1.082756314	1.238185242	2.228609189
H	-0.117989	4.397970	-1.093432	H	-0.057593555	4.532210037	-0.880062262
C	-4.830904	-0.480137	-0.397029	C	-4.774272966	-0.342243741	-0.345729951
C	-5.569079	0.012260	0.709828	C	-5.305695162	-0.081293055	0.939716480
C	-5.532984	-1.094450	-1.451230	C	-5.651465995	-0.737116309	-1.366057294
C	-6.971402	-0.089628	0.714351	C	-6.685262972	-0.202945714	1.158226237
C	-6.925730	-1.212295	-1.423587	C	-7.019604997	-0.868438408	-1.130898071
H	-4.969368	-1.457365	-2.313839	H	-5.250632389	-0.917887205	-2.367817630
C	-7.649911	-0.702382	-0.339702	C	-7.540940549	-0.599306652	0.134928899
H	-7.511637	0.315013	1.572762	H	-7.064956984	0.013518871	2.160568429
H	-7.445008	-1.690379	-2.257675	H	-7.682958243	-1.172348196	-1.945435289
H	-8.738874	-0.782709	-0.315389	H	-8.614479773	-0.695896117	0.322039265
C	-4.952993	0.639337	1.925143	C	-4.482092205	0.326921827	2.125519069
O	-5.522931	1.454135	2.631959	O	-4.912726834	1.007324697	3.040557893
O	-3.705925	0.171616	2.186216	O	-3.221779347	-0.165854940	2.085557565
H	-3.365434	0.670835	2.956556	H	-2.715987917	0.219313016	2.842451647



E= -2006.274199 Ry (\*O)

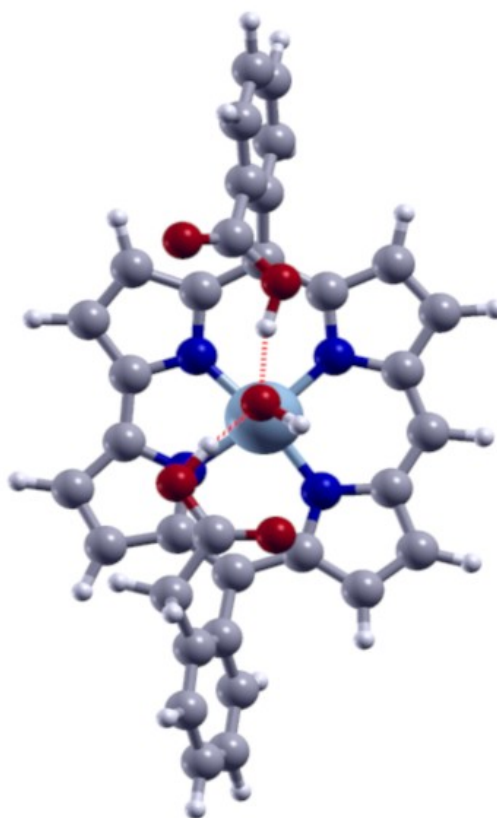
C	-0.431664	2.792005	0.409257
C	-1.475530	3.743272	0.590896
H	-1.348686	4.794029	0.841693
C	-2.676218	3.070713	0.382539
H	-3.679215	3.487474	0.438151
C	-2.367085	1.707885	0.049535
C	-3.197263	0.642379	-0.340867
C	-2.662410	-0.597955	-0.782523
C	-3.400677	-1.694617	-1.360663
H	-4.482436	-1.728483	-1.467428
C	-2.485785	-2.647318	-1.745816
H	-2.683946	-3.604117	-2.225068
C	-1.178366	-2.150298	-1.408916
C	0.048276	-2.787140	-1.643823
C	1.328633	-2.283791	-1.372626
C	2.591735	-2.901669	-1.679877
C	3.579418	-2.033600	-1.274349
C	2.929561	-0.872438	-0.712937
C	3.555002	0.321373	-0.261185
C	2.818738	1.466423	0.089140
C	3.247149	2.790799	0.444927
H	4.282585	3.108100	0.543999
C	2.112063	3.573565	0.632021

E= -869.3132766489 Ry (\*O)

C	-0.432869715	2.787735157	0.393151160
C	-1.475134959	3.734444366	0.579063995
H	-1.351883398	4.787370763	0.830061584
C	-2.672626813	3.062261879	0.374665796
H	-3.676453548	3.481122766	0.434466951
C	-2.366128657	1.703110576	0.040004082
C	-3.197309958	0.639550026	-0.344594575
C	-2.660884801	-0.595341171	-0.787506932
C	-3.393612002	-1.692833809	-1.362771766
H	-4.476910617	-1.733809366	-1.466816265
C	-2.478831129	-2.640989746	-1.747463377
H	-2.677708032	-3.600236715	-2.224610639
C	-1.174952159	-2.142492406	-1.413744561
C	0.049104576	-2.777510484	-1.645020899
C	1.326911931	-2.276811428	-1.375213536
C	2.587315749	-2.895262697	-1.677247657
C	3.573231896	-2.029996400	-1.272718799
C	2.927189106	-0.867841499	-0.717099172
C	3.551383634	0.323453930	-0.268521356
C	2.812661351	1.466286131	0.074577034
C	3.236849779	2.788128264	0.430387392
H	4.272971939	3.108588985	0.531385931
C	2.104271319	3.568438135	0.616012268

H	2.080073	4.627870	0.897251	H	2.074779261	4.624502307	0.881668002
C	0.986982	2.727443	0.416471	C	0.982024645	2.724670846	0.399140012
N	-0.991141	1.568704	0.110643	N	-0.991804002	1.566640026	0.094862882
N	-1.317413	-0.909102	-0.813713	N	-1.317807751	-0.903547835	-0.820955259
N	1.568483	-1.062113	-0.776997	N	1.568726410	-1.057454459	-0.783147918
N	1.435352	1.462363	0.111645	N	1.431358482	1.462821764	0.094433931
Mn	0.156566	0.060464	0.037317	Mn	0.155185475	0.060864608	0.026520527
H	4.654807	-2.161220	-1.373429	H	4.649744468	-2.163494867	-1.368658596
H	2.712912	-3.871970	-2.157457	H	2.710545895	-3.868720246	-2.151062769
H	0.248813	0.345926	-1.564034	H	0.255187847	0.339550730	-1.577953845
C	-4.674940	0.857622	-0.386142	C	-4.673713249	0.850820698	-0.381224829
C	-5.546711	0.256767	0.550992	C	-5.538607315	0.256617329	0.562423008
C	-5.207463	1.694300	-1.386839	C	-5.215700997	1.677312010	-1.380948502
C	-6.926104	0.504526	0.448944	C	-6.915250184	0.504266004	0.469513372
C	-6.581706	1.926624	-1.475608	C	-6.587177083	1.908030656	-1.461417381
H	-4.525267	2.151734	-2.107542	H	-4.540553507	2.132455163	-2.112440490
C	-7.446120	1.326863	-0.552469	C	-7.442880801	1.317171285	-0.530226500
H	-7.602478	0.040237	1.171903	H	-7.587374919	0.044447329	1.201967860
H	-6.975712	2.571824	-2.264394	H	-6.987793458	2.548153293	-2.253317489
H	-8.523188	1.500085	-0.611490	H	-8.522230873	1.490509658	-0.582034008
C	-5.032732	-0.611873	1.674904	C	-5.021982748	-0.607243448	1.683418866
H	-5.441277	-0.271880	2.642997	H	-5.438681955	-0.273144829	2.652167517
H	-3.938568	-0.543210	1.778458	H	-3.927362002	-0.526357597	1.791330521
C	-5.389174	-2.084726	1.545956	C	-5.360509629	-2.082164462	1.553983854
O	-6.050798	-2.602781	0.668439	O	-6.017751767	-2.606319023	0.677836130
O	-4.863083	-2.791312	2.589265	O	-4.824041695	-2.782804077	2.594117676
H	-5.118215	-3.724012	2.439880	H	-5.076067798	-3.724724588	2.438428527
H	0.001252	-3.771495	-2.116070	H	0.001734815	-3.764247588	-2.115766803
C	5.044349	0.389302	-0.258858	C	5.038759814	0.388108770	-0.257730166
C	5.678510	1.212832	-1.208482	C	5.682207275	1.200015943	-1.206254917
C	5.855842	-0.382159	0.611890	C	5.842403349	-0.376809079	0.621284899
C	7.071729	1.272253	-1.305066	C	7.072656904	1.254798291	-1.294293104
H	5.057071	1.792268	-1.895116	H	5.068193154	1.779446946	-1.902307362
C	7.256407	-0.333255	0.488386	C	7.240640149	-0.332557707	0.506502328
C	7.865838	0.491506	-0.456987	C	7.857902311	0.480341713	-0.438386534
H	7.535209	1.918588	-2.054351	H	7.542936930	1.895804339	-2.046383781
H	7.851257	-0.952932	1.162547	H	7.831264498	-0.949719906	1.189664087
H	8.954906	0.525040	-0.532285	H	8.949449501	0.510469670	-0.507809742
C	5.330945	-1.266210	1.701705	C	5.310123582	-1.249891248	1.712541951
O	4.126029	-0.864288	2.185498	O	4.107883083	-0.838283904	2.192093917
H	3.865861	-1.522651	2.861525	H	3.845776343	-1.500960581	2.875858144
O	5.934684	-2.228118	2.148085	O	5.905851391	-2.213264385	2.164783105
O	0.173887	-0.809773	1.370602	O	0.182272658	-0.808121809	1.361510218





E= -2006.9227281 Ry (\*OH)

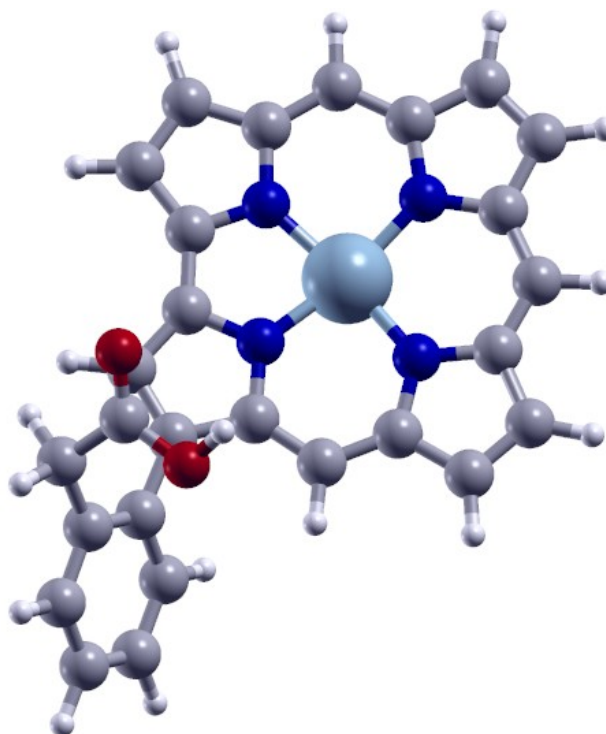
C	0.634515	-2.056175	-1.619772
C	1.715299	-2.970192	-1.825331
H	1.629168	-3.996664	-2.173837
C	2.883806	-2.295741	-1.488262
H	3.899654	-2.682772	-1.532686
C	2.522815	-0.962691	-1.077835
C	3.291793	0.107323	-0.578412
C	2.741211	1.404955	-0.312997
C	3.449515	2.594956	0.073867
H	4.522706	2.656514	0.231619
C	2.522455	3.608758	0.212906
H	2.710997	4.642909	0.494342
C	1.227259	3.050374	-0.055784
C	-0.024895	3.692943	0.012660
C	-1.296918	3.121001	-0.186834
C	-2.584334	3.735007	-0.010415
C	-3.539329	2.753531	-0.193025
C	-2.851330	1.534638	-0.519027
C	-3.418573	0.235101	-0.718548
C	-2.672252	-0.874480	-1.169011
C	-3.058253	-2.221199	-1.501728
H	-4.078558	-2.597921	-1.505892
C	-1.903002	-2.932170	-1.815083
H	-1.839127	-3.978381	-2.104270
C	-0.804728	-2.034138	-1.649551
N	1.155366	-0.865422	-1.198661

E= -870.5864125178 Ry (\*OH)

C	0.638230640	-2.024344258	-1.651767646
C	1.717093229	-2.934839906	-1.858572171
H	1.634502469	-3.959933199	-2.215944185
C	2.881451490	-2.266243676	-1.509621594
H	3.897349244	-2.657421965	-1.548567592
C	2.521723098	-0.939301657	-1.090056193
C	3.288146263	0.118988490	-0.571031728
C	2.736547466	1.411522795	-0.299410015
C	3.437087039	2.596903754	0.101871495
H	4.509646148	2.660244831	0.273958792
C	2.510612940	3.607142778	0.235654958
H	2.697341165	4.641004002	0.525553579
C	1.221207247	3.051785184	-0.047020734
C	-0.028750661	3.691020563	0.017619321
C	-1.297383465	3.120351615	-0.180814757
C	-2.582055783	3.729493611	0.002938610
C	-3.534040622	2.749173341	-0.174992684
C	-2.848617424	1.534620886	-0.507488517
C	-3.412204954	0.237082540	-0.708606467
C	-2.664004232	-0.861253180	-1.172806418
C	-3.043616437	-2.205138927	-1.510217607
H	-4.062282146	-2.590143009	-1.505909289
C	-1.890116592	-2.906164653	-1.838053013
H	-1.825552259	-3.951830427	-2.133887582
C	-0.797313423	-2.005978939	-1.677033032
N	1.157621526	-0.839308678	-1.220989006

N	1.395588	1.710828	-0.365696	N	1.393694908	1.716667479	-0.361744883
N	-1.498387	1.792051	-0.512769	N	-1.498667280	1.794343033	-0.507135026
N	-1.303587	-0.810303	-1.292719	N	-1.298969712	-0.789610583	-1.309234134
Mn	-0.072756	0.497607	-0.657406	Mn	-0.071125615	0.512941524	-0.674095205
H	-4.618319	2.855486	-0.107187	H	-4.613921854	2.851166267	-0.079567624
H	-2.749195	4.779560	0.246432	H	-2.748275052	4.774517807	0.263937963
H	0.013097	0.965705	-2.137392	H	0.011559413	0.999321700	-2.147224380
O	-0.220302	-0.114010	1.305857	O	-0.225509943	-0.146620948	1.287987458
C	4.721061	-0.133649	-0.229736	C	4.711315673	-0.127701652	-0.212810935
C	5.075266	-0.954207	0.874869	C	5.058318329	-0.969312496	0.874308604
C	5.730625	0.491785	-0.986530	C	5.725819297	0.511025802	-0.945934493
C	6.441684	-1.095244	1.176631	C	6.419494594	-1.115733465	1.182685214
C	7.081681	0.317650	-0.678423	C	7.071103677	0.331235560	-0.632152047
H	5.438922	1.111149	-1.838540	H	5.442403707	1.150235710	-1.788365391
C	7.437579	-0.477459	0.415513	C	7.418868662	-0.484471670	0.444430023
H	6.726610	-1.707399	2.037136	H	6.698804729	-1.747239978	2.033304309
H	7.848602	0.802658	-1.286637	H	7.842758986	0.830209874	-1.225754540
H	8.488603	-0.614483	0.680700	H	8.469681980	-0.627085177	0.714799590
C	4.076668	-1.729565	1.723353	C	4.059971796	-1.761781260	1.700899117
H	4.548554	-1.943295	2.696700	H	4.529005379	-1.988134579	2.674671020
H	3.861326	-2.702463	1.253526	H	3.857808445	-2.730756103	1.212806452
C	2.744332	-1.037330	2.019845	C	2.724260942	-1.083029460	2.000715087
O	2.664901	0.101484	2.468666	O	2.642071405	0.050328668	2.462443771
O	1.695822	-1.816507	1.738311	O	1.679171847	-1.856907682	1.705577831
H	0.852113	-1.219252	1.684991	H	0.830418419	-1.247458468	1.651457622
H	0.200853	0.563736	1.869899	H	0.220072589	0.517598288	1.863486727
H	-0.008046	4.751886	0.281990	H	-0.012734223	4.751477488	0.287395698
C	-4.791072	-0.038468	-0.200251	C	-4.780010796	-0.043187134	-0.188580984
C	-4.889386	-0.738074	1.031656	C	-4.875227299	-0.747256110	1.037394125
C	-5.960874	0.310527	-0.890519	C	-5.950454641	0.304084927	-0.872331182
C	-6.149966	-1.094353	1.527585	C	-6.131150298	-1.108311334	1.532713240
C	-7.216659	-0.023302	-0.367252	C	-7.201143776	-0.034879116	-0.349768096
H	-5.883042	0.826859	-1.850665	H	-5.878435253	0.828171325	-1.830812865
C	-7.310987	-0.726878	0.839239	C	-7.291798282	-0.742773748	0.850105260
H	-6.207185	-1.656544	2.462574	H	-6.185285479	-1.676906797	2.466320173
H	-8.121751	0.254742	-0.912505	H	-8.108683714	0.244883468	-0.893436052
H	-8.290613	-0.994194	1.242187	H	-8.271718650	-1.014365748	1.254436095
C	-3.633275	-1.138506	1.776925	C	-3.620144443	-1.148015921	1.780137456
O	-2.788017	-0.099866	1.881799	O	-2.775544844	-0.112933581	1.893761779
H	-1.793516	-0.328289	1.879438	H	-1.767261244	-0.333347042	1.860827245
O	-3.443179	-2.267124	2.198841	O	-3.434144343	-2.279844787	2.195333456

**Table S8:** Structures, energies, and coordinates of the complexes with the substituent R4=C<sub>6</sub>H<sub>4</sub>-CH<sub>2</sub>-COOH.



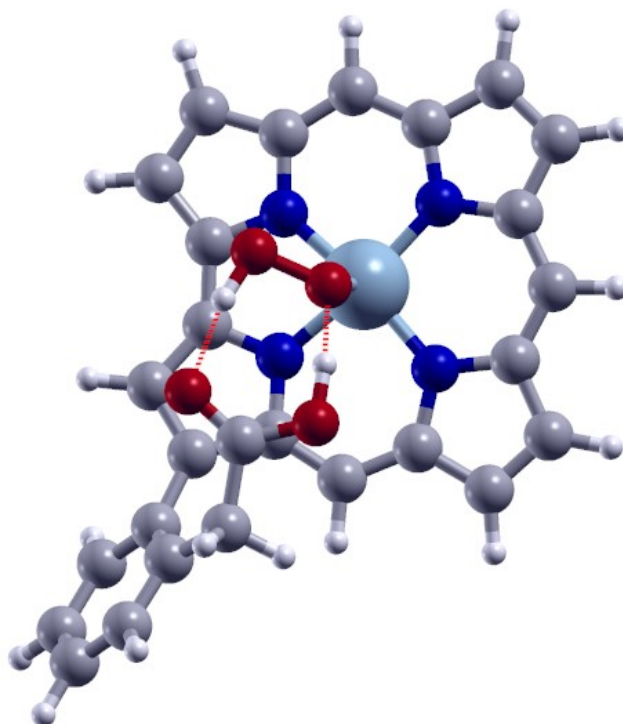
E= -1511.9112963 a.u (\*)

C	0.412367	-1.669988	-0.598470
C	1.821522	-1.742247	-0.729758
H	2.399562	-2.650145	-0.887883
C	2.327033	-0.432901	-0.654962
C	1.194836	0.446693	-0.466197
C	1.104929	1.833917	-0.265537
C	-0.100964	2.513539	-0.035902
C	-0.278245	3.918763	0.201622
H	0.530509	4.647069	0.224271
C	-1.623464	4.153328	0.398462
H	-2.106251	5.106410	0.606714
C	-2.309454	2.896329	0.286113
C	-3.683553	2.649480	0.420367
C	-4.312743	1.399648	0.326952
C	-5.710236	1.102241	0.476100
C	-5.871731	-0.257788	0.312241
C	-4.579813	-0.833030	0.061461
C	-4.273218	-2.187349	-0.136135
C	-2.971508	-2.675103	-0.343590
C	-2.447357	-3.999334	-0.510276
H	-3.038970	-4.912980	-0.516726
C	-1.060767	-3.902414	-0.648422
H	-0.360396	-4.724406	-0.779084
C	-0.726639	-2.522934	-0.569955
N	0.063989	-0.337832	-0.436833

E= -687.5085602578 Ry (\*)

C	0.412570521	-1.656128848	-0.594859192
C	1.819110231	-1.720237042	-0.727267059
H	2.401521383	-2.625906978	-0.893022471
C	2.320853989	-0.412454517	-0.646354057
C	1.185507806	0.459033714	-0.450278072
C	1.087827854	1.841208004	-0.240889449
C	-0.117202135	2.513823254	-0.008846024
C	-0.300100398	3.913633446	0.237955071
H	0.505670651	4.647383193	0.268571688
C	-1.643426037	4.141954538	0.430533718
H	-2.128740714	5.094695087	0.643005521
C	-2.324542666	2.886601307	0.306789650
C	-3.694803507	2.634545390	0.432834514
C	-4.318354064	1.386698087	0.329456864
C	-5.712693253	1.083743279	0.470437574
C	-5.868950357	-0.272337724	0.298428899
C	-4.577086836	-0.841501755	0.050516884
C	-4.264700230	-2.189603101	-0.152883713
C	-2.963236405	-2.670648398	-0.356384267
C	-2.435109999	-3.989317967	-0.527881303
H	-3.023107746	-4.907277722	-0.543177685
C	-1.051506308	-3.887835349	-0.660182482
H	-0.350062391	-4.710504638	-0.793705105
C	-0.721076701	-2.511201175	-0.573397704
N	0.059677930	-0.328408791	-0.426713043

N	-1.363084	1.907950	0.025966	N	-1.375655664	1.905318487	0.042864985
N	-3.639549	0.205716	0.078629	N	-3.641860273	0.198620529	0.076356154
N	-1.899986	-1.807860	-0.385789	N	-1.895946429	-1.801818926	-0.390900624
Mn	-1.785696	0.087259	-0.350884	Mn	-1.788781403	0.089027209	-0.342501181
H	-5.100443	-2.899143	-0.110892	H	-5.090837822	-2.905317582	-0.135491838
H	-6.799151	-0.824944	0.369057	H	-6.797700762	-0.841318139	0.347363153
H	-6.482094	1.840547	0.685642	H	-6.490670568	1.817960489	0.680449303
H	-4.322995	3.510716	0.624665	H	-4.338677355	3.493585185	0.640495378
H	2.024625	2.421397	-0.269496	H	2.005783860	2.433908151	-0.238382959
H	-1.956766	0.266726	-1.868565	H	-1.951507005	0.275090831	-1.856246507
C	3.729877	0.011641	-0.779335	C	3.720026220	0.036904994	-0.777039370
C	4.057116	0.958156	-1.771241	C	4.032705532	1.003144928	-1.750637360
C	4.755779	-0.463956	0.077906	C	4.760929562	-0.450940275	0.051352087
C	5.365583	1.421599	-1.933517	C	5.332518531	1.476172480	-1.921610979
H	3.266069	1.312471	-2.436861	H	3.232042736	1.370134040	-2.399793658
C	6.063525	0.012428	-0.099693	C	6.060124326	0.037060134	-0.134471018
C	6.376806	0.944041	-1.094772	C	6.355332108	0.989215015	-1.109691245
H	5.593337	2.147618	-2.717625	H	5.545759541	2.221422749	-2.694143740
H	6.852336	-0.349219	0.566561	H	6.862389619	-0.334226637	0.512733357
H	7.404775	1.295509	-1.209968	H	7.381245437	1.350314754	-1.231505658
C	4.473308	-1.449002	1.192255	C	4.506207615	-1.461253487	1.144363869
H	5.418059	-1.686263	1.711914	H	5.462087263	-1.700448211	1.645716704
H	4.084630	-2.407372	0.820459	H	4.124667939	-2.417344172	0.754999514
C	3.506123	-1.003476	2.281561	C	3.552371698	-1.055820396	2.257248807
O	2.835496	-1.759354	2.957122	O	2.905171413	-1.837835348	2.924558206
O	3.513676	0.346553	2.468995	O	3.541771654	0.288020850	2.475617750
H	2.877923	0.517430	3.193483	H	2.909466608	0.427425048	3.222254110

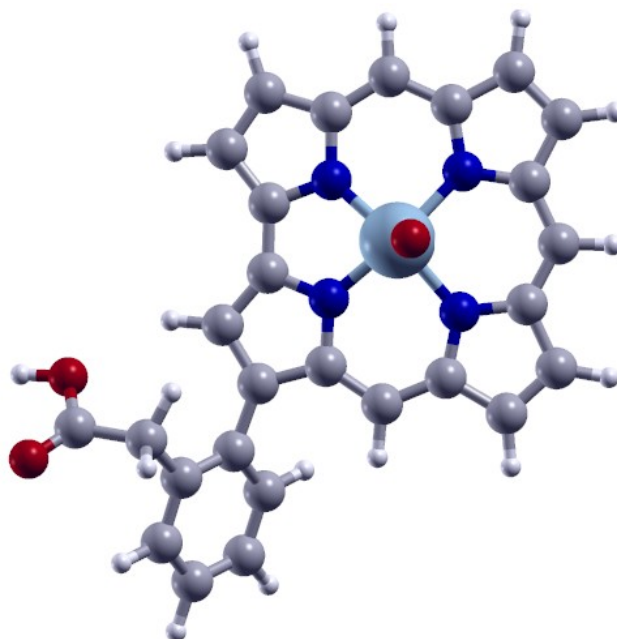


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C 0.558483 -1.826128 -0.725674

E= -753.0451199341 Ry (\*OOH)  
C 0.555654601 -1.822529000 -0.728004034

C	1.977894	-1.966889	-0.741364	C	1.972158556	-1.962514692	-0.743913640
H	2.535409	-2.892424	-0.618297	H	2.530720752	-2.889531133	-0.619923173
C	2.524054	-0.678969	-0.782794	C	2.518222210	-0.677863112	-0.783593287
C	1.412505	0.249136	-0.864757	C	1.407845990	0.248866152	-0.866957397
C	1.348728	1.647739	-0.960139	C	1.341024234	1.644018081	-0.963601790
C	0.164737	2.407491	-0.836761	C	0.158765898	2.399974252	-0.840933376
C	0.024792	3.832974	-0.938388	C	0.018072688	3.821647752	-0.943249165
H	0.837753	4.522101	-1.159095	H	0.833215138	4.509853505	-1.165096778
C	-1.300714	4.145746	-0.706869	C	-1.303548063	4.134355290	-0.710394032
H	-1.757932	5.133336	-0.705279	H	-1.761470637	5.123178854	-0.708215192
C	-1.999878	2.914910	-0.460215	C	-2.001815138	2.907486408	-0.462759572
C	-3.373490	2.729219	-0.207041	C	-3.371061687	2.723064462	-0.207640486
C	-4.041737	1.503480	-0.040944	C	-4.035040392	1.500100936	-0.040879944
C	-5.447630	1.281540	0.167803	C	-5.436724574	1.276763637	0.169313557
C	-5.648415	-0.081621	0.232729	C	-5.636394529	-0.082791489	0.234138552
C	-4.372384	-0.724432	0.063631	C	-4.364101952	-0.724756341	0.063860089
C	-4.106051	-2.111460	0.037889	C	-4.098610514	-2.107263347	0.039395105
C	-2.840437	-2.676123	-0.178939	C	-2.835828974	-2.669821490	-0.177745038
C	-2.367652	-4.036802	-0.201796	C	-2.363337047	-4.026437625	-0.199030342
H	-2.988261	-4.920650	-0.066504	H	-2.985589724	-4.909802391	-0.058968690
C	-0.992533	-4.007896	-0.415739	C	-0.991221947	-3.998194690	-0.414239673
H	-0.321842	-4.861331	-0.481711	H	-0.319775992	-4.853057612	-0.477542180
C	-0.620457	-2.631892	-0.530342	C	-0.620041097	-2.626027165	-0.531863369
N	0.260831	-0.495845	-0.810605	N	0.259467373	-0.495403615	-0.813010225
N	-1.085604	1.877960	-0.532485	N	-1.089405041	1.872311712	-0.535142925
N	-3.412602	0.268157	-0.084195	N	-3.405306009	0.266813448	-0.084913898
N	-1.748930	-1.872364	-0.394796	N	-1.746624431	-1.867924155	-0.393883731
Mn	-1.529196	0.024933	-0.318792	Mn	-1.528870113	0.025446491	-0.315945947
H	-4.953266	-2.781733	0.197431	H	-4.946756613	-2.778732079	0.201852723
H	-6.591486	-0.605292	0.377679	H	-6.580321058	-0.608056005	0.380158652
H	-6.195983	2.067156	0.251853	H	-6.185450881	2.064297359	0.253825867
H	-3.988003	3.631131	-0.160386	H	-3.987281485	3.626112282	-0.159773399
H	2.279605	2.199596	-1.107767	H	2.271275598	2.200372704	-1.112738474
H	-1.761451	-0.054929	-1.852847	H	-1.748835349	-0.059809248	-1.848905276
O	-0.871613	-0.027905	1.622088	O	-0.863999407	-0.018835142	1.621906474
O	-0.539172	-1.303908	2.157352	O	-0.509814337	-1.289699346	2.168311879
H	0.453955	-1.221230	2.289198	H	0.493751546	-1.184757129	2.292661146
C	3.953486	-0.358450	-0.597547	C	3.945008047	-0.360729808	-0.595632224
C	4.877501	-0.920806	-1.504393	C	4.869508136	-0.932502483	-1.491765049
C	4.442761	0.404301	0.499571	C	4.432947050	0.408088077	0.494572669
C	6.253047	-0.734970	-1.365935	C	6.241656111	-0.748299480	-1.350445499
H	4.485961	-1.506110	-2.340135	H	4.480408735	-1.527659443	-2.324751865
C	5.835089	0.568666	0.622505	C	5.822174133	0.571621724	0.619558068
C	6.736123	0.019017	-0.292064	C	6.722619110	0.013929371	-0.285339338
H	6.941423	-1.177153	-2.089858	H	6.931898644	-1.199680070	-2.069825040
H	6.220876	1.140342	1.471918	H	6.206385897	1.153089786	1.465923067
H	7.809631	0.171054	-0.157823	H	7.797984652	0.166118572	-0.149382811
C	3.590515	1.109971	1.551789	C	3.582371195	1.119566584	1.538996790
H	3.383475	2.145633	1.238979	H	3.371687994	2.152279134	1.211817858
H	4.193140	1.186847	2.473463	H	4.192346160	1.211042853	2.456572179
C	2.267618	0.482607	1.964894	C	2.266452898	0.489794086	1.964564261
O	2.129827	-0.718484	2.209007	O	2.140313748	-0.713020836	2.210399237
O	1.285276	1.378641	2.060821	O	1.279167808	1.374055692	2.062448411

H	0.380748	0.886076	2.034723	H	0.366152090	0.868469725	2.024293275
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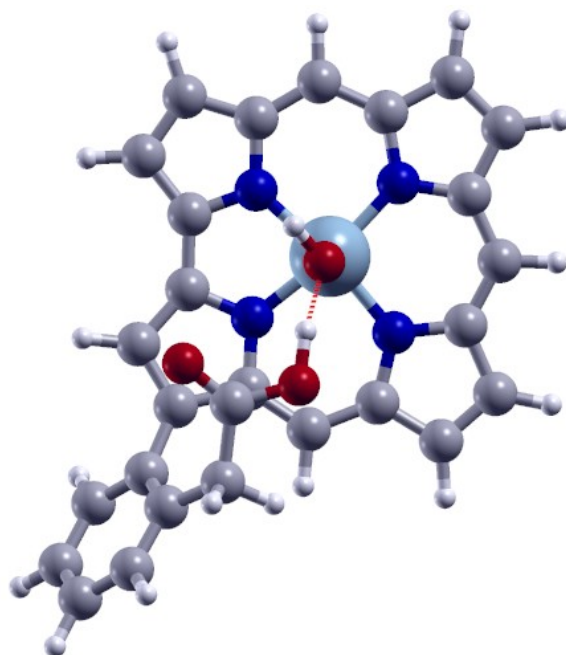


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C	0.515386	-1.373835	-0.344291
C	1.916986	-1.215176	-0.511806
H	2.632995	-1.997129	-0.754658
C	2.205970	0.145926	-0.347509
C	0.947954	0.814984	-0.079604
C	0.640969	2.164698	0.102960
C	-0.676082	2.657815	0.204173
C	-1.083334	4.040176	0.251588
H	-0.400402	4.887405	0.271601
C	-2.459263	4.064936	0.238001
H	-3.111843	4.935676	0.255091
C	-2.910948	2.697809	0.188640
C	-4.237031	2.244629	0.131548
C	-4.663860	0.913327	0.017281
C	-6.018095	0.441325	-0.124161
C	-5.962410	-0.928327	-0.242551
C	-4.573274	-1.311031	-0.178442
C	-4.039576	-2.604171	-0.348401
C	-2.670583	-2.876800	-0.404190
C	-1.951520	-4.080062	-0.714750
H	-2.407122	-5.049847	-0.905827
C	-0.594424	-3.772630	-0.745392
H	0.226888	-4.450204	-0.967288
C	-0.477778	-2.385487	-0.439280
N	-0.042448	-0.148216	-0.053631
N	-1.805890	1.868884	0.182613
N	-3.813548	-0.174079	-0.004806
N	-1.735541	-1.874476	-0.212397
Mn	-1.884938	-0.085671	0.406220
H	-4.742587	-3.424838	-0.505309

E= -719.6668246049 Ry (*O)			
C	0.510826385	-1.373805051	-0.356558563
C	1.909709263	-1.215524737	-0.523100296
H	2.624561910	-1.999703633	-0.768455183
C	2.202470987	0.141894412	-0.358236893
C	0.946729487	0.810710342	-0.090805245
C	0.641219731	2.157408367	0.091404861
C	-0.671200578	2.651316682	0.196191893
C	-1.077269960	4.030673268	0.247247181
H	-0.394058809	4.879968899	0.265675809
C	-2.449672581	4.056722655	0.241143945
H	-3.100596293	4.930776319	0.263863890
C	-2.903613256	2.693456150	0.192141882
C	-4.227370601	2.243035535	0.143402552
C	-4.657160092	0.916107135	0.029783612
C	-6.009808956	0.446281611	-0.105670067
C	-5.957108252	-0.919581504	-0.228239765
C	-4.571313883	-1.305013300	-0.172200355
C	-4.039319306	-2.593928498	-0.347473522
C	-2.673581323	-2.866603107	-0.408921821
C	-1.959024688	-4.068079083	-0.721883004
H	-2.416333097	-5.038854664	-0.913333404
C	-0.604253162	-3.765089964	-0.755318877
H	0.213520305	-4.448165887	-0.980971523
C	-0.481856084	-2.381515571	-0.449623835
N	-0.043268977	-0.149526885	-0.064853274
N	-1.800401746	1.865816827	0.179443301
N	-3.811548404	-0.171286256	0.001507116
N	-1.736332760	-1.869097236	-0.219854627
Mn	-1.882414100	-0.083848464	0.403292241
H	-4.744435052	-3.414766003	-0.504363862



H	-6.790816	-1.620467	-0.381411	H	-6.790229119	-1.609407740	-0.364539437
H	-6.900822	1.077661	-0.138099	H	-6.894286129	1.083334366	-0.112748899
H	-5.016994	3.009723	0.145003	H	-5.006745243	3.010626523	0.163283146
H	1.456137	2.890517	0.110551	H	1.457730736	2.883621626	0.096227631
H	-2.113507	0.259200	-1.175437	H	-2.123613407	0.255015164	-1.181148581
C	3.512928	0.818115	-0.478317	C	3.510736433	0.810271504	-0.485233827
C	3.628562	1.899338	-1.381507	C	3.635069881	1.883728063	-1.391606798
C	4.657958	0.434115	0.265900	C	4.650271892	0.433814453	0.266412118
C	4.833979	2.579714	-1.557204	C	4.837609052	2.563183888	-1.562739835
H	2.754652	2.179824	-1.974294	H	2.765032604	2.164003759	-1.992644001
C	5.863686	1.132281	0.080089	C	5.853063467	1.132258129	0.085410779
C	5.960488	2.194497	-0.821229	C	5.956324144	2.186207519	-0.818520224
H	4.895195	3.403114	-2.272746	H	4.903035392	3.384370867	-2.282938724
H	6.740083	0.831685	0.661411	H	6.727409419	0.837640981	0.675773832
H	6.910745	2.718476	-0.947237	H	6.907895579	2.712635413	-0.940204989
C	4.627727	-0.682793	1.301112	C	4.619562677	-0.675856107	1.303383176
H	3.600656	-1.043298	1.449767	H	3.590954846	-1.038426755	1.447042437
H	5.017662	-0.310373	2.259287	H	5.002114124	-0.298959546	2.264539688
C	5.521408	-1.837452	0.889102	C	5.513414368	-1.833105094	0.905834113
O	6.659514	-2.024870	1.273079	O	6.632650175	-2.041037232	1.330296421
O	4.909040	-2.664549	-0.013877	O	4.925335211	-2.637021568	-0.030665451
H	5.574496	-3.342795	-0.249223	H	5.599267847	-3.326008004	-0.247607940
O	-2.132920	-0.007187	1.974588	O	-2.130730060	-0.010141566	1.972628200



E= -1587.6669876 a.u (*OH)				E= -720.9339275902 Ry (*OH)			
C	-0.570953	1.848804	-0.654364	C	0.570315448	-1.848852249	-0.652220170
C	-1.990893	1.979655	-0.705726	C	1.988245149	-1.976622251	-0.702461567
H	-2.556439	2.902255	-0.600917	H	2.555501685	-2.899478465	-0.592857532
C	-2.525912	0.689280	-0.733536	C	2.522907218	-0.689703497	-0.731183252
C	-1.404148	-0.231908	-0.783255	C	1.401963455	0.230179601	-0.786571270
C	-1.331809	-1.625754	-0.880105	C	1.327093152	1.618761384	-0.887121955
C	-0.135194	-2.382091	-0.792285	C	0.131038524	2.373152072	-0.799842474
C	0.015536	-3.806259	-0.916857	C	-0.020410988	3.794692270	-0.924760884



H	-0.795494	-4.501500	-1.124432	H	0.792256873	4.490572092	-1.132724140
C	1.350395	-4.105776	-0.725562	C	-1.351828493	4.093128964	-0.729806714
H	1.819406	-5.087452	-0.748509	H	-1.823389377	5.075645737	-0.750333433
C	2.038825	-2.868108	-0.477078	C	-2.039010117	2.857600961	-0.480742798
C	3.411487	-2.667805	-0.230966	C	-3.406575734	2.658192913	-0.231510067
C	4.071892	-1.438100	-0.025954	C	-4.064229247	1.431715699	-0.025188134
C	5.478118	-1.207860	0.178337	C	-5.467822619	1.201626229	0.178758244
C	5.661453	0.155564	0.289021	C	-5.651374328	-0.158519208	0.289909416
C	4.372011	0.781832	0.152058	C	-4.364696551	-0.784329006	0.154051459
C	4.081585	2.169184	0.159657	C	-4.074089581	-2.168464461	0.162843282
C	2.808287	2.727383	-0.030942	C	-2.804688724	-2.724219693	-0.027784854
C	2.334247	4.086775	-0.104468	C	-2.330588490	-4.080004275	-0.096623770
H	2.951893	4.975805	0.008149	H	-2.950868332	-4.968427084	0.019845744
C	0.964395	4.048537	-0.347863	C	-0.963448306	-4.043183357	-0.339745254
H	0.295907	4.898427	-0.462807	H	-0.294861472	-4.895603227	-0.449550147
C	0.593513	2.667573	-0.425541	C	-0.591673819	-2.665959059	-0.423044996
N	-0.258219	0.521858	-0.709969	N	0.257192755	-0.525585116	-0.710859920
N	1.109284	-1.844557	-0.522172	N	-1.108736751	1.837566943	-0.526843862
N	3.431529	-0.215815	-0.023170	N	-3.426115439	0.210555027	-0.019982406
N	1.714415	1.915160	-0.220637	N	-1.710123018	-1.913205048	-0.219746805
Mn	1.519364	0.001239	-0.195976	Mn	-1.515701825	-0.007419789	-0.198935315
H	4.924960	2.847629	0.306713	H	-4.918542423	-2.848242076	0.311610199
H	6.598454	0.687552	0.442073	H	-6.589680545	-0.691566508	0.443754384
H	6.237576	-1.985627	0.228098	H	-6.227049730	1.982216763	0.227840524
H	4.037115	-3.563439	-0.213437	H	-4.034114035	3.555076891	-0.213821392
H	-2.261994	-2.182174	-1.014317	H	2.256726537	2.179360707	-1.022948795
H	1.815961	0.150831	-1.732817	H	-1.827989718	-0.136917290	-1.731195713
O	1.063909	-0.044287	1.712409	O	-1.057896270	0.072320865	1.717163342
C	-3.951003	0.349545	-0.558149	C	3.945614355	-0.353382129	-0.554876750
C	-4.878777	0.859724	-1.490233	C	4.872693493	-0.876162198	-1.475586373
C	-4.423006	-0.389109	0.563014	C	4.417597366	0.396542015	0.555173073
C	-6.250150	0.641631	-1.353815	C	6.240781116	-0.662162264	-1.338715664
H	-4.496592	1.428324	-2.341890	H	4.490720189	-1.455610844	-2.322111785
C	-5.811569	-0.583427	0.682084	C	5.803151246	0.585894184	0.675372949
C	-6.719507	-0.088522	-0.257425	C	6.708941882	0.077250853	-0.252886085
H	-6.945564	1.041268	-2.095562	H	6.936891847	-1.075041328	-2.074772148
H	-6.188260	-1.133550	1.549485	H	6.179110066	1.146455758	1.538686909
H	-7.789889	-0.263424	-0.124865	H	7.780830881	0.251327304	-0.119955877
C	-3.544749	-1.018716	1.637783	C	3.543231520	1.036471596	1.621449285
H	-3.256628	-2.039806	1.340916	H	3.253921606	2.055419050	1.312707957
H	-4.158427	-1.130800	2.547913	H	4.160433563	1.162661611	2.529363351
C	-2.274244	-0.273187	2.068759	C	2.276777774	0.293996086	2.066090820
O	-2.241898	0.925427	2.308121	O	2.253590394	-0.903467100	2.311822861
O	-1.234217	-1.110138	2.172112	O	1.234652306	1.122516216	2.170446606
H	-0.331070	-0.600673	2.150093	H	0.318578164	0.606674074	2.139732427
H	1.214596	0.807652	2.156471	H	-1.195062620	-0.788000333	2.167495461