

Supporting Information

Defining the Conditional Basis of Silicon Phthalocyanine Near-IR Uncaging

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3. Effect of the umbelliferone ligand on the triplet excited state of SiPc **1**
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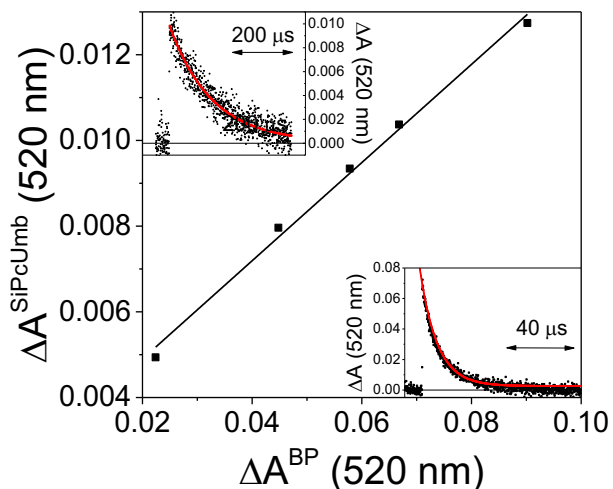


Figure S1. Comparative actinometry of **1** in argon-saturated PBS vs. benzophenone standard in acetonitrile. Plot shows the T_1 - T_n absorption change at 520 nm at varying laser energies. All solutions are argon saturated and have identical absorbance at 355 nm. All absorption changes are extrapolated to $t = 0$ after the laser pulse. Inset shows a pair of kinetic traces for **1** (top) and

BP (bottom) measured at equal incident laser energy.

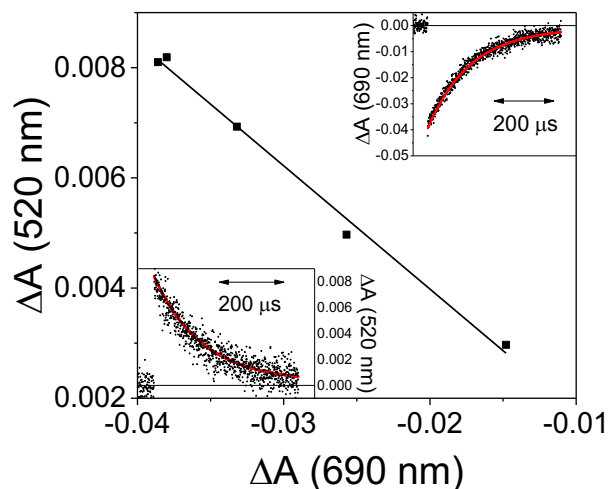
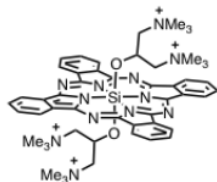


Figure S2. T_1 - T_n absorption of **1** (520 nm) as a function of ground-state depletion (690 nm) in argon-saturated PBS. Transients were measured at varying laser energies (two shown) and ΔA 's are extrapolated to $t = 0$ after laser excitation.

Effect of the umbelliferone ligand on the triplet excited state of SiPc **1**.

Model compound **SiPcM1** was used to examine the effect of the umbelliferone ligand on the excited states of SiPc **1**.

SiPcM1:



Stock solutions of **SiPcM1** and **1** were prepared in DMSO, then diluted into PBS. The optical densities of the 2 PBS solutions were matched (0.35) and transient absorption was carried out using 355-nm excitation as described above. Each solution was deoxygenated by Argon bubbling for about 30 minutes. The T_1 - T_n absorption and decay of the 2 compounds are shown in Figure S3.

As seen in Figure S3, the T_1 - T_n absorption signal is 3.5 times higher for the model compound (**SiPcM1**). Since the structure of the SiPc core is the same for all three compounds, it is reasonable to assume that they have the same T_1 - T_n extinction coefficient. This is also supported by identical T_1 - T_n spectra for the compounds (Figure 1a and Figure S4, albeit with different intensities). Thus, we conclude that relative Φ_T 's decrease in the order **SiPcM1** (1.00) and **1** (0.285).

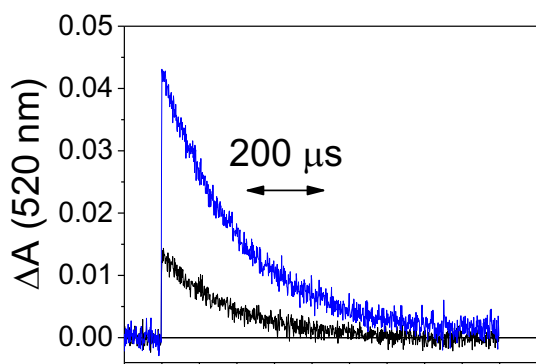


Figure S3. T_1 - T_n absorption of SiPcM1 (Blue) and **1** (Black) in argon-saturated PBS using 355-nm excitation. The optical densities of the solutions were matched at 355 nm.

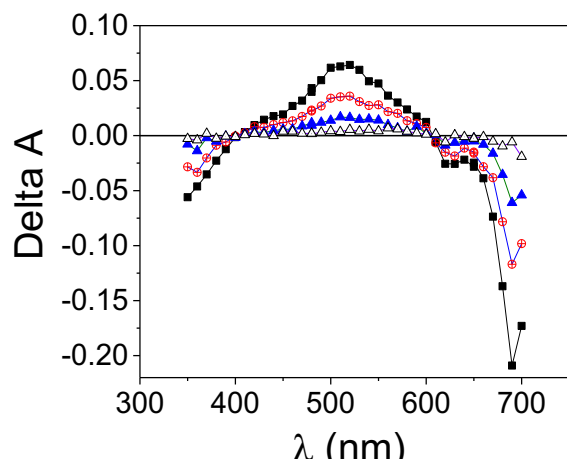
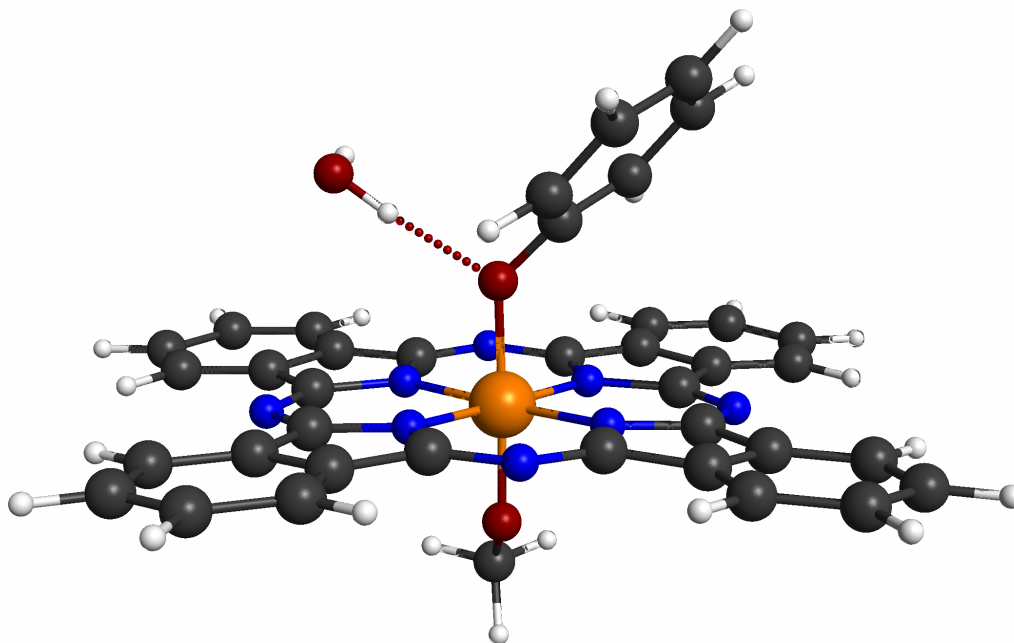


Figure S4. Transient absorption spectra obtained after 355-nm pulsed excitation of SiPcM1 in argon-saturated PBS (0, 117, 289 and 600 μ s in order of decreasing ΔA).

Quantum Chemistry Data: Absolute Energies and Structures (Å)

1a. Neutral SiPc(OMe)(OPh)--HOH: reactant for OPh displacement



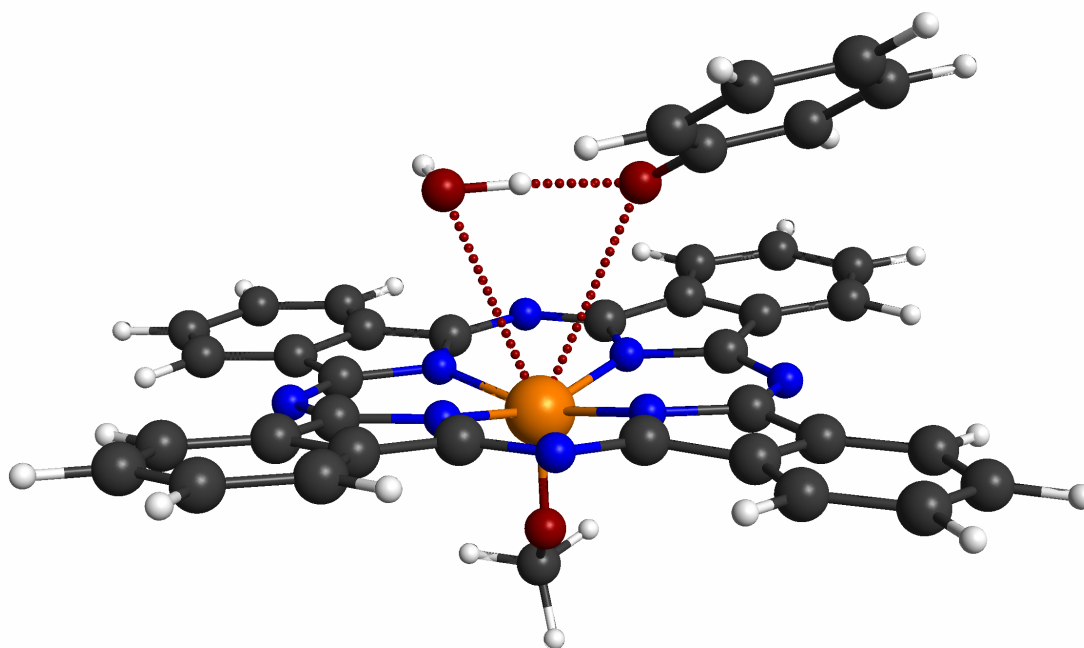
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N	7.0	-0.1445659664	-1.6034215434	-0.2125357789
N	7.0	1.1512363926	0.3703326805	1.1776617733
N	7.0	-1.3279115083	0.2867566363	-1.8099867973
C	6.0	-1.7766936246	1.3777881266	-2.5253642981
C	6.0	-1.9341203325	-0.8382863947	-2.3336868410
C	6.0	1.6873029182	1.4988961297	1.7623633042
C	6.0	1.6880987572	-0.7292628785	1.8183859337
C	6.0	-0.6812364331	3.0426553839	-1.3440812648
C	6.0	0.6834293788	3.0959907262	0.4199371165
C	6.0	-0.9241565798	-2.4374282266	-0.9928904092
C	6.0	0.5975171722	-2.3970398283	0.6395489253
N	7.0	-1.4712561554	2.6486194658	-2.3260683149
N	7.0	1.4710118272	2.7584832670	1.4263452721
N	7.0	-1.7595823191	-2.0935886784	-1.9574059923
N	7.0	1.4524967874	-2.0039766084	1.5672225792
C	6.0	0.4897944463	4.4741544222	0.0056216745
C	6.0	-0.3647725170	4.4399892403	-1.1079826066
C	6.0	2.5908384797	1.1139132743	2.8344530586
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C	6.0	0.2939641448	-3.7948108178	0.3920134360
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C	6.0	3.3761297483	-0.9941173645	3.7849921788
C	6.0	4.1544987102	-0.2489703663	4.6710967742
C	6.0	4.1504280201	1.1607426785	4.6398115751
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C	6.0	-1.1881433142	-5.0266777792	-1.1093010775
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C	6.0	-3.4244872923	1.6381259044	-4.5271320826
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C	6.0	-4.2532729228	0.8967698433	-5.3685323255
C	6.0	-4.3594279291	-0.5042401030	-5.2420696090
H	1.0	-3.3393335602	2.7161186385	-4.6209363703
H	1.0	-4.8284884545	1.4049383970	-6.1372749194
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H	1.0	-0.5452023910	7.7514960494	-1.7431692022
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H	1.0	3.3627306053	2.9471798711	3.6941097174
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H	1.0	-1.0867539540	-7.1616680169	-0.8853373183
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H	1.0	1.5983163620	-1.5927859776	-2.2270092517
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C	6.0	-3.5075194787	1.5245571156	0.5528634053
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H	1.0	-2.6223095119	3.6115853562	3.7025267708
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H	1.0	-1.6848066074	-1.0680540352	2.0417045709
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1b. Neutral SiPc(OMe)(PhO-H-OH): transition state for OPh displacement



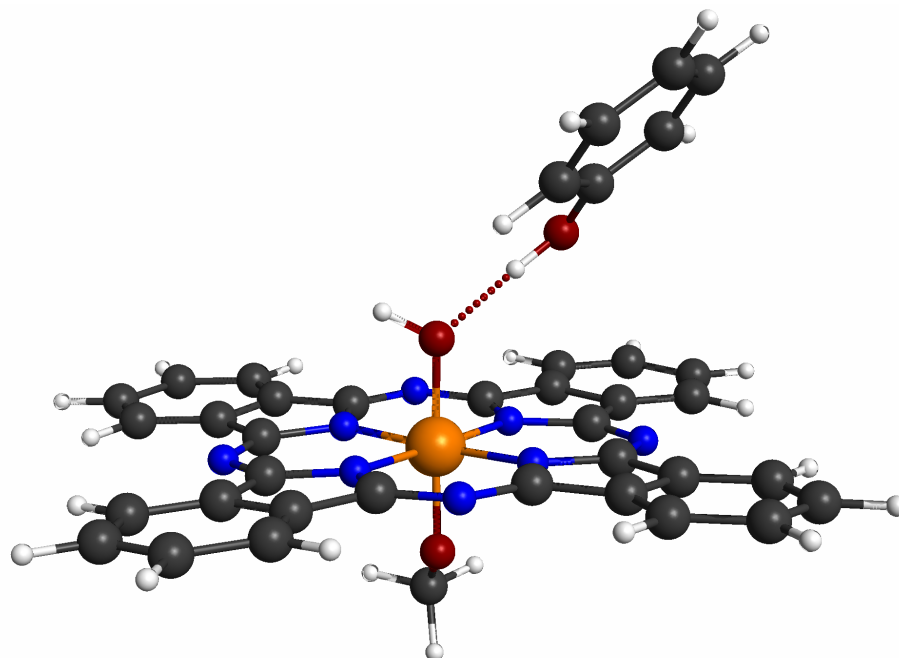
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N	7.0	1.2679536052	0.1582407886	1.0914630314
N	7.0	-1.1960711027	0.0663730350	-1.7351726400
C	6.0	-1.7992591944	1.1659414640	-2.3467398427
C	6.0	-1.8307856781	-1.0565896978	-2.2651109540
C	6.0	1.6825021098	1.2784486084	1.8096463550
C	6.0	1.8305880069	-0.9388934034	1.7438754634
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C	6.0	0.9050997009	-2.5899796173	0.4659616701
N	7.0	-1.5086810635	2.4370021603	-2.1842062286
N	7.0	1.4294645571	2.5395945086	1.5403975115
N	7.0	-1.5635742026	-2.3187322090	-2.0111472679
N	7.0	1.7121653831	-2.2083639417	1.4281256063
C	6.0	0.4316502987	4.2408605995	0.1461857530
C	6.0	-0.4013350783	4.2089021991	-0.9774776772
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H	1.0	-1.9610724237	-0.0045424539	1.6232261569
H	1.0	-1.8545033074	-1.5289423043	1.9070274950

1c. Neutral SiPc(OMe)(OH)--HOPh: product for OPh displacement



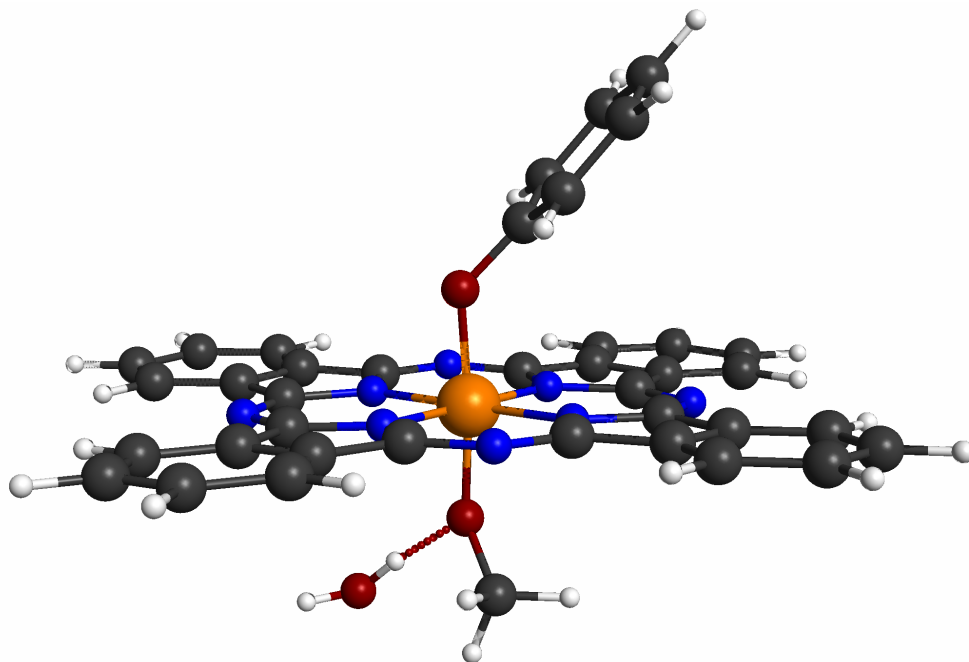
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N	7.0	1.4219822039	0.1267612279	1.1636798775
N	7.0	-1.1361574326	0.0808418387	-1.7643293314
C	6.0	-1.6091275504	1.1801941884	-2.4502077179
C	6.0	-1.7500651113	-1.0396216069	-2.2891448540
C	6.0	1.9564140453	1.2506708882	1.7558892151
C	6.0	1.9712820784	-0.9781282839	1.7818789154
C	6.0	-0.4912566686	2.8350554146	-1.2749482500
C	6.0	0.9090535533	2.8648885853	0.4617036841
C	6.0	-0.7243937229	-2.6558516589	-0.9773198090
C	6.0	0.8334440876	-2.6348467155	0.6247798968
N	7.0	-1.3049306435	2.4498548070	-2.2423363625
N	7.0	1.7168710755	2.5140509227	1.4471693057
N	7.0	-1.5720884499	-2.2986431110	-1.9273530273
N	7.0	1.7145803024	-2.2510358015	1.5331316824
C	6.0	0.6839635161	4.2517230956	0.0881547053
C	6.0	-0.1937517292	4.2327333413	-1.0080845231
C	6.0	2.8858178634	0.8566722317	2.8027669258
C	6.0	2.8994924545	-0.5481498674	2.8146554527
C	6.0	0.5114793584	-4.0284065137	0.3776467066

C	6.0	-0.4742165090	-4.0412768006	-0.6243031628
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C	6.0	-2.5544028223	0.7518781425	-3.4673465367
C	6.0	1.1693815709	5.4536656219	0.6090286479
C	6.0	-0.6176076397	5.4151697078	-1.6195572539
C	6.0	0.7472786213	6.6354544996	-0.0002102338
C	6.0	-0.1347571235	6.6164553267	-1.1002276061
C	6.0	3.6776023191	1.5968776862	3.6841658032
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C	6.0	4.4954470267	-0.5217690482	4.5885368381
C	6.0	4.4826776497	0.8881370957	4.5763777384
C	6.0	0.9909775377	-5.2155602088	0.9394544844
C	6.0	-1.0109202806	-5.2416983209	-1.0994496631
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C	6.0	-3.2999939477	1.4602021621	-4.4129008999
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C	6.0	-4.2386898040	-0.6759502766	-5.1407777154
H	1.0	-3.2237177447	2.5401239351	-4.4910638598
H	1.0	-4.7377887665	1.2439776598	-5.9956820489
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H	1.0	-3.5630073891	-2.4616341291	-4.1112460446
H	1.0	-1.2964600896	5.3960578051	-2.4663053708
H	1.0	-0.4425587938	7.5565795626	-1.5492360390
H	1.0	1.1029792956	7.5898760984	0.3776682326
H	1.0	1.8478491385	5.4637623617	1.4562659144
H	1.0	3.6647858522	2.6822089868	3.6719249444
H	1.0	5.1122219517	1.4305544245	5.2760690834
H	1.0	5.1342112186	-1.0409142543	5.2974529401
H	1.0	3.7088906218	-2.3449478931	3.7146965669
H	1.0	1.7522448694	-5.2009459437	1.7129363537
H	1.0	0.8042187540	-7.3554187402	0.8789783384
H	1.0	-0.9274212176	-7.3780168420	-0.8829006699
H	1.0	-1.7708638899	-5.2470186882	-1.8743752451
O	8.0	1.4936424403	0.0822187575	-1.4059706276
O	8.0	-3.6107177243	1.2674713526	0.2619836038
C	6.0	1.6969041480	-0.7567120921	-2.5232809006
H	1.0	2.6482495481	-0.4766993529	-2.9895676325
H	1.0	1.7594320246	-1.8181810445	-2.2435181347
H	1.0	0.9059042981	-0.6469567090	-3.2792495642
C	6.0	-3.9992602059	2.2398494127	1.1278867368
C	6.0	-5.2017459206	2.9143909397	0.8603528708
C	6.0	-3.2533992117	2.5836627925	2.2680941358
C	6.0	-5.6469944658	3.9181766743	1.7205871267
C	6.0	-3.7112928679	3.5904649699	3.1211154937
C	6.0	-4.9068999277	4.2652016998	2.8566762669

H	1.0	-5.7699415566	2.6411273145	-0.0248091685
H	1.0	-6.5789316146	4.4338851188	1.5006894498
H	1.0	-5.2570216882	5.0482274035	3.5237013038
H	1.0	-3.1247409718	3.8478429854	4.0001309700
H	1.0	-2.3228734038	2.0614922164	2.4724116829
O	8.0	-1.1678372459	0.2550653751	0.8408701462
H	1.0	-2.7209741426	0.9027463044	0.5150064272
H	1.0	-1.2481089268	-0.5207957013	1.4176848358

2a. Neutral SiPc(OPh)(OMe)--HOH: reactant for OMe displacement



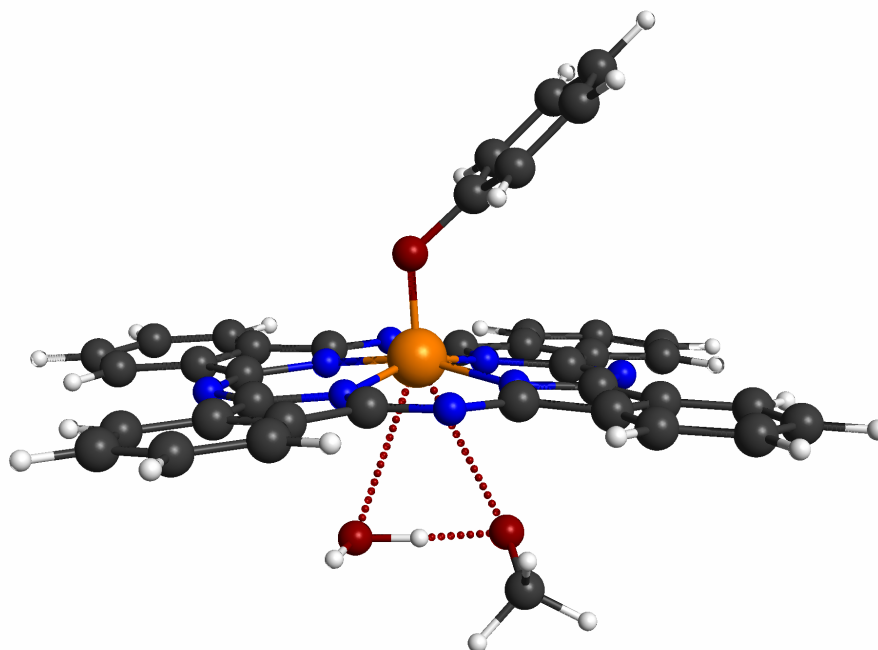
$E = -2453.86727 \text{ hartree}$

ATOM	CHARGE	X	Y	Z
SI	14.0	-0.0589498846	0.0992167026	-0.0581812635
N	7.0	-0.0353725220	2.0331469636	-0.0986935777
N	7.0	-0.0922720284	-1.8337505737	-0.0133328066
N	7.0	1.2426947444	0.1148724581	1.3819610121
N	7.0	-1.3668632358	0.0923668797	-1.4916924051
C	6.0	-1.8676362292	1.1986181425	-2.1489862662
C	6.0	-1.9425445503	-1.0268220473	-2.0588430753
C	6.0	1.7751892010	1.2335081216	1.9907799360
C	6.0	1.7956235490	-0.9951707367	1.9869445148
C	6.0	-0.7567415379	2.8435020698	-0.9568438240
C	6.0	0.6915945067	2.8590551241	0.7424773452
C	6.0	-0.8791967218	-2.6524683033	-0.7958180325
C	6.0	0.6640342351	-2.6409530140	0.8116715957
N	7.0	-1.5891187358	2.4678662234	-1.9121777806
N	7.0	1.5201947459	2.4999569250	1.7072132065
N	7.0	-1.7358545816	-2.2915515283	-1.7354245380
N	7.0	1.5412435366	-2.2659558466	1.7259224672
C	6.0	0.4301723113	4.2462815445	0.4086935276
C	6.0	-0.4784440530	4.2363474718	-0.6624939964
C	6.0	2.7098368256	0.8290459278	3.0268578221
C	6.0	2.7261504918	-0.5756537924	3.0209924878
C	6.0	0.3457280193	-4.0355961286	0.5553681609

C	6.0	-0.6305124707	-4.0424030910	-0.4536071079
C	6.0	-2.8517936460	-0.6258345554	-3.1191810322
C	6.0	-2.8014882891	0.7763453303	-3.1783198054
C	6.0	0.9092885214	5.4457711772	0.9442158166
C	6.0	-0.9411736206	5.4256910444	-1.2337693038
C	6.0	0.4493822508	6.6318893800	0.3748440102
C	6.0	-0.4645946062	6.6219843376	-0.7005415959
C	6.0	3.5043462120	1.5607721657	3.9132569097
C	6.0	3.5359066286	-1.2961815371	3.9024564972
C	6.0	4.3305491471	-0.5673566539	4.7872712264
C	6.0	4.3147934019	0.8429179343	4.7926588830
C	6.0	0.8190839185	-5.2243061837	1.1161464110
C	6.0	-1.1680545395	-5.2379356239	-0.9363908794
C	6.0	-0.6970246086	-6.4262522578	-0.3776632053
C	6.0	0.2843399086	-6.4195049608	0.6348538046
C	6.0	-3.5695233040	1.4927459946	-4.0995425603
C	6.0	-3.6717928068	-1.3601156251	-3.9796858361
C	6.0	-4.3901634431	0.7615664317	-4.9583816178
C	6.0	-4.4408427147	-0.6465906158	-4.8989784646
H	1.0	-3.5274444774	2.5765181494	-4.1413072985
H	1.0	-5.0022905079	1.2842909213	-5.6878226200
H	1.0	-5.0914584877	-1.1834501685	-5.5834395725
H	1.0	-3.7074112141	-2.4438230479	-3.9304104932
H	1.0	-1.6438190996	5.4131779242	-2.0608694573
H	1.0	-0.8008588536	7.5666960447	-1.1183742794
H	1.0	0.7991741923	7.5840209920	0.7637419152
H	1.0	1.6119899465	5.4486349185	1.7713690105
H	1.0	3.4891609131	2.6460842134	3.9140394902
H	1.0	4.9463449084	1.3779654465	5.4961439932
H	1.0	4.9738947069	-1.0936017485	5.4866845076
H	1.0	3.5445454789	-2.3815487400	3.8947732469
H	1.0	1.5737311665	-5.2144154207	1.8961934935
H	1.0	0.6276890299	-7.3643946532	1.0465845082
H	1.0	-1.0917073809	-7.3761597493	-0.7270869200
H	1.0	-1.9234513395	-5.2384050555	-1.7157890475
O	8.0	1.2154622038	-0.0499394101	-1.2450902800
O	8.0	-1.3190158169	0.0568611887	1.1687592376
C	6.0	2.2426868459	0.8818568205	-1.5420676356
H	1.0	2.9541252804	0.3852652842	-2.2102868138
H	1.0	1.8527612398	1.7722880912	-2.0512834666
H	1.0	2.7882212815	1.2005374108	-0.6433898409
C	6.0	-2.4624324986	0.7760015395	1.3397890550
C	6.0	-3.6825459662	0.2939708795	0.8359729007
C	6.0	-2.4589560602	1.9577493821	2.0998838221
C	6.0	-4.8684207424	0.9925305523	1.0709530038
C	6.0	-3.6492565193	2.6515311168	2.3289691454
C	6.0	-4.8593433947	2.1772837985	1.8136538995

H	1.0	-3.6908397717	-0.6357416484	0.2746673736
H	1.0	-5.8038117836	0.6050592804	0.6739911257
H	1.0	-5.7839108478	2.7188068863	1.9949311858
H	1.0	-3.6289035275	3.5652508212	2.9183895606
H	1.0	-1.5227998335	2.3140974506	2.5193805546
O	8.0	2.2611732563	-2.4048434013	-2.3211311226
H	1.0	1.8092178845	-1.6161899034	-1.9495667274
H	1.0	2.8961916537	-2.6496876764	-1.6308545812

2b. Neutral SiPc(OPh)(MeO-H-OH): transition state for OMe displacement



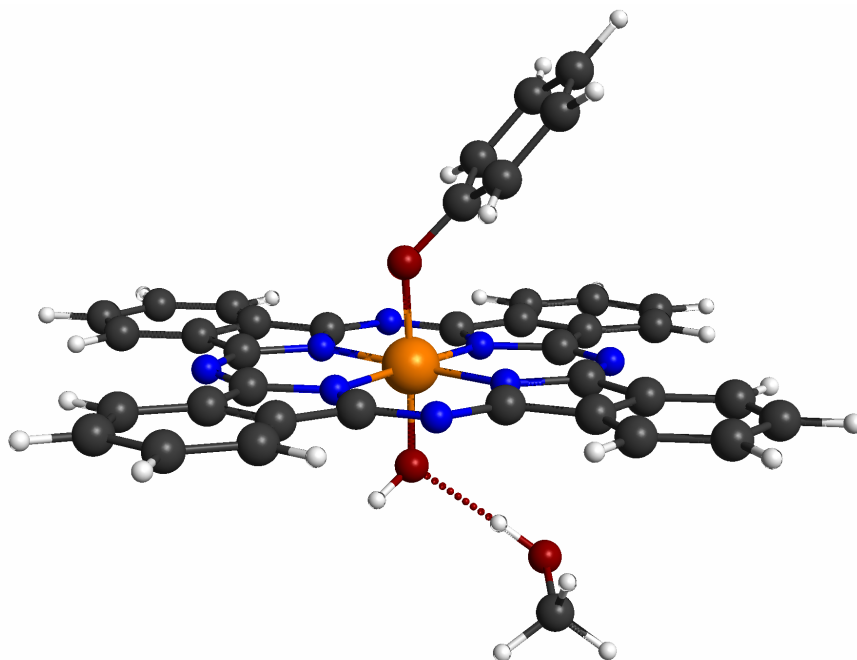
$E = -2453.78154 \text{ hartree}$

ATOM	CHARGE	X	Y	Z
SI	14.0	-0.3128740654	-0.0036112089	0.2028841398
N	7.0	-0.0651887330	1.8771177467	-0.0259214246
N	7.0	-0.1781685743	-1.9026066536	0.0840669622
N	7.0	1.1962808216	-0.0103119904	1.3661266222
N	7.0	-1.3624711494	-0.0176210782	-1.3826117433
C	6.0	-1.8280355829	1.0874607193	-2.0961827360
C	6.0	-1.9681525377	-1.1315754707	-1.9710378994
C	6.0	1.7606028869	1.1056962218	1.9934037802
C	6.0	1.7947183124	-1.1235319684	1.9612344002
C	6.0	-0.7158960534	2.7048685262	-0.9413846426
C	6.0	0.7069041415	2.7167464935	0.7639683895
C	6.0	-0.9688766951	-2.7431809239	-0.6963966136
C	6.0	0.6280309888	-2.7386549760	0.8465026700
N	7.0	-1.5610409596	2.3534398584	-1.8791708725
N	7.0	1.5244029066	2.3695965937	1.7378451816
N	7.0	-1.8179728115	-2.3921732048	-1.6353588373
N	7.0	1.5417327817	-2.3879963962	1.7249047332
C	6.0	0.5191275277	4.0978826737	0.3764086377
C	6.0	-0.3707836374	4.0878386565	-0.7037526326
C	6.0	2.7208392555	0.6911695914	2.9891097729
C	6.0	2.7513685013	-0.7080339128	2.9600426428
C	6.0	0.3231810152	-4.1230231702	0.5747352321

C	6.0	-0.6912844503	-4.1260405712	-0.3907720574
C	6.0	-2.8136197555	-0.7260451249	-3.0674889018
C	6.0	-2.7220633877	0.6687870631	-3.1483147220
C	6.0	1.0536607799	5.2905145269	0.8723120541
C	6.0	-0.7647016934	5.2712564742	-1.3359494052
C	6.0	0.6601022360	6.4723763715	0.2468307605
C	6.0	-0.2364680903	6.4632037871	-0.8436359301
C	6.0	3.5313043412	1.4215700787	3.8652408934
C	6.0	3.5913403434	-1.4383810668	3.8079840643
C	6.0	4.3970558757	-0.7147063180	4.6832274284
C	6.0	4.3670785553	0.6977279806	4.7117747770
C	6.0	0.8444122607	-5.3151683944	1.0903104592
C	6.0	-1.2244430968	-5.3212486939	-0.8863293785
C	6.0	-0.7104420608	-6.5088575744	-0.3721026416
C	6.0	0.3111726343	-6.5060251355	0.6042381989
C	6.0	-3.4251060985	1.3923813709	-4.1185843387
C	6.0	-3.6114188995	-1.4583349674	-3.9542561903
C	6.0	-4.2220770498	0.6673362258	-5.0000589270
C	6.0	-4.3140454862	-0.7407386136	-4.9184808978
H	1.0	-3.3480136216	2.4731119646	-4.1769899778
H	1.0	-4.7846569716	1.1901915440	-5.7681042134
H	1.0	-4.9455526018	-1.2706335229	-5.6257361541
H	1.0	-3.6768124171	-2.5394363151	-3.8888499863
H	1.0	-1.4526034479	5.2575753476	-2.1750761758
H	1.0	-0.5177106291	7.4052763523	-1.3053264168
H	1.0	1.0503370377	7.4216340822	0.6025768890
H	1.0	1.7449720223	5.2921769583	1.7087201461
H	1.0	3.5034965888	2.5061313598	3.8828050202
H	1.0	5.0090936374	1.2267069592	5.4100532035
H	1.0	5.0618468083	-1.2437959783	5.3597481654
H	1.0	3.6090447520	-2.5229881345	3.7816923342
H	1.0	1.6306156775	-5.3068560083	1.8380942915
H	1.0	0.6854907597	-7.4538995313	0.9800948012
H	1.0	-1.0998788918	-7.4589490131	-0.7264845439
H	1.0	-2.0074020374	-5.3182058546	-1.6376175720
O	8.0	1.2945285380	1.0594035530	-2.3550711707
O	8.0	-1.5004847428	0.0110907403	1.4032590138
C	6.0	2.3424379569	1.9401199676	-2.2095690647
H	1.0	3.3455448558	1.4537488897	-2.2441537527
H	1.0	2.3635857916	2.7316145062	-2.9922294289
H	1.0	2.3329852633	2.4977638294	-1.2404984072
C	6.0	-2.6313822901	0.7972461389	1.4973102625
C	6.0	-3.8345412508	0.3523457542	0.9373004833
C	6.0	-2.5884621004	2.0008904429	2.2100911524
C	6.0	-4.9895782078	1.1254092785	1.0753119353
C	6.0	-3.7492698634	2.7669823021	2.3416834143
C	6.0	-4.9513989027	2.3361685525	1.7730862234

H	1.0	-3.8604246340	-0.5967756862	0.4103377425
H	1.0	-5.9210415840	0.7762992792	0.6373172653
H	1.0	-5.8517603251	2.9351252694	1.8772096382
H	1.0	-3.7107737190	3.7021567023	2.8942063135
H	1.0	-1.6554435886	2.3210509610	2.6642948753
O	8.0	2.1608292107	-1.1267928992	-1.5099095774
H	1.0	1.8063181295	-0.2263461724	-1.9300134871
H	1.0	2.8758464602	-0.8338671947	-0.9248161894

2c. Neutral SiPc(OPh)(OH)--HOMe: product for OMe displacement



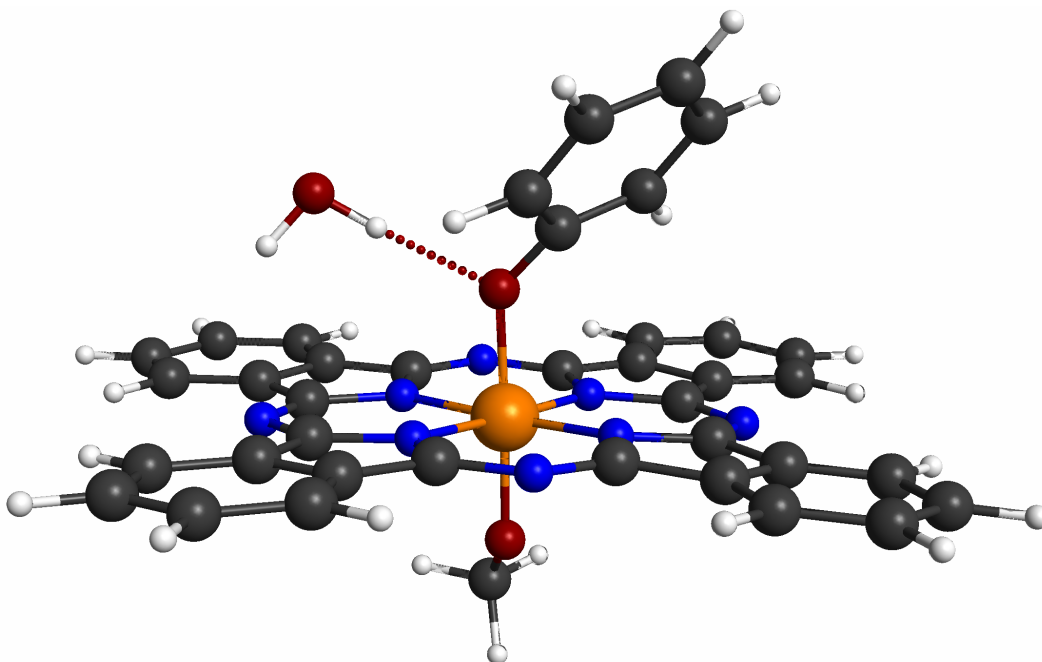
$E = -2453.87073$ hartree

ATOM	CHARGE	X	Y	Z
SI	14.0	-0.0557724991	-0.0500186515	0.0046561922
N	7.0	0.0255065396	1.8903437387	-0.0595404274
N	7.0	-0.1430878876	-1.9891061607	0.0992012664
N	7.0	1.2699292923	-0.0596532607	1.4291206687
N	7.0	-1.3370143440	-0.0405207606	-1.4286042055
C	6.0	-1.8302264386	1.0732097515	-2.0835039763
C	6.0	-1.9195819451	-1.1566889212	-2.0009347860
C	6.0	1.8300547952	1.0579813559	2.0220059203
C	6.0	1.7452534992	-1.1718399845	2.0998119862
C	6.0	-0.6827324759	2.7083874501	-0.9165285555
C	6.0	0.7977389816	2.7001021718	0.7501036609
C	6.0	-0.9163674147	-2.7982197033	-0.7064817237
C	6.0	0.5684965738	-2.8051661129	0.9539981461
N	7.0	-1.5410405242	2.3401588232	-1.8506482213
N	7.0	1.6247744515	2.3258053731	1.7107846081
N	7.0	-1.7366211334	-2.4236062614	-1.6731773400
N	7.0	1.4366836178	-2.4379905592	1.8804992029
C	6.0	0.5773869403	4.0930133688	0.4010960248
C	6.0	-0.3562115161	4.0981113358	-0.6485838489
C	6.0	2.7181857951	0.6473255148	3.0940034485
C	6.0	2.6657636359	-0.7556636634	3.1426578583
C	6.0	0.2331597727	-4.1958443282	0.6953652584

C	6.0	-0.7027463836	-4.1912712917	-0.3517857967
C	6.0	-2.8175649132	-0.7450852800	-3.0644298754
C	6.0	-2.7629281974	0.6573573510	-3.1149516092
C	6.0	1.1039519089	5.2828569646	0.9111326987
C	6.0	-0.7962543098	5.2934483734	-1.2229735094
C	6.0	0.6653556679	6.4766477562	0.3389949863
C	6.0	-0.2727956452	6.4818678094	-0.7141956496
C	6.0	3.5203203200	1.3757005840	3.9771080601
C	6.0	3.4145790183	-1.4781765377	4.0758594042
C	6.0	4.2180513704	-0.7530891875	4.9548863969
C	6.0	4.2700965561	0.6560916745	4.9064083860
C	6.0	0.6692494266	-5.3900151751	1.2741198864
C	6.0	-1.2359797917	-5.3804769121	-0.8548971637
C	6.0	-0.8029511658	-6.5741112685	-0.2770859207
C	6.0	0.1374944854	-6.5787588963	0.7734474923
C	6.0	-3.5233807279	1.3808465590	-4.0378416444
C	6.0	-3.6341622511	-1.4727553249	-3.9347266577
C	6.0	-4.3394637817	0.6566590662	-4.9058607012
C	6.0	-4.3940329569	-0.7523838794	-4.8551653742
H	1.0	-3.4776437876	2.4646639315	-4.0734860757
H	1.0	-4.9449782825	1.1846807079	-5.6370033141
H	1.0	-5.0403414249	-1.2833436458	-5.5482429119
H	1.0	-3.6721878408	-2.5566122294	-3.8918720856
H	1.0	-1.5184286342	5.2932082898	-2.0332125333
H	1.0	-0.5918543107	7.4313131462	-1.1347912793
H	1.0	1.0512366792	7.4220853375	0.7096686257
H	1.0	1.8251359037	5.2739127133	1.7222056244
H	1.0	3.5554493233	2.4597756496	3.9369731014
H	1.0	4.9060909504	1.1876548772	5.6085435803
H	1.0	4.8151246395	-1.2804459382	5.6934463994
H	1.0	3.3699375090	-2.5620744517	4.1109577785
H	1.0	1.3941063505	-5.3896199747	2.0820226019
H	1.0	0.4524338423	-7.5275219186	1.1987053666
H	1.0	-1.1950844187	-7.5192897710	-0.6418135279
H	1.0	-1.9585569956	-5.3720224317	-1.6647873374
O	8.0	1.5021235364	1.5056044264	-3.4250803770
O	8.0	-1.2764727858	0.0004806976	1.2651509005
C	6.0	2.5719763396	2.3695272438	-3.0806005721
H	1.0	3.5120548585	1.8264317469	-2.8908617771
H	1.0	2.7412617637	3.0460578537	-3.9253753577
H	1.0	2.3507804152	2.9854106346	-2.1949122505
C	6.0	-2.4348950947	0.7052675782	1.3921286358
C	6.0	-3.6413671067	0.1918672869	0.8870616252
C	6.0	-2.4550164717	1.9116005851	2.1117851754
C	6.0	-4.8384943785	0.8835480934	1.0831735622
C	6.0	-3.6566485855	2.5970476831	2.3036488504
C	6.0	-4.8536926208	2.0910427785	1.7880973084

H	1.0	-3.6316789362	-0.7555082964	0.3562771155
H	1.0	-5.7636710298	0.4723024742	0.6862127983
H	1.0	-5.7872039932	2.6263303222	1.9395675752
H	1.0	-3.6549299072	3.5293227734	2.8635015265
H	1.0	-1.5276605835	2.2938596893	2.5283796689
O	8.0	1.1940951767	-0.1693612040	-1.2178185775
H	1.0	1.3583262944	0.8993110601	-2.6648185803
H	1.0	2.0800483388	-0.2285112231	-0.8270245496

3a. Anion SiPc⁻(OMe)(OPh)--HOH: reactant for OPh displacement



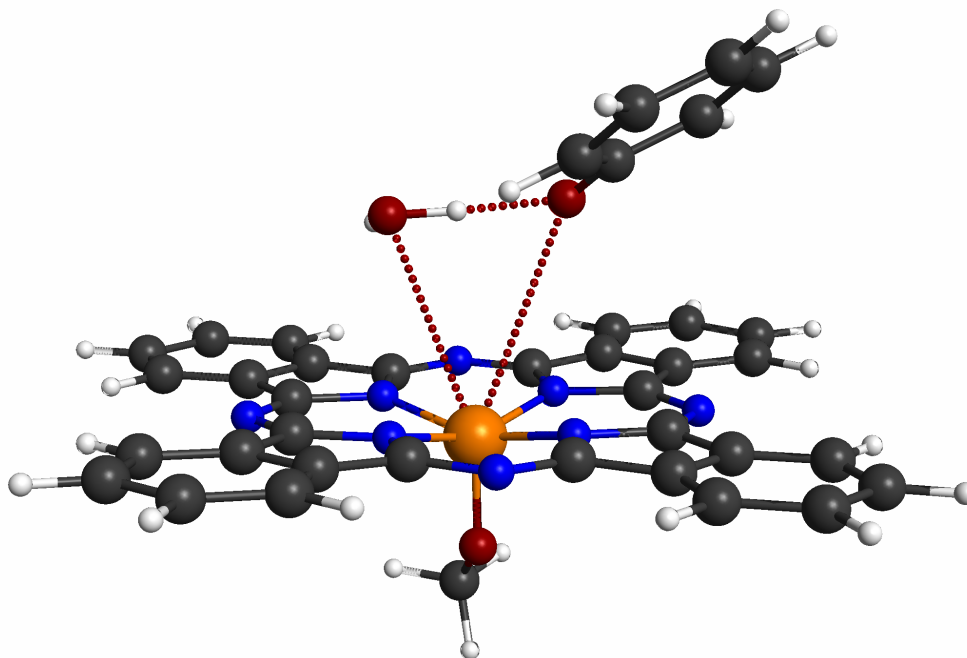
$E = -2453.98745$ hartree

ATOM	CHARGE	X	Y	Z
SI	14.0	0.1356540372	0.4784290701	-0.3729226936
N	7.0	0.3109050880	2.3943228531	-0.5333955066
N	7.0	-0.0912137072	-1.4255555363	-0.1592333646
N	7.0	1.4443358016	0.4921305338	1.0736357481
N	7.0	-1.2134028522	0.4797022913	-1.7735164781
C	6.0	-1.6037007216	1.5718356263	-2.5278095380
C	6.0	-1.9464142996	-0.6105059825	-2.2050490207
C	6.0	2.1008443987	1.5974884034	1.5748452891
C	6.0	1.9016237282	-0.6152934537	1.7651776845
C	6.0	-0.2950473079	3.1883836952	-1.5058347117
C	6.0	1.1702547917	3.2075699219	0.1954951534
C	6.0	-0.9981911408	-2.2294911265	-0.8449500946
C	6.0	0.6105716086	-2.2414219012	0.7229768170
N	7.0	-1.1592186624	2.8337570970	-2.4193121332
N	7.0	1.9782685574	2.8707636151	1.1671646948
N	7.0	-1.8547396548	-1.8767577238	-1.7679567324
N	7.0	1.5179136743	-1.8920977289	1.6002928785
C	6.0	1.0859392678	4.5766219975	-0.3058013543
C	6.0	0.1774366914	4.5631016747	-1.3714060018
C	6.0	3.0003296774	1.1945622503	2.6190077904
C	6.0	2.8751061168	-0.2103362060	2.7380939877
C	6.0	0.1534384963	-3.6190124962	0.5773988289

C	6.0	-0.8552743706	-3.6106165110	-0.3953767871
C	6.0	-2.8365135228	-0.2081935523	-3.2552623334
C	6.0	-2.6149397720	1.1748094472	-3.4638669994
C	6.0	1.7266334632	5.7533613433	0.0862058467
C	6.0	-0.1230315528	5.7273580393	-2.0813527512
C	6.0	1.4281816334	6.9205245083	-0.6201040274
C	6.0	0.5140302540	6.9074487219	-1.6916537533
C	6.0	3.8911403088	1.9111153928	3.4358577424
C	6.0	3.6377042262	-0.9233102143	3.6795280347
C	6.0	4.5162588815	-0.2082343182	4.4829215080
C	6.0	4.6433227767	1.1995809146	4.3615617951
C	6.0	0.5384564578	-4.8025150377	1.2115367698
C	6.0	-1.5109940431	-4.7857843911	-0.7688700695
C	6.0	-1.1278302013	-5.9711229600	-0.1384930010
C	6.0	-0.1147138146	-5.9792430462	0.8405766660
C	6.0	-3.3398167844	1.8802938364	-4.4408622084
C	6.0	-3.7825654031	-0.9106965152	-4.0217499351
C	6.0	-4.2739914854	1.1798945850	-5.1917512157
C	6.0	-4.4939429011	-0.2069193257	-4.9840656264
H	1.0	-3.1694596870	2.9414086025	-4.5986589363
H	1.0	-4.8488462643	1.6988111329	-5.9544916104
H	1.0	-5.2334094184	-0.7229314365	-5.5909794702
H	1.0	-3.9486359697	-1.9719552660	-3.8600697465
H	1.0	-0.8273788648	5.7119554337	-2.9076273875
H	1.0	0.3030763779	7.8320733313	-2.2223731130
H	1.0	1.9080680779	7.8549223119	-0.3414114466
H	1.0	2.4314682227	5.7557470449	0.9121672748
H	1.0	3.9856651822	2.9890273285	3.3402386175
H	1.0	5.3415357297	1.7265385509	5.0067303382
H	1.0	5.1196173164	-0.7330734534	5.2191593210
H	1.0	3.5396330070	-2.0012905831	3.7707519983
H	1.0	1.3193473240	-4.8026557667	1.9659524348
H	1.0	0.1608057500	-6.9182230793	1.3132632593
H	1.0	-1.6173949665	-6.9039652338	-0.4052162032
H	1.0	-2.2914161683	-4.7732318214	-1.5236498183
O	8.0	1.4427663645	0.3153382430	-1.5140495067
O	8.0	-1.1733255095	0.6201397368	0.8738389517
C	6.0	1.5382691386	-0.6404209348	-2.5448382430
H	1.0	2.4608415284	-0.4485750123	-3.1078029961
H	1.0	1.5858370201	-1.6712327393	-2.1630512578
H	1.0	0.6968037018	-0.5808215714	-3.2515982868
C	6.0	-1.7714721260	1.7306013527	1.3932404787
C	6.0	-2.8713119266	2.3300882670	0.7572495905
C	6.0	-1.3455031169	2.2337787122	2.6346425851
C	6.0	-3.5160269769	3.4204915452	1.3469172564
C	6.0	-1.9963777792	3.3220029949	3.2177159449
C	6.0	-3.0833327692	3.9252948558	2.5771209461

H	1.0	-3.2179126538	1.9287972146	-0.1899934314
H	1.0	-4.3662408144	3.8745348483	0.8426031864
H	1.0	-3.5890772598	4.7721822732	3.0335574415
H	1.0	-1.6534963650	3.6968922220	4.1795917571
H	1.0	-0.5189353867	1.7443399941	3.1397020019
O	8.0	-1.1638213239	-1.1075138212	3.1798572575
H	1.0	-1.1660098582	-0.5624936284	2.3652546984
H	1.0	-0.3083285026	-1.5623713438	3.1373337089

3b. Anion SiPc⁻(OMe)(PhO-H-OH): transition state for OPh displacement



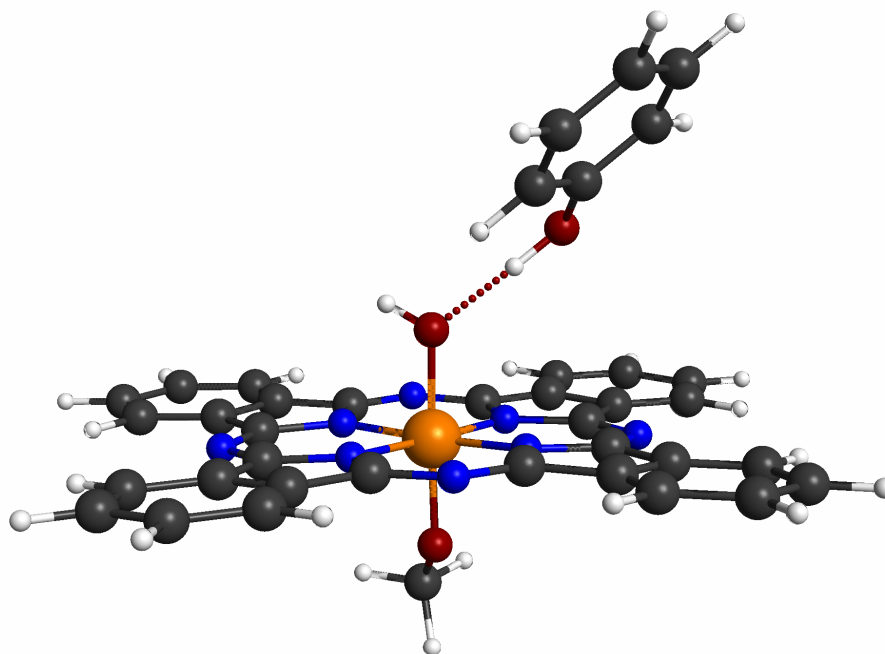
$E = -2453.94127$ hartree

ATOM	CHARGE	X	Y	Z
SI	14.0	0.5377896244	0.2473408006	-0.6442793989
N	7.0	0.4507574962	2.1438346737	-0.5422966779
N	7.0	0.1381647026	-1.5856277860	-0.2723497117
N	7.0	1.5989728840	0.2792261879	0.9562431729
N	7.0	-1.0381369658	0.2845008296	-1.7431245737
C	6.0	-1.5570356368	1.3996157950	-2.4077154540
C	6.0	-1.7687901283	-0.8087029535	-2.2196064407
C	6.0	2.2422429981	1.3838572762	1.5133502177
C	6.0	2.0672053644	-0.8281752740	1.6712715678
C	6.0	-0.2556434254	2.9921209198	-1.4177794540
C	6.0	1.2915483765	2.9885306106	0.2004896560
C	6.0	-0.7462163108	-2.4275655483	-0.9766640950
C	6.0	0.8393175463	-2.4361573953	0.6112974502
N	7.0	-1.1647371640	2.6658416545	-2.2833524300
N	7.0	2.1205970764	2.6590301828	1.1450605273
N	7.0	-1.6212467304	-2.0875366505	-1.8749807782
N	7.0	1.7330421505	-2.1033549085	1.4914598939
C	6.0	1.1303379531	4.3677142083	-0.2263600751
C	6.0	0.1684188531	4.3690435778	-1.2368878366
C	6.0	3.1082401791	0.9804429508	2.5733720246
C	6.0	2.9984687073	-0.4212724967	2.6714428555
C	6.0	0.4064671206	-3.8093973821	0.4375899282

C	6.0	-0.5820217208	-3.8042658987	-0.5488288499
C	6.0	-2.7403434704	-0.3853121488	-3.1731454381
C	6.0	-2.6026015448	1.0124768459	-3.2954846187
C	6.0	1.7465597236	5.5481547655	0.1964968121
C	6.0	-0.2213932812	5.5526344937	-1.8693210905
C	6.0	1.3649772317	6.7329512332	-0.4337376027
C	6.0	0.3922223510	6.7349135353	-1.4544693424
C	6.0	3.9622253279	1.7046261073	3.4258713076
C	6.0	3.7404304827	-1.1408571934	3.6274794001
C	6.0	4.5830750377	-0.4231400464	4.4619108854
C	6.0	4.6943206016	0.9904401536	4.3616983022
C	6.0	0.7969214123	-4.9940278367	1.0701631072
C	6.0	-1.2228558230	-4.9818372675	-0.9458842362
C	6.0	-0.8337148998	-6.1664775301	-0.3220123199
C	6.0	0.1649558691	-6.1721669426	0.6745978619
C	6.0	-3.4205100275	1.7473220358	-4.1753822309
C	6.0	-3.7000586824	-1.0895709317	-3.9249248396
C	6.0	-4.3602477421	1.0483862450	-4.9161324021
C	6.0	-4.4998505195	-0.3612519171	-4.7912570716
H	1.0	-3.3118511246	2.8237794565	-4.2664047878
H	1.0	-5.0065459485	1.5834228069	-5.6067325772
H	1.0	-5.2503686332	-0.8721908828	-5.3883569437
H	1.0	-3.8035025421	-2.1658438437	-3.8256460720
H	1.0	-0.9715282133	5.5474400260	-2.6537997930
H	1.0	0.1182183209	7.6752744051	-1.9248391452
H	1.0	1.8238080711	7.6715919845	-0.1354745664
H	1.0	2.4941274969	5.5383567386	0.9833963177
H	1.0	4.0425255617	2.7844483318	3.3457548564
H	1.0	5.3662451870	1.5162088131	5.0346864050
H	1.0	5.1727946594	-0.9469084616	5.2095223245
H	1.0	3.6526457970	-2.2205115697	3.7017561343
H	1.0	1.5632878512	-4.9911959156	1.8387623000
H	1.0	0.4431856943	-7.1130288637	1.1414204865
H	1.0	-1.3068467230	-7.1027635876	-0.6048555129
H	1.0	-1.9926090179	-4.9688286761	-1.7110143370
O	8.0	1.7610321186	0.1477954642	-1.7837611355
O	8.0	-2.6479814822	1.5111639517	1.0089862032
C	6.0	1.8768835315	-0.8591965368	-2.7858071142
H	1.0	2.7481317007	-0.6147900432	-3.4001398191
H	1.0	2.0265362894	-1.8522962385	-2.3451747398
H	1.0	0.9909123903	-0.8851230764	-3.4323259140
C	6.0	-2.8414768402	2.6431345090	1.6135401880
C	6.0	-3.9151212246	3.5187367199	1.2448688974
C	6.0	-2.0222274340	3.1037961335	2.6961595560
C	6.0	-4.1441055699	4.7282023343	1.8966828601
C	6.0	-2.2649942572	4.3143725142	3.3415058939
C	6.0	-3.3258752484	5.1476267849	2.9561256546

H	1.0	-4.5598960112	3.2019305897	0.4262343548
H	1.0	-4.9766867344	5.3559433272	1.5777290739
H	1.0	-3.5091970305	6.0911957957	3.4647432199
H	1.0	-1.6143570397	4.6191065223	4.1618706592
H	1.0	-1.1898712521	2.4739295379	3.0053445030
O	8.0	-1.3316444597	-0.3487944219	2.3490123993
H	1.0	-1.7893252298	0.4010519020	1.8503309556
H	1.0	-1.5965746210	-1.1392112360	1.8550909823

3c. Anion SiPc⁻(OMe)(OH)--HOPh: product for OPh displacement



$E = -2453.99889$ hartree

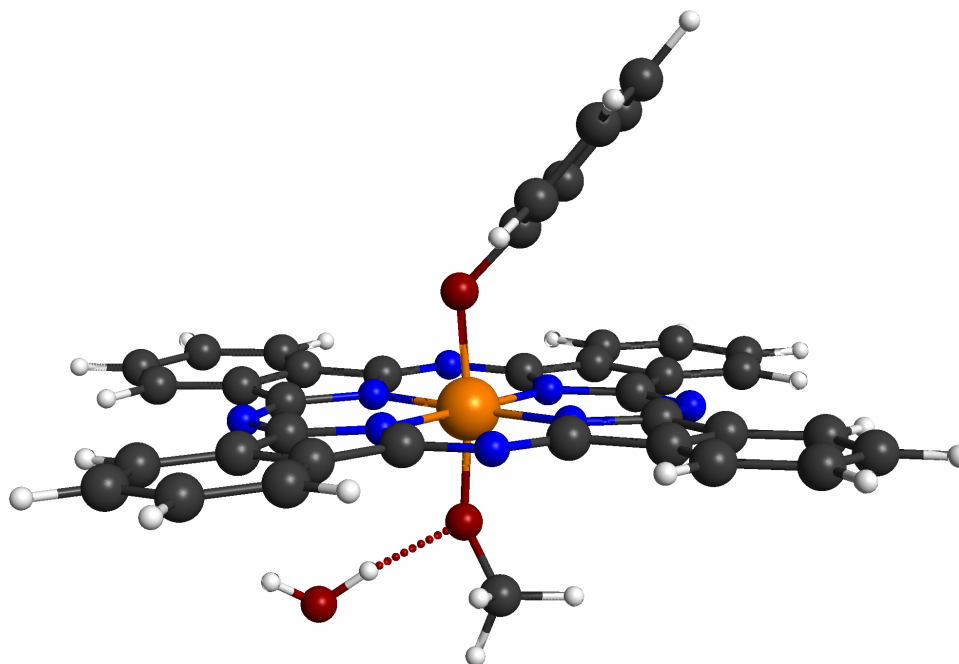
COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
SI	14.0	0.3174921202	0.2385279899	-0.3748943496
N	7.0	0.4469792894	2.1511438524	-0.4985137214
N	7.0	0.1139409700	-1.6869836475	-0.1797068251
N	7.0	1.6592233910	0.2308508774	1.0427624341
N	7.0	-1.0533643969	0.2250709134	-1.7652077073
C	6.0	-1.4953981806	1.3280754659	-2.4706745680
C	6.0	-1.7622441740	-0.8731711289	-2.2134749628
C	6.0	2.2983669836	1.3390573066	1.5561717096
C	6.0	2.1614111947	-0.8838835845	1.6900845367
C	6.0	-0.2204699187	2.9554838278	-1.4180506936
C	6.0	1.2825658498	2.9661704779	0.2526885308
C	6.0	-0.7736310414	-2.4987960114	-0.8843067258
C	6.0	0.8589095512	-2.5097949186	0.6667247466
N	7.0	-1.0929128276	2.6006987614	-2.3245424783
N	7.0	2.1217030939	2.6215856685	1.1962552446
N	7.0	-1.6371810197	-2.1464932131	-1.8019364056
N	7.0	1.7950686289	-2.1632117605	1.5114273885
C	6.0	1.1303447037	4.3507832782	-0.1890899094
C	6.0	0.1979519871	4.3428115622	-1.2349413228
C	6.0	3.2418986629	0.9312461086	2.5599294140
C	6.0	3.1564482160	-0.4797124377	2.6422450965

C	6.0	0.4237918399	-3.8920879685	0.4984940567
C	6.0	-0.5977653958	-3.8847223232	-0.4618436257
C	6.0	-2.6826691238	-0.4673874593	-3.2371862801
C	6.0	-2.5090505712	0.9282748304	-3.4042273775
C	6.0	1.7320024089	5.5365953621	0.2360049017
C	6.0	-0.1658816198	5.5216214308	-1.8888110594
C	6.0	1.3704467030	6.7181256075	-0.4150526537
C	6.0	0.4320999152	6.7105699712	-1.4653562939
C	6.0	4.1376757666	1.6472616844	3.3716222994
C	6.0	3.9627802281	-1.1977519110	3.5420740193
C	6.0	4.8460083362	-0.4829022826	4.3408945242
C	6.0	4.9335274555	0.9304704524	4.2562600099
C	6.0	0.8384507365	-5.0809616523	1.1040064059
C	6.0	-1.2358437224	-5.0653059149	-0.8495974904
C	6.0	-0.8233197950	-6.2549575571	-0.2469093773
C	6.0	0.2024862521	-6.2624419728	0.7191063260
C	6.0	-3.2774427497	1.6414188364	-4.3407720739
C	6.0	-3.6240602988	-1.1734357901	-4.0057916421
C	6.0	-4.2061663410	0.9369743314	-5.0954941130
C	6.0	-4.3785884287	-0.4616898677	-4.9291410261
H	1.0	-3.1448748068	2.7123930469	-4.4654503930
H	1.0	-4.8142107485	1.4626287115	-5.8273045211
H	1.0	-5.1157287300	-0.9809586908	-5.5362032666
H	1.0	-3.7553602967	-2.2438231769	-3.8747930162
H	1.0	-0.8886954779	5.5099980288	-2.6990554590
H	1.0	0.1715723527	7.6462139511	-1.9530619296
H	1.0	1.8195531759	7.6593452471	-0.1092048353
H	1.0	2.4562146612	5.5352852251	1.0450619562
H	1.0	4.2020917328	2.7296215109	3.3046226236
H	1.0	5.6365233000	1.4576571299	4.8960865950
H	1.0	5.4834571696	-1.0123365362	5.0444417455
H	1.0	3.8947139743	-2.2801282615	3.6051375343
H	1.0	1.6291422606	-5.0809146072	1.8481780651
H	1.0	0.5011312454	-7.2048583183	1.1705388490
H	1.0	-1.2994251479	-7.1914943813	-0.5249294347
H	1.0	-2.0258077710	-5.0530903289	-1.5944638733
O	8.0	1.6032920600	0.1059852451	-1.5432768316
O	8.0	-3.1084515451	2.0474661423	0.6147526810
C	6.0	1.6968656539	-0.8423628350	-2.5802958404
H	1.0	2.5975711152	-0.6225368769	-3.1679733005
H	1.0	1.7851573677	-1.8730552746	-2.2049090178
H	1.0	0.8347171412	-0.8051915900	-3.2629527012
C	6.0	-3.1850495803	3.0039961877	1.5719639765
C	6.0	-4.2844058784	3.8790822804	1.5377200439
C	6.0	-2.2225076177	3.1472444944	2.5869502238
C	6.0	-4.4155240706	4.8791850005	2.5009812997
C	6.0	-2.3669781308	4.1528794313	3.5456273057

C	6.0	-3.4598582730	5.0249430637	3.5130758237
H	1.0	-5.0219211410	3.7599633827	0.7483404903
H	1.0	-5.2711190569	5.5495401010	2.4599588893
H	1.0	-3.5652061553	5.8057437086	4.2614284879
H	1.0	-1.6153278055	4.2539295404	4.3255137392
H	1.0	-1.3734606798	2.4700612559	2.6102941584
O	8.0	-0.9503740175	0.4878821885	0.8535828213
H	1.0	-2.2759206752	1.5015912172	0.7124857516
H	1.0	-1.2438826595	-0.3581205929	1.2256023959

4a. Anion SiPc⁻(OPh)(OMe)--HOH: reactant for OMe displacement



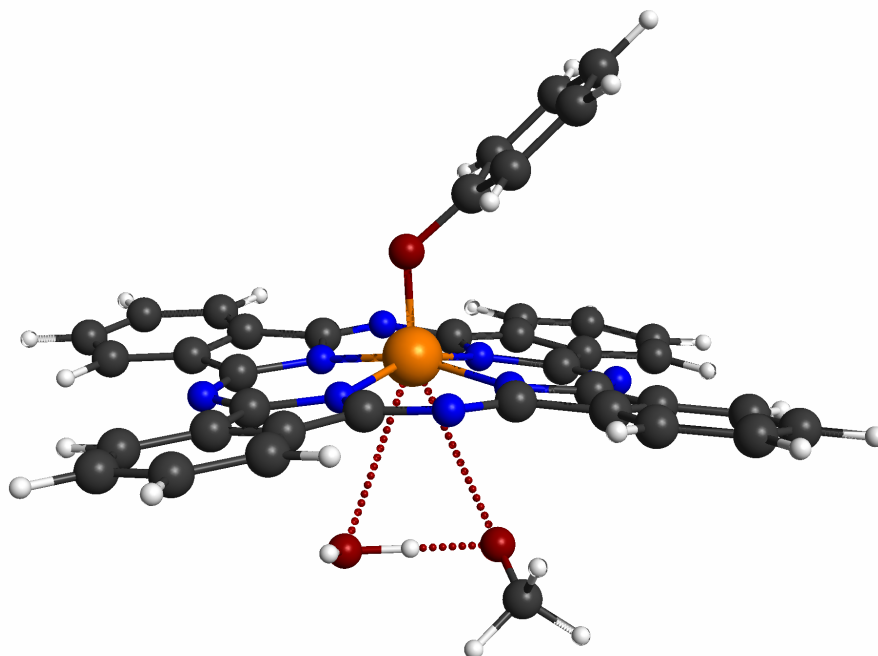
$E = -2453.98921 \text{ hartree}$

ATOM	CHARGE	X	Y	Z
SI	14.0	-0.0934330973	0.0604562356	-0.1245496674
N	7.0	-0.1044250706	1.9886321750	-0.1432781943
N	7.0	-0.1068966464	-1.8667876322	-0.0823078043
N	7.0	1.1892831411	0.0881481494	1.3448066924
N	7.0	-1.3815383667	0.0468878862	-1.5836976775
C	6.0	-1.8874754675	1.1495291073	-2.2435058572
C	6.0	-1.9632778901	-1.0777808897	-2.1410886057
C	6.0	1.7021211448	1.2117076695	1.9671718195
C	6.0	1.7704639759	-1.0180866560	1.9331067082
C	6.0	-0.8160752766	2.8012766776	-1.0249983736
C	6.0	0.6009832541	2.8277567360	0.7213822980
C	6.0	-0.8977638312	-2.6965982518	-0.8694458939
C	6.0	0.6597616919	-2.6739434711	0.7459563580
N	7.0	-1.6152680397	2.4402149746	-1.9939415370
N	7.0	1.4181606357	2.4942759187	1.6853380701
N	7.0	-1.7480759073	-2.3585553211	-1.8035164643
N	7.0	1.5330887724	-2.3107157483	1.6517812504
C	6.0	0.3243625562	4.2180205711	0.3790163699
C	6.0	-0.5523128728	4.2015910777	-0.7131938540
C	6.0	2.6360073710	0.8180965270	2.9823347859
C	6.0	2.6822151690	-0.5968985047	2.9580182632
C	6.0	0.3461220638	-4.0758472273	0.4820636347

C	6.0	-0.6330629378	-4.0891894002	-0.5197045362
C	6.0	-2.8627703874	-0.6863460176	-3.1884099259
C	6.0	-2.8116515351	0.7266706065	-3.2559164282
C	6.0	0.7762218205	5.4207925897	0.9271391820
C	6.0	-1.0105730045	5.3870283490	-1.2926566895
C	6.0	0.3212775972	6.6077988394	0.3503316347
C	6.0	-0.5625942497	6.5912215117	-0.7469453609
C	6.0	3.4291939353	1.5484910031	3.8845956895
C	6.0	3.5166425032	-1.3060717300	3.8389895337
C	6.0	4.2968950634	-0.5775637637	4.7270809765
C	6.0	4.2536851654	0.8406391459	4.7489973708
C	6.0	0.8287017428	-5.2612698603	1.0396250867
C	6.0	-1.1615783919	-5.2892481262	-0.9993464905
C	6.0	-0.6815877527	-6.4776034390	-0.4445749939
C	6.0	0.3027104789	-6.4639356685	0.5627884246
C	6.0	-3.5943803693	1.4328669881	-4.1854398570
C	6.0	-3.6939145219	-1.4186680274	-4.0540474883
C	6.0	-4.4150404262	0.7026996635	-5.0349495914
C	6.0	-4.4641398055	-0.7139647944	-4.9696113160
H	1.0	-3.5549915355	2.5173864102	-4.2327580984
H	1.0	-5.0318547073	1.2211085368	-5.7645313618
H	1.0	-5.1178758957	-1.2531510860	-5.6503950885
H	1.0	-3.7306730210	-2.5030450423	-4.0016106500
H	1.0	-1.6908278414	5.3675731821	-2.1387459251
H	1.0	-0.8988001954	7.5324774088	-1.1735992982
H	1.0	0.6527474628	7.5616972885	0.7518958781
H	1.0	1.4575145924	5.4276198515	1.7725942566
H	1.0	3.3946340479	2.6341084035	3.9001188590
H	1.0	4.8786192098	1.3786265650	5.4572201137
H	1.0	4.9534137566	-1.0984924006	5.4192344808
H	1.0	3.5479040650	-2.3917208564	3.8193111704
H	1.0	1.5868936141	-5.2442252570	1.8166736525
H	1.0	0.6560720308	-7.4055475627	0.9745680859
H	1.0	-1.0722446858	-7.4296597409	-0.7939512677
H	1.0	-1.9202896806	-5.2939807824	-1.7760777199
O	8.0	1.2309282446	-0.0756578308	-1.2847988419
O	8.0	-1.4149262186	-0.0376674725	1.0660942223
C	6.0	2.1704330239	0.9378255719	-1.5922099102
H	1.0	2.9662717147	0.4876759146	-2.1972326335
H	1.0	1.7200842195	1.7559488901	-2.1704910121
H	1.0	2.6347976801	1.3635379232	-0.6920220356
C	6.0	-2.4196819742	0.8117365183	1.3876978841
C	6.0	-3.6965982521	0.6434358310	0.8210671529
C	6.0	-2.2393091668	1.8101329353	2.3623552633
C	6.0	-4.7602558565	1.4573024842	1.2166621036
C	6.0	-3.3072953052	2.6215773071	2.7504968814
C	6.0	-4.5737585559	2.4529208684	2.1811326873

H	1.0	-3.8418150351	-0.1389093949	0.0816370298
H	1.0	-5.7411557510	1.3096601832	0.7698186212
H	1.0	-5.4038373534	3.0840414451	2.4879049968
H	1.0	-3.1487590184	3.3878619615	3.5063608659
H	1.0	-1.2584284532	1.9312419975	2.8124128397
O	8.0	2.9504883426	-2.2687706421	-1.4913297871
H	1.0	2.2643256606	-1.5657446597	-1.4341398596
H	1.0	3.1072965439	-2.4957435123	-0.5619137944

4b. Anion SiPc⁻(OPh)(MeO-H-OH): transition state for OMe displacement



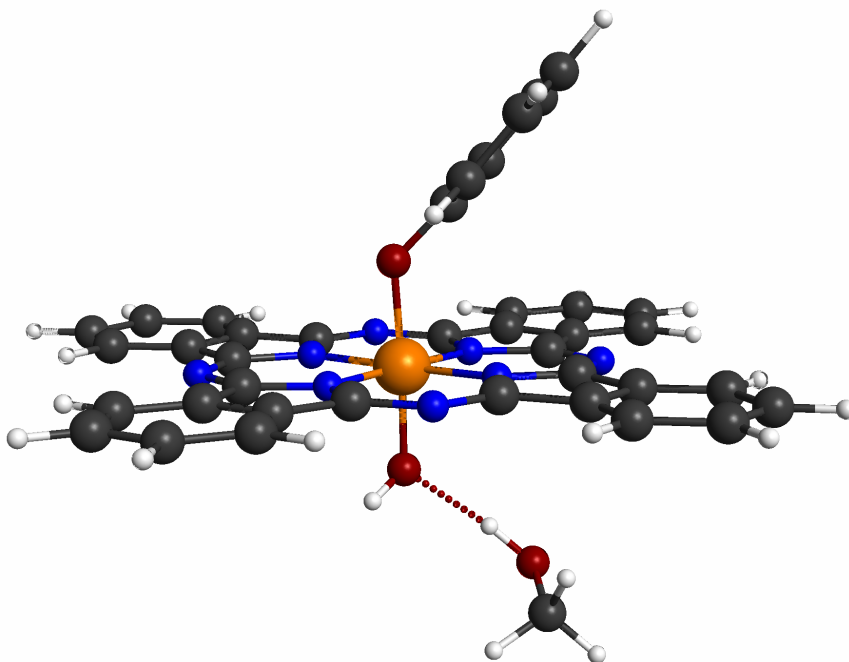
$E = -2453.91200$ hartree

ATOM	CHARGE	X	Y	Z
SI	14.0	-0.3225419297	-0.0248651609	0.1855568426
N	7.0	-0.0818419772	1.8455622681	-0.0370359282
N	7.0	-0.1693124135	-1.9103307238	0.0505975598
N	7.0	1.1865629456	-0.0298635014	1.3557084749
N	7.0	-1.3602175252	-0.0387107323	-1.4127551666
C	6.0	-1.7682870251	1.0586278890	-2.1733195029
C	6.0	-2.0148344887	-1.1479256098	-1.9594681967
C	6.0	1.7183919154	1.0843499318	2.0132700570
C	6.0	1.8449291105	-1.1417322979	1.8932554998
C	6.0	-0.6972926578	2.6815399828	-0.9839246656
C	6.0	0.6248319196	2.6980549421	0.8222057036
C	6.0	-1.0348826677	-2.7554496138	-0.6652342204
C	6.0	0.6624318894	-2.7586247739	0.7974826184
N	7.0	-1.4729219421	2.3398144374	-1.9659546292
N	7.0	1.4223471143	2.3663937892	1.7960370862
N	7.0	-1.9048458828	-2.4188568389	-1.5714281654
N	7.0	1.6014735362	-2.4247091809	1.6314901589
C	6.0	0.4067372309	4.0863864796	0.4479169796
C	6.0	-0.3967366357	4.0735091236	-0.6937929972
C	6.0	2.7088980423	0.6778390022	2.9545669931
C	6.0	2.7990123799	-0.7277829725	2.8682804721
C	6.0	0.3006464069	-4.1462765379	0.5656145600

C	6.0	-0.7744228509	-4.1430299423	-0.3263936245
C	6.0	-2.8209387531	-0.7524118571	-3.0665906511
C	6.0	-2.6553413459	0.6413948683	-3.2094438379
C	6.0	0.8711283978	5.2822692759	0.9996934881
C	6.0	-0.7717999119	5.2579445758	-1.3319504272
C	6.0	0.4964099988	6.4695522239	0.3686641331
C	6.0	-0.3136827226	6.4574479905	-0.7845727761
C	6.0	3.5225103789	1.4031576422	3.8464256203
C	6.0	3.6980287281	-1.4476012180	3.6788190282
C	6.0	4.4923737711	-0.7282573234	4.5571884948
C	6.0	4.4055221466	0.6888555090	4.6401910013
C	6.0	0.8172272263	-5.3399294123	1.0774863899
C	6.0	-1.3735790667	-5.3326375715	-0.7499909746
C	6.0	-0.8643973762	-6.5265304119	-0.2392329007
C	6.0	0.2186716060	-6.5300872130	0.6639898953
C	6.0	-3.3250254352	1.3504069112	-4.2250798178
C	6.0	-3.6549119595	-1.4773028209	-3.9395571913
C	6.0	-4.1469027961	0.6320522365	-5.0789426310
C	6.0	-4.3108374900	-0.7731403858	-4.9367646363
H	1.0	-3.1959364847	2.4233314313	-4.3307563434
H	1.0	-4.6783857406	1.1468833804	-5.8749262121
H	1.0	-4.9637837862	-1.3001039954	-5.6274816200
H	1.0	-3.7769783120	-2.5504821880	-3.8283812462
H	1.0	-1.3935524570	5.2419808308	-2.2217342791
H	1.0	-0.5844297867	7.3995024545	-1.2534383325
H	1.0	0.8356659146	7.4206919601	0.7697783204
H	1.0	1.4985429343	5.2844040888	1.8856209162
H	1.0	3.4526107480	2.4850164833	3.9066816446
H	1.0	5.0457465558	1.2168400644	5.3417651594
H	1.0	5.1965631092	-1.2524515308	5.1976897656
H	1.0	3.7606481282	-2.5295801542	3.6126453145
H	1.0	1.6515390124	-5.3359327201	1.7719249744
H	1.0	0.5906551926	-7.4779994082	1.0430860058
H	1.0	-1.3079380427	-7.4715882881	-0.5404497409
H	1.0	-2.2058717595	-5.3230538405	-1.4468204902
O	8.0	1.4999401974	1.0344373616	-2.4664700159
O	8.0	-1.5388582102	-0.0305877409	1.3747779632
C	6.0	2.4424253513	2.0158490399	-2.2804645748
H	1.0	3.4791672289	1.6250272833	-2.1248161121
H	1.0	2.5293357225	2.7239617153	-3.1414933804
H	1.0	2.2536057043	2.6708271649	-1.3955611093
C	6.0	-2.6378351949	0.7886711530	1.4842886696
C	6.0	-3.8486641541	0.4110808421	0.8892494656
C	6.0	-2.5717092585	1.9599945825	2.2500326546
C	6.0	-4.9820894530	1.2110343899	1.0490507795
C	6.0	-3.7106739441	2.7542865387	2.4031805734
C	6.0	-4.9186620702	2.3869840420	1.8027773288

H	1.0	-3.8927602876	-0.5086990056	0.3138049176
H	1.0	-5.9174631896	0.9113404923	0.5829456516
H	1.0	-5.8022187933	3.0076140036	1.9246936160
H	1.0	-3.6515129564	3.6634945205	2.9964565294
H	1.0	-1.6342793552	2.2347482397	2.7245157363
O	8.0	2.5009162422	-1.0021206016	-1.4338744073
H	1.0	2.0654844117	-0.1457926763	-1.9025642611

4c. Anion SiPc⁻(OPh)(OH)--HOMe: product for OMe displacement



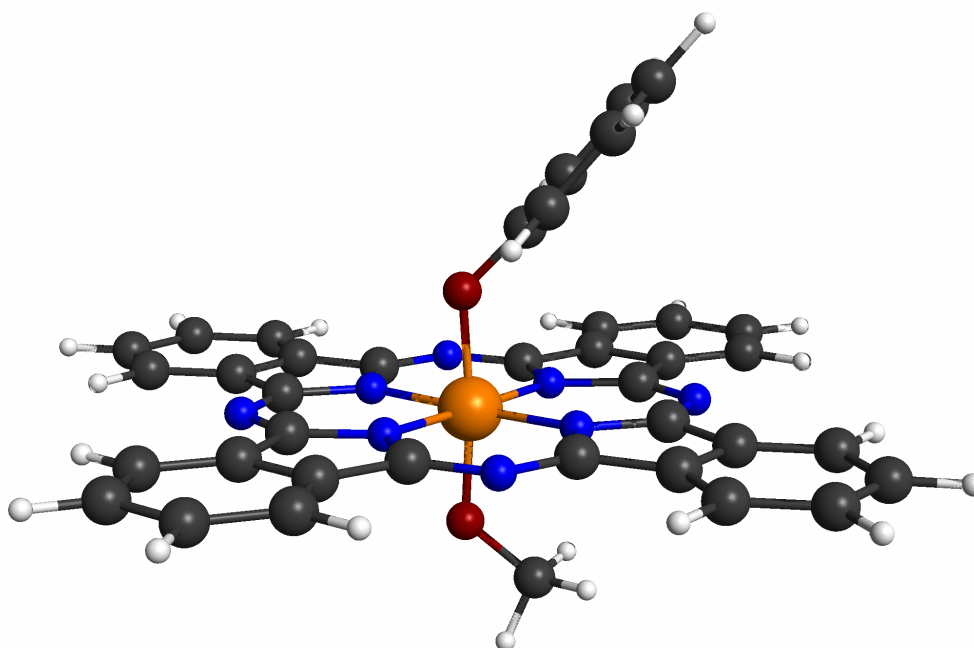
$E = -2453.99218$ hartree

SI	14.0	-0.0862716635	-0.0830686827	-0.0344810326
N	7.0	-0.0601819450	1.8511346328	-0.0651149994
N	7.0	-0.1256198421	-2.0207300169	0.0408607007
N	7.0	1.1897680664	-0.0706197989	1.4459886518
N	7.0	-1.3150364830	-0.0929752151	-1.5241517943
C	6.0	-1.8253205165	1.0140534003	-2.1741776710
C	6.0	-1.8900467410	-1.2184417808	-2.0942450022
C	6.0	1.7279898752	1.0551788563	2.0529786845
C	6.0	1.6923622219	-1.1802144627	2.1043052310
C	6.0	-0.7433260647	2.6635018787	-0.9633096390
C	6.0	0.6963296572	2.6805906368	0.7600253603
C	6.0	-0.8841836694	-2.8459637919	-0.7821459035
C	6.0	0.5815761127	-2.8307324379	0.9155590768
N	7.0	-1.5540557214	2.3043666697	-1.9235320339
N	7.0	1.5054450471	2.3383508252	1.7279609399
N	7.0	-1.6880578000	-2.5001117269	-1.7540083611
N	7.0	1.4170305312	-2.4710338069	1.8577326642
C	6.0	0.4708966419	4.0729682124	0.3852622047
C	6.0	-0.4273892962	4.0627484087	-0.6896505793
C	6.0	2.6031629679	0.6568317824	3.1147384322
C	6.0	2.5819727194	-0.7587773063	3.1469266398
C	6.0	0.2622280575	-4.2313758620	0.6465211590
C	6.0	-0.6552048442	-4.2399946581	-0.4126904617
C	6.0	-2.7805997746	-0.8205543682	-3.1448235653

C	6.0	-2.7400758951	0.5936934927	-3.1955388367
C	6.0	0.9775823967	5.2705712806	0.8945036536
C	6.0	-0.8519888444	5.2496152757	-1.2900514814
C	6.0	0.5548948345	6.4598626282	0.2972341654
C	6.0	-0.3498883774	6.4497353925	-0.7823482244
C	6.0	3.3960636517	1.3853292128	4.0201892020
C	6.0	3.3518388846	-1.4703633310	4.0841442985
C	6.0	4.1340789030	-0.7441877307	4.9712633124
C	6.0	4.1557353611	0.6751657783	4.9390704702
C	6.0	0.6977554350	-5.4186797967	1.2374845337
C	6.0	-1.1689573779	-5.4370937073	-0.9153059745
C	6.0	-0.7372268843	-6.6272586541	-0.3256683763
C	6.0	0.1857355054	-6.6184581096	0.7381102024
C	6.0	-3.5200933697	1.3049203964	-4.1238980253
C	6.0	-3.6010437229	-1.5486906237	-4.0250767388
C	6.0	-4.3288087856	0.5791163001	-4.9878030432
C	6.0	-4.3684099759	-0.8390302650	-4.9384477937
H	1.0	-3.4872962238	2.3901281176	-4.1584541351
H	1.0	-4.9432268010	1.1011357669	-5.7168235210
H	1.0	-5.0128450087	-1.3748259559	-5.6307205552
H	1.0	-3.6308173520	-2.6337912249	-3.9851089959
H	1.0	-1.5482451426	5.2354326033	-2.1231511584
H	1.0	-0.6598771319	7.3922385521	-1.2258025212
H	1.0	0.9289943211	7.4100781256	0.6690669113
H	1.0	1.6754237611	5.2723204816	1.7264099050
H	1.0	3.4109114049	2.4711636619	3.9943426253
H	1.0	4.7798184000	1.2108244371	5.6498637871
H	1.0	4.7413849499	-1.2663033294	5.7061855189
H	1.0	3.3322369954	-2.5562096236	4.1063148523
H	1.0	1.4092723330	-5.4057234831	2.0576480506
H	1.0	0.5026828044	-7.5613727159	1.1757446439
H	1.0	-1.1182717041	-7.5769625048	-0.6917431308
H	1.0	-1.8801578904	-5.4382846137	-1.7358487213
O	8.0	1.6299692191	1.4255093896	-3.4324831283
O	8.0	-1.4245861758	-0.1503818448	1.1313447254
C	6.0	2.6412583483	2.3380130977	-3.0475013566
H	1.0	3.5685977005	1.8358115237	-2.7245161461
H	1.0	2.8855491112	2.9575566125	-3.9180823796
H	1.0	2.3214846180	3.0100612372	-2.2353285285
C	6.0	-2.3996222067	0.7394827626	1.4384335012
C	6.0	-3.6744813035	0.6140982241	0.8573126824
C	6.0	-2.1931306188	1.7360700137	2.4091036574
C	6.0	-4.7120156374	1.4691324031	1.2346648050
C	6.0	-3.2349998742	2.5888434780	2.7791939396
C	6.0	-4.5000269462	2.4631712301	2.1954530911
H	1.0	-3.8381844771	-0.1662683553	0.1195681238
H	1.0	-5.6921226391	1.3555627212	0.7763097955

H	1.0	-5.3097550819	3.1265264325	2.4882632701
H	1.0	-3.0573465929	3.3543736535	3.5315401004
H	1.0	-1.2131968142	1.8242842192	2.8688492725
O	8.0	1.2356683925	-0.1532819010	-1.2039012384
H	1.0	1.4201012263	0.8718495408	-2.6439434118
H	1.0	2.0943380716	-0.1356966131	-0.7532402032

5. SiPc(OPh)(OMe): isolated neutral species; no H₂O molecule



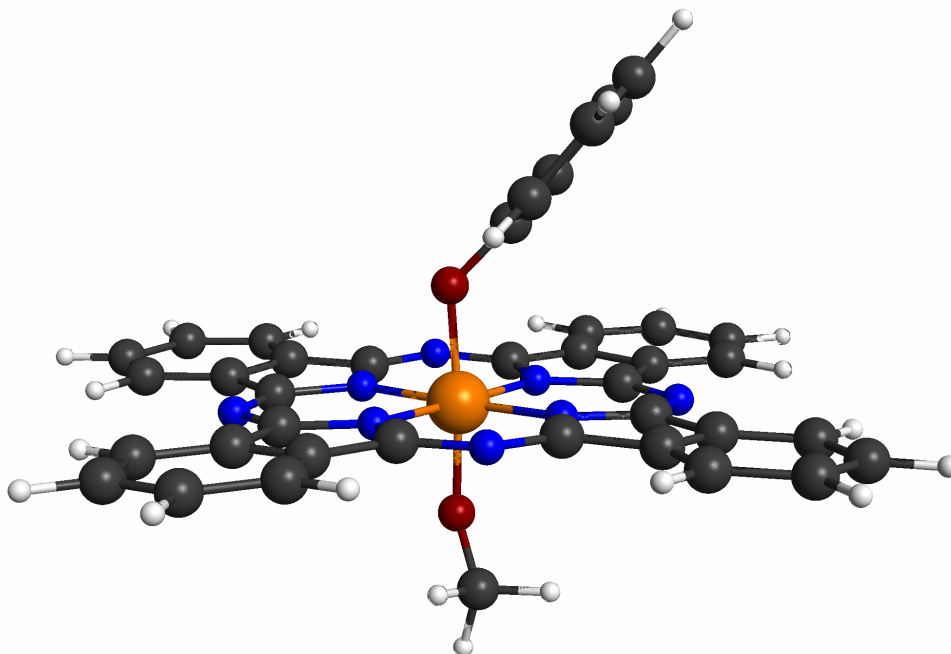
$E = -2377.47880 \text{ hartree}$

ATOM	CHARGE	X	Y	Z
SI	14.0	-0.0179648652	0.0776096813	-0.2144735456
N	7.0	-0.0376000420	2.0159560701	-0.2407478973
N	7.0	-0.0325966927	-1.8575430469	-0.1568832473
N	7.0	1.2438019804	0.1015171383	1.2606464324
N	7.0	-1.3104230453	0.0621049505	-1.6668822425
C	6.0	-1.8608926640	1.1629562014	-2.2918932407
C	6.0	-1.8583495886	-1.0668515078	-2.2437352294
C	6.0	1.7938920565	1.2281530926	1.8368903019
C	6.0	1.7680405738	-0.9985345280	1.9051624930
C	6.0	-0.7642596941	2.8196651476	-1.1005372598
C	6.0	0.7306021328	2.8434428010	0.5563582531
C	6.0	-0.7811654744	-2.6817404242	-0.9725102674
C	6.0	0.6845435243	-2.6568817604	0.7060404151
N	7.0	-1.6097820912	2.4365873704	-2.0410856876
N	7.0	1.5693342474	2.4904473091	1.5156963670
N	7.0	-1.6173205856	-2.3291379591	-1.9333272260
N	7.0	1.5165125524	-2.2724657455	1.6591525042
C	6.0	0.4860964848	4.2291721933	0.2002650000
C	6.0	-0.4570751579	4.2145749586	-0.8405464540
C	6.0	2.7056826931	0.8386883882	2.9005025054
C	6.0	2.6883788098	-0.5647783194	2.9444550062
C	6.0	0.3939487743	-4.0553185551	0.4332119746

C	6.0	-0.5302244725	-4.0705800572	-0.6239916819
C	6.0	-2.7914163466	-0.6771449515	-3.2872063538
C	6.0	-2.7928160117	0.7277374554	-3.3174604531
C	6.0	1.0047219120	5.4298259130	0.6941004205
C	6.0	-0.9137219943	5.4002273011	-1.4233299666
C	6.0	0.5498579421	6.6130273668	0.1139821743
C	6.0	-0.3978350407	6.5983346412	-0.9312930156
C	6.0	3.5017994455	1.5828291363	3.7746261084
C	6.0	3.4657381568	-1.2720693486	3.8641136576
C	6.0	4.2626220350	-0.5308944447	4.7373991716
C	6.0	4.2807361731	0.8782191295	4.6929173074
C	6.0	0.8504638508	-5.2400469214	1.0156614820
C	6.0	-1.0299603742	-5.2711795516	-1.1345646908
C	6.0	-0.5755453170	-6.4555337998	-0.5541391169
C	6.0	0.3528380391	-6.4400798513	0.5070152028
C	6.0	-3.5944727086	1.4343231840	-4.2176605497
C	6.0	-3.5936409441	-1.4221632807	-4.1563114142
C	6.0	-4.3952265474	0.6920635483	-5.0852390811
C	6.0	-4.3949485740	-0.7182779486	-5.0545622241
H	1.0	-3.5914547835	2.5195775993	-4.2374337675
H	1.0	-5.0312146051	1.2071642273	-5.7995442607
H	1.0	-5.0316565974	-1.2639768510	-5.7451363287
H	1.0	-3.5902398500	-2.5072595561	-4.1293989251
H	1.0	-1.6418570108	5.3842464328	-2.2280690676
H	1.0	-0.7291113796	7.5403321920	-1.3592212488
H	1.0	0.9305774331	7.5659582848	0.4705974672
H	1.0	1.7344008286	5.4360305922	1.4975828267
H	1.0	3.5121144261	2.6675946551	3.7370616447
H	1.0	4.9132268799	1.4230924879	5.3880272884
H	1.0	4.8806523775	-1.0468798815	5.4667380236
H	1.0	3.4485501790	-2.3569529003	3.8949168996
H	1.0	1.5641297967	-5.2237139208	1.8333354986
H	1.0	0.6844603476	-7.3819325633	0.9350675128
H	1.0	-0.9425110374	-7.4089151066	-0.9237870879
H	1.0	-1.7454565722	-5.2782731149	-1.9507741976
O	8.0	1.3247356960	0.0009963539	-1.2985762218
O	8.0	-1.3320004833	-0.0201623304	0.9624073443
C	6.0	1.5366337537	0.7035514266	-2.5036120435
H	1.0	2.4945105438	0.3755052181	-2.9230325073
H	1.0	0.7545462363	0.5024644003	-3.2497960932
H	1.0	1.5908713909	1.7915639740	-2.3501446216
C	6.0	-2.3429655100	0.8324489675	1.2794720739
C	6.0	-3.6241460529	0.6338718621	0.7371457210
C	6.0	-2.1518585930	1.8633445179	2.2151842763
C	6.0	-4.6851187781	1.4611778772	1.1118371289
C	6.0	-3.2173009209	2.6876893370	2.5827519360
C	6.0	-4.4883950476	2.4950735251	2.0323810728

H	1.0	-3.7782652649	-0.1802218557	0.0347556137
H	1.0	-5.6705121021	1.2932866603	0.6832990397
H	1.0	-5.3158147558	3.1374433395	2.3217482922
H	1.0	-3.0520167820	3.4817611930	3.3072556096
H	1.0	-1.1686918845	2.0009537602	2.6553216787

6. SiPc⁻(OPh)(OMe): isolated anion radical species; no H₂O molecule



$E = -2377.59896 \text{ hartree}$

ATOM	CHARGE	X	Y	Z
SI	14.0	0.0221198490	0.0618530711	-0.1889161610
N	7.0	0.0129054398	1.9942882004	-0.2157167717
N	7.0	-0.0075742516	-1.8671437556	-0.1266006051
N	7.0	1.2667773771	0.0957224058	1.3136322825
N	7.0	-1.2569906628	0.0386154803	-1.6574603852
C	6.0	-1.7438961293	1.1396878926	-2.3353263453
C	6.0	-1.8395399585	-1.0859381415	-2.2092827115
C	6.0	1.7686547534	1.2223134116	1.9377761389
C	6.0	1.8166619556	-1.0090872244	1.9355899558
C	6.0	-0.6597420292	2.7985933527	-1.1336989097
C	6.0	0.7266165716	2.8345976561	0.6355762603
C	6.0	-0.7891950004	-2.6989102599	-0.9167304872
C	6.0	0.7390418247	-2.6692812950	0.7267524227
N	7.0	-1.4523595888	2.4299630816	-2.1055296457
N	7.0	1.5152454161	2.5048859140	1.6255645543
N	7.0	-1.6313435561	-2.3660488904	-1.8616977208
N	7.0	1.5802979626	-2.3017295529	1.6592915417
C	6.0	0.4943616847	4.2233376429	0.2514301251
C	6.0	-0.3634749090	4.2003793031	-0.8561070747
C	6.0	2.6630422920	0.8333235051	2.9902647307
C	6.0	2.6956765553	-0.5825398617	2.9865640261
C	6.0	0.4302116805	-4.0729340182	0.4634482378

C	6.0	-0.5301221290	-4.0911344866	-0.5567324998
C	6.0	-2.7256506887	-0.6983239701	-3.2704255983
C	6.0	-2.6610887955	0.7137411813	-3.3529637762
C	6.0	0.9712320710	5.4276803925	0.7736100454
C	6.0	-0.7759457093	5.3816567623	-1.4768108996
C	6.0	0.5615974829	6.6106837815	0.1555392069
C	6.0	-0.3023507109	6.5878403099	-0.9571547206
C	6.0	3.4341511905	1.5685265647	3.9076886066
C	6.0	3.4942062972	-1.2868334334	3.9043161454
C	6.0	4.2531846495	-0.5534695276	4.8066298028
C	6.0	4.2238620564	0.8653649847	4.8076373193
C	6.0	0.9002321818	-5.2562089288	1.0364108029
C	6.0	-1.0524114092	-5.2931276635	-1.0380018262
C	6.0	-0.5850923851	-6.4792385852	-0.4674253522
C	6.0	0.3808722338	-6.4609759571	0.5573791977
C	6.0	-3.4263260293	1.4153511113	-4.3005315869
C	6.0	-3.5526423854	-1.4329967109	-4.1376835007
C	6.0	-4.2433065361	0.6826711278	-5.1515521403
C	6.0	-4.3063433898	-0.7325648650	-5.0703855170
H	1.0	-3.3762930172	2.4988599156	-4.3606277839
H	1.0	-4.8462468848	1.1980299298	-5.8948750928
H	1.0	-4.9567635013	-1.2738622847	-5.7527386515
H	1.0	-3.5991798824	-2.5164337622	-4.0735784019
H	1.0	-1.4404294388	5.3581156526	-2.3353390033
H	1.0	-0.6026669483	7.5256432269	-1.4169977640
H	1.0	0.9140321884	7.5657276538	0.5360528593
H	1.0	1.6376853092	5.4388719911	1.6308584341
H	1.0	3.4100376136	2.6545921194	3.9070346221
H	1.0	4.8315786773	1.4069297547	5.5281090266
H	1.0	4.8816462447	-1.0706726061	5.5271831095
H	1.0	3.5151629440	-2.3729538206	3.9009695985
H	1.0	1.6434448771	-5.2359094557	1.8277970122
H	1.0	0.7247852720	-7.4006428361	0.9815596916
H	1.0	-0.9715558614	-7.4326958906	-0.8177478433
H	1.0	-1.7976665178	-5.3011376782	-1.8276991374
O	8.0	1.3278615942	-0.0564120158	-1.3404235799
O	8.0	-1.3249092313	-0.0198875571	0.9842866448
C	6.0	2.4182792203	0.8237592478	-1.4759944532
H	1.0	3.1102365990	0.4061340252	-2.2192475560
H	1.0	2.1141457098	1.8221704876	-1.8249743330
H	1.0	2.9754005461	0.9509561447	-0.5355401617
C	6.0	-2.3228864673	0.8451302792	1.2795417908
C	6.0	-3.5950336293	0.6835481449	0.6993754564
C	6.0	-2.1452952510	1.8559718933	2.2424856278
C	6.0	-4.6546903039	1.5146455332	1.0692756041
C	6.0	-3.2089289725	2.6846718605	2.6050370012
C	6.0	-4.4699060160	2.5221133793	2.0216877029

H	1.0	-3.7395267472	-0.1068560866	-0.0315785916
H	1.0	-5.6312536363	1.3715374503	0.6114095354
H	1.0	-5.2967495999	3.1669584299	2.3081364993
H	1.0	-3.0512571555	3.4600718072	3.3518257609
H	1.0	-1.1688980255	1.9735155608	2.7030657486