Supporting Information

Ligand release of silicon phthalocyanine dyes triggered by X-ray irradiation

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MATERIALS AND METHODS

Reagents and general information

Compounds **1-4** were synthesized according to literature methods.[1] General chemicals were of the best grade available, supplied by FUJIFILM Wako Pure Chemical Corporation (Osaka, Japan), Tokyo Chemical Industries Co, Ltd. (Tokyo, Japan), KANTO CHEMICAL Co., INC. (Tokyo, Japan) and Sigma-Aldrich Co. LLC (St. Louis, MO, USA), and were used without further purification. MALDI-TOF mass spectra (MS) were recorded with an AB SCIEX TOF/TOF 5800 mass spectrometer (Tokyo, Japan), High performance liquid chromatography (HPLC) analyses were carried out on an HPLC system (Shimadzu Corporation, Kyoto, Japan) equipped with reverse-phase columns, Inertsil ODS-3 (4.6 mm × 250 mm) (GL Sciences Inc., Tokyo, Japan), using eluent A (0.1 M triethylammonium acetic acid (TEAA)) and eluent B (99% CH_3CN/1% H_2O). X-rays were generated by a CLINAC (Varian Medical Systems, Palo Alto, CA, USA) or an X-Rad iR-225 (Precision X-Ray, North Branford, CT, USA).

X-ray irradiation of phthalocyanine derivatives

For irradiation with CLINAC, a 5 μM solution of compounds **1-4** in 0.1 M phosphate buffer (pH7.0) without or with 0.1 M HCOONa was prepared in a vial. The solution was bubbled with Ar or N_2O gas through the septum cap of the sealed vial to remove oxygen. For irradiation with the X-Rad iR-225, a 500 μM solution of compound **1-4** in 0.1 M phosphate buffer (pH7.0) without or with 1 M HCOONa was filled into a gas-permeable polymethylpentene (TPXTM) tube (0.76 mm I.D. × 1.0 O.D. × 60 mm long, Toho Kasei Sangyo Co.,Ltd, Tokyo, Japan), which was then sealed at both end; this TPX tube was then placed into a 5ϕ ESR tube (5 mm O.D. × 250 mm long, S-5-ESR-250S, Norell Inc., Morganton, NC, USA). Ar or N_2O gas was supplied to the ESR tube through a long capillary glass tube to remove oxygen from the sample, and the tube was subsequently sealed.

After the samples were prepared, each solution was irradiated using the CLINAC or X-Rad iR-225. The irradiated solution was analyzed by HPLC (eluent A/eluent B = 75/25 to 60/40 in 5 min, 60/40 to 0/100 in 10 min for compound **2**; eluent A/eluent B = 80/20 to 0/100 in 10 min for compounds **1**, **3** and **4**). Methylene blue (MB) was used as an internal standard. X-rays were generated using the X-Rad iR-225 at a dose rate of 210 Gy/min, if not otherwise described. All the experiments were carried out at room temperature. Fig. 3e, Fig. 4a, and Fig. 5b were made from single measurement. Data in Fig. 3b represents the mean (n = 2). Data in Fig. 4b and Fig. 5d represents the mean ± SEM (n = 3 or 4).

For MS analysis, a solution of 5 μM compound **2** in 0.1 M sodium phosphate buffer (pH7.0) with 0.1 M HCOONa was prepared with [^{18}O]H_2O (Taiyo Nippon Sanso Corp., Tokyo, Japan) or H_2O. The solution was bubbled with Ar through the septum cap of the sealed vial. The solution was then irradiated using the CLINAC at 20 Gy. After irradiation, the solution was analyzed by MALDI-TOF

MS.

ESR measurement

As previously described, 5φ ESR quartz tube with a TPX capillary tube containing a phthalocyanine derivative solution (0.1 M phosphate buffer pH 7.0) with 1 M HCOONa was sealed under Ar or N_2O gas. The ESR measurement area at the bottom of the ESR quartz tube was covered by a lead plate and shielded against the scatter X-rays, and the TPX capillary tube containing the sample was placed on the opposite side of the quartz tube such that only the TPX capillary tube was irradiated with X-rays. This configuration was used to avoid undesired glass-derived radicals in the measurement area of the ESR quartz tube as a result of X-ray irradiation.

After compounds **1-4** were exposed to 210 Gy X-rays at room temperature, the TPX tube was quickly moved to the bottom of the ESR quartz tube and placed in the ESR cavity, where the temperature was maintained at 110 K using a temperature controller (ES-DVT3; JEOL, Tokyo, Japan); ESR spectra of the frozen-samples were then recorded. In the case of analysis of the decay kinetics of anion radicals in compound **2**, the ESR quartz tube containing the sample was placed in the ESR cavity at room temperature immediately after irradiation, and ESR spectra at 298 K were recorded 2.5, 5, 10, 15, and 30 min after X-ray irradiation. All ESR spectra were recorded using a JEOL-RE1X spectrometer. The EPR parameters were as follows: incident microwave power, 10 mW; microwave frequency, 9.4335 GHz; modulation frequency, 100 kHz; field modulation amplitude, 0.1 mT; time constant, 0.3 s; scan range, 336.79 ± 5 mT; sweep time, 8 min/10 mT; receiver gain, 5.0×10^2. The line width, intensity, and g-value of the EPR signal were estimated using the signal of a co-mounted Mn^{2+} marker (ES-DM1; JEOL) in the cavity and the Win-Rad software (Radical Research, Tokyo, Japan). The concentration of IR700 anion radicals was estimated using a standard curve created by the double integration of the EPR signals of DPPH in methanol.

Quantum chemical calculation

All density functional theory (DFT) calculations were performed using Gaussian16[2] with the long-range and dispersion corrected ωB97X-D functional.[3] The spin-unrestricted self-consistent field calculations were performed for singlet-state calculations. The aug-cc-pVDZ basis set[4] was adopted for N and O atoms, whereas the cc-pVDZ basis set[5,6] was used for all other atoms. The water solvent effect was considered using the integral equation formalism variant of the polarizable continuum model (IEFPCM).[7] The normal mode analyses were performed at the optimized structures to confirm the stability, whereas the thermally corrected Gibbs energies at 298.15 K and 1 atm were evaluated using Grimme's qRRHO approximation[8] implemented in the Goodvibes program.[9]

SUPPORTING DATA

Molecular geometry (.xyz) files containing optimized molecular coordinates by the quantum chemical calculation and its energy are available via the following website: https://github.com/k-masato/SiPc_X-ray_structures. The data are also shown below.

Geometry optimized cartesian coordinates of SiPc(OX)$_2$ of compound **1** (neutral).
E=-7641.668735 (radical: -7641.805457) / qh-G(298.15K)=-7640.411472 (wB97X-D/(aug-)cc-pVDZ, water solv.)

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C    1.0443861193    -5.7585804706   -0.9733241723
C    0.5109762645    -4.5687035807   -0.4761574749
C    -0.5119580258   -4.5686250617    0.4758344522
C    -1.045616813    -5.7584219692    0.9729306819
C    -0.5170057077   -6.9460578293    0.4791120766
C    0.7937924451    -3.1755293815   -0.7699543711
N    -0.0002292349   -2.3686260569   -0.0000567598
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C	0.3855492887	6.0734405234	-0.5881006096
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O	-1.3478269227	-0.3980412905	-1.0875168225
Si	-1.9273999783	-0.9832997969	-2.5550327904
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O   -9.8549843166    0.5005135781    -2.4339246262
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O   -7.6465222485   -4.6056354705     1.306019786
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O	1.3476150234	-0.3981744787	1.0875706329
Si	1.9277916289	-0.9847049806	2.5543281264
C	3.6508810525	-0.2574849453	2.808523892
C	4.6182338309	-0.5012496601	1.6377045169
C	4.6074841428	0.7009354352	0.7085729115
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C	7.0387380242	0.744570014	0.0015212023
C	7.4150506036	1.8231694959	1.0240442418
C	7.3767436981	1.4483376309	2.5054297877
S	8.5091699111	0.112286163	2.9796618172
O	9.8550086294	0.5002260438	2.4337913513
O	8.4616366468	0.0755724203	4.4805243029
O	7.9690275079	-1.1463804472	2.3486569371
C	5.3707393662	-0.630107282	-1.2386553542
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H	3.6103061647	0.8187948927	0.2592551328
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H   4.8698803527   3.8815353543   -2.9902077418

H   3.4144033389   3.8141993213   -1.9531367543

H   0.6247505015   0.6005203976   3.9827512153

Geometry optimized cartesian coordinates of SiPc(OX)$_2$ of compound **1** (radical).

E=-7641.812208 / qh-G(298.15K)=-7640.556707 (wB97X-D/(aug-)cc-pVDZ, water solv.)

Si   0.0002329381   -0.3926689618   0.0019722662

C   -0.5357678112   -6.9144419427   0.4727931732

C   -1.0792434119   -5.7207026316   0.9435427705

C   -0.5276949854   -4.5338880736   0.4662220842

C   0.5242994936   -4.5361248113   -0.4464541175

C   1.0747292527   -5.7252730409   -0.9192372244

C   0.5301279616   -6.9166934584   -0.4439346376

C   -0.8180808353   -3.1318886137   0.7651204644

N   -0.0006626038   -2.3213226453   0.0056634196

C   0.8160013922   -3.1355493664   -0.750701933

N   -1.6637905132   -2.7849514313   1.6910530814

C   -1.816253324   -1.4999384952   2.0586048558

N   1.2549506171   -0.39959021   -1.4719209285

C   1.670672345   0.6992954184   -2.1782228131

C   2.5166515121   0.2866782367   -3.2543222266

C   2.6079844793   -1.1175500363   -3.1734953567

C   1.8156868382   -1.5094714043   -2.0504041703

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N   1.3884458001   1.9900831964   -1.9237444128
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H   1.3792876631   4.9354576299   -2.1109331257
O   1.3553069121   -0.3497323639   1.1105271956
Si   1.8706994111   -0.9229085077   2.596987449
C   3.6418402522   -0.3073374171   2.8518752592
C   4.574214735   -0.5557916367   1.6557622048
C   4.5494938009   0.6523348556   0.7336172275
N   5.522904147   0.6142105568   -0.4220907666

C	6.9742263834	0.6938264572	0.0091197538
C	7.3617181969	1.757520013	1.0437799639
C	7.3427155854	1.3594462224	2.5194609594
S	8.4917206614	0.0268820368	2.9617219783
O	9.8292980517	0.4363473475	2.4104621825
O	8.4590875046	-0.0335321709	4.4625899805
O	7.9585784541	-1.2273553691	2.3166480344
C	5.2877305503	-0.6590775646	-1.232910576
C	6.0557837496	-1.9165481776	-0.8378056629
C	5.3936813799	-3.1085969296	-1.5205580782
S	6.0985840613	-4.68723296	-0.9909241917
O	5.3350210262	-5.7302886677	-1.7601320392
O	7.5588147494	-4.6410298329	-1.3513084339
O	5.8660139119	-4.7636949097	0.4937457303
C	5.1639702489	1.730146957	-1.3876090213
C	5.2101370481	3.1723106572	-0.9031077684
C	4.4734119178	4.0264168289	-1.929582823
S	4.6983765121	5.7968111316	-1.6320754506
O	4.3021309051	6.0364854245	-0.201335518
O	3.7950606384	6.4785624131	-2.6220111127
O	6.1573368299	6.0704123543	-1.8817196927
C	0.8606191833	-0.2916089163	4.0524510513
C	1.9277949181	-2.8070868169	2.6361312728
H	2.4845540781	-3.1395841319	3.5264977967
H	2.4325353295	-3.2143553013	1.7453598276
H	0.9195826143	-3.2439413907	2.689470127
H	3.6405696535	0.760220395	3.1331907676
H	4.0248576913	-0.8469328455	3.733996455
H	5.6006350195	-0.7607265743	1.9915587064
H	4.2402674975	-1.4498923069	1.1075919247
H	3.5477600942	0.7653312216	0.2933375029
H	4.7688655577	1.5640669	1.3005322602
H	7.5328721535	0.854810947	-0.9211187222
H	7.2499825325	-0.2882065679	0.4023727014
H	6.7659798639	2.6709050985	0.9435735073
H	8.3909975341	2.052645066	0.7947105986

H	7.6648288248	2.2157624327	3.1270042243
H	6.3593163584	1.0406256246	2.8887430428
H	5.5143128144	-0.4140195326	-2.2780334077
H	4.2072800462	-0.8332384203	-1.1671371985
H	6.052753672	-2.0810655181	0.245683823
H	1.4217741534	-0.4814059422	4.9816324072
H	7.1036488301	-1.8473869913	-1.1591371947
H	5.5095407468	-3.0746559629	-2.6124009392
H	4.3201779097	-3.1764108919	-1.2852166103
H	5.8344728421	1.6104132215	-2.2481615805
H	4.1467664321	1.4918597434	-1.719870553
H	4.7218756609	3.299637313	0.0722047362
H	6.2471769561	3.5236708026	-0.8225866232
H	-0.1136985645	-0.793965249	4.1389652042
H	4.8455766625	3.8559602951	-2.9503870063
H	3.3918276986	3.8304754962	-1.9100195102
H	0.6877159709	0.7931166949	3.9738947541
O	-1.3548080759	-0.3527214967	-1.1067345279
Si	-1.8707424207	-0.9310976782	-2.5909903043
C	-3.6413148329	-0.3148631017	-2.8482139183
C	-4.5739034063	-0.5578974742	-1.6511535008
C	-4.5480775588	0.6537186331	-0.733628762
N	-5.521524175	0.6208986668	0.42221197
C	-6.9727716646	0.7002318078	-0.0093022707
C	-7.3592561196	1.7603233105	-1.0480273604
C	-7.340625477	1.3565868543	-2.5221739809
S	-8.4908519556	0.0233943066	-2.9593345966
O	-9.8280506461	0.4361889709	-2.4096409137
O	-8.4582813389	-0.0427866998	-4.4599606913
O	-7.958856363	-1.2288578333	-2.3094731025
C	-5.2875379383	-0.6495101297	1.2378773253
C	-6.0567441595	-1.907769812	0.8475525705
C	-5.3956859457	-3.0978391523	1.5347583562
S	-6.1019924643	-4.677816305	1.0110198173
O	-5.3393556597	-5.7186769241	1.7841091052
O	-7.5621771379	-4.6289693623	1.3712391434

O	-5.8695019157	-4.7600171777	-0.4733563089
C	-5.1615523516	1.7401660689	1.3834782017
C	-5.2063469593	3.1805184494	0.8934946792
C	-4.468876085	4.0378130956	1.9167710622
S	-4.6920445894	5.8072818426	1.6124816262
O	-4.2953897345	6.0411027124	0.1808890784
O	-3.7881670878	6.4919014606	2.5999240251
O	-6.150761199	6.0832818286	1.8609067902
C	-0.8600854451	-0.3063029585	-4.0488578896
C	-1.9295981521	-2.815355905	-2.6229478532
H	-2.4865604843	-3.1507152834	-3.5121137899
H	-2.4348393143	-3.2187557515	-1.7307007057
H	-0.9217933887	-3.2533633138	-2.6744947296
H	-3.6390547202	0.7516148595	-3.1335890551
H	-4.0248432392	-0.8574567109	-3.7282715422
H	-5.6005125165	-0.7631832421	-1.9861567568
H	-4.240761988	-1.4501986784	-1.0995716628
H	-3.546241259	0.7674795027	-0.2937794513
H	-4.7666155032	1.5634808222	-1.3040196414
H	-7.5312640626	0.8653061241	0.9203112344
H	-7.2494565528	-0.2830384241	-0.3987936903
H	-6.7626520807	2.673520351	-0.9513129239
H	-8.3882552952	2.0573750707	-0.8000940656
H	-7.6619558156	2.2108662211	-3.1329905174
H	-6.3575187025	1.0354560579	-2.8902321358
H	-5.5139117984	-0.4002624512	2.2820535508
H	-4.2072477252	-0.8249155987	1.1727876459
H	-6.0539225756	-2.0763818491	-0.235306646
H	-1.4214109926	-0.4991489383	-4.977307846
H	-7.1045301051	-1.8364457931	1.168670332
H	-5.5115056968	-3.0597188274	2.6264679582
H	-4.3222452154	-3.1674777485	1.2996631757
H	-5.8321757849	1.62434014	2.2444717964
H	-4.1445764583	1.5021930081	1.716658187
H	-4.7179096017	3.3036803566	-0.0822647187
H	-6.2430506362	3.5325465749	0.8115794903

H   0.1137743404   -0.8098750537   -4.1334378897

H   -4.8413214228   3.8716339585   2.9381780874

H   -3.3874850927   3.8407250785   1.8980691137

H   -0.686192179   0.778557161   -3.9744577104

Geometry optimized cartesian coordinates of SiPc(OX)$_2$ of compound **2** (neutral).

E=-6981.505364 (radical: -6981.643334) / qh-G(298.15K)=-6980.330872 (wB97X-D/(aug-)cc-pVDZ, water solv.)

Si   -0.5608989914   -0.3924483435   0.5846048614

C   -1.3371021315   -6.8918564316   0.7967193315

C   -0.5481127574   -5.8935432832   0.2356372842

C   -0.8681713048   -4.5736532385   0.5584572811

C   -1.9295206653   -4.2673653519   1.4159214465

C   -2.7282043368   -5.2671043759   1.9739183001

C   -2.4169568569   -6.5825668278   1.6473012614

C   -0.2936894583   -3.3045008898   0.1518255772

N   -0.9545653273   -2.2754693607   0.7706281201

C   -1.9423653667   -2.8220564028   1.5479671534

N   0.6741978697   -3.2155988118   -0.7396686988

C   1.1273374658   -2.0566738084   -1.1729527789

N   -1.896502508   0.0200292403   1.9121750187

C   -2.156549226   1.2568985901   2.4354989624

C   -3.1790082579   1.1511896898   3.4604800301

C   -3.5310198315   -0.2001384051   3.5272179921

C   -2.7036073821   -0.8868675443   2.5519538516

C   -3.8027141116   2.1071179683   4.2660926423

C   -4.8000920984   1.6611438003   5.1251248073

C   -5.1579365063   0.2991655401   5.1885987795

C   -4.5249253543   -0.652433277   4.3975934243

N   -2.7625284272   -2.1899863128   2.3647334005

C   2.1162725539   -1.9510566957   -2.2304164014

C   2.3349822977   -0.5848018107   -2.4300141158

C   1.4848230137   0.1081499351   -1.4788658454

N   0.7752812468   -0.8016034867   -0.7439101416

C   2.8090609543   -2.91532625   -2.9653053135

C   3.7338920706   -2.460173338   -3.897787642

C   3.9517039206   -1.0826452668   -4.1025265801
C   3.2528089139   -0.1247377348   -3.3774720594
N   1.4821899578   1.4229560084   -1.3587000569
N   -0.1649077415   1.4879491574   0.4010210083
C   0.7297721623   2.0430237932   -0.4743017923
C   0.7589757708   3.4876535308   -0.302389566
C   -0.1619499082   3.7802628394   0.7058845483
C   -0.7212556065   2.5053278514   1.129778496
C   1.497166298   4.4891485254   -0.931086452
C   1.2698651348   5.7983158972   -0.5147801413
C   0.3350217176   6.0944638915   0.4947153018
C   -0.3951247098   5.0895169454   1.1240384825
N   -1.6284197169   2.413479355   2.0789823211
H   2.2323238343   4.2543354041   -1.7015530396
H   -1.1188455556   -7.9371615824   0.5735375953
H   0.2933547426   -6.1334971955   -0.4154329519
H   -3.569330086   -5.028116384   2.6257330121
H   -3.0186015834   -7.3941562896   2.0589687256
H   -3.5198750368   3.1586910094   4.2162270285
H   -5.3174231869   2.3763406107   5.7657006399
H   -5.9457127087   -0.0110608303   5.8761560569
H   -4.7944259584   -1.7077789133   4.4459643152
H   2.6327128544   -3.9794702848   -2.8066773953
H   4.3019974481   -3.1806710515   -4.487443636
H   4.6829190706   -0.7657232827   -4.8470839279
H   3.4148213971   0.9416515428   -3.5351309682
H   1.8276076447   6.6133633477   -0.9782615366
H   0.1823370281   7.1336804299   0.7894758712
H   -1.12655304   5.3154472907   1.9006709745
O   -1.787300136   -0.2059162395   -0.6412984409
C   -1.9650510111   -1.0190795864   -1.7765192141
C   -3.3018985229   -0.7212239325   -2.4409379499
C   -4.5002095353   -0.8609281612   -1.4906022247
C   -4.7196015093   0.4415650712   -0.7348819226
N   -5.9702423241   0.5434879598   0.1075984509
C   -7.2486110042   0.574290009   -0.7043898903

C	-7.3282212602	1.5514402724	-1.880852809
C	-6.8850500811	1.0467136094	-3.2540132922
S	-7.8656310603	-0.3334201718	-3.9074494976
O	-9.3021501048	0.0980324957	-3.8078449628
O	-7.3922144408	-0.511050211	-5.3218947531
O	-7.5561570753	-1.5249888232	-3.0363156362
C	-6.0310838997	-0.6152875149	1.0965357316
C	-6.6556796022	-1.9326982749	0.6487646282
C	-6.2667624175	-2.9948091794	1.6728476132
S	-6.8220471556	-4.6510413154	1.2044482584
O	-6.3573165667	-5.5421689492	2.3228832304
O	-8.3202127252	-4.5775207631	1.0910052856
O	-6.1509282472	-4.9513091188	-0.1079756581
C	-5.8304906242	1.7680848965	1.003210304
C	-5.5306380364	3.1220524975	0.3641039299
C	-4.8736102682	4.0190303832	1.4082846421
S	-4.6686932692	5.7166694996	0.8152003461
O	-3.9108558836	5.6115178292	-0.4798972322
O	-3.8966252256	6.4164064122	1.8989925797
O	-6.0584782529	6.2634125042	0.6326159237
H	-1.1561676153	-0.8593247194	-2.5127622584
H	-1.9501378189	-2.0906233256	-1.50265145
H	-3.2807334853	0.2888533702	-2.8836084683
H	-3.4196232071	-1.4265462761	-3.2770321491
H	-5.4009020472	-1.1290264432	-2.0613706918
H	-4.2966349409	-1.6862589177	-0.7913184967
H	-3.8746863521	0.6267884007	-0.0598676848
H	-4.7578253835	1.2734530752	-1.445620095
H	-8.0366604118	0.8011642657	0.0241671244
H	-7.4142438659	-0.4399678788	-1.0796090035
H	-6.7936208978	2.4860431168	-1.6780958588
H	-8.3874357235	1.8346942506	-1.959638271
H	-7.0085090854	1.8499963769	-3.9925900429
H	-5.8406305306	0.712326595	-3.2984308338
H	-6.5759300095	-0.2446848125	1.9736640259
H	-4.9900425248	-0.7754973042	1.398623789

H	-6.3058535263	-2.2451812851	-0.3415092287
H	-7.7497004721	-1.8497103193	0.6049547465
H	-6.7055030976	-2.7963121129	2.6610891962
H	-5.1746422973	-3.0749745059	1.7832051207
H	-6.757368603	1.8227823717	1.587824971
H	-5.0189907959	1.507155129	1.6944059926
H	-4.8439516909	3.039069247	-0.4871194946
H	-6.4562876725	3.594794853	0.0106301087
H	-5.4683862811	4.0941340725	2.3301380365
H	-3.8613797613	3.669367177	1.6607227723
O	0.6853499529	-0.4826058691	1.8011588101
C	0.5742480088	-1.0743607028	3.0733335058
C	1.9456487307	-1.1981167896	3.7224563314
C	2.9604453538	-1.9625275985	2.8596423052
C	3.6374393264	-1.0100021446	1.884764534
N	4.7943071579	-1.5587645604	1.0818305879
C	6.0160046726	-1.87847174	1.9181358804
C	6.5157087301	-0.8097679261	2.8945205598
C	5.9679167945	-0.8402913872	4.321314162
S	6.3631748465	-2.3462387179	5.253579167
O	7.8495540745	-2.5313570842	5.1268393701
O	5.9145283316	-2.062290464	6.6587276594
O	5.5823697674	-3.4634158267	4.6080187911
C	4.3601230771	-2.8103916598	0.3270761458
C	4.4412120496	-4.1601827346	1.0326960383
C	3.6244247907	-5.155129926	0.2134306375
S	3.5032491387	-6.7766474076	1.0051661572
O	2.6815043658	-7.6059878048	0.0575797368
O	4.9131521002	-7.2777939979	1.1591373294
O	2.8210844827	-6.537201031	2.3244139234
C	5.1050535707	-0.5641103646	-0.0297760758
C	5.3737074766	0.8945645351	0.3331767012
C	5.0845153311	1.7597317119	-0.8894985526
S	5.5719615305	3.4841227856	-0.6368783276
O	4.8668290878	3.9330949061	0.6132965147
O	5.1064780459	4.203489844	-1.8723267989

O   7.0694171725   3.4751789411   -0.4887546406

H   -0.0829816117   -0.4802860164   3.7344268138

H   0.1360862546   -2.0875303783   3.0022489953

H   2.3324572567   -0.1951835553   3.9697343211

H   1.8129408298   -1.7266060182   4.6781897588

H   3.7084262129   -2.4478537059   3.5029816324

H   2.4271021524   -2.7584387546   2.3177756114

H   2.9039552724   -0.6385671158   1.1583086853

H   4.0241492115   -0.1432294555   2.4305659216

H   6.800166874   -2.1144292623   1.1882921963

H   5.7899664077   -2.7891520704   2.4807345354

H   6.3762189109   0.2040072042   2.5029683019

H   7.6042982441   -0.9495810012   2.9559215495

H   6.4226406772   -0.0263962521   4.9016618331

H   4.8782210286   -0.7290974052   4.390638422

H   4.9700660509   -2.849223642   -0.5839993917

H   3.3273074447   -2.6051790888   0.0237815743

H   4.0414927117   -4.1227328175   2.0522203733

H   5.4819793656   -4.5044981273   1.0953139331

H   4.0642885615   -5.3334964346   -0.7781128603

H   2.584710738   -4.819161273   0.0809968748

H   5.9593462248   -0.9808151214   -0.577950583

H   4.2313136124   -0.6159427587   -0.6916755513

H   4.7346892868   1.2454431658   1.1527431042

H   6.4205828186   1.0309215111   0.6342087456

H   5.6336118699   1.4219263738   -1.7803745703

H   4.0087257341   1.7874034611   -1.1186312142

Geometry optimized cartesian coordinates of SiPc(OX)$_2$ of compound **2** (radical).

E=-6981.649613 / qh-G(298.15K)=-6980.479211 (wB97X-D/(aug-)cc-pVDZ, water solv.)

Si   -0.5424972789   -0.3027615349   0.5760374917

C   -1.2894047691   -6.8185197995   0.81203878

C   -0.4745443451   -5.814884637   0.2918406162

C   -0.8192827469   -4.4959923394   0.5815376911

C   -1.93129969   -4.1897421154   1.3649361597

C   -2.753818158   -5.1886381476   1.8825528462

C	-2.4180836103	-6.5092823005	1.5908996643
C	-0.2251684611	-3.2203455358	0.1824114097
N	-0.9303625029	-2.1844032267	0.7610322357
C	-1.9622502133	-2.7331783247	1.4954057592
N	0.7612429976	-3.1467095492	-0.6633251946
C	1.1988920268	-1.9649268684	-1.1361489599
N	-1.8920263318	0.1060138706	1.89534077
C	-2.1132734464	1.332348142	2.4670996911
C	-3.1246062308	1.2193187969	3.4717111272
C	-3.5232426349	-0.1330941586	3.4841920379
C	-2.7285790489	-0.7978152676	2.5003034226
C	-3.7405388576	2.1609685435	4.3182224053
C	-4.7535506689	1.7180615546	5.1475179328
C	-5.1568652925	0.3563463073	5.1569755247
C	-4.5485195925	-0.5778437892	4.340218271
N	-2.807567729	-2.1222751843	2.2738385195
C	2.1518837225	-1.8613559359	-2.1956024641
C	2.3158558993	-0.4844995787	-2.4514567267
C	1.4691833431	0.2013386559	-1.5253955478
N	0.8073503951	-0.7098632754	-0.743444856
C	2.8871175174	-2.8237296345	-2.9132636131
C	3.7809117736	-2.3731725708	-3.8661671682
C	3.9440784951	-0.9866690246	-4.1269395723
C	3.21837959	-0.0357601551	-3.4346811024
N	1.4227751125	1.5425522263	-1.4336379349
N	-0.1556091442	1.5739944487	0.3915195651
C	0.6939392105	2.1395575834	-0.5352377044
C	0.7117548266	3.5924707476	-0.3566710123
C	-0.1332020909	3.8720186021	0.7152547719
C	-0.6792466255	2.5895677177	1.1627905407
C	1.3910984833	4.6047576614	-1.0306142703
C	1.1934001262	5.9124141233	-0.5901076587
C	0.3420683215	6.1943098052	0.4923367123
C	-0.3350827496	5.176070502	1.1614835812
N	-1.5485554427	2.505236771	2.1281759436
H	2.0542739549	4.378675762	-1.8663530042

H	-1.0498457649	-7.8637403494	0.6098990378
H	0.4032736263	-6.0565190509	-0.308975796
H	-3.6323188194	-4.9500085593	2.4835796935
H	-3.0400784887	-7.3192269336	1.9754070732
H	-3.4302118034	3.2067449976	4.3091465025
H	-5.2565037723	2.4237831386	5.8107564135
H	-5.9612693968	0.0471220156	5.8265138654
H	-4.8553572309	-1.6250024799	4.3454499535
H	2.7587063727	-3.8882734785	-2.7108281253
H	4.3734323778	-3.0920632335	-4.4345710014
H	4.657370315	-0.6719367306	-4.8905149591
H	3.3431983968	1.0296240135	-3.6332091757
H	1.7079633235	6.7333312759	-1.092133964
H	0.2100971501	7.2292690574	0.8119594148
H	-1.0011056804	5.3884239094	1.9985585971
O	-1.7636740787	-0.1247926369	-0.6774786203
C	-1.9227808729	-0.9637828194	-1.7904601504
C	-3.279565739	-0.7308307628	-2.4427436918
C	-4.4587093959	-0.8946934104	-1.4727008049
C	-4.6789416276	0.3933442242	-0.6919476319
N	-5.9385129107	0.4833900322	0.1392122071
C	-7.2083562189	0.5428057151	-0.6831460396
C	-7.2633225752	1.5302375558	-1.852947317
C	-6.8157552824	1.0300309084	-3.2263048487
S	-7.8122305066	-0.3274200698	-3.9021920038
O	-9.2430538163	0.1250493111	-3.8092397604
O	-7.3311871665	-0.4967071067	-5.3153915292
O	-7.5285487178	-1.533756394	-3.0430646833
C	-6.0153509729	-0.6971299749	1.1005202124
C	-6.638862018	-2.0014898267	0.6144838798
C	-6.2511940406	-3.0871877638	1.6137588945
S	-6.8120312591	-4.7312011682	1.1142341279
O	-6.3444446902	-5.6481265815	2.2109968934
O	-8.3112681477	-4.654216966	1.0103002589
O	-6.1496434748	-5.0076538874	-0.2082220335
C	-5.7971224654	1.6860985534	1.0632788826

C	-5.5159304743	3.0548589251	0.4483304855
C	-4.8916784344	3.94956437	1.5141526382
S	-4.7429236913	5.6657594374	0.9622171729
O	-3.9548493459	5.6222426284	-0.318626463
O	-4.0219328434	6.3727190342	2.0764480126
O	-6.1490571579	6.1643301242	0.7624839469
H	-1.1274464814	-0.7903397832	-2.5404322005
H	-1.8637740139	-2.0300053839	-1.5008682206
H	-3.3058420269	0.2713868016	-2.9041596552
H	-3.3859673022	-1.4560036369	-3.2638818258
H	-5.3654306013	-1.1633320587	-2.0338824463
H	-4.2362996086	-1.7271980057	-0.7865421546
H	-3.8402073403	0.5589044055	-0.0049278987
H	-4.7060602764	1.2405025643	-1.385195147
H	-7.9998051813	0.7758705021	0.0399937477
H	-7.3881061811	-0.4649546497	-1.0687955627
H	-6.7151031845	2.4543489345	-1.6394416064
H	-8.3172234603	1.8310370262	-1.9385007581
H	-6.9188750526	1.8415813195	-3.9590164212
H	-5.7766359589	0.6787023133	-3.2628375048
H	-6.5705753373	-0.3442531152	1.9784805126
H	-4.9795627384	-0.8677188599	1.4142639373
H	-6.2826349171	-2.2889409526	-0.3809899858
H	-7.7329032977	-1.9189026537	0.5660241928
H	-6.6860094459	-2.9081751275	2.6075869543
H	-5.1585581316	-3.1658947701	1.719380853
H	-6.7205729171	1.7229352709	1.6549145201
H	-4.9774568392	1.4158249196	1.7415647849
H	-4.816284302	2.9960445777	-0.394602314
H	-6.4463686681	3.5140832928	0.0892471294
H	-5.4914988921	3.9837883621	2.4351812926
H	-3.8700380937	3.6267736934	1.764037271
O	0.6981109744	-0.3867369668	1.8202574541
C	0.5585686494	-0.9967863456	3.07577121
C	1.9222237872	-1.1966081717	3.7247472845
C	2.9045070584	-1.9874614452	2.8484661747

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C   3.5816134628   -1.0593188613   1.8498699934
N   4.7426425482   -1.6271041583   1.0655867958
C   5.964880901    -1.9174795919   1.9106334495
C   6.4474138894   -0.8308585679   2.8764934196
C   5.8928458779   -0.8494058444   4.3008364033
S   6.3029732648   -2.3363607089   5.2564426523
O   7.7919469745   -2.5067272316   5.1357836945
O   5.848861017    -2.036232174    6.6567628718
O   5.5364434333   -3.4725334692   4.6276674249
C   4.3135716364   -2.900352638    0.3456051602
C   4.3943901015   -4.2288498439   1.0905615683
C   3.5738279556   -5.2417382189   0.2979307177
S   3.4644566651   -6.8490180146   1.1173435673
O   2.6323647248   -7.6966601404   0.1946229288
O   4.8767123092   -7.3480418203   1.2620517444
O   2.7989806423   -6.5910572463   2.441979597
C   5.0482720783   -0.6609844605   -0.0717782508
C   5.3499022551   0.7971952895    0.2650870025
C   5.0852933975   1.648479501     -0.9724440827
S   5.6423829945   3.3559799808    -0.7575715399
O   4.9509538176   3.8650450761    0.4778641405
O   5.2130092599   4.0670048631    -2.0110514581
O   7.1380750523   3.29149216      -0.6013318086
H   -0.0756774161  -0.3887350247   3.7488980048
H   0.0754131147   -1.988322179    2.9885437374
H   2.3568209101   -0.2178074691   3.9914179957
H   1.7676228359   -1.7381584662   4.670414515
H   3.6543659654   -2.4799443728   3.4843936752
H   2.3473749892   -2.7784409396   2.3218761532
H   2.8490502224   -0.7098063069   1.1122757944
H   3.9652582207   -0.1772879064   2.3731712122
H   6.7558168034   -2.1528598579   1.1876852786
H   5.7500559993   -2.8236393749   2.4845086037
H   6.2974224221   0.1765487256    2.473081091
H   7.5373429159   -0.9569115969   2.9448709624
H   6.3338352952   -0.0217712517   4.8723799423
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H   4.8013989868   -0.7519364161   4.3622950765

H   4.9282812871   -2.9641727298   -0.5608600462

H   3.2824754625   -2.7067747468   0.0297342077

H   3.9928858296   -4.1620629896   2.1078259936

H   5.4342647984   -4.5741970452   1.16464206

H   4.0051006608   -5.4367594316   -0.6944321205

H   2.5345374824   -4.9041646533   0.1670979941

H   5.8886859181   -1.1002864745   -0.623926572

H   4.1626991616   -0.7100607386   -0.7185629851

H   4.7163216937   1.1759055509   1.0766574864

H   6.3990095089   0.9135073324   0.567379669

H   5.6142917889   1.2719968346   -1.8599564561

H   4.0100012502   1.7113308596   -1.1964255037

Geometry optimized cartesian coordinates of SiPc(OH)(OX) of compound **1** (neutral).
E=-4874.840062 (radical: -4874.974716) / qh-G(298.15K)=-4874.015567 (wB97X-D/(aug-)cc-pVDZ, water solv.)

Si   2.2995755843   0.5324052686   0.859015759

C   4.2803898551   -5.6881216832   0.7373868035

C   4.6810876694   -4.3984021705   0.4039315637

C   3.8275237604   -3.3535321832   0.7595715577

C   2.6230594324   -3.591605967   1.4272808178

C   2.2122502077   -4.8839144333   1.7566227598

C   3.0606538944   -5.927463539   1.3996574222

C   3.8924774229   -1.9192912779   0.5301089388

N   2.7804392618   -1.3183396113   1.046505419

C   2.0063688719   -2.2918049387   1.6305598053

N   4.8837930746   -1.353405483   -0.1353877406

C   4.8646888655   -0.0799900652   -0.4711014952

N   0.7414795079   0.2499020467   1.9734452269

C   -0.1096356993   1.218932594   2.4299553242

C   -1.0561682487   0.6372694127   3.3634865003

C   -0.7524283566   -0.7269256558   3.4316782312

C   0.3774810545   -0.9366287481   2.5466634165

C   -2.1225582839   1.18178393   4.0848343679

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C   -2.8783858862    0.3111935452    4.8601790898
C   -2.57317325    -1.063996063    4.9267949142
C   -1.5041691337   -1.6016157758    4.2202264876
N    0.9138039498   -2.1275110751    2.3423795512
C    5.9221640565    0.5413661296   -1.2548815304
C    5.5323965479    1.8674911318   -1.4593337284
C    4.2530793783    2.0269116821   -0.7845058406
N    3.8840842651    0.8403343508   -0.2100411842
C    7.1144416124    0.0436334978   -1.7802556389
C    7.9022110069    0.9239438898   -2.5159573289
C    7.5091713552    2.2597469749   -2.7221255778
C    6.3181170517    2.7523275294   -2.1971608708
N    3.5995165568    3.1697062366   -0.7630054731
N    1.8271945996    2.4021853243    0.6867269493
C    2.4746965255    3.3252752907   -0.0883201846
C    1.7615815404    4.5907081864   -0.0447021577
C    0.6640802057    4.3973437678    0.7996889133
C    0.7300276469    3.0155834705    1.2450419479
C    2.0073613187    5.8235426619   -0.6508419035
C    1.1130380673    6.8541680737   -0.3813632252
C    0.0073818862    6.6583660903    0.4684563999
C   -0.2354703751    5.4289883373    1.0723912089
N   -0.1473885242    2.4914678987    2.0727673938
H    2.8651329972    5.9675640419   -1.308197663
H    4.9172375573   -6.5341220982    0.4750071974
H    5.6183622154   -4.2085074127   -0.1195393706
H    1.2558753501   -5.0695485203    2.2481679723
H    2.7751970332   -6.9546371279    1.6315790368
H   -2.3531396773    2.2462189736    4.0325439078
H   -3.7235564972    0.6958902274    5.4323576656
H   -3.1888568251   -1.7148650419    5.5488808684
H   -1.2596275627   -2.6627732888    4.2737746451
H    7.4128009157   -0.9925963708   -1.6197132652
H    8.8429242347    0.5748383987   -2.944027341
H    8.1528624404    2.9187358303   -3.3064657465
H    6.0075602117    3.7853153715   -2.3554754713
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H	1.2671925614	7.8337435554	-0.8361454808
H	-0.6756319469	7.4889338124	0.6527846854
H	-1.1015521613	5.2828763166	1.7188510601
O	3.2362152574	0.8357414228	2.3042376403
O	1.3387821545	0.1836653659	-0.5365577288
Si	1.4342203542	-0.4044087216	-2.1127623141
C	-0.3239823752	-0.4130721402	-2.8011981112
C	-1.3629242999	-1.0437017626	-1.8559911849
C	-2.0218931498	0.0564908384	-1.0412722101
N	-3.1913419833	-0.3550563272	-0.1786055709
C	-4.3952031973	-0.8121229784	-0.9780176074
C	-4.8764323574	0.0805371425	-2.1263210348
C	-4.2945516493	-0.1679576497	-3.5180304642
S	-4.6818551054	-1.7941594328	-4.2235824334
O	-6.1767526223	-1.932320347	-4.1472302555
O	-4.158953665	-1.7406465506	-5.6308947713
O	-3.9618601456	-2.8097296799	-3.372747589
C	-2.7617632864	-1.4642636734	0.7779421571
C	-2.8534429303	-2.914255499	0.3137774974
C	-2.1015247884	-3.7696640298	1.3296684433
S	-1.9174106726	-5.4872625433	0.7964584379
O	-1.1892747898	-6.1633573374	1.9258562461
O	-3.309242803	-6.0179298801	0.5870295305
O	-1.1148766374	-5.4362728231	-0.4749454869
C	-3.5279505951	0.8040891266	0.7480090259
C	-3.8271355205	2.1757303	0.1524930223
C	-3.6198854723	3.2199980846	1.2445661133
S	-4.1298503314	4.8731099492	0.7128626636
O	-3.4118553427	5.1340466766	-0.5818641932
O	-3.6976077872	5.7862777856	1.827023068
O	-5.6239079729	4.8115639263	0.546916201
C	2.5034454124	0.666966946	-3.22776969
C	2.0469325554	-2.1846119035	-2.1455547977
H	1.8401697143	-2.6147979299	-3.1382560072
H	1.5333430786	-2.8055010559	-1.3939980917
H	3.1307952688	-2.2562778556	-1.9746726976

H   -0.6266317028   0.6067836841   -3.0949173583

H   -0.2781858409   -0.9910222169   -3.7387802187

H   -2.1183744876   -1.6064005605   -2.4227637912

H   -0.869894783   -1.7633579851   -1.1850784137

H   -1.2846177425   0.5168268052   -0.367117512

H   -2.3920270373   0.8399825598   -1.710815009

H   -5.1944355202   -0.9277086173   -0.2355754449

H   -4.1589490957   -1.8015451735   -1.3802174371

H   -4.754550273   1.1451212199   -1.8999237763

H   -5.9625110037   -0.0787631632   -2.1886548645

H   -4.72985687   0.5508860342   -4.2250307729

H   -3.2026993349   -0.0716643881   -3.5770899403

H   -3.367942534   -1.3446060403   1.6848613489

H   -1.72533116   -1.2163139499   1.0362298803

H   -2.410117591   -3.0615527671   -0.6776588511

H   2.2793457181   0.4239949639   -4.2787039674

H   -3.8995312855   -3.2435990064   0.2648342964

H   -2.6167224742   -3.8060372026   2.2997798422

H   -1.0729893905   -3.4128795457   1.4902391386

H   -4.374184143   0.4665377911   1.3594540285

H   -2.6550411186   0.8847443476   1.4062827492

H   -3.1605942153   2.4223665441   -0.6834944876

H   -4.8632971251   2.2285554859   -0.2056451123

H   3.57941696   0.495935514   -3.0718615053

H   -4.2137022715   3.0045961681   2.1446996618

H   -2.5591561508   3.2988128983   1.5265843589

H   2.2905140178   1.7363872931   -3.073849029

H   3.3173630175   1.766481545   2.5239667893

Geometry optimized cartesian coordinates of SiPc(OH)(OX) of compound **1** (radical).

E=-4874.981124 / qh-G(298.15K)=-4874.159798 (wB97X-D/(aug-)cc-pVDZ, water solv.)

Si   -0.9007689849   -0.3105365437   0.8259659951

C   -1.0670831587   -6.8487241053   1.0987267912

C   -0.2779512042   -5.7793758646   0.6791860797

C   -0.7329614788   -4.4942890195   0.9671738945

C   -1.9284945441   -4.2846517237   1.6509556445

C	-2.727099437	-5.3475369081	2.0681898233
C	-2.2780929402	-6.6352552526	1.7801547927
C	-0.201697329	-3.1707627799	0.6340847871
N	-1.0488616091	-2.2018607035	1.1183232127
C	-2.0887984268	-2.8364653028	1.778025242
N	0.8867384025	-3.0211607429	-0.0692043446
C	1.2884977321	-1.8119876663	-0.4932662379
N	-2.4410412498	-0.0001592105	1.9655696
C	-2.9129246774	1.221097129	2.3732050825
C	-3.9515536265	1.0379949117	3.3342723076
C	-4.1081939146	-0.3571099221	3.489881748
C	-3.1559850888	-0.9666381428	2.6214370871
C	-4.7816713545	1.9385705241	4.0329427549
C	-5.7570884786	1.4137860479	4.8578014187
C	-5.9147590935	0.0093430068	5.0133923095
C	-5.098104167	-0.8815597153	4.3446338823
N	-3.0431526103	-2.3035874806	2.4763542707
C	2.4487023557	-1.621143492	-1.3153046548
C	2.5156900609	-0.2424456242	-1.5930784836
C	1.3974903037	0.3591065981	-0.9266547642
N	0.6744216275	-0.6053122881	-0.2754031063
C	3.4042580262	-2.5102041901	-1.8356140824
C	4.4117606344	-1.9846348384	-2.6265785423
C	4.4792257785	-0.5968852329	-2.9055944079
C	3.5401698723	0.2842982592	-2.3969345989
N	1.1461741869	1.6767654562	-0.9729999332
N	-0.7282365422	1.5979861275	0.5491043027
C	0.1695382442	2.2128591451	-0.2947733776
C	-0.0882645001	3.6535224406	-0.3153404757
C	-1.1559148346	3.8832050019	0.5509501901
C	-1.5523391653	2.5781281281	1.082574587
C	0.5340985133	4.6973563743	-0.997321758
C	0.0485861808	5.9853882249	-0.7814115404
C	-1.0263049833	6.2173464622	0.0939109024
C	-1.6443982368	5.1694341878	0.7737108138
N	-2.5282711733	2.435734518	1.9264870096

H	1.368680537	4.5087342061	-1.6736477988
H	-0.7457513614	-7.8704465714	0.8897800145
H	0.6567549189	-5.938484239	0.1402332092
H	-3.675005717	-5.1761181869	2.5810316328
H	-2.8774330774	-7.495006025	2.0844172742
H	-4.6584588788	3.0163272859	3.9144396629
H	-6.4200491441	2.0850139254	5.4066016866
H	-6.6951936225	-0.3654804658	5.6779383556
H	-5.2141104382	-1.9596060681	4.4661302243
H	3.348579165	-3.5785716942	-1.6216856249
H	5.1704347637	-2.6473284768	-3.0468448649
H	5.2882398332	-0.2214326835	-3.5348134853
H	3.5883390076	1.3529551972	-2.6114376082
H	0.5082420217	6.8293974958	-1.2982393533
H	-1.384662722	7.2375419686	0.241273676
H	-2.4834362917	5.3555129389	1.4454828108
O	0.1354546576	-0.2426242041	2.2526031397
O	-1.9635325722	-0.3893086041	-0.5574055089
Si	-2.0875086179	-1.0788809157	-2.0799134968
C	-3.7550168974	-0.5282231839	-2.7852243082
C	-4.9181641389	-0.6849850559	-1.7899426327
C	-5.1106961893	0.6209606193	-1.0369089322
N	-6.3080745154	0.6849734434	-0.1183633555
C	-7.6311050918	0.6304459276	-0.854347239
C	-7.8252927542	1.5623934154	-2.0560415444
C	-7.4427909599	1.0368831385	-3.4397407618
S	-8.4178476126	-0.382315475	-4.0110747538
O	-9.8583298543	0.0315616722	-3.8921899189
O	-7.9786307545	-0.6080971352	-5.4301739046
O	-8.0692250987	-1.5343769427	-3.1031498837
C	-6.2293109295	-0.4542706328	0.8969219455
C	-6.8621874738	-1.7952453718	0.5414514616
C	-6.4244483203	-2.8065301194	1.5972643234
S	-6.8944240601	-4.4991415654	1.1737303152
O	-6.4556713074	-5.3296239953	2.3491937931
O	-8.387078171	-4.4915378223	0.9812799241

O	-6.1465092956	-4.8295618456	-0.0898176809
C	-6.1852332574	1.9337086344	0.7399164411
C	-6.0824637249	3.2972529703	0.0675547689
C	-5.5237238874	4.278355641	1.0930350491
S	-5.5630063403	5.9861213525	0.4985300253
O	-4.8787347402	5.9796996489	-0.8405345268
O	-4.8213338518	6.7775798266	1.5406326472
O	-7.018326505	6.3582314387	0.4036730563
C	-0.7387415027	-0.5292685552	-3.2704754897
C	-2.1303553005	-2.9613003836	-1.993328103
H	-2.4761621515	-3.3638181876	-2.9587556759
H	-2.8204315261	-3.3127315328	-1.2092332027
H	-1.1356165279	-3.3840876041	-1.7904773951
H	-3.6957525061	0.5086266316	-3.1594441529
H	-3.939677868	-1.1560204604	-3.6724433895
H	-5.8456198021	-0.9720624061	-2.3057262987
H	-4.6901009718	-1.4942852484	-1.0799930308
H	-4.228418227	0.8252842959	-0.4125106321
H	-5.2170948274	1.4482386202	-1.7472473714
H	-8.3863545062	0.847561909	-0.0886385624
H	-7.7739998757	-0.4011055646	-1.1885031445
H	-7.3207111995	2.5243781274	-1.9182388975
H	-8.8987504209	1.7995912616	-2.0770800981
H	-7.6311079771	1.8189836887	-4.1874806529
H	-6.3921558901	0.7334159878	-3.5339665249
H	-6.6871033274	-0.0807631732	1.8214910329
H	-5.1571126131	-0.5781977339	1.0915638273
H	-6.551468025	-2.1494846854	-0.4483417633
H	-1.0464063821	-0.77049267	-4.3007779599
H	-7.9577090668	-1.7243608105	0.5417557401
H	-6.8797018106	-2.5995422077	2.5758231646
H	-5.3307168715	-2.834258057	1.7198395439
H	-7.0481140613	1.9184359759	1.4179161843
H	-5.2843800123	1.7614984552	1.3408545446
H	-5.4091398491	3.2850683618	-0.7992450687
H	-7.0691385256	3.6455403848	-0.2647214075

H   0.2189487886   -1.0358323783   -3.0772369006

H   -6.1091167397   4.2804666097   2.0241242805

H   -4.4748879793   4.0486734432   1.3335531641

H   -0.5761129886   0.5581320003   -3.2070789343

H   0.4907307047   0.6378306454   2.3912886982

Geometry optimized cartesian coordinates of SiPc(OH)(OX) of compound **2** (neutral).

E=-4544.758755 (radical: -4544.893683) / qh-G(298.15K)=-4543.975110 (wB97X-D/(aug-)cc-pVDZ, water solv.)

Si   2.2090234469   0.6272357366   0.8935552585

C   3.9094006053   -5.670097009   0.5128690794

C   4.3139701472   -4.3950545917   0.1342809032

C   3.5371086554   -3.3214628267   0.5746032465

C   2.4019415288   -3.5196302375   1.3662231048

C   1.9889919134   -4.7989755159   1.7437905369

C   2.75988597   -5.8692039289   1.3035422852

C   3.6357252663   -1.8897099305   0.3514137981

N   2.6102964055   -1.2500149091   0.9903190705

C   1.8513392754   -2.2026451994   1.627216091

N   4.5825900823   -1.3531151852   -0.4005081017

C   4.6064898097   -0.0701423374   -0.688568446

N   0.6936802991   0.3771187732   2.0756141026

C   -0.131093443   1.3549525288   2.5580868469

C   -1.0956516802   0.776758646   3.4750228798

C   -0.8219013745   -0.5943100152   3.5182512431

C   0.3025126752   -0.8131365507   2.628560771

C   -2.1546678151   1.3306280762   4.2003567371

C   -2.9327049561   0.4614466669   4.9549206411

C   -2.6578874122   -0.9212477744   4.9960210189

C   -1.5974606644   -1.4684176714   4.2843203537

N   0.8021722165   -2.0125633498   2.3972951659

C   5.6150656044   0.5226483834   -1.5555680102

C   5.284204732   1.8745362875   -1.6751977811

C   4.0880814887   2.076445806   -0.8699753908

N   3.7153009078   0.8935649393   -0.29283652

C   6.7208525468   -0.0172381354   -2.2115321635

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C   7.4840152679    0.8482636756    -2.9897245975
C   7.1507509536    2.2104346767    -3.1101299849
C   6.0453871308    2.7449300011    -2.4548843499
N   3.503644642     3.2510078388    -0.7521809261
N   1.7971164617    2.5170736264    0.7929378776
C   2.442094235     3.437026633     0.0110095813
C   1.7887826485    4.729933717     0.1305621882
C   0.7179101441    4.5507797546    1.0103713055
C   0.7464482377    3.1547583908    1.4104092905
C   2.0542503425    5.9709264508    -0.4503988224
C   1.2067644846    7.0224752627    -0.1175730304
C   0.1246086348    6.83900967      0.7651360293
C   -0.1381196212   5.6011899736    1.3427039343
N   -0.130952427    2.6381283755    2.2413484114
H   2.8903950683    6.1056986738    -1.1368528911
H   4.4873707781    -6.5366530792   0.1886171544
H   5.1975524544    -4.2357371625   -0.4841380568
H   1.0886785598    -4.9553962644   2.3395294423
H   2.4689470822    -6.886129482    1.5710349629
H   -2.3627776067   2.4003409078    4.1672574447
H   -3.773009147    0.8528657092    5.5297476625
H   -3.2916836753   -1.5704143589   5.6015355479
H   -1.3784100631   -2.5361008045   4.3148207548
H   6.9738713717    -1.0733719639   -2.116249239
H   8.3581152079    0.4665005896    -3.5191197465
H   7.7729894184    2.8567362077    -3.7307219653
H   5.7816042745    3.7988342624    -2.5457272881
H   1.3782298694    8.0093260518    -0.5498657433
H   -0.5228897595   7.6864823442    0.9950617521
H   -0.9886923098   5.4548984677    2.0095566932
O   3.2461242433    0.8482489983    2.2758887899
O   1.1254569671    0.383907588     -0.4529879984
C   1.3850459189    -0.3547821092   -1.6214554183
C   0.1076080158    -0.5226912467   -2.4324639374
C   -1.0430193825   -1.1370878957   -1.6214990895
C   -1.813830369    -0.0391708986   -0.9028760437
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N   -3.0778059973   -0.4498258299   -0.1843133992
C   -4.1906414559   -0.8836635001   -1.116092537
C   -4.5216823918   0.020090862   -2.3076927389
C   -3.7867008776   -0.2413725228   -3.6227172669
S   -4.10409527   -1.8682385487   -4.3609430863
O   -5.5989801254   -1.99101029   -4.4599062371
O   -3.4184034917   -1.8288422646   -5.696965694
O   -3.4986048944   -2.8853080923   -3.426378721
C   -2.7755172984   -1.5746528674   0.7997180914
C   -2.8102635842   -3.0153972576   0.2995927475
C   -2.123143163   -3.882688629   1.3495960258
S   -2.0069118641   -5.6177275807   0.8531641642
O   -1.3048013512   -6.2978387615   1.9962124327
O   -3.419865205   -6.0956367749   0.6589200714
O   -1.2067685038   -5.6283665663   -0.4205537431
C   -3.5007399989   0.7038276518   0.7150635059
C   -3.6934354485   2.0892382122   0.1056804428
C   -3.5915558773   3.1225610716   1.2235615301
S   -4.0528303772   4.7805071263   0.6628308035
O   -3.1996033639   5.0647977893   -0.5419649427
O   -3.7549166588   5.681465046   1.8291664948
O   -5.5190398213   4.711110062   0.3316778451
H   2.1489883626   0.1405222069   -2.2484016489
H   1.7676657584   -1.3633221038   -1.3750190971
H   -0.1981081477   0.4499501973   -2.8535225703
H   0.3392907329   -1.1749501169   -3.2875250709
H   -1.7108602772   -1.7061722989   -2.2839724831
H   -0.6168144025   -1.8476757238   -0.897044626
H   -1.1681531875   0.4333232752   -0.1520137795
H   -2.1042911898   0.7355979067   -1.619767876
H   -5.0710372856   -0.9910940571   -0.4702499098
H   -3.9239279749   -1.8746094794   -1.4946858006
H   -4.405146064   1.0821260773   -2.0649306935
H   -5.5960716833   -0.1177007436   -2.4958229261
H   -4.1289583328   0.4777211222   -4.3788894895
H   -2.6945408792   -0.1571257916   -3.5550371816

H	-3.4941074203	-1.4674827933	1.6218188708
H	-1.7820639411	-1.334784841	1.1963723165
H	-2.2948366336	-3.1380120879	-0.6595610358
H	-3.8461932406	-3.3544546916	0.1657829894
H	-2.6644119067	-3.8781768426	2.3065753398
H	-1.0861335704	-3.5617342681	1.5313073928
H	-4.4243717166	0.3784443448	1.2099637506
H	-2.7161523401	0.7531489937	1.480337507
H	-2.9289796904	2.324647922	-0.6452759732
H	-4.6790128208	2.1685647334	-0.3712709997
H	-4.2669169601	2.8973733967	2.0617355578
H	-2.5620166798	3.2047883969	1.603756771
H	3.3749505764	1.7678527372	2.5187267053

Geometry optimized cartesian coordinates of SiPc(OH)(OX) of compound **2** (radical).

E=-4544.900094 / qh-G(298.15K)=-4544.118775 (wB97X-D/(aug-)cc-pVDZ, water solv.)

Si	2.1836765564	0.681416337	0.8779435554
C	3.8641924534	-5.6436219136	0.5980947064
C	4.2870732758	-4.3674720805	0.2324971449
C	3.4952617092	-3.2905392962	0.6276762185
C	2.3258361165	-3.4790675414	1.3620391846
C	1.8945722366	-4.7531175144	1.7284396338
C	2.680843813	-5.833469746	1.3331629943
C	3.615679883	-1.8510491628	0.3894586834
N	2.5612623242	-1.1978117954	0.9867223418
C	1.7628355299	-2.1508022114	1.6012607828
N	4.577192107	-1.3495655611	-0.3365929015
C	4.6072389535	-0.0469268059	-0.6620850117
N	0.6508977134	0.4551291083	2.0478470296
C	-0.1363487671	1.4521528373	2.5597335339
C	-1.0979469171	0.8969252922	3.4562568119
C	-0.8764542178	-0.4975620313	3.4617476182
C	0.2181283385	-0.7338940915	2.5792053042
C	-2.1445411748	1.4646062287	4.2112675791
C	-2.9532555578	0.613340507	4.9382712067
C	-2.7346986805	-0.7915107427	4.937658206

C   -1.7026892544   -1.3565147953   4.2144317963
N   0.7036806482   -1.9663199068   2.327427731
C   5.599207261   0.5148998926   -1.5333825284
C   5.257819028   1.8708204043   -1.7012114417
C   4.0773117433   2.0904163845   -0.9168020819
N   3.7092269592   0.9220166196   -0.3003583948
C   6.7201500044   -0.0340784848   -2.1783207841
C   7.4778173874   0.8024103706   -2.9801829704
C   7.1355396525   2.1673161562   -3.1481386609
C   6.0318020492   2.7143799078   -2.5165133979
N   3.4782344301   3.2889536038   -0.8192691802
N   1.8054166643   2.5761909476   0.7736924128
C   2.4495026241   3.4831019138   -0.0433721856
C   1.8089079952   4.7937344385   0.0833871977
C   0.7652522817   4.6430385321   0.9941663383
C   0.7721784796   3.2415388895   1.4128388312
C   2.0735701376   6.0221000823   -0.5198849153
C   1.2524101977   7.0949687844   -0.1784566578
C   0.1960899863   6.9398041217   0.7363705665
C   -0.0644874892   5.7090917947   1.3359010074
N   -0.0997781268   2.7637846495   2.2475126822
H   2.8907059248   6.1350392877   -1.2333774266
H   4.4562735474   -6.5124899622   0.3061472938
H   5.1998310876   -4.2132269666   -0.3441189699
H   0.9695041803   -4.9051958477   2.2860947366
H   2.3721028109   -6.8466343328   1.5961257938
H   -2.3108384614   2.5428731674   4.2110368324
H   -3.7764369204   1.0208933509   5.5276950985
H   -3.3966187512   -1.4302932334   5.5251138923
H   -1.5329187667   -2.4344481521   4.2147866408
H   6.9811031741   -1.0853359137   -2.0475579942
H   8.3558258293   0.4086484374   -3.495363356
H   7.757286442   2.794625645   -3.7894808676
H   5.7670111003   3.7647940898   -2.6460890321
H   1.4271470461   8.0727097266   -0.6305004203
H   -0.4329158641   7.7989343854   0.9756207013

H	-0.8970525026	5.5785931285	2.0286865927
O	3.2223881649	0.9079327988	2.2798016648
O	1.1096217419	0.4512236906	-0.498140208
C	1.3849198867	-0.3159580358	-1.6389536891
C	0.1106564584	-0.5474121778	-2.4416326719
C	-1.0180648107	-1.1817037716	-1.6157137455
C	-1.7828630128	-0.1041398109	-0.8599207104
N	-3.0480173435	-0.5323685066	-0.1518649837
C	-4.1656635766	-0.9388447357	-1.088407956
C	-4.50571981	-0.0054810829	-2.2541194726
C	-3.777242617	-0.2310984269	-3.5788709141
S	-4.1015800398	-1.8357707648	-4.3608971057
O	-5.5976386112	-1.9623596391	-4.4398881545
O	-3.4390515515	-1.7522895876	-5.7068680094
O	-3.4778794141	-2.8795779005	-3.4691472114
C	-2.7441799192	-1.6845543681	0.7993244172
C	-2.7850932017	-3.1085129827	0.2547612271
C	-2.0914911349	-4.0098698143	1.2710725139
S	-1.9623667845	-5.72143093	0.703634513
O	-1.2589646765	-6.4476912538	1.8175571785
O	-3.3718331414	-6.2017783349	0.4854976887
O	-1.1608115261	-5.6744614441	-0.5690631627
C	-3.4630403669	0.5985736512	0.7793853203
C	-3.6828696894	1.9913528595	0.1942110324
C	-3.5421545035	3.0165678199	1.3150026705
S	-4.0479091886	4.6714618921	0.789532825
O	-3.2396123248	4.9851335313	-0.4398279528
O	-3.7282921365	5.5668587709	1.9552789283
O	-5.5237760172	4.584218299	0.5046029552
H	2.1350903084	0.1783102806	-2.2855830203
H	1.797467383	-1.3062514328	-1.3664974372
H	-0.2317657467	0.4038043023	-2.8842215297
H	0.3593293724	-1.2121012262	-3.2829509054
H	-1.6943416103	-1.7426453186	-2.2769777279
H	-0.5724587244	-1.9021950693	-0.9119155731
H	-1.1337669933	0.3395758586	-0.0948438954

H   -2.0701237845   0.6950380016   -1.5513510451

H   -5.0423279418   -1.0625659996   -0.4403411894

H   -3.9038376174   -1.9197982823   -1.4950572746

H   -4.3910595895   1.050112093   -1.9850427293

H   -5.5805938097   -0.1423871972   -2.4403719308

H   -4.1213899248   0.5093150906   -4.3133355416

H   -2.6846813998   -0.1513144887   -3.5127708133

H   -3.4599663487   -1.5992042484   1.6264758861

H   -1.7500583673   -1.458354861   1.2019289751

H   -2.2734978871   -3.2005465522   -0.7098076167

H   -3.8216380328   -3.4430796283   0.1145106609

H   -2.633162592   -4.0481216933   2.2270904424

H   -1.0594247431   -3.6813181218   1.4668738867

H   -4.3756152865   0.2559244441   1.283430482

H   -2.6637183739   0.6415890114   1.5302882208

H   -2.948298487   2.23732911   -0.5825983245

H   -4.6857107847   2.0709863513   -0.2459435645

H   -4.1760930989   2.7757807391   2.1807048783

H   -2.4975628188   3.10898967   1.6494985346

H   3.3382441639   1.8372155524   2.4889999057

Geometry optimized cartesian coordinates of SiPc(OH)$_2$ (neutral).

E=-2108.010805 (radical: -2108.143028) / qh-G(298.15K)=-2107.615651 (wB97X-D/(aug-)cc-pVDZ, water solv.)

C   -6.4765850112   -0.5326356529   0.4703105352

C   -5.2924918094   -1.2546943976   0.3747684241

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N   -1.9113441154   0.1731334106   0.0979374621

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Si   0.0295324924   0.181888029   -0.0092818622

N   0.0222062951   2.1098685587   0.0100020168
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C   -0.6750757616   4.3099901028   0.0666772726
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C   -0.6775887753   -6.3426211095   0.0457371261
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N   2.3904392559   -2.1989966915   -0.1868758402
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C   4.1455567845   -0.5233949559   -0.3376696224
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C   5.3335280097   -1.2504617382   -0.4296600269
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H   5.3287492388   -2.3407891263   -0.4309125239
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H   -5.2870769104   -2.3449199266   0.3737507548
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H   -1.2105466054   7.6420505547   0.1161156977

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H   2.5342666422   -5.1464958665   -0.1938328877

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H   0.1721759141   -0.5977835749   2.1534491245

Geometry optimized cartesian coordinates of SiPc(OH)$_2$ (radical).

E=-2108.149222 / qh-G(298.15K)=-2107.758009 (wB97X-D/(aug-)cc-pVDZ, water solv.)

C   -6.4953294872   -0.5300768071   0.4400056948

C   -5.3058973934   -1.2499283572   0.3520943324

C   -4.1188280683   -0.5239805858   0.2640806191

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C   -5.3056340822   1.5958452386   0.3562968244

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N   -1.9101799986   0.1742981116   0.090657975

C   -2.7202228123   1.290172181   0.1690599564

N   -2.3698915346   -2.1969007557   0.1721464717

C   -1.0807034452   -2.5774001239   0.099633336

Si   0.0317882825   0.1829954503   -0.0109501154

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C   1.1291118673   2.9248502795   -0.0623628992

C   0.726294829   4.2978057824   -0.0205448038

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C   -1.3960082435   -5.1576168002    0.1303461608
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C    4.1581468153   -0.5200491226   -0.3553113259
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C    6.5327309213   -0.5240955766   -0.5534263521
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O    0.1436368034    0.2442714455    1.7451232752
O   -0.0318635475    0.1735647216   -1.7701486445
H   -7.4448222408   -1.0635014173    0.5092065195
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H   -5.2993201408    2.6865144657    0.3593449648
H   -7.4446572615    1.4094545176    0.512980762
H    2.5344399804    5.5047543338   -0.146158622
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H -0.9357319303   0.1697883278   -2.0921565418

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