

Supporting Information for

Optical Properties of Phthalocyanine and Naphthalocyanine Compounds

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Atomic Coordinates for PBE/DNP optimized structures

		SINC	singlet
N	1.266146986	-0.125378824	0.023371571
C	1.014885305	-1.464579252	-0.216414864
C	-0.412070470	-1.716606528	-0.091272399
C	-1.011750213	-0.474259792	0.243275971
C	0.067549355	0.498020820	0.314666312
C	5.965314888	0.981830751	-0.408944526
C	7.036670576	1.963600688	-0.382715404
C	6.428556318	3.212595388	-0.082822201
C	5.006095060	2.955325387	0.065511844
N	4.762471268	1.606548269	-0.123417182
C	5.412064929	-2.585080074	-1.043860968
C	4.138255017	-3.213772164	-0.989593133
C	3.180443984	-2.177467703	-0.645496550
N	3.842410508	-0.972116132	-0.499216151
C	5.191454039	-1.184457644	-0.726706969
N	6.173023397	-0.296026045	-0.684051426
N	1.883670293	-2.414258117	-0.519517497
N	2.188674757	2.448647942	0.408336690
C	0.846187571	2.653236333	0.664467411
C	0.625381395	4.050263654	0.996513372
C	1.889897813	4.690105090	0.905844814
C	2.845346679	3.661629672	0.528268798
N	4.134038656	3.906892180	0.360865529
N	-0.135687460	1.767306944	0.621476875
Si	3.008517494	0.738741036	-0.041908116
C	7.172950253	4.370399622	0.035995427
C	8.578969040	4.295208937	-0.144170764
C	9.199345811	3.023184610	-0.452765620
C	8.401973181	1.852792564	-0.567550756
C	10.612140881	2.980674025	-0.624025236
C	11.381257150	4.120485753	-0.503233790
C	10.774383255	5.365729801	-0.198247754

C	9.406797857	5.447898232	-0.027679109
C	2.037714420	6.034111214	1.187428854
C	0.892641359	6.774379668	1.585447463
C	-0.394911524	6.121307859	1.682702364
C	-0.510269545	4.739625018	1.374425788
C	-1.518467238	6.887711589	2.098932564
C	-1.393042248	8.228342615	2.410043067
C	-0.131496061	8.867932170	2.315137620
C	0.981974516	8.156924004	1.909465676
C	-2.376428731	-0.353953090	0.416431475
C	-3.185920324	-1.509854999	0.241426283
C	-2.573787460	-2.776568919	-0.099894949
C	-1.164848181	-2.860984979	-0.261725138
C	3.986416652	-4.559696587	-1.260203110
C	5.138521795	-5.318156580	-1.600092234
C	6.436358771	-4.678625885	-1.656751535
C	6.555009183	-3.293948107	-1.363059773
C	7.567211491	-5.466075739	-2.016239269
C	7.437555767	-6.808522527	-2.313735166
C	6.166188520	-7.434731190	-2.252776470
C	5.046391422	-6.705425537	-1.906211307
C	-3.411522351	-3.914361601	-0.277678816
C	-4.781080070	-3.822631596	-0.126854340
C	-5.379880694	-2.581825022	0.206653530
C	-4.600551344	-1.457037626	0.389763867
H	6.692502249	5.321904472	0.269900835
H	8.864175394	0.890398223	-0.793769854
H	11.082819738	2.022813010	-0.856390157
H	12.462746633	4.063515405	-0.635814961
H	11.391088372	6.260340610	-0.102205425
H	8.935481305	6.404857175	0.206869986
H	3.011308058	6.520003233	1.116054780
H	-1.472325467	4.232469751	1.451257862
H	-2.487596197	6.392126731	2.176068098
H	-2.265532936	8.797174937	2.733609163
H	-0.039859625	9.927298067	2.561384156
H	1.951825545	8.651264170	1.833085917
H	-2.829953531	0.604386085	0.674889061
H	-0.692184041	-3.808053220	-0.527533023
H	3.004245203	-5.032051105	-1.221710170
H	7.526897349	-2.801103687	-1.403365505
H	8.545769686	-4.984675703	-2.058717052
H	8.315000081	-7.393758933	-2.593081343
H	6.073001601	-8.496875658	-2.485583482
H	4.067561156	-7.186016173	-1.862228547
H	-2.946508215	-4.867216179	-0.540056673
H	-5.406175905	-4.704925533	-0.269163725
H	-6.463071533	-2.517366524	0.320387227
H	-5.064750855	-0.503696291	0.651739931
O	2.768117238	1.089019439	-1.690001806
Si	2.856283044	1.090871943	-3.318012742
O	1.654861766	2.137849933	-3.833190595
C	4.542275423	1.697006882	-3.892012797
H	5.327161078	1.011161410	-3.537636574
H	4.621176808	1.734501886	-4.990056604
H	4.769900025	2.700162632	-3.499260656
C	2.518248374	-0.633511996	-3.982364275

H	1.520716828	-0.982210789	-3.676653286
H	3.258180107	-1.362235944	-3.617993582
H	2.553887049	-0.650080367	-5.083495208
C	1.689792607	2.933973382	-5.015050258
H	2.725066104	3.234751503	-5.257846043
H	1.127955332	3.858127007	-4.799998907
C	1.061293167	2.218838976	-6.211399205
H	0.026413566	1.939233957	-5.960464694
H	1.610801399	1.279195661	-6.394355076
C	1.074114814	3.079826230	-7.474188006
H	0.491337734	4.000845233	-7.340231685
H	2.108789881	3.383712919	-7.715926653
N	0.480864214	2.386662302	-8.610928041
H	0.757589380	1.425051082	-8.784665440
C	-0.353600403	2.999962230	-9.511060910
O	-0.705606388	4.176909990	-9.398934946
C	-0.796630097	2.117827169	-10.677141846
H	-0.641750775	1.052245410	-10.442264708
H	-0.129052373	2.353050484	-11.524230792
C	-2.248043538	2.371768165	-11.092550912
H	-2.373779800	3.451364535	-11.261348977
H	-2.917287914	2.114567092	-10.254869879
C	-2.660936432	1.586384994	-12.339569287
H	-2.528322774	0.505331348	-12.156350038
H	-1.981096510	1.839501687	-13.172209194
C	-4.107226055	1.849886382	-12.770842629
H	-4.238752019	2.929594084	-12.957062984
H	-4.786695032	1.600553038	-11.937577825
C	-4.531717505	1.067125857	-14.017325783
H	-4.400346520	-0.012900346	-13.829403180
H	-3.853663063	1.316388087	-14.852477973
C	-5.978832960	1.335905622	-14.441739887
H	-6.115698012	2.418548083	-14.605049389
H	-6.658296414	1.065205363	-13.615750522
C	-6.403772247	0.580419052	-15.706907185
H	-6.268947496	-0.502070786	-15.541637170
H	-5.719197849	0.866735820	-16.525082740
C	-7.855407260	0.871080006	-16.103260420
H	-8.535539211	0.598648833	-15.282511779
H	-7.993636317	1.955108372	-16.246034725
C	-8.436152956	0.210979610	-17.351168792
O	-9.643368581	0.281032916	-17.604698526
N	-7.561769806	-0.445798474	-18.174853036
H	-6.576077707	-0.465778273	-17.935816157
C	-7.998275377	-1.055824381	-19.425972324
H	-8.958751150	-1.557894859	-19.238990942
H	-7.267192194	-1.822165176	-19.712749636
C	-8.174518535	-0.038150495	-20.559556434
H	-7.227216039	0.508807877	-20.715007838
H	-8.925953813	0.703348192	-20.249271829
C	-8.614305460	-0.678010289	-21.872612988
H	-8.838673550	0.109106771	-22.613820078
H	-9.537629761	-1.257145431	-21.725710767
O	-7.661885717	-1.617275288	-22.398945631
H	-6.859419557	-1.116148399	-22.624870527
O	3.212255186	0.373793834	1.611366593
Si	3.878653068	0.472568384	3.110172900

O	2.766179264	0.019199443	4.269937512
C	5.376548062	-0.664445690	3.172114787
H	6.144538956	-0.328369458	2.459333367
H	5.831662596	-0.677059783	4.174195237
H	5.120458827	-1.699865882	2.900297245
C	4.303039744	2.228473384	3.597297889
H	3.397143100	2.852115114	3.625062730
H	5.018324313	2.696386697	2.906094556
H	4.744943432	2.242810403	4.604989757
C	2.341226027	-1.311498119	4.561364653
H	3.098016618	-2.050924348	4.245089353
H	1.412488520	-1.529808587	4.004749062
C	2.100033561	-1.423321183	6.063876714
H	1.303207061	-0.721285073	6.351000307
H	3.019353280	-1.090119345	6.573911973
C	1.731928232	-2.834546825	6.525509101
H	0.798095568	-3.178032565	6.062081828
H	2.524579118	-3.548284409	6.245095363
N	1.508815836	-2.891246329	7.964869026
H	2.237611719	-2.530185009	8.574148103
C	0.299013536	-3.210422843	8.531199038
O	-0.671092579	-3.585957118	7.870873356
C	0.270114813	-3.072718881	10.056980638
H	0.649056478	-2.072296330	10.329696597
H	0.986169263	-3.796349472	10.483059915
C	-1.119690634	-3.287097538	10.654305555
H	-1.446399287	-4.317556184	10.444243671
H	-1.835632949	-2.635834269	10.129580773
C	-1.169909572	-3.010642333	12.159415636
H	-0.851182372	-1.970036111	12.350736107
H	-0.441614821	-3.654641073	12.684393371
C	-2.560536382	-3.225847724	12.765590686
H	-2.866442625	-4.274739339	12.609367529
H	-3.292366111	-2.609191762	12.215179452
C	-2.640531652	-2.889643414	14.258793068
H	-2.335024679	-1.839484936	14.410970929
H	-1.909762201	-3.505466794	14.812801573
C	-4.035503800	-3.097973132	14.856299141
H	-4.339113901	-4.150113719	14.720296482
H	-4.766105329	-2.493226383	14.291820430
C	-4.127199248	-2.731451795	16.343764334
H	-3.820439824	-1.678846731	16.470156784
H	-3.397541942	-3.347919567	16.899246688
C	-5.533621760	-2.930966553	16.917434576
H	-6.268357823	-2.370449956	16.319301175
H	-5.831206220	-3.988733172	16.827828901
C	-5.802252196	-2.532967115	18.368548036
O	-6.953797026	-2.487369796	18.815395774
N	-4.711647222	-2.245754628	19.143981966
H	-3.785823206	-2.292569202	18.733200169
C	-4.843211687	-1.842851360	20.540554173
H	-5.666040418	-1.115304018	20.609807113
H	-3.918043440	-1.332052586	20.838219442
C	-5.123113602	-3.011338789	21.492707059
H	-4.333198307	-3.775685184	21.386895102
H	-6.070880751	-3.487003223	21.197288973
C	-5.215454551	-2.566641877	22.948399665

H	-5.518326280	-3.415616198	23.586408685
H	-5.981583479	-1.786004735	23.058125171
O	-4.002531162	-1.970096862	23.441999755
H	-3.323685674	-2.666332547	23.452300033

SiNc-(OSi(CH₃)₃)₂ singlet

N	-1.845596750	-0.838800620	0.013332102
C	-2.115931682	-2.177084465	-0.203041207
C	-3.546623739	-2.405444715	-0.072901365
C	-4.128832351	-1.146351991	0.229957601
C	-3.035395442	-0.188280289	0.273198444
C	2.892636624	0.149385600	-0.244663528
C	3.992141473	1.091271566	-0.130224987
C	3.417121636	2.343646469	0.213749157
C	1.981938489	2.126271842	0.307101832
N	1.702881428	0.797320208	0.036541124
C	2.262302145	-3.374910561	-1.023252069
C	0.977417876	-3.981214836	-0.980866350
C	0.039607976	-2.932366234	-0.616282944
N	0.725728631	-1.745365488	-0.440129197
C	2.069003838	-1.978736446	-0.669498795
N	3.070621666	-1.118582130	-0.577812629
N	-1.262085342	-3.144063914	-0.496408090
N	-0.866099564	1.708847513	0.467147069
C	-2.217314457	1.955722286	0.619659692
C	-2.418163344	3.363783547	0.918915984
C	-1.125998222	3.955695560	0.965189982
C	-0.178960149	2.893458661	0.665480121
N	1.127651453	3.093440256	0.599735897
N	-3.219856130	1.096028809	0.533439331
Si	-0.072917838	-0.020401113	0.021934078
C	4.198683589	3.467990975	0.398930164
C	5.605798090	3.352544398	0.238421080
C	6.190597784	2.074220557	-0.109043185
C	5.355147725	0.940625296	-0.293972274
C	7.603920098	1.989150476	-0.260844515
C	8.409192082	3.096311011	-0.085375935
C	7.835816111	4.349040223	0.249340435
C	6.469963803	4.471357911	0.408579770
C	-0.959737234	5.296622173	1.251668744
C	-2.113434907	6.091700849	1.493016659
C	-3.428714938	5.489803025	1.433456239
C	-3.560150501	4.106124790	1.142127286
C	-4.567748400	6.311173058	1.670935893
C	-4.429118679	7.653802868	1.960835102
C	-3.139893066	8.242330792	2.029051140
C	-2.012434587	7.477706481	1.801794956
C	-5.489859297	-1.004867752	0.413363995
C	-6.314341739	-2.156217601	0.301944262
C	-5.721342180	-3.440077759	-0.008798985
C	-4.316257763	-3.545557267	-0.192422903
C	0.804472394	-5.319766530	-1.271601045

C	1.943684921	-6.095438528	-1.616238631
C	3.253380783	-5.477775644	-1.659919166
C	3.392269979	-4.098282910	-1.350812343
C	4.371687469	-6.281307117	-2.019095366
C	4.222942177	-7.620298517	-2.322633925
C	2.941275063	-8.226436090	-2.272779422
C	1.831930148	-7.478857543	-1.930792163
C	-6.572883994	-4.574741579	-0.117564451
C	-7.937142686	-4.464360596	0.063518371
C	-8.518378273	-3.208564560	0.370840484
C	-7.724583564	-2.084160478	0.482155222
H	3.745816655	4.427689952	0.666650976
H	5.786540813	-0.028259697	-0.563981785
H	8.045511414	1.022181166	-0.525407045
H	9.493149384	3.009442175	-0.205474172
H	8.481774040	5.220792220	0.388979994
H	6.027238300	5.437360940	0.674471612
H	0.037917162	5.743772145	1.288174660
H	-4.548861019	3.640146693	1.102532164
H	-5.561631442	5.855012218	1.623479519
H	-5.315087554	8.270328199	2.140133655
H	-3.040398917	9.307007428	2.261439580
H	-1.017638432	7.932049836	1.849761737
H	-5.929136390	-0.029657683	0.645597329
H	-3.856309381	-4.510400178	-0.427857336
H	-0.188399697	-5.777543186	-1.241053679
H	4.375978489	-3.621242216	-1.378376574
H	5.361287975	-5.814753090	-2.053536217
H	5.095344958	-8.220995734	-2.597456862
H	2.832100349	-9.288630476	-2.511605153
H	0.841407859	-7.943624269	-1.898235808
H	-6.121681844	-5.544742076	-0.353279748
H	-8.573134220	-5.350441309	-0.022275189
H	-9.600312989	-3.130633449	0.513902796
H	-8.174547667	-1.113738338	0.718514223
O	-0.229502449	0.336259153	-1.623581111
Si	-0.367802810	0.700988730	-3.220651145
C	-2.193002801	0.696681474	-3.692180888
C	0.357778627	2.413329965	-3.531841439
H	0.235251303	2.715116185	-4.587059105
H	1.436286878	2.449536995	-3.299410334
H	-0.140870812	3.177513840	-2.909935521
C	0.563031842	-0.585504534	-4.237702601
H	0.144178319	-1.596159839	-4.090404418
H	1.631440724	-0.624901040	-3.961623805
H	0.506061660	-0.359079431	-5.317483140
O	0.033565763	-0.399576932	1.672956225
Si	0.667785334	-0.622438533	3.179883238
C	-0.751016761	-1.115773270	4.316355771
C	1.962020509	-1.994682096	3.150126594
H	2.344767905	-2.197223232	4.167192717
H	2.828402366	-1.738085663	2.516748335
H	1.536955866	-2.938048985	2.766169859
C	1.453873184	0.970704147	3.817400534
H	0.735262403	1.809169707	3.800676896
H	2.332092388	1.272142220	3.221826268
H	1.790961025	0.847130158	4.862109566

H	-2.649904190	-0.297455202	-3.544808194
H	-2.340338897	0.974519749	-4.750448896
H	-2.763644507	1.414663698	-3.077873296
H	-0.409830342	-1.270709317	5.354970772
H	-1.228892842	-2.050925999	3.979300099
H	-1.531856166	-0.335377148	4.335801596

SiNc-(OSi(CH₃)₃)₂ triplet

N	-1.885129412	-0.880423507	0.064986408
C	-2.164883952	-2.244453132	-0.112940564
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C	-4.171405396	-1.169378420	0.194074836
C	-3.067800557	-0.220921662	0.262472996
C	2.828784076	0.104572942	-0.347779766
C	3.930449735	1.054849941	-0.284247906
C	3.374470352	2.300652043	0.112424227
C	1.950061873	2.089682164	0.250162177
N	1.655625409	0.742118221	-0.027894527
C	2.201251165	-3.449446713	-0.941071616
C	0.924357641	-4.065028218	-0.834489840
C	-0.010109306	-3.014963143	-0.499890479
N	0.684833625	-1.799210899	-0.391746175
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N	3.022556180	-1.174218992	-0.650898777
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C	-1.142469414	3.911946462	0.956169328
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Si	-0.116632565	-0.071294773	0.019492383
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C	5.571616403	3.295526839	0.057106403
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C	7.806180314	4.274890396	-0.003579402
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C	-3.436614595	5.423901438	1.540193075
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C	-6.378138592	-2.131745564	0.170304325
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C	-8.604418232	-3.130263354	0.130940924
C	-7.789960073	-2.018910720	0.246434196
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H	5.685016949	-0.057195807	-0.844773393
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H	8.464121293	5.133235701	0.141684813
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H	-0.217989859	-5.888311552	-0.992693153
H	4.301147736	-3.677652360	-1.347645438
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H	2.822213145	-9.397630085	-2.210397636
H	0.826810973	-8.064814445	-1.594041089
H	-6.220764474	-5.547699986	-0.283452822
H	-8.681753030	-5.284733924	-0.142635633
H	-9.688583391	-3.023116049	0.192319901
H	-8.228042991	-1.029880542	0.399317623
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H	2.132842617	0.269035268	-3.616521089
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Si	0.714779482	-0.597499559	3.164586638
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C	2.054077146	-1.924219406	3.083079975
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H	1.640203605	-2.886509577	2.743396528
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H	0.729690623	1.828501593	3.793443265
H	2.314434160	1.344883717	3.153153136
H	1.853911127	0.898166485	4.809026022

H	-2.059605850	-0.571748860	-4.115400211
H	-1.896669612	0.940383668	-5.041839555
H	-2.733263837	0.943001177	-3.471825568
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SiNc-(OH)₂

singlet

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C	2.057764638	2.144523201	0.293665007
N	1.786499164	0.807962743	0.061394341
C	2.335309727	-3.372388234	-0.975384239
C	1.047350557	-3.975708480	-0.951634125
C	0.103708136	-2.919922345	-0.630144250
N	0.787812854	-1.727107135	-0.471204004
C	2.140742970	-1.968564771	-0.653300641
N	3.142751284	-1.107576329	-0.569115399
N	-1.199152484	-3.130392105	-0.523318387
N	-0.790414500	1.704447572	0.534605869
C	-2.138242238	1.942195287	0.721312912
C	-2.337059438	3.341757369	1.055153812
C	-1.046398024	3.939239566	1.074976642
C	-0.102070860	2.891001426	0.725026037
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C	7.630164687	2.111925817	-0.636405870
C	8.416148437	3.244496870	-0.552608621
C	7.837613493	4.491781639	-0.206836572
C	6.485979542	4.580758579	0.061641405
C	-0.877142557	5.274263792	1.387616637
C	-2.029585330	6.056948778	1.671911065
C	-3.345214716	5.451226609	1.632741599
C	-3.477478997	4.070580141	1.328314763
C	-4.482143875	6.268663659	1.893479510
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C	0.877094788	-5.319528987	-1.221212928
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C	1.913456117	-7.493043525	-1.813049944
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C	-8.472587829	-3.156616164	0.279596227
C	-7.668924267	-2.042773525	0.420548677
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H	6.037949578	5.538831031	0.335546522
H	0.117164051	5.723090215	1.410597921
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H	-2.952568433	9.261454791	2.471934755
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