SUPPORTING INFORMATION

Theoretical study on photophysical properties of double helicenes entwined with two perylene diimides

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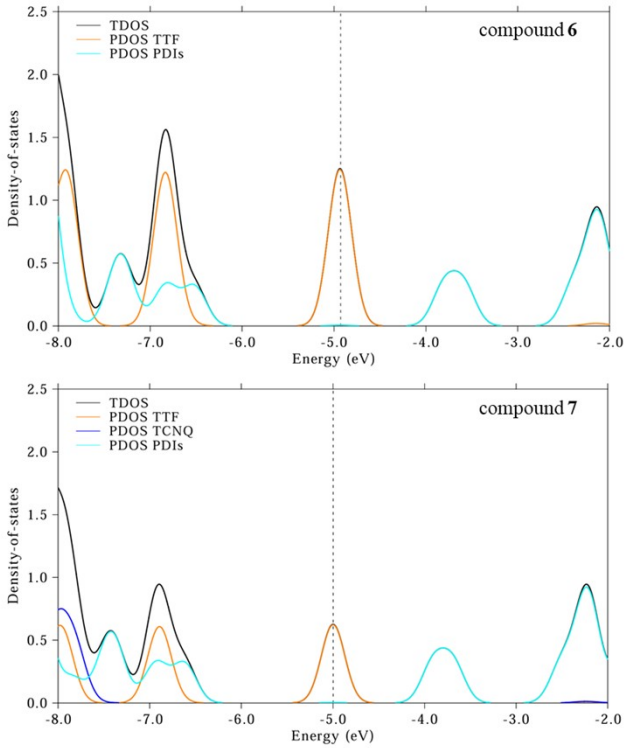


Fig. S1 Plot of DOS of compounds **6** and **7**. The dashed line represents the HOMO level.

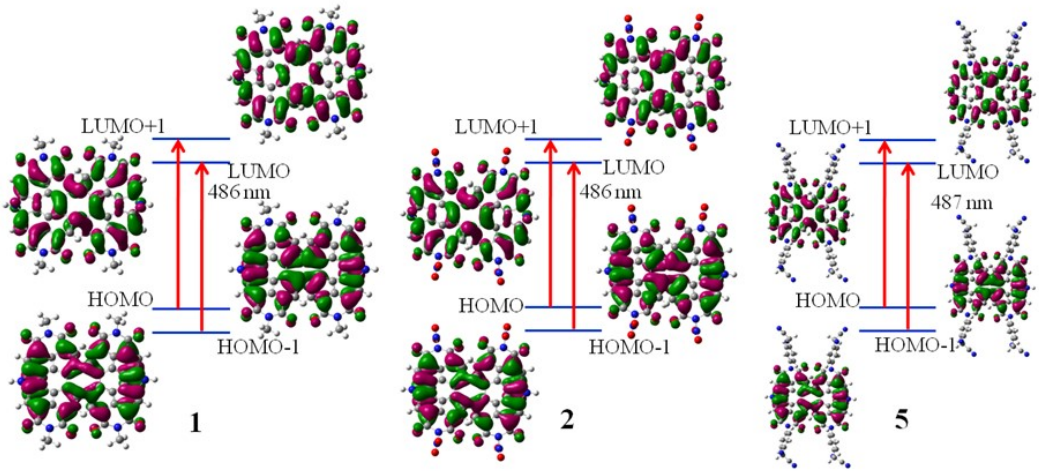
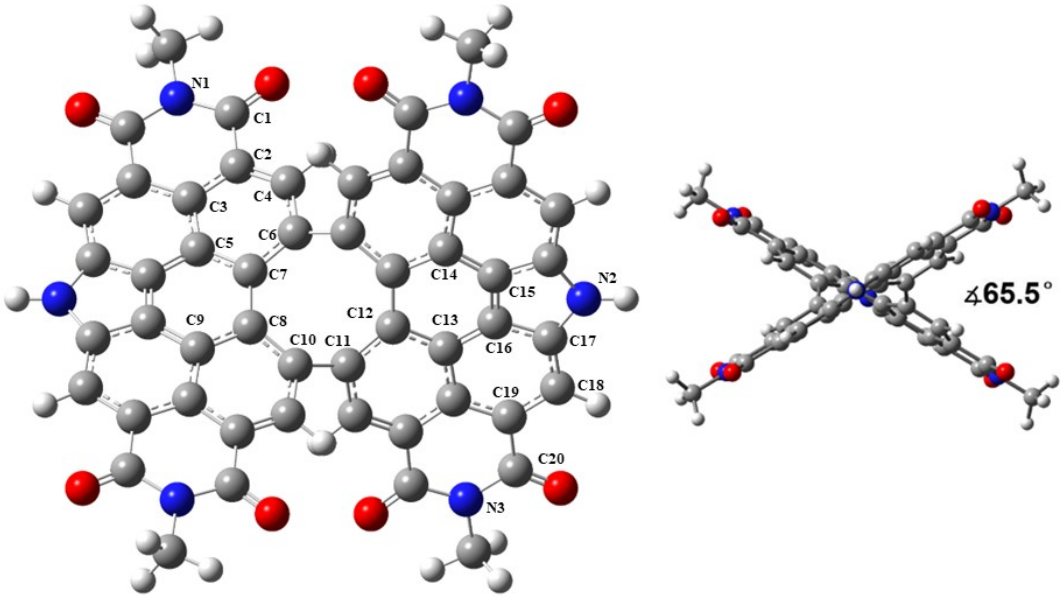


Fig. S2 Molecular orbital isosurfaces involved in the major electron transitions of compounds **1**, **2** and **5**.

Table S1 The main concerned bond length (Å), bond angles (°), and the torsion angle (°) defined by the central benzene rings in each PDI subunit for compounds **1**-**7** calculated at the PBE0/6-311g(d) level.



	1	**2**	**3**	**4**	**5**	**6**	**7**
N1-C1	1.402	1.405	1.393	1.393	1.410	1.418	1.417
C1-C2	1.476	1.473	1.470	1.471	1.474	1.473	1.474
C2-C3	1.397	1.401	1.399	1.398	1.398	1.398	1.398
C2-C4	1.385	1.385	1.384	1.384	1.385	1.385	1.385
C3-C5	1.340	1.401	1.399	1.398	1.400	1.400	1.401
C4-C6	1.420	1.419	1.420	1.420	1.420	1.419	1.419
C5-C7	1.430	1.430	1.430	1.4292	1.429	1.429	1.430
C6-C7	1.404	1.403	1.403	1.404	1.404	1.403	1.403
C7-C8	1.481	1.480	1.481	1.480	1.481	1.481	1.481
C8-C10	1.404	1.403	1.403	1.403	1.404	1.403	1.404
C10-C11	1.496	1.496	1.495	1.495	1.495	1.495	1.495
C12-C13	1.430	1.430	1.430	1.430	1.430	1.430	1.429
C13-C16	1.380	1.381	1.381	1.381	1.380	1.380	1.380
C14-C15	1.380	1.381	1.381	1.3801	1.380	1.380	1.380
C15-C16	1.371	1.372	1.371	1.371	1.371	1.371	1.371
C16-C17	1.388	1.389	1.388	1.389	1.389	1.389	1.389
C17-N2	1.398	1.395	1.397	1.396	1.397	1.397	1.397
C17-C18	1.408	1.407	1.408	1.406	1.408	1.408	1.408
C18-C19	1.394	1.394	1.394	1.395	1.394	1.394	1.395
C19-C20	1.478	1.475	1.473	1.473	1.478	1.476	1.477
C20-N3	1.401	1.407	1.395	1.408	1.414	1.420	1.414
C6-C7-C8	127.4	127.0	127.3	127.3	127.3	127.3	127.2
C7-C8-C10	127.4	127.0	127.3	127.1	127.3	127.2	127.3
C8-C10-C11	127.2	127.2	127.1	127.1	127.3	127.3	127.2
C5-C9-C13-C14	65.5	66.2	66.0	65.7	65.4	65.6	65.5

Table S2 The β_{HRS} values ($\times 10^{-30}$ esu) of the compounds **1**-**7** calculated at the functionals PBE0, M06-2X, CAM-B3LYP and BHandHLYP and the basis set 6-311G(d).

Compounds	PBE0	M06-2X	CAM-B3LYP	BHandHLYP
1	5.07	4.29	4.46	4.52
2	5.05	4.50	4.59	4.82
3	3.37	3.44	3.58	3.79
4	10.18	8.03	7.91	7.74
5	7.43	6.40	6.70	6.69
6	21.11	4.30	5.33	5.04
7	93.51	9.40	8.18	8.71

Table S3 Cartesian coordinates (Å) for the optimized S_0 geometry of compound **1** using the PBE0 with 6-311G(d) basis set.

C	-5.605659	-2.107989	1.418213	C	4.116657	0.550561	0.409743
C	-5.427209	-0.933848	0.661080	C	0.625737	1.571996	0.408692
C	-4.116663	-0.550604	0.409663	C	0.795751	2.754755	1.176319
C	-2.947038	-1.180031	0.785013	C	1.998517	3.150070	1.736889
C	-3.136590	-2.382243	1.476636	C	3.136555	2.382184	1.476735
C	-4.459159	-2.799846	1.805877	C	4.459133	2.799809	1.805968
C	-1.695539	-0.667723	0.321382	C	5.605627	2.107980	1.418289
C	-0.625753	-1.572066	0.408647	C	5.427198	0.933828	0.661170
C	-0.795782	-2.754824	1.176264	C	4.605661	-4.057592	-2.564538
C	-1.998562	-3.150145	1.736797	N	3.431531	-4.758986	-2.867246
C	-4.116928	0.548658	-0.410154	C	2.126387	-4.408883	-2.495444
C	-2.947563	1.178669	-0.785430	C	2.124275	4.409590	2.495499
C	-1.695841	0.666891	-0.321796	N	3.429249	4.760317	2.867317
C	-5.427645	0.931503	-0.661253	C	4.603666	4.059242	2.564964
C	-5.606629	2.105687	-1.418175	O	1.175143	-5.103633	-2.778196
C	-4.460463	2.798035	-1.805894	O	5.680144	-4.491653	-2.923311
C	-3.137673	2.380917	-1.476810	O	1.172699	5.103930	2.778176
C	-2.000007	3.149410	-1.736834	O	5.677963	4.493873	2.923642
C	-0.797044	2.754538	-1.176371	C	3.617192	-5.992441	-3.619707
C	-0.626485	1.571754	-0.408913	C	3.614372	5.993868	3.619728
C	-2.124335	-4.409688	2.495350	N	6.231202	0.001293	0.000085
N	-3.429307	-4.760328	2.867289	N	-6.231202	-0.001320	-0.000016
C	-4.603729	-4.059277	2.564885	H	-6.569972	-2.519679	1.696898
C	-4.605584	4.057454	-2.564786	H	0.053131	-3.419161	1.301077
N	-3.431507	4.759153	-2.866999	H	-6.571137	2.517070	-1.696685
C	-2.126380	4.409080	-2.495093	H	0.051550	3.419298	-1.301053
O	-5.677999	-4.493740	2.923798	H	-2.634501	-6.426570	3.797783
O	-1.172733	-5.103855	2.778348	H	-4.236978	-6.687373	3.053266
O	-5.680074	4.491605	-2.923426	H	-4.114799	-5.780057	4.564804

O	-1.175063	5.103575	-2.778244	H	-4.240759	6.685508	-3.053076
C	-3.614412	-5.993764	3.619900	H	-4.116674	5.778724	-4.564779
C	-3.617159	5.992604	-3.619444	H	-2.637495	6.426299	-3.796520
C	0.797071	-2.754545	-1.176448	H	-0.051540	-3.419288	-1.301209
C	0.626501	-1.571790	-0.408930	H	6.571182	-2.517117	-1.696516
C	1.695852	-0.666937	-0.321763	H	-0.053166	3.419090	1.301131
C	2.947583	-1.178675	-0.785405	H	6.569947	2.519689	1.696974
C	3.137703	-2.380903	-1.476843	H	4.238294	-6.686608	-3.052097
C	2.000041	-3.149368	-1.736953	H	4.119410	-5.778851	-4.563645
C	4.116926	-0.548672	-0.410092	H	2.637328	-6.424639	-3.799328
C	5.427661	-0.931521	-0.661187	H	4.236862	6.687434	3.052939
C	5.606663	-2.105706	-1.418103	H	2.634458	6.426681	3.797607
C	4.460490	-2.798046	-1.805843	H	4.114827	5.780325	4.564625
C	1.695530	0.667656	0.321439	H	7.236513	0.001463	0.000202
C	2.947020	1.179973	0.785101	H	-7.236512	-0.001459	0.000107

Table S4 Cartesian coordinates (Å) for the optimized S_0 geometry of compound **2** using the PBE0 with 6-311G(d) basis set.

C	-2.088560	5.609646	1.438294	C	0.547065	-4.116868	0.413180
C	-0.924801	5.428907	0.667684	C	1.561583	-0.623557	0.412782
C	-0.547015	4.116850	0.413403	C	2.737582	-0.784899	1.189418
C	-1.176741	2.948482	0.794118	C	3.129632	-1.984486	1.758858
C	-2.373369	3.134758	1.497899	C	2.373548	-3.134814	1.497495
C	-2.778571	4.464666	1.833055	C	2.778788	-4.464735	1.832558
C	-0.664857	1.698856	0.324778	C	2.088728	-5.609700	1.437840
C	-1.561537	0.623541	0.412992	C	0.924879	-5.428934	0.667372
C	-2.737441	0.784854	1.189780	C	-4.023174	-4.627395	-2.608315
C	-3.129422	1.984419	1.759311	N	-4.683307	-3.416667	-2.889023
C	0.547384	4.116811	-0.413356	C	-4.380314	-2.092487	-2.529409
C	1.177013	2.948394	-0.794085	C	4.380054	-2.093004	2.529372
C	0.665013	1.698804	-0.324776	N	4.682913	-3.417226	2.888940
C	0.925310	5.428841	-0.667573	C	4.022684	-4.627880	2.608144
C	2.089106	5.609495	-1.438147	O	-5.101599	-1.180193	-2.838148
C	2.779016	4.464462	-1.832930	O	-4.476585	-5.675868	-2.991024
C	2.373680	3.134581	-1.497825	O	5.101417	-1.180794	2.838179
C	3.129642	1.984184	-1.759236	O	4.475989	-5.676409	2.990826
C	2.737539	0.784639	-1.189747	N	-0.000300	-6.232290	-0.000154
C	1.561599	0.623411	-0.412996	N	0.000297	6.232288	0.000075
C	-4.379751	2.092907	2.529978	H	-2.492035	6.575788	1.722914
N	-4.682569	3.417119	2.889623	H	-3.397780	-0.066985	1.317774
C	-4.022374	4.627786	2.608793	H	2.492686	6.575608	-1.722716
C	4.022860	4.627489	-2.608623	H	3.397807	-0.067255	-1.317742
N	4.682956	3.416772	-2.889462	H	-3.397967	0.067301	-1.317335

C	4.380007	2.092579	-2.529860	H	-2.492896	-6.575547	-1.722659
O	-4.475627	5.676303	2.991569	H	3.397938	0.066935	1.317362
O	-5.101074	1.180683	2.838834	H	2.492236	-6.575852	1.722379
O	4.476228	5.675976	-2.991346	H	-0.000348	-7.238140	-0.000176
O	5.101259	1.180298	-2.838715	H	0.000340	7.238138	0.000084
C	-2.737684	-0.784597	-1.189448	N	-5.931783	-3.570135	-3.664600
C	-1.561653	-0.623399	-0.412830	N	-5.930913	3.570708	3.665391
C	-0.665054	-1.698795	-0.324760	N	5.931356	-3.570844	3.664557
C	-1.177110	-2.948367	-0.794055	N	5.931343	3.570270	-3.665183
C	-2.373862	-3.134528	-1.497658	O	6.909757	3.740293	-3.007945
C	-3.129855	-1.984121	-1.758935	O	5.794322	3.502241	-4.846526
C	-0.547435	-4.116798	-0.413447	O	6.909717	-3.740959	3.007229
C	-0.925392	-5.428819	-0.667664	O	5.794443	-3.502779	4.845927
C	-2.089282	-5.609444	-1.438104	O	-5.793857	3.502612	4.846722
C	-2.779238	-4.464397	-1.832764	O	-6.909329	3.740850	3.008194
C	0.664894	-1.698870	0.324634	O	-6.910115	-3.740178	-3.007252
C	1.176836	-2.948513	0.793864	O	-5.794901	-3.502035	-4.845950

Table S5 Cartesian coordinates (Å) for the optimized S_0 geometry of compound **3** using the PBE0 with 6-311G(d) basis set.

C	-5.606170	-2.103252	1.421789	C	4.115622	0.547745	0.411980
C	-5.426545	-0.930561	0.662931	C	0.625321	1.570025	0.409985
C	-4.115661	-0.548155	0.411468	C	0.793998	2.752426	1.178376
C	-2.946343	-1.177008	0.790806	C	1.995166	3.144072	1.744450
C	-3.135178	-2.375120	1.486977	C	3.135105	2.374876	1.487173
C	-4.460043	-2.793149	1.814705	C	4.459972	2.793087	1.814669
C	-1.695061	-0.666348	0.323359	C	5.606113	2.103243	1.421739
C	-0.625369	-1.570372	0.409816	C	5.426502	0.930393	0.663125
C	-0.794079	-2.752760	1.178201	C	4.608018	-4.046573	-2.574636
C	-1.995256	-3.144309	1.744347	N	3.423095	-4.704436	-2.904202
C	-4.115614	0.547896	-0.412130	C	2.125244	-4.397170	-2.502393
C	-2.946237	1.176836	-0.791188	C	2.125326	4.396972	2.502248
C	-1.695007	0.666092	-0.323645	N	3.423260	4.704547	2.903566
C	-5.426474	0.930643	-0.663220	C	4.608136	4.046526	2.574160
C	-5.606019	2.103620	-1.421653	O	1.208403	-5.146661	-2.771110
C	-4.459846	2.793463	-1.814500	O	5.674540	-4.523571	-2.911214
C	-3.135005	2.375173	-1.486998	O	1.208565	5.146567	2.770806
C	-1.995028	3.144390	-1.744092	O	5.674691	4.523552	2.910616
C	-0.793889	2.752625	-1.178037	N	6.230374	-0.000136	-0.000066
C	-0.625280	1.570108	-0.409814	N	-6.230393	0.000118	-0.000078
C	-2.125470	-4.397171	2.502189	H	-6.571499	-2.514247	1.698163
N	-3.423298	-4.704035	2.904555	H	0.054807	-3.417807	1.300228
C	-4.608221	-4.046437	2.574393	H	-6.571318	2.514875	-1.697750

C	-4.607952	4.046976	-2.573893	H	0.055038	3.417646	-1.299904
N	-3.422945	4.704625	-2.903699	H	-0.054993	-3.417736	-1.300397
C	-2.125192	4.397474	-2.501520	H	6.571356	-2.514473	-1.698373
O	-5.674809	-4.523435	2.910835	H	-0.054915	3.417436	1.300421
O	-1.208760	-5.146956	2.770391	H	6.571431	2.514403	1.697909
O	-5.674432	4.524191	-2.910189	H	7.235768	-0.000085	-0.000147
O	-1.208200	5.146785	-2.770383	H	-7.235787	0.000052	-0.000232
C	0.793931	-2.752742	-1.178341	N	3.555075	-5.815765	-3.743683
C	0.625284	-1.570378	-0.409899	H	4.464407	-6.218924	-3.544113
C	1.695016	-0.666400	-0.323457	H	2.810629	-6.456581	-3.489425
C	2.946266	-1.177091	-0.790973	N	-3.555241	-5.815360	3.743996
C	3.135048	-2.375199	-1.487169	H	-4.465841	-6.216694	3.546310
C	1.995082	-3.144350	-1.744493	H	-2.812846	-6.457751	3.487634
C	4.115611	-0.548247	-0.411697	N	3.555192	5.815968	3.742870
C	5.426479	-0.930721	-0.663148	H	4.465310	6.217982	3.544470
C	5.606049	-2.103428	-1.421993	H	2.811950	6.457658	3.487316
C	4.459900	-2.793290	-1.814882	N	-3.555026	5.816094	-3.742982
C	1.695021	0.665987	0.323648	H	-4.462908	6.221331	-3.541043
C	2.946281	1.176662	0.791173	H	-2.808525	6.455316	-3.490649

Table S6 Cartesian coordinates (Å) for the optimized S_0 geometry of compound **4** using the PBE0 with 6-311G(d) basis set.

C	5.726505	-1.715913	-0.877677	C	-4.055720	0.912552	-0.823453
C	5.470199	-0.555645	-0.125415	C	-0.581712	1.935240	-0.470056
C	4.138049	-0.184497	0.005492	C	-0.672043	3.118256	-1.250648
C	3.013093	-0.812734	-0.491160	C	-1.814244	3.515539	-1.924533
C	3.269125	-2.006046	-1.178615	C	-2.975301	2.750309	-1.777384
C	4.625988	-2.407729	-1.383996	C	-4.260474	3.169379	-2.235739
C	1.722064	-0.299147	-0.150906	C	-5.439058	2.477749	-1.965394
C	0.661564	-1.196107	-0.348527	C	-5.335357	1.301493	-1.195912
C	0.899748	-2.369274	-1.109185	C	-4.866585	-3.645690	2.145790
C	2.150199	-2.760041	-1.558304	N	-3.689570	-4.303347	2.551770
C	4.055675	0.912956	0.823269	C	-2.334869	-4.003738	2.322954
C	2.855292	1.546122	1.076963	C	-1.868471	4.774536	-2.683828
C	1.656878	1.033291	0.490843	N	-3.137716	5.133899	-3.131104
C	5.335279	1.302001	1.195730	C	-4.333276	4.428180	-3.000285
C	5.438880	2.478221	1.965282	O	-1.460057	-4.724355	2.728313
C	4.260222	3.169715	2.235678	O	-5.947832	-4.099006	2.425670
C	2.975079	2.750512	1.777378	O	-0.911002	5.479477	-2.926269
C	1.813965	3.515620	1.924604	O	-5.348532	4.862735	-3.506553
C	0.671767	3.118259	1.250767	N	-6.202714	0.376831	-0.611455
C	0.581549	1.935283	0.470103	N	6.202708	0.377414	0.611255
C	2.335184	-4.003632	-2.322864	H	6.716346	-2.116272	-1.070617

N	3.689907	-4.303088	-2.551763	H	0.064479	-3.028184	-1.324485
C	4.866877	-3.645224	-2.145973	H	6.372139	2.890354	2.334369
C	4.332948	4.428464	3.000306	H	-0.186291	3.781581	1.290714
N	3.137324	5.134256	3.130993	H	-0.064209	-3.028120	1.324612
C	1.868058	4.774516	2.684087	H	-6.716167	-2.116881	1.070428
O	5.948153	-4.098602	-2.425629	H	0.185936	3.781686	-1.290529
O	1.460430	-4.724378	-2.728112	H	-6.372349	2.889808	-2.334488
O	5.348111	4.863037	3.506675	H	-7.204025	0.383606	-0.704237
O	0.910470	5.479199	2.926773	H	7.204026	0.384320	0.703961
C	-0.899540	-2.369316	1.109224	N	-3.920378	-5.543670	3.316125
C	-0.661447	-1.196165	0.348516	N	3.920823	-5.543482	-3.315976
C	-1.722029	-0.299317	0.150827	N	-3.238850	6.394728	-3.728237
C	-3.013019	-0.813029	0.491026	N	3.238402	6.395015	3.728070
C	-3.268962	-2.006341	1.178510	O	3.976510	-5.398390	-4.497585
C	-2.149970	-2.760192	1.558298	O	4.020194	-6.528842	-2.653797
C	-4.138014	-0.184905	-0.005677	O	-4.019799	-6.529094	2.654048
C	-5.470135	-0.556158	0.125231	O	-3.975949	-5.398469	4.497728
C	-5.726358	-1.716431	0.877516	H	2.347422	6.572474	4.179200
C	-4.625790	-2.408154	1.383849	H	3.985758	6.333351	4.410915
C	-1.656954	1.033150	-0.490898	H	-3.986862	6.333191	-4.410295
C	-2.855397	1.545877	-1.077065	H	-2.348130	6.571951	-4.179875

Table S7 Cartesian coordinates (Å) for the optimized S_0 geometry of compound **5** using the PBE0 with 6-311G(d) basis set.

C	2.282981	4.871774	-2.918186	H	-3.397484	-0.274058	-1.287321
C	1.105156	4.945025	-2.149898	H	-2.699209	-6.760060	0.231431
C	0.685511	3.768222	-1.544148	H	-0.196488	-6.989107	2.055440
C	1.281423	2.523681	-1.572388	H	0.225663	6.891973	-2.030363
C	2.487498	2.477426	-2.282128	C	-5.860323	4.556627	2.409198
C	2.941802	3.643659	-2.965473	C	-5.932299	4.528691	3.794505
C	0.733420	1.467591	-0.780073	C	-6.957761	4.951934	1.660522
C	1.605074	0.390306	-0.557162	C	-7.108485	4.890851	4.431876
C	2.789516	0.302954	-1.334632	H	-5.068770	4.222619	4.374230
C	3.217929	1.288278	-2.208458	C	-8.134280	5.319830	2.297642
C	-0.413807	4.028255	-0.766900	H	-6.891774	4.982104	0.578912
C	-1.077061	3.029308	-0.083464	C	-8.213834	5.287077	3.684836
C	-0.600032	1.684553	-0.173082	H	-7.155073	4.875515	5.516370
C	-0.758722	5.366969	-0.897301	H	-8.985010	5.639692	1.704798
C	-1.927593	5.783169	-0.231553	C	-6.087286	-4.332633	-2.462095
C	-2.653075	4.811666	0.457381	C	-6.149908	-4.296860	-3.847672
C	-2.273691	3.438368	0.518104	C	-7.207975	-4.673151	-1.720805
C	-3.069873	2.438266	1.082721	C	-7.339391	-4.596859	-4.492704
C	-2.708432	1.116003	0.886277	H	-5.268704	-4.033677	-4.421768

C	-1.532340	0.705717	0.205233	C	-8.397863	-4.979062	-2.365601
C	4.475043	1.153454	-2.966738	H	-7.149989	-4.709796	-0.638963
N	4.866305	2.298373	-3.691639	C	-8.467600	-4.938853	-3.753181
C	4.202843	3.546063	-3.729553	H	-7.378856	-4.576084	-5.577365
C	-3.908272	5.209190	1.128025	H	-9.267084	-5.257105	-1.778493
N	-4.643081	4.174356	1.750561	C	5.863990	-2.604659	4.567216
C	-4.324260	2.800817	1.767024	C	6.956328	-3.381118	4.205684
O	4.663815	4.468114	-4.360389	C	5.927806	-1.780924	5.681212
O	5.140835	0.145882	-2.978470	C	8.113374	-3.335179	4.966746
O	-4.308821	6.349099	1.155603	H	6.896890	-4.027150	3.337468
O	-5.046564	1.996366	2.305712	C	7.089702	-1.728070	6.437504
C	2.742462	-0.554042	1.379408	H	5.071106	-1.175916	5.955359
C	1.569487	-0.579295	0.580329	C	8.183035	-2.508637	6.083712
C	0.637894	-1.608369	0.788390	H	8.966119	-3.944703	4.681909
C	1.114919	-2.691321	1.590335	H	7.133990	-1.084795	7.310516
C	2.307572	-2.707659	2.323320	C	6.084638	2.194867	-4.444414
C	3.101163	-1.559065	2.262240	C	6.125838	1.404933	-5.582225
C	0.452821	-3.901620	1.554315	C	7.215775	2.884586	-4.030317
C	0.793911	-5.095871	2.175162	C	7.304128	1.295867	-6.307912
C	1.959463	-5.083646	2.965044	H	5.238266	0.870841	-5.902166
C	2.684567	-3.893549	3.019367	C	8.390527	2.781360	-4.757378
C	-0.696680	-1.753363	0.162381	H	7.174732	3.509057	-3.145246
C	-1.245984	-3.070148	0.068336	C	8.439135	1.983811	-5.897395
C	-0.647869	-4.102895	0.761855	H	7.327020	0.677695	-7.199382
C	-1.568964	-0.725120	-0.227666	H	9.267281	3.335983	-4.437228
C	-2.757706	-1.071102	-0.922461	C	-9.790936	-5.196393	-4.477275
C	-3.190454	-2.371557	-1.119842	H	-10.254363	-4.224942	-4.704579
C	-2.457798	-3.413025	-0.544123	C	-9.526181	5.612584	4.401527
C	-2.916717	-4.761640	-0.480937	H	-10.033585	4.665619	4.637989
C	-2.256511	-5.769655	0.220744	C	9.486298	-2.460199	6.877810
C	-1.072459	-5.418109	0.896776	H	9.936197	-3.461324	6.871704
C	3.933087	-3.861182	3.808538	C	9.767876	1.828718	-6.640373
N	4.661653	-2.650085	3.784241	H	10.406099	1.141741	-6.065400
C	4.346365	-1.487726	3.047261	C	10.500492	3.094230	-6.737588
C	-4.456757	-2.664844	-1.815518	C	9.619510	1.236746	-7.970435
N	-4.855515	-4.017506	-1.795037	C	9.286769	-2.096270	8.281433
C	-4.186597	-5.089597	-1.161628	C	10.454935	-1.552953	6.251419
O	5.063349	-0.516723	3.072208	C	-10.757841	-5.933243	-3.662087
O	4.331618	-4.805952	4.449283	C	-9.602193	-5.876296	-5.761333
O	-5.125409	-1.822793	-2.365706	C	-10.456874	6.383011	3.575386
O	-4.651021	-6.205072	-1.187735	C	-9.310066	6.297374	5.678674
N	-0.164168	-6.026558	1.766256	N	-9.439252	-6.378756	-6.783495
N	0.196252	5.926984	-1.748981	N	-11.521819	-6.485208	-3.002228

H	2.721160	5.708143	-3.452479	N	-9.127186	6.802795	6.695994
H	3.427970	-0.566205	-1.213475	N	-11.193770	6.961260	2.907291
H	-2.311122	6.797978	-0.239962	N	9.115274	-1.820168	9.385181
H	-3.395566	0.354981	1.241853	N	11.212247	-0.859143	5.732285
H	3.427921	0.280296	1.270518	N	11.083021	4.085652	-6.777701
H	2.339623	-5.939759	3.512275	N	9.495007	0.743823	-9.002559

Table S8 Cartesian coordinates (Å) for the optimized S_0 geometry of compound **6** using the PBE0 with 6-311G(d) basis set.

C	1.825283	-2.014824	-5.644781	H	2.192160	-2.389768	-6.594411
C	0.654440	-1.249091	-5.488815	H	3.403421	-1.295094	-0.095563
C	0.330878	-0.867251	-4.193598	H	-2.848499	0.985745	-6.707809
C	1.021082	-1.114021	-3.023975	H	-3.425669	1.294954	-0.036155
C	2.220504	-1.816642	-3.197682	H	3.374234	1.287706	-0.481079
C	2.575590	-2.279856	-4.499545	H	2.808810	2.338521	6.112188
C	0.565947	-0.519034	-1.806062	H	-3.417804	-1.334536	0.122079
C	1.519443	-0.486031	-0.776900	H	-2.182432	-1.060142	6.705073
C	2.698577	-1.262908	-0.920063	H	0.344058	0.710701	7.069124
C	3.041034	-1.948367	-2.073409	H	-0.363143	-0.777846	-7.311016
C	-0.772625	-0.053477	-4.226775	C	-5.715792	-3.342121	4.086027
C	-1.345842	0.447603	-3.075731	C	-6.912949	-2.843562	4.385777
C	-0.770075	0.119189	-1.809404	S	-5.535585	-5.098247	4.108272
C	-1.215160	0.063218	-5.537551	H	-7.131301	-1.785193	4.446191
C	-2.394814	0.804681	-5.739124	S	-8.190259	-3.962415	4.762946
C	-3.032124	1.316174	-4.608995	C	-7.261198	-5.396122	4.300457
C	-2.554728	1.125052	-3.278227	C	-7.825725	-6.603980	4.122613
C	-3.259414	1.510631	-2.133724	S	-9.555670	-6.900444	4.330309
C	-2.806018	1.075219	-0.899595	S	-6.902345	-8.039732	3.667469
C	-1.617869	0.322784	-0.709917	C	-9.509609	-8.490411	3.601858
C	4.300896	-2.706353	-2.169682	C	-8.317014	-9.002632	3.304267
N	4.595087	-3.218191	-3.457977	H	-10.455828	-8.995513	3.455556
C	3.829941	-3.046901	-4.641953	H	-8.152335	-9.985015	2.880368
C	-4.289589	2.069579	-4.789810	C	6.057940	3.991316	2.767927
N	-4.930376	2.509565	-3.601546	C	7.296947	3.504653	2.766928
C	-4.516037	2.268139	-2.267555	S	5.871513	5.744399	2.670557
O	4.208841	-3.511330	-5.688589	H	7.533688	2.448520	2.769718
O	5.049890	-2.887323	-1.243572	S	8.616199	4.635424	2.685149
O	-4.768152	2.313993	-5.869662	C	7.589563	6.061729	2.894381
O	-5.167746	2.660919	-1.333657	C	8.083225	7.278024	3.188234
C	2.754894	1.245846	0.409104	S	9.809377	7.593553	3.398569
C	1.573019	0.460611	0.379557	S	7.063878	8.706625	3.390868
C	0.725193	0.483402	1.497876	C	9.574050	9.188449	4.078060
C	1.295654	1.074579	2.668076	C	8.340068	9.688980	4.074276

C	2.502148	1.783818	2.726174	H	10.452431	9.705973	4.442027
C	3.206036	1.927739	1.526735	H	8.068876	10.672889	4.435186
C	0.725931	0.818331	3.898967	C	5.777605	-3.989942	-3.573789
C	1.174010	1.196066	5.157803	C	6.962681	-3.512284	-3.946643
C	2.350967	1.967157	5.201446	S	5.655917	-5.724509	-3.270840
C	2.981910	2.242500	3.988828	H	7.146874	-2.475559	-4.197241
C	-0.602017	-0.160142	1.629583	S	8.283588	-4.633647	-4.094610
C	-1.048833	-0.496559	2.945022	C	7.392516	-5.994290	-3.395960
C	-0.365443	-0.000604	4.036627	C	7.992094	-7.134582	-3.009538
C	-1.553096	-0.361947	0.617673	S	9.732924	-7.404967	-3.152925
C	-2.715845	-1.116927	0.920649	S	7.108566	-8.501534	-2.322165
C	-3.044860	-1.558182	2.191585	C	9.727551	-8.853003	-2.171390
C	-2.230417	-1.177998	3.262611	C	8.548168	-9.345920	-1.798147
C	-2.572932	-1.378314	4.632924	H	10.687120	-9.296835	-1.938788
C	-1.827761	-0.871739	5.697282	H	8.409206	-10.249017	-1.217655
C	-0.676091	-0.125141	5.384113	C	-6.106476	3.282476	-3.764955
C	4.240991	3.013437	4.009039	C	-7.334601	2.783670	-3.884494
N	4.880051	3.204588	2.755997	S	-5.923066	5.034374	-3.877458
C	4.462138	2.698571	1.498774	H	-7.563612	1.725944	-3.868032
C	-4.282743	-2.315703	2.445908	S	-8.646324	3.898257	-4.133371
N	-4.561311	-2.568015	3.812552	C	-7.657833	5.342108	-3.865547
C	-3.803643	-2.137311	4.933996	C	-8.188422	6.564446	-3.682586
O	5.106889	2.893001	0.499865	S	-9.929043	6.871570	-3.687164
O	4.727352	3.467524	5.014986	S	-7.206009	8.010345	-3.425728
O	-5.026333	-2.700839	1.579859	C	-9.781964	8.500237	-3.065480
O	-4.168763	-2.392028	6.054956	C	-8.558232	9.012079	-2.948192
N	0.290355	0.614371	6.069679	H	-10.699246	9.026011	-2.833083
N	-0.317596	-0.675650	-6.311743	H	-8.335626	-10.014817	-2.606347

Table S9 Cartesian coordinates (Å) for the optimized S_0 geometry of compound **7** using the PBE0 with 6-311G(d) basis set.

C	1.485646	-3.661126	-4.757671	H	-3.924239	1.143521	-0.555820
C	0.307468	-2.898780	-4.870814	H	2.885741	1.077584	-0.829033
C	-0.050303	-2.142313	-3.762880	H	2.154927	4.121221	5.096052
C	0.609847	-2.011271	-2.557793	H	-3.910427	-1.299826	0.409846
C	1.816196	-2.719035	-2.479987	H	-2.850133	1.035982	6.599843
C	2.207137	-3.553575	-3.569223	H	-0.330514	2.848029	6.456038
C	0.120281	-1.078290	-1.591092	H	-0.666416	-3.022091	-6.771832
C	1.046987	-0.720427	-0.599927	C	5.477981	4.689663	1.476428
C	2.231780	-1.491018	-0.469625	C	6.718573	4.240776	1.653938
C	2.607027	-2.492065	-1.349574	S	5.287416	6.325919	0.840150
C	-1.157392	-1.392692	-4.068314	H	6.959526	3.239714	1.987576
C	-1.763062	-0.572212	-3.138582	S	8.034680	5.307588	1.258803

C	-1.218376	-0.488229	-1.819785	C	6.996530	6.718224	1.005202
C	-1.568450	-1.689690	-5.360891	C	7.475658	7.973367	0.937202
C	-2.749196	-1.064351	-5.804787	S	9.192934	8.359972	1.092106
C	-3.418563	-0.241144	-4.899294	S	6.444331	9.383796	0.677697
C	-2.971028	-0.007790	-3.565753	C	8.929622	10.081288	1.262344
C	-3.707403	0.701529	-2.613015	C	7.694092	10.541604	1.075836
C	-3.282258	0.675483	-1.295124	H	9.793987	10.695026	1.481540
C	-2.095022	0.033295	-0.855642	H	7.407227	11.584439	1.121483
C	3.871792	-3.229003	-1.179205	C	5.394871	-4.855597	-2.092020
N	4.203278	-4.103860	-2.243448	C	6.587158	-4.488699	-2.556286
C	3.469178	-4.311211	-3.440831	S	5.279358	-6.422859	-1.288385
C	-4.680966	0.397779	-5.323287	H	6.769868	-3.570251	-3.099061
N	-5.350493	1.174284	-4.350290	S	7.922665	-5.578010	-2.323838
C	-4.964285	1.363388	-3.005212	C	7.022224	-6.681629	-1.272795
O	3.877992	-5.067153	-4.286944	C	7.619512	-7.638382	-0.539930
O	4.595233	-3.110944	-0.223256	S	9.367040	-7.902879	-0.539395
O	-5.138404	0.278817	-6.436350	S	6.725643	-8.750704	0.501525
O	-5.635309	2.022909	-2.248637	C	9.340781	-8.987714	0.832693
C	2.245899	1.306963	0.016934	C	8.153784	-9.368916	1.300567
C	1.068452	0.537804	0.207692	H	10.295812	-9.321422	1.217961
C	0.194248	0.896102	1.245313	H	8.002998	10.057721	2.121948
C	0.734423	1.827023	2.186370	C	-6.355854	-1.944047	4.736753
C	1.935405	2.534353	2.046252	C	-7.467640	-1.169718	5.036266
C	2.666944	2.307431	0.876694	C	-6.402127	-3.320954	4.888648
C	0.136650	1.958942	3.423364	C	-8.629193	-1.776139	5.487637
C	0.549996	2.717234	4.510538	H	-7.422017	-0.092342	4.925555
C	1.721956	3.478044	4.337205	C	-7.566493	-3.929988	5.334877
C	2.381547	3.369325	3.113465	H	-5.528593	-3.919659	4.656369
C	-1.133625	0.311080	1.540297	C	-8.683173	-3.158999	5.635235
C	-1.612033	0.397027	2.884507	H	-9.490394	-1.163210	5.734914
C	-0.956459	1.213376	3.783701	H	-7.592781	-5.008087	5.455630
C	-2.059887	-0.204521	0.620321	C	-6.566004	1.815929	-4.764114
C	-3.229030	-0.837871	1.116990	C	-7.686076	1.051398	-5.060267
C	-3.589834	-0.861306	2.453936	C	-6.613881	3.198190	-4.866911
C	-2.802046	-0.158637	3.369917	C	-8.854642	1.674680	-5.467704
C	-3.183038	0.078630	4.723342	H	-7.639196	-0.028661	-4.983019
C	-2.465876	0.897989	5.594709	C	-7.786796	3.822617	-5.266088
C	-1.303721	1.515329	5.093731	H	-5.735188	3.787650	-4.631185
C	3.636402	4.123368	2.919807	C	-8.907634	3.061021	-5.572199
N	4.303883	3.924344	1.682891	H	-9.729100	1.073861	-5.700619
C	3.919045	3.047994	0.636827	H	-7.818276	4.904258	-5.349774
C	-4.833831	-1.510152	2.906048	C	-9.997878	-3.819163	6.056690
N	-5.151925	-1.318616	4.266819	H	-10.639453	-3.907937	5.167489

C	-4.428473	-0.551072	5.207972	C	-10.221506	3.713116	-5.996130
O	4.585779	2.930818	-0.359675	C	-10.743363	-3.013611	7.027193
O	4.096452	4.872396	3.745417	N	-11.337380	-2.357939	7.762766
O	-5.548025	-2.161059	2.181403	C	-9.819130	-5.177338	6.572441
O	-4.829964	-0.432218	6.341837	N	-9.671811	-6.255150	6.947130
N	-0.356495	2.441507	5.536675	C	-10.030826	5.005227	-6.656955
N	-0.647227	-2.618343	-5.851122	N	-9.867456	6.014357	-7.185051
H	1.878834	-4.304077	-5.538044	C	-11.135335	3.856748	-4.856818
H	2.914911	-1.261521	0.341715	N	-11.850548	3.937247	-3.958819
H	-3.181444	-1.198020	-6.790811	H	-10.717834	3.057074	-6.722720