

Supporting Information

Heavy atom effect on Zn(II) phthalocyanines derivatives: a theoretical exploration of the photophysical properties

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- Cartesian coordinates of compounds **A,B** and **1-7**.

-S1-

C	-3.230885	-2.681914	-0.445499
C	-3.934201	-1.450538	-0.429907
C	-5.331301	-1.413500	-0.561897
C	-5.995557	-2.640759	-0.617910
C	-5.306014	-3.847726	-0.631258
C	-3.910799	-3.901476	-0.590521
C	-1.824732	-2.349204	-0.234568
C	-2.929719	-0.412699	-0.210307
H	-7.080214	-2.640151	-0.713353
H	-5.858592	-4.780128	-0.737462
N	-1.695361	-0.992557	-0.148701
N	-0.859826	-3.242095	-0.059395
C	0.423145	-2.962848	0.122812
C	1.460117	-3.963840	0.361001
C	2.689370	-3.260035	0.376211
C	1.423536	-5.358984	0.515370
C	2.359983	-1.855875	0.143268
C	3.905082	-3.937363	0.553160
C	2.649912	-6.020673	0.609020
C	3.857221	-5.330221	0.632283
H	2.647831	-7.102995	0.727756
H	4.788435	-5.877329	0.771754
N	1.004866	-1.729741	0.044720
N	-3.205064	0.870078	-0.012117
C	-2.307978	1.830163	0.165565
C	-2.637062	3.231887	0.413820
C	-1.407648	3.935524	0.406780
C	-3.852547	3.907858	0.597626
C	-0.370861	2.937026	0.157925
C	-1.370674	5.329006	0.576064
C	-3.804299	5.299612	0.692875
C	-2.596754	5.989946	0.677439
H	-4.735427	5.845282	0.838399
H	-2.594313	7.070897	0.808071
N	-0.952766	1.705010	0.065980
N	0.912167	3.218321	-0.020924
C	1.876991	2.327708	-0.207356
C	3.283099	2.662760	-0.414999
C	3.986253	1.431160	-0.414637
C	3.963270	3.883778	-0.545523
C	2.981694	0.390984	-0.207040
C	5.383256	1.395255	-0.547595
C	5.358542	3.830199	-0.586548
C	6.047830	2.623055	-0.588033
H	5.911457	4.763651	-0.681267
H	7.132494	2.623447	-0.683407
N	1.747480	0.970102	-0.137974
Zn	0.026020	-0.011559	-0.080511
N	3.257062	-0.893981	-0.023715
S	5.512511	-3.190436	0.668063
S	-6.346028	0.042152	-0.645724
S	-5.460042	3.159769	0.703089
S	0.090049	6.336117	0.652802
S	3.234691	5.498120	-0.650736
S	6.397974	-0.059097	-0.650153
C	-5.620797	0.902098	-2.074687
H	-4.635616	1.307937	-1.825414
H	-5.567173	0.228821	-2.936664
H	-6.301025	1.729352	-2.302663
C	5.233467	-1.996868	2.001648
H	5.018982	-1.005145	1.599148
H	4.441665	-2.346433	2.669586
C	5.671362	-0.904066	-2.087297
H	4.688063	-1.316100	-1.840652
H	5.613358	-0.220719	-2.941037
H	6.353659	-1.726344	-2.326814
C	-5.181661	1.955995	2.027642
H	-4.965993	0.967821	1.617273
H	-4.390450	2.300712	2.698769
S	-0.037026	-6.366777	0.583706
S	-3.182033	-5.514644	-0.713008
C	-0.897367	-5.645483	2.014026
H	-0.225672	-5.600513	2.877706
H	-1.297089	-4.657215	1.767490
H	-1.729016	-6.321856	2.236418
C	-2.046838	-5.306394	-2.117246
H	-2.556821	-4.798262	-2.942690
H	-1.147398	-4.765705	-1.808267
H	-1.770034	-6.317986	-2.431598
C	2.097359	5.302994	-2.055191
H	2.606336	4.802573	-2.885949
H	1.198577	4.759066	-1.749655
H	1.819995	6.317431	-2.359688
C	0.949448	5.604706	2.078533
H	0.278075	5.555595	2.942238
H	1.347453	4.617407	1.825834
H	1.782523	6.278082	2.304655
I	-6.981657	1.708896	3.240196
I	7.032968	-1.759694	3.217096