Supporting Information

Rational molecular engineering of pyrene-based D–A–π–A–D donor molecules for high-performance photovoltaics

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Table 1: Optimized coordinates of the designed compounds in the gas phase employing the HSEH1PBE/6-31G(d,p) level of theory.

S1

Atoms	Coordinates (Å)		
	X	Y	Z
C	11.788229	1.632761	2.698857
C	10.418813	1.590632	2.930453
C	9.561283	0.939498	2.034757
C	10.106146	0.316643	0.878055
C	11.511929	0.357827	0.653451
C	12.331156	1.022720	1.574016
C	8.148794	0.863323	2.246802
C	9.250972	-0.348160	-0.046837
C	7.842050	-0.375584	0.170906
C	7.331108	0.236235	1.362180
C	7.013933	-1.040079	-0.763463
C	7.600289	-1.686200	-1.858007
C	8.968857	-1.662552	-2.071038
C	9.816947	-0.990915	-1.184432
C	11.233411	-0.934902	-1.384994
C	12.044141	-0.287348	-0.509027
H	13.117741	-0.251174	-0.674066
H	11.648159	-1.425813	-2.261415
H	7.736110	1.318139	3.143462

H	12.438998	2.143352	3.402432
H	9.998588	2.064460	3.813592
H	13.403196	1.055253	1.398691
H	6.266146	0.186441	1.557018
H	6.953760	-2.188782	-2.571604
H	9.392278	-2.157784	-2.940674
C	-7.277940	1.509906	-1.517330
C	-8.598099	1.871113	-1.716609
C	-9.628508	1.248642	-1.002512
C	-9.292569	0.256942	-0.038796
C	-7.929196	-0.108951	0.174150
C	-6.918982	0.508280	-0.605378
C	-11.003989	1.583940	-1.210196
C	-10.330273	-0.366873	0.711970
C	-11.692116	-0.018102	0.481246
C	-11.992318	0.975504	-0.504641
C	-12.695004	-0.652734	1.225002
H	-13.733099	-0.387016	1.043879
C	-12.375283	-1.606844	2.183636
C	-11.049296	-1.946271	2.423064
C	-10.014398	-1.339636	1.700386
C	-8.637284	-1.644203	1.934731
C	-7.646731	-1.058024	1.212553
H	-6.611860	-1.291113	1.436419
H	-8.391326	-2.352216	2.721914
H	-11.241672	2.341848	-1.951935
H	-6.497184	1.994905	-2.092656
H	-8.845819	2.637402	-2.446092
H	-13.033330	1.237600	-0.674047
H	-13.166529	-2.087180	2.751432
H	-10.801707	-2.687328	3.178407
S	0.058046	-0.167936	-0.548408
C	1.174182	-1.494356	-0.409124
C	-1.316042	-1.219135	-0.377178
C	0.489065	-2.680963	-0.208315

C	-0.902397	-2.527354	-0.190504
C	4.710252	0.053378	-0.582023
C	3.267639	-0.061111	-0.515979
C	5.544138	-1.107126	-0.630226
C	2.615963	-1.338716	-0.496001
C	4.874663	-2.312956	-0.638781
C	3.467132	-2.427562	-0.574586
C	-2.690517	-0.754985	-0.437938
C	-3.056426	0.630098	-0.379011
C	-4.442076	1.051218	-0.425848
C	-5.505606	0.098021	-0.524731
C	-3.753778	-1.633119	-0.560956
C	-5.104634	-1.221947	-0.596726
S	3.809313	2.257859	-0.566326
S	-3.093280	3.007431	-0.241684
N	5.134169	1.318657	-0.620485
N	2.648601	1.117898	-0.496930
N	-2.201745	1.646135	-0.275631
N	-4.587597	2.376297	-0.351676
H	5.459879	-3.226994	-0.685807
H	3.046396	-3.427294	-0.593367
H	0.979478	-3.634642	-0.053754
H	-1.586396	-3.350118	-0.019303
H	-3.552002	-2.694587	-0.659111
H	-5.864831	-1.987759	-0.717853

S2

C	-17.866359	4.091743	1.612969
C	-16.521138	3.907583	1.907722
C	-15.782502	2.898569	1.276850
C	-16.422738	2.057124	0.325318
C	-17.804568	2.248063	0.036508
C	-18.503110	3.271606	0.688891
C	-14.402648	2.664614	1.569891

C	-15.688265	1.027957	-0.330818
C	-14.299310	0.848711	-0.056146
C	-13.698139	1.688007	0.940211
C	-13.587347	-0.171533	-0.732822
C	-14.277027	-1.012110	-1.615358
C	-15.626138	-0.844621	-1.878081
C	-16.353638	0.177887	-1.258849
C	-17.743302	0.390281	-1.528145
C	-18.437112	1.382188	-0.912373
H	-19.491583	1.533683	-1.127359
H	-18.234460	-0.265226	-2.242416
H	-13.923688	3.280715	2.326502
H	-18.424919	4.879332	2.109835
H	-16.027909	4.546210	2.635639
H	-19.556378	3.417089	0.464178
H	-12.660675	1.517170	1.205241
H	-13.721222	-1.790227	-2.130224
H	-16.127801	-1.500713	-2.584282
C	13.459690	3.107493	0.314290
C	14.732430	3.648401	0.378369
C	15.860834	2.846330	0.175756
C	15.677027	1.467195	-0.125971
C	14.363512	0.913739	-0.199588
C	13.247334	1.748088	0.051887
C	17.189404	3.372112	0.259519
C	16.816784	0.645099	-0.357905
C	18.128148	1.193740	-0.265214
C	18.274481	2.582164	0.052749
C	19.233047	0.363185	-0.489407
H	20.232249	0.783896	-0.414569
C	19.062380	-0.979601	-0.805444
C	17.787147	-1.521779	-0.907049
C	16.653485	-0.728997	-0.687940
C	15.325119	-1.245249	-0.805282
C	14.236356	-0.464372	-0.578020

H	13.241993	-0.878166	-0.704329
H	15.198955	-2.284363	-1.098167
H	17.311144	4.426183	0.494483
H	12.597132	3.738191	0.508250
H	14.863893	4.703073	0.604641
H	19.277935	2.993846	0.121186
H	19.931236	-1.607852	-0.977257
H	17.656919	-2.570373	-1.160953
S	-0.062978	-1.064072	0.096085
C	-1.224336	-2.355573	0.130961
C	1.281915	-2.160551	0.185100
C	-0.576161	-3.570006	0.225099
C	0.827829	-3.461372	0.254955
H	-1.102196	-4.517686	0.231833
H	1.495063	-4.314684	0.287656
C	-12.134333	-0.381364	-0.559709
C	-11.228263	0.681141	-0.709538
C	-9.879227	0.422823	-0.572609
C	-9.352145	-0.857790	-0.273890
C	-11.630897	-1.663703	-0.297978
C	-10.270218	-1.908208	-0.151689
C	-7.893582	-0.736367	-0.240066
C	-7.614607	0.718737	-0.567476
C	-6.896359	-1.639296	0.055263
C	-5.438561	-1.553486	-0.018180
C	-7.178672	-3.018138	0.621782
C	-4.912245	-2.776682	0.470113
C	-4.514579	-0.608462	-0.481983
C	-3.155031	-0.881835	-0.434533
C	-2.653311	-2.090435	0.075175
C	-3.564858	-3.057703	0.536323
N	-8.838846	1.319018	-0.721535
N	-5.954719	-3.597036	0.851830
O	-6.561801	1.322837	-0.661008
O	-8.232322	-3.567677	0.883220

H	-11.582332	1.676135	-0.960628
H	-12.329785	-2.485216	-0.174725
H	-9.916725	-2.901875	0.078497
H	-4.866082	0.335942	-0.868940
H	-2.462330	-0.140699	-0.821967
H	-3.215856	-3.994198	0.958734
C	2.973011	-0.409011	-0.328203
C	4.286873	0.006252	-0.293228
C	2.653963	-1.677612	0.186480
C	5.344124	-0.774433	0.237606
C	3.689228	-2.474840	0.703840
C	5.007632	-2.043478	0.728187
C	6.582341	-0.015823	0.064804
C	6.160369	1.267731	-0.626829
C	7.883407	-0.268137	0.440069
C	9.138683	0.437486	0.175838
C	8.268217	-1.425404	1.343068
C	10.165929	-0.244286	0.873689
C	9.523071	1.537667	-0.600792
C	10.856181	1.928416	-0.641340
C	11.855764	1.249362	0.070096
C	11.493428	0.133845	0.842535
N	4.797234	1.194716	-0.773971
N	9.618410	-1.311119	1.559289
H	2.207147	0.220744	-0.771223
H	3.450297	-3.444311	1.127871
H	5.777204	-2.671961	1.150254
H	8.777596	2.085985	-1.156247
H	11.137697	2.776982	-1.257087
H	12.237982	-0.398874	1.425784
O	7.586406	-2.300331	1.845041
O	6.815090	2.229458	-0.983056
H	-8.921012	2.296494	-0.946979
H	-5.875964	-4.523641	1.236712
H	4.274049	1.938474	-1.205427

H	10.116010	-1.966787	2.138515

S3

C	11.831741	-0.144963	-3.128151
C	10.460735	-0.266664	-3.319002
C	9.588254	-0.323615	-2.224979
C	10.120004	-0.257000	-0.907258
C	11.527068	-0.139625	-0.721319
C	12.361404	-0.082527	-1.844437
C	8.172504	-0.458212	-2.381879
C	9.249850	-0.310981	0.219074
C	7.840803	-0.411084	0.031645
C	7.341294	-0.499989	-1.308861
C	6.996167	-0.457060	1.163332
C	7.564189	-0.443130	2.440966
C	8.934604	-0.346635	2.627704
C	9.799776	-0.268512	1.531841
C	11.218343	-0.152164	1.689373
C	12.044199	-0.086627	0.613510
H	13.118960	0.003450	0.747771
H	11.622143	-0.116476	2.697805
H	7.769509	-0.530748	-3.388712
H	12.494297	-0.100301	-3.987434
H	10.050840	-0.318851	-4.324191
H	13.434612	0.009871	-1.700056
H	6.273152	-0.612487	-1.457380
H	6.904799	-0.480215	3.303483
H	9.345887	-0.320753	3.633254
C	-7.377120	1.854610	1.077055
C	-8.718526	2.179264	1.173989
C	-9.701474	1.331170	0.651105
C	-9.296553	0.136147	-0.006486
C	-7.911619	-0.194141	-0.110867
C	-6.950036	0.670880	0.463450

C	-11.096811	1.631372	0.756535
C	-10.285221	-0.727607	-0.558953
C	-11.667750	-0.406451	-0.436522
C	-12.038231	0.799696	0.240221
C	-12.621291	-1.275513	-0.981639
H	-13.675296	-1.029212	-0.884018
C	-12.233219	-2.435951	-1.640607
C	-10.886721	-2.753674	-1.771995
C	-9.899163	-1.915518	-1.239984
C	-8.503275	-2.198689	-1.371081
C	-7.558915	-1.380537	-0.837614
H	-6.508353	-1.611955	-0.975302
H	-8.206137	-3.086237	-1.923779
H	-11.388474	2.547047	1.264175
H	-6.631982	2.518539	1.501010
H	-9.020031	3.096911	1.671892
H	-13.094696	1.038811	0.329163
H	-12.987014	-3.096897	-2.057999
H	-10.586122	-3.658786	-2.293027
S	0.052151	0.297813	0.514712
C	1.193980	-0.961118	0.894114
C	-1.305388	-0.766287	0.759230
C	0.531362	-2.150640	1.140406
C	-0.863702	-2.041942	1.064588
H	1.037790	-3.087053	1.342943
H	-1.526114	-2.887869	1.205279
C	5.521857	-0.553129	1.055493
C	4.735369	0.478271	0.463786
C	3.311060	0.364826	0.411356
C	2.640784	-0.778626	0.953301
C	4.842995	-1.624904	1.605168
C	3.445283	-1.733604	1.561223
C	-3.125154	0.888070	0.107708
C	-4.511721	1.230239	0.018293
C	-2.704374	-0.363254	0.660964

C	-5.511901	0.328339	0.489833
C	-3.712888	-1.200905	1.120870
C	-5.070605	-0.867572	1.031101
C	4.604218	2.518698	-0.544631
C	3.197419	2.402188	-0.610475
C	-2.578031	2.890211	-0.843022
C	-3.947726	3.218836	-0.948191
N	5.357439	1.582255	-0.022034
N	2.570516	1.350694	-0.142830
N	-2.182028	1.750548	-0.331934
N	-4.892231	2.412014	-0.529625
H	5.103132	3.405930	-0.931000
H	2.593538	3.191492	-1.054274
H	5.414815	-2.415521	2.082642
H	2.985351	-2.596742	2.030070
H	-3.451197	-2.140900	1.594093
H	-5.804124	-1.562551	1.429031
H	-1.810796	3.579215	-1.191196
H	-4.255869	4.164909	-1.390361

S4

C	-11.611495	2.636576	2.133769
C	-10.236821	2.610962	2.334334
C	-9.431013	1.691273	1.651360
C	-10.034033	0.776486	0.744410
C	-11.445120	0.804592	0.551834
C	-12.211282	1.743419	1.253620
C	-8.015189	1.624895	1.842965
C	-9.232010	-0.165135	0.037949
C	-7.817528	-0.182387	0.219899
C	-7.247815	0.732965	1.164608
C	-7.041847	-1.125112	-0.495396
C	-7.686061	-2.042298	-1.334191
C	-9.059961	-2.029694	-1.510346

C	-9.856296	-1.093004	-0.843257
C	-11.276458	-1.043143	-1.017131
C	-12.036478	-0.134130	-0.353758
H	-13.113598	-0.106398	-0.496130
H	-11.736132	-1.754757	-1.697997
H	-7.558408	2.305935	2.556345
H	-12.221912	3.356979	2.670153
H	-9.771764	3.306768	3.027626
H	-13.287330	1.764566	1.102576
H	-6.178998	0.700036	1.339722
H	-7.079718	-2.757756	-1.881979
H	-9.528567	-2.743098	-2.182933
C	7.150169	1.354189	-1.762248
C	8.450012	1.742457	-2.032129
C	9.511961	1.295107	-1.237850
C	9.227924	0.458934	-0.121654
C	7.885129	0.066289	0.162316
C	6.843351	0.496881	-0.696665
C	10.868522	1.658634	-1.511721
C	10.297075	0.019909	0.711205
C	11.639197	0.393543	0.413299
C	11.887534	1.224504	-0.725734
C	12.673827	-0.057837	1.242289
H	13.696815	0.226217	1.010170
C	12.403889	-0.854878	2.348434
C	11.097222	-1.216519	2.652876
C	10.031854	-0.790976	1.849513
C	8.672198	-1.121538	2.143663
C	7.652049	-0.712397	1.344616
H	6.630238	-0.956364	1.612470
H	8.463781	-1.701969	3.038706
H	11.066450	2.294806	-2.370365
H	6.343692	1.700423	-2.399552
H	8.657378	2.391281	-2.878849
H	12.913764	1.506160	-0.946333

H	13.219063	-1.194361	2.980510
H	10.888731	-1.834113	3.522476
S	-0.090112	-0.339460	-0.514993
C	-1.199891	-1.637094	-0.185377
C	1.291479	-1.346319	-0.200467
C	-0.506407	-2.783649	0.160212
C	0.885794	-2.620983	0.153060
H	-0.990052	-3.717270	0.421823
H	1.575996	-3.413965	0.415723
C	-5.570786	-1.202482	-0.387174
C	-4.697279	-0.116802	-0.662068
C	-3.280655	-0.250980	-0.604713
C	-2.641303	-1.476714	-0.264347
C	-4.925735	-2.388626	-0.080900
C	-3.522139	-2.521754	-0.015689
C	2.998746	0.502673	-0.504815
C	4.347707	0.944611	-0.616311
C	2.656271	-0.866721	-0.321426
C	5.448656	0.048663	-0.538189
C	3.751509	-1.719885	-0.269903
C	5.088114	-1.279418	-0.369778
N	-4.984653	1.145550	-1.036265
N	-2.733457	0.931439	-0.938286
H	-5.532453	-3.262072	0.140663
H	-3.125258	-3.496273	0.248272
H	3.583514	-2.787131	-0.170029
H	5.872330	-2.029973	-0.346612
N	-3.791165	1.675980	-1.170140
H	-3.687239	2.639483	-1.451277
N	2.195194	1.576972	-0.597393
N	4.338279	2.283136	-0.774205
N	3.054333	2.558617	-0.753976
H	2.732235	3.509836	-0.851384

S5

C	-12.159881	2.060951	1.233689
C	-10.817425	2.373419	1.409708
C	-9.816561	1.473488	1.022512
C	-10.186912	0.227919	0.444052
C	-11.565472	-0.086533	0.274181
C	-12.532104	0.844614	0.673074
C	-8.424999	1.754486	1.199594
C	-9.184655	-0.701041	0.042707
C	-7.805014	-0.380221	0.201387
C	-7.468335	0.872706	0.810171
C	-6.828959	-1.317997	-0.205601
C	-7.238863	-2.552304	-0.720945
C	-8.579476	-2.867437	-0.876535
C	-9.573322	-1.954344	-0.510435
C	-10.966524	-2.244234	-0.669632
C	-11.919262	-1.351021	-0.298006
H	-12.973242	-1.583732	-0.425127
H	-11.246275	-3.203225	-1.097650
H	-8.143577	2.696629	1.662704
H	-12.923460	2.770406	1.538417
H	-10.530494	3.323347	1.852864
H	-13.583364	0.603134	0.540358
H	-6.422010	1.108495	0.968508
H	-6.479747	-3.265150	-1.030087
H	-8.867053	-3.828261	-1.294670
C	7.326051	2.115489	0.920440
C	8.667504	2.405661	1.093869
C	9.649925	1.447721	0.817069
C	9.247152	0.173126	0.329444
C	7.862818	-0.123557	0.146719
C	6.898269	0.859736	0.472337
C	11.043254	1.714276	1.006250
C	10.237661	-0.803680	0.023870
C	11.617716	-0.512655	0.223460

C	11.984976	0.776572	0.726030
C	12.572601	-1.491579	-0.079007
H	13.624540	-1.267491	0.076831
C	12.188450	-2.732399	-0.573234
C	10.845014	-3.022985	-0.778041
C	9.856025	-2.075340	-0.486777
C	8.465273	-2.330763	-0.701274
C	7.518214	-1.403417	-0.403193
H	6.474554	-1.622374	-0.600280
H	8.174929	-3.289407	-1.123109
H	11.332966	2.691851	1.382491
H	6.579734	2.867278	1.153076
H	8.968224	3.383646	1.459824
H	13.039707	0.991675	0.875832
H	12.943101	-3.478609	-0.803131
H	10.548219	-3.992436	-1.169293
S	-0.033686	0.322985	-0.231730
C	-1.144795	-0.839783	0.429374
C	1.311336	-0.459899	0.544068
C	-0.484572	-1.774563	1.209579
C	0.895569	-1.561816	1.273211
H	-1.019173	-2.575576	1.703872
H	1.599536	-2.172614	1.823749
N	-5.375827	0.845483	-1.542267
N	-2.593570	1.075920	-1.212446
C	-4.674718	1.782149	-2.131920
C	-3.274052	1.907256	-1.963459
C	-4.693869	-0.020928	-0.747486
C	-3.283613	0.093175	-0.595113
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H	-5.053946	-2.758979	1.192171
N	2.250226	1.862023	-0.933589

N	4.988110	2.490542	-1.002616
C	2.707043	2.895996	-1.596995
C	4.088077	3.205889	-1.631505
C	3.150828	1.100950	-0.275772
C	4.538581	1.417303	-0.300255
C	5.450095	0.582906	0.405054
C	2.705374	-0.047147	0.456270
N	3.582062	-0.802406	1.108310
C	4.885090	-0.491492	1.078485
H	5.532422	-1.149395	1.655059
H	4.441021	4.065283	-2.199559
H	1.986169	3.513891	-2.128346
H	-2.724227	2.702597	-2.462423
H	-5.212200	2.478534	-2.773681

S6

C	8.166823	5.476745	-1.365151
C	7.131125	4.659669	-1.800534
C	6.918763	3.403333	-1.218466
C	7.774121	2.964713	-0.170347
C	8.839307	3.806291	0.262240
C	9.013188	5.055764	-0.346172
C	5.882535	2.523390	-1.657299
C	7.571828	1.692000	0.437163
C	6.493602	0.855569	0.017164
C	5.683553	1.312115	-1.073349
C	6.300562	-0.396737	0.659225
C	7.214216	-0.803926	1.646357
C	8.267445	-0.000312	2.036309
C	8.460539	1.262297	1.462528
C	9.523088	2.125195	1.875886
C	9.703357	3.345037	1.305629
H	10.513877	3.992055	1.630383
H	10.188259	1.780370	2.663068
H	5.255567	2.834909	-2.488537

H	8.318333	6.448433	-1.825561
H	6.474671	4.987628	-2.602006
H	9.824960	5.695946	-0.011252
H	4.908027	0.662022	-1.461067
H	7.070330	-1.768768	2.117737
H	8.946068	-0.339020	2.814368
C	-5.043717	1.791726	-1.422324
C	-5.871162	2.894173	-1.533355
C	-7.090257	2.945885	-0.847049
C	-7.450452	1.855926	-0.004722
C	-6.591748	0.724307	0.121417
C	-5.387044	0.688238	-0.625860
C	-7.979242	4.060519	-0.965846
C	-8.674076	1.910437	0.722425
C	-9.542000	3.031282	0.584069
C	-9.154627	4.100093	-0.285959
C	-10.742884	3.058439	1.304099
H	-11.404323	3.913609	1.193732
C	-11.088067	2.012118	2.151436
C	-10.242770	0.919458	2.300564
C	-9.033634	0.848545	1.597291
C	-8.129335	-0.249617	1.739878
C	-6.967257	-0.308614	1.039271
H	-6.297867	-1.148623	1.176725
H	-8.388097	-1.045066	2.433715
H	-7.691175	4.880707	-1.618042
H	-4.121102	1.755082	-1.994494
H	-5.586241	3.723653	-2.174656
H	-9.821840	4.951934	-0.387419
H	-12.022708	2.050728	2.702931
H	-10.512635	0.106102	2.968826
S	0.328010	-1.255909	-0.181947
C	1.477237	-2.568330	-0.148617
C	-1.010954	-2.348317	-0.422648
C	0.828123	-3.780731	-0.321090

C	-0.560139	-3.657815	-0.474951
C	5.188520	-1.295246	0.369120
C	2.876971	-2.343107	0.040092
C	5.211722	-2.691495	0.289456
C	3.914887	-3.286001	0.095427
C	-2.357878	-1.879436	-0.533255
C	-4.479643	-0.455788	-0.588684
C	-3.525975	-2.622771	-0.765451
C	-4.717951	-1.814222	-0.801374
H	1.375306	-4.714520	-0.329724
H	-1.245241	-4.482453	-0.623541
S	3.547733	-0.764574	0.234333
S	-2.785780	-0.215898	-0.356970
N	6.335890	-3.455259	0.358646
N	3.759398	-4.628984	-0.023205
N	-3.574244	-3.965262	-0.960095
N	-5.936728	-2.359245	-1.068220
C	6.147814	-4.743837	0.242129
C	4.860424	-5.332599	0.052082
C	-4.762983	-4.457818	-1.198369
C	-5.941750	-3.651616	-1.260369
H	7.027041	-5.384217	0.291229
H	4.771751	-6.413750	-0.037662
H	-4.837946	-5.532035	-1.357331
H	-6.899847	-4.120970	-1.478057

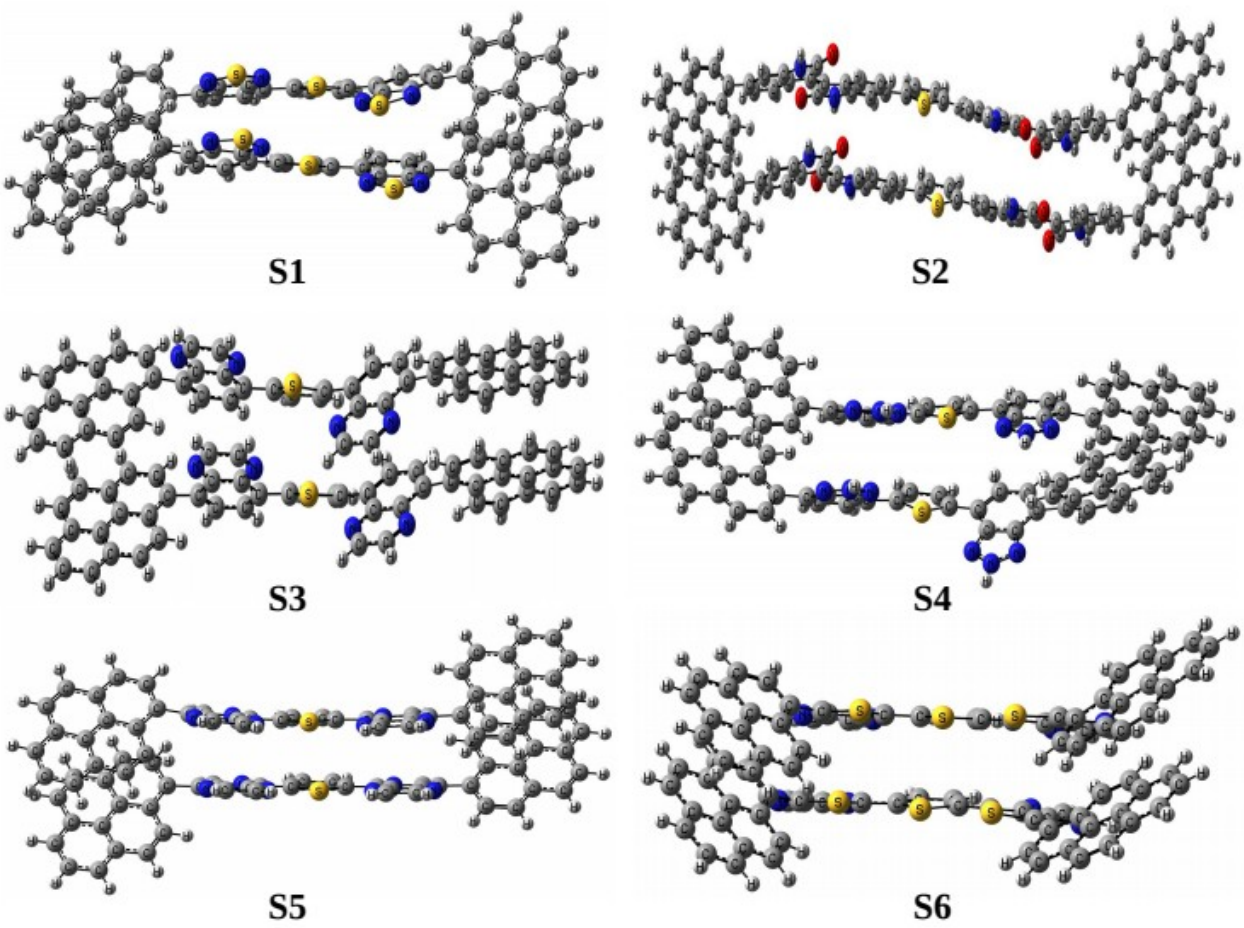

Fig. 1: Structural representations of the optimized π-stacked dimers of the studied compounds.