Supporting Information

Photoelectron Spectroscopy of Molecular Anion of Alq_3: An Estimation of Reorganization Energy for Electron Transport in the Bulk

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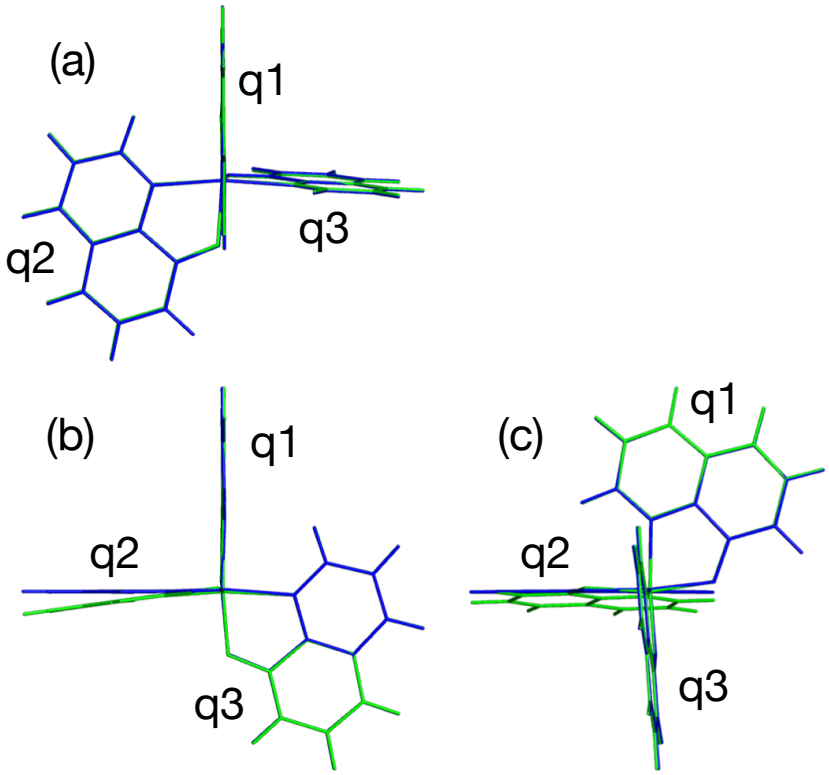


Figure S1. Comparison of structures of **1** (green) and **3** (blue). (a) Top, (b) front, and (c) side view.

Table S1. Three-dimensional coordinates of optimized structures.

Meridional Alq_3

Anion (**3**)				Neutral (**1**)			
elem.	x	y	z	elem.	x	y	z
Al	-0.1335458920	-0.2259536672	0.2346971464	Al	0.1153728857	-0.2364896887	-0.2009130130
C	2.1887328255	-1.7953235005	0.0420251512	C	-2.2898512475	-1.7053980298	0.0229470908
C	2.3356603506	-0.5556353675	2.0132170748	C	-2.3458459487	-0.6149390210	-2.0239128844
C	1.3703203082	-2.0782085897	-1.0991899171	C	-1.5187182518	-1.9020616232	1.2176936536
C	3.4540679626	-2.4041343433	0.2399571993	C	-3.5285440212	-2.3598964768	-0.2020740733
C	3.5948012795	-1.1007188124	2.2842421749	C	-3.5800753630	-1.2172942218	-2.3371991290
H	1.8587097702	0.1566083848	2.6749257639	H	-1.8436648570	0.0586100039	-2.7079555400
C	1.8534701630	-3.0085291161	-2.0247083143	C	-2.0412792793	-2.7680984252	2.1726312903
C	3.9047203055	-3.3341883242	-0.7301020428	C	-4.0193537310	-3.2311718277	0.8018015126
C	4.1621734941	-2.0221816426	1.4134779890	C	-4.1660328712	-2.0785477098	-1.4350021147
H	4.1146533086	-0.7961802237	3.1856485438	H	-4.0504114224	-0.9971593460	-3.2873316022
C	3.1052877019	-3.6186165658	-1.8267517373	C	-3.2762221152	-3.4147746175	1.9511840526
H	1.2493467944	-3.2471330285	-2.8928271842	H	-1.4818366299	-2.9474630012	3.0830818720
H	4.8690669974	-3.8152050596	-0.6042123082	H	-4.9621459500	-3.7451705616	0.6565843529
H	5.1371226050	-2.4529326578	1.6175180319	H	-5.1158083747	-2.5512604806	-1.6637841092
H	3.4557731321	-4.3351586971	-2.5643810888	H	-3.6490784356	-4.0856215194	2.7182330851
N	1.6444509784	-0.8937638778	0.9162469879	N	-1.7317736755	-0.8509236846	-0.8761806237
O	0.2301401184	-1.4330608345	-1.1925977032	O	-0.3883676599	-1.2415227381	1.3161998149
C	0.7260349559	2.4498828693	-0.0104677111	C	-0.5741506283	2.5585422991	-0.0298576671
C	1.2489188848	1.3699730577	-2.0238004546	C	-1.1152658504	1.6233033980	2.0204228903
C	0.1347002653	2.2898850702	1.2758595859	C	-0.0437053631	2.2759709437	-1.3325552434
C	1.2991000555	3.6758382238	-0.4332277118	C	-1.0016739150	3.8564011794	0.3570106260
C	1.8375220394	2.5325316136	-2.5125316309	C	-1.5689571210	2.8703173954	2.4949656757
H	1.2088332631	0.4570699345	-2.6040931483	H	-1.1363709908	0.7301939708	2.6332685410
C	0.1042401033	3.3979396619	2.1305312382	C	0.0517643366	3.3424901804	-2.2220310689
C	1.2548506586	4.7691780138	0.4660024040	C	-0.8874876568	4.9078832138	-0.5849945308
C	1.8715920707	3.6972471961	-1.7412116517	C	-1.5115470024	3.9754300393	1.6728553667
H	2.2701245847	2.5172959913	-3.5073656827	H	-1.9582852686	2.9428492164	3.5028694170
C	0.6630276749	4.6172943740	1.7143251391	C	-0.3687350144	4.6327247795	-1.8358664375
H	-0.3485993408	3.2945225342	3.1103684351	H	0.4530491340	3.1670758828	-3.2129783097
H	1.6861327881	5.7204117390	0.1703442981	H	-1.2046381612	5.9090842352	-0.3183692159
H	2.3288602152	4.6056666188	-2.1184493307	H	-1.8563659718	4.9419607226	2.0261593775
H	0.6341677687	5.4646530443	2.3937701301	H	-0.2795693323	5.4383719416	-2.5572322414
O	-0.3396778827	1.0909913486	1.5673667863	O	0.2981748317	1.0361185016	-1.5793840222
N	0.6865260555	1.3145622996	-0.7906656735	N	-0.6320663073	1.4794845086	0.7952822654
C	-2.9588400043	-0.6889237913	0.0032005180	C	2.8611709064	-0.8610966421	-0.0109200079
C	-2.4417981348	0.9646334352	-1.5313286718	C	2.5201517422	0.9112549061	1.4415509680
C	-2.4105780211	-1.5637921562	1.0123026626	C	2.2317637710	-1.7513932741	-0.9461401797
C	-4.3395287131	-0.6829725331	-0.3341898936	C	4.2479080887	-0.9380307199	0.2922974716
C	-3.7899686067	1.0469916423	-1.9361693338	C	3.8799564661	0.9133275654	1.8057335544
H	-1.6753143430	1.5898600939	-1.9735678623	H	1.8268893157	1.6205522820	1.8768374915
C	-3.3121161269	-2.4225166620	1.6513992142	C	3.0402715320	-2.7064031182	-1.5561204897
C	-5.2067590918	-1.5723077524	0.3473342892	C	5.0269562483	-1.9263088087	-0.3563427488
C	-4.7284042327	0.2315057853	-1.3437469478	C	4.7358376622	-0.0027838653	1.2356377975
H	-4.0686009298	1.7532836390	-2.7091934297	H	4.2330181312	1.6366076334	2.5301077006
C	-4.6775819000	-2.4117673900	1.3123352945	C	4.4149358577	-2.7788281082	-1.2548616982
H	-2.9367774798	-3.0952811621	2.4135270642	H	2.5936917145	-3.3925447746	-2.2655184390

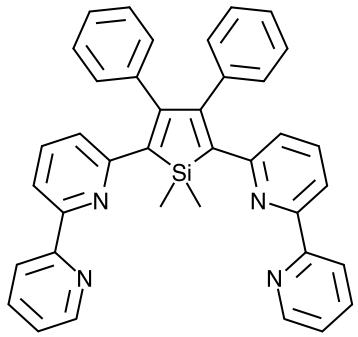
H	-6.2641960802	-1.5867722662	0.1078321471	H	6.0861615887	-2.0040471212	-0.1415728782
H	-5.7711417020	0.2821308350	-1.6432968924	H	5.7871979522	-0.0157784863	1.5044244351
H	-5.3416083159	-3.0943676999	1.8352360958	H	5.0110321761	-3.5370252651	-1.7521817424
N	-2.0491549658	0.1223786337	-0.5926272897	N	2.0286864054	0.0535186556	0.5616192166
O	-1.1402037157	-1.4920103182	1.2464142468	O	0.9491926710	-1.5998352980	-1.1520295092

Facial Alq_3

Anion (**4**)				Neutral (**2**)			
elem.	x	y	z	elem.	x	y	z
Al	-0.0270965730	-0.0416127843	-0.6848958956	Al	0.0008390752	-0.0021248909	-0.6971962189
C	2.0848590375	-1.8633492520	-0.0746361654	C	-2.4680788469	1.2737121638	-0.0244228821
C	0.4716879791	-2.1999379362	1.5688089605	C	-0.9804784582	1.9464506849	1.6184932140
C	2.4136698384	-1.1282915195	-1.2614128264	C	-2.6317136302	0.4674347408	-1.2019766677
C	2.9570522227	-2.8426876738	0.4760285312	C	-3.5236042541	2.0696889081	0.5016823080
C	1.2574224308	-3.1863580635	2.1748503077	C	-1.9588585986	2.7693764991	2.2095337603
H	-0.4962306118	-1.9270462444	1.9704949417	H	0.0185910491	1.8847707390	2.0329151695
C	3.6486875442	-1.3964262192	-1.8646783025	C	-3.8851488241	0.4775051678	-1.8092787580
C	4.1933122761	-3.0778476127	-0.1720851436	C	-4.7764880618	2.0486652660	-0.1556103403
C	2.4978378745	-3.5127313356	1.6427252193	C	-3.2193700971	2.8284178248	1.6572930318
H	0.8810286789	-3.6879241058	3.0592431986	H	-1.7038365595	3.3469134602	3.0893475074
C	4.5113040289	-2.3584230306	-1.3159980202	C	-4.9294397526	1.2617112059	-1.2816852693
H	3.9181833184	-0.8523687941	-2.7624437644	H	-4.0376201276	-0.1198255860	-2.6998978627
H	4.8767826424	-3.8187040935	0.2290291723	H	-5.5952324405	2.6474361673	0.2253771513
H	3.1184710146	-4.2735822505	2.1049744321	H	-3.9854255843	3.4573856623	2.0992163041
H	5.4606227446	-2.5458167641	-1.8098796095	H	-5.8892830655	1.2468256425	-1.7875241524
N	0.8711562182	-1.5466043273	0.4701347293	N	-1.2288624785	1.2185034633	0.5399708468
O	1.5386307065	-0.2593582323	-1.6924580642	O	-1.5973739739	-0.2160262602	-1.6134018367
C	0.5941557732	2.6587836293	-0.0118170360	C	0.1312764996	-2.7778110984	-0.0242888504
C	1.6921484274	1.3506241920	1.5699668052	C	-1.1940454045	-1.8255112207	1.6193518213
C	-0.2628642501	2.6389971564	-1.1597793479	C	0.9103140712	-2.5165343405	-1.2025693153
C	1.1091277214	3.8699489035	0.5254707751	C	-0.0291212349	-4.0896732365	0.5027403779
C	2.2534627455	2.4878354960	2.1584773044	C	-1.4160691648	-3.0840014470	2.2115238953
H	1.9028838549	0.3604586488	1.9541401709	H	-1.6402572164	-0.9293868291	2.0335655851
C	-0.6100517138	3.8693204539	-1.7306690255	C	1.5280999721	-3.6071272819	-1.8099886479
C	0.7358881285	5.0879779453	-0.0920493268	C	0.6153292624	-5.1642388734	-0.1546851069
C	1.9687578442	3.7495237911	1.6522853807	C	-0.8368803017	-4.2052029359	1.6594069048
H	2.9116837284	2.3654086449	3.0113379792	H	-2.0426908704	-3.1516976383	3.0921044451
C	-0.1089128679	5.0654193918	-1.1930785384	C	1.3720586073	-4.9034362598	-1.2816743649
H	-1.2593350022	3.8756765071	-2.5984936276	H	2.1207526625	-3.4406919067	-2.7012329565
H	1.1176610126	6.0253532514	0.2986745675	H	0.5069950306	-6.1725400244	0.2269097947
H	2.3965177153	4.6400285700	2.1011689753	H	-0.9974416050	-5.1828884273	2.1022248045
H	-0.3897075108	6.0040190735	-1.6626404084	H	1.8646683440	-5.7272900111	-1.7876326205
O	-0.6584414303	1.4707443561	-1.5935891000	O	0.9842594664	-1.2791829799	-1.6145411480
N	0.8686405680	1.4228773185	0.5131040407	N	-0.4405468549	-1.6770038946	0.5400089194
C	-2.6857415188	-0.8211986035	0.0005538168	C	2.3375041200	1.5016009101	-0.0223240758
C	-1.9855913510	0.5902195379	1.7121606214	C	2.1802019671	-0.1268221562	1.6172584349
C	-2.2950652337	-1.4676706814	-1.2187122443	C	1.7203011970	2.0466921652	-1.1993508859
C	-3.9851577288	-0.9682164501	0.5533749267	C	3.5522674534	2.0209013294	0.5059956242
C	-3.2387287705	0.5014532721	2.3323222846	C	3.3801239300	0.3118255539	2.2101845504
H	-1.1942940358	1.1993515885	2.1314333707	H	1.6296409025	-0.9638028214	2.0296279021
C	-3.2487696527	-2.2705290263	-1.8531117027	C	2.3524904502	3.1306879397	-1.8037638504
C	-4.9163987808	-1.7885199583	-0.1291686495	C	4.1572704575	3.1199585646	-0.1483995246

C	-4.2409205001	-0.2716756971	1.7665215221	C	4.0583073481	1.3774847401	1.6608225518
H	-3.4086424215	1.0490433102	3.2523945478	H	3.7537488119	-0.1983360847	3.0892735242
C	-4.5342286504	-2.4175993310	-1.3036803412	C	3.5514303212	3.6461517019	-1.2739387266
H	-2.9770655305	-2.7696344771	-2.7760130253	H	1.9107128118	3.5617179867	-2.6938759582
H	-5.9158341129	-1.9152699993	0.2731744384	H	5.0833571058	3.5321248858	0.2343619033
H	-5.2177420506	-0.3458338664	2.2334534518	H	4.9843406554	1.7287948651	2.1044197801
H	-5.2515141335	-3.0462329482	-1.8237792417	H	4.0159207786	4.4875981118	-1.7775310346
N	-1.7034483289	-0.0605017831	0.5786941488	N	1.6729261969	0.4528587892	0.5395703175
O	-1.0785723147	-1.2642679771	-1.6477582135	O	0.6136243826	1.4896056710	-1.6130243604

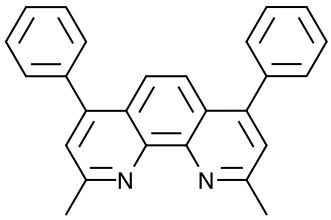
Table S2. Three-dimensional coordinates of optimized structures of BBDDS (2,5-bis(2,2'-bipyridin-6-yl)-1,1-dimethyl-3,4-diphenylsilole).



Anion				Neutral			
elem.	x	y	z	elem.	x	y	z
C	-0.1443260816	-2.2408479359	0.0192120532	C	-0.1511550501	-2.2306848420	0.1016432808
C	1.2478063732	-2.0185132331	0.0003266590	C	1.1966681620	-2.0302711398	0.0484000089
C	1.6762874753	-0.6331793025	0.0058831094	C	1.6408743735	-0.5946455286	-0.0423539650
C	0.6528645590	0.3362993570	-0.0173291032	C	0.6417551230	0.3316853358	-0.0997973517
Si	-1.0073125615	-0.5620604189	-0.0013183494	Si	-1.0378890137	-0.5526050492	-0.0013731198
C	-2.0645899958	-0.2753355449	1.5406591936	C	-2.0265088795	-0.2047776699	1.5582522244
H	-2.4175661860	0.7590748911	1.5549669121	H	-2.3933227864	0.8232848927	1.5329891164
H	-2.9224439055	-0.9534783997	1.5328264126	H	-2.8767659471	-0.8904970199	1.6093571585
H	-1.4840199398	-0.4558014332	2.4505285194	H	-1.4166753561	-0.3348176340	2.4563888159
C	-2.0367907689	-0.2033408281	-1.5470338309	C	-2.0451463957	-0.2831005213	-1.5645699403
H	-2.9120992071	-0.8578364185	-1.5635417738	H	-2.9284192350	-0.9245069327	-1.5415439622
H	-2.3619811747	0.8407238091	-1.5413201597	H	-2.3595999842	0.7628677867	-1.6177589140
H	-1.4527451635	-0.3830965958	-2.4548170166	H	-1.4654585871	-0.5209833514	-2.4605780077
C	3.1266553567	-0.2986463726	0.0829258882	C	3.1011343235	-0.2819167460	-0.0316601468
C	4.0313371898	-0.6394152211	-0.9354045726	C	3.9266391326	-0.6075674263	-1.1157941293
C	3.6326982077	0.3870934585	1.2001698931	C	3.6742806372	0.3544917150	1.0771070690
C	5.3825999543	-0.3111450595	-0.8412187657	C	5.2834820155	-0.2915275347	-1.0978468560
H	3.6652911165	-1.1633001863	-1.8105837304	H	3.5017730072	-1.1038938335	-1.9807305187
C	4.9821116202	0.7141674270	1.2988878674	C	5.0326276819	0.6633928881	1.0996954976
H	2.9466342892	0.6648918150	1.9927439619	H	3.0456177251	0.6110565542	1.9226743702
C	5.8677554246	0.3667638050	0.2767854370	C	5.8419230492	0.3441635871	0.0103967562
H	6.0585355902	-0.5858273036	-1.6450743021	H	5.9054479340	-0.5453135635	-1.9492645400
H	5.3448839714	1.2410719624	2.1760578426	H	5.4582560497	1.1547564913	1.9678868638
H	6.9199057894	0.6216098375	0.3510818154	H	6.8988618262	0.5856272390	0.0258292623
C	2.2562617868	-3.1135731355	-0.0723118587	C	2.2253855774	-3.1128487749	0.0421609859
C	3.1920186223	-3.3420615709	0.9493151472	C	3.0870443960	-3.3090442436	1.1293152769
C	2.2904185839	-3.9663996758	-1.1885881955	C	2.3427528708	-3.9628343228	-1.0653707864
C	4.1222683501	-4.3760155894	0.8592160012	C	4.0285594306	-4.3359736427	1.1154817503
H	3.1828190118	-2.7021110519	1.8238221180	H	3.0137700035	-2.6586421194	1.9933604319
C	3.2198321090	-4.9983268436	-1.2832243188	C	3.2895550425	-4.9847255474	-1.0838333190
H	1.5699153678	-3.8091394808	-1.9836816668	H	1.6817859389	-3.8205117375	-1.9132467420
C	4.1436092907	-5.2105865780	-0.2578808993	C	4.1341928437	-5.1770641132	0.0084262403
H	4.8326158334	-4.5301179477	1.6655546136	H	4.6824108874	-4.4768028215	1.9691833613
H	3.2246313950	-5.6389233166	-2.1597358474	H	3.3662711675	-5.6314651210	-1.9511259474
H	4.8683727551	-6.0150414409	-0.3289944538	H	4.8702746080	-5.9731147786	-0.0037969982

C	0.7399095970	1.7591730873	-0.1950810201	C	0.7276985740	1.7872303983	-0.2794100756
C	1.8925418324	2.4940309678	-0.6126908837	C	1.8305144598	2.4850345262	-0.8105681279
C	-0.4751796277	3.7614046903	-0.1229881551	C	-0.4801927105	3.7658271595	-0.0880960429
C	1.8278930058	3.8647170843	-0.7517486231	C	1.7465013036	3.8606352553	-0.9659695648
H	2.8121452703	1.9770559074	-0.8410632233	H	2.7244679319	1.9573297020	-1.1077280968
C	0.6311912831	4.5427514874	-0.4876419283	C	0.5824189737	4.5253275361	-0.5917883017
C	-1.7947636875	4.4169029747	0.1357176218	C	-1.7681154230	4.4156922302	0.3033819832
H	2.7040099292	4.4148399781	-1.0832724206	H	2.5792912107	4.4120588857	-1.3889135066
H	0.5488668436	5.6153335285	-0.6132463876	H	0.4856912525	5.5955309276	-0.7259580479
C	-1.8612526031	5.6323228151	0.8374695016	C	-1.7762062846	5.6657100360	0.9375458172
C	-4.0816446329	4.3796205476	-0.0847463085	C	-4.0592818223	4.3120076667	0.3655360914
C	-3.0982023205	6.2193402199	1.0719598243	C	-2.9934240846	6.2387248665	1.2885576939
H	-0.9518912308	6.0874268137	1.2105817165	H	-0.8444330716	6.1654118310	1.1727977545
C	-4.2435952373	5.5824879649	0.6007762756	C	-4.1667884167	5.5510369280	0.9957550041
H	-4.9493100188	3.8485665781	-0.4703737364	H	-4.9519859068	3.7430519595	0.1189320088
H	-3.1683526014	7.1517019542	1.6230437871	H	-3.0234486639	7.2001630295	1.7892203101
H	-5.2323166862	5.9972988960	0.7613666730	H	-5.1391779344	5.9558506551	1.2498501408
C	-0.8764097012	-3.4642078459	0.1958086013	C	-0.9025954620	-3.4803893860	0.2800649634
C	-0.3413324591	-4.7210830534	0.6164417268	C	-0.3880796915	-4.6784407533	0.8141144308
C	-3.0095108500	-4.4308266741	0.1177182391	C	-3.0160202722	-4.4316905235	0.0828100999
C	-1.1690271046	-5.8157626642	0.7539010916	C	-1.2345813987	-5.7662298839	0.9678507403
H	0.7088078358	-4.8133600005	0.8483424594	H	0.6467248874	-4.7473083564	1.1147237297
C	-2.5386901718	-5.7000070476	0.4851972904	C	-2.5694311371	-5.6579927778	0.5892004907
C	-4.4678902562	-4.2270863466	-0.1459636857	C	-4.4446555523	-4.2413136909	-0.3135262049
H	-0.7575933944	-6.7641316667	1.0877313291	H	-0.8599367633	-6.6911179303	1.3929532326
H	-3.2126218171	-6.5386751242	0.6094471311	H	-3.2539328188	-6.4865590931	0.7219723994
C	-5.2066920079	-5.1934256367	-0.8491579783	C	-5.1550131999	-5.2691123296	-0.9489754369
C	-6.3350668405	-2.9049321440	0.0670589784	C	-6.2769588024	-2.8622242214	-0.3830541943
C	-6.5582834205	-4.9797937288	-1.0882851652	C	-6.4820342850	-5.0551842126	-1.3045373940
H	-4.7118685291	-6.0828514096	-1.2197547940	H	-4.6673210232	-6.2078600711	-1.1816892063
C	-7.1456251046	-3.8069975384	-0.6202055711	C	-7.0631794242	-3.8248199465	-1.0148719384
H	-6.7526360471	-1.9763483452	0.4503840869	H	-6.6933415914	-1.8883630673	-0.1387908528
H	-7.1407868317	-5.7102863086	-1.6405381555	H	-7.0480013065	-5.8322796662	-1.8062662644
H	-8.1953531560	-3.5913053737	-0.7844474570	H	-8.0934795244	-3.6101940224	-1.2725486408
N	-0.4313794528	2.4401205041	0.0124226309	N	-0.4068543583	2.4400922798	0.0495313460
N	-2.9011074081	3.8057576543	-0.3160888376	N	-2.8988441827	3.7500373295	0.0265794268
N	-2.2269278524	-3.3651471281	-0.0162123258	N	-2.2065410143	-3.3790143525	-0.0532376074
N	-5.0374528350	-3.0975743852	0.3028406218	N	-5.0029982889	-3.0532226824	-0.0397438547

Table S3. Three-dimensional coordinates of optimized structures of BCP (bathocuproine).

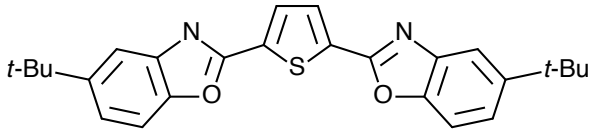


Anion				Neutral			
elem.	x	y	z	elem.	x	y	z
C	-4.1436397365	-4.5047846485	0.2994610061	C	-4.1416003940	-4.4825119502	0.1619719407
C	-2.7839766970	-4.6113368276	0.0882119526	C	-2.7702108910	-4.5882269278	0.0439079888
C	-2.0098933405	-3.4183192646	-0.0258880508	C	-2.0082228304	-3.3825180081	0.0098924010
C	-2.7008944848	-2.1648195842	0.1241804829	C	-2.7134585608	-2.1540565838	0.1375565638
C	-4.7390969838	-3.2229132385	0.4229820815	C	-4.7544480105	-3.2137851462	0.2719504258
C	-0.6248245154	-3.4058911158	-0.3178972360	C	-0.5911275370	-3.3609504095	-0.1932949837
C	-1.9690361850	-0.9051458467	0.0306207571	C	-1.9682140107	-0.8984985941	0.1176960374
C	-0.5415501871	-0.9515815285	-0.1344030760	C	-0.5539498817	-0.9324176596	-0.0288632770
C	0.0685571785	-2.2174706080	-0.3675540940	C	0.1031564524	-2.1912487591	-0.2117972472
C	0.1820948254	0.2964137751	-0.1519272757	C	0.1397187968	0.3143052064	-0.0336401693
C	-0.6184838953	1.4738462056	-0.1464159445	C	-0.6083873702	1.4701028388	0.0678136654
C	-1.9919611124	1.4050688322	-0.0244064124	C	-2.0139787663	1.4032469960	0.1989180295
H	-0.1097279623	-4.3361140904	-0.5238534953	H	-0.0707109558	-4.2961164986	-0.3547141848
H	-4.7507086839	-5.3988837820	0.4030918248	H	-4.7517765721	-5.3784771345	0.1979421255
H	1.1191900997	-2.2446273994	-0.6256125140	H	1.1709955318	-2.2041396030	-0.3878048724
H	-0.1395194194	2.4462305846	-0.1653572551	H	-0.1138219995	2.4353618009	0.0743431211
C	-2.8397155977	2.6538233702	0.0218233905	C	-2.8252594333	2.6679495595	0.3275439736
H	-3.5781771296	2.6421941789	-0.7875882782	H	-3.8856907915	2.4210176789	0.3559772059
H	-3.4027194718	2.6989588436	0.9607862812	H	-2.5647725680	3.2077616486	1.2440464262
H	-2.2337013162	3.5597578883	-0.0686791179	H	-2.6375570636	3.3447539975	-0.5119598147
C	-6.2249689768	-3.0997418658	0.6715312230	C	-6.2513072854	-3.1041178936	0.4188482901
H	-6.5148463272	-3.5805404347	1.6139867021	H	-6.5875753466	-3.5696843499	1.3512640270
H	-6.4944748302	-2.0445196922	0.7195043299	H	-6.5421848533	-2.0545340900	0.4267556539
H	-6.8066170694	-3.5776886526	-0.1261761607	H	-6.7670626500	-3.6124837446	-0.4018973570
C	1.6347586189	0.4151649881	-0.1686851160	C	1.6230240055	0.4054049813	-0.1403774669
C	2.2715277442	1.5030117523	-0.8291506088	C	2.2126637096	1.1265533180	-1.1867926957
C	2.4990707860	-0.4789956363	0.5194057789	C	2.4563449989	-0.1841634246	0.8203680831
C	3.6496149826	1.6699812371	-0.8138941101	C	3.5979190390	1.2497919040	-1.2749822253
H	1.6635721263	2.2057499382	-1.3874879100	H	1.5801294461	1.5807772040	-1.9413830715
C	3.8755063344	-0.3035188741	0.5374649036	C	3.8404631434	-0.0545846974	0.7361563420
H	2.0687416701	-1.2955426745	1.0856234796	H	2.0150148263	-0.7312111227	1.6458423095
C	4.4775169660	0.7694983370	-0.1339652886	C	4.4162102161	0.6603706504	-0.3133961208
H	4.0877208762	2.5080376717	-1.3493968721	H	4.0368463573	1.8048652786	-2.0965783367
H	4.4901336788	-1.0041572415	1.0960753569	H	4.4693805329	-0.5084439982	1.4939925377
H	5.5541924185	0.8998624206	-0.1241573272	H	5.4938676636	0.7580152870	-0.3799960069
C	-2.1676371378	-5.9648831083	-0.0029740509	C	-2.1410743253	-5.9361964147	-0.0400671865
C	-1.1909181595	-6.3800643196	0.9136725535	C	-1.2110842593	-6.3629003065	0.9181024579
C	-2.5834505133	-6.8730034527	-0.9859221452	C	-2.5060716596	-6.8233830456	-1.0610429597
C	-0.6535494685	-7.6644694638	0.8532478407	C	-0.6629225497	-7.6417076184	0.8561678380

H	-0.8612786136	-5.6881055717	1.6799793310
C	-2.0442813318	-8.1585256392	-1.0501325658
H	-3.3277975311	-6.5592519943	-1.7094581315
C	-1.0776332017	-8.5593282471	-0.1300846370
H	0.0958572674	-7.9678540027	1.5769731989
H	-2.3757916372	-8.8432216364	-1.8240877404
H	-0.6558308471	-9.5577505846	-0.1793091724
N	-2.6726498733	0.2428013158	0.0888055508
N	-4.0394372259	-2.1103080630	0.3438023511

H	-0.9309112042	-5.6943875030	1.7243499280
C	-1.9518558164	-8.1002466222	-1.1270863785
H	-3.2182240641	-6.5032970689	-1.8135119068
C	-1.0291833704	-8.5138099721	-0.1682816162
H	0.0472223856	-7.9587176252	1.6118396324
H	-2.2401702097	-8.7704014819	-1.9293027349
H	-0.5995586142	-9.5079450838	-0.2176123747
N	-2.6644286285	0.2539438136	0.2303965454
N	-4.0568885222	-2.0920165758	0.2675052278

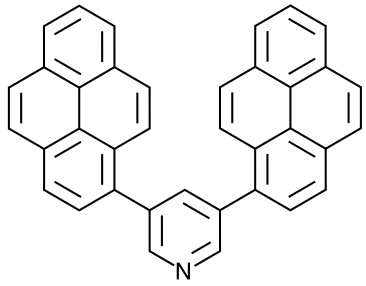
Table S4. Three-dimensional coordinates of optimized structures of BtBBT (2,5-bis(5-*tert*-butyl-2-benzoxazolyl)thiophene).



Anion				Neutral			
elem.	x	y	z	elem.	x	y	z
C	0.0930843911	0.4720461561	-0.0003111972	C	0.1242212769	0.4858104430	-0.0003085438
C	1.5015833859	0.5336861929	-0.0004639622	C	1.5040172887	0.5191225117	-0.0004718831
C	2.0087888743	1.8199973706	0.0001419083	C	2.0205073420	1.8289813961	0.0001462354
C	1.0214122254	2.8263549714	0.0007980001	C	1.0347744706	2.7950440534	0.0007812946
S	-0.5983154078	2.1048508600	0.0006334886	S	-0.5583646482	2.0890972886	0.0006204134
H	2.1025205174	-0.3657619504	-0.0010132632	H	2.1014140112	-0.3818211073	-0.0010218943
H	3.0618800174	2.0672455974	0.0001328332	H	3.0720313544	2.0797398505	0.0001397269
C	-0.6992819980	-0.6842652990	-0.0008121289	C	-0.7048013293	-0.6922901958	-0.0008168158
C	-2.5899569541	-1.7909109149	-0.0011454988	C	-2.5818990938	-1.7782793819	-0.0011420497
C	-1.4948506687	-2.6765179512	-0.0017502418	C	-1.5011359885	-2.6662997621	-0.0017454448
C	-3.8985991684	-2.2133770775	-0.0011973817	C	-3.8969624826	-2.1944155506	-0.0011900306
C	-1.7353229503	-4.0531422910	-0.0024387855	C	-1.7260475593	-4.0407517803	-0.0024345754
C	-4.1178120010	-3.6044468012	-0.0018967545	C	-4.1018860734	-3.5771885363	-0.0018861972
H	-4.7249954516	-1.5125118442	-0.0007241844	H	-4.7247531943	-1.4968298201	-0.0007188718
C	-3.0594764921	-4.5278428119	-0.0025162958	C	-3.0451190958	-4.5123135314	-0.0025109741
H	-0.8906924382	-4.7320085743	-0.0029026597	H	-0.8797263198	-4.7159366738	-0.0028964411
H	-5.1421091256	-3.9515378430	-0.0019463887	H	-5.1239895967	-3.9292775870	-0.0019385368
C	1.2314728168	4.2122751556	0.0014957197	C	1.2329145291	4.2219076955	0.0015025604
C	0.6049011785	6.3114948043	0.0026792813	C	0.6021686062	6.2967635564	0.0026742500
C	2.0097250360	6.2113558679	0.0024401852	C	1.9981563916	6.2081774477	0.0024418983
C	-0.0632278462	7.5134203955	0.0033987414	C	-0.0749734818	7.4984453377	0.0033946087
C	2.7735189886	7.3816295211	0.0029524639	C	2.7718410482	7.3662430063	0.0029460116
C	0.7259632759	8.6797423299	0.0039061069	C	0.7189991265	8.6489506798	0.0038921614
H	-1.1455693599	7.5651884233	0.0035698186	H	-1.1560958765	7.5535622441	0.0035675826
C	2.1297031557	8.6323188676	0.0036946263	C	2.1295976392	8.6111699388	0.0036843813
H	3.8541732184	7.3013379954	0.0027664970	H	3.8512184243	7.2821065763	0.0027580848
H	0.2142133264	9.6325111784	0.0044745030	H	0.2122638249	9.6038754547	0.0044604960
N	2.3752368417	4.8860050451	0.0016968370	N	2.3607179610	4.8643843877	0.0016891461
N	-0.3231479111	-1.9573053534	-0.0015261136	N	-0.3190024634	-1.9315947043	-0.0015140747
O	0.0975674542	5.0418440106	0.0020808952	O	0.1057052021	5.0161682478	0.0020689860
O	-2.0942171484	-0.5166884640	-0.0005435385	O	-2.0707444129	-0.5034769838	-0.0005418863
C	-3.3035267849	-6.0514525666	-0.0032815372	C	-3.2990996543	-6.0334859051	-0.0032729463
C	-2.6655340146	-6.6804844192	-1.2641050816	C	-2.6623946480	-6.6604828561	-1.2655931656
C	-2.6652173814	-6.6818008293	1.2567239430	C	-2.6620711562	-6.6618009025	1.2582284548
C	-4.8005537248	-6.4139253816	-0.0032833063	C	-4.7990276192	-6.3820376449	-0.0032627529
H	-3.1076869080	-6.2588115318	-2.1713092497	H	-3.0981659538	-6.2359752456	-2.1742723058
H	-1.5896905892	-6.4974518223	-1.3048003360	H	-1.5836097206	-6.4930921639	-1.3031333585
H	-2.8249324601	-7.7648789935	-1.2766495683	H	-2.8327948548	-7.7414557300	-1.2793688450
H	-3.1071450081	-6.2610783198	2.1644789558	H	-3.0976098327	-6.2382430146	2.1674621541
H	-2.8246095185	-7.7662084413	1.2681741354	H	-2.8324675149	-7.7427876776	1.2709185335
H	-1.5893644022	-6.4988069984	1.2973415564	H	-1.5832766950	-6.4944488608	1.2956671489

H	-4.9152128367	-7.5025842214	-0.0038386125	H	-4.9200959680	-7.4685778158	-0.0038148563
H	-5.3112647527	-6.0266143009	0.8826932693	H	-5.3085772377	-5.9957614927	0.8838038331
H	-5.3114869082	-6.0256871402	-0.8887258545	H	-5.3088045813	-5.9948349015	-0.8897945830
C	2.9912000049	9.9124636708	0.0042519757	C	2.9821734676	9.8963104909	0.0042445886
C	3.8875503056	9.9364892206	1.2645578008	C	3.8761944526	9.9197274018	1.2660484192
C	3.8872078835	9.9378167401	-1.2562712270	C	3.8758567576	9.9210514255	-1.2577731962
C	2.1444381517	11.1991143380	0.0050450790	C	2.1237905132	11.1747667089	0.0050301589
H	3.2771252886	9.9298573246	2.1721171236	H	3.2684996723	9.9066682892	2.1750795716
H	4.5489687794	9.0684379576	1.3046665400	H	4.5504363759	9.0611014910	1.3029971005
H	4.5111588161	10.8378414136	1.2769459833	H	4.4894276424	10.8260870049	1.2796748411
H	3.2765361202	9.9321444106	-2.1636710540	H	3.2679186858	9.9089464991	-2.1666548796
H	4.5108159140	10.8391796747	-1.2678776987	H	4.4890867812	10.8274246678	-1.2706125307
H	4.5486122941	9.0698060394	-1.2974754001	H	4.5500882655	9.0624645478	-1.2958034036
H	2.8036492175	12.0730512471	0.0054169076	H	2.7768714505	12.0515292443	0.0054028763
H	1.5063099102	11.2648016132	-0.8805437977	H	1.4872169854	11.2404179358	-0.8816497539
H	1.5065494223	11.2638670413	0.8908753226	H	1.4874541074	11.2394872963	0.8919486587

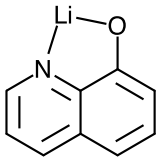
Table S5. Three-dimensional coordinates of optimized structures of DPP (3,5-di(1-pyrenyl)pyridine).



Anion				Neutral			
elem.	x	y	z	elem.	x	y	z
C	-2.2144035335	-2.2060015418	0.0183477756	C	-2.0264128147	-2.1976088204	0.0664979270
C	-0.8035741126	-2.2315209476	0.0064558367	C	-0.6243101111	-2.2185432637	0.0486811198
C	-0.1559440504	-0.9897201837	-0.0000539178	C	0.0283126346	-0.9833433357	-0.0028457581
C	-0.8881588815	0.2040915210	0.0144805144	C	-0.7098385323	0.2034611899	-0.0331460898
C	-2.2935146192	0.0806292177	0.0455384094	C	-2.1069866200	0.0851199463	-0.0082396147
N	-2.9402379748	-1.0865539779	0.0424095665	N	-2.7543390340	-1.0801725225	0.0396241918
H	0.9268079180	-0.9520636061	-0.0165671109	H	1.1118220044	-0.9456400487	-0.0193829773
H	-2.7685408740	-3.1405177888	0.0007660539	H	-2.5799040746	-3.1321945338	0.0920827348
H	-2.9104291463	0.9744179473	0.0809799499	H	-2.7246103829	0.9789538398	-0.0159506426
C	-0.2461231652	1.5330635100	-0.0588962141	C	-0.0645354612	1.5404430523	-0.1306818063
C	0.8196355074	1.9377310642	0.8064060692	C	0.8657054243	2.0089320677	0.8295355578
C	-0.7014635138	2.4403592128	-1.0305199147	C	-0.3934113360	2.3586871809	-1.2187528128
C	1.4372555551	3.2178779051	0.6092663857	C	1.4758395015	3.2892859391	0.6429286888
C	1.2791690455	1.1428276739	1.9000440145	C	1.2064131808	1.2678992675	2.0146805154
C	-0.1207555843	3.6821602634	-1.2150576367	C	0.1906319797	3.6045452848	-1.3988901371
H	-1.5118830985	2.1329778941	-1.6833169639	H	-1.1057157141	1.9937029332	-1.9502695537
C	2.5214432023	3.6334922394	1.4461998447	C	2.4246783032	3.7793369272	1.5906845041
C	0.9686421771	4.0966965067	-0.4167312221	C	1.1368484229	4.0901233966	-0.4875619146
C	2.3129112095	1.5432780562	2.7046544758	C	2.1058683090	1.7393686785	2.9182646057
H	0.7867011021	0.2011173972	2.1042660596	H	0.7203796410	0.3179232074	2.1938119878
H	-0.4848976270	4.3414682680	-1.9967610385	H	-0.0766984137	4.2073206862	-2.2602844926
C	2.9816811141	2.7845477220	2.5008526028	C	2.7588873738	3.0028445313	2.7383891532
C	3.1491496254	4.9043796782	1.2373292101	C	3.0425835513	5.0514746447	1.3971523142
C	1.6118005738	5.3538430104	-0.5978922145	C	1.7727410644	5.3662008631	-0.6553477235
H	2.6330802889	0.9107063131	3.5268994573	H	2.3384556219	1.1598104322	3.8056355635
C	4.0581881475	3.2110297832	3.3096032015	C	3.6963116193	3.5011298900	3.6554084406
C	4.2218852813	5.2850659868	2.0731830261	C	3.9756959628	5.5079075878	2.3396035025
C	2.6621705381	5.7427668339	0.1911171977	C	2.6841024055	5.8245048197	0.2416894661
H	1.2495944768	6.0082725144	-1.3854456488	H	1.5072937291	5.9625520515	-1.5220052594
C	4.6636494337	4.4436338428	3.0895729951	C	4.2979422604	4.7393359744	3.4543604667
H	4.4067501967	2.5629962243	4.1072043475	H	3.9479956509	2.9085961587	4.5285675099
H	4.6986218667	6.2468563490	1.9125799822	H	4.4466284935	6.4738431743	2.1909239270
H	3.1399658102	6.7048969693	0.0326699503	H	3.1567479034	6.7907524421	0.0998273923
H	5.4908087477	4.7546053586	3.7206296241	H	5.0211384479	5.1095915564	4.1722903180
C	-0.0688462677	-3.5126110548	0.0588355480	C	0.1150183105	-3.5073434747	0.1250837261
C	0.9955943644	-3.8431933984	-0.8389544511	C	1.0458666097	-3.9110707245	-0.8635381715

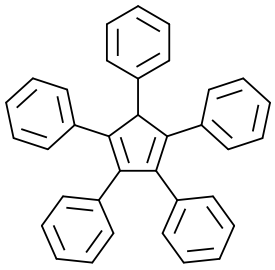
C	-0.4302633025	-4.4483123306	1.0429157313	C	-0.1228805797	-4.3453103647	1.2218047090
C	1.7063552025	-5.0771410473	-0.6620738654	C	1.7489076877	-5.1457290233	-0.6969734733
C	1.3652826441	-3.0194509387	-1.9452389263	C	1.2979699705	-3.1494092424	-2.0577305399
C	0.2406445114	-5.6465839617	1.2083651136	C	0.5515500726	-5.5473766803	1.3827344022
H	-1.2398155539	-4.1972712595	1.7204190125	H	-0.8361985091	-4.0299347068	1.9750798884
C	2.7907961129	-5.4173336650	-1.5320811406	C	2.7001793884	-5.5696597924	-1.6737287785
C	1.3313815481	-5.9852983253	0.3767893956	C	1.5010058744	-5.9669894961	0.4424740006
C	2.3993546245	-3.3479857722	-2.7813856836	C	2.2000555238	-3.5581884335	-2.9888097123
H	0.8026045413	-2.1144371216	-2.1333689594	H	0.7418586781	-2.2356978126	-2.2209566749
H	-0.0528459745	-6.3287634164	2.0000981584	H	0.3531359975	-6.1663592510	2.2512368189
C	3.1586206057	-4.5395903955	-2.5993627827	C	2.9444803745	-4.7730359771	-2.8302621199
C	3.5113284652	-6.6413312990	-1.3437724428	C	3.4106097035	-6.7955742218	-1.5004697972
C	2.0655229703	-7.1945442945	0.5369452423	C	2.2288603442	-7.1956115813	0.5894458697
H	2.6496210146	-2.6955751429	-3.6123304328	H	2.3646483178	-2.9648089941	-3.8822423617
C	4.2370162679	-4.8911281039	-3.4409778651	C	3.8858796579	-5.2059417964	-3.7759559508
C	4.5819572647	-6.9474745227	-2.2123147767	C	4.3440259729	-7.1870554112	-2.4714077634
C	3.1158494557	-7.5104089819	-0.2841019464	C	3.1421023228	-7.5904228699	-0.3354383329
H	1.7738021899	-7.8717163778	1.3344718015	H	2.0320375430	-7.8080491117	1.4631581918
C	4.9330483916	-6.0784680775	-3.2407966861	C	4.5779532938	-6.3991296335	-3.5946527051
H	4.5152705197	-4.2212948355	-4.2481386713	H	4.0690458920	-4.5982758494	-4.6557514146
H	5.1290155192	-7.8736587571	-2.0673255968	H	4.8852606212	-8.1177696541	-2.3381760919
H	3.6639212744	-8.4368609210	-0.1413001423	H	3.6848586306	-8.5213367766	-0.2090736389
H	5.7602037035	-6.3319049562	-3.8970833126	H	5.3029130404	-6.7189920597	-4.3346841945

Table S6. Three-dimensional coordinates of optimized structures of Liq ((8-quinolinolato)lithium).



Anion				Neutral			
elem.	x	y	z	elem.	x	y	z
C	-4.8855619516	0.8160341977	-0.0124906871	C	-4.8740028111	0.8181993477	0.0003411088
C	-3.4751631432	0.8191378890	-0.0213318951	C	-3.4713349797	0.8126411624	0.0001603574
C	-2.8305613933	2.1207931752	-0.0018780240	C	-2.8268920065	2.1187280506	0.0002593054
C	-3.5950771466	3.3274390532	0.0055350695	C	-3.5928315711	3.3271199868	0.0005242695
C	-5.0088461227	3.2512381022	0.0089927605	C	-5.0049961504	3.2559969626	0.0006955749
C	-5.6228897454	2.0069130788	0.0036205135	C	-5.6107426179	2.0134928572	0.0006012435
H	-5.3867417150	-0.1462162568	-0.0199093191	H	-5.3815278571	-0.1395466845	0.0002728858
C	-2.8697312063	4.5525553217	0.0071221863	C	-2.8670047212	4.5424299652	0.0005988672
H	-5.5935981715	4.1655448052	0.0198249598	H	-5.5895382906	4.1685045887	0.0008969723
H	-6.7087197348	1.9504397149	0.0090982868	H	-6.6946995446	1.9533119945	0.0007319448
C	-1.4817297003	4.5280517470	-0.0195788572	C	-1.4909167948	4.5318344299	0.0004214956
C	-0.8157631431	3.2988660644	-0.0077930198	C	-0.8215298972	3.2937050839	0.0001654500
H	-3.4115195436	5.4933359486	0.0213967649	H	-3.4107877774	5.4819696800	0.0007979409
H	-0.9043067623	5.4465367972	-0.0360865514	H	-0.9189091167	5.4516653807	0.0004752327
H	0.2703861905	3.2608796333	0.0014217831	H	0.2642786712	3.2601380390	0.0000225228
N	-1.4531002884	2.1209541441	0.0140385017	N	-1.4573158893	2.1315839745	0.0000863262
O	-2.7509927037	-0.2601774125	-0.0365344324	O	-2.7466303826	-0.2640752324	-0.0000837367
Li	-1.0244623487	0.2116039667	0.0712887298	Li	-1.0529968930	0.2062303830	-0.0002309912

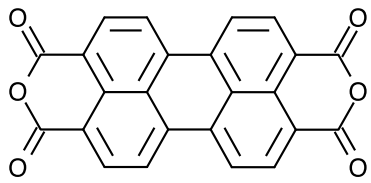
Table S7. Three-dimensional coordinates of optimized structures of PPCPD (1,2,3,4,5-pentaphenyl-1,3-cyclopentadiene).



Anion				Neutral			
elem.	x	y	z	elem.	x	y	z
C	0.4218596477	0.4641694935	0.0772343762	C	0.4071580289	0.4057363549	0.0127450079
H	1.5138676668	0.5831680970	0.1404837615	H	1.5025492187	0.3459897041	0.0727161141
C	-0.0001526864	-0.3701584571	-1.1394965836	C	-0.0772993267	-0.4079051160	-1.1794946869
C	-0.7630293915	-1.4464661622	-0.6745330060	C	-0.8022701417	-1.4666947556	-0.7271975390
C	-0.0721441253	-0.3549382835	1.2696941848	C	-0.1499653513	-0.3564998929	1.2088123416
C	-0.8426982413	-1.4215091543	0.7663043101	C	-0.8489292672	-1.4325598134	0.7581180619
C	-0.1830286882	1.8728026981	-0.0098743073	C	0.0272000032	1.8800441995	-0.0622219563
C	0.6171770515	3.0096053274	-0.1504998550	C	0.9978746835	2.8782090429	0.0413459209
C	-1.5721397661	2.0486050533	0.0277956100	C	-1.3093228426	2.2602954904	-0.2338944191
C	0.0560766483	4.2845292919	-0.2473199741	C	0.6461599353	4.2274432106	-0.0175763846
H	1.6969791587	2.8978752310	-0.1793900740	H	2.0382046110	2.6012010692	0.1773018101
C	-2.1384583119	3.3159642358	-0.0665593130	C	-1.6639981865	3.6043954315	-0.2930393221
H	-2.2061672713	1.1755546788	0.1336124079	H	-2.0737642475	1.4955688237	-0.3210239308
C	-1.3260489373	4.4440201168	-0.2048568530	C	-0.6861323445	4.5948644783	-0.1835976218
H	0.7015010340	5.1505273974	-0.3577986211	H	1.4146551601	4.9880053932	0.0660432992
H	-3.2178952663	3.4266483671	-0.0329269921	H	-2.7039360171	3.8813851079	-0.4272765933
H	-1.7675351076	5.4325238822	-0.2795280642	H	-0.9625325034	5.6421402025	-0.2314461124
C	0.4225863886	-0.1200977714	2.6052874381	C	0.2027606743	-0.0315561691	2.6091478539
C	0.3583923764	-1.0853022406	3.6529130155	C	0.7766826580	-1.0147934533	3.4330292737
C	1.0840264148	1.0966257070	2.9405233841	C	0.0056690325	1.2491218116	3.1508790740
C	0.8824357613	-0.8402475527	4.9131033236	C	1.1343587947	-0.7317307733	4.7477301334
H	-0.0883058827	-2.0498368694	3.4610491236	H	0.9465523129	-2.0070083446	3.0326627977
C	1.6067899477	1.3325145204	4.2057855303	C	0.3609652864	1.5299476467	4.4685935772
H	1.1660848555	1.8782249608	2.1981191701	H	-0.4412156577	2.0257847878	2.5444955903
C	1.5109008710	0.3737083378	5.2176392743	C	0.9267408770	0.5429403727	5.2731148735
H	0.8117232366	-1.6163869860	5.6703501603	H	1.5785754897	-1.5078141728	5.3613982303
H	2.0927294670	2.2838116639	4.4053803061	H	0.1909768976	2.5242668530	4.8670282846
H	1.9174901530	0.5601429310	6.2058508086	H	1.2041906193	0.7643935315	6.2976569710
C	-1.6477532526	-2.3719162667	1.5573987821	C	-1.5352723591	-2.4454233977	1.5956627749
C	-1.5383692325	-3.7674364358	1.4027571116	C	-1.2718052159	-3.8144663807	1.4423606358
C	-2.5789766216	-1.8992800897	2.5041995852	C	-2.4661842292	-2.0510745700	2.5672814926
C	-2.3248578537	-4.6424507891	2.1476456306	C	-1.9083799363	-4.7571292570	2.2456133738
H	-0.8207787147	-4.1644771596	0.6951154295	H	-0.5600126811	-4.1423999330	0.6939071679
C	-3.3644303270	-2.7724859794	3.2481816273	C	-3.1080536169	-2.9941486984	3.3658096844
H	-2.6726842981	-0.8290018979	2.6497234807	H	-2.6844486369	-0.9971843028	2.6946248758
C	-3.2461054788	-4.1543176790	3.0752813444	C	-2.8300438563	-4.3512398312	3.2097291644

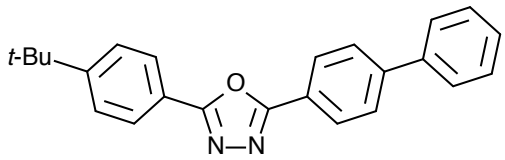
H	-2.2132265732	-5.7130600974	2.0056810240	H	-1.6855215234	-5.8105077759	2.1161037500
H	-4.0744205884	-2.3741894856	3.9666343355	H	-3.8258753187	-2.6680900990	4.1104607380
H	-3.8570362686	-4.8367424783	3.6569736360	H	-3.3286784976	-5.0860828179	3.8318527058
C	-1.3635817876	-2.5097774472	-1.5098844303	C	-1.4380261987	-2.5262901570	-1.5476572834
C	-2.7417255259	-2.7864114985	-1.4780727316	C	-2.8094004823	-2.7963973337	-1.4370530314
C	-0.5633158858	-3.2900233151	-2.3637925494	C	-0.6783417534	-3.2875940611	-2.4469039595
C	-3.2933266597	-3.7997913588	-2.2584036972	C	-3.4060334935	-3.7853681538	-2.2152847316
H	-3.3817914302	-2.1964998784	-0.8325087355	H	-3.4120963094	-2.2258227660	-0.7397838258
C	-1.1127343289	-4.3026656298	-3.1437745358	C	-1.2731024150	-4.2818652525	-3.2194237153
H	0.5007862888	-3.0883350334	-2.4085042727	H	0.3841776707	-3.0943268344	-2.5388804741
C	-2.4835790018	-4.5667756038	-3.0963510957	C	-2.6401840625	-4.5326030621	-3.1089701779
H	-4.3611651336	-3.9898865489	-2.2122910163	H	-4.4695442956	-3.9747815789	-2.1201640477
H	-0.4687962245	-4.8899432086	-3.7911070335	H	-0.6679528523	-4.8611403386	-3.9081432920
H	-2.9130382596	-5.3556156623	-3.7051825877	H	-3.1039125339	-5.3057961541	-3.7112622889
C	0.3041784388	0.0400359544	-2.4931536440	C	0.2042558915	0.0014186644	-2.5659701551
C	1.4485671192	0.8371706786	-2.7669606608	C	1.4623349900	0.5226246291	-2.9128019069
C	-0.5003052679	-0.2894215458	-3.6185309044	C	-0.7719880185	-0.0812338437	-3.5735853889
C	1.7717828405	1.2508452831	-4.0527798214	C	1.7404922458	0.9261782199	-4.2158048216
H	2.1049811550	1.1141471143	-1.9512297273	H	2.2372115132	0.5990819567	-2.1588075834
C	-0.1724320047	0.1275418504	-4.9006211037	C	-0.4952264180	0.3262035536	-4.8744371530
H	-1.4067067657	-0.8606226080	-3.4724812612	H	-1.7575561149	-0.4571722285	-3.3298629085
C	0.9691633796	0.9008073483	-5.1419588775	C	0.7632884393	0.8286709886	-5.2043413925
H	2.6637802636	1.8514526932	-4.2080366273	H	2.7224756940	1.3173513727	-4.4583652935
H	-0.8257320471	-0.1425373001	-5.7255832014	H	-1.2679757286	0.2574837604	-5.6322769772
H	1.2185709341	1.2274168608	-6.1457897841	H	0.9774295966	1.1457859616	-6.2187403740

Table S8. Three-dimensional coordinates of optimized structures of PTCDA (perylenetetracarboxylic dianhydride).



Anion				Neutral			
elem.	x	y	z	elem.	x	y	z
C	-9.6667082820	-3.5174266529	-0.8070932634	C	-9.6732381724	-3.5266528424	-0.8084376594
C	-8.6734888624	-2.4944265422	-0.5579303123	C	-8.6646036663	-2.4877745555	-0.5554056858
C	-8.9905716504	-1.1284797167	-0.8369333873	C	-8.9862161128	-1.1239936124	-0.8358408064
C	-10.2680351715	-0.7517104295	-1.3568629822	C	-10.2615046194	-0.7424844501	-1.3555203675
C	-7.3896288320	-2.7974346785	-0.0443137133	C	-7.4003034811	-2.7866043784	-0.0495595931
C	-8.0049342227	-0.1132881650	-0.5896708041	C	-8.0064631748	-0.1148629928	-0.5900544343
C	-6.7358956035	-0.4713845122	-0.0750793039	C	-6.7373971225	-0.4690774851	-0.0759076917
C	-6.4489414631	-1.8157707425	0.1901666934	C	-6.4465826383	-1.7942473488	0.1885129948
C	-5.7292510752	0.5495224904	0.1793293669	C	-5.7177375822	0.5687224247	0.1813550826
C	-7.3130305616	2.2804704670	-0.6142052826	C	-7.2946002330	2.2921121401	-0.6087192967
C	-8.3046752819	1.2431699210	-0.8610988109	C	-8.3025457104	1.2415097081	-0.8601130374
C	-9.5627198894	1.5873476778	-1.3699582209	C	-9.5423716274	1.5892123054	-1.3626079350
C	-10.5154379378	0.6188327926	-1.6104683174	C	-10.5055503004	0.6071920212	-1.6054195579
H	-11.4732579451	0.9295703431	-2.0036305025	H	-11.4608751537	0.9253623753	-1.9985301339
H	-9.7702588897	2.6314512780	-1.5702552935	H	-9.7544843517	2.6317824265	-1.5644288023
H	-7.1252781551	-3.8224352099	0.1748805460	H	-7.1288768035	-3.8091793690	0.1719845898
H	-5.4714398055	-2.0668245770	0.5836208320	H	-5.4706618054	-2.0501067004	0.5819471608
C	-11.6300691931	-5.5123066777	-1.3028547004	C	-11.6321971488	-5.5106469727	-1.3038448169
C	-9.4193070471	-4.8879693924	-0.5534838219	C	-9.4291923098	-4.8763293763	-0.5585389535
C	-10.3720257287	-5.8564840745	-0.7939922319	C	-10.3923711005	-5.8583496179	-0.8013502758
H	-8.4614877303	-5.1987067209	-0.1603197835	H	-8.4738672402	-5.1944998038	-0.1654289594
H	-10.1644879719	-6.9005872795	-0.5936918213	H	-10.1802583125	-6.9009197616	-0.5995296024
C	-10.9441712757	-3.1406575276	-1.3270242829	C	-10.9485267489	-3.1451436537	-1.3281170416
C	-11.9298087776	-4.1558490544	-1.5742866636	C	-11.9282797237	-4.1542742615	-1.5739033145
C	-11.2612535152	-1.7747108803	-1.6060288210	C	-11.2701393100	-1.7813626771	-1.6085518332
C	-13.1988457810	-3.7977532163	-2.0888824887	C	-13.1973458696	-3.8000597340	-2.0880497899
C	-12.5451120002	-1.4717032300	-2.1196495644	C	-12.5344397701	-1.4825327606	-2.1143971873
C	-13.4857987702	-2.4533673513	-2.3541315938	C	-13.4881605491	-2.4748898091	-2.3524699318
H	-12.8094619660	-0.4467029240	-2.3388457242	H	-12.8058667094	-0.4599576842	-2.3359406604
H	-14.4632991774	-2.2023139098	-2.7475890976	H	-14.4640815310	-2.2190304099	-2.7459036946
C	-12.6217142757	-6.5496071046	-1.5497472699	C	-12.6401427596	-6.5612493632	-1.5552381944
C	-14.2054900718	-4.8186602910	-2.3432918041	C	-14.2170053748	-4.8378596467	-2.3453126832
O	-13.8503358954	-6.1339630520	-2.0560816016	O	-13.8647716470	-6.1488312628	-2.0597021754
O	-6.0844068727	1.8648257592	-0.1078764897	O	-6.0699714253	1.8796940670	-0.1042550989
O	-4.6163163496	0.3616895256	0.6157473729	O	-4.6200143388	0.3610734998	0.6144479395
O	-7.4569938463	3.4663293476	-0.8075414988	O	-7.4576826625	3.4624268916	-0.8073428749
O	-15.3184233166	-4.6308277857	-2.7797137812	O	-15.3147285216	-4.6302107471	-2.7784057932
O	-12.4777528073	-7.7354654154	-1.3564061957	O	-12.4770603900	-7.7315640979	-1.3566144859

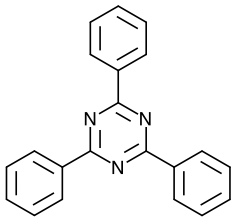
Table S9. Three-dimensional coordinates of optimized structures of t-Bu-PBD (2-(4-*tert*-butylphenyl)-5-(4-biphenyl)-1,3,4-oxadiazole).



Anion				Neutral			
elem.	x	y	z	elem.	x	y	z
C	-0.0956154932	0.4437704662	-0.1167136188	C	-0.0957838851	0.4579709772	-0.2017016008
C	0.4934696676	2.5273239265	-0.1212327542	C	0.4852168992	2.5167546035	-0.2111429843
O	-0.6289059626	1.7155556573	-0.0595588745	O	-0.6181941386	1.7174381487	-0.1027733019
C	-0.9611064709	-0.6997397123	-0.0767095099	C	-0.9796472718	-0.6959455595	-0.1281773666
C	-2.3649372215	-0.5669580340	0.0195700611	C	-2.3635675373	-0.5502998421	0.0355025396
C	-0.4363513133	-2.0091597802	-0.1320133750	C	-0.4454467662	-1.9856066055	-0.2213222016
C	-3.1829619688	-1.6863307502	0.0577617659	C	-3.1810837944	-1.6701366523	0.1033240058
H	-2.8014199194	0.4234324492	0.0638236638	H	-2.7969447527	0.4395292979	0.1094448527
C	-1.2715581558	-3.1161068141	-0.0921622509	C	-1.2772379556	-3.0978303355	-0.1512733923
H	0.6368585796	-2.1372882722	-0.2061358506	H	0.6232463740	-2.1074825568	-0.3480440724
C	-2.6703106424	-2.9948972411	0.0040040541	C	-2.6633058616	-2.9718598349	0.0126775824
H	-4.2547468295	-1.5299227697	0.1319780461	H	-4.2468569596	-1.5203444992	0.2301512036
H	-0.8124260139	-4.0962674521	-0.1375448889	H	-0.8246537718	-4.0773732057	-0.2268007809
C	0.3548827621	3.9403054817	-0.0873129643	C	0.3367033535	3.9629703187	-0.1499665718
C	-0.9134013831	4.5741467155	0.0199456592	C	-0.9173378774	4.5621263519	0.0241404681
C	1.4949930596	4.7888188319	-0.1594598482	C	1.4712919670	4.7793506103	-0.2662725914
C	-1.0254689237	5.9487285075	0.0490786146	C	-1.0311951249	5.9454086357	0.0807562777
H	-1.8048437235	3.9621430281	0.0930052926	H	-1.8004013066	3.9435035403	0.1252549350
C	1.3679116465	6.1588338358	-0.1218443425	C	1.3473838276	6.1590738831	-0.2083559531
H	2.4739364926	4.3344064527	-0.2568489566	H	2.4404653492	4.3183330444	-0.4106874889
C	0.1037939791	6.8069686602	-0.0178630340	C	0.0956250808	6.7729396669	-0.0336308252
H	-2.0154625627	6.3769521057	0.1616009070	H	-2.0065723004	6.3896112861	0.2414251644
H	2.2681233119	6.7571217971	-0.2089068135	H	2.2318799134	6.7743985616	-0.3246594983
C	-0.0226059454	8.2609697487	0.0200508980	C	-0.0297813781	8.2498853683	0.0290220451
C	1.0660254972	9.1017196379	0.3682170907	C	0.9225586825	9.0251234161	0.7079719595
C	-1.2409491433	8.9194245608	-0.2887678469	C	-1.1034727599	8.9091651953	-0.5885689727
C	0.9444289940	10.4845323073	0.4028685553	C	0.8044691336	10.4109158466	0.7685371606
H	2.0147496324	8.6566156015	0.6430941666	H	1.7476092048	8.5364198122	1.2136201702
C	-1.3595588660	10.3021623191	-0.2483814486	C	-1.2205258216	10.2951374999	-0.5297767908
H	-2.0999956213	8.3332275912	-0.5926485659	H	-1.8375514632	8.3337735626	-1.1411594929
C	-0.2695361748	11.1084684846	0.0967339615	C	-0.2673288442	11.0522249035	0.1495243432
H	1.8048605272	11.0850072836	0.6840115428	H	1.5465902403	10.9897933662	1.3069779030
H	-2.3115703555	10.7598537133	-0.5016807729	H	-2.0527560104	10.7850263562	-1.0229382132
H	-0.3632164339	12.1884412474	0.1258085041	H	-0.3586569564	12.1314181192	0.1957704402
C	-3.6216869632	-4.2013901177	0.0496290999	C	-3.6086744847	-4.1820265882	0.0934360458
C	-2.8693902679	-5.5437576574	-0.0144482265	C	-2.8569190208	-5.5211085848	-0.0167607868
H	-2.1811021206	-5.6621668875	0.8270193774	H	-2.1317742015	-5.6495731665	0.7914328790
H	-3.5853901114	-6.3709769657	0.0220831651	H	-3.5706015260	-6.3467086570	0.0476292029
H	-2.2949965865	-5.6419021923	-0.9397882382	H	-2.3298370253	-5.6161065247	-0.9699948924

C	-4.4380879522	-4.1768627593	1.3642288031	C	-4.3570445114	-4.1592534304	1.4471917896
H	-5.0279283512	-3.2616296839	1.4539265972	H	-4.9537804252	-3.2522804831	1.5680577548
H	-5.1282092050	-5.0275591757	1.4076032692	H	-5.0344481373	-5.0156716218	1.5183373490
H	-3.7741854630	-4.2295267028	2.2317048126	H	-3.6541662710	-4.2116030275	2.2831383246
C	-4.5974118548	-4.1455846154	-1.1504261822	C	-4.6351397454	-4.1082169796	-1.0615980162
H	-4.0483823234	-4.1759512360	-2.0957798997	H	-4.1326197076	-4.1245959747	-2.0325655694
H	-5.2891836492	-4.9957478204	-1.1273556368	H	-5.3161946000	-4.9635219704	-1.0166139529
H	-5.1918185349	-3.2289300215	-1.1422203747	H	-5.2387166387	-3.1990345317	-1.0125374768
N	1.2147774202	0.4844454552	-0.2045682796	N	1.1934866087	0.4850203298	-0.3552511179
N	1.5940234677	1.7908413756	-0.2076987638	N	1.5698047283	1.8188285098	-0.3610738954

Table S10. Three-dimensional coordinates of optimized structures of TPT (2,4,6-triphenyl-1,3,5-triazine).



Anion				Neutral			
elem.	x	y	z	elem.	x	y	z
C	-1.2667598911	-0.3023487332	0.0000000358	C	0.9978258073	0.3893538472	0.0012027044
C	0.9206288480	-0.9604329490	-0.0000001714	C	0.9982121459	2.6598635190	-0.0003310719
C	0.3936668579	1.2642291673	-0.0000000129	C	-0.9683095033	1.5249452781	-0.0001931360
C	1.9204265941	-2.0198660965	-0.0000003100	C	1.7404802609	3.9449985819	-0.0009616787
C	3.3062727413	-1.7317971010	-0.0000003972	C	1.0489816903	5.1643047064	-0.0020061861
C	1.5372280269	-3.3825745912	-0.0000003594	C	3.1421873920	3.9553322663	-0.0005202314
C	4.2497275299	-2.7477486068	-0.0000005205	C	1.7461596335	6.3678815644	-0.0025959346
H	3.6136642898	-0.6937266062	-0.0000003599	H	-0.0326878600	5.1522126485	-0.0023438890
C	2.4904130009	-4.3945056582	-0.0000004722	C	3.8363112365	5.1606742955	-0.0011121337
H	0.4808336439	-3.6168391411	-0.0000002886	H	3.6722563533	3.0123659039	0.0002860285
C	3.8560704725	-4.0945870055	-0.0000005577	C	3.1410443511	6.3699321110	-0.0021510885
H	5.3062381263	-2.4946572372	-0.0000005952	H	1.2019445281	7.3055795319	-0.0034031658
H	2.1661118888	-5.4315691892	-0.0000004948	H	4.9204880351	5.1578737823	-0.0007633855
H	4.5971686752	-4.8871434284	-0.0000006517	H	3.6833962804	7.3089596019	-0.0026116543
C	-2.7256691921	-0.6472833828	0.0000001093	C	1.7396366575	-0.8960349006	0.0023079127
C	-3.1432798901	-1.9839366274	0.0000001420	C	3.1413419032	-0.9068942535	0.0027675307
C	-3.6964466220	0.3620637950	0.0000001564	C	1.0477004346	-2.1150983995	0.0029058889
C	-4.4994102328	-2.3041799417	0.0000002179	C	3.8350329395	-2.1124805919	0.0038036853
H	-2.3827521237	-2.7541508997	0.0000000961	H	3.6717696913	0.0358686601	0.0023035912
C	-5.0532042046	0.0421156230	0.0000002170	C	1.7444474544	-3.3189214205	0.0039416512
H	-3.3601293143	1.3908242926	0.0000001445	H	-0.0339657670	-2.1026247615	0.0025483736
C	-5.4608802154	-1.2921671731	0.0000002493	C	3.1393311908	-3.3214908858	0.0043936020
H	-4.8076430802	-3.3451132697	0.0000002445	H	4.9192109093	-2.1100581843	0.0041519957
H	-5.7941713579	0.8355796348	0.0000002421	H	1.1998932910	-4.2564229403	0.0043973566
H	-6.5175044182	-1.5414614376	0.0000002911	H	3.6813429165	-4.2607138329	0.0052012893
C	0.8147207628	2.6648132104	0.0000000326	C	-2.4524072602	1.5252110251	-0.0006673421
C	2.1808940845	3.0261916116	-0.0000000613	C	-3.1621736225	2.7339728855	-0.0017162029
C	-0.1392640602	3.7075834518	0.0000001749	C	-3.1626618835	0.3167259194	-0.0000719529
C	2.5694661701	4.3575797510	-0.0000000250	C	-4.5530917999	2.7325008132	-0.0021594958
H	2.9196659435	2.2347814294	-0.0000001683	H	-2.6105290669	3.6644796564	-0.0021730529
C	0.2584462155	5.0406974729	0.0000002141	C	-4.5535798536	0.3187808380	-0.0005173857
H	-1.1878716470	3.4408700911	0.0000002446	H	-2.6114278705	-0.6140234781	0.0007373734
C	1.6127775871	5.3835649542	0.0000001086	C	-5.2527577089	1.5257805563	-0.0015618715
H	3.6270153355	4.6056267372	-0.0000001015	H	-5.0927081616	3.6728521802	-0.0029716449
H	-0.4961228477	5.8223808401	0.0000003179	H	-5.0935794070	-0.6213519409	-0.0000500157
H	1.9197737469	6.4243696525	0.0000001408	H	-6.3371546491	1.5259937849	-0.0019082455
N	1.3299280594	0.3154935734	-0.0000001320	N	-0.3400749635	2.7075774338	-0.0007914847
N	-0.9626307553	0.9977376276	0.0000000743	N	-0.3404808816	0.3421059598	0.0008067785
N	-0.4146921237	-1.3226054772	-0.0000000760	N	1.7082851567	1.5244897585	0.0006631782