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Crystal Structure and Modeled Charge Carrier Mobility for Benzobis(thiadiazole) Derivatives

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1. Single Point Energy

Table S1. Single Point Energies (Hartree) for λ_e Calculated from B3LYP/6-311++G(2df,2p)

	1	**2**	**3**	**4**	**5**	**6**
E (NG)[a]	-3485.77093832	-3485.77009517	-3485.75435444	-3636.26095939	-3636.26115693	-3636.25235434
E_- (AG)[b]	-3485.88105709	-3485.87738941	-3485.85578094	-3636.36746468	-3636.36828562	-3636.35240945
E* (NEonAG)[c]	-3485.76453112	-3485.76391837	-3485.74713867	-3636.25489289	-3636.25526054	-3636.24625507
E_-* (AEonNG)[d]	-3485.88032046	-3485.87721844	-3485.85474372	-3636.36688931	-3636.36754709	-3636.35238980

[a] Neutral ground state. [b] Anion radical ground state. [c] Neutral energy based on anion radical geometry. [d] Anion radical energy based on neutral geometry.

Table S2. Single Point Energies (Hartree) for λ_h Calculated from B3LYP/6-311++G(2df,2p)

	1	**2**	**3**	**4**	**5**	**6**
E (NG)[a]	-3485.77093832	-3485.77009517	-3485.75435444	-3636.26095939	-3636.26115693	-3636.25235434
E_+ (CG)[b]	-3485.5334596	-3485.53409718	-3485.51994865	-3636.02784639	-3636.02673598	-3636.02283642
E* (NEonCG)[c]	-3485.76646118	-3485.76527093	-3485.74918319	-3636.25608171	-3636.25635416	-3636.24653362
E_+* (CEonNG)[d]	-3485.5289402	-3485.52993414	-3485.51547345	-3636.02264124	-3636.02212266	-3636.01801236

[a] Neutral ground state. [b] Cation radical ground state. [c] Neutral energy based on cation radical geometry. [d] Cation radical energy based on neutral geometry.

2. Optimized Geometry

Table S3. Optimized Geometry for Neutral Ground State (NG) of **1** (B3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	-1.16428395	3.14919948	0.90895307	S	1.16428395	-3.14919948	-0.90895307
N	0.29076379	2.69044462	0.34554606	N	-0.29076379	-2.69044462	-0.34554606
C	0.24788706	1.36020095	0.14066045	C	-0.24788706	-1.36020095	-0.14066045
C	-1.06194072	0.78025415	0.48424055	C	1.06194072	-0.78025415	-0.48424055
N	-1.92913883	1.7127876	0.92829242	N	1.92913883	-1.7127876	-0.92829242
C	1.35440729	0.6109659	-0.35413679	C	-1.35440729	-0.6109659	0.35413679
S	2.9766809	2.91905445	-0.49671213	S	-2.9766809	-2.91905445	0.49671213
C	2.6327326	1.19688064	-0.68723865	C	-2.6327326	-1.19688064	0.68723865
C	3.76620987	0.55050495	-1.18335447	C	-3.76620987	-0.55050495	1.18335447
H	3.78114491	-0.51006541	-1.38483654	H	-3.78114491	0.51006541	1.38483654
C	4.86304357	1.40474496	-1.40241816	C	-4.86304357	-1.40474496	1.40241816
H	5.80629137	1.06081809	-1.81079411	H	-5.80629137	-1.06081809	1.81079411
C	4.6092769	2.72882117	-1.08641435	C	-4.6092769	-2.72882117	1.08641435
C	5.52027636	3.87040067	-1.19640968	C	-5.52027636	-3.87040067	1.19640968
C	5.04130695	5.19078109	-1.32371486	C	-5.04130695	-5.19078109	1.32371486
H	3.97236873	5.37575006	-1.35920972	H	-3.97236873	-5.37575006	1.35920972
C	5.91817833	6.26457363	-1.43207631	C	-5.91817833	-6.26457363	1.43207631
H	5.52854216	7.27188338	-1.53683714	H	-5.52854216	-7.27188338	1.53683714
C	7.3007039	6.0454634	-1.42303473	C	-7.3007039	-6.0454634	1.42303473
C	7.79565995	4.74372488	-1.29641817	C	-7.79565995	-4.74372488	1.29641817
H	8.86573715	4.56942452	-1.28181486	H	-8.86573715	-4.56942452	1.28181486
C	6.91539471	3.67188013	-1.1807674	C	-6.91539471	-3.67188013	1.1807674
H	7.31497364	2.67109154	-1.05678099	H	-7.31497364	-2.67109154	1.05678099
C	8.23648195	7.2198443	-1.50163055	C	-8.23648195	-7.2198443	1.50163055
F	7.83625763	8.13188462	-2.42558972	F	-7.83625763	-8.13188462	2.42558972
F	8.31336437	7.88887992	-0.31707899	F	-8.31336437	-7.88887992	0.31707899
F	9.50157304	6.85516248	-1.82321422	F	-9.50157304	-6.85516248	1.82321422

Table S4. Optimized Geometry for Anion Radical Ground State (AG) of **1** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	-1.26112039	3.22557553	0.5902567	S	1.26112039	-3.22557553	-0.5902567
N	0.25345162	2.71786707	0.1529985	N	-0.25345162	-2.71786707	-0.1529985
C	0.22162293	1.38434131	0.05322339	C	-0.22162293	-1.38434131	-0.05322339
C	-1.10738592	0.81347533	0.35486678	C	1.10738592	-0.81347533	-0.35486678
N	-2.01264191	1.75036149	0.66734856	N	2.01264191	-1.75036149	-0.66734856
C	1.35883785	0.59688342	-0.30789083	C	-1.35883785	-0.59688342	0.30789083
S	2.95396347	2.91361393	-0.53885201	S	-2.95396347	-2.91361393	0.53885201
C	2.64703844	1.17286059	-0.60028647	C	-2.64703844	-1.17286059	0.60028647
C	3.82605117	0.51059568	-0.96335022	C	-3.82605117	-0.51059568	0.96335022
H	3.86201509	-0.5638566	-1.06307049	H	-3.86201509	0.5638566	1.06307049
C	4.92068276	1.36463142	-1.18063989	C	-4.92068276	-1.36463142	1.18063989
H	5.89580377	0.9923345	-1.47635318	H	-5.89580377	-0.9923345	1.47635318
C	4.63928815	2.71110193	-0.99775533	C	-4.63928815	-2.71110193	0.99775533
C	5.53416906	3.84791196	-1.14524009	C	-5.53416906	-3.84791196	1.14524009
C	5.07261301	5.18305727	-1.03898096	C	-5.07261301	-5.18305727	1.03898096
H	4.021798	5.37233094	-0.84489885	H	-4.021798	-5.37233094	0.84489885
C	5.93151355	6.26399868	-1.18712826	C	-5.93151355	-6.26399868	1.18712826
H	5.54163432	7.27395341	-1.10426642	H	-5.54163432	-7.27395341	1.10426642
C	7.2928371	6.05899467	-1.45306411	C	-7.2928371	-6.05899467	1.45306411
C	7.77508802	4.74732706	-1.55836474	C	-7.77508802	-4.74732706	1.55836474
H	8.82633593	4.5717959	-1.76116708	H	-8.82633593	-4.5717959	1.76116708
C	6.91383326	3.66777401	-1.40697219	C	-6.91383326	-3.66777401	1.40697219
H	7.31744966	2.66452904	-1.48932744	H	-7.31744966	-2.66452904	1.48932744
C	8.21084136	7.2320793	-1.57141252	C	-8.21084136	-7.2320793	1.57141252
F	7.67536214	8.24481295	-2.31190798	F	-7.67536214	-8.24481295	2.31190798
F	8.51615075	7.79266004	-0.35926485	F	-8.51615075	-7.79266004	0.35926485
F	9.4021038	6.916723	-2.14685555	F	-9.4021038	-6.916723	2.14685555

Table S5. Optimized Geometry for Cation Radical Ground State (CG) of **1** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.01649327	0.96016138	0.01963609	C	-8.62551767	1.04729885	-0.30208286
C	0.38998414	1.35879121	0.01605872	C	-9.54613098	0.04242547	0.01985113
C	1.47719688	0.40458211	0.00576914	C	-9.09971911	-1.24470185	0.33874695
C	1.01580162	-0.96241431	0.01020974	C	-7.73903174	-1.52706745	0.3354434
C	-0.39063366	-1.36106266	0.01588283	N	1.84775211	-2.00775179	0.0100272
C	-1.47790176	-0.40683199	0.01533634	S	0.94459544	-3.36849978	0.01736609
N	-1.84841831	2.00548096	0.02774957	N	-0.54178349	-2.6899867	0.02049465
S	-0.94515764	3.3662131	0.03143808	C	11.0279773	-0.3383746	-0.0085625
N	0.5412127	2.6876982	0.02243707	F	11.31509427	-1.59083294	-0.42165082
C	-2.84578363	-0.76607203	0.01105504	F	11.53549887	-0.19482965	1.24011646
C	2.84515181	0.76352017	-0.00651636	F	11.70260918	0.52092988	-0.80936322
S	4.16223231	-0.42102262	0.00500085	C	-11.02712537	0.34168487	-0.03017003
C	5.37139922	0.83425798	-0.01668318	F	-11.73684599	-0.4846636	0.76883409
C	4.77733165	2.10672573	-0.0232908	F	-11.50928665	0.19412816	-1.28968898
C	3.3914098	2.07289544	-0.02111435	F	-11.294449	1.61125252	0.35120015
S	-4.16343701	0.4177188	0.0320629	H	5.3461763	3.02724664	-0.05690267
C	-5.3721244	-0.83813268	0.01337777	H	2.76492703	2.95238836	-0.0387319
C	-4.77720585	-2.11027448	0.00067943	H	-5.34546154	-3.03115357	-0.03232174
C	-3.39146791	-2.07569598	-0.00372481	H	-2.76465861	-2.95481833	-0.02642853
C	6.79253499	0.52269221	-0.02407666	H	7.41338781	2.51265185	0.58970914
C	-6.79357795	-0.52808944	0.01212885	H	9.81440162	2.00443639	0.56983166
C	7.74073987	1.51841112	0.30791851	H	8.96964168	-2.04420772	-0.62271304
C	9.09864854	1.23263597	0.30682238	H	6.56204734	-1.54707775	-0.63636067
C	9.54343085	-0.05369674	-0.02711702	H	-6.56728392	1.55130056	-0.5737239
C	8.62287691	-1.05209028	-0.35841872	H	-8.97364946	2.0439668	-0.54982733
C	7.2619884	-0.76625839	-0.35635154	H	-9.81333173	-2.01838337	0.5986865
C	-7.26587515	0.76539914	-0.30478141	H	-7.41015437	-2.52315882	0.60875053

Table S6. Optimized Geometry for Neutral Ground State (NG) of **2** (B3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	-0.45453937	3.42745589	-0.38020202	S	0.45465629	-3.42749031	0.37916052
S	-4.07460484	1.00947314	0.10823824	S	4.07475851	-1.00944436	-0.10950972
F	-10.6829251	-0.58396945	-1.67957012	F	10.67879064	0.58456741	1.68345717
F	-10.06215198	-2.06339221	-0.2069463	F	10.06296321	2.06291609	0.20772243
F	-11.47923087	-0.4983685	0.3444164	F	11.48056916	0.496483	-0.33827222
N	0.9201313	2.55692586	-0.36205743	N	-0.91999775	-2.55692707	0.36111176
N	-1.54704446	2.24087285	-0.17050824	N	1.54715122	-2.24088008	0.16954238
C	0.58406124	1.26265163	-0.18698737	C	-0.58393338	-1.26263841	0.18614511
C	-0.87327044	1.07879393	-0.0740842	C	0.87339807	-1.07877618	0.07322574
C	-1.51239387	-0.18051912	0.11585315	C	1.51252811	0.18054222	-0.11661318
C	-2.94424012	-0.34374931	0.22380768	C	2.94438821	0.34382877	-0.22437792
C	-3.65809899	-1.52706605	0.41834744	C	3.65824666	1.52727693	-0.41814362
H	-3.16808886	-2.48335035	0.523629	H	3.16821472	2.48360534	-0.52290971
C	-5.05389569	-1.35231844	0.4746297	C	5.05405598	1.35257739	-0.47442069
H	-5.74403144	-2.16989278	0.64830382	H	5.74422925	2.17023797	-0.64754621
C	-5.45580664	-0.03581954	0.32834819	C	5.45595312	0.03599326	-0.32894472
C	-6.8216707	0.49585066	0.340407	C	6.82184226	-0.49561881	-0.34123448
C	-7.9064985	-0.33964322	0.01109839	C	7.90647564	0.33941471	-0.01022331
H	-7.72758124	-1.36806745	-0.27953186	H	7.72734846	1.36738747	0.28190538
C	-9.2119048	0.14800694	0.03746488	C	9.2119447	-0.1481254	-0.03681994
C	-9.47189021	1.48125084	0.3761146	C	9.47212692	-1.48081212	-0.37741852
H	-10.49040306	1.85329936	0.39362825	H	10.49065781	-1.85278348	-0.39513116
C	-8.40259529	2.31873539	0.69441444	C	8.40298038	-2.31787425	-0.69741628
H	-8.59000098	3.35285537	0.96631638	H	8.59056006	-3.35156033	-0.97084498
C	-7.0952321	1.83515363	0.68050932	C	7.09559157	-1.83440228	-0.68326286
H	-6.27986633	2.49698622	0.9558606	H	6.28034804	-2.4958356	-0.95993467
C	-10.35246677	-0.74872674	-0.36894229	C	10.35204904	0.7482037	0.37175334

Table S7. Optimized Geometry for Anion Radical Ground State (AG) of **2** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	0.43575327	-3.48207934	-0.16788357	S	-0.43574996	3.48215032	0.16779915
S	4.05559005	-1.03100946	0.03474958	S	-4.05560721	1.03104328	-0.03480993
F	10.36344598	1.39712826	-1.36046149	F	-10.36346662	-1.39719106	1.36050564
F	10.3671635	1.76107091	0.78261	F	-10.36709027	-1.76117424	-0.78255897
F	11.59640854	0.16546361	-0.05178983	F	-11.59640754	-0.16558104	0.05176325
N	-0.95147168	-2.57506046	-0.15125514	N	0.95147354	2.57512806	0.15119403
N	1.54509316	-2.25443698	-0.08204117	N	-1.54508817	2.2545044	0.08198435
C	-0.59572592	-1.2852141	-0.07831782	C	0.59573043	1.28528117	0.07824663
C	0.86997214	-1.10007811	-0.03722955	C	-0.86996805	1.10014528	0.03715657
C	1.50428948	0.17801263	0.04286953	C	-1.50428521	-0.1779468	-0.04293687
C	2.93693738	0.33919398	0.08613736	C	-2.93693186	-0.33914245	-0.08618753
C	3.67044477	1.52729713	0.16957825	C	-3.67042027	-1.52725821	-0.16961372
H	3.18311026	2.4895893	0.21708114	H	-3.18306925	-2.48954218	-0.21711776
C	5.06526121	1.34203761	0.19241538	C	-5.06524017	-1.3420242	-0.19241613
H	5.75929366	2.17227934	0.2721145	H	-5.75925788	-2.1722811	-0.27208429
C	5.46358078	0.01629307	0.12821848	C	-5.46358274	-0.01628672	-0.12820931
C	6.817434	-0.52378278	0.13680293	C	-6.81744506	0.52376573	-0.13674969
C	7.93911344	0.32102099	-0.00552969	C	-7.93911069	-0.32106369	0.00554141
H	7.7949518	1.38715318	-0.14110491	H	-7.79493392	-1.38720303	0.14104254
C	9.23680163	-0.19143841	0.01437013	C	-9.2368064	0.19137727	-0.01431058
C	9.47101469	-1.56305176	0.16395477	C	-9.47104268	1.56299615	-0.16380961
H	10.48174816	-1.95308444	0.1748371	H	-10.48178218	1.95301412	-0.17465732
C	8.36880495	-2.41204413	0.29776275	C	-8.36884733	2.41201263	-0.29758126
H	8.52532023	-3.48044377	0.41715875	H	-8.52537966	3.48041718	-0.41691138
C	7.07173457	-1.90802794	0.28785299	C	-7.07176923	1.90801571	-0.28771425
H	6.23756141	-2.59223286	0.40752562	H	-6.23760829	2.59224172	-0.40735154
C	10.38250901	0.7674642	-0.15068696	C	-10.38249673	-0.76755047	0.15071778

Table S8. Optimized Geometry for Cation Radical Ground State (CG) of **2** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	-0.41085683	3.46478449	-0.24320367	S	0.41086503	-3.46456438	0.24340833
S	-4.0461176	1.06595014	0.05699975	S	4.04605616	-1.06585339	-0.05694253
F	-10.20686497	-1.40002846	-1.43469707	F	10.20704082	1.39976765	1.43455955
F	-10.32825162	-1.77373475	0.70548776	F	10.32826167	1.77352415	-0.70562527
F	-11.52657345	-0.18629466	-0.19157096	F	11.52659609	0.18601362	0.19129208
N	0.9510515	2.56265543	-0.22643726	N	-0.95105031	-2.56244832	0.22648643
N	-1.51386625	2.2669419	-0.11250432	N	1.51387353	-2.26673764	0.11255167
C	0.59593071	1.27783521	-0.11778772	C	-0.59592129	-1.27762809	0.11787712
C	-0.85437083	1.10664812	-0.05037918	C	0.85437867	-1.10644173	0.05047182
C	-1.52143707	-0.16677215	0.07118382	C	1.52144631	0.16697395	-0.07110139
C	-2.92720472	-0.30553273	0.13663654	C	2.92721722	0.3056876	-0.13658995
C	-3.66842859	-1.50859983	0.26261971	C	3.66850449	1.50871115	-0.26262267
H	-3.18545087	-2.47171067	0.33661803	H	3.18558101	2.47184726	-0.3366378
C	-5.04211793	-1.32573832	0.293118	C	5.0421832	1.32577126	-0.29314724
H	-5.74319434	-2.14262154	0.40817252	H	5.74330213	2.14261253	-0.40823967
C	-5.43319516	0.01967615	0.19721686	C	5.43318945	-0.01966182	-0.19721668
C	-6.78869295	0.54892857	0.20654029	C	6.78865755	-0.54899006	-0.20654935
C	-7.88310675	-0.31487144	-0.00227494	C	7.88312496	0.31476061	0.00218932
H	-7.72141342	-1.36987439	-0.19104513	H	7.72149586	1.36978361	0.19090212
C	-9.18535502	0.17981549	0.00608998	C	9.18534555	-0.17999882	-0.00618194
C	-9.42830162	1.53951665	0.2210313	C	9.42821103	-1.53972599	-0.22105102
H	-10.44486625	1.91554779	0.22726212	H	10.44475449	-1.91581423	-0.22728701
C	-8.3493943	2.40653824	0.42767161	C	8.34925021	-2.40669889	-0.42761662
H	-8.53252043	3.46175822	0.60053019	H	8.5323131	-3.46193874	-0.60042093
C	-7.04748142	1.92279601	0.42028551	C	7.04736463	-1.92288361	-0.4202259
H	-6.22620124	2.60928536	0.60097309	H	6.22604201	-2.60933766	-0.60085446
C	-10.32162674	-0.78955898	-0.2286358	C	10.32167606	0.78932428	0.22847289

Table S9. Optimized Geometry for Neutral Ground State (NG) of **3** (B3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	0.50756674	3.28624915	-1.01641677	C	-6.98905602	-1.82515628	-1.18494609
N	-0.87624521	2.44046623	-0.89052311	H	-6.13795448	-2.29559554	-1.66633749
N	1.57750429	2.16112192	-0.53333238	C	-7.81861481	1.30610527	0.85354395
C	-0.56203317	1.20318366	-0.45369982	F	-6.77718806	1.32238716	1.71724566
C	-1.50386169	0.15839488	-0.21565091	F	-7.67252209	2.38882621	0.03632749
C	-0.88732226	-1.04068722	0.24286965	F	-8.93345014	1.54565066	1.59028036
C	0.5620601	-1.20292841	0.4530544	S	4.08145715	0.99114446	0.06068818
C	1.5038631	-0.15807159	0.21521645	C	2.92991802	-0.29939488	0.41710166
C	0.88735233	1.04094425	-0.24350242	C	3.61983991	-1.41557011	0.8881794
S	-0.50748188	-3.28613666	1.01532628	H	3.11455545	-2.32508788	1.17657737
N	0.87630636	-2.44029651	0.88962077	C	5.0180237	-1.24330978	0.95770805
N	-1.57744681	-2.1609403	0.53247774	H	5.69416141	-2.00833942	1.31658955
S	-4.08137959	-0.99109801	-0.06175119	C	5.43850768	0.00544406	0.54630953
C	-2.92996291	0.29984007	-0.41712396	C	6.79523406	0.58894698	0.53889988
C	-3.62002853	1.41645639	-0.88694433	C	7.92125757	-0.01108771	-0.0787469
H	-3.11483718	2.32627341	-1.17456521	C	9.17688861	0.60301161	-0.00601329
C	-5.01821836	1.24419704	-0.95640117	H	10.0252652	0.130081	-0.48595238
H	-5.69445024	2.00957961	-1.31435092	C	9.34345323	1.81996259	0.653772
C	-5.4385652	-0.0049943	-0.54620606	H	10.32487377	2.28131502	0.69754589
C	-6.79524771	-0.58859794	-0.53914556	C	8.23998235	2.43656473	1.24314313
C	-7.92124075	0.01075504	0.07921412	H	8.35032952	3.38659224	1.75740034
C	-9.17684643	-0.60335425	0.00603077	C	6.98904856	1.82609999	1.18354896
H	-10.02519509	-0.13093959	0.48653235	H	6.13791426	2.2970536	1.66439038
C	-9.34340524	-1.81967593	-0.6549064	C	7.81859692	-1.30717215	-0.85184417
H	-10.324799	-2.28105344	-0.69902172	F	6.77741745	-1.32405263	-1.71583357
C	-8.23995357	-2.43564292	-1.24498403	F	7.67202885	-2.38906484	-0.03363852
H	-8.35030094	-3.38518344	-1.76014072	F	8.93360191	-1.54766617	-1.58802291

Table S10. Optimized Geometry for Anion Radical Ground State (AG) of **3** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	0.45805364	3.3803571	-0.83989125	C	-6.90733343	-1.97134878	-0.88624644
N	-0.93259736	2.48790917	-0.70738787	H	-6.006553	-2.47336598	-1.22259261
N	1.55724817	2.2004195	-0.45764553	C	-8.02965927	1.3552516	0.64748079
C	-0.58622582	1.24052383	-0.36072767	F	-7.06981826	1.55303511	1.57723006
C	-1.4994771	0.15803714	-0.14865316	F	-7.90317665	2.36096289	-0.27251126
C	-0.87550739	-1.07450426	0.21483804	F	-9.21653796	1.60014352	1.27751865
C	0.58620063	-1.24022242	0.36108435	S	4.05351241	1.03661538	0.01047423
C	1.49946288	-0.15775073	0.1489329	C	2.92931689	-0.29691579	0.29621901
C	0.87548208	1.07480875	-0.21447659	C	3.65373886	-1.43566617	0.6593755
S	-0.45809128	-3.38000744	0.84040186	H	3.16167084	-2.36862611	0.89036059
N	0.93256634	-2.48757834	0.7078432	C	5.04918117	-1.24715953	0.7022085
N	-1.55727659	-2.20010592	0.45803253	H	5.73446545	-2.03224431	0.99434837
S	-4.05351114	-1.03646561	-0.01070588	C	5.45553332	0.03639853	0.38256963
C	-2.92932346	0.29716244	-0.29610772	C	6.78832819	0.64461309	0.40307258
C	-3.6537431	1.43590283	-0.65927719	C	7.99575822	0.01955836	-0.02557668
H	-3.16167787	2.36891171	-0.89007281	C	9.22453139	0.68545259	0.09060327
C	-5.04917632	1.24733146	-0.7023587	H	10.12661958	0.18325246	-0.23834415
H	-5.73447699	2.03240635	-0.99449445	C	9.30457786	1.98246745	0.59043451
C	-5.45550231	-0.03626312	-0.38284727	H	10.26700565	2.4790759	0.66656345
C	-6.78828141	-0.64457595	-0.40363216	C	8.12743646	2.6299742	0.97555759
C	-7.99575277	-0.0198191	0.02531655	H	8.15932574	3.6450267	1.36238191
C	-9.22445746	-0.68579188	-0.09111212	C	6.90752648	1.9715848	0.88512388
H	-10.12659222	-0.18384021	0.2380883	H	6.00680213	2.47385452	1.22123636
C	-9.30437254	-1.98260043	-0.59150285	C	8.02957338	-1.35580365	-0.64709821
H	-10.26675567	-2.47926605	-0.66782173	F	7.06974211	-1.55394359	-1.57678936
C	-8.12718563	-2.62982592	-0.97693543	F	7.90293788	-2.36107407	0.2733804
H	-8.15898691	-3.64471726	-1.36418829	F	9.21643651	-1.60111113	-1.27698561

Table S11. Optimized Geometry for Cation Radical Ground State (CG) of **3** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	0.47305004	3.33010357	-0.95518428	C	-6.93641066	-1.89397468	-1.07550346
N	-0.8993945	2.4537046	-0.83179003	H	-6.07821942	-2.39157849	-1.51500026
N	1.54899116	2.18929782	-0.49932695	C	-7.81660764	1.34565162	0.78706037
C	-0.56940832	1.22218227	-0.42752622	F	-6.74911319	1.41232552	1.62074007
C	-1.51199973	0.14810319	-0.20246822	F	-7.70004688	2.38728215	-0.08565194
C	-0.8710001	-1.06878722	0.23419812	F	-8.91348084	1.59104221	1.53060019
C	0.56941394	-1.22136135	0.42991536	S	4.05534459	1.04117571	0.05159521
C	1.51205311	-0.14741734	0.20444604	C	2.90996906	-0.26933523	0.38557103
C	0.87100037	1.06962193	-0.23177139	C	3.62419686	-1.41274398	0.82572664
S	-0.47313334	-3.32900231	0.95840757	H	3.12343195	-2.32887334	1.101811
N	0.8993599	-2.45271007	0.8347192	C	5.00065157	-1.23719686	0.87813612
N	-1.54903733	-2.18834683	0.5021017	H	5.69101	-2.00281535	1.20467388
S	-4.05509565	-1.04090998	-0.05034356	C	5.41109603	0.04519336	0.49473236
C	-2.90983608	0.26968246	-0.38443012	C	6.76255694	0.62360718	0.48691864
C	-3.62407259	1.41263002	-0.82577001	C	7.90180555	-0.01554788	-0.07039585
H	-3.12337257	2.32872146	-1.10209263	C	9.1515389	0.60168713	0.0022512
C	-5.00044418	1.23667998	-0.87898178	H	10.01056276	0.11067232	-0.43905471
H	-5.69080161	2.00189741	-1.20646331	C	9.30342531	1.84840028	0.61393359
C	-5.4108017	-0.04558119	-0.49504324	H	10.2851541	2.3078418	0.66211071
C	-6.76213778	-0.62431704	-0.48777346	C	8.19067103	2.4970966	1.14629735
C	-7.90188863	0.01491464	0.06842323	H	8.29365156	3.46750512	1.62104295
C	-9.15142418	-0.60266205	-0.00467502	C	6.93752437	1.89288495	1.07527351
H	-10.01085555	-0.1115933	0.43577264	H	6.07974763	2.39044303	1.5156192
C	-9.30261827	-1.84977614	-0.61571788	C	7.81578858	-1.34582177	-0.78980035
H	-10.28421285	-2.30946496	-0.66426402	F	6.74762843	-1.41187145	-1.62267879
C	-8.18937401	-2.49851954	-1.14699291	F	7.6998106	-2.38797718	0.08238213
H	-8.29181236	-3.46923045	-1.62123594	F	8.91204916	-1.59088745	-1.53435253

Table S12. Optimized Geometry for Neutral Ground State (NG) of **4** (B3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	0.99449004	-3.17611889	1.0113867	S	-0.99449004	3.17611889	-1.0113867
N	1.76670001	-1.75048241	1.15370706	N	-1.76670001	1.75048241	-1.15370706
C	0.97806439	-0.80067585	0.61079007	C	-0.97806439	0.80067585	-0.61079007
C	-0.28063742	-1.35844669	0.08613586	C	0.28063742	1.35844669	-0.08613586
N	-0.36632076	-2.69050894	0.26430817	N	0.36632076	2.69050894	-0.26430817
C	1.30178606	0.58800961	0.54196222	C	-1.30178606	-0.58800961	-0.54196222
S	2.91536776	2.87298899	0.94008498	S	-2.91536776	-2.87298899	-0.94008498
C	2.53049454	1.15191056	1.05246482	C	-2.53049454	-1.15191056	-1.05246482
C	3.58101895	0.48404436	1.68345075	C	-3.58101895	-0.48404436	-1.68345075
H	3.55828837	-0.57982224	1.86609145	H	-3.55828837	0.57982224	-1.86609145
C	4.64714132	1.32138463	2.06387177	C	-4.64714132	-1.32138463	-2.06387177
H	5.52339305	0.95947054	2.5894391	H	-5.52339305	-0.95947054	-2.5894391
C	4.45078733	2.65327827	1.74185816	C	-4.45078733	-2.65327827	-1.74185816
C	5.34854384	3.78366041	1.99593755	C	-5.34854384	-3.78366041	-1.99593755
C	4.86230415	5.1009391	2.11678191	C	-4.86230415	-5.1009391	-2.11678191
H	3.79665041	5.29173476	2.03943128	H	-3.79665041	-5.29173476	-2.03943128
C	5.72297585	6.16790835	2.36535798	C	-5.72297585	-6.16790835	-2.36535798
H	5.34457925	7.17863335	2.46972636	H	-5.34457925	-7.17863335	-2.46972636
C	7.08644903	5.92007914	2.49409087	C	-7.08644903	-5.92007914	-2.49409087
C	7.60365301	4.63141849	2.39089917	C	-7.60365301	-4.63141849	-2.39089917
H	8.6701806	4.46754479	2.49865148	H	-8.6701806	-4.46754479	-2.49865148
C	6.73585482	3.5730532	2.13440524	C	-6.73585482	-3.5730532	-2.13440524
H	7.14169064	2.57340334	2.02173149	H	-7.14169064	-2.57340334	-2.02173149
O	7.95392697	6.98133474	2.82543681	O	-7.95392697	-6.98133474	-2.82543681
F	7.58158949	8.30892933	1.04089107	F	-7.58158949	-8.30892933	-1.04089107
F	9.29168621	8.63095417	2.35660125	F	-9.29168621	-8.63095417	-2.35660125
F	9.259899	6.93122351	0.98854265	F	-9.259899	-6.93122351	-0.98854265
C	8.50534162	7.69248822	1.81637169	C	-8.50534162	-7.69248822	-1.81637169

Table S13. Optimized Geometry for Anion Radical Ground State (AG) of **4** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	1.15473494	-3.23886634	0.72061384	S	-1.15473494	3.23886634	-0.72061384
N	1.89729362	-1.76907119	0.91126151	N	-1.89729362	1.76907119	-0.91126151
C	1.04582734	-0.82340299	0.49106322	C	-1.04582734	0.82340299	-0.49106322
C	-0.23467545	-1.38309935	0.00970194	C	0.23467545	1.38309935	-0.00970194
N	-0.28653576	-2.71762929	0.09156892	N	0.28653576	2.71762929	-0.09156892
C	1.30809752	0.58496905	0.49319335	C	-1.30809752	-0.58496905	-0.49319335
S	2.87094554	2.89001837	0.95968685	S	-2.87094554	-2.89001837	-0.95968685
C	2.54819117	1.14992242	0.96645989	C	-2.54819117	-1.14992242	-0.96645989
C	3.6599293	0.47973758	1.48687973	C	-3.6599293	-0.47973758	-1.48687973
H	3.67610044	-0.59533592	1.58565462	H	-3.67610044	0.59533592	-1.58565462
C	4.71834166	1.32759826	1.8639898	C	-4.71834166	-1.32759826	-1.8639898
H	5.6373908	0.94925494	2.29947422	H	-5.6373908	-0.94925494	-2.29947422
C	4.47127543	2.67464043	1.65294981	C	-4.47127543	-2.67464043	-1.65294981
C	5.34108768	3.80959886	1.93827431	C	-5.34108768	-3.80959886	-1.93827431
C	4.87209502	5.14285179	1.88066031	C	-4.87209502	-5.14285179	-1.88066031
H	3.83513277	5.33555677	1.6253502	H	-3.83513277	-5.33555677	-1.6253502
C	5.70480369	6.22418185	2.15944821	C	-5.70480369	-6.22418185	-2.15944821
H	5.32866842	7.24097228	2.11825797	H	-5.32866842	-7.24097228	-2.11825797
C	7.03169167	5.98830755	2.50321656	C	-7.03169167	-5.98830755	-2.50321656
C	7.53559187	4.69258934	2.58373816	C	-7.53559187	-4.69258934	-2.58373816
H	8.57173267	4.53057493	2.86157117	H	-8.57173267	-4.53057493	-2.86157117
C	6.69748306	3.61969251	2.29431883	C	-6.69748306	-3.61969251	-2.29431883
H	7.10401369	2.61520877	2.33946052	H	-7.10401369	-2.61520877	-2.33946052
O	7.85882688	7.08361709	2.87076378	O	-7.85882688	-7.08361709	-2.87076378
F	7.87694559	8.163044	0.88902954	F	-7.87694559	-8.163044	-0.88902954
F	9.28330827	8.6803336	2.47550074	F	-9.28330827	-8.6803336	-2.47550074
F	9.51649271	6.81845923	1.36222498	F	-9.51649271	-6.81845923	-1.36222498
C	8.6067959	7.66091618	1.91564022	C	-8.6067959	-7.66091618	-1.91564022

Table S14. Optimized Geometry for Cation Radical Ground State (CG) of **4** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
C	0.38853151	1.40904347	-0.04057607	C	9.52191249	0.0976033	0.55534949
C	-1.01267687	0.99645707	-0.10425134	C	9.10349368	1.37042822	0.16289925
C	-1.46260979	-0.37387159	-0.07247485	C	7.74289595	1.63548971	0.07398685
C	-0.3696846	-1.31657203	0.02407998	N	-0.5099203	-2.64612058	0.06385469
C	1.03138134	-0.90388903	0.0898137	S	0.97961954	-3.30924204	0.17340346
C	1.48097385	0.46670246	0.06460565	N	1.87047764	-1.94002173	0.17576782
N	0.52929063	2.73825985	-0.0887803	O	-10.86379693	0.26551332	-0.71227125
S	-0.95994856	3.40123335	-0.20265651	C	-11.66681754	0.24122634	0.39004993
N	-1.85140461	2.03235735	-0.19641488	F	-12.90761409	0.50764003	-0.00736597
C	2.84317851	0.8394364	0.13473421	F	-11.65054449	-0.96181242	1.00342463
C	-2.82542053	-0.74621549	-0.13089641	F	-11.29599737	1.15832389	1.31068168
S	-4.1489093	0.42263555	-0.27407672	O	10.88215547	-0.16423924	0.72138155
C	-5.34878441	-0.84353472	-0.27641863	C	11.61197302	-0.52227494	-0.37378949
C	-4.74405768	-2.10805958	-0.1781601	F	12.85972022	-0.7478691	0.02732459
C	-3.36158483	-2.05934921	-0.09574106	F	11.12994134	-1.63935552	-0.96016321
S	4.16841763	-0.33084212	0.24929588	F	11.62499285	0.4444455	-1.31793707
C	5.36605733	0.93657767	0.28094387	H	-5.30445666	-3.0336237	-0.14308266
C	4.76120989	2.2017792	0.19577419	H	-2.73023105	-2.93059872	-0.00299648
C	3.37826313	2.15340094	0.11892862	H	5.31920049	3.12927986	0.21761258
C	-6.76833206	-0.54875683	-0.37065978	H	2.74485582	3.02621033	0.06129823
C	6.78513683	0.64100315	0.38128408	H	-6.58405895	1.5735556	0.05813149
C	-7.26417332	0.76161178	-0.17877996	H	-9.00494209	2.03744857	-0.12134913
C	-8.6228195	1.03396522	-0.26894374	H	-9.76238397	-2.09835576	-0.99206616
C	-9.50617947	-0.01055503	-0.54799628	H	-7.34491036	-2.58995162	-0.84367496
C	-9.05238982	-1.31369219	-0.75672162	H	6.53846308	-1.41081362	1.05231013
C	-7.69222447	-1.57891718	-0.66472703	H	8.96412348	-1.87628592	1.19734002
C	7.2467065	-0.63280282	0.78578233	H	9.83790444	2.13210008	-0.07186984
C	8.60531114	-0.90482881	0.87674861	H	7.42348668	2.6181781	-0.25373306

Table S15. Optimized Geometry for Neutral Ground State (NG) of **5** (B3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	0.48102093	-3.37956933	-0.67013663	S	-0.48103983	3.37871572	0.67000458
S	4.06136009	-1.03443062	0.26291237	S	-4.06114836	1.0339932	-0.26293702
F	11.43231248	-0.32408197	-1.16736684	F	-11.4321949	0.32517937	1.16752253
F	9.99905971	1.21829172	-1.70106432	F	-9.99926831	-1.21752019	1.70115241
F	11.81524974	1.75031677	-0.61419463	F	-11.81560678	-1.74912449	0.61432319
O	10.26057937	0.68793301	0.47371604	O	-10.26073146	-0.68706296	-0.47361067
N	1.5581448	-2.22102038	-0.29139209	N	-1.55818184	2.2201821	0.29126065
N	-0.89418497	-2.5098241	-0.64697451	N	0.89417022	2.50897644	0.64684478
C	0.87798246	-1.07071058	-0.12487485	C	-0.87801524	1.06987603	0.12474996
C	-0.57067217	-1.23859342	-0.33394999	C	0.57063257	1.23775531	0.33382343
C	1.50354005	0.16370436	0.21503146	C	-1.50358009	-0.16452466	-0.21515498
C	2.92691176	0.31142954	0.41650492	C	-2.92697385	-0.3120836	-0.41660175
C	3.6287695	1.47280939	0.74303144	C	-3.62907403	-1.47332062	-0.74312672
H	3.13397206	2.42076483	0.89221361	H	-3.13448114	-2.42137434	-0.89234713
C	5.01846472	1.28667903	0.86854411	C	-5.01873693	-1.28690192	-0.86859291
H	5.698018	2.08505735	1.14384537	H	-5.69846172	-2.08513511	-1.14389145
C	5.42732135	-0.01708824	0.64653174	C	-5.42732638	0.0169431	-0.64654497
C	6.78891764	-0.55631491	0.70241174	C	-6.78881228	0.5564544	-0.70237869
C	7.89304772	0.29919634	0.51773659	C	-7.89311704	-0.29882876	-0.51769156
H	7.7565148	1.35260461	0.30365565	H	-7.75679955	-1.35227017	-0.30363653
C	9.18027942	-0.21418785	0.58689823	C	-9.18024232	0.21482938	-0.58680511
C	9.43533539	-1.56031035	0.83684614	C	-9.43502127	1.56101161	-0.83671373
H	10.45538148	-1.92182266	0.89383034	H	-10.45499269	1.92274065	-0.89365887
C	8.34174801	-2.41258682	1.00852097	C	-8.34125942	2.41306134	-1.00840021
H	8.50996075	-3.46652739	1.20683939	H	-8.50925536	3.46704223	-1.20668831
C	7.03861654	-1.92208909	0.94521922	C	-7.03823003	1.92228656	-0.94514777
H	6.20668085	-2.59954682	1.10920863	H	-6.20615585	2.59957266	-1.1091436
C	10.85716745	0.82296221	-0.73161231	C	-10.8573161	-0.82198429	0.73173136

Table S16. Optimized Geometry for Anion Radical Ground State (AG) of **5** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	0.33480328	-3.49661229	-0.06501152	S	-0.33480323	3.49669381	0.06497111
S	4.02383943	-1.146477	0.08775845	S	-4.02386451	1.14651532	-0.08781271
F	11.61744133	0.06656172	-0.97316589	F	-11.61740228	-0.06660937	0.97328643
F	10.26308222	1.76433619	-0.93498488	F	-10.2630229	-1.76436914	0.93515496
F	11.95850146	1.69549223	0.43738374	F	-11.95848442	-1.69562022	-0.43716489
O	10.28903816	0.35762002	0.82880297	O	-10.28904959	-0.35774904	-0.82870799
N	1.47905233	-2.29986647	-0.00658555	N	-1.4790499	2.29994656	0.00654581
N	-1.02522319	-2.54963009	-0.08402503	N	1.02522346	2.5497113	0.08398535
C	0.83777381	-1.12549939	-0.0004601	C	-0.83777203	1.12557888	0.00042022
C	-0.63245893	-1.26901326	-0.04530573	C	0.63246143	1.26909327	0.04526572
C	1.50875119	0.13555859	0.04399938	C	-1.50874883	-0.13548041	-0.04403961
C	2.94546879	0.25656874	0.08249258	C	-2.94546467	-0.2565081	-0.08253446
C	3.71282214	1.42557274	0.12228212	C	-3.71279359	-1.42552808	-0.12231971
H	3.25343651	2.40264875	0.12103037	H	-3.25338665	-2.40259432	-0.12106461
C	5.10160177	1.20110456	0.15451152	C	-5.10157755	-1.20109002	-0.15455158
H	5.82140065	2.01304805	0.16799492	H	-5.82135758	-2.01305013	-0.16803523
C	5.46125622	-0.1371315	0.14047329	C	-5.46126066	0.1371387	-0.14051989
C	6.79945938	-0.71292057	0.16094538	C	-6.79947547	0.71290001	-0.16099623
C	7.9278644	0.08989116	0.44960435	C	-7.92787255	-0.08995142	-0.4495779
H	7.81883849	1.14181889	0.6846155	H	-7.81883426	-1.14189354	-0.68451862
C	9.19440887	-0.47086155	0.45519815	C	-9.19442729	0.4707772	-0.45518115
C	9.42869665	-1.82182548	0.21102472	C	-9.42873602	1.82175191	-0.21108701
H	10.43499387	-2.22247227	0.24388355	H	-10.43504176	2.22237686	-0.24394924
C	8.31653001	-2.62222388	-0.06886534	C	-8.31657859	2.62218846	0.06872986
H	8.45644633	-3.68080782	-0.26868374	H	-8.4565102	3.68078233	0.26848498
C	7.03222112	-2.08421898	-0.09771507	C	-7.03225869	2.08421002	0.09758415
H	6.1929015	-2.73209342	-0.32889779	H	-6.19294711	2.73211675	0.32870542
C	11.00165359	0.94914759	-0.1436607	C	-11.00162866	-0.94923209	0.14380973

Table S17. Optimized Geometry for Cation Radical Ground State (CG) of **5** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.59611728	1.25018709	-0.28833443	C	7.86702167	-0.20799519	0.53303275
C	0.84783254	1.10754659	-0.10884534	C	-6.99025646	-2.05277761	-0.68169756
C	1.51467983	-0.13709682	0.18677488	C	-8.2871947	-2.55315356	-0.72722098
C	0.59618658	-1.25009203	0.28809311	C	-9.384173	-1.68777234	-0.67359002
C	-0.84776304	-1.10745154	0.10860345	C	-9.1501033	-0.31636136	-0.56867018
C	-1.51461285	0.1371933	-0.18699769	C	-7.86696409	0.20815057	-0.53288399
N	-0.95255369	2.51167339	-0.5533524	O	10.23731145	-0.56635513	0.58418603
S	0.40076257	3.42658564	-0.57474447	C	10.78889369	-0.9211192	-0.60946788
N	1.50141497	2.264525	-0.2479228	F	11.79936569	-1.75002861	-0.35916979
N	0.95262275	-2.51158059	0.55309469	F	9.90026846	-1.54965903	-1.41427859
S	-0.40069079	-3.4264972	0.57446376	F	11.25514611	0.14371371	-1.29638376
N	-1.50134423	-2.26443228	0.24766394	O	-10.23721329	0.56659317	-0.5837894
C	-2.91411759	0.24875052	-0.35654798	C	-10.78905806	0.92073834	0.60992882
C	2.91418003	-0.24864214	0.35636466	F	-11.79927155	1.75003158	0.35985629
S	4.02511571	1.12400234	0.21132607	F	-9.90051664	1.54856562	1.4153781
C	5.40826726	0.11684881	0.54470494	F	-11.25576101	-0.14441583	1.29604823
C	5.02227343	-1.2180219	0.74856884	H	5.72158692	-2.00920649	0.98726338
C	3.65503407	-1.422635	0.64940571	H	3.17589428	-2.38052142	0.78797642
S	-4.02506601	-1.12388208	-0.21147205	H	-5.72153358	2.00934782	-0.98733639
C	-5.40821477	-0.1167107	-0.54480298	H	-3.17582165	2.38063673	-0.78813088
C	-5.02221651	1.21815872	-0.74866449	H	6.15455631	2.7423888	0.74503636
C	-3.65496928	1.4227559	-0.6495474	H	8.45064872	3.62234911	0.81300853
C	6.75598821	0.66252323	0.58580206	H	10.40184657	2.05962086	0.71423056
C	-6.75594371	-0.66237014	-0.58586264	H	7.7451867	-1.28042495	0.44564665
C	6.9902816	2.05294508	0.68148241	H	-6.15454112	-2.7422186	-0.74541508
C	8.28721031	2.55334076	0.72704585	H	-8.45065078	-3.62214893	-0.81331259
C	9.38419909	1.68796191	0.67360712	H	-10.40182355	-2.05942291	-0.71419162
C	9.15015256	0.31653568	0.56885081	H	-7.74511357	1.28056829	-0.44535081

Table S18. Optimized Geometry for Neutral Ground State (NG) of **6** (B3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	0.61471868	-1.7570601	2.93744037	S	-0.61471868	1.7570601	-2.93744037
N	0.23916256	-0.19163748	2.71045088	N	-0.23916256	0.19163748	-2.71045088
C	0.09948995	0.00619251	1.3857435	C	-0.09948995	-0.00619251	-1.3857435
C	0.32342754	-1.22397657	0.60634157	C	-0.32342754	1.22397657	-0.60634157
N	0.62186823	-2.2767691	1.39518426	N	-0.62186823	2.2767691	-1.39518426
C	-0.22734104	1.27092662	0.81692466	C	0.22734104	-1.27092662	-0.81692466
S	-0.30181566	2.50243492	3.35769935	S	0.30181566	-2.50243492	-3.35769935
C	-0.43781417	2.47015054	1.59805967	C	0.43781417	-2.47015054	-1.59805967
C	-0.74727836	3.74786135	1.12965943	C	0.74727836	-3.74786135	-1.12965943
H	-0.8583052	3.96684885	0.07839851	H	0.8583052	-3.96684885	-0.07839851
C	-0.88436432	4.70836261	2.14765258	C	0.88436432	-4.70836261	-2.14765258
H	-1.10347746	5.75114285	1.94950532	H	1.10347746	-5.75114285	-1.94950532
C	-0.67968681	4.20635659	3.42346561	C	0.67968681	-4.20635659	-3.42346561
C	-0.83043951	4.96191567	4.67352065	C	0.83043951	-4.96191567	-4.67352065
C	-0.12938032	4.69084448	5.86421792	C	0.12938032	-4.69084448	-5.86421792
C	-0.31362511	5.4280486	7.03011663	C	0.31362511	-5.4280486	-7.03011663
H	0.24110297	5.15558808	7.92033252	H	-0.24110297	-5.15558808	-7.92033252
C	-1.20346872	6.50205706	7.03368043	C	1.20346872	-6.50205706	-7.03368043
H	-1.34931551	7.08045282	7.94028928	H	1.34931551	-7.08045282	-7.94028928
C	-1.91214858	6.80997932	5.86918054	C	1.91214858	-6.80997932	-5.86918054
H	-2.62020642	7.63296657	5.86150424	H	2.62020642	-7.63296657	-5.86150424
C	-1.73424462	6.04659917	4.71922092	C	1.73424462	-6.04659917	-4.71922092
H	-2.32184378	6.2693239	3.83536911	H	2.32184378	-6.2693239	-3.83536911
O	0.73410756	3.57675783	5.90027595	O	-0.73410756	-3.57675783	-5.90027595
C	2.07111088	3.78998497	5.87954532	C	-2.07111088	-3.78998497	-5.87954532
F	2.46600099	4.56077539	4.84381549	F	-2.46600099	-4.56077539	-4.84381549
F	2.67462967	2.60012084	5.78387357	F	-2.67462967	-2.60012084	-5.78387357
F	2.52317236	4.39547271	7.00754447	F	-2.52317236	-4.39547271	-7.00754447

Table S19. Optimized Geometry for Anion Radical Ground State (AG) of **6** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	0.75491128	-1.7400896	2.95679293	S	-0.75491128	1.7400896	-2.95679293
N	0.33128481	-0.15813228	2.70888281	N	-0.33128481	0.15813228	-2.70888281
C	0.14858144	0.01169291	1.39451157	C	-0.14858144	-0.01169291	-1.39451157
C	0.37205591	-1.22377706	0.61402145	C	-0.37205591	1.22377706	-0.61402145
N	0.71599024	-2.26507146	1.38462505	N	-0.71599024	2.26507146	-1.38462505
C	-0.22343653	1.26134038	0.8103039	C	0.22343653	-1.26134038	-0.8103039
S	-0.23795945	2.50377011	3.34798144	S	0.23795945	-2.50377011	-3.34798144
C	-0.43281418	2.45819113	1.59066081	C	0.43281418	-2.45819113	-1.59066081
C	-0.79344845	3.72901054	1.13063532	C	0.79344845	-3.72901054	-1.13063532
H	-0.941876	3.93119318	0.08053721	H	0.941876	-3.93119318	-0.08053721
C	-0.92664	4.68816746	2.14927864	C	0.92664	-4.68816746	-2.14927864
H	-1.18458363	5.72260453	1.94699235	H	1.18458363	-5.72260453	-1.94699235
C	-0.6661021	4.20819797	3.42500615	C	0.6661021	-4.20819797	-3.42500615
C	-0.81115766	4.96743319	4.66416255	C	0.81115766	-4.96743319	-4.66416255
C	-0.13966453	4.69445412	5.87531154	C	0.13966453	-4.69445412	-5.87531154
C	-0.33407822	5.43287019	7.03932426	C	0.33407822	-5.43287019	-7.03932426
H	0.19926946	5.14422508	7.9379012	H	-0.19926946	-5.14422508	-7.9379012
C	-1.1980597	6.52776438	7.03294461	C	1.1980597	-6.52776438	-7.03294461
H	-1.3506424	7.10770656	7.93783283	H	1.3506424	-7.10770656	-7.93783283
C	-1.87230762	6.84813882	5.84926199	C	1.87230762	-6.84813882	-5.84926199
H	-2.56296901	7.68666309	5.8238209	H	2.56296901	-7.68666309	-5.8238209
C	-1.69122336	6.0787596	4.70547422	C	1.69122336	-6.0787596	-4.70547422
H	-2.26104751	6.31351824	3.81326915	H	2.26104751	-6.31351824	-3.81326915
O	0.7138667	3.56794798	5.94029842	O	-0.7138667	-3.56794798	-5.94029842
C	2.0460327	3.76759085	5.94604888	C	-2.0460327	-3.76759085	-5.94604888
F	2.48005886	4.54920163	4.93448222	F	-2.48005886	-4.54920163	-4.93448222
F	2.6497285	2.57646218	5.8585726	F	-2.6497285	-2.57646218	-5.8585726
F	2.48584486	4.36007024	7.09718683	F	-2.48584486	-4.36007024	-7.09718683

Table S20. Optimized Geometry for Cation Radical Ground State (CG) of **6** (UB3LYP/6-31+G(d,p))

Atom	X	Y	Z	Atom	X	Y	Z
S	1.12367427	-1.59498032	2.9020292	S	-1.12367427	1.59498032	-2.9020292
N	0.55177603	-0.08353155	2.66985656	N	-0.55177603	0.08353155	-2.66985656
C	0.25317993	0.04846246	1.37450866	C	-0.25317993	-0.04846246	-1.37450866
C	0.52323806	-1.16620102	0.60668954	C	-0.52323806	1.16620102	-0.60668954
N	1.01583581	-2.14926019	1.36844445	N	-1.01583581	2.14926019	-1.36844445
C	-0.27502386	1.26902188	0.81463539	C	0.27502386	-1.26902188	-0.81463539
S	-0.20693929	2.53698785	3.31987183	S	0.20693929	-2.53698785	-3.31987183
C	-0.51775655	2.4347825	1.57928461	C	0.51775655	-2.4347825	-1.57928461
C	-1.01463814	3.67832768	1.11268325	C	1.01463814	-3.67832768	-1.11268325
H	-1.25597542	3.84846691	0.07403241	H	1.25597542	-3.84846691	-0.07403241
C	-1.14447571	4.63595775	2.10395754	C	1.14447571	-4.63595775	-2.10395754
H	-1.48926977	5.64195495	1.90416657	H	1.48926977	-5.64195495	-1.90416657
C	-0.75565621	4.19175551	3.38207978	C	0.75565621	-4.19175551	-3.38207978
C	-0.83299909	4.98059071	4.60551516	C	0.83299909	-4.98059071	-4.60551516
C	-0.16341886	4.65223845	5.807945	C	0.16341886	-4.65223845	-5.807945
C	-0.27800796	5.42506726	6.95679261	C	0.27800796	-5.42506726	-6.95679261
H	0.23686177	5.1205002	7.8595672	H	-0.23686177	-5.1205002	-7.8595672
C	-1.06067997	6.5809513	6.93272754	C	1.06067997	-6.5809513	-6.93272754
H	-1.15111257	7.18563733	7.82910935	H	1.15111257	-7.18563733	-7.82910935
C	-1.73717195	6.94205106	5.76332858	C	1.73717195	-6.94205106	-5.76332858
H	-2.36020106	7.82994968	5.74382178	H	2.36020106	-7.82994968	-5.74382178
C	-1.62800635	6.15319844	4.62609305	C	1.62800635	-6.15319844	-4.62609305
H	-2.18667457	6.4313403	3.74062418	H	2.18667457	-6.4313403	-3.74062418
O	0.57211613	3.46047328	5.83951497	O	-0.57211613	-3.46047328	-5.83951497
C	1.9271031	3.51397288	6.00283225	C	-1.9271031	-3.51397288	-6.00283225
F	2.51330647	4.33546646	5.10927604	F	-2.51330647	-4.33546646	-5.10927604
F	2.39712291	2.27693485	5.82879051	F	-2.39712291	-2.27693485	-5.82879051
F	2.28585463	3.93637234	7.23176232	F	-2.28585463	-3.93637234	-7.23176232

3. XRD data

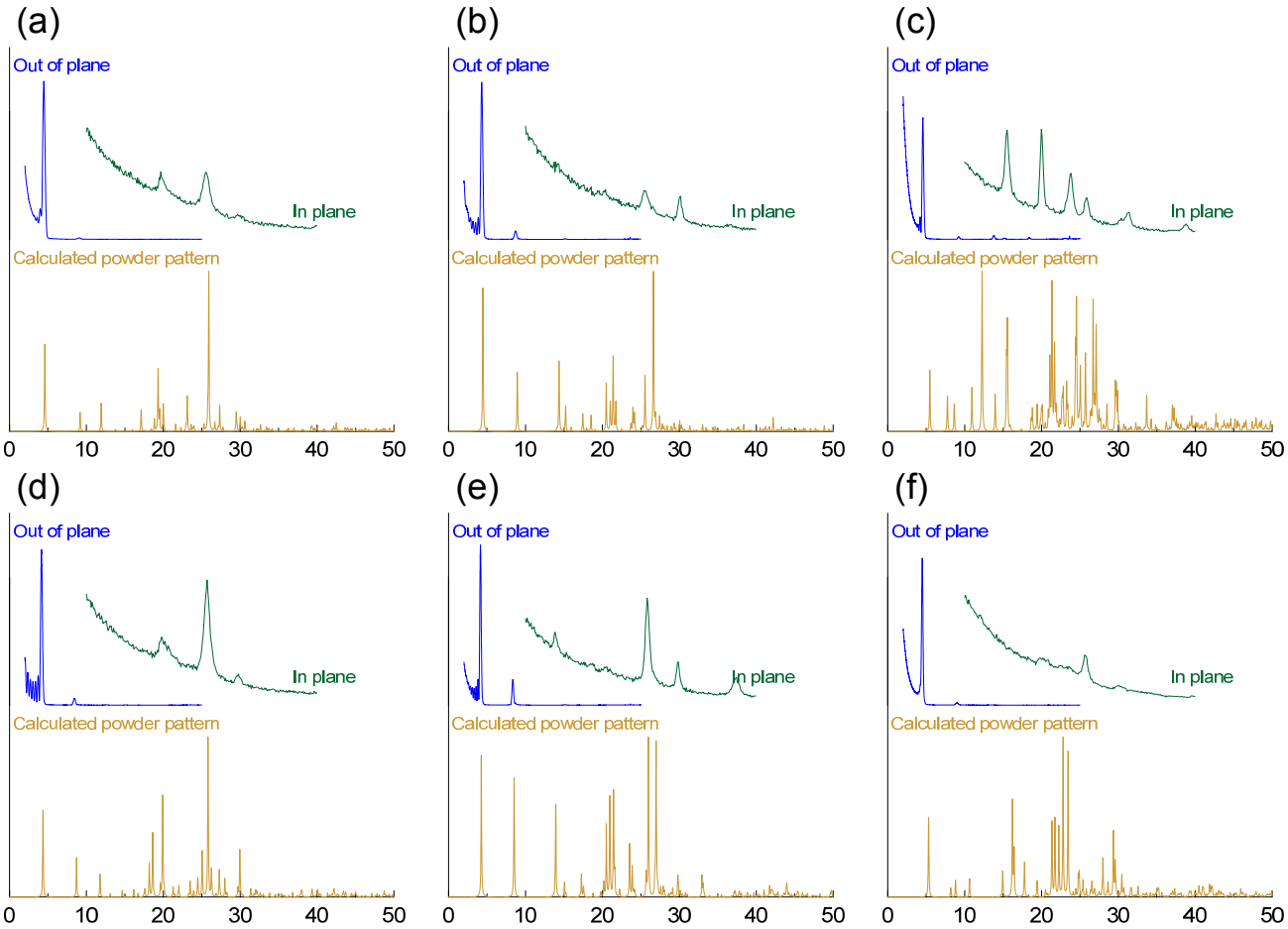

Figure S1. Out-of-plane and in-plane X-ray diffraction of thin-films and simulated pattern from the single crystal XRD data for compounds **1**–**6**.[1]

1 M. Mamada, H. Shima, Y. Yoneda, T. Shimano, N. Yamada, K. Kakita, T. Machida, Y. Tanaka, S. Aotsuka, D. Kumaki and S. Tokito, *Chem. Mater.*, 2015, **27**, 141.