Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Electron transfer in complexes of B^{II} cations with organic π-acceptors: A combined experimental and quantum-chemical study

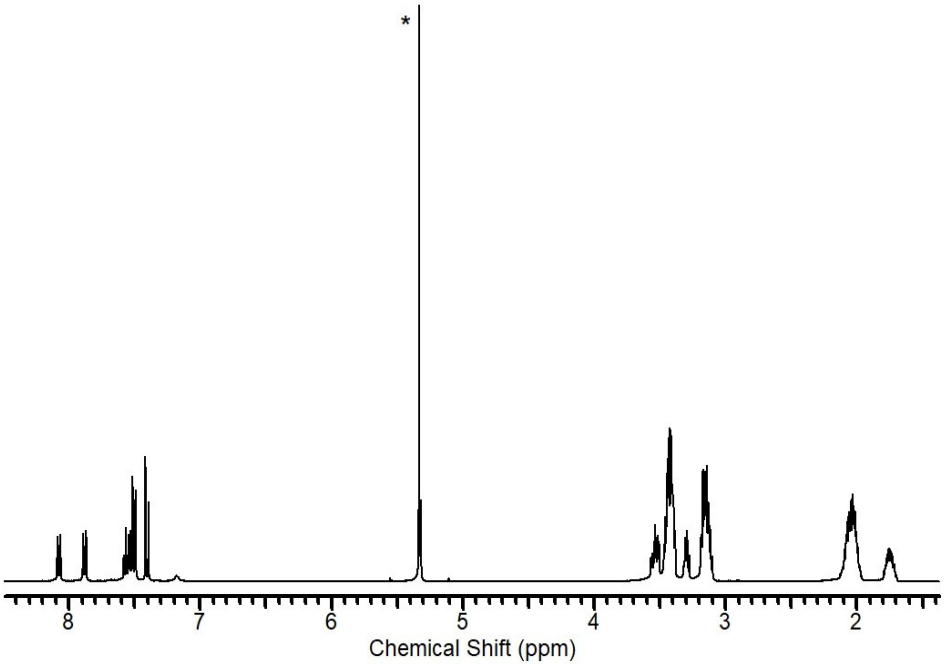
Daniel Vogler, Nina Wolf, Elisabeth Kaifer, Hans-Jörg Himmel

Content

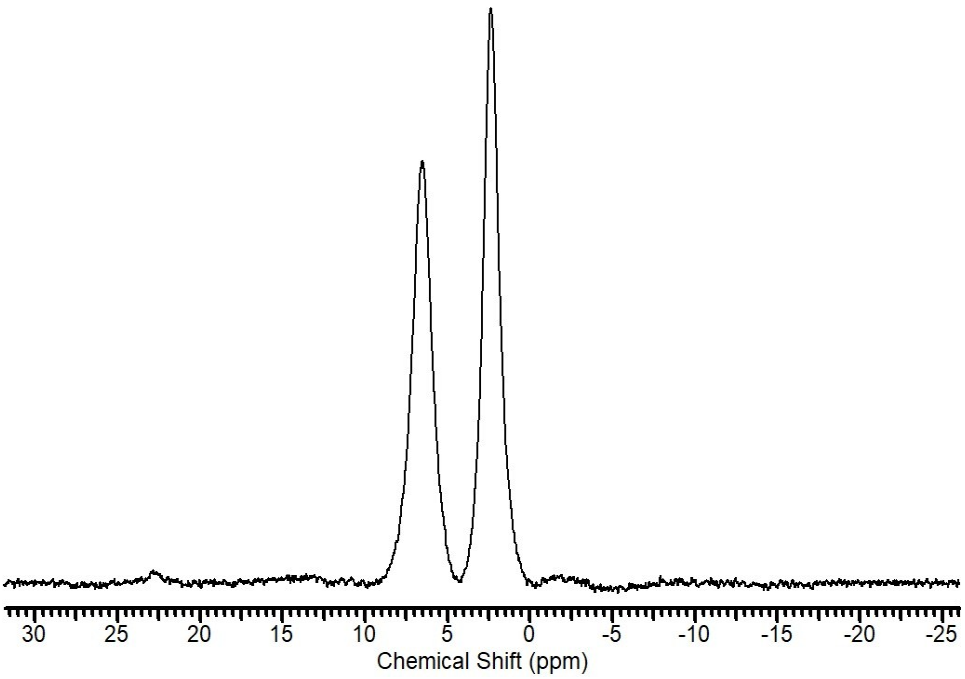
1 Analytical data

1a) Analytical data for compound **4**(OTf)

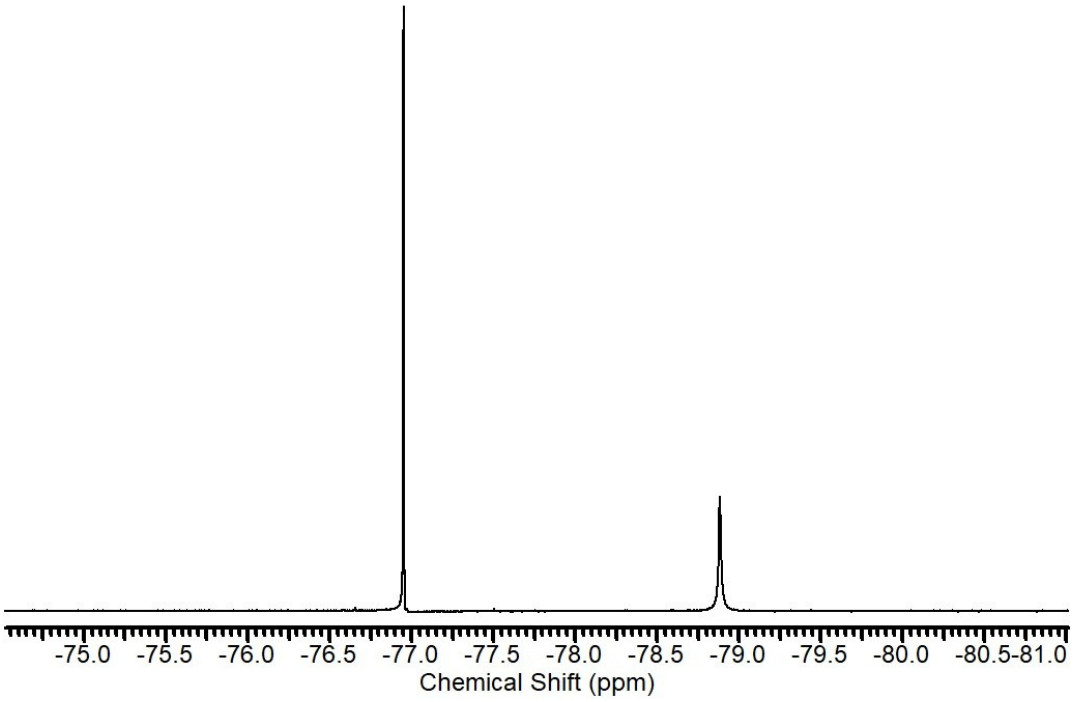
^{1}H NMR spectrum (400 MHz, CH_2Cl_2) for **4**(OTf). The asterisk denotes a solvent signal.



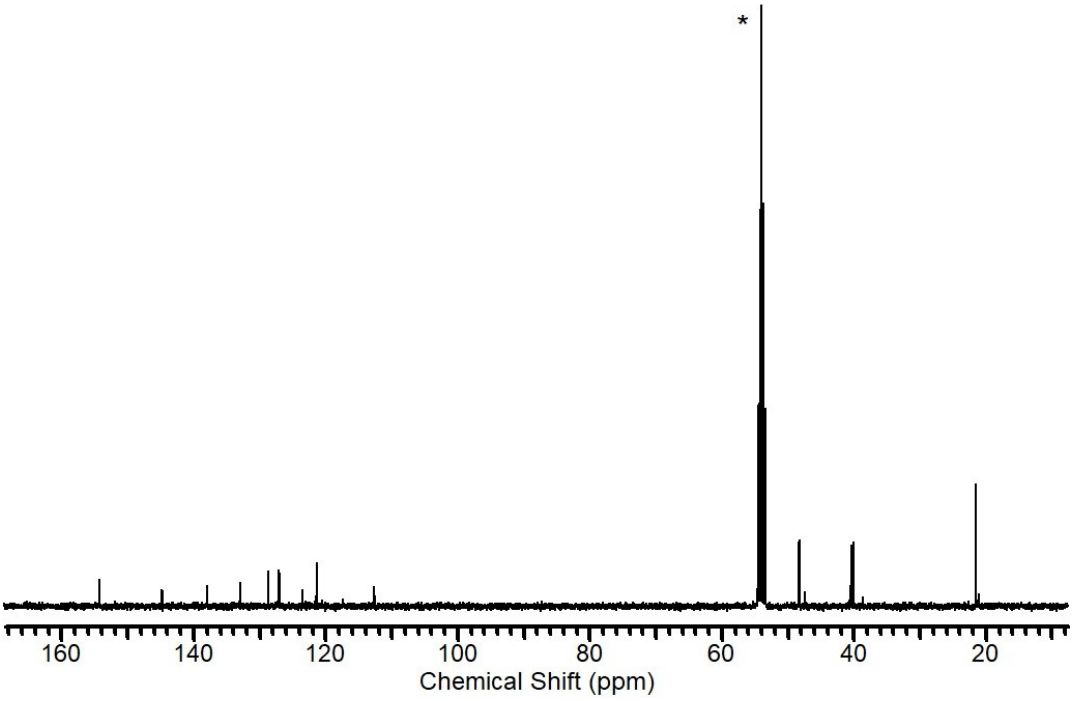
^{11}B NMR spectrum (128 MHz, CD_2Cl_2) for **4**(OTf).



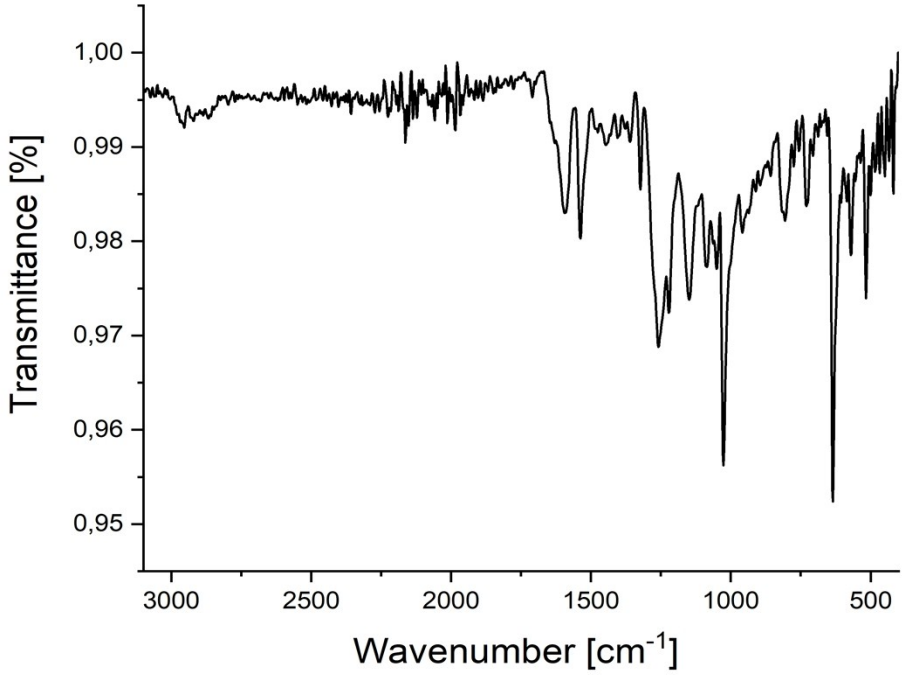
^{19}F NMR spectrum (376 MHz, CD_2Cl_2) for **4**(OTf).



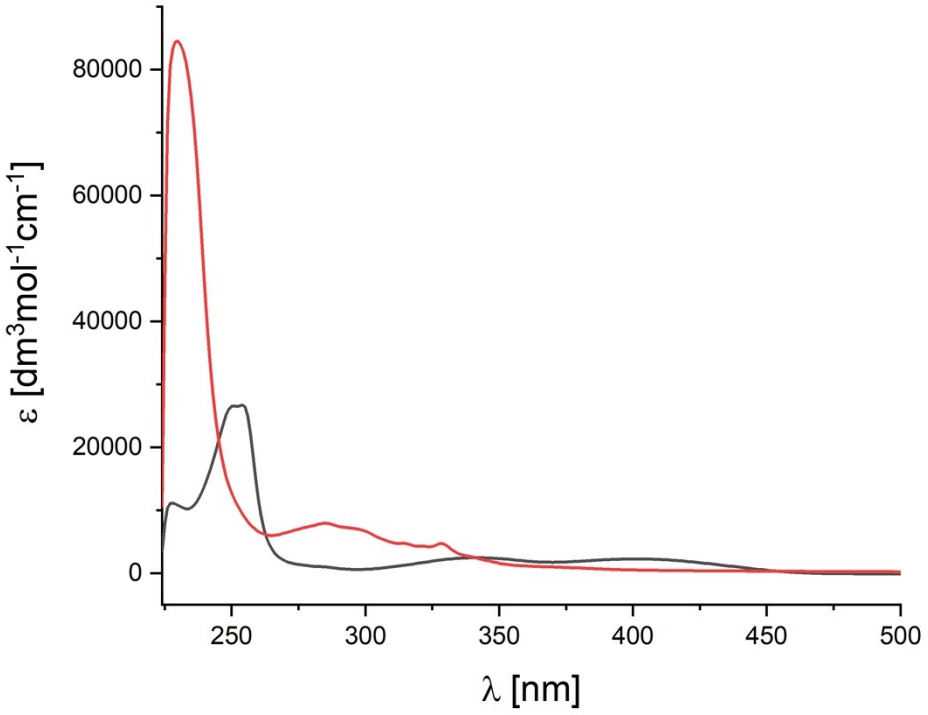
^{13}C NMR spectrum (100 MHz, CD_2Cl_2) for **4**(OTf). The asterisk denotes a solvent signal.



IR spectrum (powder) of **4**(OTf).

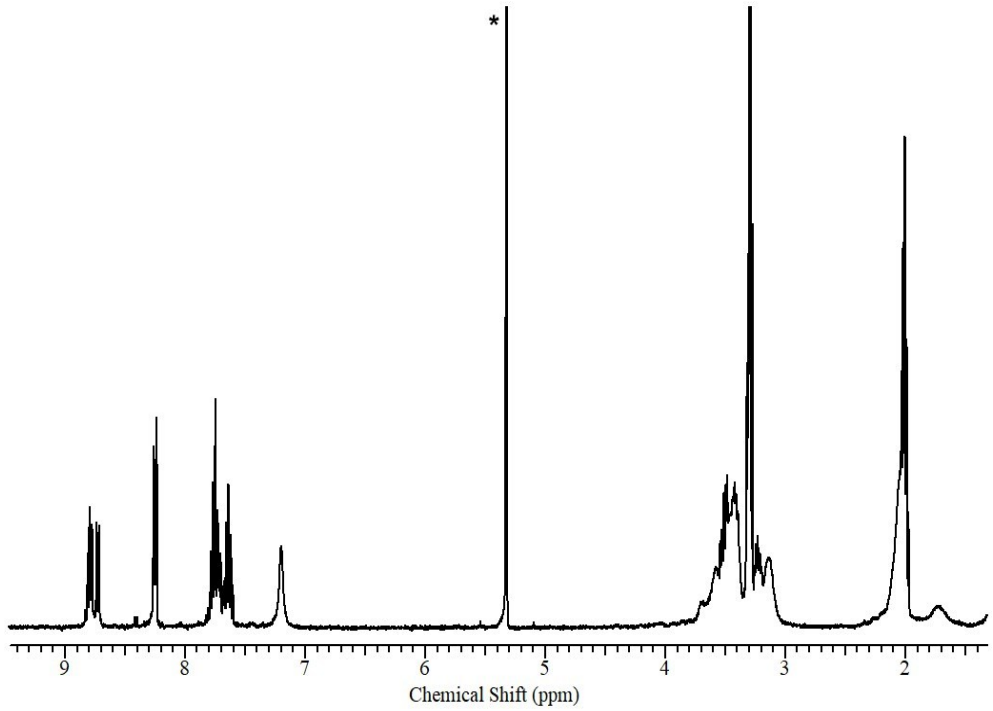


UV-Vis spectra (CH_2Cl_2) for **4**(OTf) (red) and 1,2-naphthalene-dione (**S_3**, black).

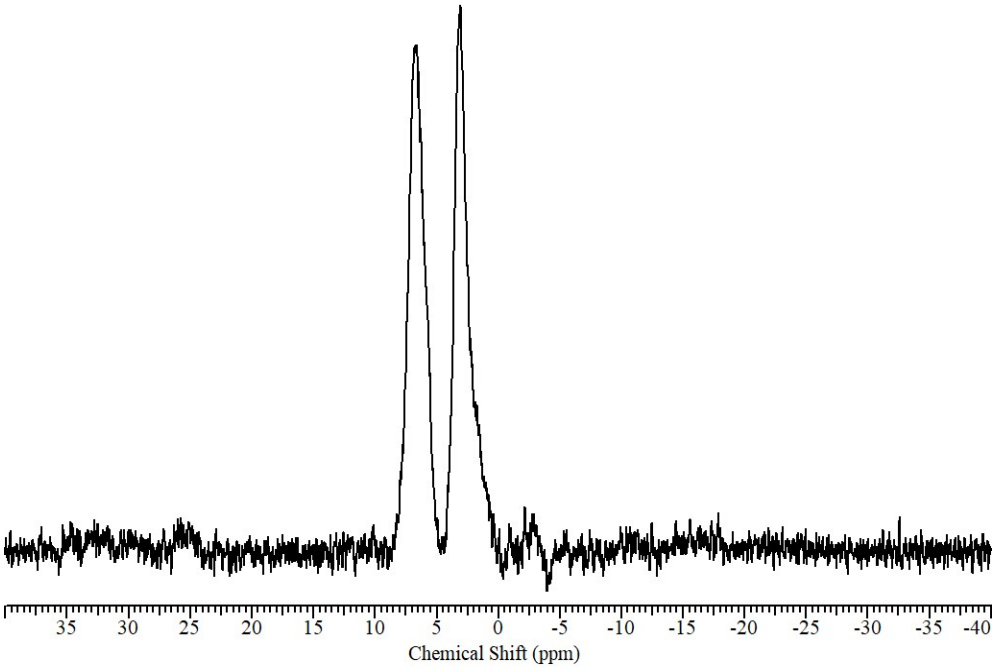


1b) Analytical data for compound **5**(OTf)

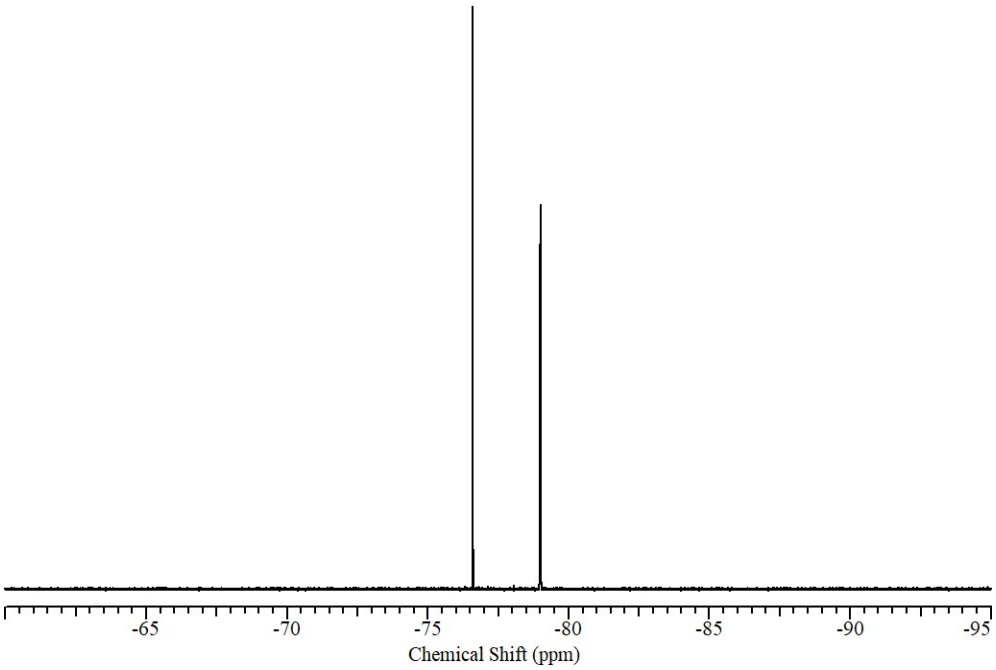
^{1}H NMR spectrum (400 MHz, CH_2Cl_2) for **5**(OTf). The asterisk denotes a solvent signal.



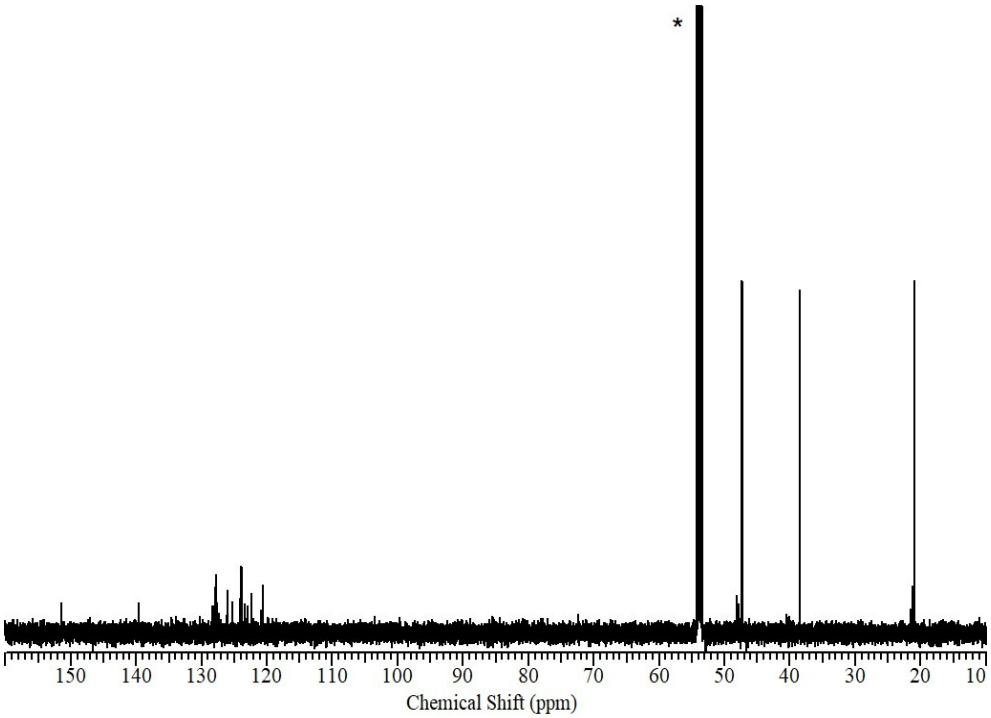
^{11}B NMR spectrum (128 MHz, CD_2Cl_2) for **5**(OTf).



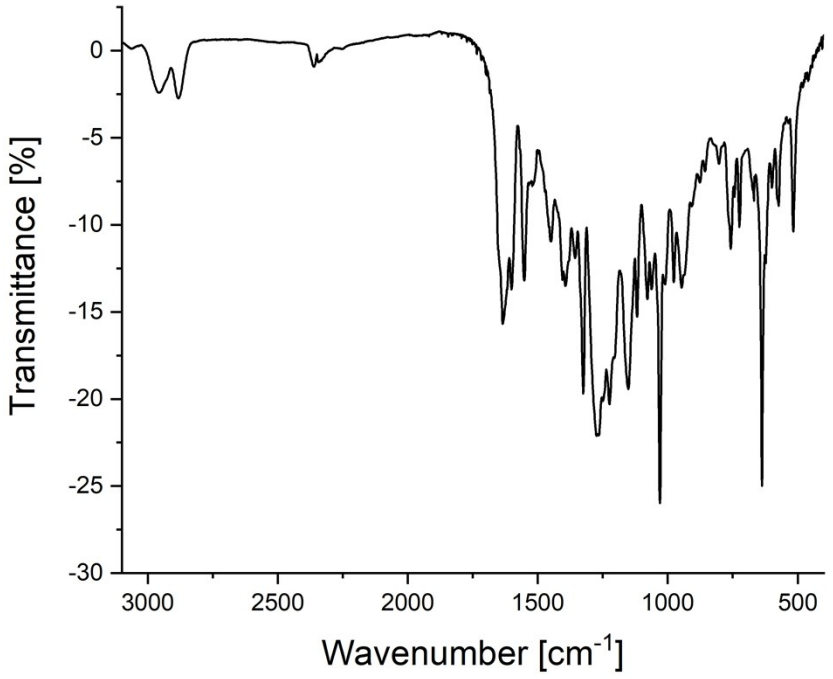
^{19}F NMR spectrum (376 MHz, CD_2Cl_2) for **5**(OTf).



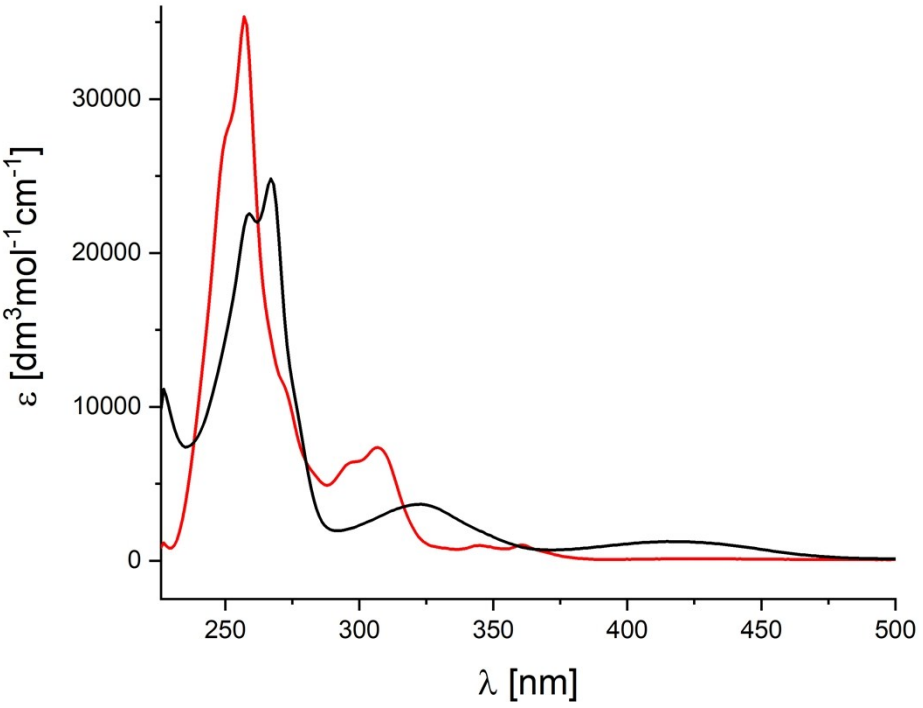
^{13}C NMR spectrum (100 MHz, CD_2Cl_2) for **5**(OTf). The asterisk denotes a solvent signal.



IR spectrum (KBr disk) of **5**(OTf).

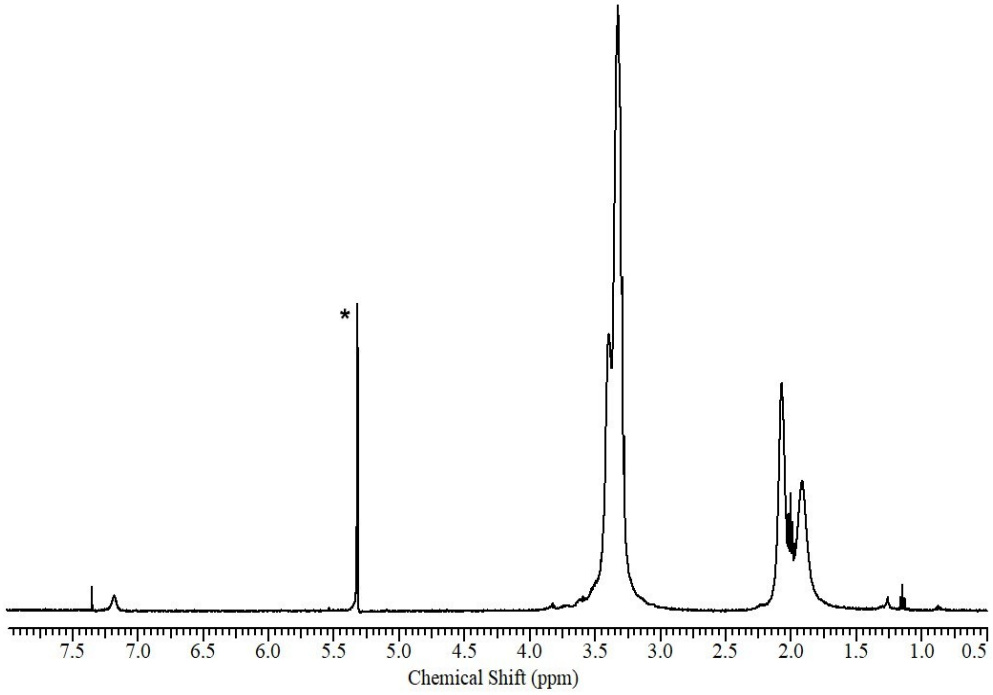


UV-Vis spectra (CH_2Cl_2) for **5**(OTf) (red) and 9,10-phenanthrene-dione (**S_4**, black).

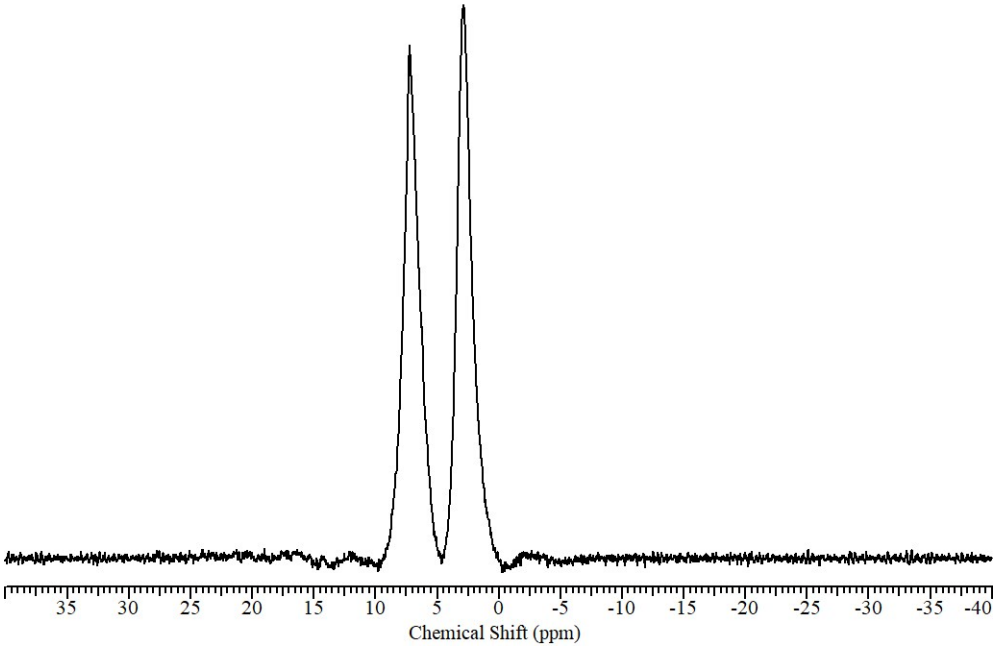

30000
20000
10000
0
ε [dm3mol-1cm-1]
250
300
350
400
450
500
λ [nm]

1c) Analytical data for compound **6**(OTf)

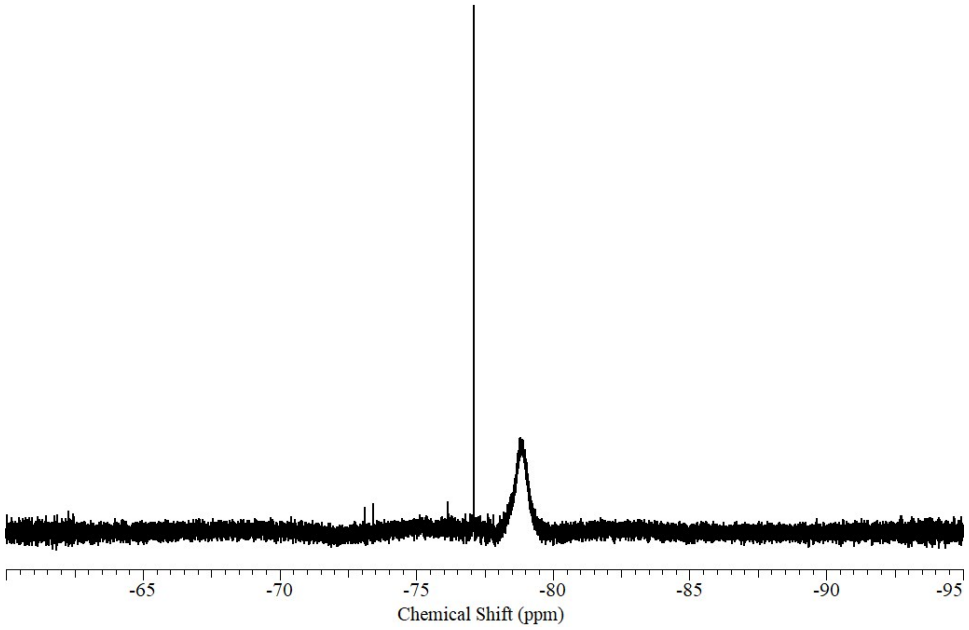
^{1}H NMR spectrum (400 MHz, CH_2Cl_2) for **6**(OTf). The asterisk denotes a solvent signal.



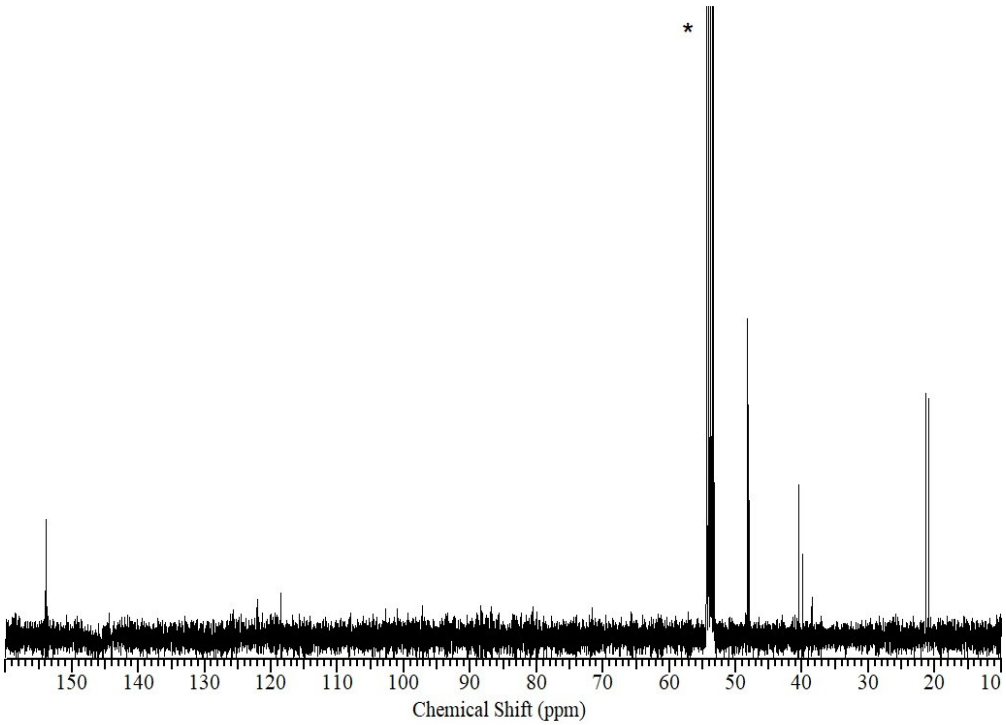
^{11}B NMR spectrum (128 MHz, CD_2Cl_2) for **6**(OTf).



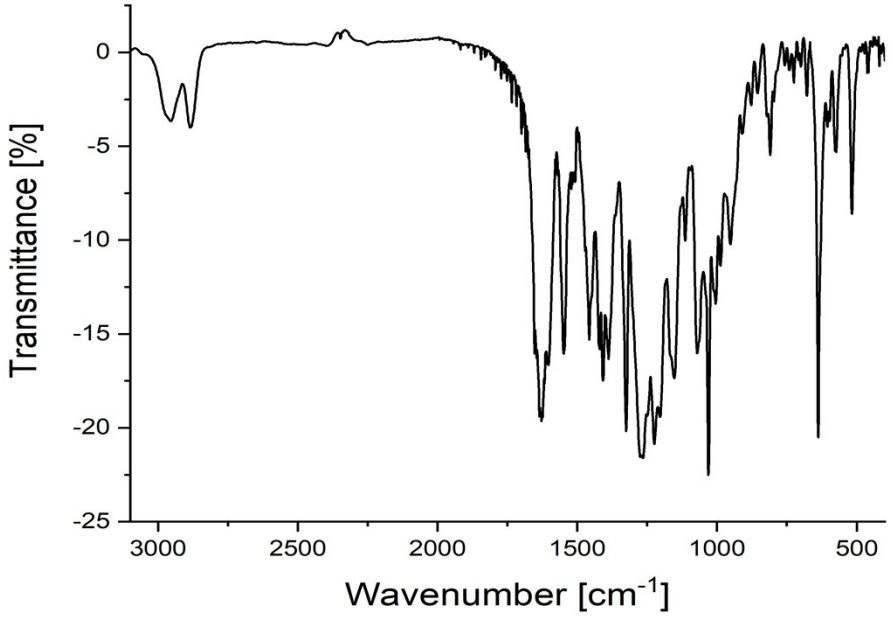
^{19}F NMR spectrum (376 MHz, CD_2Cl_2) for **6**(OTf).



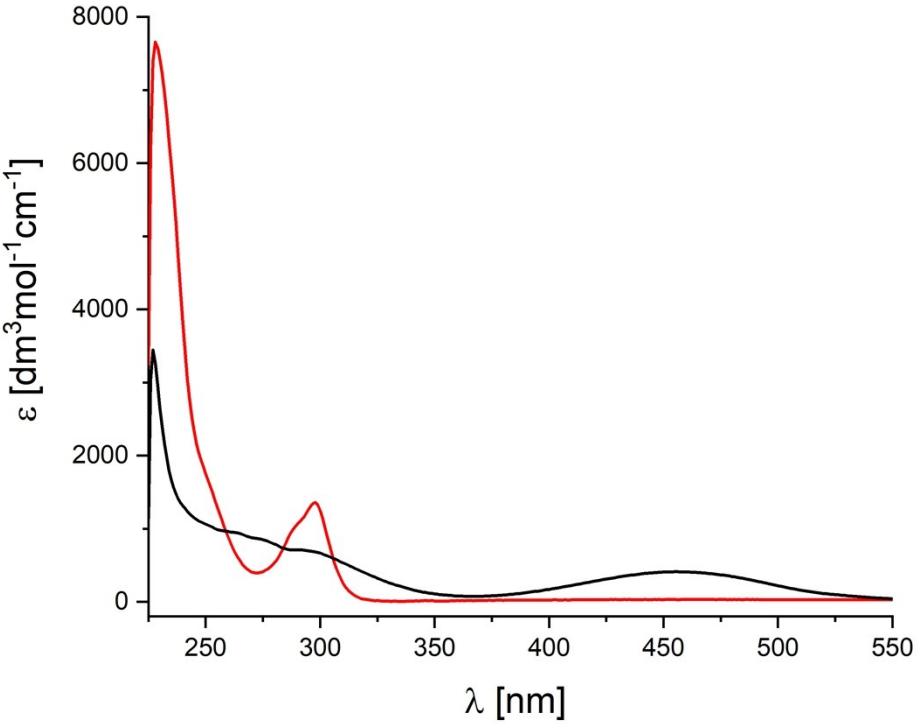
^{13}C NMR spectrum (100 MHz, CD_2Cl_2) for **6**(OTf).



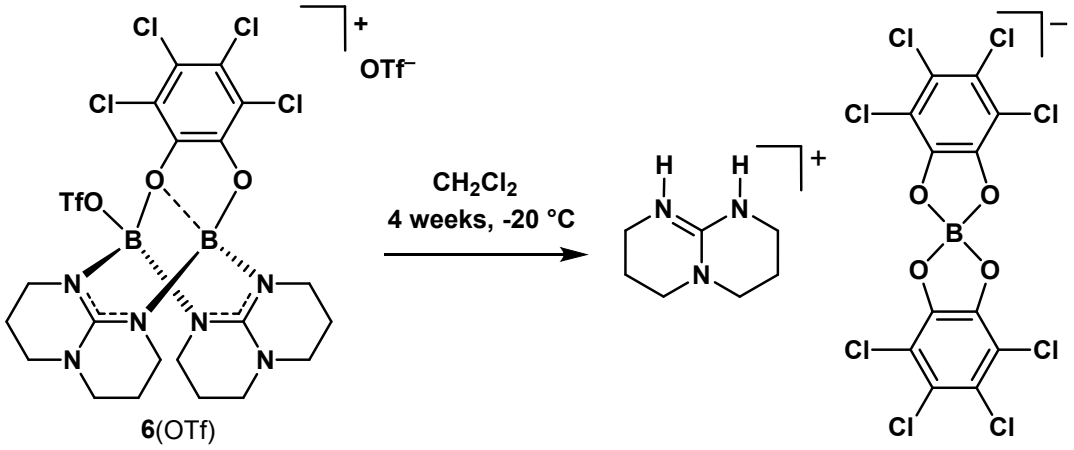
IR spectrum (KBr disk) of **6**(OTf).



UV/Vis spectra (CH_2Cl_2) for **6**(OTf) (red) and 3,4,5,6-tetrachloro-benzoquinone (**S_2**, black).



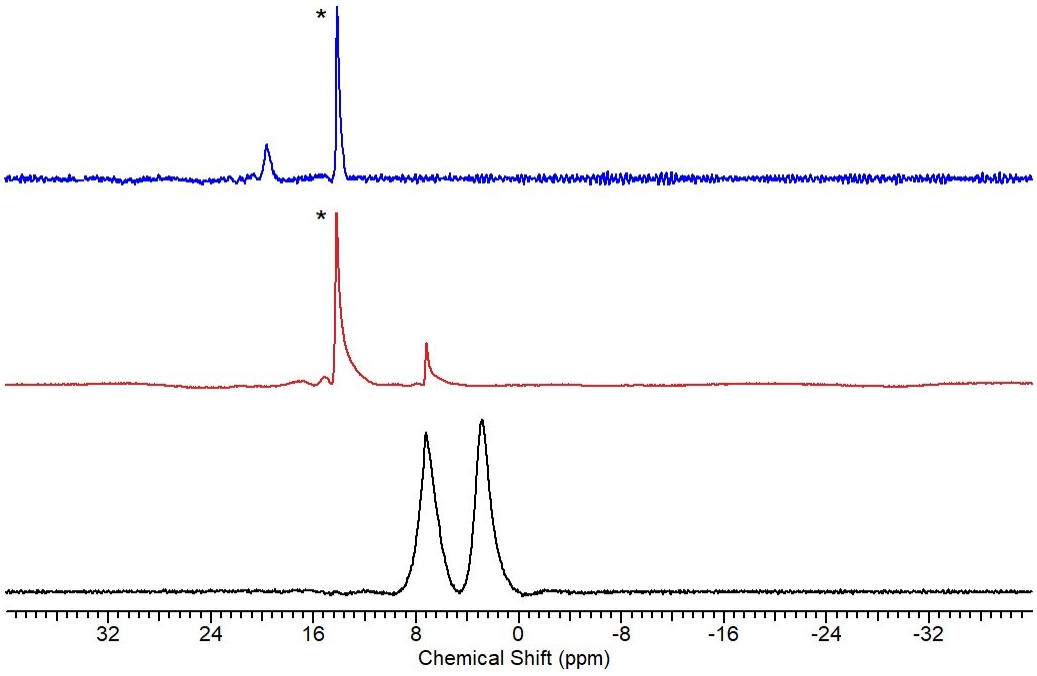
2. Decomposition of **6**(OTf)



6(OTf)

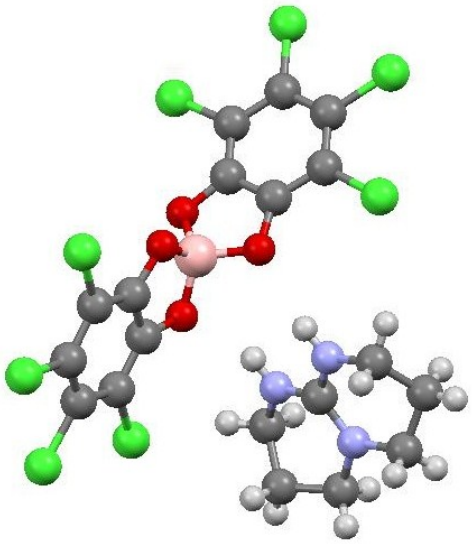
+ other products

^{11}B NMR spectra (128 MHz, CD_2Cl_2) of **6**(OTf) immediately after preparation of a solution in CH_2D_2 (black), after storage under argon atmosphere at -20 °C for four weeks (red) and of the crystals of the decomposition product (blue). The asterisk marks the signal of the boron atom of the crytallized structure at δ = 14.1 ppm.[1]



[1] C. Feuvrie, I. Ledoux, J. Zyss, H. Le Bozec, O. Maury, *C. R. Chimie*, 2005, **8**, 1243-1248.

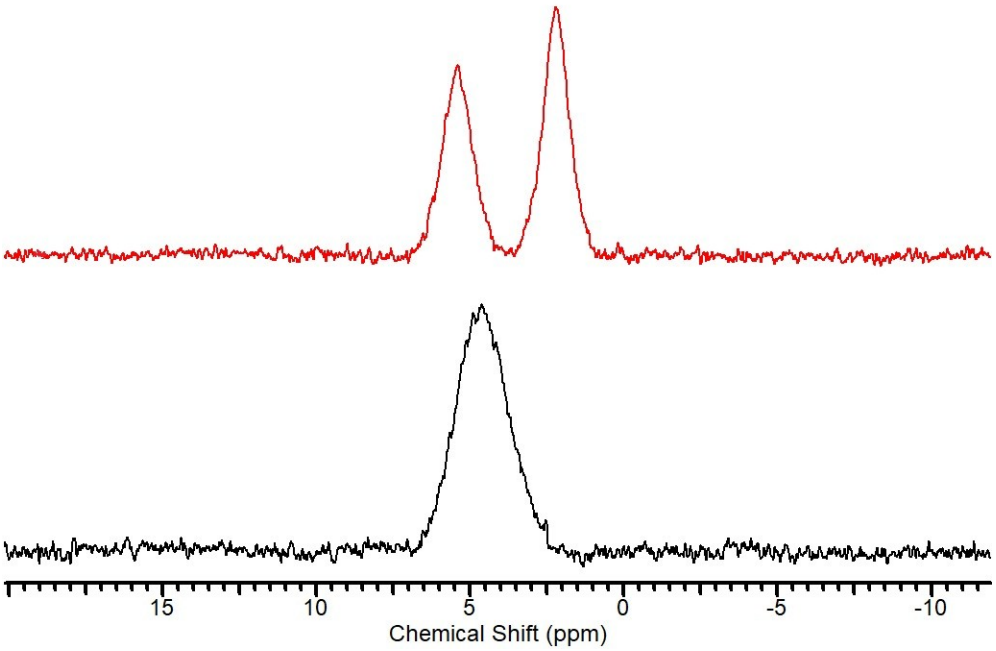
Illustration of the structure of one cation-anion pair from the crystals formed during the decomposition of **6**(OTf) in dichloromethane solution.



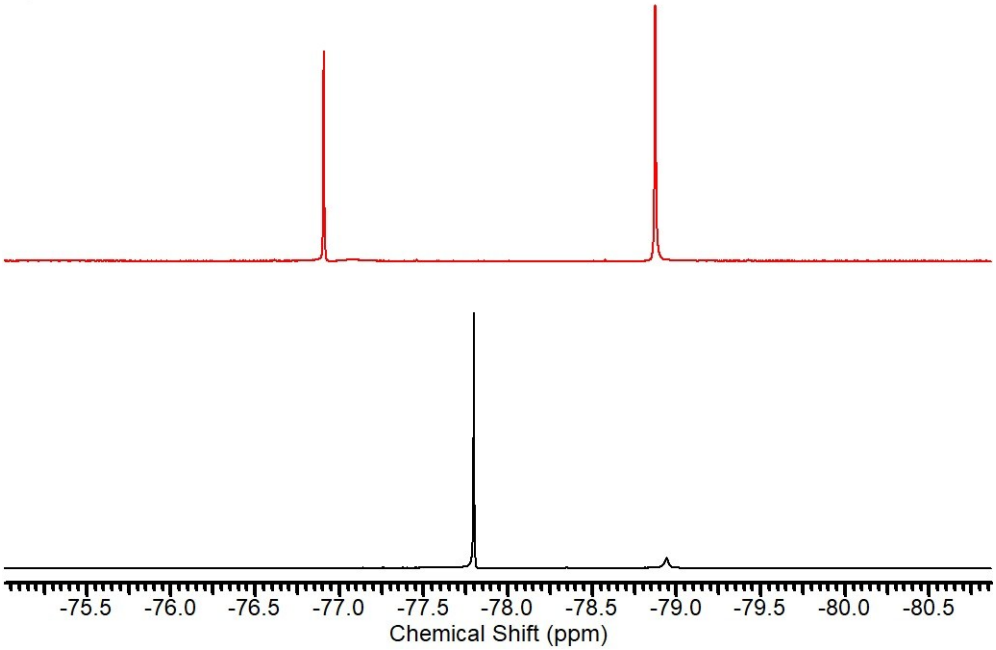
Crystal data for $C_{20}H_{16}BCl_{10}N_3O_4$, M_r = 727.67, 0.60 x 0.45 x 0.20, monoklin, space group P 21/n, a = 15.239(3), b = 11.928(2), c = 16.177(3) Å, α = 90.00°, β = 105.52(3)°, γ = 90.00°, V = 2833.2(11) Å^3, Z = 4, ρ_{cald} = 1.706 Mg·m^3, Mo-K_α radiation (λ = 0.71073 Å), T = 120 K, θ_{range} = 2.145 - 30.074°. Reflections collected 8281, independent reflections 6272, R_{int} = 0.0483. Final R indices [I > 2σ(I)]: R = 0.0570, wR = 0.1017.

3. Analytical data for reaction of compound **2** with 2,2'-dichlorobenzil (**S_5**)

^{11}B NMR spectra (128 MHz, CD_2Cl_2) for compound **2** (black) and the product of the reaction of **2** with **S_5** (red), denoted **7**(OTf)

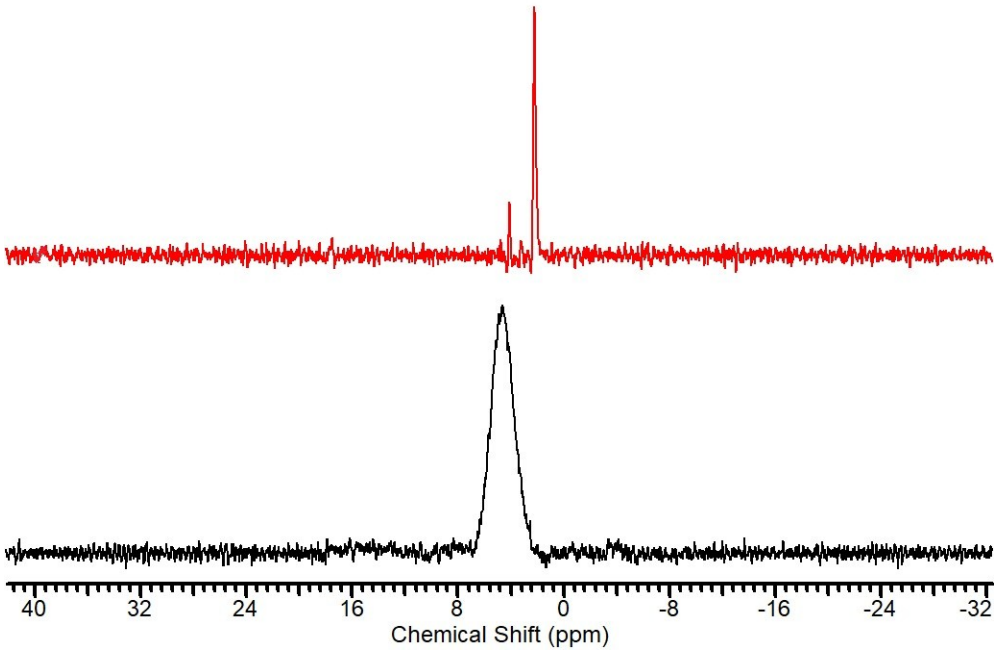


^{19}F NMR spectra (376 MHz, CD_2Cl_2) for compound **2** (black) and the product of the reaction of **2** with **S_5** (red), denoted **7**(OTf)



4. Analytical data for reaction of compound **2** with benzil (**S_6**)

^{11}B NMR spectra (128 MHz, CD_2Cl_2) for compound **2** (black) and the product of the reaction of **2** with **S_6** (red).



^{19}F NMR spectra (376 MHz, CD_2Cl_2) for compound **2** (black) and the product of the reaction of **2** with **S_6** (red).

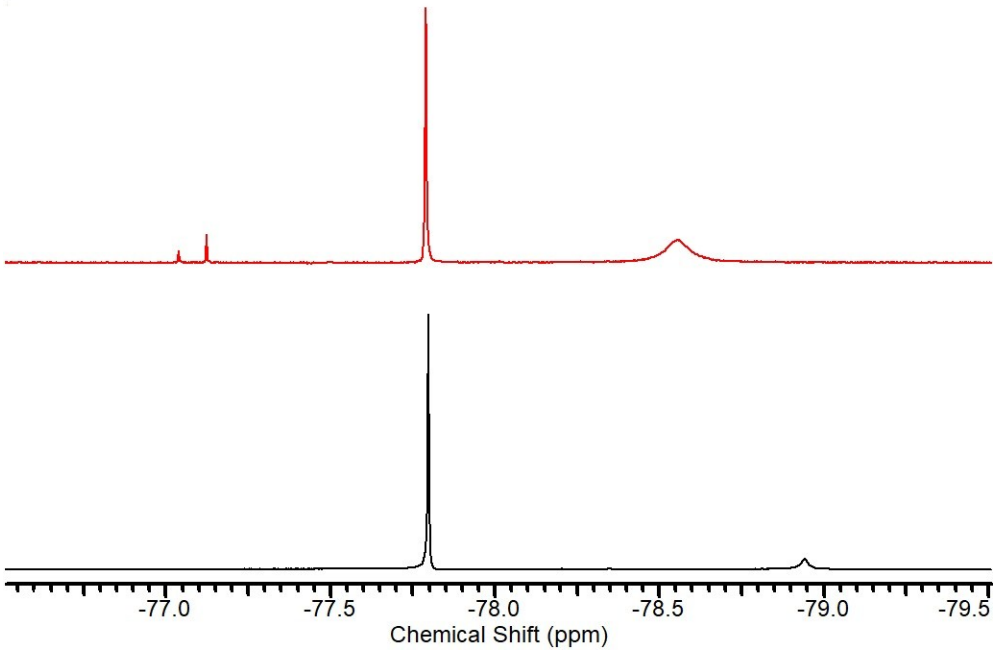
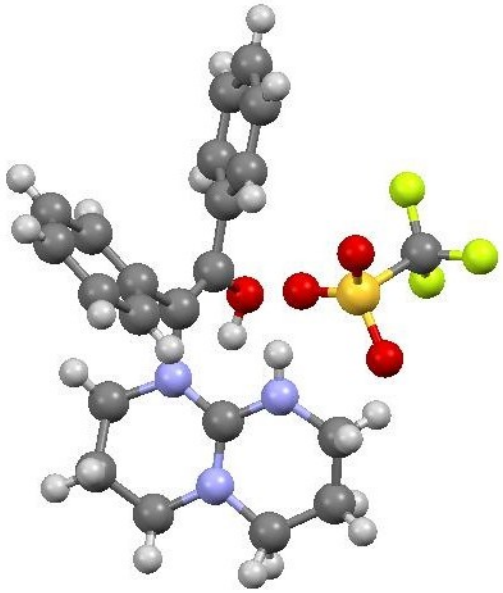
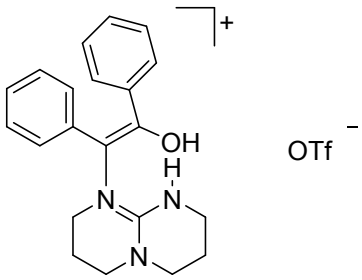


Illustration of the structure of one cation-anion pair in the crystals precipitating from the reaction mixture containing compound **2** and $\mathbf{S_6}$.

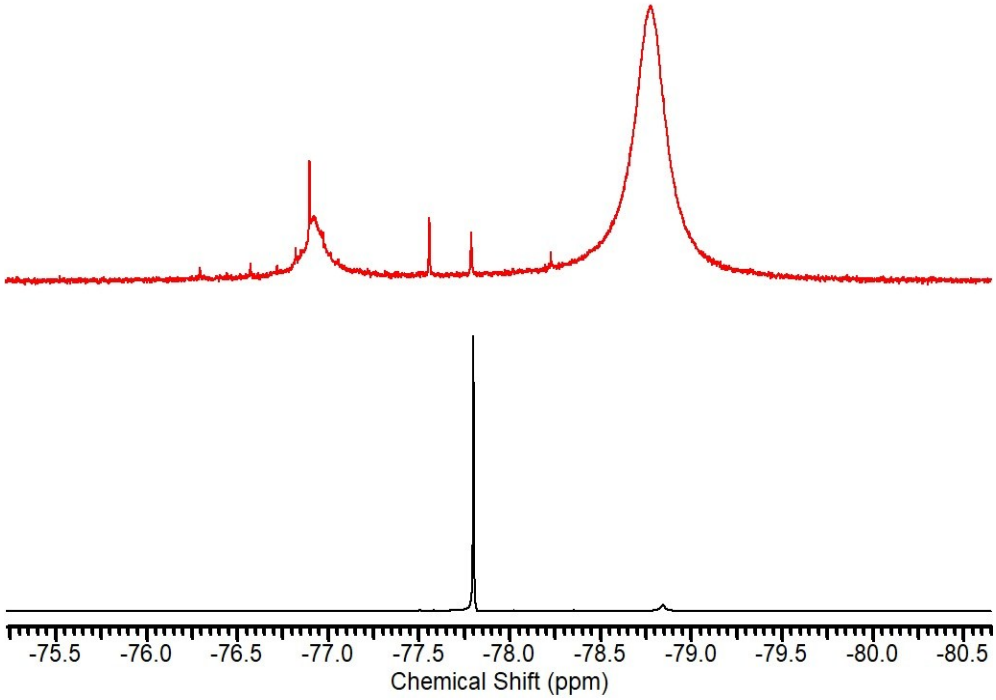




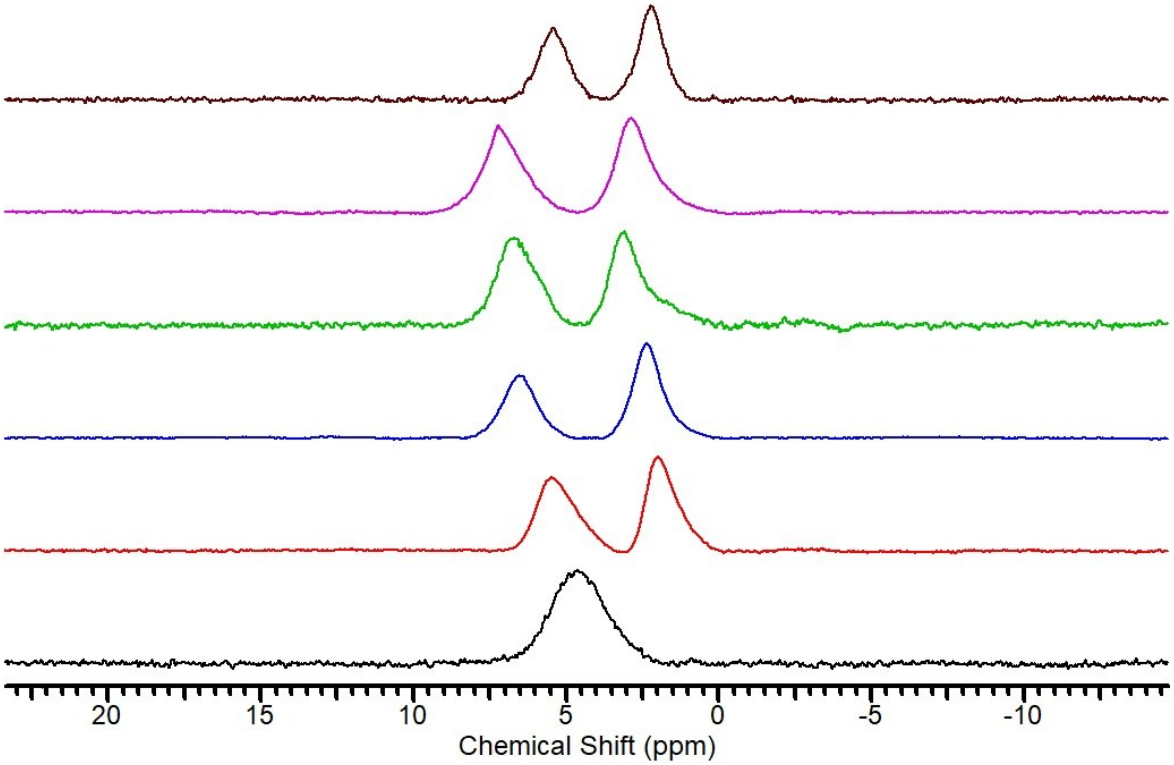
Crystal data for $C_{22}H_{24}F_3N_3O_4S$, M_r = 483.50, 0.80 x 0.70 x 0.60 mm, monoclinic, space group P 21/n, a = 22.713(5), b = 9.776(2), c = 23.112(5) Å, α = 90.00°, β = 119.37°, γ = 90.00°, V = 4472.2(19) Å^3, Z = 8, ρ_{cald} = 1.436 Mg·m^{-3}, Mo-K_α radiation (λ = 0.71073 Å), T = 120 K, θ_{range} = 1.761 - 30.099°. Reflections collected 13102, independent reflections 8759, R_{int} = 0.0604. Final R indices [$I > 2\sigma(I)$]: R = 0.0935, wR = 0.1528.

5. Analytical data for reaction of compound **2** with 1,2-acenaphthylene-dione (**S_7**)

^{19}F NMR spectra (376 MHz, CD_2Cl_2) for compound **2** (black) and the product of the reaction between **2** and **S_7** (red).

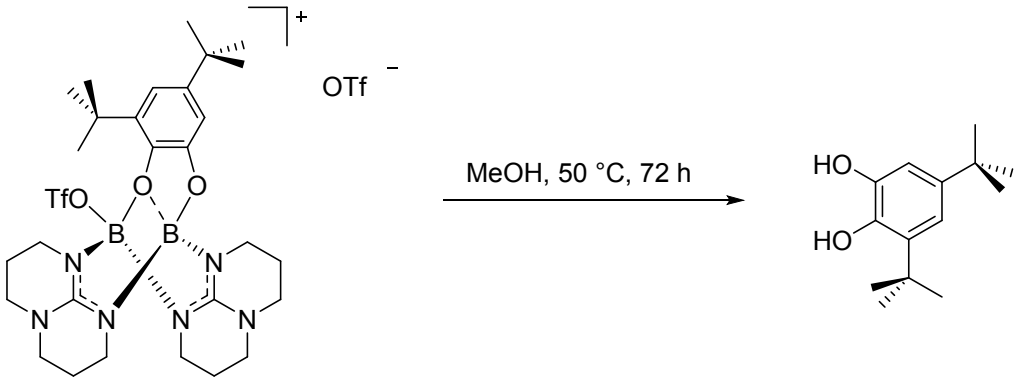


Comparison between the ^{11}B NMR spectra (128 MHz, CD_2Cl_2) for compound **2** (black), **3**(OTf) (red), **4**(OTf) (blue), **5**(OTf) (green), **6**(OTf) (magenta) and the product of the reaction between **2** and $\mathbf{S_5}$ (brown), denoted **7**(OTf).

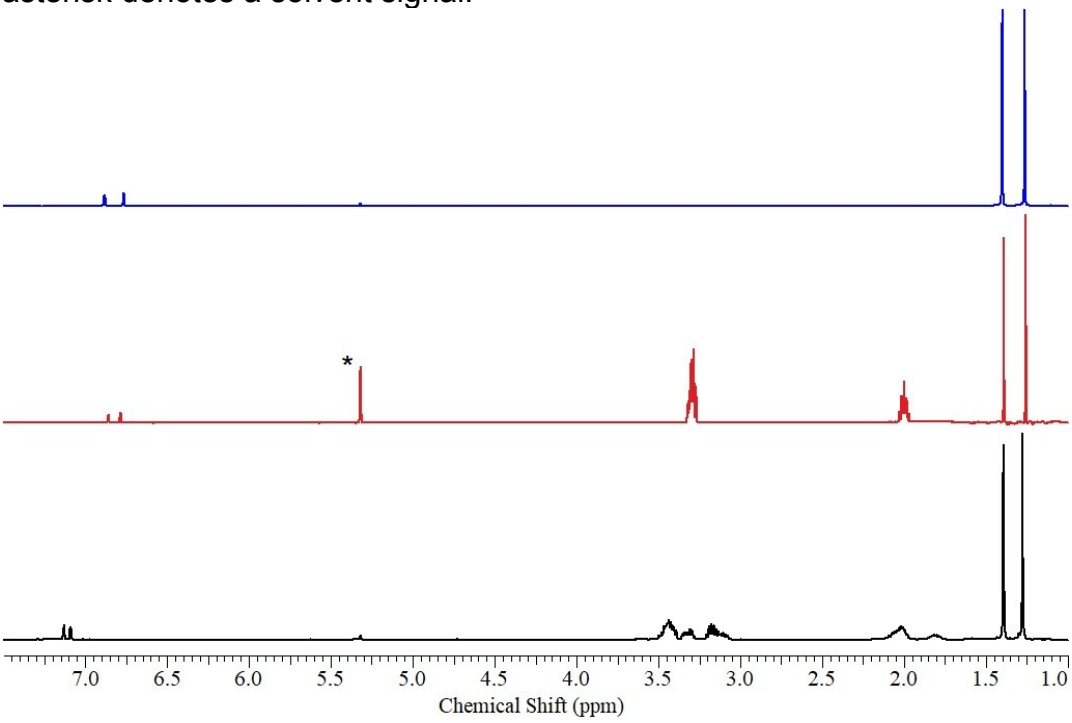


6. Separation of the catechol (shown exemplary for **3**(OTf))

Reaction of **3**(OTf) with MeOH.

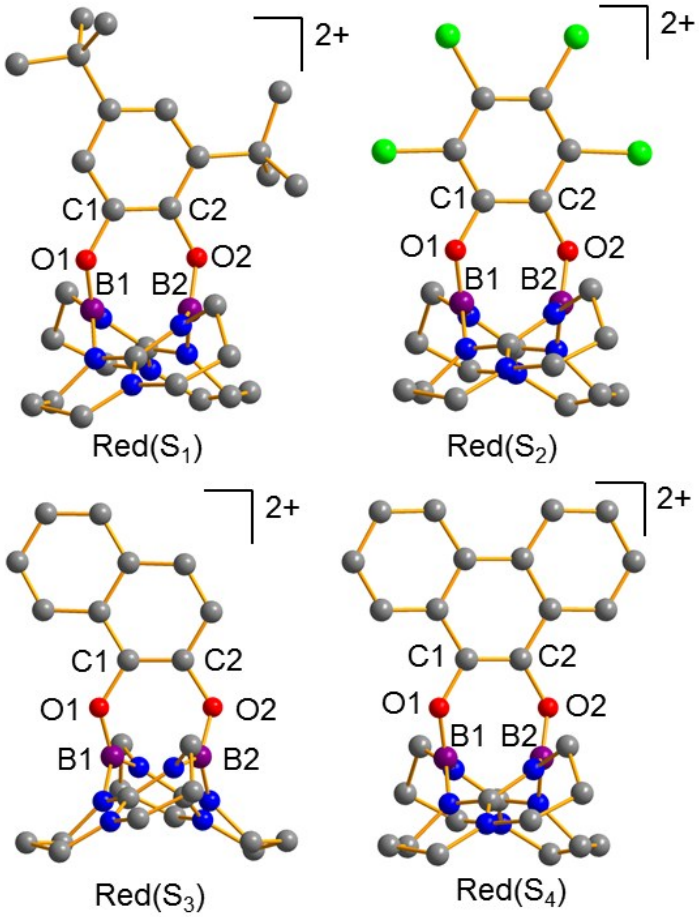


^{1}H NMR spectra (128 MHz, CD_2Cl_2) of **3**(OTf) after synthesis (black), after reaction with MeOH (red) and of the 3,5-di-*tert*-butyl-*o*-catechol (blue). The asterisk denotes a solvent signal.



7. Results of the quantum-chemical calculations

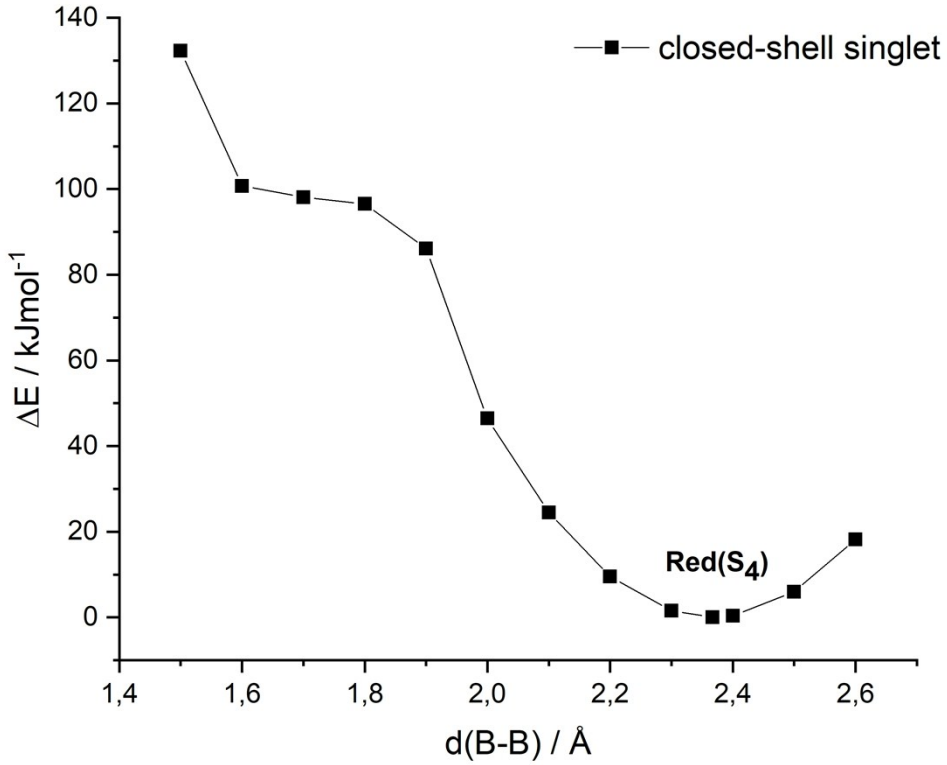
Illustration of the global-energy minima for **Red(S_1)** – **Red(S_4)** calculated with B3LYP/def2-TZVP.



Structural parameters (in Å) for the seven products of complexation and two-electron transfer, **Red(S_1)** – **Red(S_7)**, from B3LYP/def2-TZVP calculations.

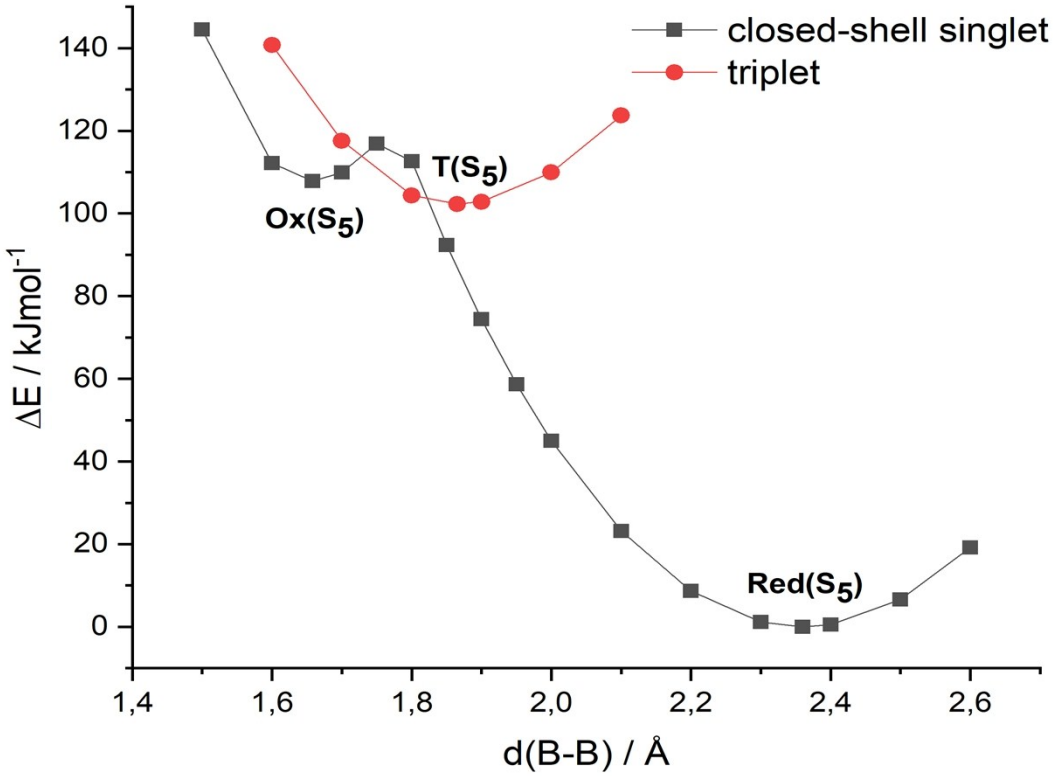
bond	**Red(S_1)**	**Red(S_2)**	**Red(S_3)**	**Red(S_4)**	**Red(S_5)**	**Red(S_6)**	**Red(S_7)**
B1···B2	2.359	2.368	2.372	2.367	2.360	2.357	2.417
B1-O1	1.344	1.352	1.348	1.346	1.346	1.342	1.354
B2-O2	1.343	1.352	1.347	1.346	1.346	1.342	1.354
O1-C1	1.400	1.381	1.396	1.396	1.401	1.410	1.385
O2-C2	1.401	1.381	1.396	1.396	1.400	1.410	1.385
C1-C2	1.399	1.399	1.382	1.366	1.342	1.353	1.374

Calculated energy of the complex between the dication $\{[B(hpp)]_2\}^{2+}$ and **S_4** as a function of the boron-boron distance.

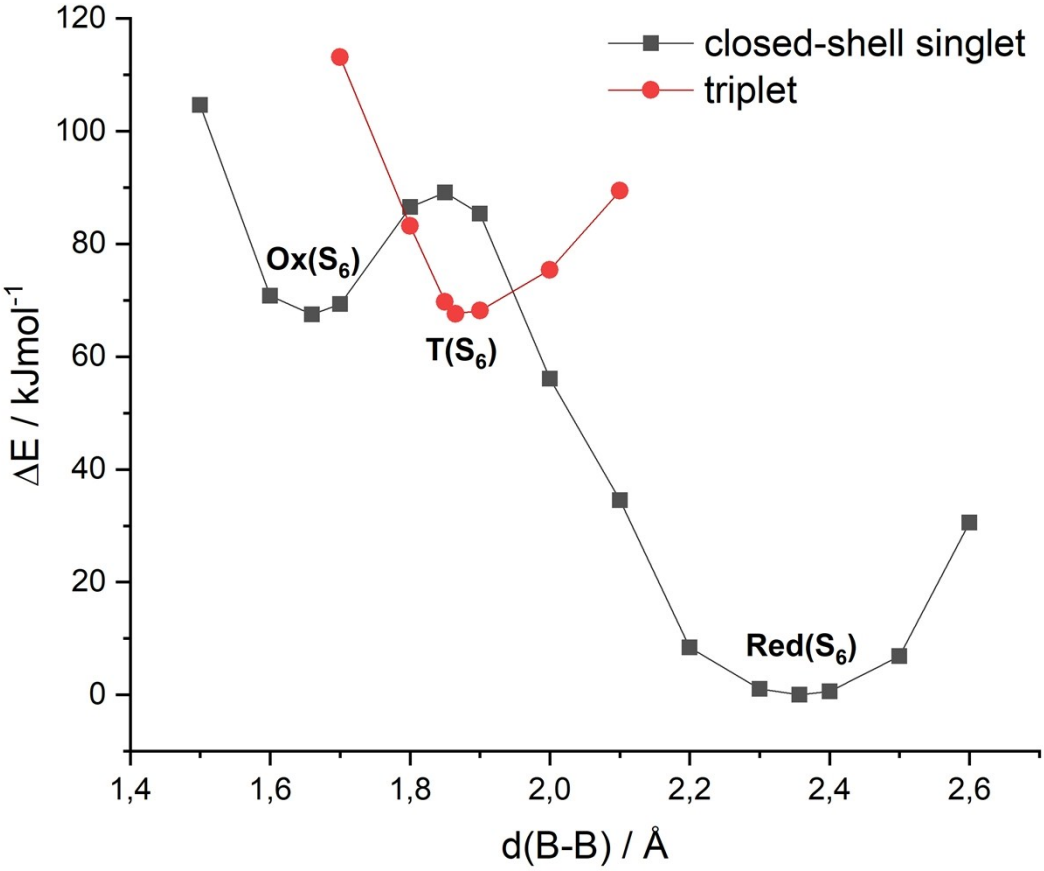


Analogue calculations were carried out for the complex between the dication $\{[B(hpp)]_2\}^{2+}$ and the substrates **S_5** and **S_6**. Contrary to the results of the complex between the dication $\{[B(hpp)]_2\}^{2+}$ and the 9,10-phenanthrene-dione, the calculations found for both substrates two minima with distances between the two boron atoms of 1.658 and 2.360 Å for **S_5** and 1.660 and 2.357 Å for **S_6**. The calculated structures for the first minima actually comply to the structures **Ox(S_5)** and **Ox(S_6)**, and the calculated structures for the second minimum comply again to the structures **Red(S_5)** and **Red(S_6)**.

Calculated energy of the complex between the dication $\{[B(hpp)]_2\}^{2+}$ and 2,2'-dichlorobenzil (**S_5**) as a function of the boron-boron distance.



Calculated energy of the complex between the dication $\{[B(hpp)]_2\}^{2+}$ and benzil (**S_6**) as a function of the boron-boron distance.



Validation of the calculational method for compounds **Ox(S_7)** and **Red(S_7)**.

Method	**Ox(S_7)** / Hartree	**Red(S_7)** / Hartree	ΔE / kJ mol^{-1}
B3LYP/def2-TZVP	-1536.817811847	-1536,833984858	42.46
B3LYP-D3/def2-TZVP	-1536.896880403	-1536.917768073	54.84
DLPNO-CCSD(T)/ cc-pVQZ	-1534.925771936	-1534.950895172	65.96

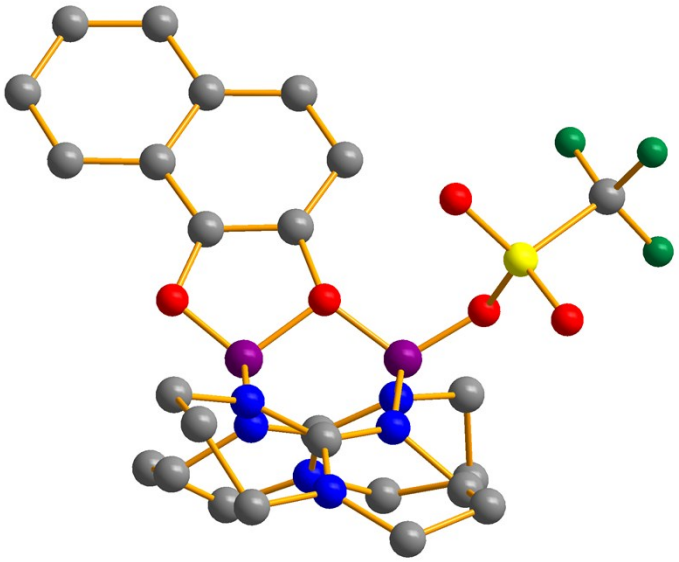
In the case of the calculation with DLPNO-CCSD(T)/cc-pVQZ, the energy was calculated at the structure optimized with B3LYP/def2-TZVP.

Cartesian coordinates and structures for all minima

A) Calculations on the cations 4-7 with BP86/def2-SVP

Cation 4

Illustration of the molecular structure of the cation **4**



E = -2421.343426 Hartree

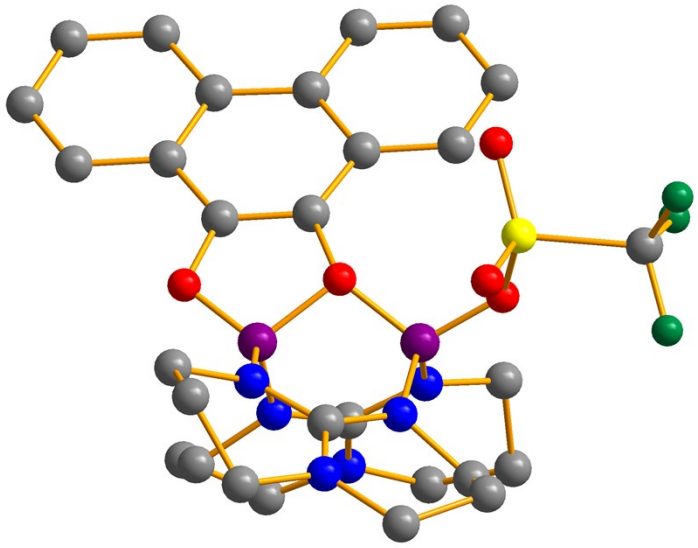
Cartesian coordinates (in Å):

S	0.118177	2.162391	9.426975
F	0.106824	3.429091	7.066529
F	-0.692623	4.567610	8.749609
F	1.465399	4.287453	8.547406
O	0.425300	-3.169346	7.794448
O	0.787728	-0.901116	8.329498
O	1.458772	1.439341	8.806323
O	-1.090599	1.427099	9.037474
O	0.364692	2.586143	10.813403
N	0.779747	-2.507640	10.183723
N	1.818726	-0.427152	10.486243
N	1.112810	-1.690963	12.370458
N	2.720671	-2.485011	8.495907
N	3.151637	-0.194694	8.286697
N	4.794629	-1.760903	7.615128
C	1.226430	-1.537057	11.022510
C	-0.117100	-3.600369	10.606142
H	-0.955204	-3.664385	9.881227

H	0.438028	-4.564281	10.540997
C	-0.625262	-3.384700	12.027662
H	-1.421765	-2.608648	12.048013
H	-1.066662	-4.325676	12.417633
C	0.538997	-2.934285	12.907093
H	1.322915	-3.726731	12.974015
H	0.198163	-2.720544	13.940758
C	1.632735	-0.727743	13.353995
H	0.866520	-0.603408	14.150588
H	2.533932	-1.175224	13.837450
C	1.963303	0.616186	12.717408
H	1.043599	1.208705	12.535445
H	2.611429	1.201517	13.403130
C	2.663816	0.392502	11.380399
H	3.653256	-0.104633	11.523051
H	2.844661	1.363653	10.881833
C	3.559866	-1.484351	8.124429
C	3.234038	-3.863464	8.511166
H	3.839577	-4.038194	9.432172
H	2.364636	-4.549249	8.543669
C	4.073439	-4.117541	7.260571
H	4.479281	-5.151015	7.253869
H	3.432056	-4.002135	6.360032
C	5.225464	-3.119118	7.240962
H	5.684250	-3.061951	6.227987
H	6.032495	-3.435466	7.943414
C	5.804909	-0.723070	7.347252
H	6.780481	-1.091113	7.738092
H	5.917536	-0.621151	6.241996
C	5.436063	0.618188	7.971775
H	5.622766	0.606682	9.068337
H	6.071416	1.416391	7.533686
C	3.957263	0.891134	7.708287
H	3.764828	0.974101	6.612258
H	3.627655	1.841198	8.167966
C	0.132783	-2.361489	6.724992
C	0.360742	-1.013070	6.975319
C	0.102034	0.013341	6.051841
H	0.254715	1.069322	6.306283
C	-0.385554	-0.380594	4.805887
H	-0.602790	0.385378	4.044508
C	-0.629290	-1.753486	4.487678
C	-1.137005	-2.153566	3.213424
H	-1.340319	-1.377029	2.457476
C	-1.377494	-3.490165	2.925196
H	-1.772034	-3.776460	1.936800
C	-1.122343	-4.497404	3.898646
H	-1.322429	-5.553489	3.654908
C	-0.628058	-4.156338	5.150456
H	-0.432958	-4.928405	5.910907
C	-0.371545	-2.790671	5.468589
C	0.265893	3.733517	8.359547
B	1.174791	-2.349840	8.725239
B	1.806329	0.030017	8.993345

Cation 5

Illustration of the molecular structure of the cation **5**



E = -2574.875108 Hartree

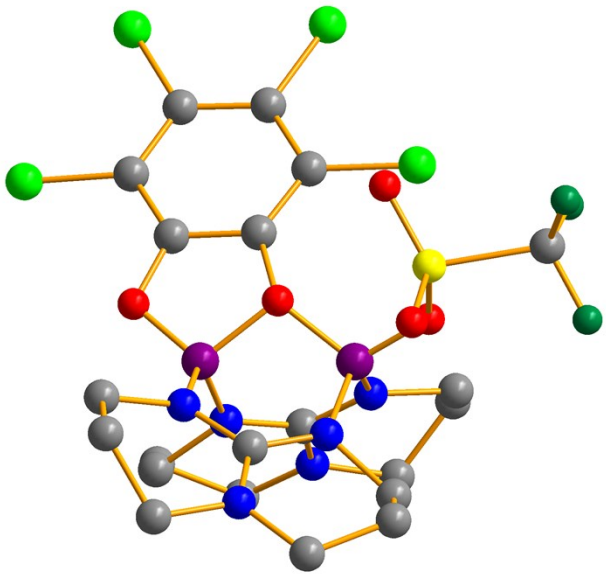
Cartesian coordinates (in Å):

S	8.038434	11.803123	9.286616
F	6.269212	10.620928	7.681072
F	5.876633	12.728916	8.104068
F	5.457783	11.214251	9.622637
O	12.495633	10.233941	12.050092
O	10.327648	10.382621	11.114501
O	8.140740	10.276441	9.911022
O	8.936483	11.970807	8.132889
O	7.990535	12.786163	10.370182
N	12.277821	10.019915	9.599521
N	10.193307	9.337872	8.844282
N	11.931893	9.745245	7.280522
N	11.440404	8.146949	11.174259
N	9.117145	8.256003	10.886166
N	10.085754	6.327707	11.857925
C	11.465461	9.715197	8.556623
C	13.564843	10.724419	9.444227
H	14.387946	10.033914	9.737736
H	13.591342	11.574700	10.157109
C	13.763623	11.199783	8.007282
H	14.827543	11.472136	7.845046
H	13.151641	12.106267	7.805506
C	13.342193	10.089054	7.045761
H	13.430504	10.421128	5.991116
H	13.988305	9.186105	7.164605
C	11.123263	9.376262	6.108810

H	11.490207	8.394417	5.725050
H	11.310965	10.127383	5.310340
C	9.635101	9.311438	6.438785
H	9.104560	8.751201	5.640239
H	9.205921	10.331976	6.492189
C	9.436657	8.631095	7.792571
H	8.365870	8.644776	8.071807
H	9.757507	7.562496	7.753649
C	10.216104	7.572875	11.317577
C	12.629390	7.321947	11.437519
H	13.496574	8.001985	11.548393
H	12.832402	6.652146	10.568145
C	12.419918	6.500859	12.708827
H	13.304813	5.866502	12.926665
H	12.279981	7.189667	13.569968
C	11.194668	5.613965	12.514780
H	11.448870	4.721057	11.896056
H	10.821328	5.233081	13.492284
C	8.804664	5.601999	11.896635
H	8.444510	5.580695	12.952300
H	9.005304	4.547001	11.602505
C	7.753834	6.231371	10.987777
H	7.963952	5.993274	9.921546
H	6.755789	5.811379	11.233242
C	7.773574	7.744887	11.189425
H	7.057020	8.256511	10.518792
H	7.485769	8.006298	12.234719
C	11.579051	10.593983	12.997967
C	10.276343	10.639399	12.544520
C	9.158867	10.946631	13.388891
C	7.797012	10.956339	12.978065
H	7.548660	10.759815	11.931347
C	6.773462	11.242639	13.877262
H	5.728740	11.253365	13.526577
C	7.073430	11.529218	15.226399
H	6.266537	11.758588	15.940519
C	8.399034	11.526953	15.653113
H	8.607929	11.753008	16.708574
C	9.479559	11.241958	14.774684
C	10.866228	11.240788	15.248848
C	11.232863	11.558176	16.586746
H	10.460653	11.835259	17.318814
C	12.562722	11.536814	17.005083
H	12.806554	11.793391	18.048706
C	13.598714	11.193811	16.103413
H	14.646830	11.182929	16.443443
C	13.285190	10.877688	14.785216
H	14.072901	10.616482	14.062203
C	11.933322	10.900463	14.348798
C	6.269335	11.571512	8.625615
B	11.723131	9.682491	10.964522
B	9.400168	9.576059	10.168568

Cation 6

Illustration of the molecular structure of the cation **6**



E = = -4105.807399 Hartree

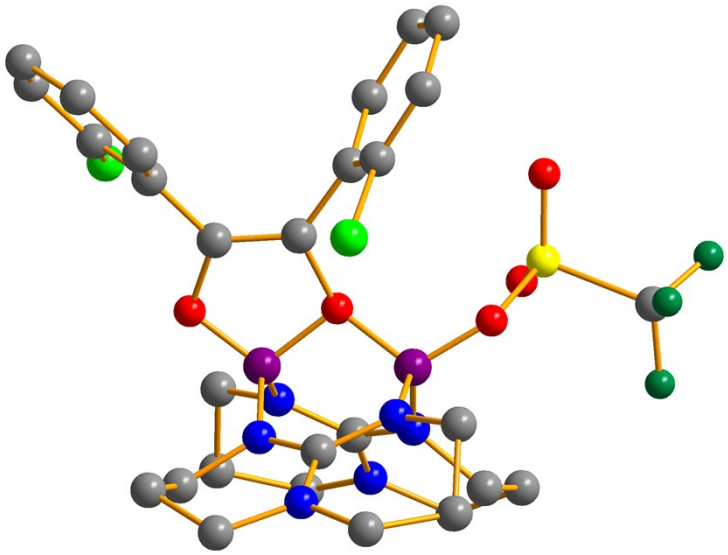
Cartesian coordinates (in Å):

C	-1.625149	-0.813314	-0.310024
C	-3.803382	-1.666419	-1.070933
C	-3.864231	-0.440262	-1.976138
C	-2.483076	-0.191477	-2.567941
H	-3.579919	-2.588862	-1.658279
H	-4.773840	-1.831760	-0.559509
H	-4.600091	-0.598829	-2.792106
H	-4.201066	0.442245	-1.388824
H	-2.258811	-0.956391	-3.347467
H	-2.433523	0.799956	-3.059800
C	-3.083324	-2.057663	1.292263
C	-0.716367	-1.555363	1.831683
C	-2.141827	-1.542950	2.374961
H	-4.138500	-1.810537	1.541966
H	-2.228357	-2.184891	3.276732
H	-3.020800	-3.168821	1.211621
H	-2.412665	-0.507150	2.674060
H	-0.013246	-1.135901	2.578165
N	-0.627343	-0.727691	0.615709
N	-1.433455	-0.237645	-1.531864
N	-2.785335	-1.470817	-0.025920
H	-0.390258	-2.598839	1.607977
B	0.577390	0.270446	0.602713

N	1.917265	-0.368192	0.339785
C	2.037739	-0.989620	-0.862483
C	3.031375	-0.237808	1.301167
N	1.054809	-0.782935	-1.776883
N	3.087154	-1.815698	-1.110575
C	4.340200	-0.741677	0.699599
H	2.781070	-0.818318	2.217840
H	3.111993	0.825513	1.608552
C	0.966661	-1.721442	-2.916482
B	-0.039284	0.335394	-1.797476
C	4.079434	-2.047489	-0.049574
C	3.247837	-2.574246	-2.360753
H	5.087943	-0.897304	1.505184
H	4.762504	0.005722	-0.007626
C	2.355084	-2.032897	-3.471533
H	0.346155	-1.246672	-3.700445
H	0.445822	-2.653913	-2.591967
H	3.726910	-2.847626	0.644713
H	5.003865	-2.418166	-0.537599
H	4.317052	-2.518490	-2.660735
H	3.023595	-3.647380	-2.151128
H	2.284804	-2.783089	-4.287102
H	2.781277	-1.100412	-3.893064
O	0.266480	1.269732	-0.575576
O	-0.030603	1.064856	-3.050776
S	1.255940	1.978592	-3.546420
O	2.447250	1.137148	-3.742272
C	0.527970	2.337190	-5.269205
F	0.388391	1.184037	-5.930253
F	-0.655263	2.939459	-5.152502
F	1.386937	3.128439	-5.904358
O	0.581652	1.133107	1.765599
C	-0.475284	2.298377	0.069495
C	-0.193877	2.198570	1.448567
C	-0.698676	3.130569	2.363909
C	-1.511918	4.182046	1.871716
C	-1.824759	4.257868	0.492139
C	-1.312041	3.302430	-0.435722
Cl	-1.785394	3.410929	-2.095076
Cl	-2.856498	5.522563	-0.080826
Cl	-2.140836	5.352051	2.973948
Cl	-0.324954	2.955336	4.041750
O	1.322570	3.226135	-2.781258

Cation 7

Illustration of the molecular structure of the cation **7**



E = -3495.052324 Hartree

Cartesian coordinates (in Å):

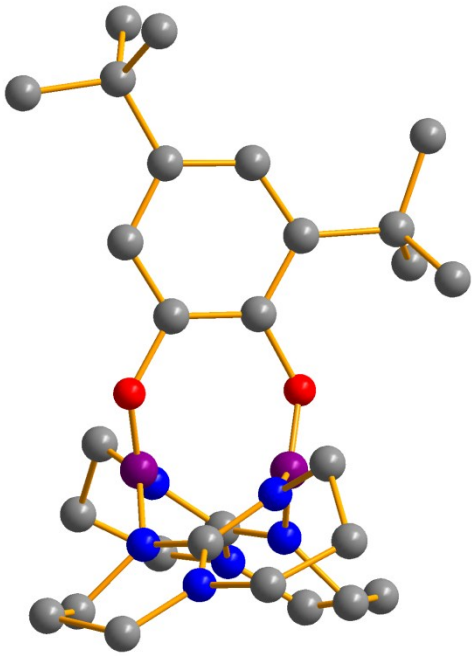
S	5.439819	6.977396	7.620765
F	3.793579	7.236147	9.708074
F	5.390290	5.765718	9.956971
F	3.653951	5.293217	8.719982
O	5.129811	9.115470	2.375345
O	4.803657	8.402814	4.591193
O	6.321187	8.003128	8.178908
O	4.160733	7.695815	6.898712
O	5.951810	5.857738	6.813516
N	4.626295	6.723413	2.806364
N	3.612063	6.270394	4.855643
N	4.174458	4.485752	3.396908
N	2.814574	8.537643	3.082524
N	2.450046	8.479150	5.394723
N	0.798991	9.402190	3.969885
B	4.340915	8.178988	3.139140
B	3.768502	7.695993	5.486145
C	4.151230	5.814771	3.691486
C	5.458139	6.289339	1.678460
H	6.493520	6.062353	2.025731
H	5.538141	7.133312	0.966954
C	4.816969	5.055184	1.046278
H	3.822022	5.326849	0.629669
H	5.434414	4.667815	0.208575
C	4.674543	3.967999	2.110127

H	3.973162	3.172642	1.771243
H	5.657065	3.473440	2.295385
C	3.751450	3.434362	4.336653
H	4.555459	2.665023	4.378141
H	2.851220	2.937047	3.903844
C	3.454512	3.981413	5.728905
H	4.392898	4.131958	6.299135
H	2.822629	3.257036	6.284626
C	2.749394	5.331080	5.592523
H	1.772648	5.217293	5.063362
H	2.534859	5.761465	6.587770
C	2.020079	8.816710	4.148033
C	2.269359	8.722841	1.729891
H	1.616330	7.860152	1.454955
H	3.120658	8.742278	1.021432
C	1.484071	10.030941	1.662190
H	2.169532	10.879134	1.877697
H	1.058642	10.191249	0.649191
C	0.355854	9.968576	2.685215
H	-0.056147	10.983781	2.885518
H	-0.488614	9.348339	2.301114
C	-0.177599	9.562745	5.058796
H	-1.179664	9.291913	4.655553
H	-0.222988	10.641119	5.341540
C	0.173616	8.707601	6.270512
H	-0.441704	9.025556	7.138329
H	-0.055447	7.636776	6.072616
C	1.660329	8.873917	6.571473
H	1.890656	9.927752	6.849246
H	1.978012	8.243002	7.422225
C	5.662477	10.018873	3.255497
C	5.464843	9.710945	4.567615
C	4.492587	6.267203	9.114461
C	6.374537	11.194301	2.710655
C	7.465019	11.060141	1.814157
C	5.969568	12.499785	3.072472
C	8.111901	12.188472	1.285584
C	6.616780	13.631104	2.554906
H	5.121298	12.614030	3.765931
C	7.683955	13.473714	1.655112
H	8.957830	12.049997	0.595316
H	6.281702	14.638021	2.850401
H	8.196154	14.355676	1.237483
C	6.048766	10.304632	5.782074
C	7.386814	9.999571	6.128055
C	5.364070	11.247789	6.587593
C	8.007243	10.592453	7.235487
H	7.938250	9.281361	5.500906
C	5.968092	11.840677	7.705107
C	7.293214	11.505081	8.027995
H	9.049556	10.337390	7.483052
H	5.406406	12.572331	8.305110
H	7.770233	11.973744	8.904050
Cl	8.080631	9.475151	1.387399
Cl	3.739753	11.764165	6.147260

B) Calculations with B3LYP/def2-TZVP

Red(S_1)

Illustration of the molecular structure (dication)



E = -1621.445733 Hartree

Cartesian coordinates (in Å):

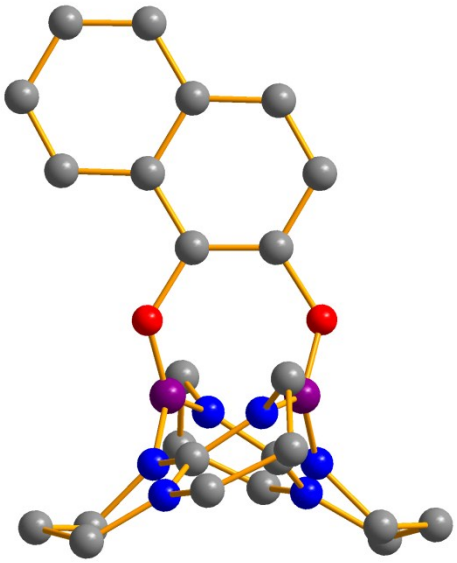
N	-1.298123	-0.782202	-1.661774
N	-2.038410	-1.416116	0.423710
N	-2.430770	-2.824352	-1.416117
N	-2.321778	1.266774	-0.532194
N	-1.415694	0.799413	1.532878
N	-2.939292	2.574331	1.318813
B	-1.140222	0.568651	-1.115668
B	-1.001996	-0.496958	0.984707
C	-1.944749	-1.711112	-0.895852
C	-0.722254	-1.242225	-2.944104
H	0.137728	-1.888768	-2.753873
H	-0.371916	-0.371968	-3.494805
C	-1.822603	-1.978051	-3.697974
H	-2.627557	-1.279891	-3.935165
H	-1.443862	-2.367848	-4.643062
C	-2.347343	-3.138567	-2.861128
H	-3.341639	-3.441914	-3.193185
H	-1.693097	-4.008953	-2.953658

C	-3.061450	-3.874312	-0.585675
H	-2.653096	-4.834311	-0.904755
H	-4.128101	-3.877991	-0.824382
C	-2.835001	-3.659850	0.904244
H	-1.835570	-3.991387	1.191176
H	-3.552594	-4.261595	1.462319
C	-2.993216	-2.183339	1.247892
H	-4.013790	-1.839627	1.057236
H	-2.769883	-1.998786	2.297177
C	-2.254251	1.578280	0.785422
C	-3.430830	1.825382	-1.330344
H	-4.357890	1.288021	-1.111998
H	-3.202956	1.683121	-2.385171
C	-3.557444	3.305615	-0.990165
H	-2.650092	3.825714	-1.302254
H	-4.393161	3.752277	-1.529160
C	-3.784100	3.476991	0.505183
H	-3.564007	4.499560	0.815152
H	-4.824406	3.272276	0.770811
C	-2.889662	2.902239	2.762156
H	-3.917344	2.995799	3.117346
H	-2.426136	3.888560	2.841626
C	-2.118120	1.876140	3.582665
H	-1.801292	2.338156	4.517940
H	-2.757291	1.029523	3.840155
C	-0.911629	1.377192	2.798220
H	-0.209556	2.186207	2.581454
H	-0.373361	0.603249	3.339422
O	0.034373	1.209854	-0.992214
O	0.269857	-0.905102	0.845586
C	1.290453	0.734926	-0.597958
C	1.414272	-0.222523	0.414278
C	2.399378	1.348315	-1.153075
C	2.683656	-0.603200	0.879076
C	3.675056	1.009626	-0.716244
C	3.772104	0.044348	0.293225
C	4.943695	1.655671	-1.290218
C	2.886577	-1.694079	1.954435
C	4.624333	2.685585	-2.383970
C	5.708044	2.371695	-0.155568
C	5.841063	0.558320	-1.902665
C	4.370747	-1.858972	2.327261
C	2.394005	-3.056773	1.416946
C	2.135172	-1.330734	3.253527
H	5.553027	3.113808	-2.761981
H	4.107347	2.234559	-3.234143
H	4.018502	3.512123	-2.005602
H	6.612216	2.835758	-0.552713
H	5.098780	3.156773	0.297208
H	6.012248	1.682420	0.632984
H	6.746659	1.006802	-2.314205
H	6.148658	-0.181462	-1.162669
H	5.328089	0.034678	-2.712132
H	2.946567	-3.340709	0.519335
H	2.562228	-3.831068	2.167768
H	1.331487	-3.048305	1.176803

H	4.977293	-2.178648	1.478942
H	4.798173	-0.941775	2.735748
H	4.459204	-2.629219	3.094001
H	2.453216	-0.356218	3.630067
H	1.053969	-1.318459	3.118331
H	2.355246	-2.070048	4.025268
H	4.757869	-0.222743	0.636516
H	2.235043	2.097772	-1.913269

Red(S_3)

Illustration of the molecular structure (dication)



E = -1460.658251 Hartree

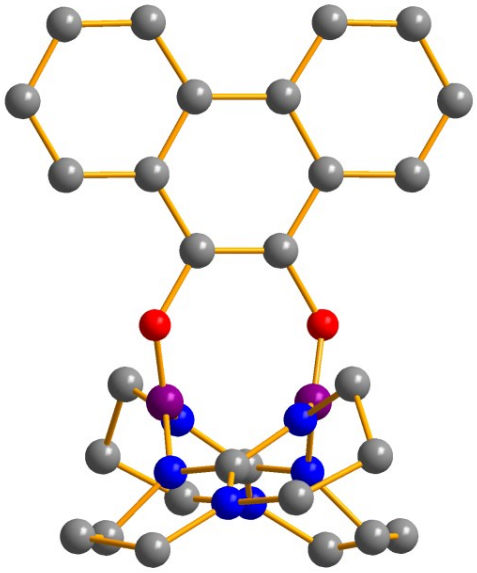
Cartesian coordinates (in Å):

N	0.576951	-1.127390	5.045629
N	-0.207033	-1.749712	7.119304
N	-0.599999	-3.147315	5.271781
N	-0.419053	0.944411	6.164064
N	0.472800	0.450109	8.228274
N	-1.008101	2.260753	8.019340
B	0.749286	0.224218	5.579995
B	0.843901	-0.858459	7.688343
C	-0.101218	-2.044991	5.800418
C	1.171936	-1.606472	3.777729
H	2.009919	-2.274199	3.991205
H	1.557711	-0.747461	3.233286

C	0.070675	-2.316713	3.001000
H	-0.711481	-1.599671	2.744756
H	0.460949	-2.717404	2.065208
C	-0.500328	-3.462829	3.827590
H	-1.496465	-3.739472	3.478283
H	0.131868	-4.350390	3.746811
C	-1.261459	-4.186574	6.092776
H	-0.867729	-5.153442	5.776349
H	-2.324820	-4.168718	5.840651
C	-1.048632	-3.979441	7.585735
H	-0.058656	-4.329301	7.883609
H	-1.783241	-4.569665	8.133850
C	-1.185261	-2.501245	7.931478
H	-2.196787	-2.138383	7.729242
H	-0.970391	-2.322735	8.983554
C	-0.347746	1.251127	7.482632
C	-1.513258	1.532248	5.365106
H	-2.452297	1.014107	5.578178
H	-1.285516	1.390336	4.310205
C	-1.608257	3.013304	5.712693
H	-0.689611	3.515562	5.404479
H	-2.433307	3.480056	5.174299
C	-1.833642	3.183763	7.208439
H	-1.592979	4.200349	7.522528
H	-2.878068	2.999155	7.472459
C	-0.944772	2.585638	9.463512
H	-1.968496	2.702603	9.822965
H	-0.458237	3.560891	9.541140
C	-0.194000	1.541506	10.281258
H	0.137642	1.996537	11.214812
H	-0.852059	0.710617	10.542190
C	0.997399	1.012980	9.492683
H	1.719872	1.803255	9.274586
H	1.516042	0.222943	10.031052
O	1.938412	0.848850	5.686908
O	2.113702	-1.291937	7.563642
C	3.167546	0.338729	6.107927
C	4.340022	0.927191	5.573334
C	3.243612	-0.610084	7.109804
C	4.305249	1.914906	4.560554
C	5.602581	0.498927	6.089443
C	4.488600	-1.025235	7.611964
C	5.473145	2.446871	4.074649
H	3.353385	2.252657	4.174563
C	5.639652	-0.477500	7.113700
C	6.721737	2.023185	4.574973
H	5.438606	3.202218	3.300216
H	7.631272	2.455024	4.178883
C	6.783240	1.072724	5.560613
H	7.739745	0.747798	5.950615
H	6.598578	-0.797706	7.500370
H	4.509528	-1.785258	8.381440

Red(S_4)

Illustration of the molecular structure (dication)



E = -1614.260399 Hartree

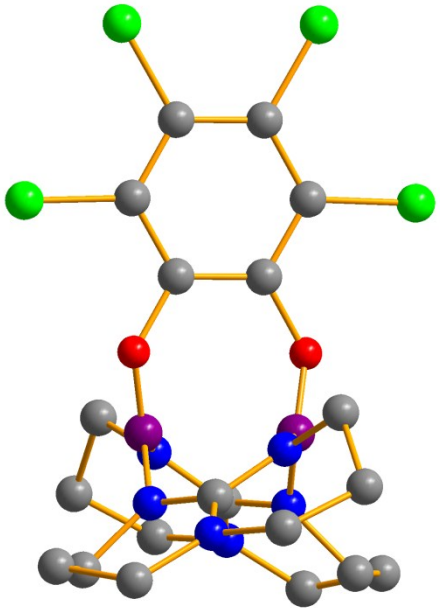
Cartesian coordinates (in Å):

N	-1.499399	-0.839060	-1.751544
N	-2.146232	-1.454705	0.370854
N	-2.697736	-2.835626	-1.448865
N	-2.368531	1.245893	-0.554710
N	-1.345838	0.724004	1.441272
N	-2.792366	2.570857	1.339304
B	-1.259161	0.504021	-1.220329
B	-1.039242	-0.588030	0.868471
C	-2.139681	-1.745926	-0.953519
C	-1.005574	-1.322441	-3.060133
H	-0.166976	-2.006397	-2.909459
H	-0.643458	-0.468002	-3.627564
C	-2.172563	-2.008222	-3.758867
H	-2.956898	-1.275202	-3.956580
H	-1.857657	-2.412204	-4.721264
C	-2.705746	-3.146822	-2.897310
H	-3.729103	-3.403034	-3.176513
H	-2.097875	-4.045784	-3.025079
C	-3.322786	-3.863857	-0.587083
H	-2.971034	-4.837561	-0.930879
H	-4.400211	-3.823960	-0.766666
C	-3.005993	-3.665830	0.888680
H	-2.006434	-4.038826	1.118804

H	-3.715452	-4.241055	1.483878
C	-3.085229	-2.185836	1.244828
H	-4.099569	-1.799823	1.110714
H	-2.797486	-2.015087	2.280618
C	-2.196172	1.546762	0.756236
C	-3.503639	1.860305	-1.271785
H	-4.436836	1.364308	-0.990845
H	-3.356888	1.714594	-2.340486
C	-3.537857	3.342672	-0.918358
H	-2.632055	3.823301	-1.292143
H	-4.388201	3.830140	-1.395591
C	-3.650417	3.515744	0.589897
H	-3.362450	4.525448	0.885913
H	-4.677599	3.356927	0.928217
C	-2.618533	2.890588	2.775410
H	-3.610924	3.031639	3.206969
H	-2.103960	3.853526	2.818953
C	-1.837002	1.826628	3.537008
H	-1.428519	2.271462	4.444637
H	-2.494969	1.011477	3.843857
C	-0.718464	1.271101	2.664787
H	0.005344	2.044147	2.395516
H	-0.180934	0.467956	3.163901
O	-0.052152	1.098747	-1.182301
O	0.207129	-1.044897	0.644905
C	1.193699	0.565309	-0.848430
C	1.321256	-0.383299	0.126465
C	2.336295	1.154786	-1.473400
C	2.603516	-0.842240	0.561037
C	3.630954	0.726194	-1.071692
C	3.766650	-0.281772	-0.034036
C	2.723810	-1.830969	1.558996
C	5.017322	-0.746319	0.419045
C	4.739048	1.316989	-1.710666
C	2.193686	2.142352	-2.469572
C	5.117516	-1.708402	1.399338
C	3.963851	-2.257705	1.973898
H	1.831887	-2.258869	1.994940
H	4.048919	-3.017059	2.740104
H	6.093786	-2.042961	1.724554
H	5.926195	-0.346286	-0.005012
H	5.740271	1.019408	-1.437006
H	1.204306	2.469531	-2.757276
C	3.301338	2.694743	-3.069474
C	4.582270	2.275800	-2.686733
H	5.454688	2.709164	-3.157802
H	3.184705	3.452320	-3.833288

Red(S_2)

Illustration of the molecular structure (dication)



E = -3145.273467 Hartree

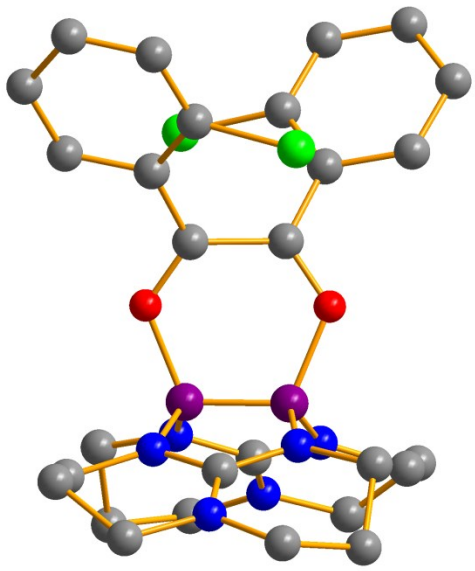
Cartesian coordinates (in Å):

N	-1.708019	-1.005470	-1.756534
N	-2.256741	-1.438550	0.438452
N	-3.012072	-2.891260	-1.246952
N	-2.358946	1.211747	-0.661215
N	-1.263454	0.750357	1.311971
N	-2.590605	2.681980	1.157122
B	-1.352333	0.346312	-1.332766
B	-1.079409	-0.610973	0.815415
C	-2.355171	-1.814580	-0.861390
C	-1.340388	-1.600346	-3.062689
H	-0.541324	-2.332598	-2.923909
H	-0.964395	-0.808589	-3.706956
C	-2.596685	-2.243551	-3.635591
H	-3.343580	-1.471037	-3.827499
H	-2.377392	-2.724603	-4.589025
C	-3.139447	-3.289323	-2.669186
H	-4.193860	-3.492422	-2.863129
H	-2.599882	-4.233310	-2.776257
C	-3.641102	-3.820810	-0.280316
H	-3.373961	-4.834725	-0.581004

H	-4.723268	-3.719993	-0.394958
C	-3.213409	-3.552648	1.155634
H	-2.225464	-3.975130	1.346985
H	-3.915045	-4.041750	1.831602
C	-3.178893	-2.051664	1.418115
H	-4.173481	-1.607931	1.322466
H	-2.810879	-1.836970	2.419746
C	-2.096525	1.585201	0.616498
C	-3.487121	1.859636	-1.363590
H	-4.434929	1.449919	-1.004199
H	-3.406534	1.636325	-2.425888
C	-3.399226	3.359933	-1.109469
H	-2.483725	3.748841	-1.558560
H	-4.238015	3.875578	-1.577429
C	-3.420767	3.637028	0.387098
H	-3.048308	4.639780	0.600784
H	-4.436497	3.573651	0.785344
C	-2.323588	3.077486	2.560628
H	-3.281642	3.314783	3.025948
H	-1.743745	4.002478	2.516794
C	-1.579442	2.009790	3.353412
H	-1.098827	2.479048	4.212080
H	-2.274318	1.262213	3.740405
C	-0.542613	1.326758	2.470880
H	0.215241	2.032049	2.121447
H	-0.036196	0.520046	2.996334
O	-0.101695	0.854647	-1.411512
O	0.129199	-1.162119	0.562321
C	1.113737	0.268785	-1.119004
C	1.243372	-0.614902	-0.042038
C	2.241724	0.687705	-1.820794
C	2.502008	-1.072843	0.340641
C	3.510073	0.225599	-1.446138
C	3.641547	-0.650313	-0.356110
Cl	2.611372	-2.161843	1.668155
Cl	2.033607	1.778839	-3.134678
Cl	4.893786	0.741065	-2.313086
Cl	5.187050	-1.214023	0.118892

Ox(S_5)

Illustration of the molecular structure (dication)



E = -2534.506124 Hartree

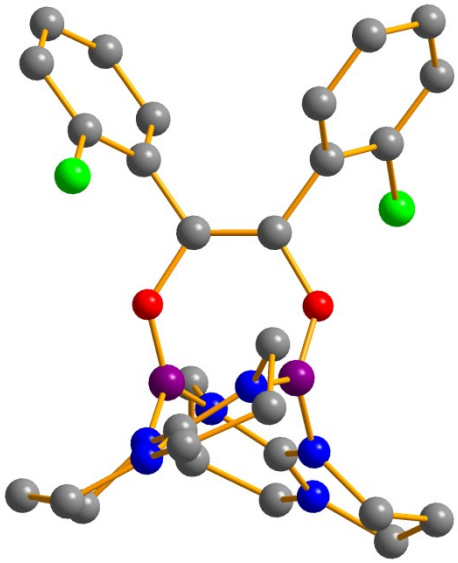
Cartesian coordinates (in Å):

N	-1.424238	-1.737795	-1.275914
N	-1.662480	-1.768686	1.012094
N	-2.060768	-3.746796	-0.213512
N	-2.110718	0.832274	1.049041
N	-3.476698	2.405950	-0.141251
B	-1.173039	-0.301231	-0.903112
B	-1.274962	-0.331103	0.751445
C	-1.719233	-2.458895	-0.160691
C	-1.447216	-2.370374	-2.598428
H	-0.455967	-2.767003	-2.843642
H	-1.679251	-1.604401	-3.338325
C	-2.482472	-3.484584	-2.634017
H	-3.485545	-3.060339	-2.545825
H	-2.434366	-4.019407	-3.582760
C	-2.228672	-4.454903	-1.493632
H	-3.069826	-5.139950	-1.377845
H	-1.337239	-5.061084	-1.683122
C	-2.321172	-4.535119	1.002361
H	-1.919947	-5.535673	0.833419
H	-3.403225	-4.635078	1.133827
C	-1.679734	-3.899734	2.223491
H	-0.594899	-4.024121	2.182316

H	-2.033971	-4.404259	3.122675
C	-2.025371	-2.418945	2.273558
H	-3.094821	-2.286398	2.471945
H	-1.480158	-1.925119	3.078344
C	-2.606668	1.395761	-0.114308
C	-2.559903	1.296242	-2.565576
H	-3.432316	0.718740	-2.891292
H	-1.759216	1.110631	-3.282019
C	-2.899751	2.778339	-2.515371
H	-1.990627	3.359595	-2.343264
H	-3.322907	3.104629	-3.465669
C	-3.899545	3.037765	-1.402092
H	-3.996120	4.108077	-1.213116
H	-4.892258	2.662508	-1.669898
C	-4.092412	2.934799	1.087346
H	-5.125598	3.191048	0.848382
H	-3.582675	3.861555	1.369042
C	-4.040551	1.918111	2.214353
H	-4.347638	2.393453	3.146141
H	-4.741005	1.103806	2.013863
C	-2.629206	1.364035	2.339913
H	-1.946998	2.143719	2.695939
H	-2.596809	0.552058	3.066242
O	0.298000	0.227324	-1.409017
O	0.204550	-0.182075	1.450816
C	1.208120	0.565866	-0.623477
C	1.260758	-0.065946	0.794568
C	2.505535	-0.545467	1.373206
C	2.654579	-0.452986	2.773927
C	3.545857	-1.144531	0.632452
C	3.816909	-0.860990	3.392172
H	1.855695	-0.008420	3.350718
C	4.709560	-1.564988	1.256542
C	4.851005	-1.406129	2.629627
H	3.928932	-0.751031	4.462250
H	5.486277	-2.039482	0.672817
H	5.766904	-1.728481	3.108081
C	2.179973	1.556785	-1.056836
C	2.753799	2.528438	-0.210312
C	2.526896	1.578584	-2.425046
C	3.684562	3.432330	-0.697242
C	3.460904	2.470744	-2.906008
H	2.080890	0.846237	-3.083295
C	4.049904	3.390601	-2.037154
H	4.097514	4.181198	-0.035549
H	3.741120	2.451521	-3.950428
H	4.784446	4.094149	-2.407519
Cl	3.343529	-1.532966	-1.049427
Cl	2.196042	2.740928	1.421933

Red(S_5)

Illustration of the molecular structure (dication)



E = -2534.547206 Hartree

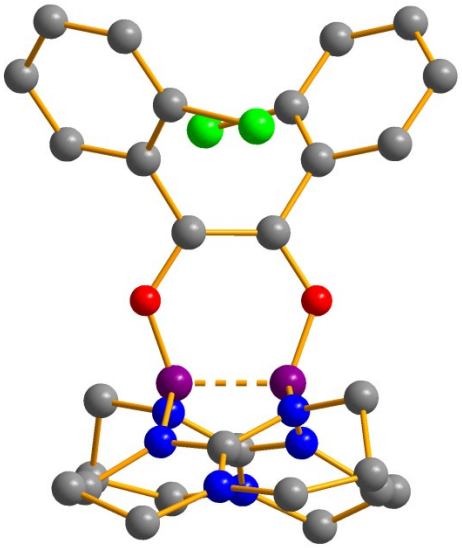
Cartesian coordinates (in Å):

N	-1.164666	-0.629996	-1.867027
N	-1.977765	-1.534314	0.088575
N	-2.209158	-2.732205	1.919074
N	-2.312766	1.237007	-0.554733
N	-1.491476	0.549144	1.484024
N	-3.045784	2.307294	1.403896
B	-1.083462	0.650028	-1.159108
B	-1.009657	-0.656095	0.804622
C	-1.803808	-1.668346	-1.249554
C	-0.498184	-0.919790	-3.155472
H	0.374764	-1.553930	-2.983645
H	-0.155052	0.019682	-3.583082
C	-1.523147	-1.603357	-4.051406
H	-2.343768	-0.912740	-4.254482
H	-1.077335	-1.866638	-5.010844
C	-2.040521	-2.871863	-3.383672
H	-3.003181	-3.170197	-3.802367
H	-1.346165	-3.701155	-3.538949
C	-2.821001	-3.901160	-1.248535
H	-2.345922	-4.796146	-1.652807
H	-3.873231	-3.928412	-1.543229
C	-2.677356	-3.851619	0.266013

H	-1.675640	-4.164245	0.565804
H	-3.386870	-4.548467	0.712620
C	-2.932163	-2.434546	0.765861
H	-3.957971	-2.118216	0.557297
H	-2.772066	-2.362240	1.840070
C	-2.313641	1.393948	0.792143
C	-3.395273	1.868177	-1.335672
H	-4.319547	1.293962	-1.226660
H	-3.115436	1.854287	-2.387514
C	-3.567949	3.296104	-0.831439
H	-2.656941	3.861901	-1.033764
H	-4.385751	3.790892	-1.355698
C	-3.869910	3.286397	0.660470
H	-3.686024	4.268472	1.098455
H	-4.917088	3.035765	0.848251
C	-3.065825	2.466738	2.876056
H	-4.109655	2.498767	3.193026
H	-2.630217	3.446093	3.088485
C	-2.305082	1.368160	3.608809
H	-2.040356	1.726211	4.603954
H	-2.933670	0.485308	3.739044
C	-1.054162	0.986207	2.828014
H	-0.363602	1.827767	2.734557
H	-0.522429	0.163070	3.300277
O	0.064630	1.304669	-0.905922
O	0.288578	-0.986491	0.676520
C	1.313118	0.827385	-0.487560
C	1.405506	-0.197515	0.374528
C	2.653431	-0.673870	1.003378
C	3.304745	0.118627	1.954045
C	3.205866	-1.924435	0.698578
C	4.459788	-0.322650	2.583850
H	2.896816	1.092648	2.192369
C	4.358086	-2.375879	1.324443
C	4.982104	-1.572057	2.271488
H	4.949866	0.306155	3.315024
H	4.766991	-3.342135	1.063343
H	5.881989	-1.925245	2.757779
C	2.450050	1.617951	-0.999538
C	2.629445	2.964498	-0.657822
C	3.371023	1.033431	-1.874877
C	3.680143	3.706414	-1.176246
C	4.427361	1.766333	-2.396890
H	3.252876	-0.009529	-2.139787
C	4.577420	3.103802	-2.050417
H	3.799078	4.741832	-0.888515
H	5.130282	1.295292	-3.070835
H	5.397659	3.683760	-2.452754
Cl	2.481850	-2.938968	-0.531808
Cl	1.554385	3.741160	0.485985

T(S_5)

Illustration of the molecular structure (dication)



E = -2534.508254 Hartree

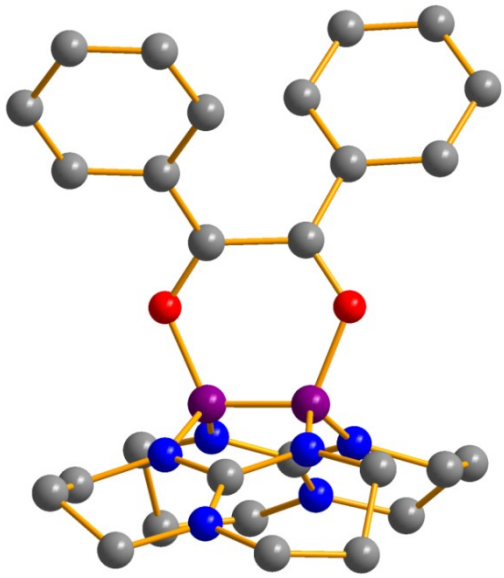
Cartesian coordinates (in Å):

N	-1.281353	-0.844731	-1.808533
N	-1.764826	-1.608265	0.280247
N	-2.272751	-2.968558	-1.574697
N	-2.122906	1.358017	-0.687263
N	-1.609640	0.727133	1.438267
N	-3.098525	2.523111	1.112728
B	-1.004829	0.392374	-1.014662
B	-0.963834	-0.387784	0.678424
C	-1.792404	-1.848415	-1.049029
C	-0.992309	-1.094135	-3.227904
H	-0.043221	-1.628517	-3.333112
H	-0.888092	-0.134214	-3.730740
C	-2.138698	-1.905328	-3.820211
H	-3.053798	-1.309537	-3.801713
H	-1.930884	-2.152063	-4.861653
C	-2.329960	-3.192509	-3.032173
H	-3.298295	-3.641994	-3.258481
H	-1.560837	-3.926131	-3.289938
C	-2.756955	-4.077219	-0.730786
H	-2.412567	-5.008124	-1.183899
H	-3.850174	-4.081507	-0.765335
C	-2.253820	-3.960234	0.699283
H	-1.197270	-4.230908	0.751614

H	-2.803384	-4.658155	1.331348
C	-2.436673	-2.534173	1.204683
H	-3.498581	-2.282947	1.286966
H	-1.989279	-2.416249	2.190712
C	-2.307550	1.570723	0.634173
C	-2.943763	2.085901	-1.666806
H	-3.895312	1.568474	-1.822421
H	-2.411441	2.096707	-2.617010
C	-3.173920	3.506009	-1.163951
H	-2.222757	4.041938	-1.142893
H	-3.838693	4.043197	-1.840806
C	-3.791810	3.475580	0.225078
H	-3.734362	4.459866	0.692308
H	-4.848248	3.195673	0.180915
C	-3.316160	2.711662	2.560083
H	-4.381529	2.892543	2.712101
H	-2.784144	3.617449	2.864733
C	-2.854650	1.511228	3.372783
H	-2.792873	1.794447	4.423811
H	-3.580347	0.698916	3.295093
C	-1.497836	1.030163	2.872162
H	-0.729702	1.791351	3.039828
H	-1.184738	0.125562	3.390675
O	0.278220	1.041108	-1.241358
O	0.423963	-0.681748	1.003781
C	1.405143	0.825504	-0.588209
C	1.499882	-0.170297	0.434732
C	2.762799	-0.725166	0.923556
C	2.971942	-0.800595	2.312174
C	3.747298	-1.269464	0.078340
C	4.143358	-1.315728	2.832006
H	2.213072	-0.408197	2.974952
C	4.923104	-1.791627	0.597929
C	5.127043	-1.799136	1.971438
H	4.297156	-1.337061	3.902408
H	5.658932	-2.214706	-0.071771
H	6.048440	-2.203951	2.369364
C	2.510357	1.698189	-0.986572
C	3.250278	2.473982	-0.075253
C	2.796135	1.840058	-2.356201
C	4.282588	3.292717	-0.510132
C	3.826140	2.650806	-2.791582
H	2.219586	1.268188	-3.070137
C	4.580027	3.367638	-1.864403
H	4.828347	3.887969	0.208738
H	4.049052	2.722605	-3.847525
H	5.389380	4.004992	-2.195945
Cl	3.471628	-1.449109	-1.633103
Cl	2.809013	2.557591	1.608719

Ox(S_6)

Illustration of the molecular structure (dication)



E = -1615.400468 Hartree

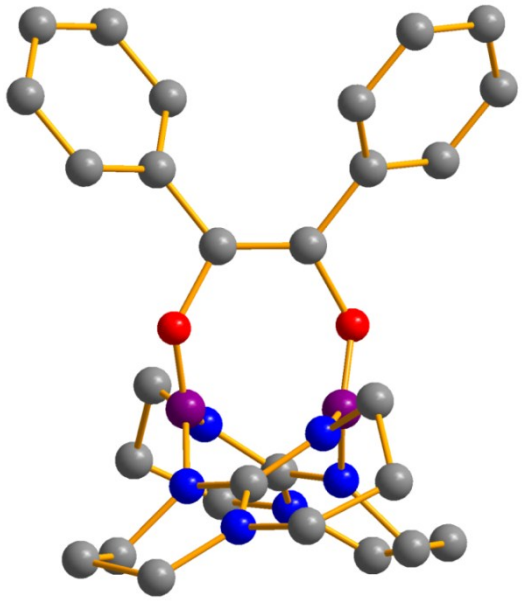
Cartesian coordinates (in Å):

N	-1.062313	-1.892243	-0.912250
N	-1.289377	-1.462854	1.334749
N	-1.695338	-3.646573	0.533630
N	-1.778355	0.619226	-1.400535
N	-1.826726	1.093143	0.848571
N	-3.178252	2.352830	-0.619629
B	-0.812723	-0.405416	-0.839879
B	-0.907582	-0.101843	0.788883
C	-1.352747	-2.373656	0.325114
C	-1.089030	-2.777687	-2.080315
H	-0.098744	-3.216562	-2.244788
H	-1.323117	-2.176121	-2.958505
C	-2.124559	-3.875818	-1.888715
H	-3.127254	-3.441622	-1.884376
H	-2.079458	-4.590379	-2.710814
C	1.867463	-4.597173	-0.577209
H	-2.708400	-5.244518	-0.323882
H	-0.976930	-5.230163	-0.644332
C	-1.953310	-4.174121	1.883187
H	-1.551669	-5.188083	1.919112
H	-3.035085	-4.246232	2.034271

C	-1.311200	-3.305690	2.950905
H	-0.226398	-3.436786	2.935243
H	-1.665734	-3.618031	3.933445
C	-1.655714	-1.845115	2.699874
H	-2.725632	-1.675633	2.865856
H	-1.113169	-1.198718	3.390385
C	-2.283012	1.388353	-0.397324
C	-2.252118	0.792450	-2.775094
H	-3.113651	0.141757	-2.963088
H	-1.455179	0.479856	-3.450527
C	-2.627891	2.245246	-3.026287
H	-1.732003	2.869934	-2.988116
H	-3.066400	2.360143	-4.017825
C	-3.624987	2.704946	-1.977038
H	-3.745598	3.788984	-2.009623
H	-4.610611	2.261763	-2.151497
C	-3.799925	3.105597	0.482313
H	-4.840911	3.283134	0.208138
H	-3.312792	4.082411	0.564353
C	-3.715182	2.341637	1.792170
H	-4.027657	2.989929	2.611047
H	-4.396414	1.487619	1.769849
C	-2.289609	1.857196	2.010775
H	-1.624759	2.708762	2.192581
H	-2.231651	1.212276	2.887558
O	0.636373	0.005274	-1.448066
O	0.553823	0.212856	1.430384
C	1.551196	0.512802	-0.751959
C	1.614027	0.188103	0.756592
C	2.854304	-0.190007	1.386969
C	2.913956	-0.238756	2.799027
C	3.977240	-0.604079	0.635555
C	4.065768	-0.658627	3.429775
H	2.057378	0.077578	3.377192
C	5.114461	-1.055423	1.279594
H	3.950697	-0.602181	-0.444419
C	5.165791	-1.071908	2.672112
H	4.118542	-0.670572	4.510258
H	5.964454	-1.391725	0.701322
H	6.065210	-1.408754	3.172004
C	2.488635	1.425297	-1.357795
C	3.277745	2.306714	-0.584718
C	2.548478	1.504127	-2.768530
C	4.091713	3.235395	-1.206638
H	3.232359	2.286782	0.494458
C	3.389566	2.411613	-3.376673
H	1.946872	0.831443	-3.363192
C	4.158815	3.281446	-2.597822
H	4.678397	3.922658	-0.612124
H	3.453549	2.452679	-4.455835
H	4.811680	3.998008	-3.080135

Red(S_6)

Illustration of the molecular structure (dication)



E = -1615.426159 Hartree

Cartesian coordinates (in Å):

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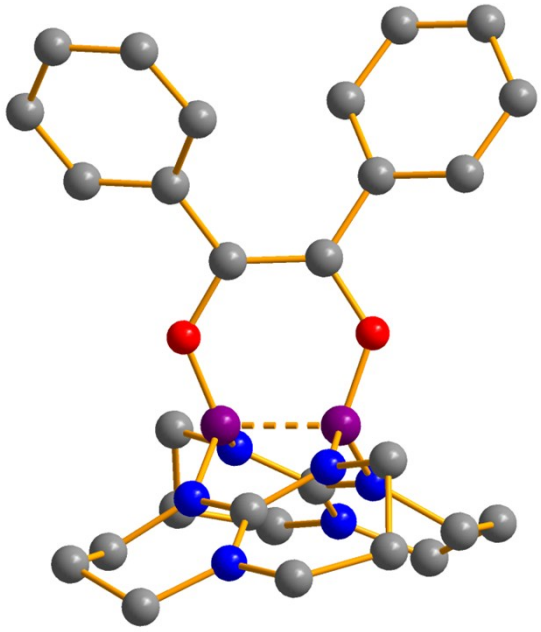
N	-1.928832	-1.542535	0.002572
N	-2.181803	-2.632205	-2.064043
N	-2.262267	1.261297	-0.505366
N	-1.461801	0.470874	1.504580
N	-3.028140	2.219151	1.499187
B	-1.031689	0.698561	-1.134295
B	-0.966099	-0.695054	0.765199
C	-1.762887	-1.607107	-1.342230
C	-0.475871	-0.760553	-3.222067
H	0.400066	-1.402817	-3.102490
H	-0.136128	0.200859	-3.600721
C	-1.513697	-1.393024	-4.140191
H	-2.335503	-0.691285	-4.294461
H	-1.081070	-1.604289	-5.118317
C	-2.025410	-2.694882	-3.535523
H	-2.992045	-2.970266	-3.960759
H	-1.333404	-3.515243	-3.741297
C	-2.808238	-3.825719	-1.453788
H	-2.346088	-4.705545	-1.903906
H	-3.860992	-3.824136	-1.748012

C	-2.664545	-3.855660	0.061339
H	-1.668651	-4.200328	0.345285
H	-3.385254	-4.562922	0.472219
C	-2.895998	-2.462198	0.633549
H	-3.917477	-2.120803	0.443458
H	-2.734131	-2.448272	1.709805
C	-2.279606	1.345220	0.848474
C	-3.348839	1.915104	-1.261212
H	-4.265453	1.322901	-1.188768
H	-3.061808	1.959088	-2.310290
C	-3.548403	3.312808	-0.687302
H	-2.646078	3.903234	-0.855774
H	-4.370684	3.820209	-1.192156
C	-3.859477	3.223987	0.800191
H	-3.692777	4.185204	1.288589
H	-4.904688	2.950797	0.966717
C	-3.069913	2.296526	2.977684
H	-4.118482	2.310187	3.279991
H	-2.639219	3.262674	3.252045
C	-2.319821	1.158479	3.659245
H	-2.075087	1.457759	4.678597
H	-2.948436	0.268487	3.725354
C	-1.053457	0.825011	2.881366
H	-0.361906	1.670664	2.857043
H	-0.527968	-0.024098	3.312806
O	0.116660	1.327617	-0.839756
O	0.331286	-1.006547	0.620299
C	1.383355	0.821106	-0.485152
C	1.459822	-0.188072	0.412483
C	2.638657	-0.638602	1.164852
C	3.512700	0.287284	1.748312
C	2.877048	-2.007217	1.349809
C	4.607422	-0.146957	2.481159
H	3.333464	1.347497	1.629303
C	3.975186	-2.436047	2.081978
H	2.208478	-2.736000	0.910520
C	4.844330	-1.508228	2.647174
H	5.273971	0.578238	2.929488
H	4.155638	-3.495533	2.209599
H	5.699823	-1.844268	3.218459
C	2.489540	1.569517	-1.097485
C	2.391778	2.956671	-1.271851
C	3.633568	0.906556	-1.559273
C	3.423514	3.663192	-1.873657
H	1.512249	3.483712	-0.925766
C	4.660759	1.617446	-2.162242
H	3.717407	-0.166255	-1.447521
C	4.561156	2.996786	-2.317941
H	3.342057	4.735710	-1.993759
H	5.538498	1.093498	-2.517584
H	5.364528	3.549104	-2.787728

T(S_6)

Illustration of the molecular structure (dication)



E = -1615.400412 Hartree

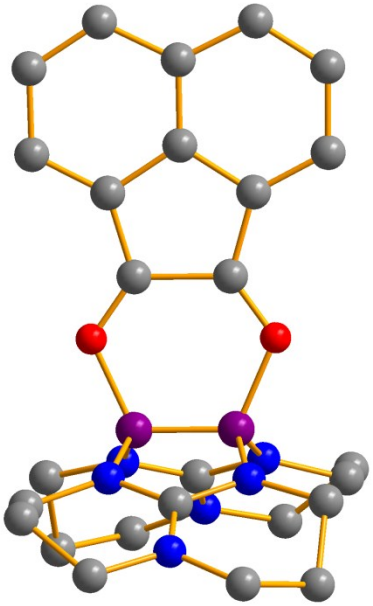
Cartesian coordinates (in Å):

N	-1.252216	-0.905866	-1.776050
N	-1.715519	-1.613330	0.336042
N	-2.225598	-3.029800	-1.475793
N	-2.116025	1.317619	-0.719599
N	-1.594386	0.755717	1.422371
N	-3.117416	2.512901	1.046134
B	-0.980234	0.359422	-1.020081
B	-0.924618	-0.370717	0.694863
C	-1.749768	-1.890615	-0.985012
C	-0.980970	-1.188586	-3.192097
H	-0.028248	-1.716350	-3.299910
H	-0.892941	-0.240905	-3.720679
C	-2.126587	-2.025378	-3.749117
H	-3.047123	-1.437893	-3.733629
H	-1.929848	-2.296920	-4.786539
C	-2.295380	-3.293288	-2.925554
H	-3.261109	-3.758709	-3.129905
H	-1.521370	-4.025432	-3.173248
C	-2.695246	-4.117656	-0.598063
H	-2.346597	-5.058608	-1.026661

H	-3.788693	-4.131898	-0.624509
C	-2.183931	-3.956234	0.824748
H	-1.124901	-4.217116	0.877491
H	-2.723883	-4.640126	1.480036
C	-2.374313	-2.517540	1.289791
H	-3.437886	-2.272850	1.372140
H	-1.922419	-2.368355	2.269590
C	-2.306360	1.562469	0.594619
C	-2.948959	2.002361	-1.718830
H	-3.890547	1.463237	-1.861819
H	-2.415873	1.997364	-2.668728
C	-3.207680	3.431198	-1.256269
H	-2.266942	3.985671	-1.248444
H	-3.881379	3.936802	-1.948476
C	-3.827271	3.426897	0.132314
H	-3.790039	4.424765	0.572165
H	-4.878192	3.125841	0.093840
C	-3.344743	2.733725	2.486892
H	-4.413645	2.900674	2.630211
H	-2.829355	3.655304	2.772587
C	-2.867746	1.561096	3.330546
H	-2.818344	1.869488	4.375134
H	-3.578429	0.734396	3.266664
C	-1.499590	1.092866	2.849243
H	-0.746487	1.871092	3.008079
H	-1.174419	0.206063	3.390666
O	0.287992	1.010159	-1.262715
O	0.460843	-0.629507	1.017786
C	1.437430	0.830373	-0.620684
C	1.545156	-0.116915	0.445837
C	2.796960	-0.649179	0.958017
C	2.864585	-1.068531	2.302017
C	3.919004	-0.850034	0.127665
C	4.025085	-1.625715	2.804932
H	2.008744	-0.930002	2.947587
C	5.067430	-1.432408	0.633504
H	3.876265	-0.583000	-0.918138
C	5.130007	-1.810618	1.972927
H	4.075860	-1.919695	3.844992
H	5.915373	-1.599833	-0.017264
H	6.034674	-2.254955	2.367460
C	2.508535	1.709545	-1.059335
C	3.469596	2.221105	-0.162973
C	2.533229	2.143829	-2.400077
C	4.425752	3.119709	-0.601439
H	3.443428	1.941480	0.880068
C	3.508654	3.021155	-2.834863
H	1.796825	1.767576	-3.096182
C	4.457188	3.513424	-1.937486
H	5.145348	3.521796	0.099303
H	3.535770	3.326872	-3.872427
H	5.214092	4.207776	-2.278765

Ox(S_7)

Illustration of the molecular structure (dication)



E = -1536.817812 Hartree

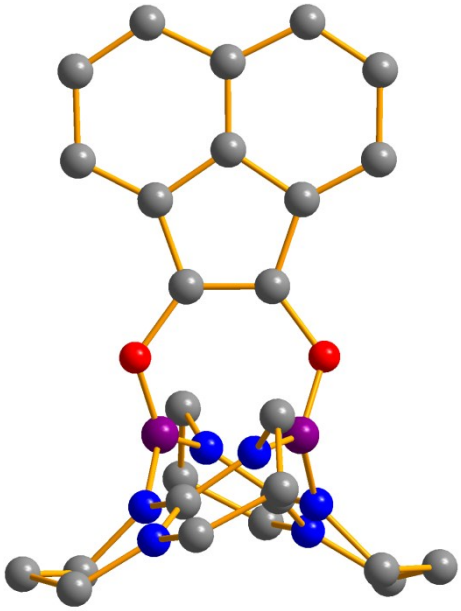
Cartesian coordinates (in Å):

N	-0.999208	-1.446298	-1.518422
N	-1.001483	-1.929946	0.729855
N	-1.388578	-3.666390	-0.821207
N	-1.776961	1.041247	-1.005527
N	-1.842417	0.538110	1.237535
N	-3.301882	2.184916	0.386359
B	-0.773870	-0.083861	-0.903803
B	-0.801782	-0.432531	0.728041
C	-1.130560	-2.387186	-0.545585
C	-1.092522	-1.821967	-2.932961
H	-0.102220	-2.082999	-3.322025
H	-1.439556	-0.954182	-3.493504
C	-2.048692	-2.992418	-3.105330
H	-3.066139	-2.677983	-2.860766
H	-2.050267	-3.334111	-4.140556
C	-1.626602	-4.133944	-2.197138
H	-2.405503	-4.896410	-2.150632
H	-0.717855	-4.617776	-2.568935
C	-1.479424	-4.690648	0.232848
H	-1.017557	-5.599593	-0.156057
H	-2.535086	-4.914076	0.416438

C	-0.787758	-4.241279	1.508065
H	0.296423	-4.263025	1.373347
H	-1.031732	-4.932546	2.314991
C	-1.232643	-2.830360	1.862510
H	-2.292554	-2.827684	2.141065
H	-0.669329	-2.453392	2.716594
C	-2.331341	1.286671	0.212991
C	-2.299878	1.707960	-2.200989
H	-3.118138	1.123061	-2.636142
H	-1.500868	1.753417	-2.941494
C	-2.784650	3.106454	-1.849705
H	-1.935581	3.727402	-1.553826
H	-3.249707	3.578028	-2.715621
C	-3.792365	3.028875	-0.716102
H	-3.986675	4.020816	-0.304917
H	-4.748531	2.628395	-1.067367
C	-3.966264	2.372462	1.687074
H	-5.021207	2.566446	1.487671
H	-3.555568	3.265238	2.169160
C	-3.805116	1.149827	2.573222
H	-4.155090	1.382261	3.579167
H	-4.418581	0.329779	2.192327
C	-2.343583	0.729012	2.602519
H	-1.743960	1.482678	3.124582
H	-2.222855	-0.209125	3.143823
O	0.663902	0.479721	-1.446171
O	0.603355	-0.116012	1.506547
C	1.612652	0.634458	-0.663396
C	1.579832	0.325750	0.883646
C	3.640071	1.112930	0.279652
C	4.971699	1.524985	0.390068
C	2.879037	0.653988	1.388088
C	3.562857	1.542052	-2.107024
C	5.593673	1.955623	-0.811547
C	5.538973	1.462092	1.690237
C	3.459342	0.603384	2.644778
C	4.902593	1.959650	-2.013930
H	3.049621	1.556015	-3.059584
H	6.625098	2.286492	-0.790269
C	4.798124	1.014499	2.773780
H	6.567295	1.768690	1.839714
H	2.906268	0.259170	3.508847
H	5.409443	2.294453	-2.909020
H	5.264193	0.979774	3.749346
C	2.929885	1.116359	-0.950831

Red(S_7)

Illustration of the molecular structure (dication)



E = -1536.833985 Hartree

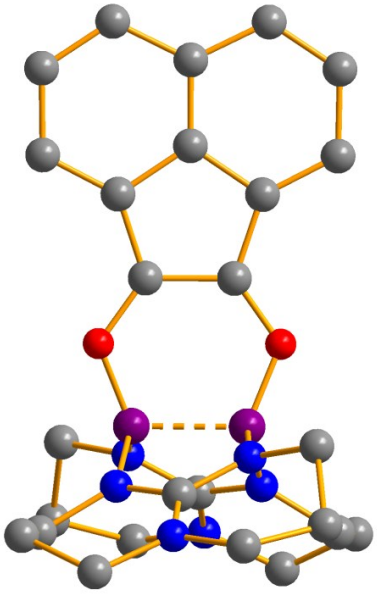
Cartesian coordinates (in Å):

N	-1.200219	-0.525636	-1.916270
N	-1.992008	-1.565435	-0.020466
N	-2.236431	-2.625943	-2.102560
N	-2.410728	1.235617	-0.513881
N	-1.465010	0.465397	1.439280
N	-3.098929	2.150656	1.537642
B	-1.176373	0.740061	-1.187545
B	-1.011853	-0.726180	0.726338
C	-1.833872	-1.608147	-1.364490
C	-0.517864	-0.744354	-3.212291
H	0.349059	-1.392948	-3.067341
H	-0.162089	0.215775	-3.578519
C	-1.537253	-1.366143	-4.158331
H	-2.350475	-0.658271	-4.329060
H	-1.082096	-1.574476	-5.126864
C	-2.071224	-2.669105	-3.574421
H	-3.037481	-2.928030	-4.010671
H	-1.387106	-3.494951	-3.783696
C	-2.842893	-3.838074	-1.507085
H	-2.379117	-4.703093	-1.983005
H	-3.900145	-3.840613	-1.784390

C	-2.671970	-3.897583	0.004269
H	-1.664317	-4.227953	0.262580
H	-3.370929	-4.628332	0.411556
C	-2.922351	-2.522455	0.612041
H	-3.954993	-2.200236	0.452165
H	-2.736169	-2.527334	1.684464
C	-2.360032	1.310436	0.837010
C	-3.544288	1.872499	-1.214529
H	-4.438933	1.251044	-1.118807
H	-3.299397	1.944759	-2.272723
C	-3.762118	3.252457	-0.605136
H	-2.887409	3.875198	-0.800696
H	-4.621722	3.741294	-1.063984
C	-4.004431	3.128125	0.892486
H	-3.856487	4.087995	1.389057
H	-5.028342	2.807241	1.100682
C	-3.050287	2.226219	3.016735
H	-4.075601	2.174440	3.386855
H	-2.664704	3.218649	3.262072
C	-2.184344	1.141088	3.646564
H	-1.877233	1.468064	4.640259
H	-2.753310	0.217975	3.771623
C	-0.965795	0.868033	2.774055
H	-0.329610	1.750857	2.678517
H	-0.359118	0.057815	3.171773
O	-0.046048	1.456883	-0.981438
O	0.293387	-1.064697	0.600530
C	1.157764	0.916362	-0.561157
C	1.301073	-0.180046	0.254389
C	3.367837	0.701052	-0.081662
C	4.743021	0.915159	-0.035625
C	2.708116	-0.360972	0.575127
C	2.951816	2.606080	-1.482743
C	5.225416	2.039641	-0.758607
C	5.495772	-0.017060	0.728672
C	3.459333	-1.254667	1.308199
C	4.347354	2.849092	-1.452719
H	2.306245	3.272468	-2.041369
H	6.284841	2.264082	-0.765945
C	4.861565	-1.062047	1.371948
H	6.570479	0.090682	0.807466
H	3.011633	-2.091615	1.829696
H	4.733869	3.701645	-1.995473
H	5.452410	-1.762650	1.947177
C	2.461223	1.519239	-0.791009

T(S_7)

Illustration of the molecular structure (dication)



E = -1536.818060 Hartree

Cartesian coordinates (in Å):

N	-1.359602	-0.551880	-1.969691
N	-1.737076	-1.663758	-0.019237
N	-2.314007	-2.702916	-2.052505
N	-2.188396	1.422094	-0.480560
N	-1.604370	0.454359	1.495772
N	-3.151027	2.229994	1.511273
B	-1.065756	0.554755	-1.004662
B	-0.947831	-0.509068	0.556000
C	-1.823208	-1.677321	-1.366857
C	-1.124475	-0.562101	-3.421087
H	-0.177624	-1.061139	-3.649259
H	-1.042595	0.468026	-3.762691
C	-2.288814	-1.279218	-4.093756
H	-3.206397	-0.707292	-3.940288
H	-2.122638	-1.347209	-5.169142
C	-2.437578	-2.681523	-3.523126
H	-3.412897	-3.099681	-3.777735
H	-1.677399	-3.352364	-3.933413
C	-2.747259	-3.946279	-1.387625
H	-2.412209	-4.781517	-2.004575
H	-3.840802	-3.965637	-1.377307

C	-2.183756	-4.060778	0.019882
H	-1.123092	-4.317667	-0.017184
H	-2.697717	-4.864087	0.548207
C	-2.359920	-2.742389	0.763432
H	-3.420019	-2.527042	0.928696
H	-1.872723	-2.782366	1.736784
C	-2.345474	1.398998	0.860447
C	-3.057185	2.277861	-1.303340
H	-3.997478	1.763050	-1.523272
H	-2.552001	2.467038	-2.249641
C	-3.314574	3.583764	-0.561392
H	-2.379269	4.139794	-0.469892
H	-4.012571	4.205653	-1.122330
C	-3.893660	3.297379	0.814981
H	-3.851250	4.188909	1.442591
H	-4.942715	2.995655	0.746354
C	-3.340742	2.161161	2.973339
H	-4.407873	2.272816	3.172497
H	-2.833610	3.021936	3.418387
C	-2.817793	0.859410	3.561671
H	-2.736358	0.964024	4.643866
H	-3.517745	0.044807	3.363794
C	-1.460244	0.520855	2.957546
H	-0.714821	1.273493	3.232218
H	-1.098435	-0.442913	3.310779
O	0.191494	1.261454	-1.245044
O	0.447517	-0.816628	0.866839
C	1.312143	0.885495	-0.679063
C	1.436127	-0.123546	0.357125
C	3.502687	0.700503	-0.104602
C	4.882320	0.907372	-0.068328
C	2.823252	-0.243117	0.709418
C	3.137932	2.365901	-1.813740
C	5.385364	1.894889	-0.955079
C	5.606357	0.103765	0.850790
C	3.554554	-1.011780	1.596382
C	4.529761	2.592684	-1.793224
H	2.506938	2.934834	-2.484073
H	6.447151	2.107269	-0.978683
C	4.950875	-0.820479	1.649318
H	6.681104	0.211681	0.930572
H	3.084284	-1.745753	2.237762
H	4.942751	3.340101	-2.457539
H	5.530100	-1.418979	2.339802
C	2.619380	1.409690	-0.959869