Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPORTING INFORMATION

Synthesis, structure and anion binding properties of 1,8-bis(dimesitylboryl)anthracene and its monoborylated analog

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Contents

1. NMR spectra

Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) spectrum of 1-(dimesitylboryl)anthracene (**1**)

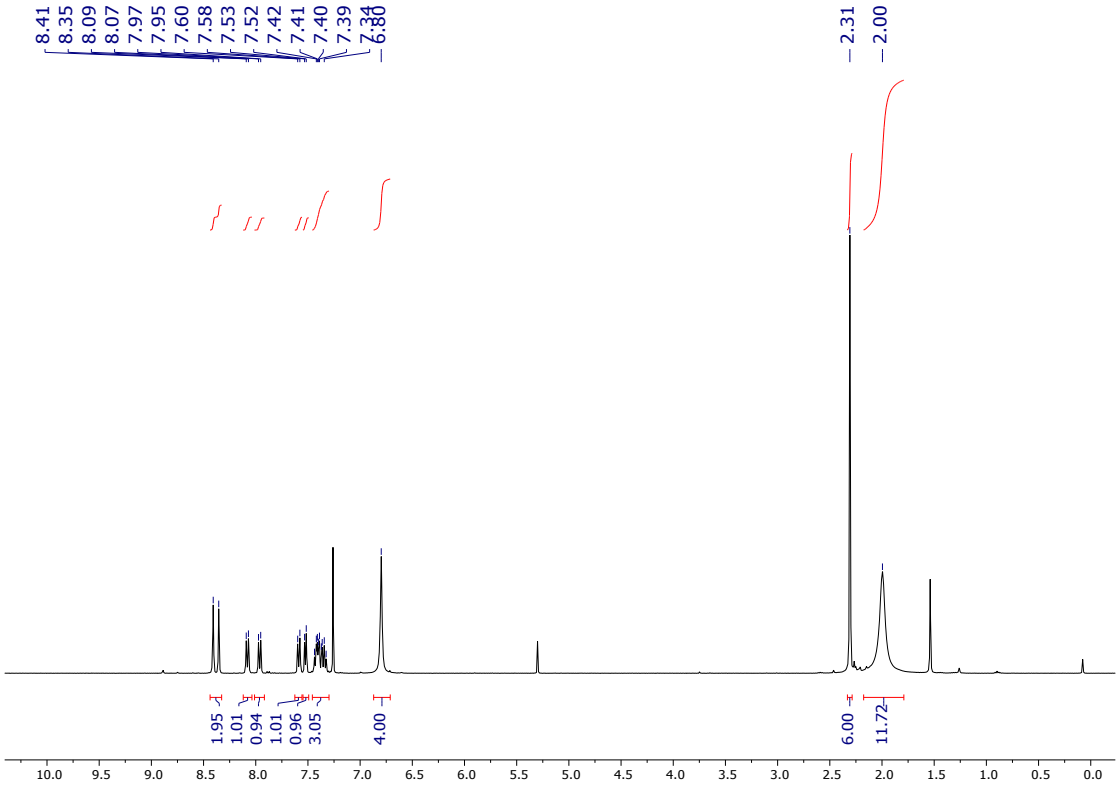


Figure S2. ^{13}C NMR (101 MHz, $CDCl_3$, 298 K) spectrum of 1-(dimesitylboryl)anthracene (**1**)

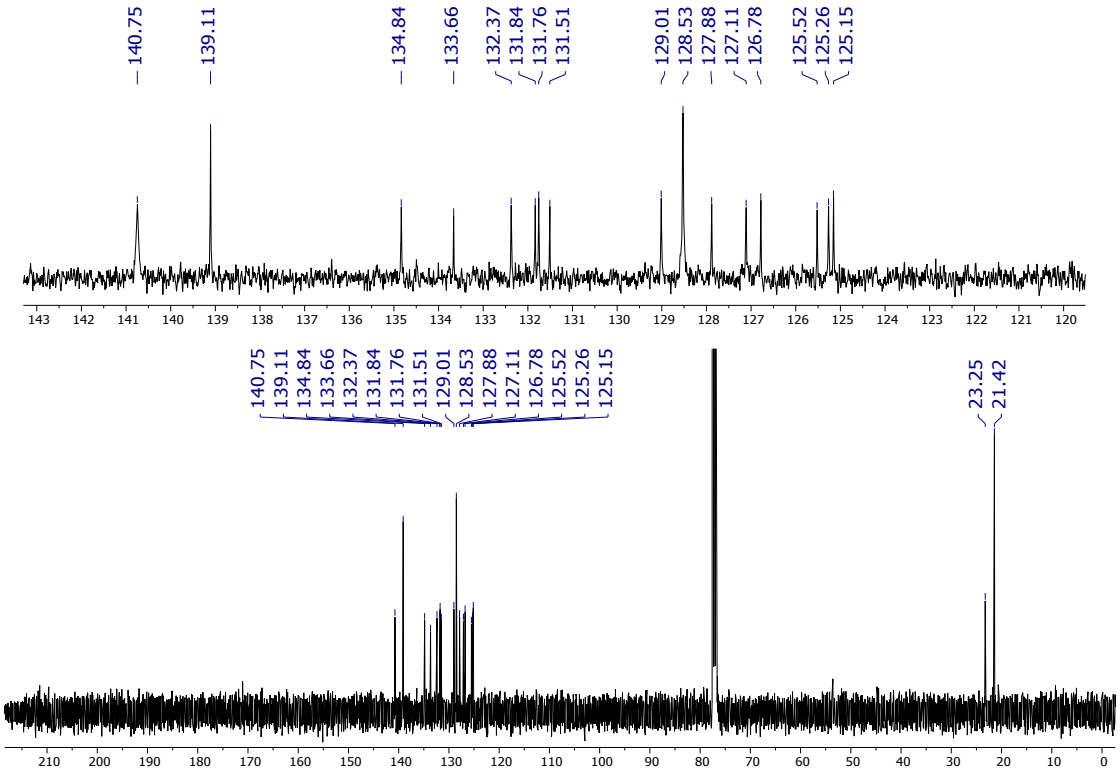


Figure S3. ^{11}B NMR (128 MHz, $CDCl_3$, 298 K) spectrum of 1-(dimesitylboryl)anthracene (**1**)

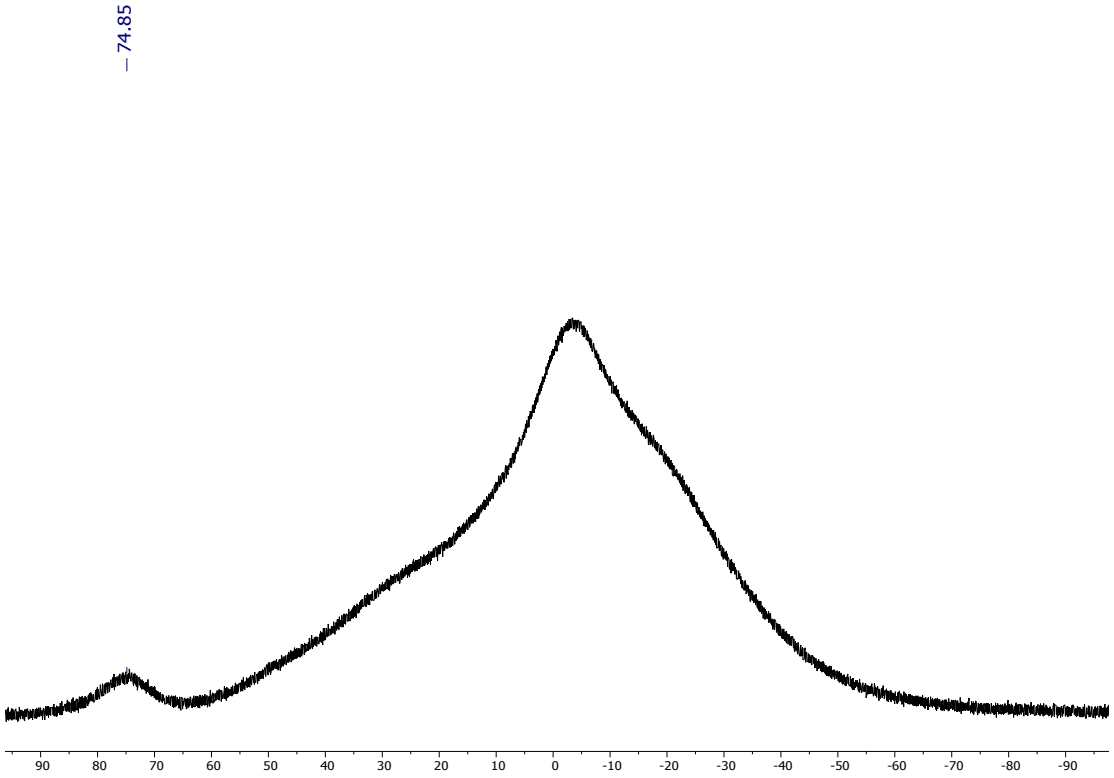


Figure S4. ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) spectrum of 1,8- bis(dimesitylboryl)anthracene (**2**)

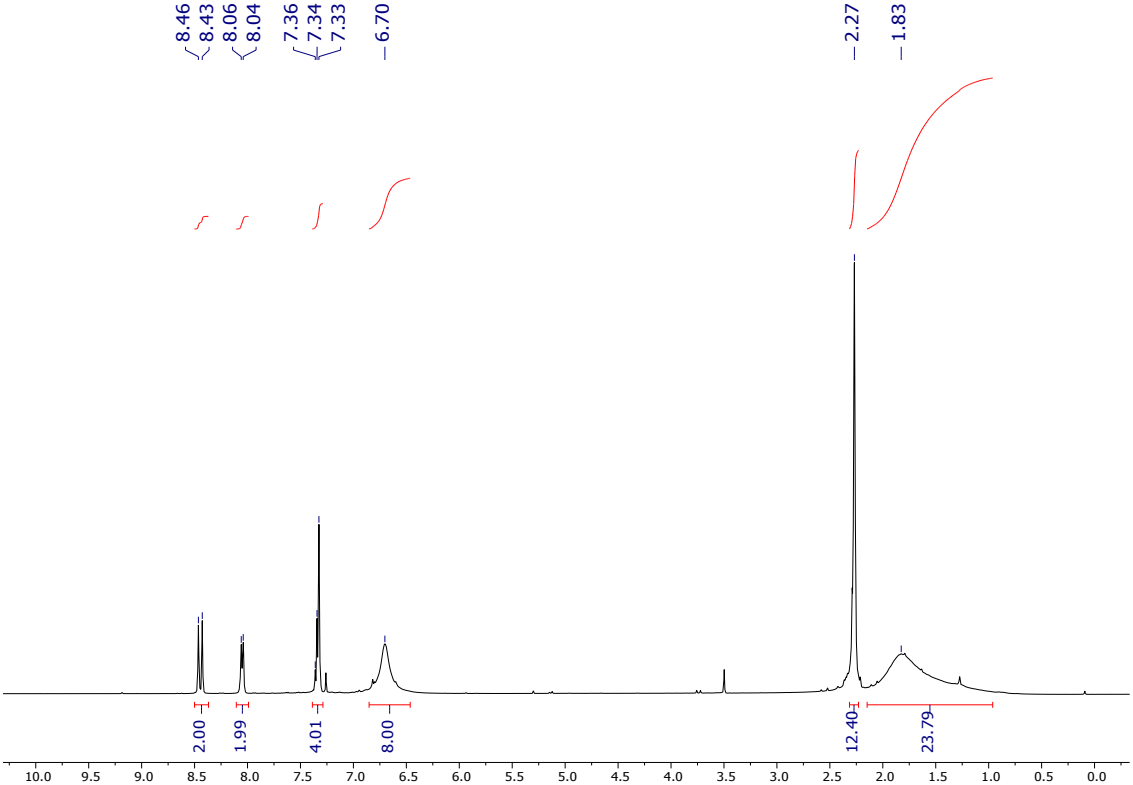


Figure S5. ^{13}C NMR (126 MHz, CD_2Cl_2, 298 K) spectrum of 1,8- bis(dimesitylboryl)anthracene (**2**)

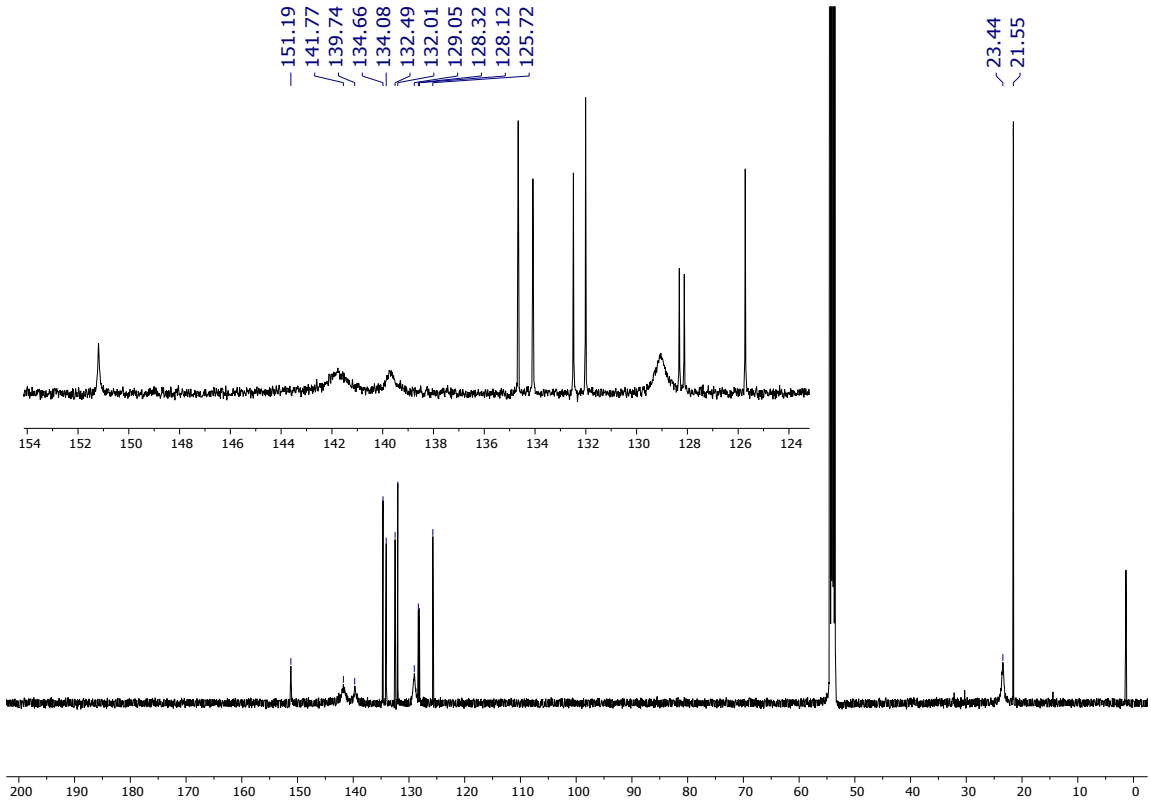
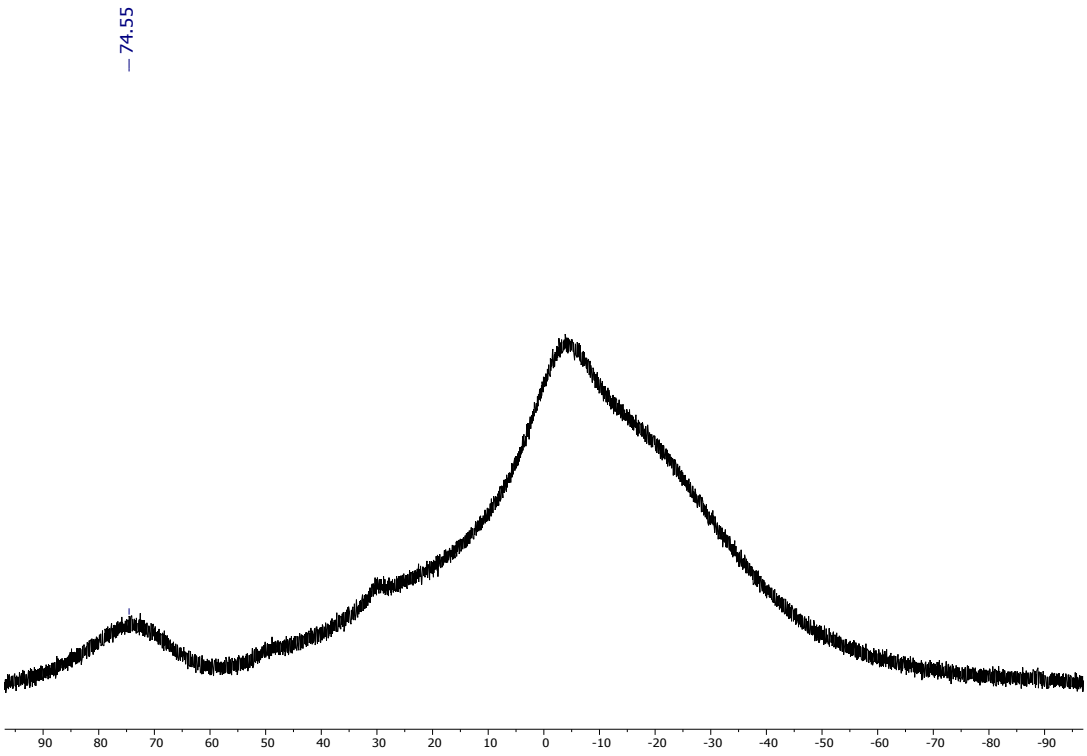


Figure S6. ^{11}B NMR (128 MHz, $CDCl_3$, 298 K) spectrum of 1,8- bis(dimesitylboryl)anthracene (**2**)



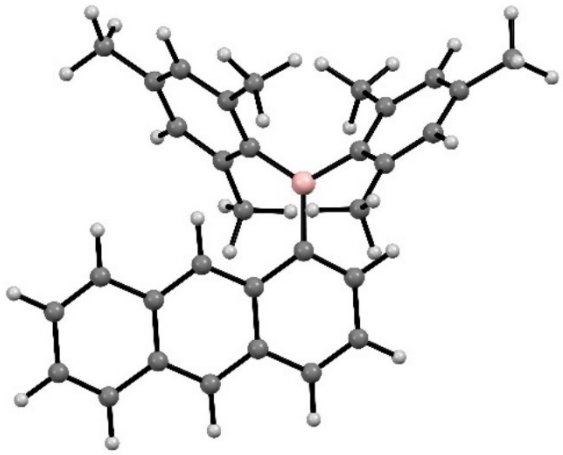
2. Solid-state structures.

X-ray refinement parameters

Compound	**1**	**2**
Empirical formula	$C_{32}H_{31}B$	$C_{50}H_{52}B_2$
Formula weight	426.38	674.53
Temperature/K	109.99	110(2)
Crystal system	monoclinic	Monoclinic
Space group	C2/c	C2/c
a/Å	40.663(5)	15.5053(18)
b/Å	8.0101(9)	19.059(2)
c/Å	15.645(2)	15.890(3)
α/°	90	90
β/°	93.812(4)	113.204(3)
γ/°	90	90
Volume/Å^3	5084.5(11)	4316.0(11)
Z	8	4
ρ_{calc}g/cm^3	1.114	1.038
μ/mm^{-1}	0.062	0.058
F(000)	1824.0	1448.0
Crystal size/mm^3	0.344 × 0.172 × 0.05	0.675 × 0.346 × 0.312
Radiation	Mo-Kα (λ = 0.71073)	Mo-Kα (λ = 0.71073)
2Θ range for data collection/°	5.22 to 54.97	5.104 to 60.064
Index ranges	-52 ≤ h ≤ 52, -10 ≤ k ≤ 10, -20 ≤ l ≤ 20	-21 ≤ h ≤ 21, -26 ≤ k ≤ 26, -22 ≤ l ≤ 22
Reflections collected	28292	27732
Independent reflections	5825 [R_{int} = 0.0636, R_{sigma} = 0.0594]	6307 [R_{int} = 0.0654, R_{sigma} = 0.0624]
Data/restraints/parameters	5825/0/304	6307/0/241
Goodness-of-fit on F^2	1.214	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0959, wR_2 = 0.2189	R_1 = 0.0834, wR_2 = 0.1990
Final R indexes [all data]	R_1 = 0.1254, wR_2 = 0.2330	R_1 = 0.1248, wR_2 = 0.2239
Largest diff. peak/hole / e Å^{-3}	1.15/-0.37	0.39/-0.44
CCDC deposition number	1946228	1946229

4. Geometry optimized structures and cartesian coordinates

S7. Optimized structure and coordinates of **1**



Atom Number	Coordinates X	Y	Z	Atom Number	Coordinates X	Y	Z
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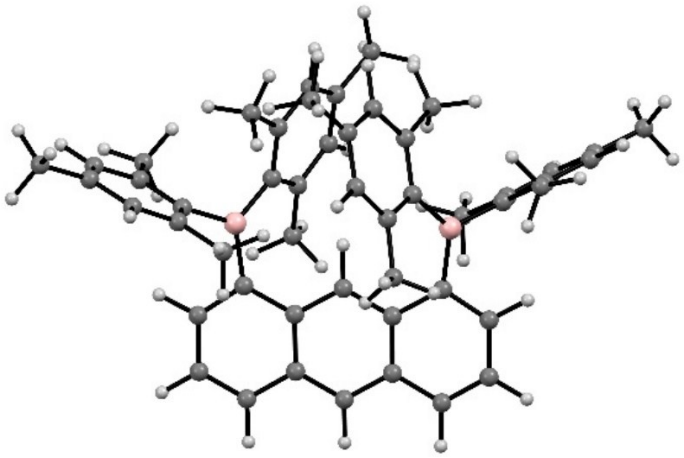
C2	5.634013	-1.329374	-0.505043	H34	7.226427	-0.369600	-1.543435
C3	1.707638	-3.308483	1.746412	H35	6.264953	-2.105197	-0.075787
C4	-3.382238	1.140869	1.606020	H36	2.360713	-4.070876	2.167390
C5	0.367217	-3.319568	1.996521	H37	-3.068645	2.093490	1.161317
C6	-1.599314	1.724495	-2.007913	H38	-4.319988	1.309969	2.145214
C7	5.328965	0.646476	-1.876370	H39	-2.617117	0.867187	2.341830
C8	-6.529482	-1.605036	-1.169874	H40	-0.070300	-4.093032	2.622561
C9	0.488222	1.099013	2.631348	H41	-2.668018	1.573524	-1.811271
C10	2.290346	-2.301807	0.911841	H42	-1.504277	2.445687	-2.826295
C11	0.502581	5.588099	0.411840	H43	-1.204269	0.764854	-2.361426
C12	3.656964	-2.308640	0.623794	H44	5.768992	1.403607	-2.520101
C13	-1.594906	-2.221717	-1.821697	H45	-7.186506	-0.728536	-1.171380
C14	-0.470666	-2.312260	1.433769	H46	-6.576299	-2.070384	-2.159655
C15	3.991026	0.667245	-1.607489	H47	-6.941371	-2.320659	-0.447277
C16	0.025963	-1.284322	0.662211	H48	1.352969	0.459598	2.414741
C17	-5.115912	-1.228655	-0.806216	H49	0.752177	1.746034	3.474027
C18	4.236686	-1.339205	-0.198667	H50	-0.322986	0.437342	2.955771
C19	-4.025585	-1.825119	-1.435392	H51	1.582473	5.717194	0.551312
C20	2.028354	-0.319180	-0.474753	H52	0.217167	6.100293	-0.512267
C21	3.398333	-0.322288	-0.761360	H53	0.005219	6.095646	1.246878
C22	-4.862980	-0.282996	0.188159	H54	4.284217	-3.093070	1.046391
C23	-3.563886	0.074731	0.546617	H55	-1.206802	-3.069854	-1.244785
C24	1.444128	-1.276958	0.360316	H56	-1.958699	-2.605907	-2.780511
C25	-0.511113	3.574507	-0.736022	H57	-0.740731	-1.566144	-2.026898
C26	0.425530	3.287804	1.443152	H58	-1.540077	-2.348185	1.639244
C27	0.131695	4.127691	0.367814	H59	3.348454	1.438556	-2.027647
C28	-0.562006	1.377351	0.308279	H60	-4.202150	-2.554748	-2.225528
C29	-2.711567	-1.515258	-1.079172	H61	1.410125	0.459022	-0.917018
C30	-2.460575	-0.548992	-0.080170	H62	-5.702974	0.197475	0.690026
C31	-0.876466	2.226411	-0.775204	H63	-0.745631	4.210701	-1.589186
C32	0.109469	1.930932	1.424935	H64	0.923487	3.703837	2.319197

S8. Optimized structure and coordinates of **2**



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C4	-3.236775	0.505485	-2.065190	H56	-5.569684	-1.255508	3.115930
C5	1.163905	-3.469415	3.435293	H57	-3.914481	-1.780262	2.751639
C6	-2.263639	-2.611447	-0.091227	H58	-4.253960	-0.072285	3.025085
C7	-0.800787	-0.297844	2.626208	H59	-7.576352	-2.130674	-2.361281
C8	0.188793	-2.522575	2.786892	H60	-8.162967	-2.451400	-0.717817
C9	0.051569	-1.213624	3.244927	H61	-8.434230	-0.872620	-1.466136
C10	-1.461975	-2.035612	1.057249	H62	-3.455365	0.242076	-3.106073
C11	-1.574385	-0.688837	1.499242	H63	-3.242375	1.600034	-1.983517
C12	-0.584321	-2.911973	1.696843	H64	-2.209245	0.176137	-1.850560
C13	-6.404559	-1.196868	-0.803074	H65	2.191522	-3.237665	3.123861
C14	-5.443623	-0.616046	-1.633268	H66	1.127797	-3.392326	4.527540
C15	-6.131090	-1.283333	0.561507	H67	0.958492	-4.507906	3.155908
C16	-4.246306	-0.116474	-1.123668	H68	-1.848948	-3.582191	-0.382629
C17	-4.927018	-0.819740	1.096522	H69	-3.313802	-2.760592	0.185775
C18	-3.969856	-0.228472	0.253162	H70	-2.247769	-1.966284	-0.975390
C19	-2.353246	4.706718	0.700961	H71	0.625897	-0.894570	4.115092
C20	-3.522329	2.614338	0.964038	H72	-0.504384	-3.935680	1.330835
C21	-3.501613	4.038520	1.002591	H73	-5.636046	-0.549834	-2.704451
C22	-1.167126	3.990051	0.348058	H74	-6.869609	-1.733300	1.225241
C23	-2.401544	1.857362	0.689382	H75	-2.316965	5.794550	0.709911
C24	-1.177170	2.553062	0.350030	H76	-4.463661	2.108135	1.173038
C25	0.864834	1.080391	-3.249668	H77	-4.407679	4.581644	1.258257
C26	4.655503	-0.990334	-2.574945	H78	0.522713	1.033816	-4.288580
C27	7.712471	-1.692731	1.366709	H79	0.215645	1.787762	-2.719038
C28	3.236882	0.506007	2.065024	H80	1.873696	1.502884	-3.244812
C29	-1.164144	-3.470298	-3.434151	H81	5.569568	-1.256529	-3.115681
C30	2.263565	-2.611455	0.091990	H82	3.914330	-1.781027	-2.751172
C31	0.000048	4.669562	-0.000605	H83	4.253954	-0.073159	-3.025127
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C34	-0.188955	-2.523319	-2.786068	H86	8.434633	-0.872389	1.465231

C35	-0.051666	-1.214515	-3.244512	H87	3.455464	0.242831	3.105967
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C37	1.574361	-0.689282	-1.499029	H89	2.209332	0.176667	1.850481
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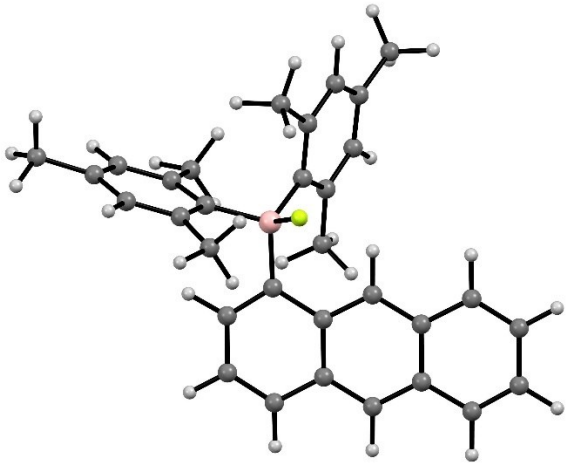
C43	4.927014	-0.820111	-1.096376	H95	2.247691	-1.966063	0.975987
C44	3.969879	-0.228604	-0.253146	H96	0.000058	5.759260	-0.000763
C45	2.353329	4.706481	-0.702216	H97	0.000004	0.788124	-0.000062
C46	3.522365	2.614012	-0.964768	H98	-0.626003	-0.895695	-4.114758
C47	3.501675	4.038184	-1.003700	H99	0.504201	-3.936018	-1.329608
C48	1.167205	3.989930	-0.349087	H100	5.636161	-0.549164	2.704500
C49	2.401579	1.857127	-0.689867	H101	6.869598	-1.733702	-1.224910
C50	1.177226	2.552939	-0.350657	H102	2.317065	5.794312	-0.711467
B51	-2.590723	0.298415	0.812813	H103	4.463682	2.107738	-1.173668
B52	2.590728	0.298142	-0.812885	H104	4.407741	4.581224	-1.259548

S9. Optimized structure and coordinates of [**1**-F]$^{-}$



Atom	Coordinates			Atom	Coordinates		
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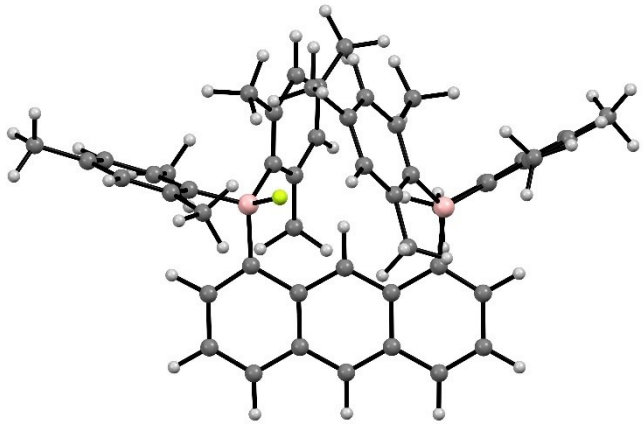
C2	-0.717158	1.278376	2.222075	H35	-3.712705	1.443031	-2.045714
C3	2.987840	0.716136	1.734607	H36	-0.892959	1.909595	3.101491
C4	6.410955	-2.238131	-0.396874	H37	-1.691071	0.913537	1.877014
C5	1.732205	-2.379003	-2.160479	H38	-0.150580	0.399589	2.542571
C6	0.558063	5.832510	0.647396	H39	3.766051	0.666224	2.506364
C7	2.198150	1.912693	-1.982205	H40	2.941466	1.746682	1.362615
C8	-0.002845	2.076785	1.147846	H41	2.024086	0.510857	2.212285
C9	0.617351	4.337348	0.454907	H42	7.001559	-1.692129	-1.145193
C10	-0.016431	3.466318	1.331345	H43	6.915821	-2.116921	0.568688
C11	1.339274	2.390473	-0.826485	H44	6.447884	-3.300055	-0.668264
C12	0.667401	1.491738	0.046979	H45	2.154711	-3.317161	-2.542116
C13	1.300635	3.771463	-0.617955	H46	0.776192	-2.596061	-1.673187
C14	4.989873	-1.734490	-0.338520	H47	1.501831	-1.727417	-3.009039
C15	4.015870	-2.210454	-1.212457	H48	-0.275159	6.278046	0.086823

C16	4.594258	-0.781879	0.592944	H49	0.416245	6.093150	1.702812
C17	2.704165	-1.727503	-1.197628	H50	1.478387	6.316237	0.298673
C18	3.287594	-0.279494	0.631468	H51	2.496838	2.761905	-2.609110
C19	2.308834	-0.707735	-0.295127	H52	3.111427	1.430037	-1.610624
C20	-1.861302	-3.046479	1.930690	H53	1.678863	1.176621	-2.599259
C21	0.299333	-2.089592	1.380115	H54	-0.539435	3.877094	2.196934
C22	-0.508281	-3.024387	2.095467	H55	1.835299	4.425107	-1.309917
C23	-2.483618	-2.118686	1.038454	H56	4.279983	-2.996823	-1.922599
C24	-0.218024	-1.158224	0.510250	H57	5.319986	-0.420554	1.324060
C25	-1.659158	-1.172749	0.327575	H58	-2.488264	-3.757800	2.466788
C26	-3.871515	-2.111148	0.863333	H59	1.377316	-2.123892	1.532948
C27	-2.300678	-0.248146	-0.508504	H60	-0.030764	-3.730579	2.773459
C28	-5.917934	-1.159773	-0.166483	H61	-4.477783	-2.836739	1.407212
C29	-5.693119	0.721883	-1.678912	H62	-1.695289	0.479343	-1.042495
C30	-6.497246	-0.236008	-0.988160	H63	-6.525937	-1.891930	0.363427
C31	-4.499597	-1.191143	0.022961	H64	-6.169359	1.451329	-2.329893
C32	-4.336326	0.719729	-1.523459	H65	-7.576862	-0.224053	-1.122077
C33	-3.690133	-0.232312	-0.672458				

S10. Optimized structure and coordinates of [**2**-F]$^{-}$



Atom	Coordinates			Atom	Coordinates		
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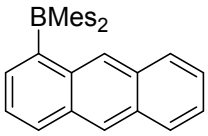
C3	4.126936	-0.788079	-2.550381	H56	1.609539	1.212866	-2.948390
C4	8.109693	-1.382549	0.428203	H57	4.939794	-0.852757	-3.284445
C5	3.940626	0.560174	2.390851	H58	3.489743	-1.673159	-2.666942
C6	-0.773947	-4.124871	-3.086763	H59	3.510058	0.081262	-2.804016
C7	2.369369	-2.699546	0.520707	H60	8.206249	-2.178854	1.177512
C8	0.755641	-0.696598	-2.316708	H61	8.533437	-1.755821	-0.510951
C9	0.053081	-3.035929	-2.452365	H62	8.733667	-0.545466	0.767611
C10	0.047750	-1.736798	-2.941502	H63	4.699299	0.814014	3.142020
C11	1.526783	-2.268845	-0.664301	H64	3.384306	1.465582	2.127772
C12	1.498475	-0.925260	-1.135041	H65	3.210138	-0.119155	2.844818
C13	0.820554	-3.281559	-1.315530	H66	-1.733219	-4.245414	-2.563134
C14	6.671190	-0.963577	0.248168	H67	-0.999482	-3.897564	-4.135029
C15	5.936924	-0.438471	1.310293	H68	-0.259912	-5.092910	-3.050223
C16	6.032525	-1.052794	-0.982535	H69	2.034495	-3.678041	0.889334
C17	4.602828	-0.049180	1.171273	H70	3.425953	-2.789293	0.235876

C18	4.694049	-0.675135	-1.149613	H71	2.310359	-1.976504	1.337098
C19	3.925050	-0.199461	-0.065062	H72	-0.521495	-1.513154	-3.846094
C20	2.106152	4.613973	-1.185033	H73	0.867409	-4.297757	-0.917149
C21	3.301241	2.505154	-1.075384	H74	6.423516	-0.314689	2.280122
C22	3.255080	3.902646	-1.363810	H75	6.589920	-1.421281	-1.845857
C23	0.928597	3.950300	-0.721015	H76	2.059508	5.682468	-1.391077
C24	2.213185	1.791374	-0.627027	H77	4.251511	1.990312	-1.209903
C25	0.981067	2.537762	-0.449943	H78	4.156106	4.401304	-1.718457
C26	-1.399503	1.570652	3.246860	H79	-1.132466	1.687464	4.302940
C27	-4.927799	-0.819651	2.478384	H80	-0.793988	2.278845	2.668605
C28	-7.547221	-2.157370	-1.614373	H81	-2.446908	1.863812	3.124970
C29	-3.114847	0.169856	-2.154643	H82	-5.864211	-1.119235	2.962177
C30	1.191374	-2.623460	4.007832	H83	-4.133212	-1.498292	2.813602
C31	-2.054598	-2.554884	0.215110	H84	-4.662494	0.180710	2.844996
C32	-0.271866	4.645071	-0.547394	H85	-7.284744	-2.751006	-2.497348
C33	-0.204036	1.898707	-0.054694	H86	-8.061831	-2.813425	-0.903900
C34	-1.126679	0.150981	2.798468	H87	-8.265404	-1.392677	-1.938304
C35	0.136233	-1.884944	3.227065	H88	-3.204693	-0.242183	-3.166106
C36	-0.217030	-0.579774	3.559134	H89	-3.185643	1.263231	-2.221305
C37	-1.435861	-1.790945	1.366926	H90	-2.101981	-0.062121	-1.796607
C38	-1.752175	-0.439612	1.669645	H91	2.192749	-2.302413	3.692841
C39	-0.493811	-2.474005	2.135363	H92	1.104714	-2.428703	5.083233
C40	-6.323680	-1.529219	-0.994053	H93	1.125534	-3.704572	3.843373
C41	-5.307321	-1.006497	-1.795726	H94	-1.593797	-3.544871	0.139305
C42	-6.185768	-1.435291	0.389616	H95	-3.135248	-2.685980	0.341712
C43	-4.186606	-0.387853	-1.243643	H96	-1.883604	-2.055252	-0.746576
C44	-5.059755	-0.847576	0.971717	H97	-0.299452	5.716093	-0.752475
C45	-4.046828	-0.314588	0.156621	H98	-0.167027	0.828068	0.128309
C46	-2.670821	4.713219	0.018683	H99	0.252785	-0.104499	4.420514
C47	-3.802459	2.644655	0.541713	H100	-0.236237	-3.497246	1.862445
C48	-3.819224	4.057948	0.354957	H101	-5.391925	-1.083172	-2.880527
C49	-1.441015	4.000938	-0.142413	H102	-6.967431	-1.841160	1.032926
C50	-2.641548	1.905081	0.461168	H103	-2.669476	5.789881	-0.147747
C51	-1.414514	2.584106	0.100258	H104	-4.741942	2.138019	0.762664
B52	2.324415	0.194298	-0.218096	H105	-4.754741	4.602508	0.463500
B53	-2.760252	0.367059	0.779170				

5. TD-DFT output

Excitation energies and oscillator strengths for **1** between 300-600 nm.



Excited State 1: Singlet-A 2.9819 eV 415.79 nm f=0.1892 <S**2>=0.000
114 ->115 0.69386
114 ->116 0.10420
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1262.57239304
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.5677 eV 347.52 nm f=0.0875 <S**2>=0.000
113 ->115 0.64911
113 ->116 0.16963
114 ->116 0.19380

Excited State 3: Singlet-A 3.5969 eV 344.69 nm f=0.0205 <S**2>=0.000
113 ->115 -0.19670
114 ->116 0.65683

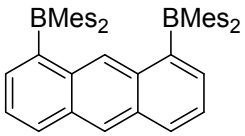
Excited State 4: Singlet-A 3.8123 eV 325.22 nm f=0.0459 <S**2>=0.000
109 ->115 -0.10747
111 ->115 -0.16171
112 ->115 0.64691
112 ->116 0.12385

Excited State 5: Singlet-A 3.8628 eV 320.97 nm f=0.0186 <S**2>=0.000
109 ->115 0.10122
111 ->115 0.63491
111 ->116 0.14004
112 ->115 0.18904
114 ->117 0.11342

Excited State 6: Singlet-A 3.9198 eV 316.30 nm f=0.0231 <S**2>=0.000
110 ->115 0.65762
110 ->116 0.15641
111 ->115 0.11923

Excited State 7: Singlet-A 3.9475 eV 314.09 nm f=0.0138 <S**2>=0.000
109 ->115 0.52504
109 ->116 -0.11190
110 ->115 0.12915
111 ->115 -0.15181
114 ->117 0.38277

Excitation energies and oscillator strengths for **2** between 300-600 nm.



Excited State 1: Singlet-A 2.9477 eV 420.61 nm f=0.2098 <S**2>=0.000
181 ->182 0.70077
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1985.84755903
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.1254 eV 396.70 nm f=0.0268 <S**2>=0.000
181 ->183 0.69833

Excited State 3: Singlet-A 3.5234 eV 351.88 nm f=0.1271 <S**2>=0.000
179 ->183 0.32205
180 ->182 0.61055
180 ->184 0.10018

Excited State 4: Singlet-A 3.5398 eV 350.25 nm f=0.0009 <S**2>=0.000
179 ->182 0.58560
179 ->184 0.10652
180 ->183 0.36212

Excited State 5: Singlet-A 3.7129 eV 333.93 nm f=0.0009 <S**2>=0.000
181 ->184 0.69135

Excited State 6: Singlet-A 3.7236 eV 332.97 nm f=0.0069 <S**2>=0.000
177 ->183 0.11909
178 ->182 0.67347

Excited State 7: Singlet-A 3.7923 eV 326.94 nm f=0.0177 <S**2>=0.000
172 ->182 -0.28884
175 ->183 -0.14021
176 ->182 0.50460
177 ->182 -0.27981
178 ->183 -0.12712
181 ->185 0.16452

Excited State 8: Singlet-A 3.8620 eV 321.04 nm f=0.0278 <S**2>=0.000
173 ->182 -0.15871
176 ->182 0.27723
177 ->182 0.40961
178 ->183 0.44414

Excited State 9: Singlet-A 3.8837 eV 319.24 nm f=0.0143 <S**2>=0.000
175 ->182 0.63536
176 ->183 -0.14758
177 ->183 0.16810
180 ->183 -0.13938

Excited State 10: Singlet-A 3.9138 eV 316.79 nm f=0.0001 <S**2>=0.000
172 ->182 0.32867
173 ->182 0.24625
176 ->182 0.31357
179 ->183 0.30136
180 ->182 -0.15486
181 ->185 -0.30077

Excited State 11: Singlet-A 3.9585 eV 313.21 nm f=0.0129 <S**2>=0.000
172 ->182 -0.28663
173 ->182 0.26602

174 ->183 -0.19761
175 ->183 0.22118
177 ->182 0.34424
178 ->183 -0.26998
179 ->183 0.17018
181 ->185 0.12769

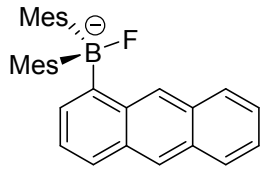
Excited State 12: Singlet-A 3.9775 eV 311.71 nm f=0.0149 <S**2>=0.000
174 ->182 0.60061
177 ->183 -0.25916
180 ->183 -0.17472

Excited State 13: Singlet-A 3.9898 eV 310.75 nm f=0.0428 <S**2>=0.000
174 ->182 0.17355
175 ->182 0.13197
176 ->183 -0.16299
179 ->182 -0.34840
179 ->184 0.12446
180 ->183 0.52240

Excited State 14: Singlet-A 4.0114 eV 309.08 nm f=0.0678 <S**2>=0.000
172 ->182 -0.18009
174 ->183 0.15454
176 ->182 -0.14015
177 ->182 -0.15062
178 ->183 0.23864
179 ->183 0.44446
180 ->182 -0.29685
180 ->184 0.12856
181 ->185 0.16290

Excited State 15: Singlet-A 4.1144 eV 301.34 nm f=0.0104 <S**2>=0.000
172 ->182 -0.14438
173 ->182 0.54219
177 ->182 -0.15010
178 ->183 0.33777
179 ->183 -0.15766

Excitation energies and oscillator strengths for [**1**-F]$^-$ between 300-600 nm.



Excited State 1: Singlet-A 3.2327 eV 383.53 nm f=0.1120 <S**2>=0.000
119 ->120 0.70103
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -1362.53693173

Copying the excited state density for this state as the 1-particle RhoCI density.

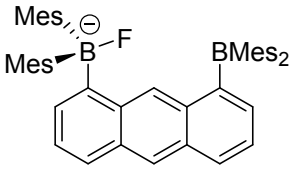
Excited State 2: Singlet-A 3.6975 eV 335.32 nm f=0.0002 <S**2>=0.000
117 ->120 0.13106
118 ->120 0.68274

Excited State 3: Singlet-A 3.8171 eV 324.82 nm f=0.0048 <S**2>=0.000
117 ->120 0.67879
118 ->120 -0.12835

Excited State 4: Singlet-A 3.9737 eV 312.01 nm f=0.0035 <S**2>=0.000
113 ->120 0.43797
115 ->120 -0.14371
116 ->120 0.15251
117 ->120 0.13291
119 ->121 0.48577

Excited State 5: Singlet-A 4.1288 eV 300.29 nm f=0.0044 <S**2>=0.000
113 ->120 -0.15015
115 ->120 -0.19105
116 ->120 0.64508
119 ->121 -0.13115

Excitation energies and oscillator strengths for [**2**-F]$^-$ between 300-600 nm.



Excited State 1: Singlet-A 2.7781 eV 446.29 nm f=0.1118 <S**2>=0.000
186 ->187 0.69942
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2085.82279722
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.3385 eV 371.37 nm f=0.0028 <S**2>=0.000
184 ->187 0.23411
185 ->187 0.66249

Excited State 3: Singlet-A 3.4211 eV 362.41 nm f=0.0283 <S**2>=0.000
184 ->187 0.12691
186 ->188 0.67521

Excited State 4: Singlet-A 3.4547 eV 358.88 nm f=0.0087 <S**2>=0.000
184 ->187 0.64334
185 ->187 -0.22933
186 ->188 -0.12956

Excited State 5: Singlet-A 3.6150 eV 342.97 nm f=0.0210 <S**2>=0.000
179 ->187 -0.12006
181 ->187 -0.15509
183 ->187 0.66262

Excited State 6: Singlet-A 3.6775 eV 337.15 nm f=0.0775 <S**2>=0.000
177 ->187 -0.11722
179 ->187 0.16077
181 ->187 0.61694
181 ->188 0.10296
183 ->187 0.19015

Excited State 7: Singlet-A 3.7951 eV 326.69 nm f=0.0328 <S**2>=0.000
177 ->187 0.10620
177 ->188 -0.10552
178 ->187 -0.20755
179 ->187 0.13765
180 ->187 0.59116
186 ->189 -0.19297

Excited State 8: Singlet-A 3.8984 eV 318.04 nm f=0.0083 <S**2>=0.000
177 ->187 0.31646
178 ->187 -0.17003
179 ->187 0.25341
180 ->187 -0.27014
180 ->188 -0.11838
183 ->187 0.11345
184 ->188 -0.13802
185 ->188 -0.29536
186 ->189 -0.25668

Excited State 9: Singlet-A 3.9211 eV 316.20 nm f=0.0059 <S**2>=0.000
177 ->187 0.27818
179 ->187 -0.12301
182 ->187 0.22239
185 ->188 0.52148
186 ->189 -0.21713

Excited State 10: Singlet-A 3.9345 eV 315.12 nm f=0.0018 <S**2>=0.000
179 ->187 -0.13720
180 ->187 0.12225
182 ->187 0.63608
185 ->188 -0.19908

Excited State 11: Singlet-A 3.9494 eV 313.93 nm f=0.0565 <S**2>=0.000
177 ->187 -0.25380
178 ->187 -0.34311
179 ->187 0.36245

180 ->187 -0.11405
181 ->187 -0.19460
182 ->187 0.12718
185 ->188 0.24626
186 ->189 0.13368

Excited State 12: Singlet-A 4.0197 eV 308.44 nm f=0.0021 <S**2>=0.000
184 ->188 0.67193
185 ->188 -0.10480

Excited State 13: Singlet-A 4.0894 eV 303.18 nm f=0.0068 <S**2>=0.000
178 ->187 0.50781
179 ->187 0.42013
181 ->187 -0.10697

6. Spectrophysical studies

UV-vis spectra and binding isotherms

Figure S11. UV-vis spectrum of **1** titrated against TBACN. The inset shows a plot of the absorbance at 389 nm as a function of fluoride concentration.

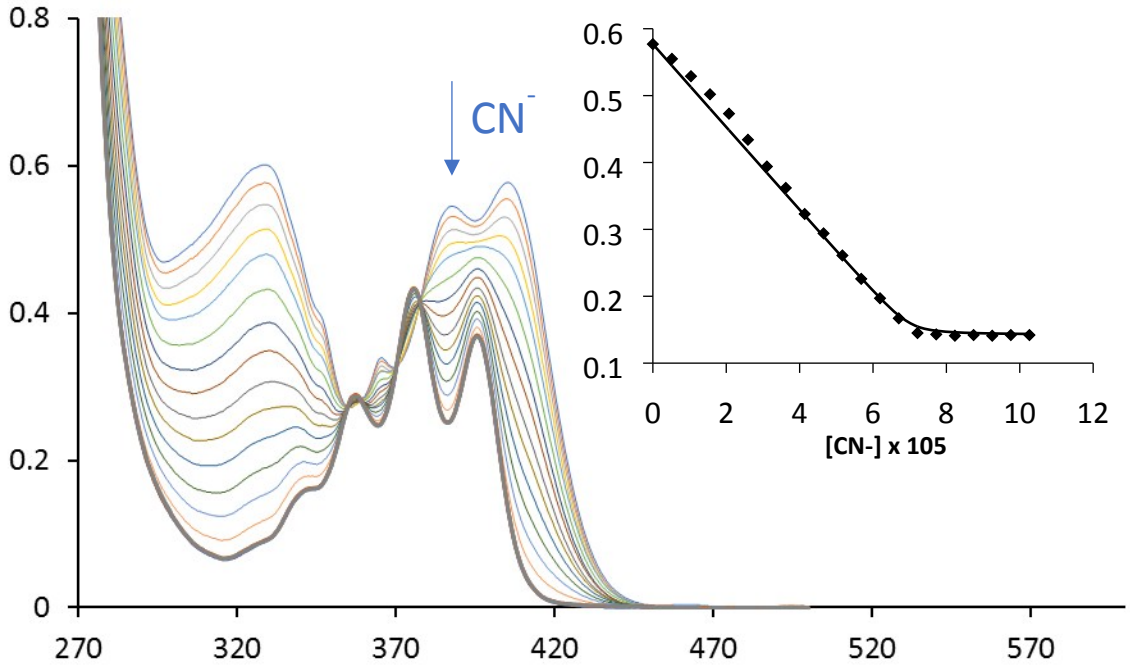
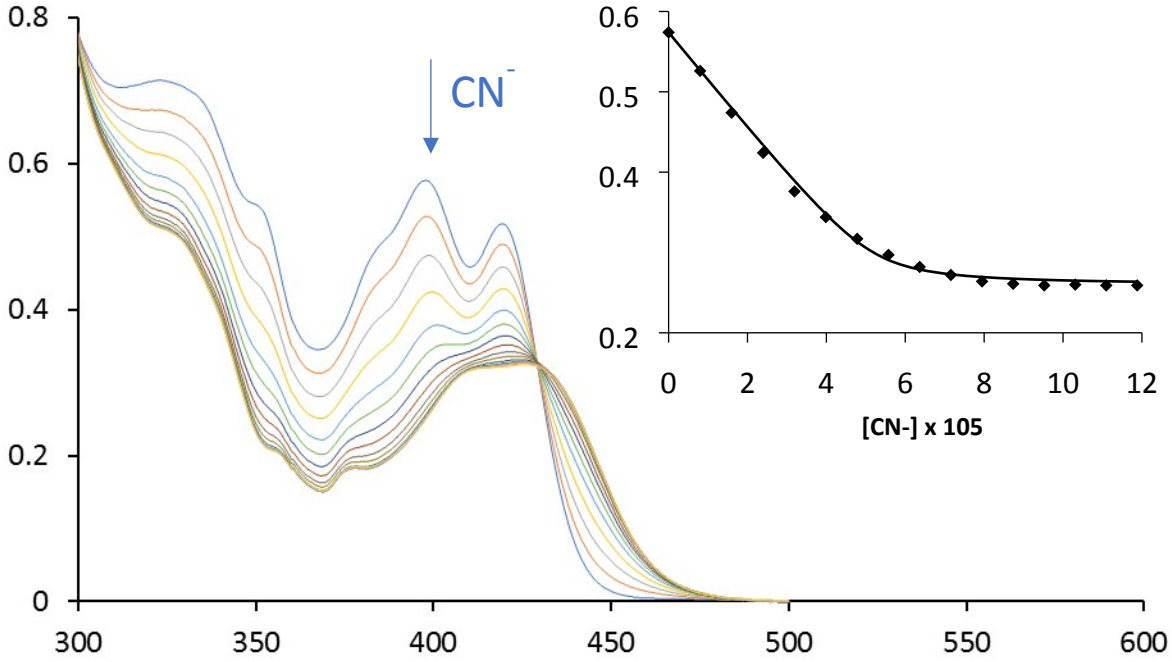


Figure S12. UV-vis spectrum of **2** titrated against TBAF. The inset shows a plot of the absorbance at 400 nm as a function of fluoride concentration.



Fluorescence emission spectra and quantum yield

Figure S13. Emission spectrum of **1** titrated against TBAF. Quantum yield determination inset

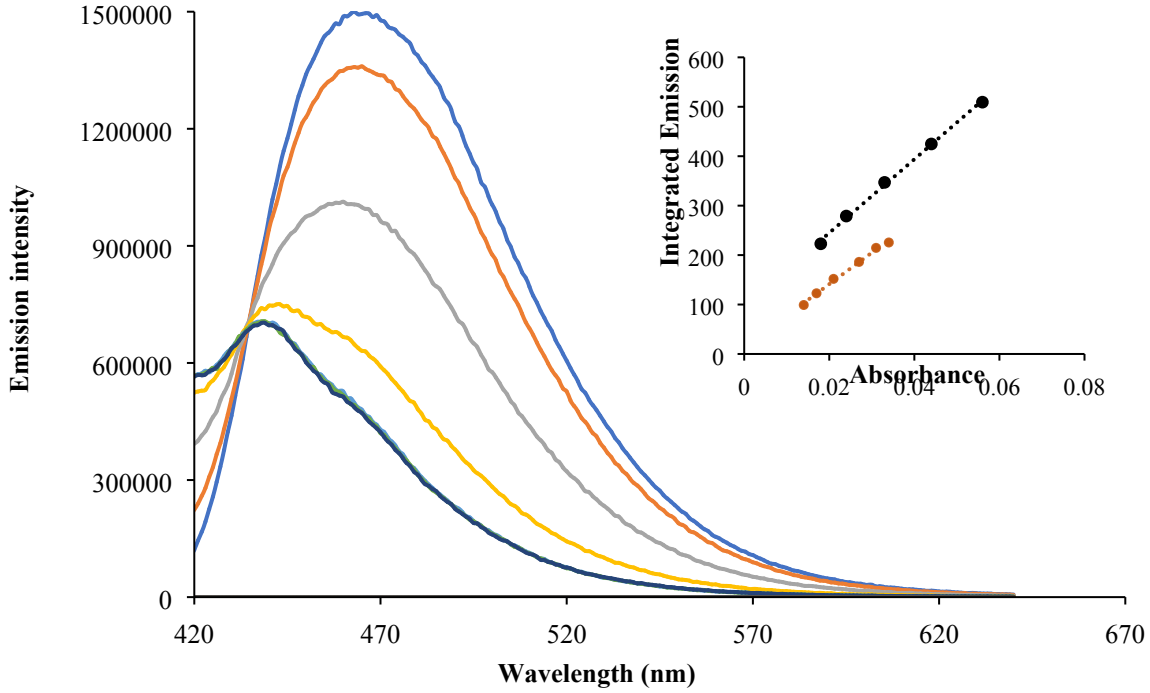


Figure S14. Emission spectrum of **2** titrated against TBAF. Quantum yield determination inset

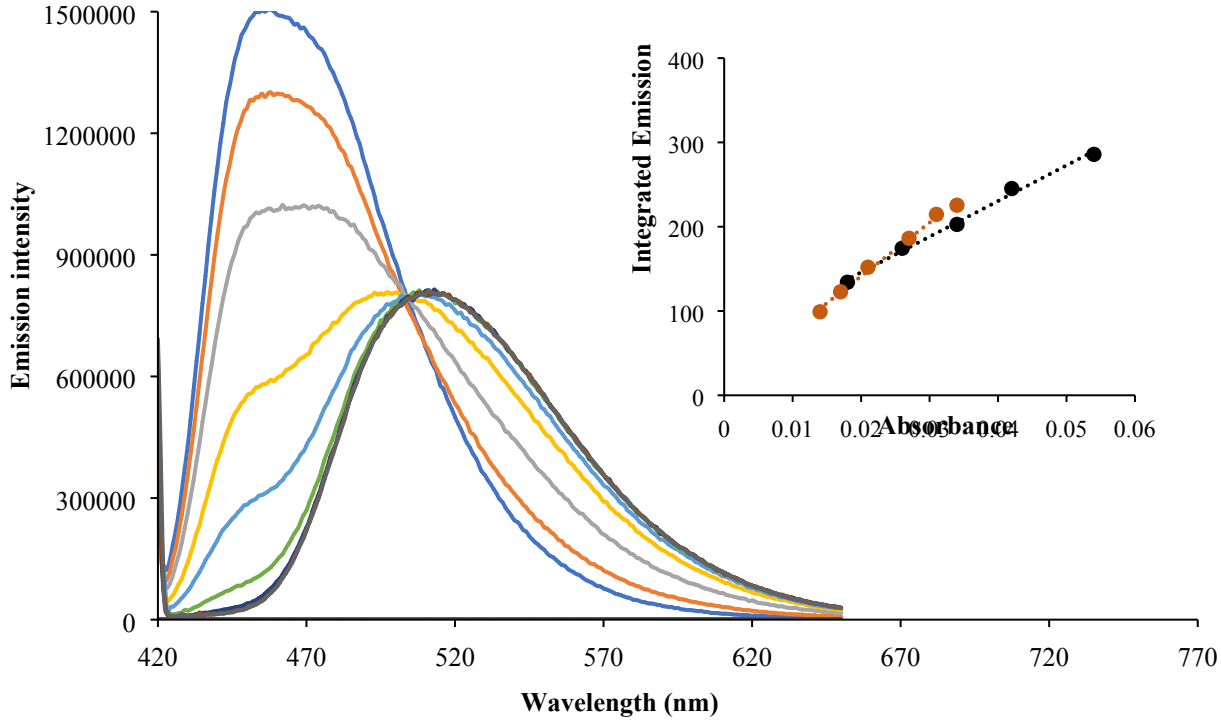
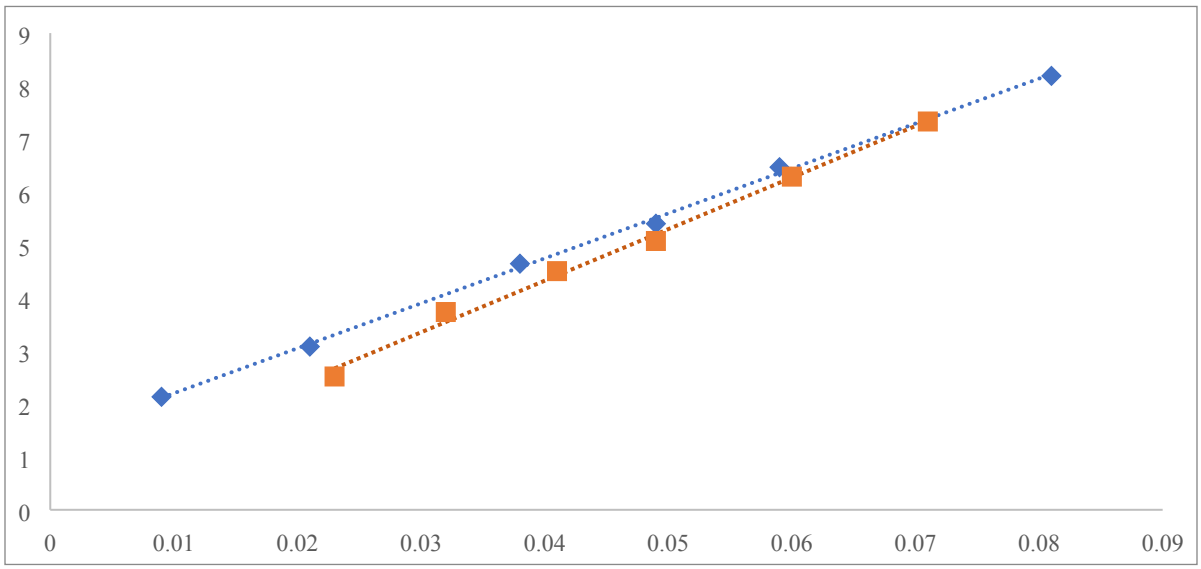
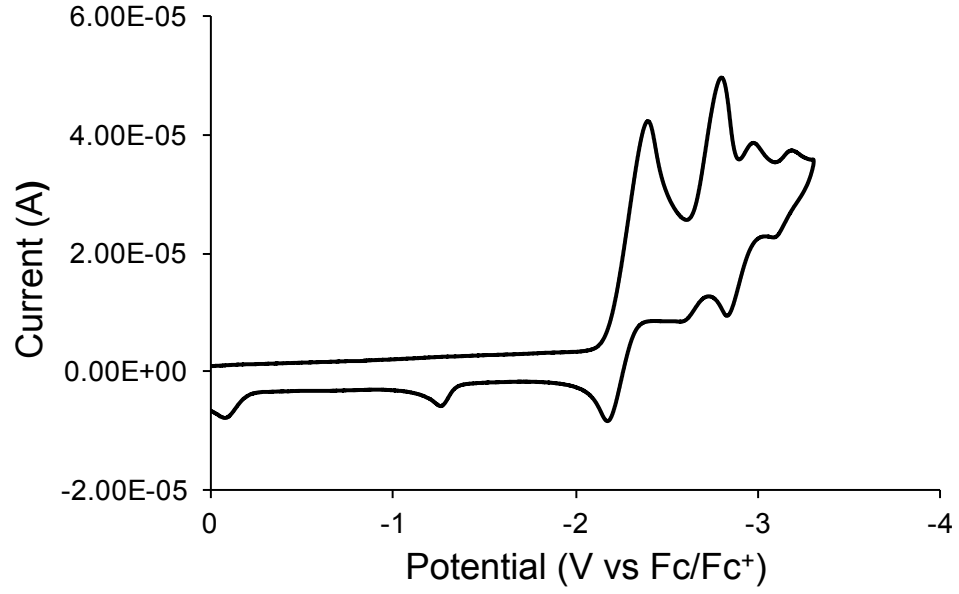


Figure S15. Quantum yield determination of [**2**-F]$^{-}$



7. Cyclic voltammograms

Figure S16. Cyclic voltammogram of **1**



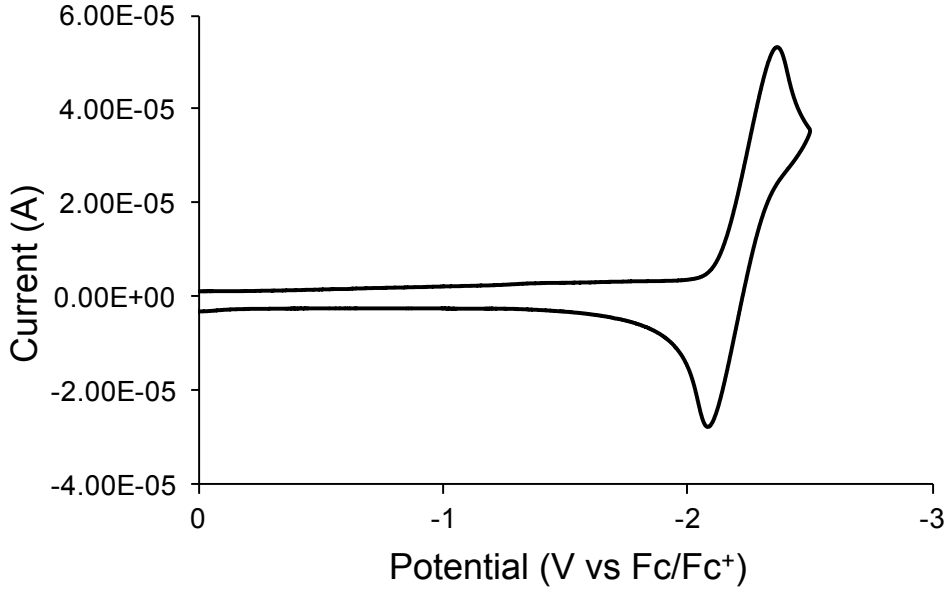
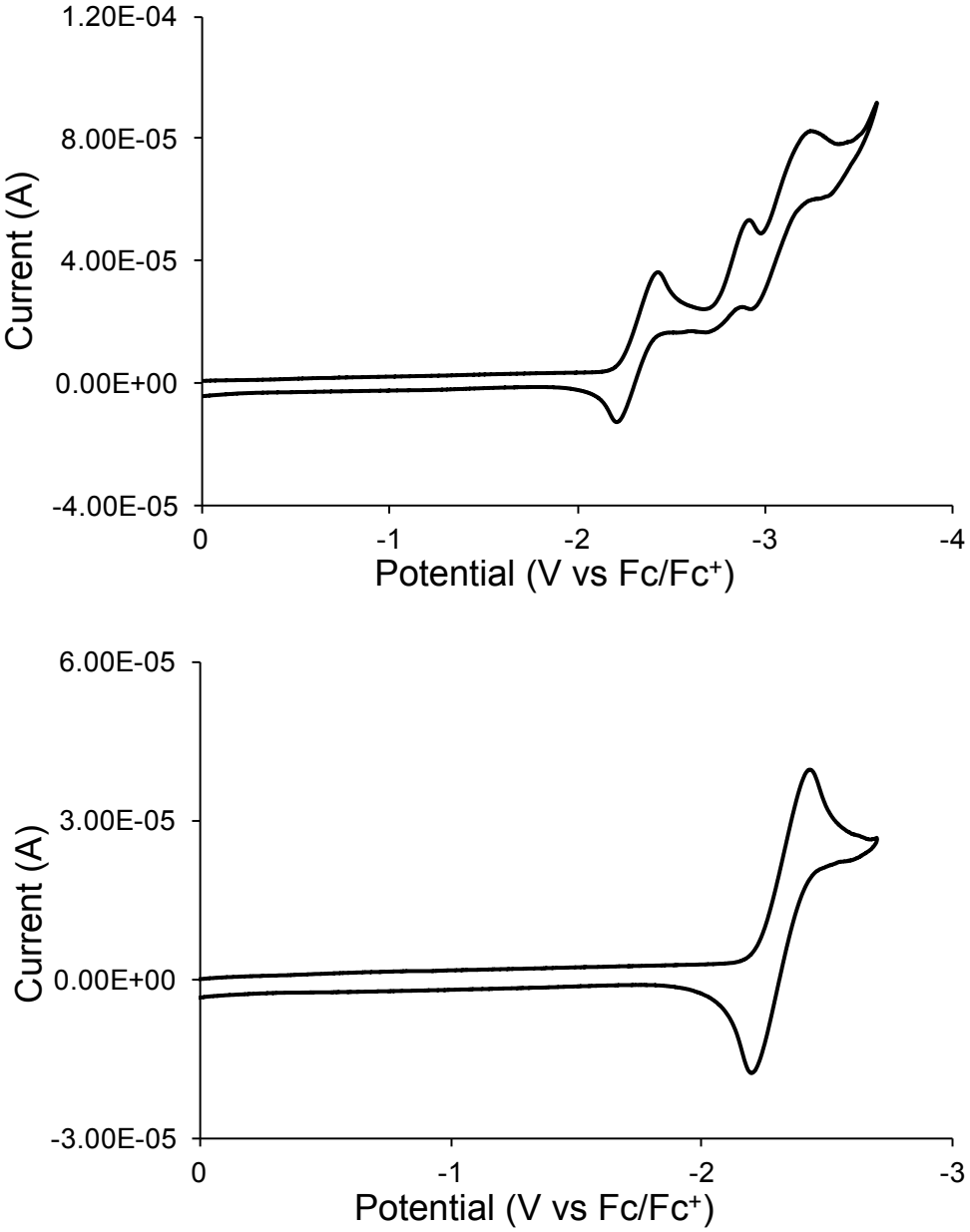


Figure S17. Cyclic voltammogram of **2**



8. Mass spectroscopic studies

Figure S18. Mass spectrum of [**1**-F]⁻

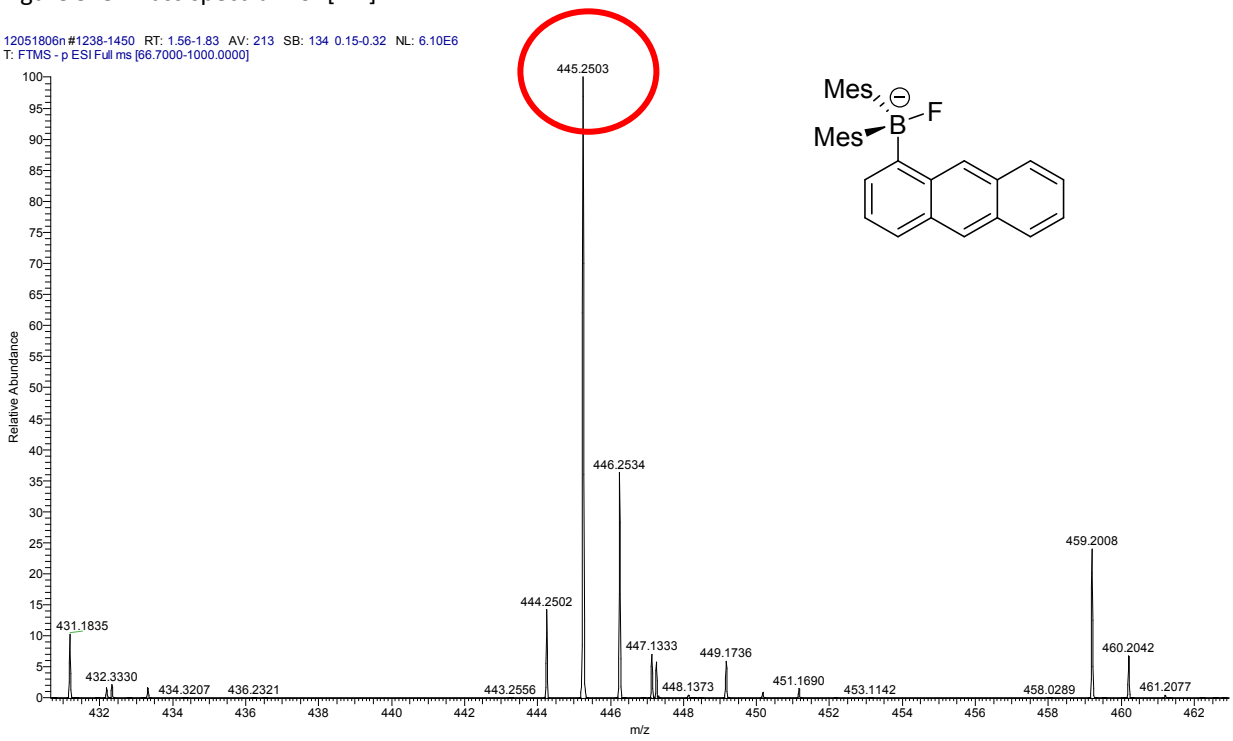


Figure S19. Mass spectrum of [**1**-CN]⁻

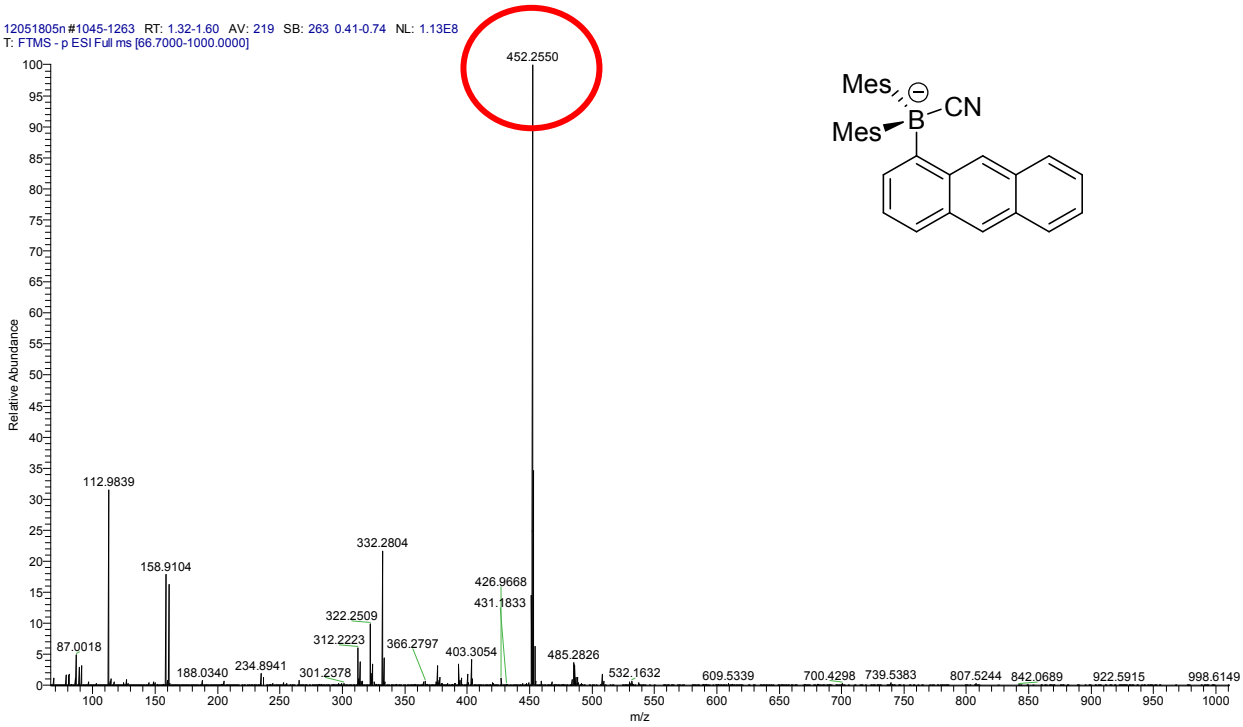


Figure S20. Mass spectrum of [**2**-F]⁻

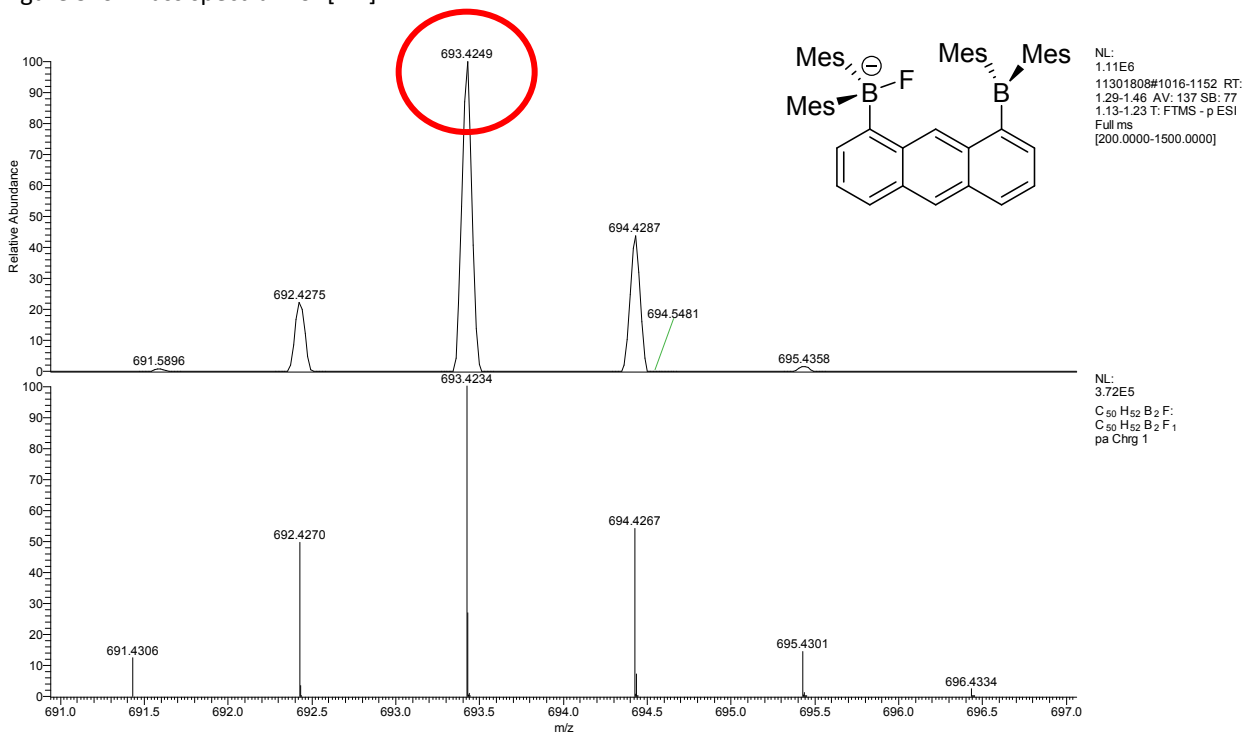


Figure S21. Mass spectrum of [**2**-CN]⁻