Electronic Supplementary Information (ESI) for:

Synthesis and Photophysical Properties of Nitrated aza–BODIPYs

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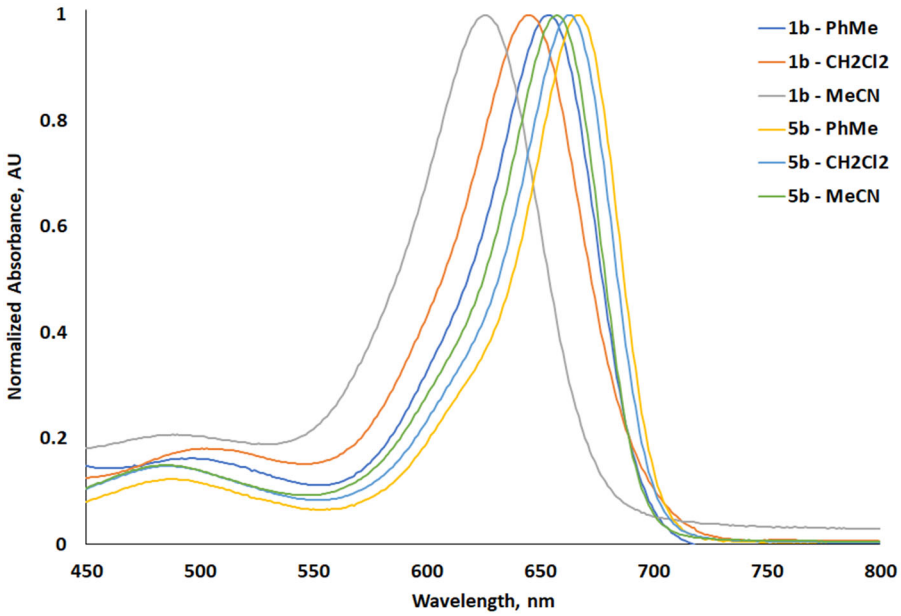


Figure S1. Absorption spectra of **1b** and **5b** in PhMe, CH_2Cl_2, and MeCN.

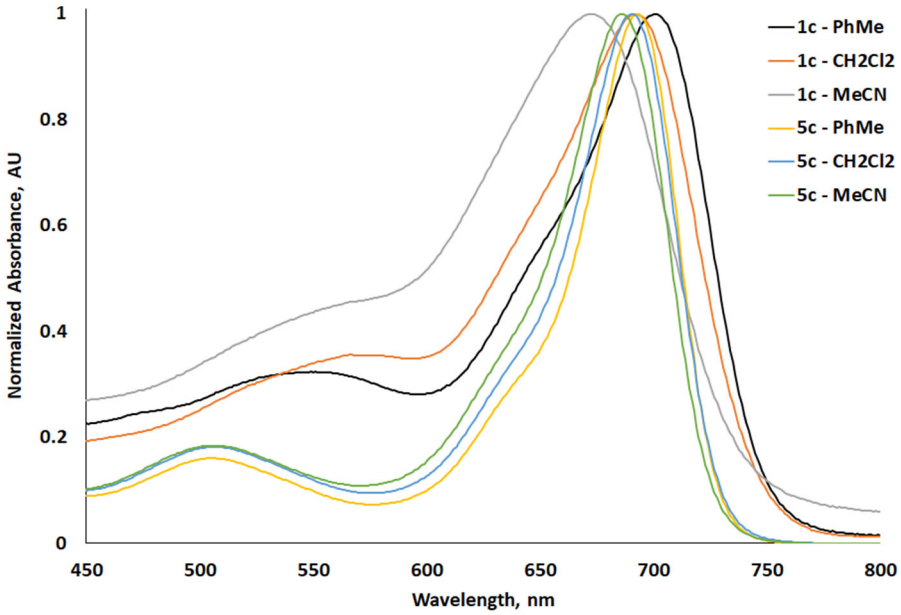


Figure S2. Absorption spectra of **1c** and **5c** in PhMe, CH_2Cl_2, and MeCN.

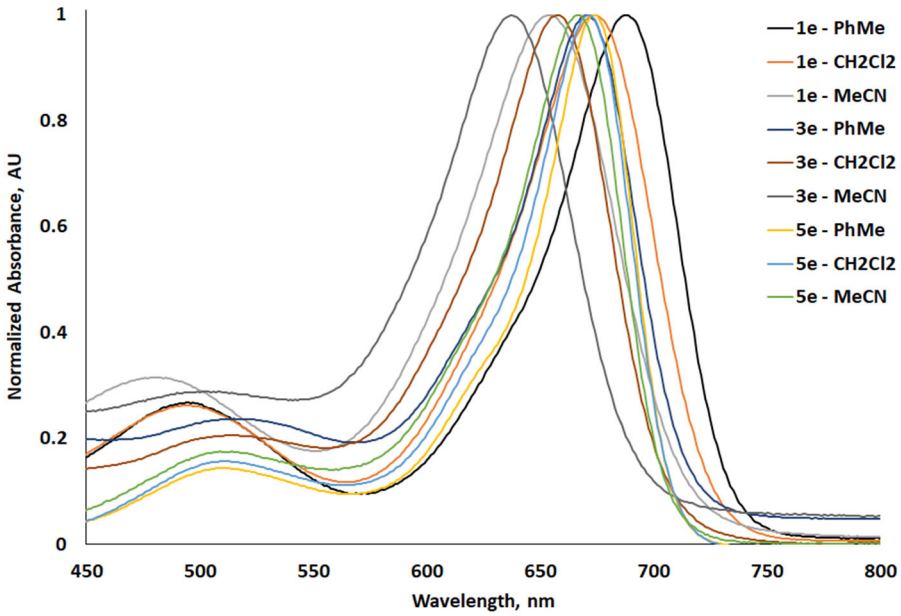


Figure S3. Absorption spectra of **1e**, **3e**, and **5e** in PhMe, CH_2Cl_2, and MeCN.

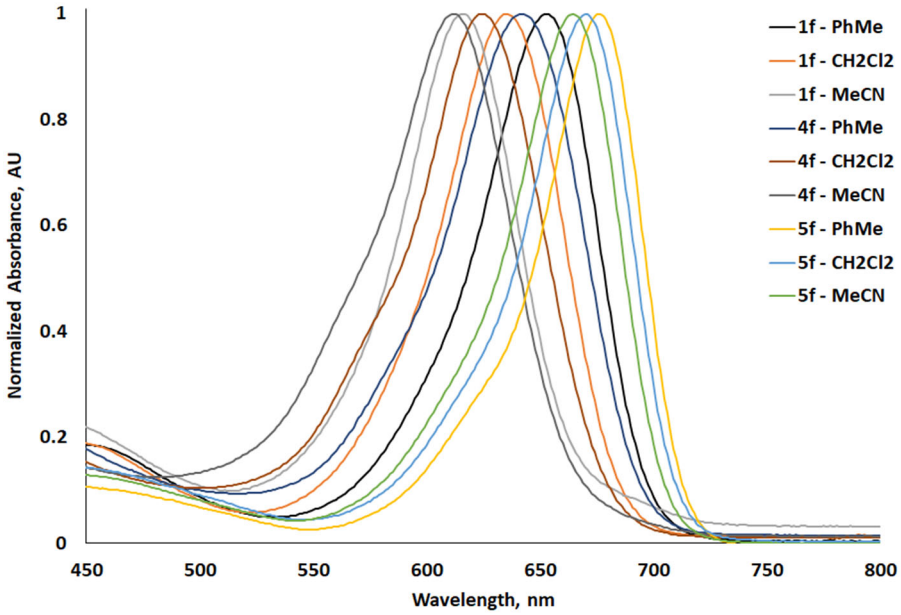


Figure S4. Absorption spectra of **1f**, **4f**, and **5f** in PhMe, CH_2Cl_2, and MeCN.

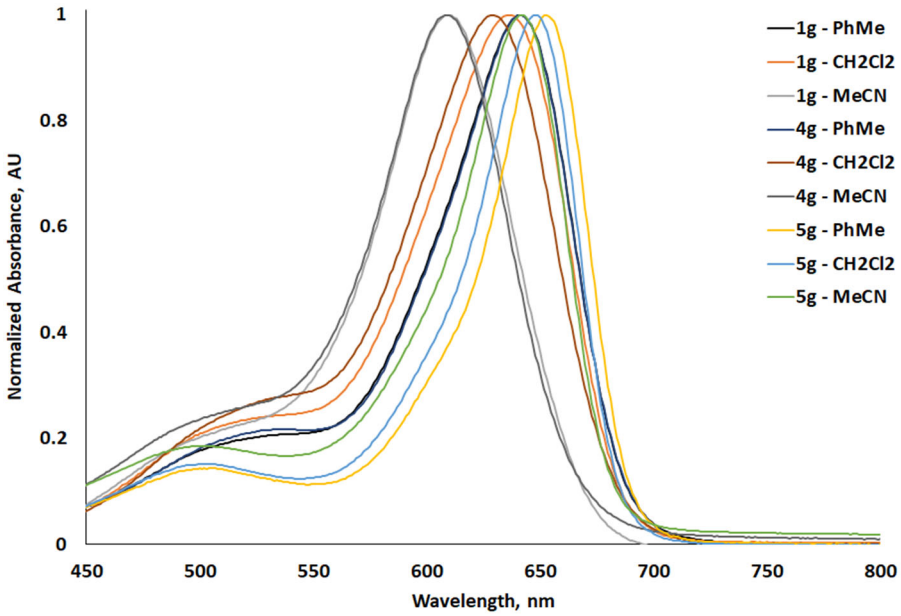


Figure S5. Absorption spectra of **1g**, **4g**, and **5g** in PhMe, CH_2Cl_2, and MeCN.

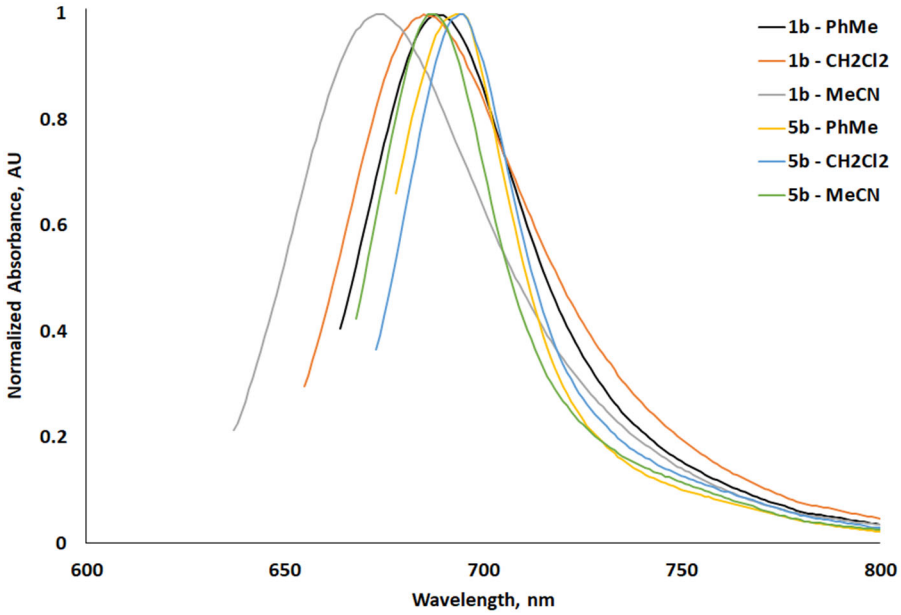


Figure S6. Emission spectra of **1b** and **5b** in PhMe, CH_2Cl_2, and MeCN.

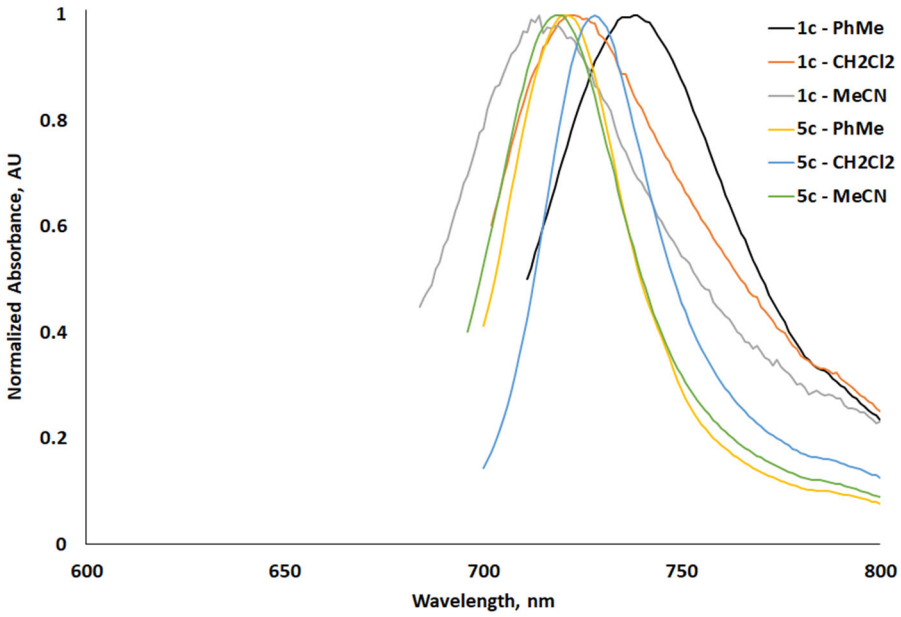


Figure S7. Emission spectra of **1c** and **5c** in PhMe, CH_2Cl_2, and MeCN.

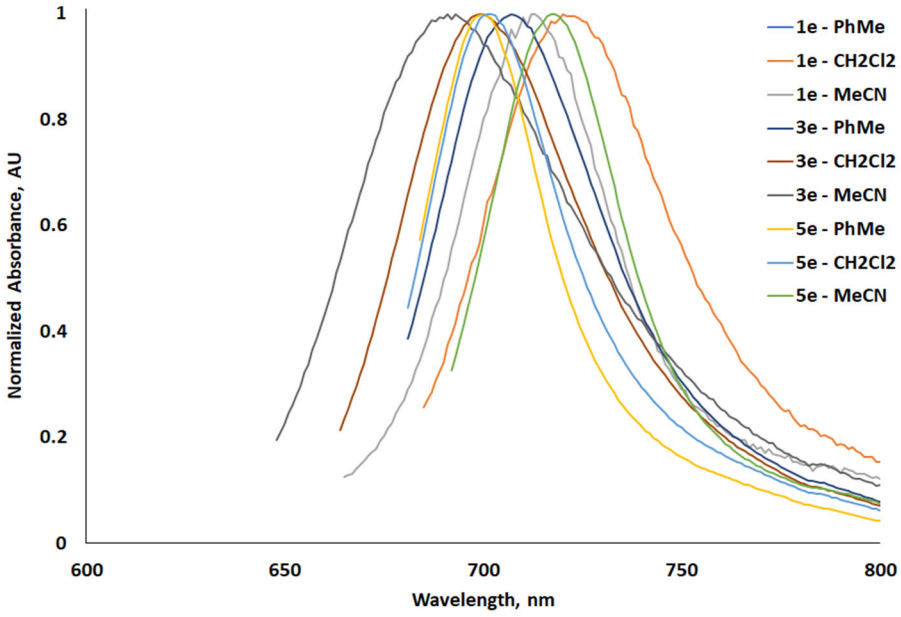


Figure S8. Emission spectra of **1e**, **3e**, and **5e** in PhMe, CH_2Cl_2, and MeCN.

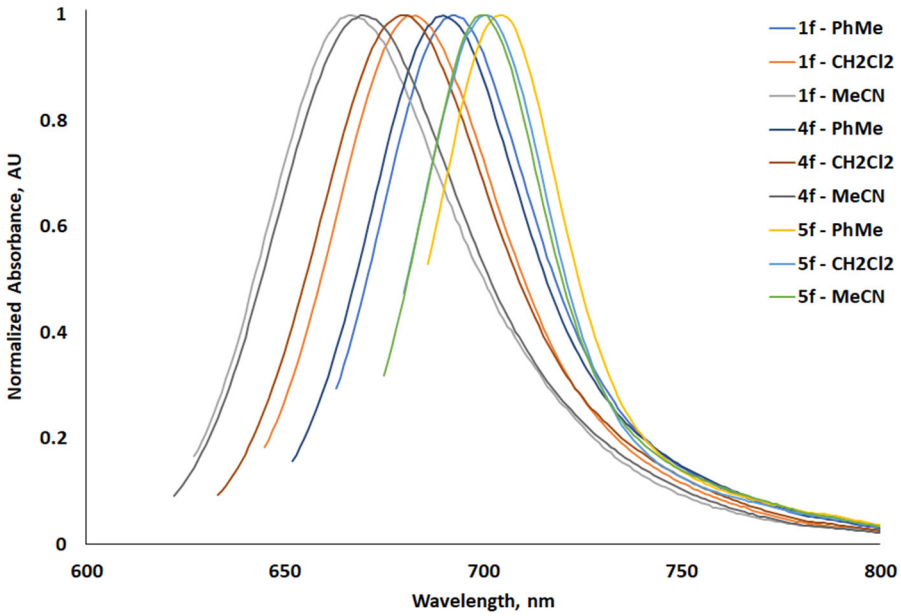


Figure S9. Emission spectra of **1f**, **4f**, and **5f** in PhMe, CH_2Cl_2, and MeCN.

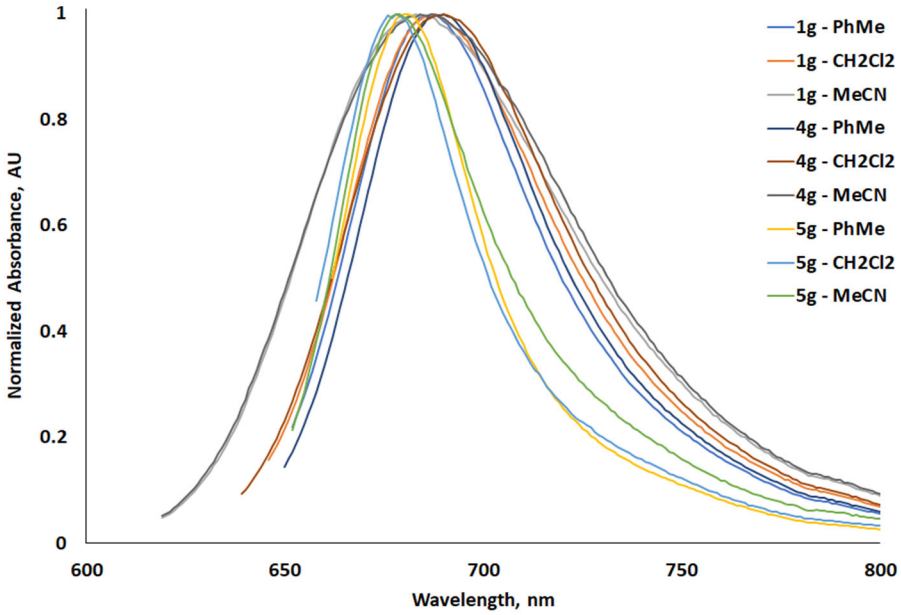


Figure S10. Emission spectra of **1g**, **4g**, and **5g** in PhMe, CH_2Cl_2, and MeCN.

Photostability Studies for **1a** and **5a**:

Solutions of **1a** and **5a** in PhMe, CH_2Cl_2, and MeCN were adjusted to have an initial absorbance of approximately 1.0 and were irradiated with a 100 W xenon lamp originating from a Newport Corporation Oriel LCS–100 Solar Simulator equipped with a Newport Corporation 91150V Reference Cell and Meter. All samples were irradiated at room temperature in an air atmosphere with a continuous flux of 1,000.0 $mW \cdot m^{-2}$ for a total of 5 hours and filtered with a 438 nm long wave pass filter. All photostability studies were performed in triplicate and averaged.

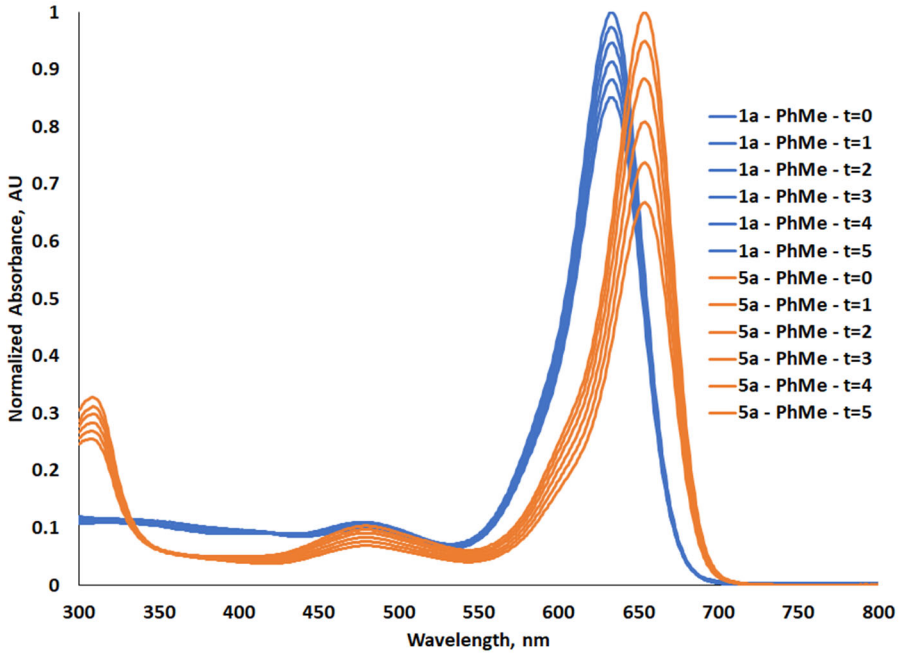


Figure S11. Photodegradation of **1a** and **5a** in PhMe.

Time (hours)	**1a** Relative Absorbance	**5a** Relative Absorbance
0	1	1
1	0.9737 ± 0.0042	0.9496 ± 0.0035
2	0.9460 ± 0.0089	0.8846 ± 0.0073
3	0.9136 ± 0.0066	0.8094 ± 0.0050
4	0.8821 ± 0.0061	0.7371 ± 0.0048
5	0.8514 ± 0.0058	0.6669 ± 0.0064

Table S1. Photodegradation absorption parameters of **1a** and **5a** in PhMe.

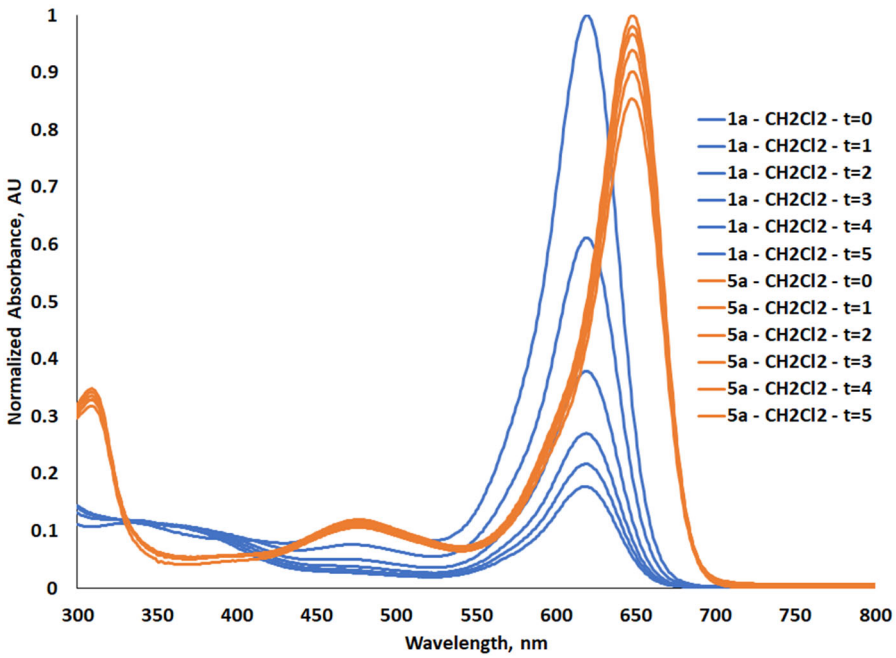


Figure S12. Photodegradation of **1a** and **5a** in CH_2Cl_2.

Time (hours)	**1a** Relative Absorbance	**5a** Relative Absorbance
0	1	1
1	0.6182 ± 0.0382	0.9815 ± 0.0038
2	0.3879 ± 0.0516	0.9659 ± 0.0059
3	0.2782 ± 0.0491	0.9380 ± 0.0074
4	0.2268 ± 0.0553	0.9008 ± 0.0072
5	0.1910 ± 0.0278	0.8530 ± 0.0104

Table S2. Photodegradation absorption parameters of **1a** and **5a** in CH_2Cl_2.

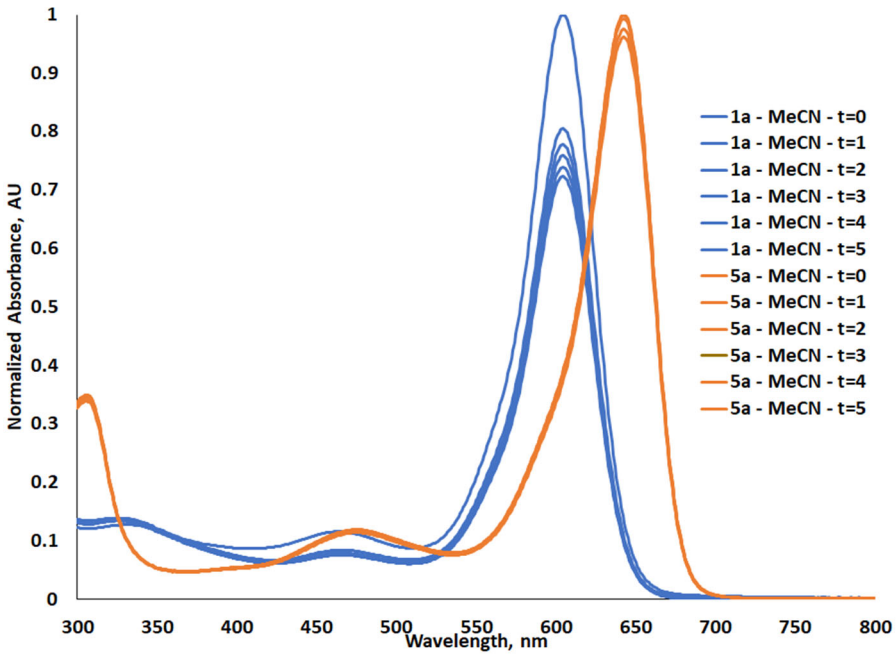


Figure S13. Photodegradation of **1a** and **5a** in MeCN.

Time (hours)	**1a** Relative Absorbance	**5a** Relative Absorbance
0	1	1
1	0.8135 ± 0.0335	0.9942 ± 0.0010
2	0.7866 ± 0.0334	0.9878 ± 0.0020
3	0.7665 ± 0.0294	0.9786 ± 0.0033
4	0.7472 ± 0.0291	0.9702 ± 0.0089
5	0.7313 ± 0.0288	0.9594 ± 0.0129

Table S3. Photodegradation absorption parameters of **1a** and **5a** in MeCN.

1a

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2028.640264	Hartree
Zero-point Energy Correction	0.468984	Hartree
Thermal Correction to Energy	0.504063	Hartree
Thermal Correction to Enthalpy	0.505007	Hartree
Thermal Correction to Free Energy	0.396935	Hartree
EE + Zero-point Energy	-2028.171280	Hartree
EE + Thermal Energy Correction	-2028.136201	Hartree
EE + Thermal Enthalpy Correction	-2028.135257	Hartree
EE + Thermal Free Energy Correction	-2028.243329	Hartree
E (Thermal)	316.304	kcal/mol
Heat Capacity (Cv)	134.904	cal/mol-kelvin
Entropy (S)	227.457	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	-0.008984	-1.674165	-0.030095
N2	0.004051	1.320179	-0.00726
N3	-1.24528	-0.721622	0.107496
N4	1.238589	-0.730289	-0.118615
C5	-1.13384	0.665202	0.080218
C6	1.136815	0.65728	-0.092344
F7	0.128397	-2.488969	1.09045
F8	-0.155808	-2.42079	-1.198269
C9	-2.548955	-1.043802	0.102695
C10	2.539819	-1.061945	-0.101273
C11	-3.300711	0.168736	0.067504
C12	3.299805	0.145816	-0.058633
C13	-2.433536	1.262515	0.068116
C14	2.441362	1.245404	-0.068416
C15	-3.074615	-2.410922	0.054752
C16	3.057543	-2.431036	-0.047672
C17	-2.697352	-3.378052	0.994809
C18	2.659063	-3.40718	-0.969813
H19	-1.999929	-3.119725	1.788693
H20	1.950898	-3.153902	-1.755752
C21	-3.231141	-4.661791	0.921894
C22	3.184974	-4.693546	-0.889213
H23	-2.942658	-5.406465	1.664628
H24	2.879983	-5.445121	-1.618258
C25	-4.128295	-4.995047	-0.09268

C26	4.095107	-5.021038	0.115719
H27	-4.538469	-6.004352	-0.149835
H28	4.499039	-6.032485	0.178976
C29	-4.503295	-4.034473	-1.033803
C30	4.490628	-4.052026	1.039668
H31	-5.200517	-4.289956	-1.832505
H32	5.197518	-4.30296	1.831256
C33	-3.989528	-2.745007	-0.955247
C34	3.984841	-2.760062	0.953006
H35	-4.280386	-1.998901	-1.696204
H36	4.291065	-2.00805	1.681738
C37	-2.658701	2.707133	0.112812
C38	2.678161	2.688035	-0.111082
C39	-1.95346	3.476789	1.05427
C40	1.985008	3.46319	-1.057077
H41	-1.285582	2.983813	1.759949
H42	1.317035	2.975538	-1.766362
C43	-2.122139	4.856492	1.104289
C44	2.165905	4.841286	-1.106853
H45	-1.581869	5.439498	1.851156
H46	1.634989	5.428527	-1.857094
C47	-2.976137	5.490262	0.2005
C48	3.020306	5.468162	-0.198575
H49	-3.103383	6.573339	0.235854
H50	3.15714	6.550068	-0.233842
C51	-3.665229	4.735809	-0.750101
C52	3.697343	4.708417	0.756405
H53	-4.325089	5.227409	-1.466146
H54	4.357269	5.194767	1.475961
C55	-3.517408	3.35275	-0.791203
C56	3.537193	3.326704	0.797615
H57	-4.051699	2.768411	-1.536762
H58	4.061671	2.738269	1.546883
N59	-4.725836	0.217841	0.237283
N60	4.727129	0.185102	-0.216696
O61	-5.338005	1.118724	-0.315856
O62	5.343416	1.068306	0.359653
O63	-5.242219	-0.634843	0.944063
O64	5.240163	-0.65742	-0.937693

1b

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2185.734507	Hartree
Zero-point Energy Correction	0.577639	Hartree
Thermal Correction to Energy	0.620473	Hartree
Thermal Correction to Enthalpy	0.621417	Hartree
Thermal Correction to Free Energy	0.491790	Hartree
EE + Zero-point Energy	-2185.156868	Hartree
EE + Thermal Energy Correction	-2185.114034	Hartree
EE + Thermal Enthalpy Correction	-2185.113090	Hartree
EE + Thermal Free Energy Correction	-2185.242717	Hartree
E (Thermal)	389.353	kcal/mol
Heat Capacity (Cv)	159.356	cal/mol-kelvin
Entropy (S)	272.822	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	-1.705169	-0.001461	-0.033131
N2	1.285286	0.005178	-0.00616
N3	-0.764423	1.241646	0.109457
N4	-0.756368	-1.243911	-0.119499
C5	0.622886	1.138534	0.088233
C6	0.630247	-1.131609	-0.098653
F7	-2.526486	-0.146784	1.083501
F8	-2.450074	0.143351	-1.204907
C9	-1.094948	2.545513	0.100424
C10	-1.078719	-2.549808	-0.098652
C11	0.11414	3.30256	0.072455
C12	0.136244	-3.298633	-0.063376
C13	1.214262	2.441293	0.081184
C14	1.230195	-2.431408	-0.080366
C15	-2.458697	3.069835	0.03745
C16	-2.436839	-3.085238	-0.03177
C17	-3.457857	2.663022	0.928739
C18	-3.452079	-2.663395	-0.898122
H19	-3.230146	1.936083	1.705129
H20	-3.24094	-1.915667	-1.659254
C21	-4.736698	3.204776	0.83803
C22	-4.725836	-3.215438	-0.801919
H23	-5.499651	2.887851	1.551611
H24	-5.501158	-2.886212	-1.496313
C25	-5.062444	4.145228	-0.144465

C26	-5.031565	-4.181304	0.162353
C27	-6.446933	4.712207	-0.256353
C28	-6.41021	-4.760849	0.279799
C29	-4.054541	4.544154	-1.035056
C30	-4.008617	-4.594032	1.029314
H31	-4.281376	5.274436	-1.814323
H32	-4.219943	-5.34306	1.794995
C33	-2.770551	4.027923	-0.941306
C34	-2.729495	-4.067615	0.929233
H35	-2.007032	4.350855	-1.650916
H36	-1.955186	-4.400974	1.622094
C37	2.654651	2.673921	0.142029
C38	2.671692	-2.656188	-0.138846
C39	3.427638	1.947615	1.064929
C40	3.441135	-1.930266	-1.065297
H41	2.938547	1.253908	1.748011
H42	2.948583	-1.242169	-1.751553
C43	4.804193	2.122362	1.128029
C44	4.818314	-2.098655	-1.127698
H45	5.381135	1.557984	1.86338
H46	5.392535	-1.53482	-1.865601
C47	5.463188	3.004198	0.261607
C48	5.48165	-2.973628	-0.257327
C49	6.947287	3.206424	0.346506
C50	6.966711	-3.168377	-0.342188
C51	4.691306	3.707543	-0.672203
C52	4.713367	-3.676452	0.679594
H53	5.182426	4.385904	-1.372903
C54	5.207854	-4.349203	1.383306
C55	3.310622	3.558508	-0.729311
C56	3.33188	-3.533632	0.736428
H57	2.735799	4.109892	-1.46975
H58	2.759907	-4.083891	1.479884
N59	0.156139	4.726068	0.25122
N60	0.188937	-4.723615	-0.232878
O61	1.04094	5.349788	-0.316208
O62	1.062126	-5.340068	0.359593
O63	-0.683957	5.232997	0.980227
O64	-0.630503	-5.237514	-0.979977
H65	-6.927558	4.385974	-1.190441
H66	-6.874627	-4.47196	1.234112
H67	-7.079506	4.391973	0.580518
H68	-7.060484	-4.41523	-0.533012
H69	-6.423826	5.810769	-0.27391
H70	-6.379958	-5.859202	0.257267
H71	7.186217	4.032312	1.033861

H72	7.210734	-3.977186	-1.047826
H73	7.452026	2.308561	0.725465
H74	7.468964	-2.26027	-0.699599
H75	7.372285	3.463375	-0.632334
H76	7.389947	-3.445546	0.631794

1c

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2486.312190	Hartree
Zero-point Energy Correction	0.599525	Hartree
Thermal Correction to Energy	0.644795	Hartree
Thermal Correction to Enthalpy	0.645739	Hartree
Thermal Correction to Free Energy	0.515088	Hartree
EE + Zero-point Energy	-2485.712665	Hartree
EE + Thermal Energy Correction	-2485.667395	Hartree
EE + Thermal Enthalpy Correction	-2485.666450	Hartree
EE + Thermal Free Energy Correction	-2485.797102	Hartree
E (Thermal)	404.615	kcal/mol
Heat Capacity (Cv)	171.372	cal/mol-kelvin
Entropy (S)	274.978	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	1.75527	0	-0.000004
N2	-1.229153	0	-0.000001
N3	0.815551	-1.241654	0.142855
N4	0.81555	1.241654	-0.142856
C5	-0.570735	-1.132556	0.124753
C6	-0.570735	1.132556	-0.124754
F7	2.542635	0.1745	1.141122
F8	2.542627	-0.174501	-1.141136
C9	1.141697	-2.550348	0.14974
C10	1.141696	2.550348	-0.149739
C11	-0.073156	-3.300258	0.144261
C12	-0.073157	3.300257	-0.14426
C13	-1.170415	-2.431975	0.144258
C14	-1.170416	2.431974	-0.144258
C15	2.494268	-3.088337	0.07592
C16	2.494267	3.088338	-0.075919
C17	3.548426	-2.612226	0.875069
C18	3.548426	2.612224	-0.875066

H19	3.367727	-1.815724	1.592667
H20	3.367728	1.815721	-1.592662
C21	4.812539	-3.164764	0.775649
C22	4.812539	3.164763	-0.775645
H23	5.627249	-2.809126	1.40665
H24	5.627249	2.809124	-1.406644
C25	5.066824	-4.197073	-0.140146
C26	5.066822	4.197075	0.140147
O27	6.332282	-4.661704	-0.16893
O28	6.33228	4.661707	0.168932
C29	4.028641	-4.677358	-0.949738
C30	4.028638	4.677362	0.949737
H31	4.196762	-5.469149	-1.676761
H32	4.196758	5.469154	1.676758
C33	2.758131	-4.130176	-0.824692
C34	2.758129	4.130179	0.824691
H35	1.962609	-4.505229	-1.470206
H36	1.962606	4.505233	1.470203
C37	-2.609281	-2.648901	0.209471
C38	-2.609282	2.6489	-0.209471
C39	-3.38199	-1.867887	1.084708
C40	-3.381991	1.867887	-1.084708
H41	-2.888283	-1.151438	1.739939
H42	-2.888284	1.151438	-1.73994
C43	-4.763336	-2.003664	1.15664
C44	-4.763337	2.003663	-1.156641
H45	-5.320611	-1.393505	1.86468
H46	-5.320611	1.393504	-1.864681
C47	-5.409464	-2.920982	0.317956
C48	-5.409465	2.920981	-0.317956
O49	-6.743135	-3.124661	0.294191
O50	-6.743137	3.124659	-0.294191
C51	-4.65422	-3.69857	-0.573801
C52	-4.654222	3.698567	0.573802
H53	-5.172019	-4.398748	-1.229832
H54	-5.17202	4.398746	1.229833
C55	-3.277656	-3.571612	-0.619594
C56	-3.277657	3.571611	0.619595
H57	-2.707496	-4.172099	-1.324031
H58	-2.707497	4.172097	1.324033
N59	-0.129771	-4.714861	0.374065
N60	-0.129773	4.714861	-0.374062
O61	-1.020902	-5.350373	-0.172093
O62	-1.020903	5.350373	0.1721
O63	0.699133	-5.206986	1.126585
O64	0.699128	5.206987	-1.126584

C65	6.63774	-5.716348	-1.071798
C66	6.637737	5.716353	1.071798
H67	6.467872	-5.407164	-2.113536
H68	6.467867	5.407171	2.113536
H69	7.699765	-5.935505	-0.925175
H70	7.699761	5.935509	0.925175
H71	6.043314	-6.613924	-0.846901
H72	6.04331	6.613928	0.846898
C73	-7.553214	-2.347899	1.165936
C74	-7.553215	2.347897	-1.165937
H75	-7.456092	-1.274629	0.944471
H76	-7.456092	1.274627	-0.944472
H77	-8.583105	-2.667742	0.980122
H78	-8.583106	2.667739	-0.980123
H79	-7.295659	-2.535506	2.218544
H80	-7.29566	2.535505	-2.218545

1e

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2336.023683	Hartree
Zero-point Energy Correction	0.588570	Hartree
Thermal Correction to Energy	0.632593	Hartree
Thermal Correction to Enthalpy	0.633537	Hartree
Thermal Correction to Free Energy	0.503468	Hartree
EE + Zero-point Energy	-2335.435113	Hartree
EE + Thermal Energy Correction	-2335.391090	Hartree
EE + Thermal Enthalpy Correction	-2335.390146	Hartree
EE + Thermal Free Energy Correction	-2335.520214	Hartree
E (Thermal)	396.958	kcal/mol
Heat Capacity (Cv)	165.342	cal/mol-kelvin
Entropy (S)	273.752	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	-2.043186	-0.00007	0.019071
N2	0.946269	-0.002029	0.003189
N3	-1.096878	1.244082	0.102184
N4	-1.099877	-1.243746	-0.09682
C5	0.289742	1.13452	0.091086
C6	0.287017	-1.13747	-0.085812
F7	-2.805045	-0.129832	1.181593

F8	-2.849752	0.129336	-1.111315
C9	-1.421886	2.549217	0.070164
C10	-1.427824	-2.548221	-0.071716
C11	-0.21091	3.302292	0.039852
C12	-0.219066	-3.304372	-0.046283
C13	0.888873	2.435272	0.070526
C14	0.882999	-2.439106	-0.072188
C15	-2.785498	3.072338	-0.013197
C16	-2.793924	-3.066732	0.009822
C17	-3.793792	2.674714	0.871533
C18	-3.794478	-2.678495	-0.887489
H19	-3.573548	1.957697	1.659322
H20	-3.566513	-1.972725	-1.683218
C21	-5.073279	3.211093	0.758473
C22	-5.076085	-3.210685	-0.777056
H23	-5.843734	2.901159	1.467069
H24	-5.840548	-2.908413	-1.495404
C25	-5.390451	4.136462	-0.240839
C26	-5.402565	-4.122476	0.231619
C27	-6.774861	4.698777	-0.376055
C28	-6.789572	-4.679161	0.364398
C29	-4.373626	4.524912	-1.125967
C30	-4.392966	-4.502217	1.128637
H31	-4.593841	5.242639	-1.918728
H32	-4.620336	-5.209977	1.928325
C33	-3.089295	4.014085	-1.009978
C34	-3.106614	-3.9955	1.015685
H35	-2.318427	4.328837	-1.715253
H36	-2.340859	-4.303755	1.72931
C37	2.327074	2.651575	0.129266
C38	2.320948	-2.657814	-0.131867
C39	3.098031	1.890895	1.024577
C40	3.093375	-1.895707	-1.024582
H41	2.602514	1.193863	1.69899
H42	2.599128	-1.196256	-1.697425
C43	4.479298	2.025387	1.093758
C44	4.474604	-2.031618	-1.093221
H45	5.034871	1.433373	1.818311
H46	5.031323	-1.438401	-1.815911
C47	5.127818	2.918955	0.231313

C48	5.121495	-2.928014	-0.232576
O49	6.46113	3.119308	0.203162
O50	6.454635	-3.129951	-0.203913
C51	4.374649	3.674592	-0.681387
C52	4.366804	-3.685176	0.67762
H53	4.894597	4.355613	-1.355578
H54	4.885484	-4.368582	1.350377
C55	2.998118	3.55095	-0.723626
C56	2.990377	-3.560197	0.719048
H57	2.429874	4.13453	-1.443441
H58	2.420928	-4.145346	1.436657
N59	-0.166427	4.72462	0.210283
N60	-0.178366	-4.725649	-0.222878
O61	0.752772	5.338191	-0.313834
O62	0.749547	-5.341639	0.282955
O63	-1.036645	5.246725	0.892826
O64	-1.060563	-5.24535	-0.891955
C65	7.269632	2.366749	1.097748
C66	7.264607	-2.375952	-1.095899
H67	7.17146	1.287822	0.906693
H68	7.167549	-1.297412	-0.902059
H69	8.29994	2.680258	0.903905
H70	8.294432	-2.691136	-0.902179
H71	7.010834	2.58478	2.144119
H72	7.006327	-2.590873	-2.143047
H73	-7.238527	4.372396	-1.318564
H74	-7.263371	-4.329225	1.293367
H75	-6.755083	5.797519	-0.391768
H76	-6.772396	-5.777197	0.406645
H77	-7.420469	4.375895	0.449791
H78	-7.425166	-4.374717	-0.476115

1f

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2780.742715	Hartree
Zero-point Energy Correction	0.532212	Hartree
Thermal Correction to Energy	0.578566	Hartree
Thermal Correction to Enthalpy	0.579510	Hartree
Thermal Correction to Free Energy	0.440847	Hartree
EE + Zero-point Energy	-2780.210503	Hartree
EE + Thermal Energy Correction	-2780.164149	Hartree
EE + Thermal Enthalpy Correction	-2780.163205	Hartree
EE + Thermal Free Energy Correction	-2780.301868	Hartree
E (Thermal)	363.055	kcal/mol
Heat Capacity (Cv)	172.520	cal/mol-kelvin
Entropy (S)	291.841	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	2.643909	-0.002761	-0.057897
N2	-0.348245	-0.004354	-0.009274
N3	1.700933	-1.244922	0.103343
N4	1.695012	1.244621	-0.119576
C5	0.31498	-1.138773	0.072197
C6	0.309498	1.131151	-0.088153
F7	3.490572	0.139262	1.036528
F8	3.353635	-0.148789	-1.249927
C9	2.029432	-2.549422	0.095511
C10	2.017585	2.550468	-0.09208
C11	0.815546	-3.303158	0.05831
C12	0.797895	3.297515	-0.041907
C13	-0.276144	-2.438328	0.054669
C14	-0.288288	2.429656	-0.051598
C15	3.390649	-3.077628	0.043478
C16	3.371292	3.091019	-0.033869
C17	4.384713	-2.669601	0.940497
C18	4.394481	2.645898	-0.880341
H19	4.153252	-1.940684	1.713794
H20	4.190765	1.877404	-1.622371
C21	5.662315	-3.21529	0.860798

C22	5.665741	3.203235	-0.790553
H23	6.42091	-2.898537	1.57896
H24	6.446678	2.85657	-1.469841
C25	5.992191	-4.159848	-0.116478
C26	5.962477	4.196619	0.148649
C27	7.375178	-4.731857	-0.216215
C28	7.337984	4.783714	0.258419
C29	4.989448	-4.559702	-1.012899
C30	4.932608	4.631592	0.996906
H31	5.220174	-5.292865	-1.788195
H32	5.137574	5.401087	1.743623
C33	3.706158	-4.041133	-0.929407
C34	3.65542	4.101373	0.90162
H35	2.947352	-4.364789	-1.643623
H36	2.877294	4.451586	1.581544
C37	-1.723158	-2.666276	0.087589
C38	-1.735644	2.653371	-0.081435
C39	-2.496818	-1.990631	1.043692
C40	-2.507754	1.98079	-1.041255
H41	-2.011247	-1.343749	1.772906
H42	-2.020848	1.337664	-1.772863
C43	-3.876756	-2.152317	1.07847
C44	-3.887623	2.141286	-1.076477
H45	-4.467756	-1.631385	1.830891
H46	-4.477498	1.622774	-1.831452
C47	-4.497213	-2.975213	0.139478
C48	-4.509713	2.960113	-0.13479
C49	-5.98223	-3.18413	0.188535
C50	-5.994968	3.167867	-0.185372
C51	-3.742367	-3.643494	-0.825267
C52	-3.756615	3.625109	0.833347
H53	-4.231275	-4.277049	-1.565103
H54	-4.246872	4.255086	1.575315
C55	-2.361025	-3.495068	-0.847158
C56	-2.375044	3.477568	0.856382
H57	-1.773318	-4.008629	-1.604183
H58	-1.788708	3.98747	1.616875
N59	0.755803	-4.729032	0.227584
N60	0.728868	4.726064	-0.196757
O61	-0.145528	-5.331625	-0.335596

O62	-0.139095	5.324295	0.420128
O63	1.595518	-5.252065	0.943189
O64	1.527132	5.25228	-0.95552
H65	7.857331	-4.423748	-1.155575
H66	7.786009	4.546419	1.23442
H67	8.007367	-4.398875	0.615851
H68	8.001992	4.398336	-0.524703
H69	7.348706	-5.830518	-0.214604
H70	7.30587	5.879423	0.178567
F71	-6.308047	-4.306186	0.873984
F72	-6.320763	4.287437	-0.874766
F73	-6.626447	-2.166105	0.790766
F74	-6.637807	2.147446	-0.784962
F75	-6.518721	-3.32102	-1.041498
F76	-6.532364	3.308201	1.043724

1g

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2780.742076	Hartree
Zero-point Energy Correction	0.532045	Hartree
Thermal Correction to Energy	0.578410	Hartree
Thermal Correction to Enthalpy	0.579354	Hartree
Thermal Correction to Free Energy	0.439483	Hartree
EE + Zero-point Energy	-2780.210031	Hartree
EE + Thermal Energy Correction	-2780.163666	Hartree
EE + Thermal Enthalpy Correction	-2780.162722	Hartree
EE + Thermal Free Energy Correction	-2780.302593	Hartree
E (Thermal)	362.958	kcal/mol
Heat Capacity (Cv)	172.509	cal/mol-kelvin
Entropy (S)	294.383	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	0.827773	-0.000001	0.000009
N2	-2.167661	0.000001	0.000002
N3	-0.122407	-1.238997	0.121797
N4	-0.122405	1.238996	-0.121792
C5	-1.50985	-1.134017	0.107136

C6	-1.509848	1.134017	-0.107132
F7	1.609481	0.146808	1.14334
F8	1.609499	-0.146809	-1.143309
C9	0.203952	-2.539649	0.127578
C10	0.203955	2.539647	-0.127577
C11	-1.000476	-3.301084	0.1138
C12	-1.000472	3.301084	-0.113803
C13	-2.102446	-2.437565	0.118761
C14	-2.102443	2.437566	-0.11876
C15	1.583379	-3.042403	0.074537
C16	1.583383	3.042401	-0.074537
C17	2.530566	-2.674829	1.034098
C18	2.530568	2.674827	-1.0341
H19	2.252924	-2.00897	1.847943
H20	2.252925	2.008969	-1.847945
C21	3.828841	-3.170875	0.957216
C22	3.828844	3.170872	-0.957218
H23	4.562842	-2.888945	1.71072
H24	4.562844	2.888944	-1.710724
C25	4.183664	-4.021402	-0.086463
C26	4.183668	4.021399	0.086462
C27	5.573112	-4.58146	-0.177302
C28	5.573117	4.581457	0.177298
C29	3.244288	-4.392649	-1.051307
C30	3.244293	4.392645	1.051307
H31	3.524773	-5.054432	-1.870787
H32	3.524779	5.054427	1.870787
C33	1.946064	-3.91156	-0.964465
C34	1.946069	3.911556	0.964466
H35	1.213674	-4.196483	-1.720052
H36	1.21368	4.196479	1.720054
C37	-3.542826	-2.659251	0.176142
C38	-3.542822	2.659254	-0.176142
C39	-4.314544	-1.906909	1.078447
C40	-4.314542	1.906911	-1.078446
H41	-3.823737	-1.208757	1.755563
H42	-3.823736	1.208757	-1.75556
C43	-5.694116	-2.065365	1.132953
C44	-5.694114	2.065369	-1.132952
H45	-6.270434	-1.484064	1.855204

H46	-6.270433	1.484066	-1.855201
C47	-6.355358	-2.952354	0.275373
C48	-6.355354	2.95236	-0.275374
C49	-7.843163	-3.131924	0.335328
C50	-7.843158	3.131934	-0.335331
C51	-5.583124	-3.683275	-0.63942
C52	-5.583119	3.683282	0.639418
H53	-6.076378	-4.368837	-1.331531
H54	-6.076372	4.368845	1.331528
C55	-4.201959	-3.553815	-0.685113
C56	-4.201955	3.55382	0.685111
H57	-3.627157	-4.127208	-1.408502
H58	-3.627152	4.127214	1.408499
N59	-1.029538	-4.722688	0.298782
N60	-1.029532	4.722687	-0.298789
O61	-1.98551	-5.340549	-0.144292
O62	-1.985506	5.340551	0.144279
O63	-0.101938	-5.234661	0.909724
O64	-0.10193	5.234658	-0.909729
F65	6.080132	-4.472356	-1.424504
F66	6.080136	4.472358	1.424501
F67	6.435681	-3.970132	0.654468
F68	6.435685	3.970126	-0.654469
F69	5.602427	-5.899599	0.129685
F70	5.602431	5.899595	-0.129693
H71	-8.099097	-4.106303	0.777551
H72	-8.09909	4.106295	-0.777597
H73	-8.316986	-2.351626	0.943455
H74	-8.316987	2.351613	-0.943424
H75	-8.285784	-3.109687	-0.669926
H76	-8.285777	3.109743	0.669924

2d

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2744.682826	Hartree
Zero-point Energy Correction	0.593834	Hartree
Thermal Correction to Energy	0.643251	Hartree
Thermal Correction to Enthalpy	0.644195	Hartree
Thermal Correction to Free Energy	0.500256	Hartree
EE + Zero-point Energy	-2744.088993	Hartree
EE + Thermal Energy Correction	-2744.039576	Hartree
EE + Thermal Enthalpy Correction	-2744.038632	Hartree
EE + Thermal Free Energy Correction	-2744.182570	Hartree
E (Thermal)	403.646	kcal/mol
Heat Capacity (Cv)	182.313	cal/mol-kelvin
Entropy (S)	302.945	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	0.903777	-0.007297	-0.098777
N2	-2.083648	-0.057739	-0.021284
N3	-0.065719	1.210556	-0.253754
N4	-0.010887	-1.234344	0.219789
C5	-1.450419	1.076184	-0.224457
C6	-1.399938	-1.163596	0.188192
F7	1.577695	-0.260626	-1.297026
F8	1.795524	0.250857	0.938772
C9	0.233021	2.516889	-0.354032
C10	0.345889	-2.522363	0.355916
C11	-0.992371	3.248254	-0.388855
C12	-0.842149	-3.307226	0.411742
C13	-2.072259	2.362719	-0.326801
C14	-1.962512	-2.471101	0.324872
C15	1.589388	3.060976	-0.347086
C16	1.731143	-2.996948	0.365363
C17	2.608515	2.557088	-1.167554
C18	2.686334	-2.503989	1.263876
H19	2.399317	1.733759	-1.846839
H20	2.406532	-1.74172	1.987544
C21	3.883206	3.09927	-1.141812

C22	3.986686	-2.984475	1.261177
H23	4.644214	2.680694	-1.795825
H24	4.697727	-2.577125	1.975723
C25	4.202008	4.170665	-0.2926
C26	4.392769	-3.980328	0.359444
O27	5.418181	4.703	-0.19601
O28	5.637389	-4.449303	0.284327
C29	3.164154	4.671126	0.529711
C30	3.416326	-4.472756	-0.538964
N31	3.377894	5.78041	1.449979
N32	3.721001	-5.509203	-1.516116
C33	1.88984	4.124879	0.504061
C34	2.11633	-3.98805	-0.535877
H35	1.144341	4.541342	1.179619
H36	1.416065	-4.396412	-1.262676
C37	-3.517073	2.551902	-0.395272
C38	-3.398032	-2.721343	0.402649
C39	-4.275957	1.726512	-1.243677
C40	-4.18909	-1.913095	1.237086
H41	-3.772889	0.991038	-1.870618
H42	-3.716301	-1.145792	1.849225
C43	-5.657335	1.857169	-1.30733
C44	-5.564195	-2.100039	1.306482
H45	-6.223775	1.21664	-1.986089
H46	-6.155647	-1.471571	1.975126
C47	-6.333933	2.790468	-0.511703
C48	-6.202361	-3.074951	0.529974
C49	-7.823631	2.943745	-0.594021
C50	-7.684446	-3.289025	0.616211
C51	-5.57505	3.59313	0.351172
C52	-5.411598	-3.861606	-0.319491
H53	-6.080067	4.314281	0.996964
H54	-5.886954	-4.615666	-0.950099
C55	-4.191037	3.490052	0.404665
C56	-4.033405	-3.702036	-0.37764
H57	-3.626372	4.118963	1.088888
H58	-3.443575	-4.320939	-1.049797
N59	-1.068075	4.648441	-0.696493
N60	-0.850293	-4.701932	0.745376
O61	-2.009884	5.283775	-0.249096

O62	-1.795276	-5.376548	0.366449
O63	-0.195979	5.121599	-1.411898
O64	0.080415	-5.135206	1.411049
C65	6.473214	4.135425	-0.971455
C66	6.628958	-3.886399	1.141659
H67	6.269007	4.240705	-2.045622
H68	6.38569	-4.072415	2.196705
H69	7.364619	4.711664	-0.708756
H70	7.558332	-4.401389	0.883079
H71	6.624223	3.078247	-0.713334
H72	6.738629	-2.808312	0.960096
H73	-8.090047	3.763131	-1.278941
H74	-7.9144	-4.14135	1.273466
H75	-8.254359	3.187413	0.385968
H76	-8.112163	-3.516321	-0.369229
H77	-8.299789	2.030147	-0.971597
H78	-8.193283	-2.407655	1.026147
O79	4.213851	6.619777	1.166151
O80	4.587284	-6.323899	-1.25131
O81	2.68201	5.816692	2.455285
O82	3.06641	-5.515267	-2.549595

3e

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2744.684354	Hartree
Zero-point Energy Correction	0.593932	Hartree
Thermal Correction to Energy	0.643322	Hartree
Thermal Correction to Enthalpy	0.644266	Hartree
Thermal Correction to Free Energy	0.501644	Hartree
EE + Zero-point Energy	-2744.090422	Hartree
EE + Thermal Energy Correction	-2744.041033	Hartree
EE + Thermal Enthalpy Correction	-2744.040088	Hartree
EE + Thermal Free Energy Correction	-2744.182710	Hartree
E (Thermal)	403.690	kcal/mol
Heat Capacity (Cv)	182.331	cal/mol-kelvin
Entropy (S)	300.173	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	2.627456	-0.004792	-0.051545
N2	-0.364163	-0.001314	-0.011431
N3	1.679407	1.233107	-0.219363
N4	1.683058	-1.23024	0.202706
C5	0.294136	1.122362	-0.194359
C6	0.297445	-1.124022	0.175023
F7	3.34577	-0.243578	-1.223309
F8	3.46681	0.222911	1.034571
C9	2.002814	2.537159	-0.296268
C10	2.009691	-2.532236	0.296639
C11	0.785541	3.286784	-0.327023
C12	0.79631	-3.285043	0.335183
C13	-0.304664	2.418498	-0.280386
C14	-0.297314	-2.419297	0.276076
C15	3.3603	3.073486	-0.262349
C16	3.371798	-3.061684	0.271383
C17	4.384091	2.571662	-1.074725
C18	4.372272	-2.589271	1.12823
H19	4.178914	1.760904	-1.770038
H20	4.146219	-1.806952	1.849261
C21	5.659246	3.124611	-1.011024
C22	5.650677	-3.136982	1.075855
H23	6.441504	2.732234	-1.663464
H24	6.415085	-2.768279	1.762418
C25	5.958017	4.169913	-0.131068
C26	5.974131	-4.147738	0.165144
C27	7.335612	4.757764	-0.053222
C28	7.356482	-4.726114	0.096486
C29	4.927111	4.660436	0.685045
C30	4.964585	-4.611544	-0.692071
H31	5.133969	5.470549	1.387009
H32	5.190422	-5.396994	-1.415931
C33	3.646513	4.134262	0.614218
C34	3.680835	-4.090724	-0.633811
H35	2.866682	4.528719	1.267417
H36	2.915407	-4.46565	-1.315051
C37	-1.74667	2.62744	-0.356247

C38	-1.739115	-2.630699	0.355281
C39	-2.51984	1.821349	-1.210454
C40	-2.51312	-1.820495	1.204543
H41	-2.026853	1.087627	-1.846618
H42	-2.021048	-1.081603	1.835431
C43	-3.895971	1.958099	-1.29145
C44	-3.889064	-1.959458	1.287865
H45	-4.446639	1.340237	-1.996627
H46	-4.440224	-1.338116	1.989597
C47	-4.57746	2.880663	-0.482409
C48	-4.5694	-2.888703	0.485783
O49	-5.893722	3.079603	-0.52821
O50	-5.885295	-3.090653	0.534667
C51	-3.795222	3.666915	0.395759
C52	-3.786374	-3.678906	-0.388146
N53	-4.404467	4.624618	1.309106
N54	-4.394636	-4.643742	-1.294543
C55	-2.411857	3.565393	0.437176
C56	-2.40323	-3.575091	-0.431252
H57	-1.866585	4.203444	1.126343
H58	-1.857238	-4.217052	-1.116203
N59	0.720057	4.692611	-0.608748
N60	0.737317	-4.688368	0.626021
O61	-0.20003	5.329611	-0.116044
O62	-0.199309	-5.325973	0.165706
O63	1.56967	5.167512	-1.346222
O64	1.609529	-5.16292	1.337206
C65	-6.662215	2.332615	-1.470012
C66	-6.65388	-2.340738	1.473931
H67	-6.600365	1.255959	-1.259823
H68	-6.596012	-1.265076	1.257542
H69	-7.692215	2.674755	-1.336982
H70	-7.683138	-2.686817	1.345339
H71	-6.332409	2.539307	-2.497338
H72	-6.321048	-2.540478	2.50168
H73	7.754149	4.641686	0.956885
H74	7.812702	-4.53261	-0.885228
H75	7.315315	5.835453	-0.269684
H76	7.333865	-5.816946	0.230056
H77	8.017359	4.276317	-0.764698

H78	8.008713	-4.297243	0.8669
O79	-5.513529	4.379945	1.752311
O80	-5.504376	-4.403779	-1.738713
O81	-3.751171	5.615379	1.602263
O82	-3.740056	-5.635488	-1.581478

4f

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2576.423830	Hartree
Zero-point Energy Correction	0.529810	Hartree
Thermal Correction to Energy	0.573398	Hartree
Thermal Correction to Enthalpy	0.574342	Hartree
Thermal Correction to Free Energy	0.442488	Hartree
EE + Zero-point Energy	-2575.894021	Hartree
EE + Thermal Energy Correction	-2575.850432	Hartree
EE + Thermal Enthalpy Correction	-2575.849488	Hartree
EE + Thermal Free Energy Correction	-2575.981342	Hartree
E (Thermal)	359.813	kcal/mol
Heat Capacity (Cv)	163.968	cal/mol-kelvin
Entropy (S)	277.510	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	-2.628997	0.384407	0.12891
N2	0.339876	0.132267	0.017105
N3	-1.813535	-0.927439	-0.096194
N4	-1.587484	1.547638	0.118533
C5	-0.428115	-0.955925	-0.067778
C6	-0.212203	1.307792	0.095148
F7	-3.556294	0.590323	-0.890157
F8	-3.261575	0.293862	1.379062
C9	-2.271787	-2.195708	-0.123758
C10	-1.770813	2.885525	0.057137
C11	-1.144246	-3.058369	-0.113582
C12	-0.496252	3.535674	0.004164
C13	0.034256	-2.288729	-0.081319
C14	0.485826	2.576864	0.059519
C15	-3.695132	-2.556548	-0.083277

C16	-3.035267	3.600331	0.060419
C17	-4.585967	-2.148139	-1.079174
C18	-4.19783	3.122352	0.6889
H19	-4.229456	-1.545432	-1.912648
H20	-4.181407	2.172286	1.216305
C21	-5.926265	-2.523578	-1.016055
C22	-5.363354	3.87775	0.676807
H23	-6.605971	-2.205373	-1.809107
H24	-6.249173	3.494971	1.187002
C25	-6.416026	-3.297537	0.039845
C26	-5.425999	5.118149	0.029573
C27	-7.862654	-3.691299	0.117277
C28	-6.691245	5.920383	-0.002348
C29	-5.513546	-3.699	1.035687
C30	-4.26417	5.592539	-0.598847
H31	-5.869164	-4.30178	1.873981
H32	-4.284545	6.554495	-1.114474
C33	-4.17267	-3.345146	0.97353
C34	-3.089507	4.858427	-0.575435
H35	-3.489017	-3.670222	1.759275
H36	-2.209662	5.248852	-1.087154
C37	1.458042	-2.64708	-0.095474
C38	1.932233	2.77814	0.065847
C39	2.301557	-2.062182	-1.049035
C40	2.796692	1.869374	0.694389
H41	1.88325	-1.393588	-1.800443
H42	2.390344	0.985821	1.182203
C43	3.665952	-2.338679	-1.05651
C44	4.169824	2.093419	0.708363
H45	4.309731	-1.888509	-1.810952
H46	4.831446	1.383972	1.203798
C47	4.19886	-3.192494	-0.094357
C48	4.693292	3.226209	0.088681
C49	5.667774	-3.489494	-0.059398
C50	6.167781	3.49997	0.107872
C51	3.372583	-3.773772	0.871088
C52	3.847167	4.141272	-0.543354
H53	3.792003	-4.4376	1.627661
H54	4.257134	5.023508	-1.035647
C55	2.010339	-3.508074	0.864961

C56	2.478376	3.916534	-0.552197
H57	1.367027	-3.962477	1.615518
H58	1.823744	4.621159	-1.065665
N59	-1.214923	-4.474449	-0.29541
O60	-0.242182	-5.141409	0.034649
O61	-2.22968	-4.948687	-0.787607
H62	-8.338255	-3.266313	1.013164
H63	-7.078694	5.991427	-1.029487
H64	-8.419249	-3.342753	-0.761436
H65	-7.469284	5.469012	0.624818
H66	-7.971823	-4.783159	0.183221
H67	-6.515049	6.9483	0.344288
F68	5.916439	-4.818671	-0.048678
F69	6.469639	4.569489	0.88209
F70	6.330786	-2.975448	-1.111699
F71	6.884718	2.464503	0.580189
F72	6.255968	-2.989	1.053841
F73	6.644945	3.781678	-1.125081
H74	-0.358255	4.61169	0.006707

4g

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2576.422113	Hartree
Zero-point Energy Correction	0.529654	Hartree
Thermal Correction to Energy	0.573262	Hartree
Thermal Correction to Enthalpy	0.574206	Hartree
Thermal Correction to Free Energy	0.442125	Hartree
EE + Zero-point Energy	-2575.892459	Hartree
EE + Thermal Energy Correction	-2575.848851	Hartree
EE + Thermal Enthalpy Correction	-2575.847907	Hartree
EE + Thermal Free Energy Correction	-2575.979988	Hartree
E (Thermal)	359.727	kcal/mol
Heat Capacity (Cv)	163.981	cal/mol-kelvin
Entropy (S)	277.988	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	0.758356	0.099768	-0.149008

N2	-2.214691	0.291369	-0.049591
N3	-0.245921	-1.072753	0.076319
N4	-0.097329	1.399302	-0.134284
C5	-1.622044	-0.89632	0.058359
C6	-1.493291	1.373194	-0.136883
F7	1.712644	0.153809	0.865187
F8	1.368742	-0.084159	-1.401128
C9	0.017395	-2.390302	0.120742
C10	0.28146	2.695093	-0.071756
C11	-1.219899	-3.082624	0.136298
C12	-0.865678	3.532479	-0.049439
C13	-2.278582	-2.149951	0.105101
C14	-1.991761	2.735021	-0.124838
C15	1.383902	-2.942372	0.086042
C16	1.653804	3.19861	-0.045148
C17	2.27729	-2.719162	1.135909
C18	2.708764	2.584399	-0.735023
H19	1.968028	-2.132037	1.998552
H20	2.529707	1.686315	-1.320506
C21	3.56094	-3.255988	1.087595
C22	3.985659	3.13425	-0.699372
H23	4.251739	-3.088644	1.912927
H24	4.796732	2.655712	-1.246429
C25	3.953888	-4.007992	-0.016828
C26	4.223276	4.293493	0.035958
C27	5.344966	-4.561017	-0.106063
C28	5.591397	4.909603	0.078338
C29	3.069396	-4.230685	-1.074424
C30	3.184118	4.917187	0.730118
H31	3.379154	-4.818076	-1.938866
H32	3.370247	5.820359	1.311414
C33	1.785963	-3.704897	-1.017825
C34	1.907848	4.376969	0.680679
H35	1.091836	-3.880615	-1.839863
H36	1.103649	4.858019	1.236872
C37	-3.734573	-2.296031	0.145508
C38	-3.381852	3.160759	-0.166067
C39	-4.480657	-1.520926	1.045988
C40	-4.387293	2.364832	-0.740464
H41	-3.964809	-0.859631	1.741914

H42	-4.131465	1.394713	-1.162436
C43	-5.869946	-1.603906	1.073331
C44	-5.7025	2.814164	-0.788954
H45	-6.426852	-1.002728	1.794954
H46	-6.464271	2.182755	-1.25078
C47	-6.56221	-2.440239	0.191882
C48	-6.067493	4.060575	-0.266507
C49	-8.059319	-2.541573	0.222382
C50	-7.490057	4.534698	-0.297736
C51	-5.812528	-3.197659	-0.720407
C52	-5.060993	4.853857	0.3059
H53	-6.328307	-3.849019	-1.429281
H54	-5.31781	5.829416	0.723917
C55	-4.425529	-3.138975	-0.740026
C56	-3.74546	4.417321	0.35399
H57	-3.86862	-3.738113	-1.458051
H58	-2.988625	5.048639	0.821694
N59	-1.329896	-4.491876	0.340972
O60	-2.407734	-5.025245	0.115983
O61	-0.344326	-5.095073	0.747853
F62	6.112068	-3.856115	-0.972493
F63	5.98859	5.164127	1.344272
F64	5.987731	-4.546909	1.07669
F65	6.532024	4.128849	-0.481224
F66	5.356534	-5.837901	-0.546958
F67	5.625479	6.094609	-0.575035
H68	-8.377044	-3.521031	0.609776
H69	-7.552884	5.581738	-0.624072
H70	-8.49988	-1.76745	0.862896
H71	-8.102212	3.921367	-0.970295
H72	-8.48452	-2.44238	-0.786035
H73	-7.938681	4.483285	0.705872
H74	-0.830257	4.616727	-0.055689

5a

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1619.994926	Hartree
Zero-point Energy Correction	0.464317	Hartree
Thermal Correction to Energy	0.493770	Hartree
Thermal Correction to Enthalpy	0.494714	Hartree
Thermal Correction to Free Energy	0.401112	Hartree
EE + Zero-point Energy	-1619.530609	Hartree
EE + Thermal Energy Correction	-1619.501156	Hartree
EE + Thermal Enthalpy Correction	-1619.500212	Hartree
EE + Thermal Free Energy Correction	-1619.593814	Hartree
E (Thermal)	309.845	kcal/mol
Heat Capacity (Cv)	117.739	cal/mol-kelvin
Entropy (S)	197.002	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	1.622979	0	0.000001
N2	-1.346299	0	0
N3	0.697605	-1.241978	0.130333
N4	0.697605	1.241978	-0.130332
C5	-0.688433	-1.134958	0.123543
C6	-0.688434	1.134957	-0.123542
F7	2.426908	0.174492	1.141189
F8	2.426908	-0.174491	-1.141188
C9	1.004672	-2.566136	0.106988
C10	1.004671	2.566136	-0.106987
C11	-0.191365	-3.323266	0.116949
C12	-0.191367	3.323265	-0.116949
C13	-1.266459	-2.447589	0.151883
C14	-1.26646	2.447589	-0.151882
C15	2.340217	-3.162555	0.072559
C16	2.340216	3.162556	-0.072559
C17	3.452447	-2.616764	0.733392
C18	3.452445	2.616765	-0.733393
H19	3.3474	-1.692298	1.294937
H20	3.347398	1.6923	-1.294938
C21	4.683494	-3.264779	0.690141
C22	4.683492	3.264782	-0.690142
H23	5.534849	-2.832594	1.217995
H24	5.534847	2.832597	-1.217997

C25	4.83268	-4.458619	-0.016639
C26	4.832678	4.458621	0.016638
H27	5.801557	-4.959203	-0.050677
H28	5.801554	4.959206	0.050676
C29	3.734536	-5.009204	-0.679526
C30	3.734534	5.009206	0.679525
H31	3.840611	-5.938063	-1.241583
H32	3.840609	5.938064	1.241583
C33	2.499749	-4.371935	-0.629753
C34	2.499747	4.371936	0.629754
H35	1.652024	-4.800461	-1.165359
H36	1.652022	4.800461	1.16536
C37	-2.686051	-2.788874	0.197954
C38	-2.686052	2.788873	-0.197954
C39	-3.629097	-1.943097	0.806614
C40	-3.629099	1.943094	-0.806613
H41	-3.299825	-1.004	1.248392
H42	-3.299826	1.003997	-1.248389
C43	-4.972823	-2.303943	0.85847
C44	-4.972824	2.30394	-0.858469
H45	-5.690377	-1.638515	1.341134
H46	-5.690378	1.638512	-1.341132
C47	-5.401699	-3.511035	0.304429
C48	-5.401701	3.511033	-0.30443
H49	-6.455586	-3.790592	0.346195
H50	-6.455588	3.79059	-0.346197
C51	-4.474005	-4.359698	-0.302977
C52	-4.474006	4.359697	0.302975
H53	-4.800384	-5.302682	-0.744207
H54	-4.800386	5.302681	0.744204
C55	-3.130358	-4.002915	-0.354277
C56	-3.13036	4.002914	0.354275
H57	-2.415721	-4.662918	-0.848397
H58	-2.415723	4.662919	0.848394
H59	-0.230296	-4.406582	0.167641
H60	-0.230298	4.406581	-0.16764

5b

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1777.087749	Hartree
Zero-point Energy Correction	0.572906	Hartree
Thermal Correction to Energy	0.610154	Hartree
Thermal Correction to Enthalpy	0.611098	Hartree
Thermal Correction to Free Energy	0.495939	Hartree
EE + Zero-point Energy	-1776.514843	Hartree
EE + Thermal Energy Correction	-1776.477595	Hartree
EE + Thermal Enthalpy Correction	-1776.476651	Hartree
EE + Thermal Free Energy Correction	-1776.591810	Hartree
E (Thermal)	382.878	kcal/mol
Heat Capacity (Cv)	142.230	cal/mol-kelvin
Entropy (S)	242.373	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	1.660558	0	0
N2	-1.306415	0	0
N3	0.737625	-1.243074	0.120461
N4	0.737625	1.243074	-0.120461
C5	-0.648527	-1.135908	0.116082
C6	-0.648527	1.135908	-0.116082
F7	2.467205	0.164471	1.142771
F8	2.467205	-0.164471	-1.142771
C9	1.045427	-2.568764	0.090455
C10	1.045427	2.568764	-0.090455
C11	-0.151365	-3.324057	0.099824
C12	-0.151365	3.324057	-0.099824
C13	-1.227414	-2.448453	0.139919
C14	-1.227414	2.448453	-0.139919
C15	2.378364	-3.165898	0.050285
C16	2.378364	3.165898	-0.050285
C17	3.504862	-2.615097	0.679673
C18	3.504862	2.615097	-0.679673
H19	3.416232	-1.680715	1.227445
H20	3.416232	1.680715	-1.227445
C21	4.732308	-3.26866	0.630105
C22	4.732308	3.26866	-0.630105
H23	5.589608	-2.825019	1.140912
H24	5.589608	2.825019	-1.140912

C25	4.89197	-4.480259	-0.051231
C26	4.89197	4.480259	0.051231
C27	6.223048	-5.168642	-0.12499
C28	6.223048	5.168642	0.12499
C29	3.76499	-5.028583	-0.680115
C30	3.76499	5.028583	0.680115
H31	3.856262	-5.971065	-1.224273
H32	3.856262	5.971065	1.224273
C33	2.533415	-4.391451	-0.626542
C34	2.533415	4.391451	0.626542
H35	1.680687	-4.835435	-1.141378
H36	1.680687	4.835435	1.141379
C37	-2.645461	-2.789997	0.187057
C38	-2.645461	2.789997	-0.187057
C39	-3.59873	-1.936511	0.765299
C40	-3.59873	1.936511	-0.765299
H41	-3.280663	-0.983801	1.185722
H42	-3.280663	0.983801	-1.185722
C43	-4.940752	-2.302765	0.817949
C44	-4.940752	2.302765	-0.817949
H45	-5.659821	-1.624611	1.282856
H46	-5.659821	1.624611	-1.282856
C47	-5.385924	-3.523168	0.297787
C48	-5.385924	3.523168	-0.297787
C49	-6.83629	-3.908418	0.335593
C50	-6.83629	3.908418	-0.335593
C51	-4.431861	-4.375262	-0.27725
C52	-4.431861	4.375262	0.27725
H53	-4.748709	-5.33402	-0.69387
H54	-4.748709	5.33402	0.69387
C55	-3.090646	-4.019317	-0.33143
C56	-3.090646	4.019317	0.33143
H57	-2.375604	-4.696566	-0.801381
H58	-2.375604	4.696566	0.801381
H59	-0.191471	-4.407418	0.146955
H60	-0.191471	4.407418	-0.146955
H61	6.64826	-5.088037	-1.136737
H62	6.64826	5.088037	1.136737
H63	6.941337	-4.726983	0.576813
H64	6.941337	4.726983	-0.576814
H65	6.129745	-6.240142	0.099616
H66	6.129745	6.240142	-0.099615
H67	-6.964634	-4.944324	0.678561
H68	-6.964634	4.944324	-0.678561
H69	-7.407667	-3.249096	1.000975
H70	-7.407667	3.249096	-1.000976

H71	-7.285216	-3.843608	-0.667095
H72	-7.285216	3.843608	0.667095

5c

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2077.663843	Hartree
Zero-point Energy Correction	0.594436	Hartree
Thermal Correction to Energy	0.634298	Hartree
Thermal Correction to Enthalpy	0.635242	Hartree
Thermal Correction to Free Energy	0.518025	Hartree
EE + Zero-point Energy	-2077.069407	Hartree
EE + Thermal Energy Correction	-2077.029545	Hartree
EE + Thermal Enthalpy Correction	-2077.028601	Hartree
EE + Thermal Free Energy Correction	-2077.145818	Hartree
E (Thermal)	398.028	kcal/mol
Heat Capacity (Cv)	154.434	cal/mol-kelvin
Entropy (S)	246.704	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	1.727896	0	0
N2	-1.234721	0	0
N3	0.80958	-1.242836	0.125422
N4	0.80958	1.242836	-0.125422
C5	-0.576625	-1.135129	0.126497
C6	-0.576625	1.135129	-0.126497
F7	2.538719	0.168522	1.142278
F8	2.538719	-0.168522	-1.142278
C9	1.118559	-2.571172	0.106031
C10	1.118559	2.571172	-0.106031
C11	-0.079401	-3.323468	0.132491
C12	-0.079401	3.323468	-0.132491
C13	-1.156095	-2.446848	0.168534
C14	-1.156095	2.446848	-0.168534
C15	2.447901	-3.169478	0.059849
C16	2.447901	3.169477	-0.059849
C17	3.600766	-2.586869	0.621995
C18	3.600766	2.586869	-0.621995
H19	3.531104	-1.6258	1.123893
H20	3.531104	1.6258	-1.123892
C21	4.823442	-3.232371	0.569544

C22	4.823443	3.232371	-0.569544
H23	5.709258	-2.781781	1.018422
H24	5.709258	2.781781	-1.018422
C25	4.94518	-4.481398	-0.057402
C26	4.94518	4.481398	0.057402
O27	6.181515	-5.025336	-0.061221
O28	6.181515	5.025336	0.061221
C29	3.81393	-5.078373	-0.627323
C30	3.81393	5.078373	0.627323
H31	3.874321	-6.040861	-1.131618
H32	3.874321	6.040861	1.131618
C33	2.58912	-4.424404	-0.557245
C34	2.58912	4.424404	0.557245
H35	1.724072	-4.894807	-1.025518
H36	1.724072	4.894807	1.025518
C37	-2.571691	-2.787621	0.228917
C38	-2.571691	2.787621	-0.228917
C39	-3.528533	-1.917031	0.771428
C40	-3.528533	1.917031	-0.771428
H41	-3.211733	-0.947805	1.153063
H42	-3.211733	0.947805	-1.153064
C43	-4.875146	-2.265525	0.844793
C44	-4.875146	2.265525	-0.844793
H45	-5.580431	-1.562086	1.283873
H46	-5.580431	1.562086	-1.283873
C47	-5.296537	-3.511229	0.365986
C48	-5.296537	3.511229	-0.365986
O49	-6.577049	-3.949021	0.387234
O50	-6.577049	3.949021	-0.387234
C51	-4.354686	-4.396441	-0.180472
C52	-4.354686	4.396441	0.180472
H53	-4.694671	-5.361551	-0.557552
H54	-4.694671	5.361551	0.557552
C55	-3.019734	-4.037501	-0.243218
C56	-3.019734	4.037501	0.243218
H57	-2.306638	-4.732896	-0.688517
H58	-2.306638	4.732896	0.688517
H59	-0.121849	-4.405907	0.194877
H60	-0.121849	4.405907	-0.194877
C61	6.349441	-6.293673	-0.678415
C62	6.349441	6.293673	0.678415
H63	6.096376	-6.250941	-1.748092
H64	6.096376	6.250941	1.748092
H65	7.408869	-6.543439	-0.564563
H66	7.408869	6.543439	0.564563
H67	5.736704	-7.060466	-0.181658

H68	5.736704	7.060466	0.181658
C69	-7.565134	-3.084042	0.926326
C70	-7.565134	3.084042	-0.926326
H71	-7.625882	-2.145398	0.355422
H72	-7.625882	2.145399	-0.355422
H73	-8.513754	-3.623558	0.842118
H74	-8.513754	3.623558	-0.842118
H75	-7.363769	-2.861339	1.984761
H76	-7.363769	2.861339	-1.984761

5d

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2336.023422	Hartree
Zero-point Energy Correction	0.588643	Hartree
Thermal Correction to Energy	0.632685	Hartree
Thermal Correction to Enthalpy	0.633629	Hartree
Thermal Correction to Free Energy	0.503188	Hartree
EE + Zero-point Energy	-2335.434779	Hartree
EE + Thermal Energy Correction	-2335.390737	Hartree
EE + Thermal Enthalpy Correction	-2335.389792	Hartree
EE + Thermal Free Energy Correction	-2335.520234	Hartree
E (Thermal)	397.016	kcal/mol
Heat Capacity (Cv)	165.370	cal/mol-kelvin
Entropy (S)	274.537	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	-1.380983	-0.001221	-0.013399
N2	1.605066	0.001955	-0.001736
N3	-0.442783	1.244365	0.105638
N4	-0.438998	-1.24606	-0.109123
C5	0.943955	1.136991	0.0817
C6	0.947378	-1.134607	-0.084864
F7	-2.184051	-0.145109	1.120254
F8	-2.152292	0.141737	-1.170148
C9	-0.771038	2.552041	0.07627
C10	-0.763735	-2.554552	-0.076205
C11	0.444167	3.301792	0.036052
C12	0.4541	-3.300759	-0.033604
C13	1.539492	2.436948	0.054489
C14	1.546685	-2.433227	-0.054114

C15	-2.122428	3.090592	0.002955
C16	-2.112921	-3.09722	-0.002178
C17	-3.163425	2.638354	0.822361
C18	-3.159663	-2.638346	-0.810868
H19	-2.973685	1.858862	1.556123
H20	-2.975799	-1.85057	-1.537263
C21	-4.438069	3.187962	0.735168
C22	-4.432639	-3.19114	-0.722228
H23	-5.216965	2.823083	1.401592
H24	-5.215916	-2.820796	-1.380442
C25	-4.696709	4.197667	-0.199807
C26	-4.684329	-4.210893	0.203858
O27	-5.895777	4.788241	-0.37366
O28	-5.881108	-4.805457	0.378177
C29	-3.662152	4.656841	-1.031755
C30	-3.644464	-4.676088	1.025877
H31	-3.877775	5.437232	-1.761536
H32	-3.854819	-5.463655	1.749446
C33	-2.394846	4.119661	-0.920064
C34	-2.378861	-4.135496	0.912623
H35	-1.607687	4.479872	-1.583897
H36	-1.588186	-4.50005	1.569802
C37	2.980912	2.668492	0.109939
C38	2.988674	-2.66097	-0.108101
C39	3.754286	1.960224	1.046223
C40	3.760848	-1.951786	-1.044759
H41	3.265314	1.27888	1.741815
H42	3.270596	-1.272474	-1.74143
C43	5.130886	2.135832	1.105124
C44	5.137861	-2.124059	-1.102619
H45	5.708274	1.585014	1.850426
H46	5.714355	-1.572633	-1.84816
C47	5.789638	3.001303	0.22186
C48	5.798226	-2.986966	-0.217981
C49	7.274066	3.203792	0.30307
C50	7.283213	-3.185631	-0.298159
C51	5.017426	3.686651	-0.724381
C52	5.027178	-3.673218	0.72851
H53	5.508102	4.351832	-1.437945
H54	5.519085	-4.336377	1.443101
C55	3.636359	3.535817	-0.778342
C56	3.645693	-3.52571	0.781534
H57	3.061156	4.0727	-1.52921
H58	3.071399	-4.063025	1.532786
N59	0.502399	4.726339	0.20849
N60	0.517274	-4.725572	-0.204221

O61	1.365767	5.342488	-0.398919
O62	1.377372	-5.339011	0.410394
O63	-0.299964	5.2412	0.973657
O64	-0.277662	-5.242753	-0.975465
C65	-6.977448	4.359304	0.443279
C66	-6.968327	-4.370406	-0.428253
H67	-6.764315	4.538602	1.507189
H68	-6.760779	-4.538341	-1.495091
H69	-7.838586	4.960897	0.136872
H70	-7.826415	-4.976985	-0.123163
H71	-7.196958	3.29396	0.280876
H72	-7.189074	-3.307277	-0.253584
H73	7.516271	4.012443	1.009507
H74	7.528164	-3.990823	-1.007591
H75	7.693291	3.484264	-0.67169
H76	7.701954	-3.468911	0.67598
H77	7.781985	2.297624	0.657599
H78	7.78937	-2.276861	-0.648557

5e

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-1927.375539	Hartree
Zero-point Energy Correction	0.583727	Hartree
Thermal Correction to Energy	0.622252	Hartree
Thermal Correction to Enthalpy	0.623196	Hartree
Thermal Correction to Free Energy	0.507280	Hartree
EE + Zero-point Energy	-1926.791812	Hartree
EE + Thermal Energy Correction	-1926.753287	Hartree
EE + Thermal Enthalpy Correction	-1926.752343	Hartree
EE + Thermal Free Energy Correction	-1926.868259	Hartree
E (Thermal)	390.469	kcal/mol
Heat Capacity (Cv)	148.294	cal/mol-kelvin
Entropy (S)	243.967	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	2.05096	0	0
N2	-0.914866	0	0
N3	1.128998	1.244479	-0.098619
N4	1.128998	-1.244479	0.098619
C5	-0.257102	1.137652	-0.100106

C6	-0.257102	-1.137652	0.100106
F7	2.859436	-0.143869	-1.145357
F8	2.859437	0.14387	1.145356
C9	1.436414	2.57057	-0.046619
C10	1.436414	-2.57057	0.046619
C11	0.241526	3.32559	-0.049843
C12	0.241526	-3.32559	0.049844
C13	-0.836726	2.450777	-0.108363
C14	-0.836726	-2.450777	0.108364
C15	2.770024	3.166438	0.008554
C16	2.770024	-3.166438	-0.008554
C17	3.898524	2.626225	-0.626192
C18	3.898525	-2.626225	0.626191
H19	3.811559	1.701017	-1.18963
H20	3.81156	-1.701016	1.189629
C21	5.126083	3.278558	-0.561621
C22	5.126084	-3.278558	0.56162
H23	5.985012	2.84311	-1.076792
H24	5.985013	-2.84311	1.07679
C25	5.283892	4.478577	0.140187
C26	5.283892	-4.478577	-0.140189
C27	6.615035	5.1652	0.229732
C28	6.615035	-5.165199	-0.229734
C29	4.154973	5.016325	0.77455
C30	4.154973	-5.016324	-0.774551
H31	4.244535	5.949573	1.334739
H32	4.244536	-5.949573	-1.33474
C33	2.92349	4.38008	0.706636
C34	2.923491	-4.380079	-0.706636
H35	2.069096	4.815283	1.226238
H36	2.069096	-4.815282	-1.226238
C37	-2.251497	2.79347	-0.159103
C38	-2.251496	-2.79347	0.159104
C39	-3.210258	1.934558	-0.71724
C40	-3.210257	-1.934559	0.717242
H41	-2.895267	0.973212	-1.119678
H42	-2.895266	-0.973213	1.119681
C43	-4.556413	2.285692	-0.780932
C44	-4.556413	-2.285692	0.780933
H45	-5.263319	1.592204	-1.232977
H46	-5.263319	-1.592205	1.232979
C47	-4.975571	3.522095	-0.276292
C48	-4.975571	-3.522096	0.276293
O49	-6.255128	3.961369	-0.286508
O50	-6.255128	-3.96137	0.286509
C51	-4.031763	4.395535	0.285996

C52	-4.031763	-4.395535	-0.285996
H53	-4.370203	5.353199	0.68284
H54	-4.370203	-5.353199	-0.68284
C55	-2.697241	4.034426	0.338708
C56	-2.697241	-4.034427	-0.338708
H57	-1.982635	4.720298	0.796089
H58	-1.982634	-4.720298	-0.796089
H59	0.203315	4.409595	-0.080852
H60	0.203316	-4.409595	0.080852
C61	-7.245673	3.108494	-0.840684
C62	-7.245672	-3.108494	0.840685
H63	-7.306438	2.158949	-0.288193
H64	-7.306437	-2.158949	0.288194
H65	-8.193237	3.647667	-0.74378
H66	-8.193237	-3.647667	0.743781
H67	-7.046637	2.906642	-1.903691
H68	-7.046637	-2.906643	1.903692
H69	7.038528	5.06526	1.240487
H70	7.038528	-5.065262	-1.240489
H71	6.522545	6.240792	0.025235
H72	6.522546	-6.240791	-0.025235
H73	7.334564	4.736739	-0.479004
H74	7.334565	-4.736737	0.479

5f

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2372.099278	Hartree
Zero-point Energy Correction	0.527325	Hartree
Thermal Correction to Energy	0.568176	Hartree
Thermal Correction to Enthalpy	0.569120	Hartree
Thermal Correction to Free Energy	0.442829	Hartree
EE + Zero-point Energy	-2371.571953	Hartree
EE + Thermal Energy Correction	-2371.531102	Hartree
EE + Thermal Enthalpy Correction	-2371.530158	Hartree
EE + Thermal Free Energy Correction	-2371.656449	Hartree
E (Thermal)	356.536	kcal/mol
Heat Capacity (Cv)	155.422	cal/mol-kelvin
Entropy (S)	265.802	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	2.700728	-0.001961	-0.00276

N2	-0.267474	0.003032	-0.012807
N3	1.778044	1.246126	-0.109963
N4	1.773179	-1.246871	0.098759
C5	0.393405	1.138876	-0.10828
C6	0.388973	-1.135051	0.08734
F7	3.505343	-0.153634	-1.145511
F8	3.498874	0.14714	1.144766
C9	2.088107	2.569942	-0.061986
C10	2.079146	-2.571781	0.053373
C11	0.888428	3.3269	-0.058998
C12	0.877085	-3.324721	0.042062
C13	-0.183126	2.451143	-0.110122
C14	-0.191906	-2.445354	0.085523
C15	3.419221	3.166654	-0.014501
C16	3.408638	-3.172878	0.015898
C17	4.5499	2.615361	-0.63654
C18	4.536023	-2.626032	0.64778
H19	4.465067	1.68283	-1.187808
H20	4.449762	-1.693774	1.199293
C21	5.777021	3.268034	-0.576996
C22	5.761402	-3.282726	0.597553
H23	6.63781	2.824778	-1.081978
H24	6.61947	-2.842939	1.110151
C25	5.932199	4.478535	0.107383
C26	5.91812	-4.493014	-0.086898
C27	7.260975	5.169813	0.187248
C28	7.245496	-5.187993	-0.157522
C29	4.801177	5.026856	0.72982
C30	4.79035	-5.037002	-0.718911
H31	4.889723	5.967664	1.277114
H32	4.880161	-5.977669	-1.26624
C33	3.569861	4.391564	0.665768
C34	3.560643	-4.397667	-0.664214
H35	2.714766	4.835371	1.176616
H36	2.708172	-4.838216	-1.182238
C37	-1.604499	2.788095	-0.14798
C38	-1.614557	-2.777752	0.114871
C39	-2.54223	1.953859	-0.777599
C40	-2.553743	-1.938783	0.737737
H41	-2.210749	1.028532	-1.244617
H42	-2.221918	-1.013306	1.204224
C43	-3.886966	2.304904	-0.822507
C44	-3.89955	-2.283118	0.770685
H45	-4.602265	1.65285	-1.323173
H46	-4.616728	-1.623849	1.259936
C47	-4.313686	3.497638	-0.239083

C48	-4.328504	-3.471827	0.178222
C49	-5.766982	3.862269	-0.243323
C50	-5.773875	-3.858363	0.258409
C51	-3.396257	4.339006	0.393557
C52	-3.410086	-4.319387	-0.442368
H53	-3.728913	5.269427	0.853892
H54	-3.744927	-5.244082	-0.911703
C55	-2.054533	3.98464	0.435527
C56	-2.065462	-3.971067	-0.472708
H57	-1.345535	4.637374	0.945533
H58	-1.356325	-4.624806	-0.981222
H59	0.847086	4.410809	-0.090929
H60	7.64559	5.15824	1.217929
H61	7.643445	-5.165593	-1.182994
H62	8.004334	4.684072	-0.456699
H63	7.982185	-4.712054	0.50125
H64	7.177796	6.224139	-0.111655
H65	7.155114	-6.245396	0.127931
F66	-5.961	5.192029	-0.372726
F67	-6.063439	-4.492925	1.421506
F68	-6.448123	3.264999	-1.240817
F69	-6.595069	-2.789262	0.197848
F70	-6.381707	3.501355	0.91044
F71	-6.141114	-4.695207	-0.732638
H72	0.831864	-4.40848	0.074126

5g

Imaginary Freq	0	
Temperature	298.150	Kelvin
Pressure	1.00000	atm
Frequencies scaled by	1.0000	
Electronic Energy (EE)	-2372.097372	Hartree
Zero-point Energy Correction	0.527335	Hartree
Thermal Correction to Energy	0.568131	Hartree
Thermal Correction to Enthalpy	0.569075	Hartree
Thermal Correction to Free Energy	0.444582	Hartree
EE + Zero-point Energy	-2371.570038	Hartree
EE + Thermal Energy Correction	-2371.529242	Hartree
EE + Thermal Enthalpy Correction	-2371.528298	Hartree
EE + Thermal Free Energy Correction	-2371.652790	Hartree
E (Thermal)	356.507	kcal/mol
Heat Capacity (Cv)	155.413	cal/mol-kelvin
Entropy (S)	262.017	cal/mol-kelvin

Cartesian Coordinates in CH_2Cl_2

Atom	X	Y	Z
B1	-0.714853	0.008008	0.002658
N2	2.253857	-0.002239	0.001375
N3	0.215302	1.244278	0.13826
N4	0.206537	-1.234752	-0.133902
C5	1.600517	1.13438	0.131402
C6	1.592528	-1.134248	-0.128224
F7	-1.520593	-0.169063	1.142277
F8	-1.520291	0.191039	-1.136302
C9	-0.085592	2.56961	0.119213
C10	-0.103289	-2.558064	-0.115465
C11	1.107872	3.324824	0.13388
C12	1.085109	-3.321292	-0.131477
C13	2.18357	2.446097	0.167366
C14	2.166654	-2.449877	-0.165398
C15	-1.423468	3.164374	0.084567
C16	-1.444886	-3.144298	-0.081149
C17	-2.529534	2.621568	0.755664
C18	-2.54796	-2.592575	-0.747439
H19	-2.421665	1.702532	1.325074
H20	-2.435959	-1.671715	-1.313052
C21	-3.762317	3.262345	0.715807
C22	-3.78636	-3.225521	-0.707452
H23	-4.610067	2.836685	1.25218
H24	-4.632919	-2.791712	-1.238138
C25	-3.909016	4.450972	0.001226
C26	-3.939135	-4.41381	0.003201
C27	-5.25171	5.112607	-0.082989
C28	-5.269381	-5.101339	0.077793
C29	-2.820974	5.003266	-0.675589
C30	-2.851731	-4.976963	0.67526
H31	-2.934017	5.929037	-1.23919
H32	-2.968698	-5.903578	1.237831
C33	-1.5884	4.36626	-0.626698
C34	-1.616226	-4.348655	0.626863
H35	-0.74557	4.794658	-1.168764
H36	-0.775396	-4.783497	1.16689
C37	3.601058	2.783529	0.215814
C38	3.58176	-2.796934	-0.215514
C39	4.554603	1.917088	0.774826
C40	4.540582	-1.936786	-0.775208
H41	4.236581	0.958498	1.181528
H42	4.228704	-0.975763	-1.180922
C43	5.897326	2.279266	0.827412

C44	5.880679	-2.308281	-0.829757
H45	6.616964	1.591965	1.27751
H46	6.604505	-1.625737	-1.280373
C47	6.342663	3.507587	0.325957
C48	6.318101	-3.539983	-0.329643
C49	7.793639	3.889016	0.363641
C50	7.766299	-3.931592	-0.369632
C51	5.388131	4.372486	-0.229555
C52	5.358311	-4.39852	0.226686
H53	5.705691	5.337324	-0.631025
H54	5.669678	-5.365767	0.62721
C55	4.046133	4.021438	-0.282925
C56	4.018866	-4.038161	0.282018
H57	3.33092	4.708713	-0.737606
H58	3.299475	-4.720672	0.737275
H59	1.147745	4.407893	0.187472
F60	-5.96261	4.67436	-1.150409
F61	-5.778563	-5.077154	1.332353
F62	-6.011733	4.87465	1.004511
F63	-6.192085	-4.543334	-0.726599
F64	-5.156425	6.451617	-0.214267
F65	-5.183201	-6.406376	-0.266961
H66	7.925848	4.91593	0.731227
H67	7.890792	-4.958826	-0.739023
H68	8.368421	3.212289	1.008118
H69	8.345091	-3.257936	-1.013739
H70	8.234691	3.848945	-0.643785
H71	8.208804	-3.896275	0.63733
H72	1.117748	-4.404562	-0.185793

UV-Vis Calculations with TD-DFT

Theory Level: TD-DFT(PBE0/jul-cc-pvDz)//DFT(PBEO/jul-cc-pvDz)

	1a			1b			1c		
Solvent	λ_{max} (nm)	Excitation Energy (eV)	Oscillator Strength	λ_{max} (nm)	Excitation Energy (eV)	Oscillator Strength	λ_{max} (nm)	Excitation Energy (eV)	Oscillator Strength
CH_2Cl_2	590.93	2.0981	0.8132	615.97	2.0128	0.7273	678.46	1.8274	0.6661
MeCN	575.41	2.1547	0.7082	611.00	2.0292	0.6741	675.55	1.8353	0.6166
PhMe	589.99	2.1015	0.8065	619.80	2.0004	0.7938	674.82	1.8373	0.7470
Gas	557.50	2.2239	0.6777	582.05	2.1301	0.6783	625.89	1.9809	0.6424

Table S4. UV-Vis of **1a–c** with CH_2Cl_2, PhMe, and MeCN as implicit solvent and gas phase.

Theory Level: TD-DFT(PBE0/jul-cc-pvDz)//DFT(B3LYP/jul-cc-pvDz)

	1a			1b			1c		
Solvent	λ_{max} (nm)	Excitation Energy (eV)	Oscillator Strength	λ_{max} (nm)	Excitation Energy (eV)	Oscillator Strength	λ_{max} (nm)	Excitation Energy (eV)	Oscillator Strength
CH_2Cl_2	595.15	2.0833	0.6976	631.54	1.9632	0.6801	698.44	1.7752	0.6238
MeCN	589.46	2.1034	0.6563	627.57	2.4153	513.33	696.29	1.7806	0.5751
PhMe	601.93	2.0598	0.7645	633.69	1.9565	0.7507	693.1	1.7888	0.7042
Gas	568.31	2.1816	0.6411	594.46	2.0857	0.6396	689.69	1.7977	.7420

Table S5. UV-Vis of **1a–c** with CH_2Cl_2, PhMe, and MeCN as implicit solvent and gas phase.

Theory Level: TD-DFT(PBE0/jul-cc-pvDz)//DFT(PBEO/jul-cc-pvDz)

	CH_2Cl_2		
Structure	λ_{max} (nm)	Excitation Energy (eV)	Oscillator Strength
1a	590.93	2.0981	0.8132
1b	615.97	2.0128	0.7082
1c	678.46	1.8274	0.8065
1e	658.16	1.8838	0.5321
1f	610.98	2.0293	0.7687

1g	605.41	2.0479	0.5549
2d	629.19	1.9705	0.6829
3e	631.74	1.9626	0.7214
4f	592.93	2.0910	0.7935
4g	598.02	2.0732	0.6227
5a	601.68	2.0606	0.8584
5b	624.93	1.9840	0.8837
5c	660.36	1.8775	0.8838
5d	651.41	1.9033	0.8709
5e	646.02	1.9192	0.7884
5f	627.38	1.9762	0.8769
5g	618.38	2.0050	0.7992

Table S6. UV-Vis of **1a–c**, **1e–g**, **2d**, **3e**, **4f–g**, and **5a–g** in CH_2Cl_2 as implicit solvent.

Theory Level: TD-DFT(PBE0/jul-cc-pvDz)//DFT(B3LYP/jul-cc-pvDz)

	CH_2Cl_2		
Structure	λ_{max} (nm)	Excitation Energy (eV)	Oscillator Strength
1a	595.15	2.0833	0.6976
1b	631.54	1.9632	0.6801
1c	698.44	1.7752	0.6238
1e	677.97	1.8287	0.4854
1f	627.2	1.9768	0.7165
1g	622.92	1.9904	0.4967
2d	646.54	1.9177	0.6348
3e	649.2	1.9098	0.6744
4f	606.67	2.0437	0.7370
4g	614.09	2.019	0.5605
5a	608.62	2.0371	0.8359
5b	632.87	1.9591	0.8569
5c	670.6	1.8489	0.8513
5d	677.57	1.8298	0.6759
5e	657.26	1.8864	0.7425
5f	634.93	1.9527	0.8540
5g	628.93	1.9714	0.7507

Table S6. UV-Vis of **1a–c**, **1e–g**, **2d**, **3e**, **4f–g**, and **5a–g** in CH_2Cl_2 as implicit solvent.

HOMO and LUMO Energies

Notes: HOMO energies taken from ground state population analysis during TD-DFT calculation at specified level of theory. LUMO energies calculated by adding excitation energy calculated during TD-DFT to the HOMO specified by the ground state population analysis.[1]

Theory Level: TD-DFT(PBE0/jul-cc-pvDz)//DFT(PBE0/jul-cc-pvDz)

	CH_2Cl_2		Acetonitrile		PhMe		Gas Phase	
Structure	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)
1a	-6.53	-4.43	-6.69	-4.53	-6.57	-4.47	-6.51	-4.29
1b	-6.42	-4.41	-6.47	-4.44	-6.32	-4.32	-6.24	-4.11
1c	-6.09	-4.27	-6.13	-4.30	-6.00	-4.16	-5.91	-3.92

Table S7. HOMO and LUMO Energies **1a–c** with CH_2Cl_2, PhMe, and MeCN as implicit solvent and gas phase.

Theory Level: TD-DFT(PBE0/jul-cc-pvDz)//DFT(PBE0/jul-cc-pvDz)

	CH_2Cl_2		Acetonitrile		PhMe		Gas Phase	
Structure	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)
1a	-6.53	-4.43	-6.69	-4.53	-6.57	-4.47	-6.51	-4.29
1b	-6.42	-4.41	-6.47	-4.44	-6.32	-4.32	-6.24	-4.11
1c	-6.09	-4.27	-6.13	-4.30	-6.00	-4.16	-5.91	-3.92

Table S8. HOMO and LUMO Energies **1a–c** with CH_2Cl_2, PhMe, and MeCN as implicit solvent and gas phase.

Theory Level: TD-DFT(PBE0/jul-cc-pvDz)//DFT(PBE0/jul-cc-pvDz)

	CH_2Cl_2	
Structure	HOMO (eV)	LUMO (eV)
1a	-6.53	-4.43
1b	-6.42	-4.41
1c	-6.09	-4.27

1e	-6.27	-4.38
1f	-6.63	-4.60
1g	-6.72	-4.67
2d	-6.56	-4.59
3e	-6.54	-4.58
4f	-6.42	-4.32
4g	-6.47	-4.40
5a	-5.96	-3.90
5b	-5.78	-3.79
5c	-5.53	-3.65
5d	-5.61	-3.70
5e	-5.68	-3.76
5f	-5.97	-3.99
5g	-6.08	-4.07

Table S9. HOMO and LUMO Energies of **1a–c**, **1e–g**, **2d**, **3e**, **4f–g**, and **5a–g** in CH_2Cl_2 as implicit solvent

Theory Level: TD-DFT(PBE0/jul-cc-pvDz)//DFT(PBE0/jul-cc-pvDz)

	CH_2Cl_2	
Structure	HOMO (eV)	LUMO (eV)
1a	-6.46	-4.38
1b	-5.77	-3.73
1c	-5.90	-4.12
1e	-6.07	-4.24
1f	-6.43	-4.45
1g	-6.52	-4.53
2d	-6.37	-4.45
3e	-6.35	-4.44
4f	-6.22	-4.17
4g	-6.27	-4.25
5a	-5.96	-3.90
5b	-5.58	-3.62
5c	-5.34	-3.49
5d	-6.00	-4.17
5e	-5.48	-3.60
5f	-5.78	-3.82
5g	-5.88	-3.91

Table S10. HOMO and LUMO Energies of **1a–c**, **1e–g**, **2d**, **3e**, **4f–g**, and **5a–g** in CH_2Cl_2 as implicit solvent

Molecular Orbital Diagrams

Theory Level: TD-DFT(PBE0/jul-cc-pvDz)//DFT(PBE0/jul-cc-pvDz)

Notes: Natural Transition Orbitals (NTO) calculated for the first excited state found during the TD-DFT calculations. HOMO and LUMO visualized using GaussView.

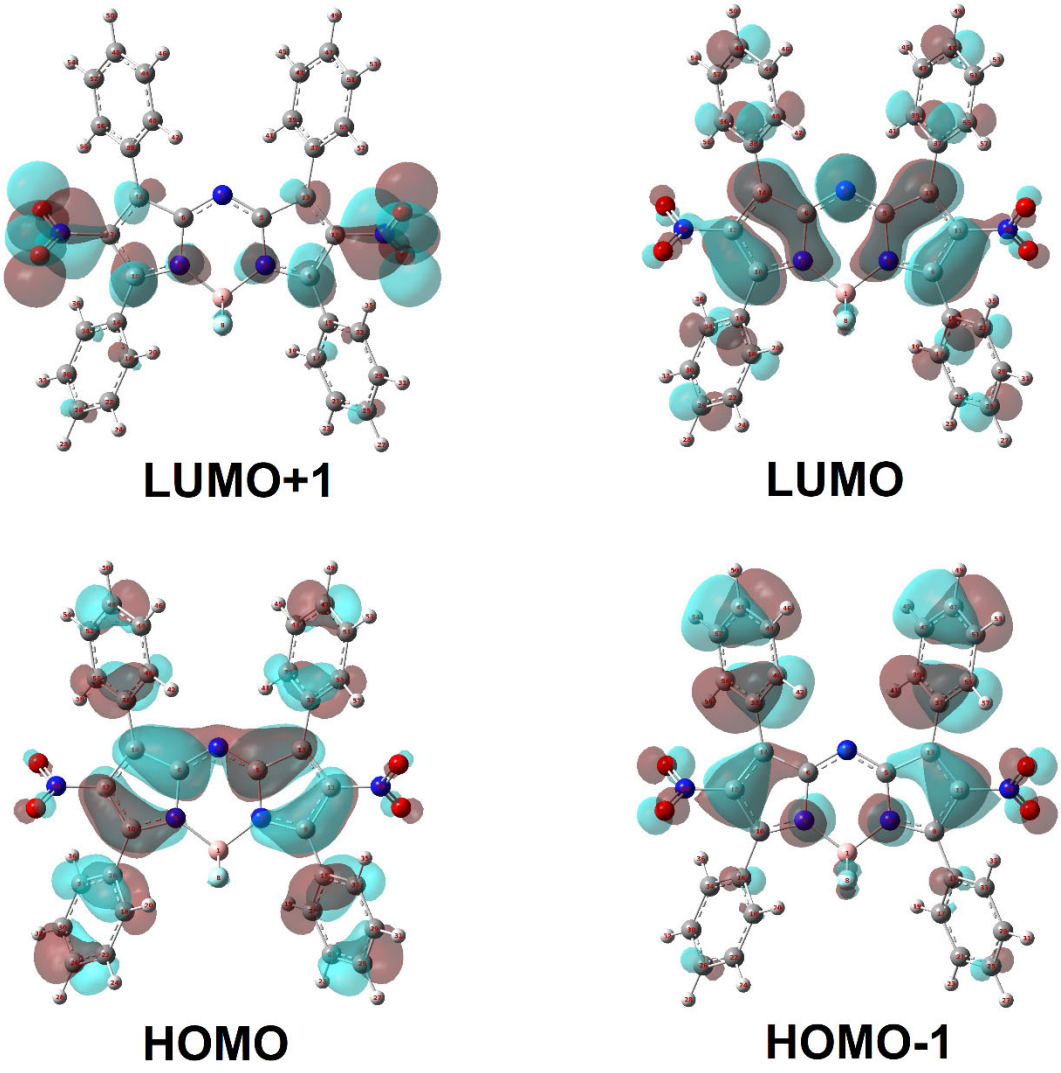


Figure S14. Frontier Molecular Oribtal Plots of **1a**.

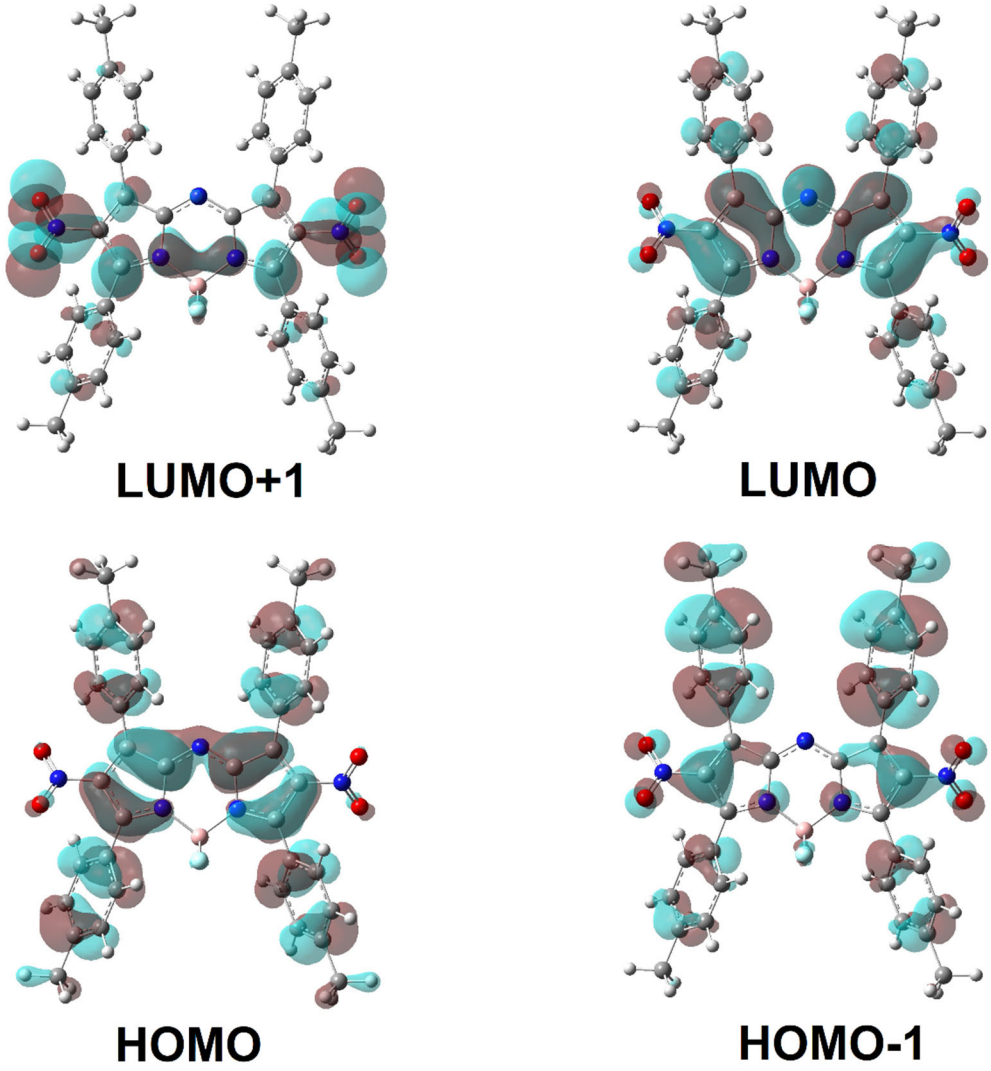


Figure S15. Frontier Molecular Oribtal Plots of **1b**.

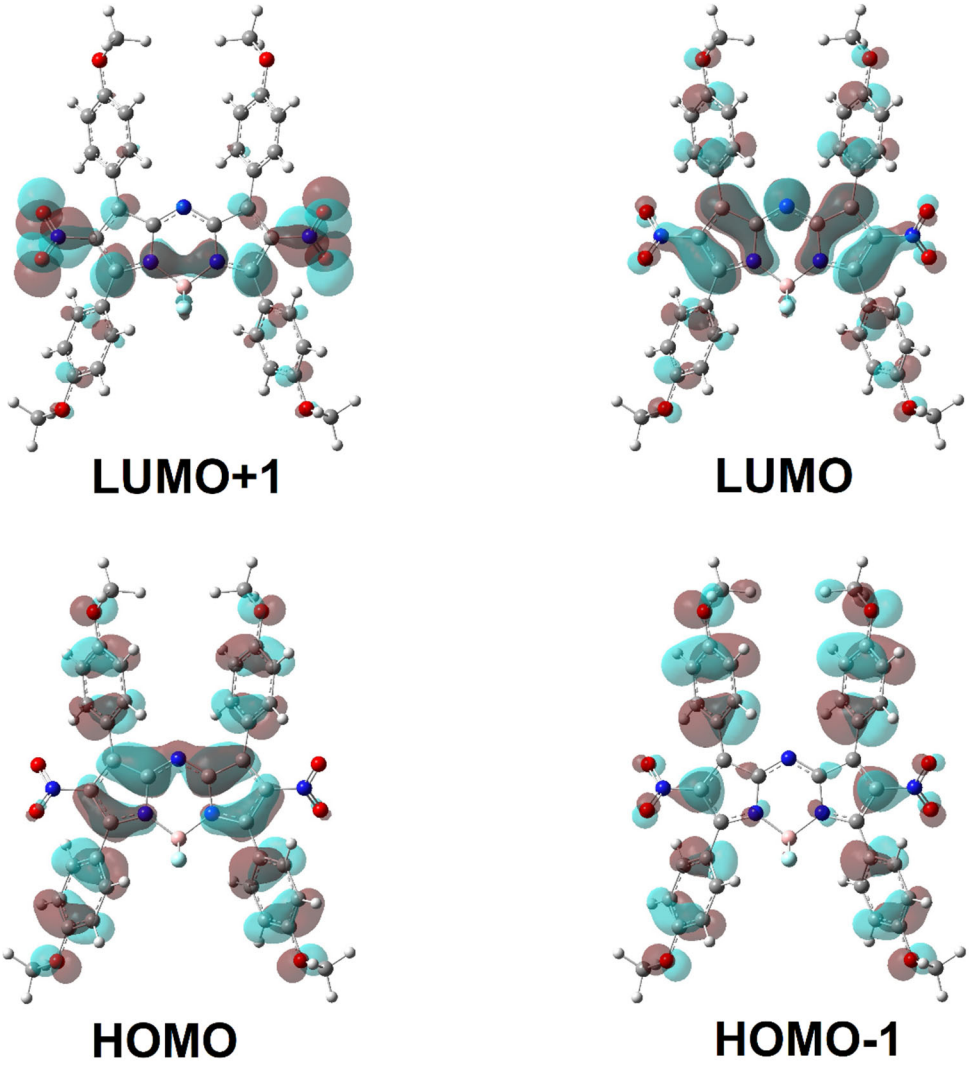


Figure S16. Frontier Molecular Oribtal Plots of **1c**.

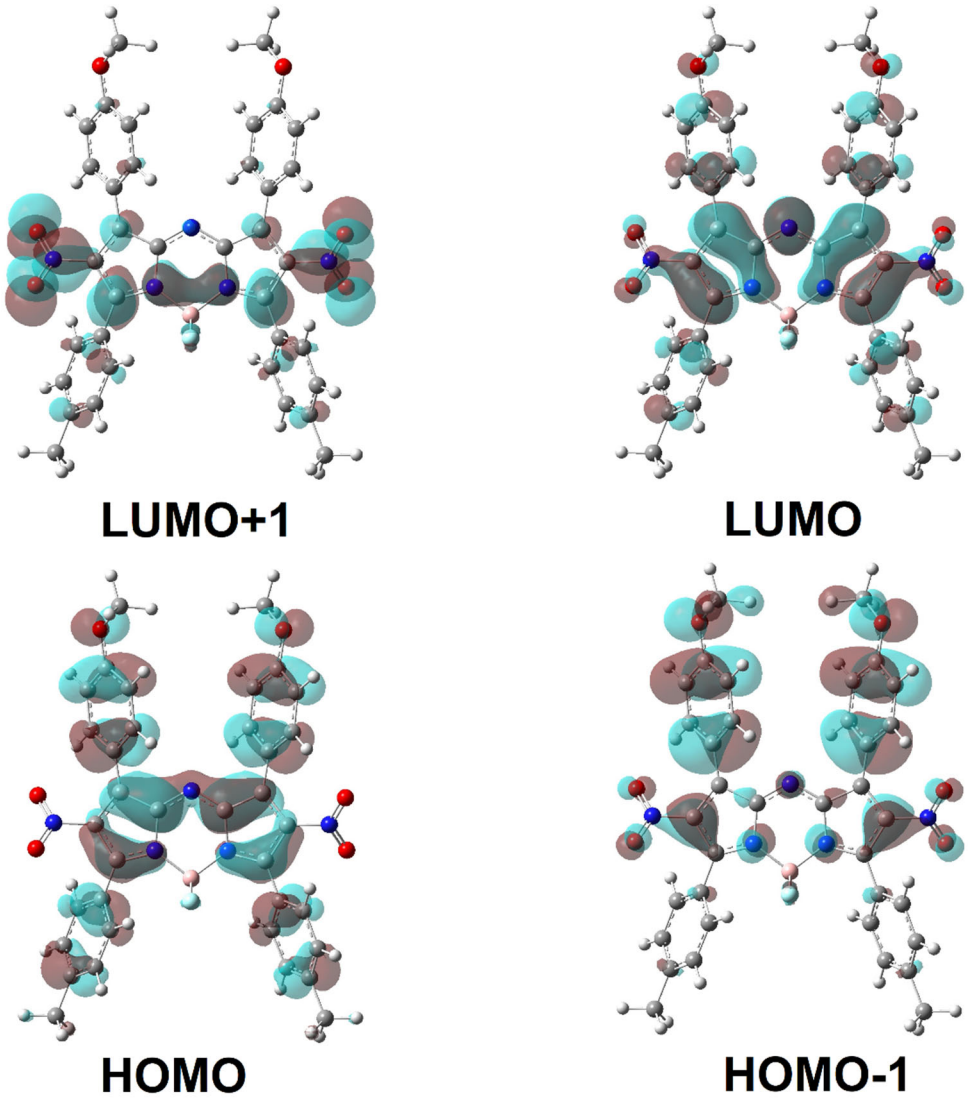


Figure S17. Frontier Molecular Oribtal Plots of **1e**.

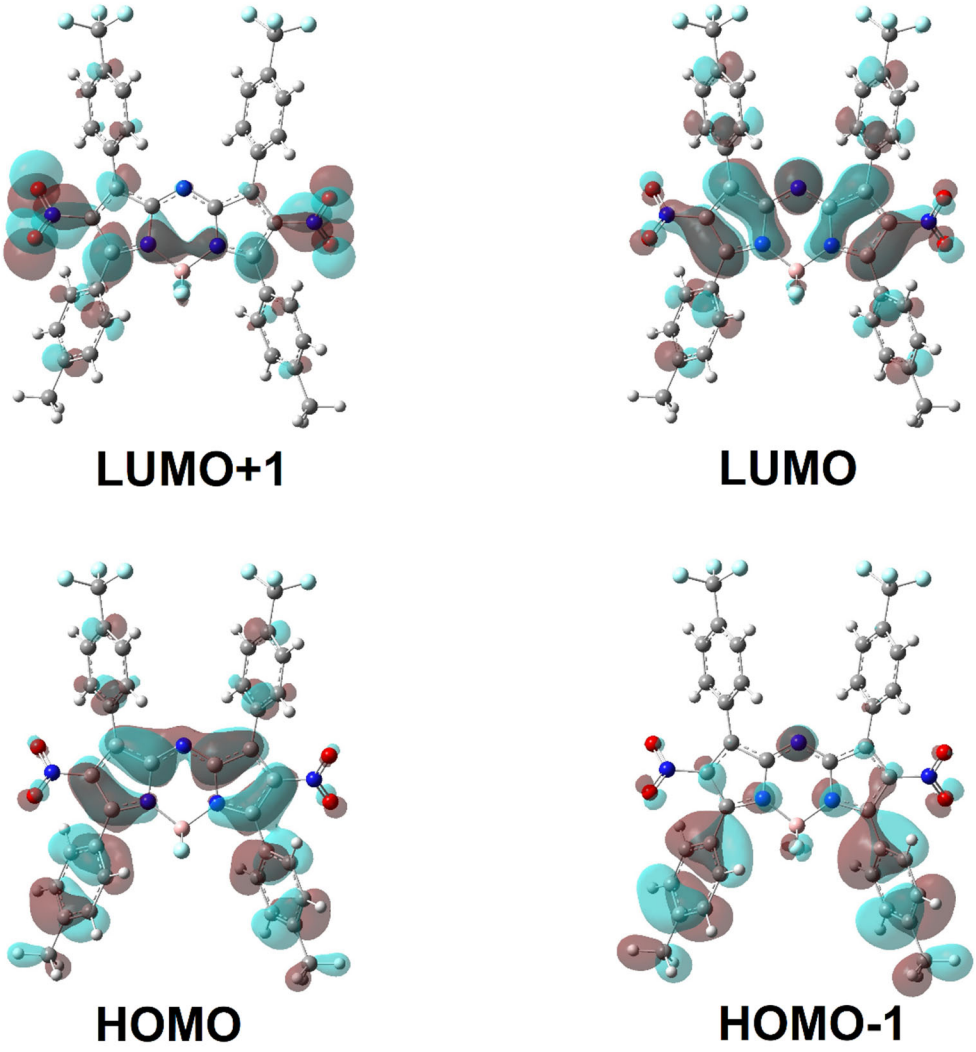


Figure S18. Frontier Molecular Oribtal Plots of **1f**.

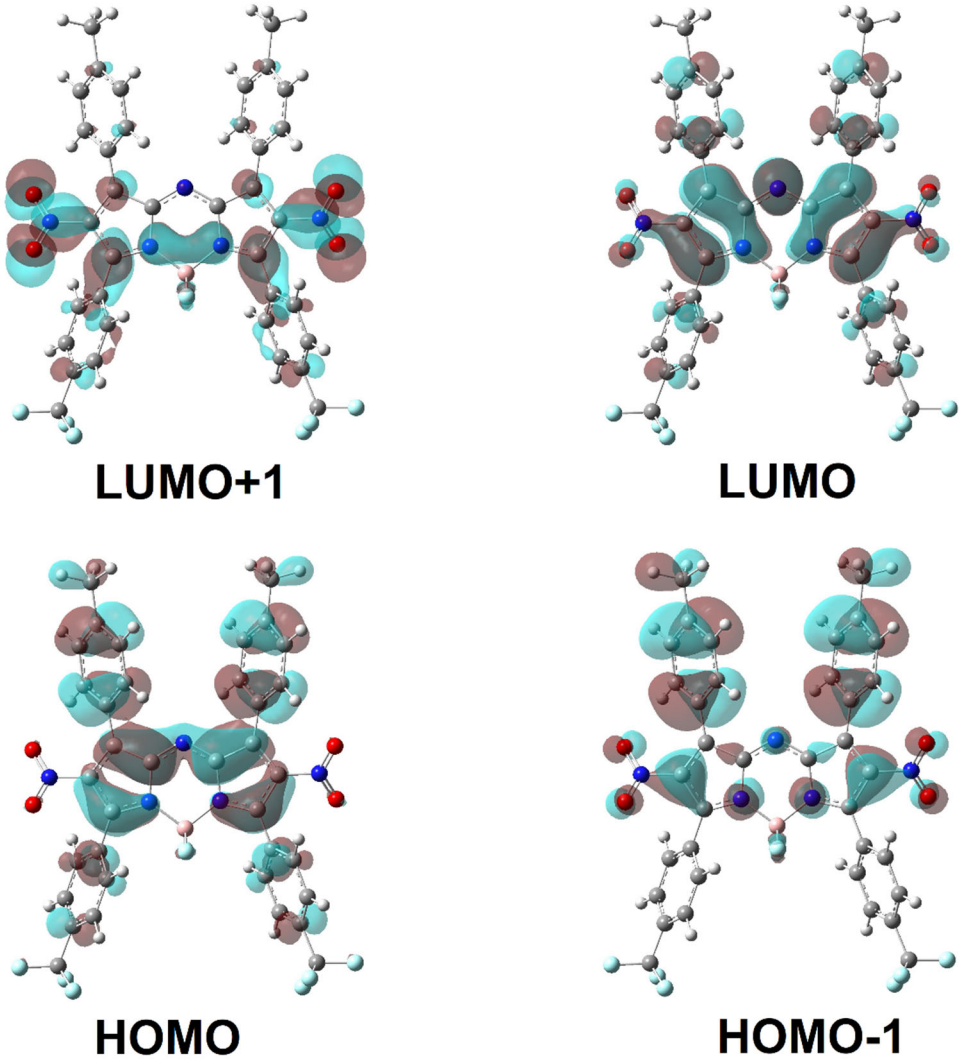


Figure S19. Frontier Molecular Oribtal Plots of **1g**.

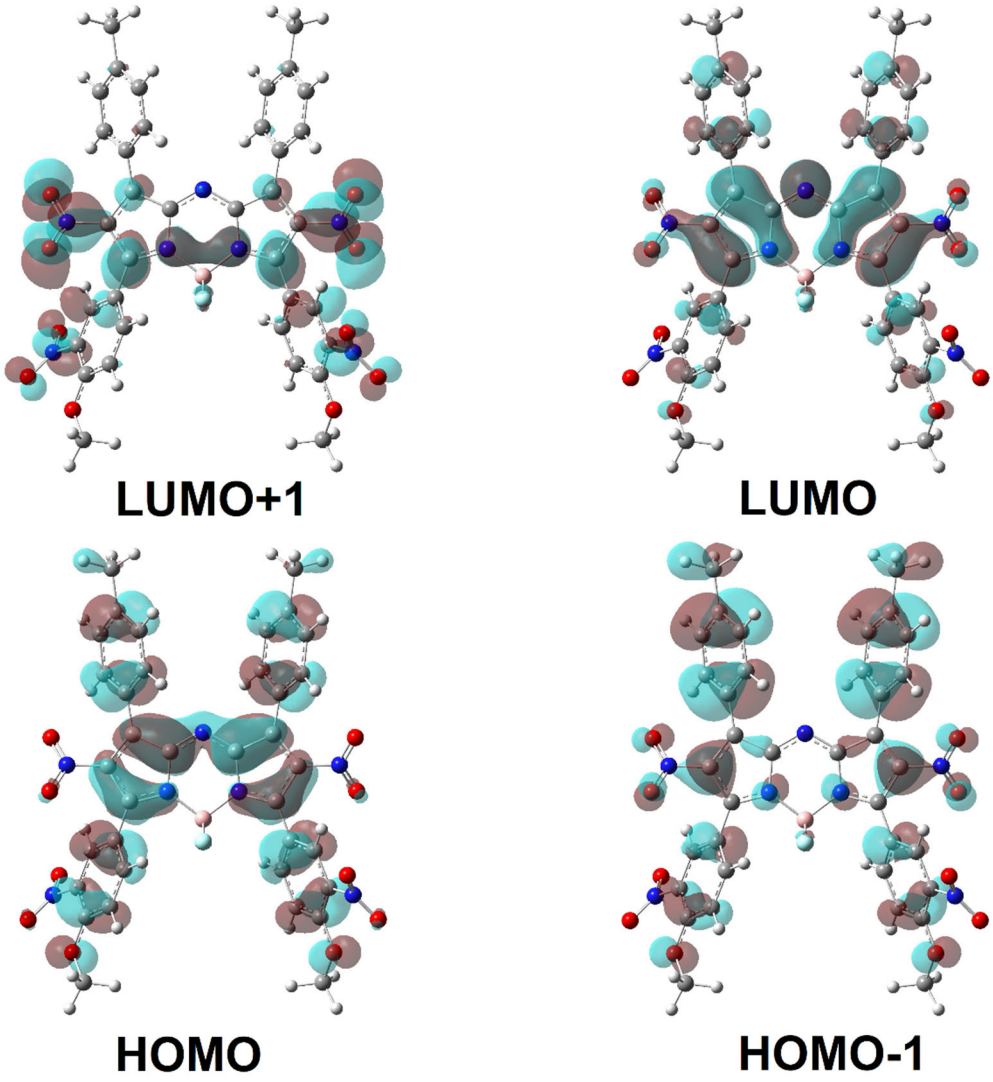


Figure S20. Frontier Molecular Oribtal Plots of **2d**.

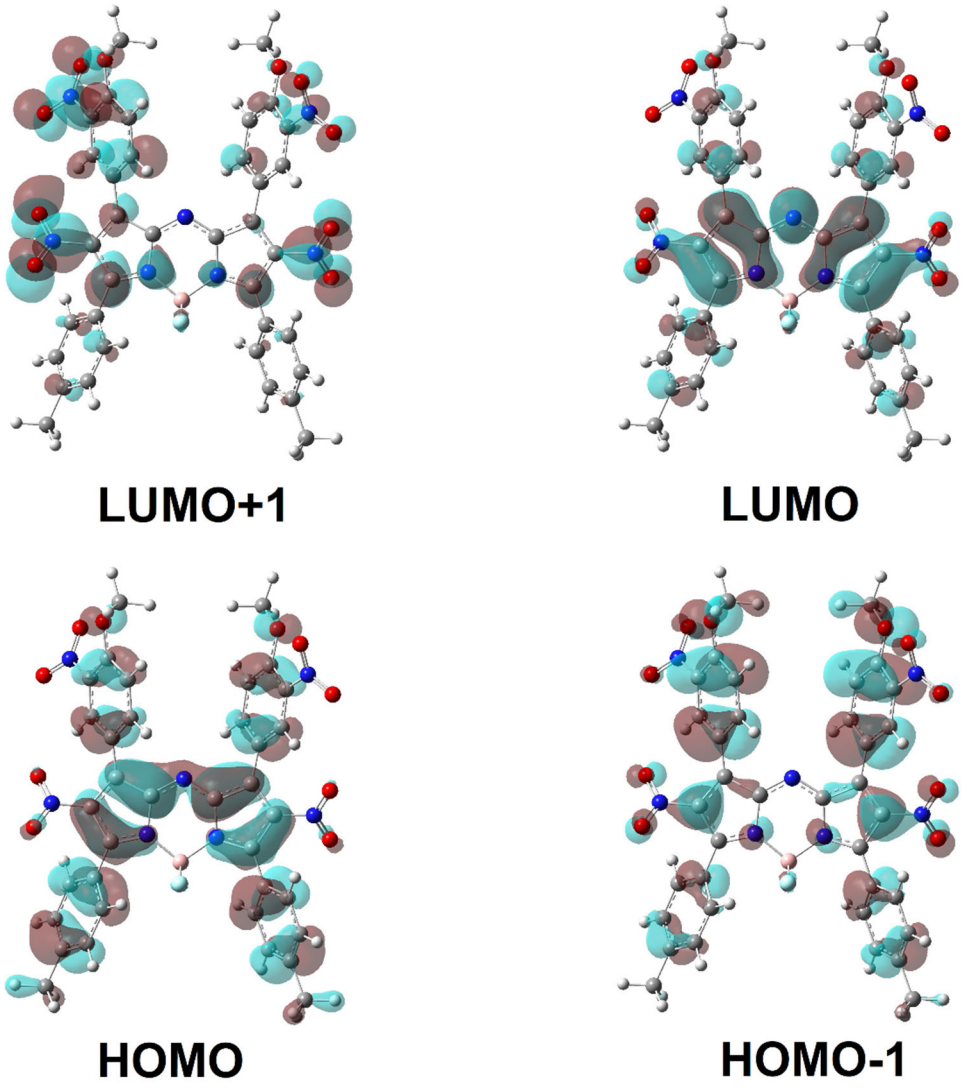


Figure S21. Frontier Molecular Oribtal Plots of **3e**.

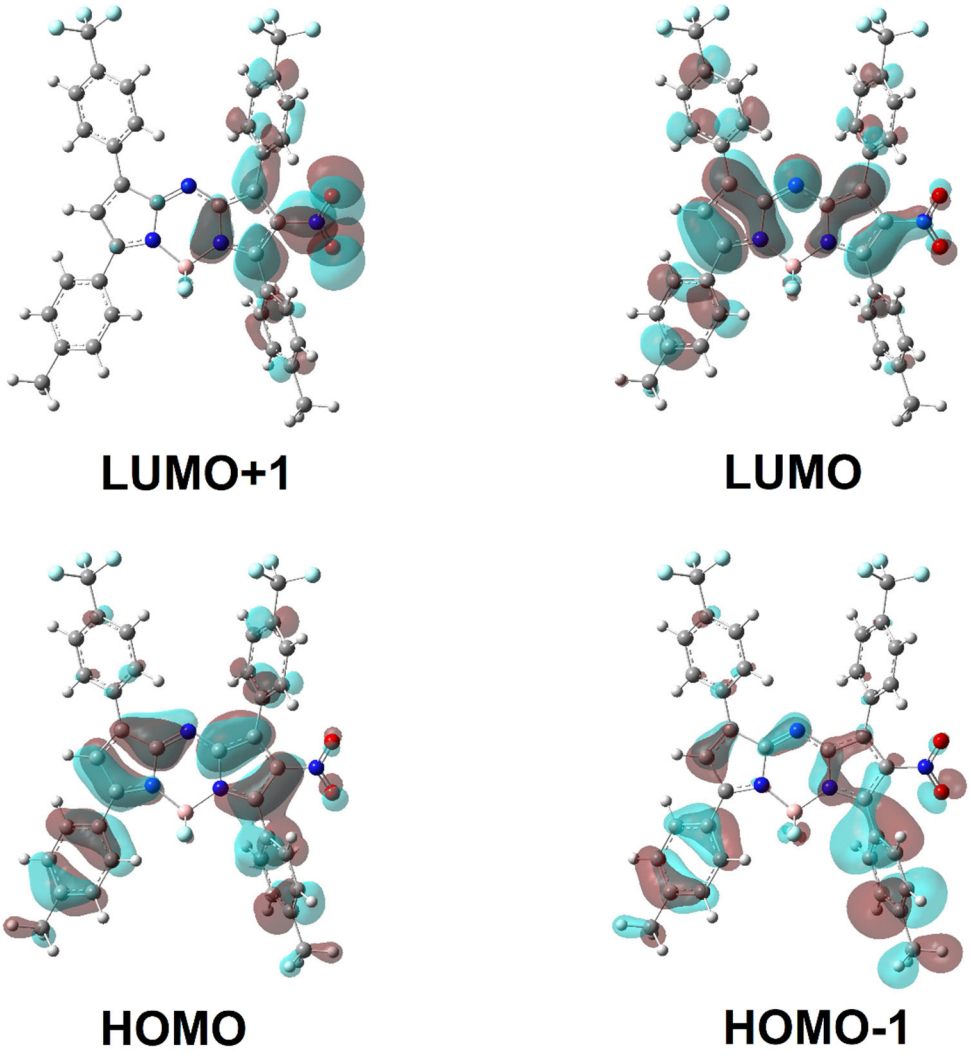


Figure S22. Frontier Molecular Oribtal Plots of **4f**.

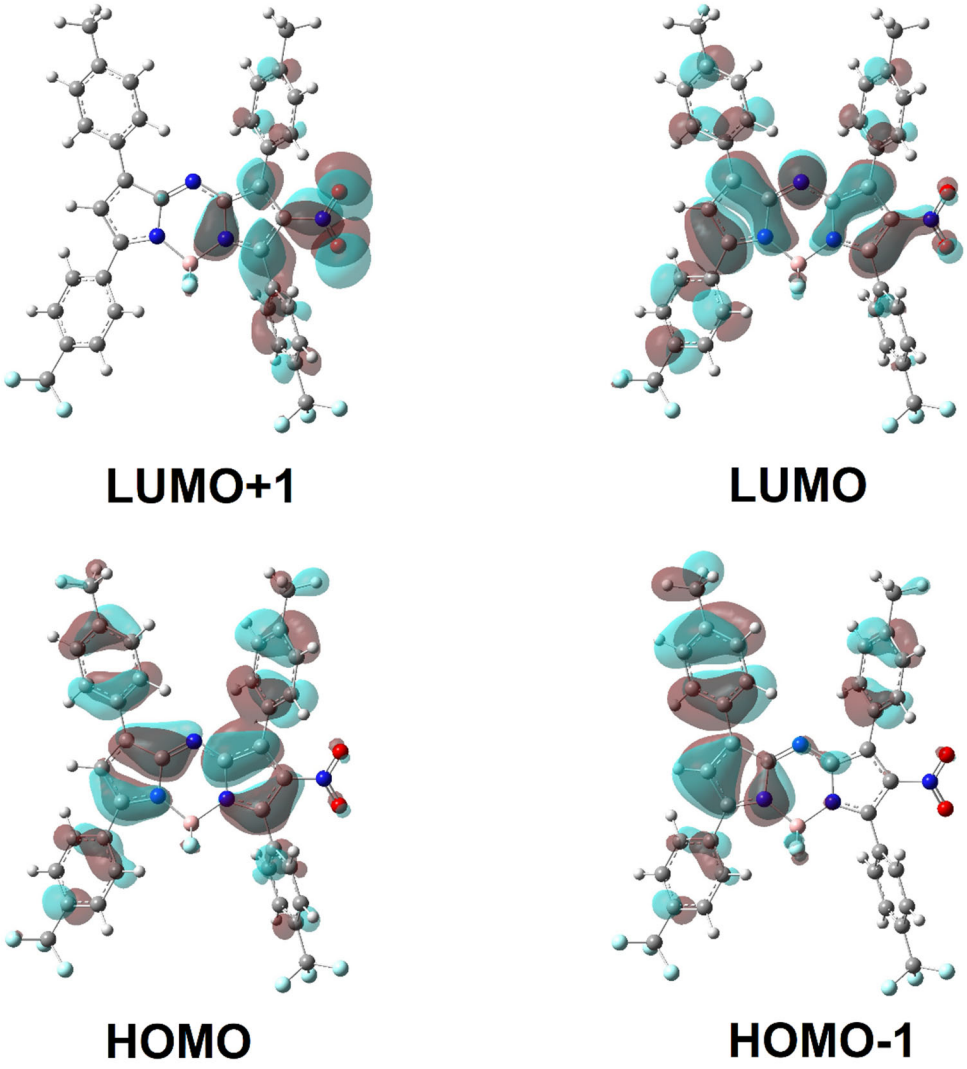


Figure S23. Frontier Molecular Oribtal Plots of **4g**.

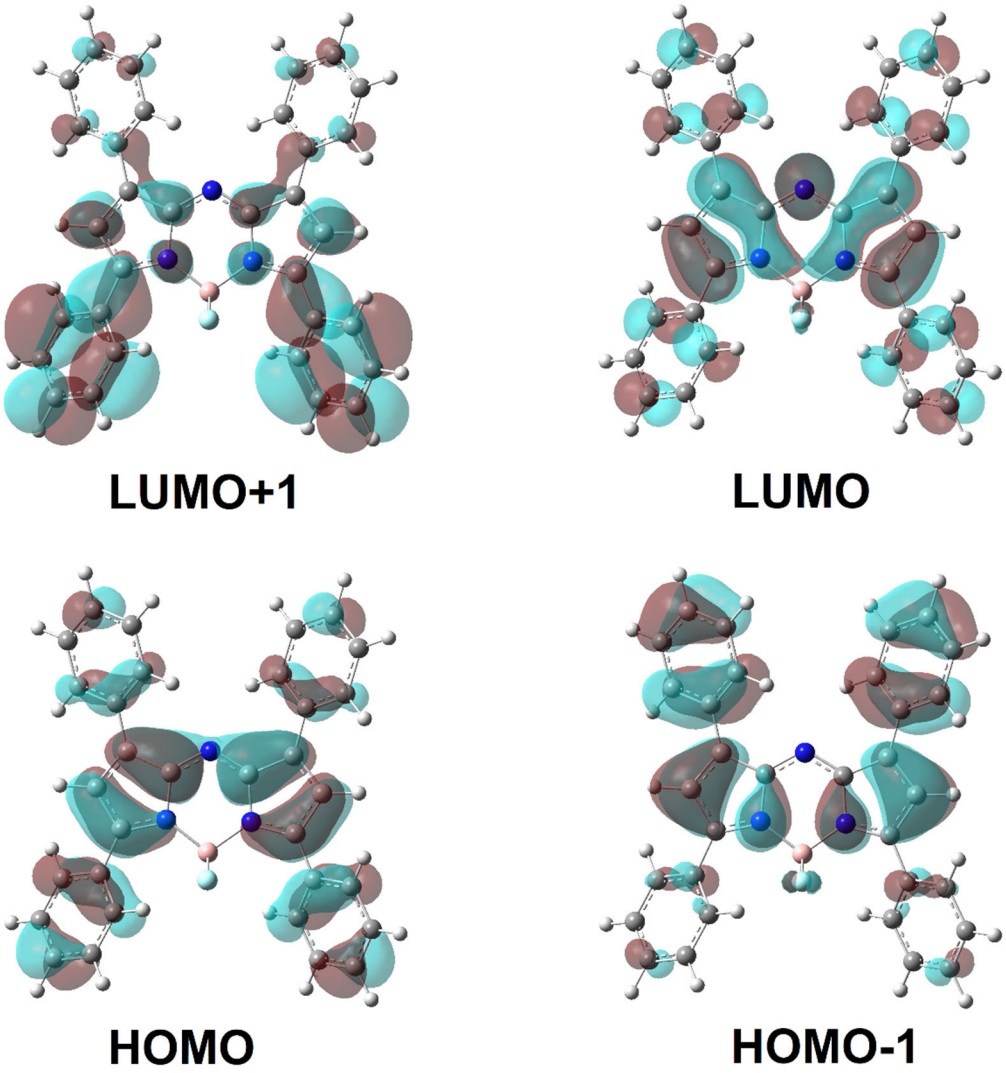


Figure S24. Frontier Molecular Oribtal Plots of **5a**.

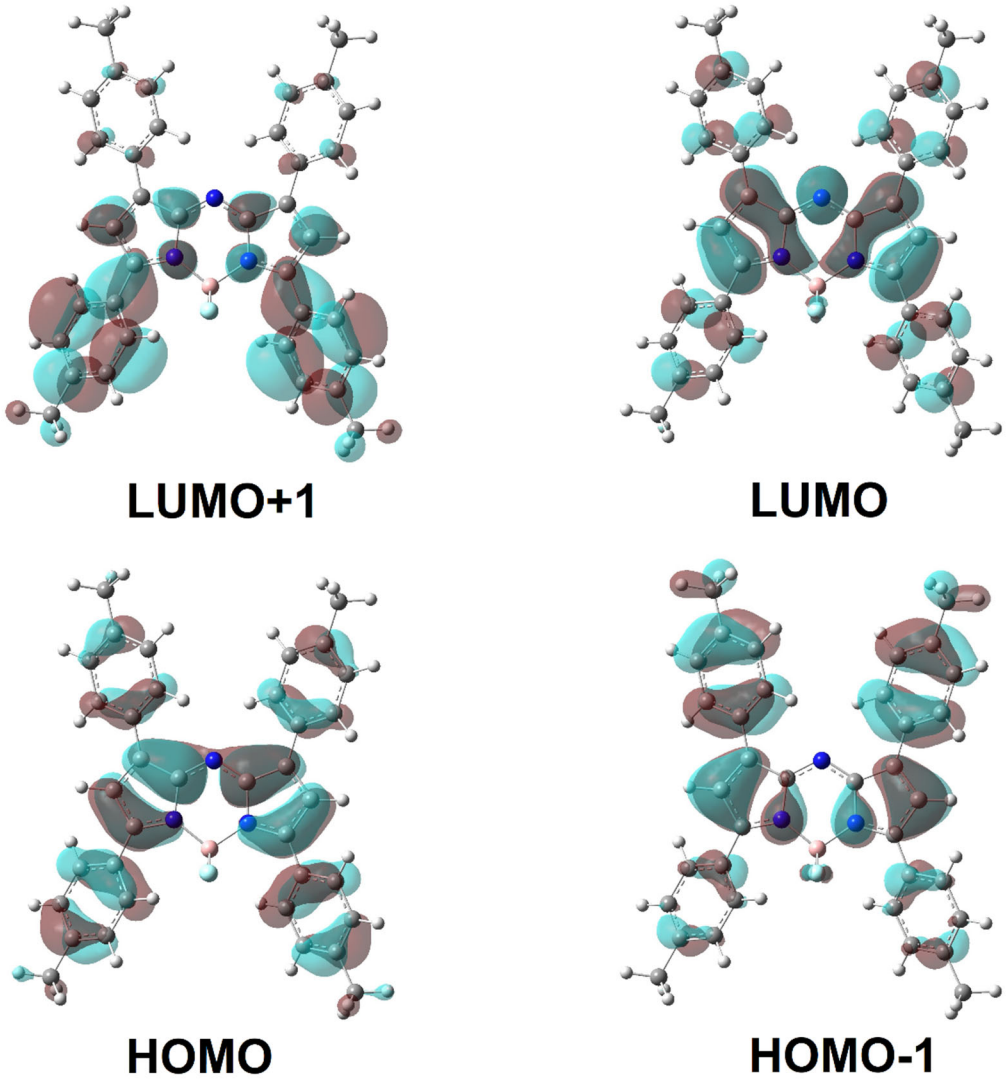


Figure S25. Frontier Molecular Oribtal Plots of **5b**.

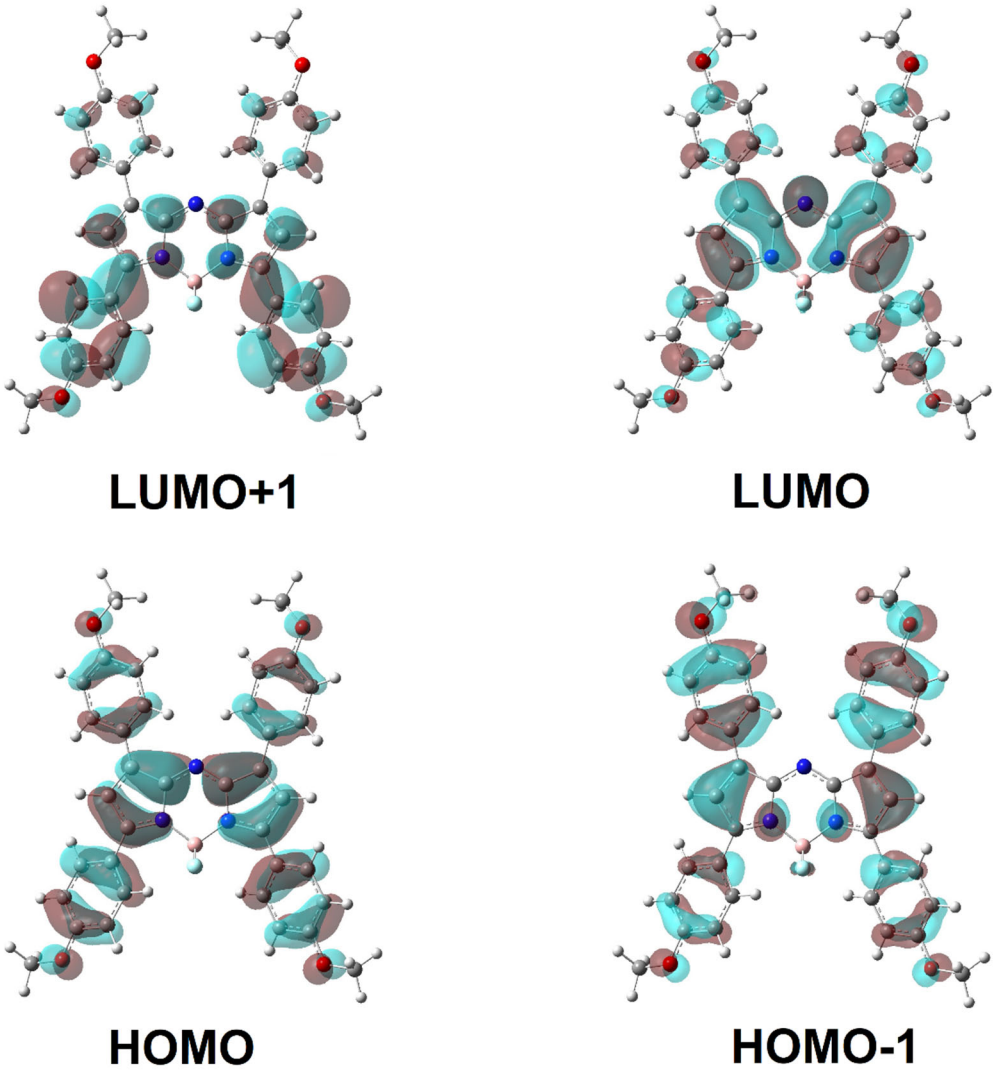


Figure S26. Frontier Molecular Oribtal Plots of **5c**.

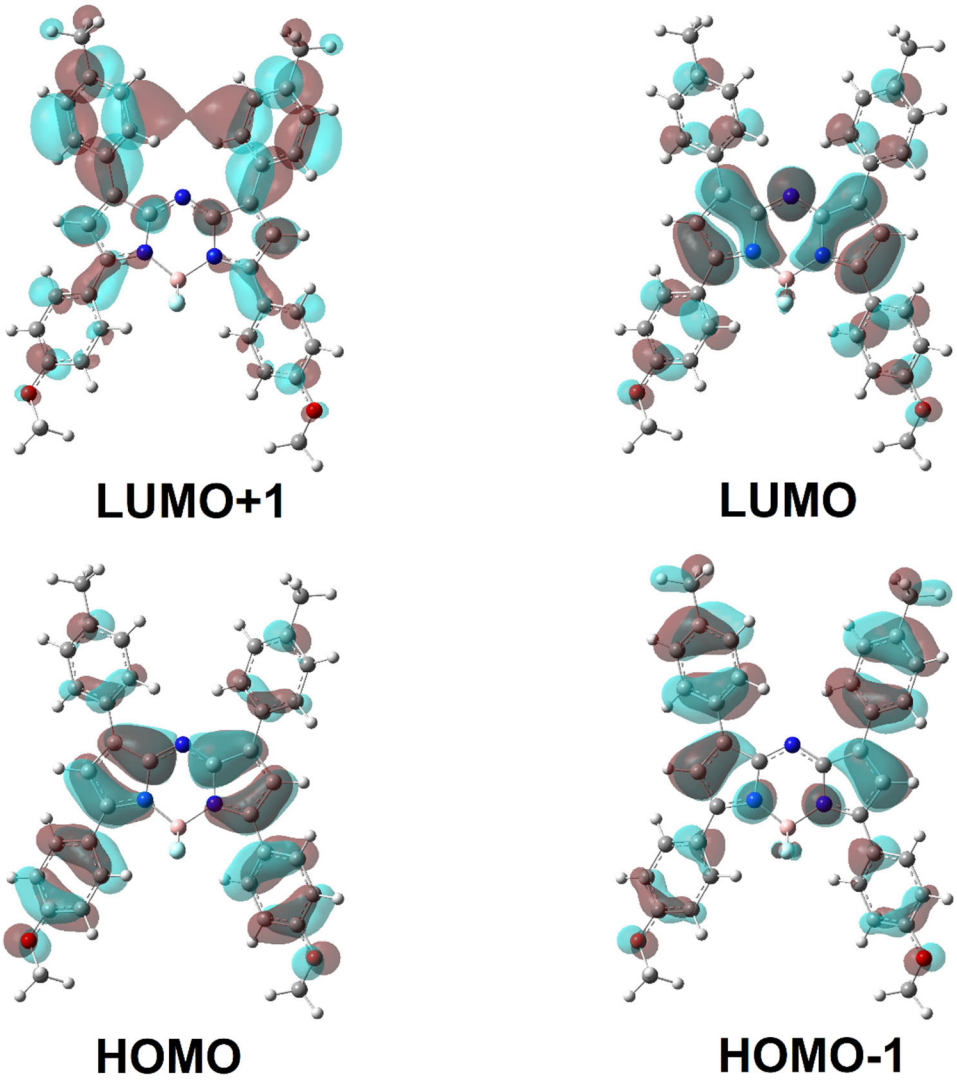


Figure S27. Frontier Molecular Oribtal Plots of **5d**.

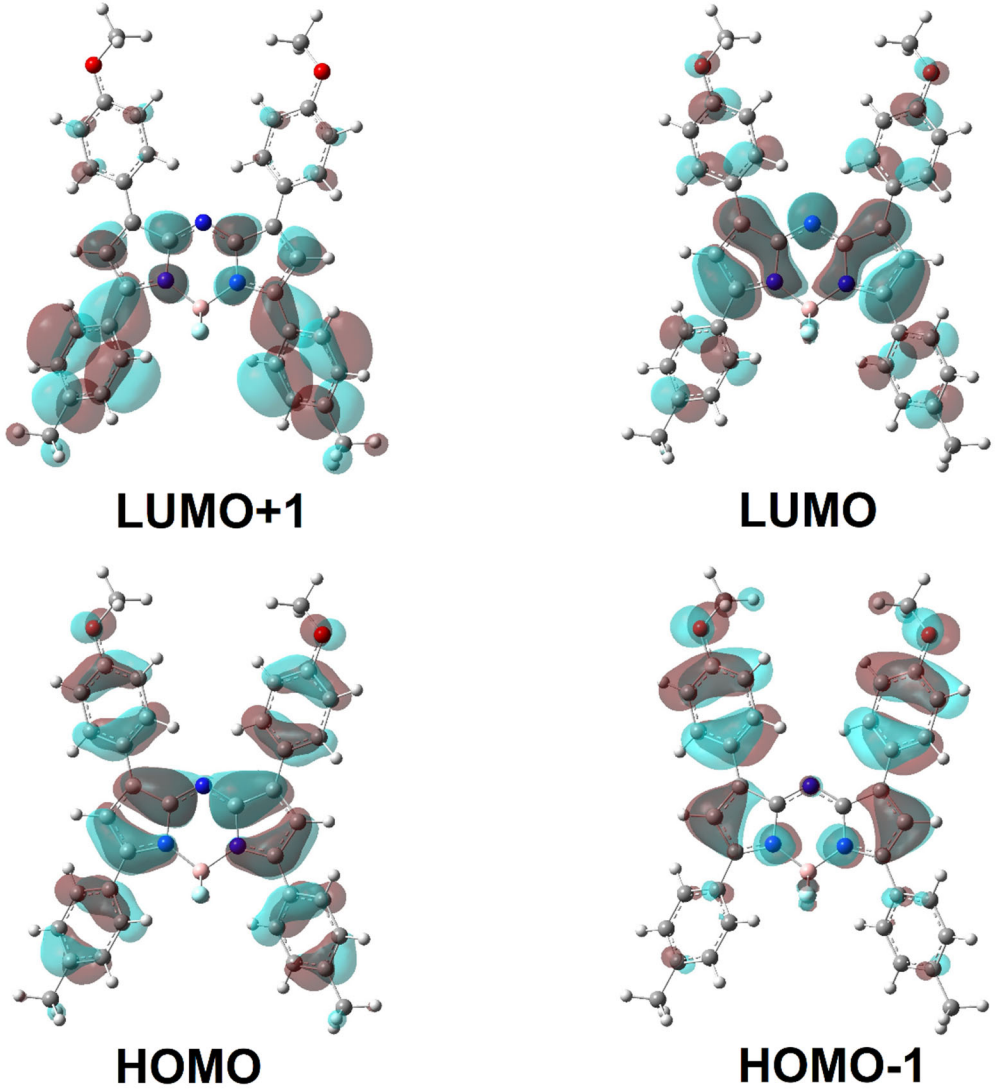


Figure S28. Frontier Molecular Oribtal Plots of **5e**.

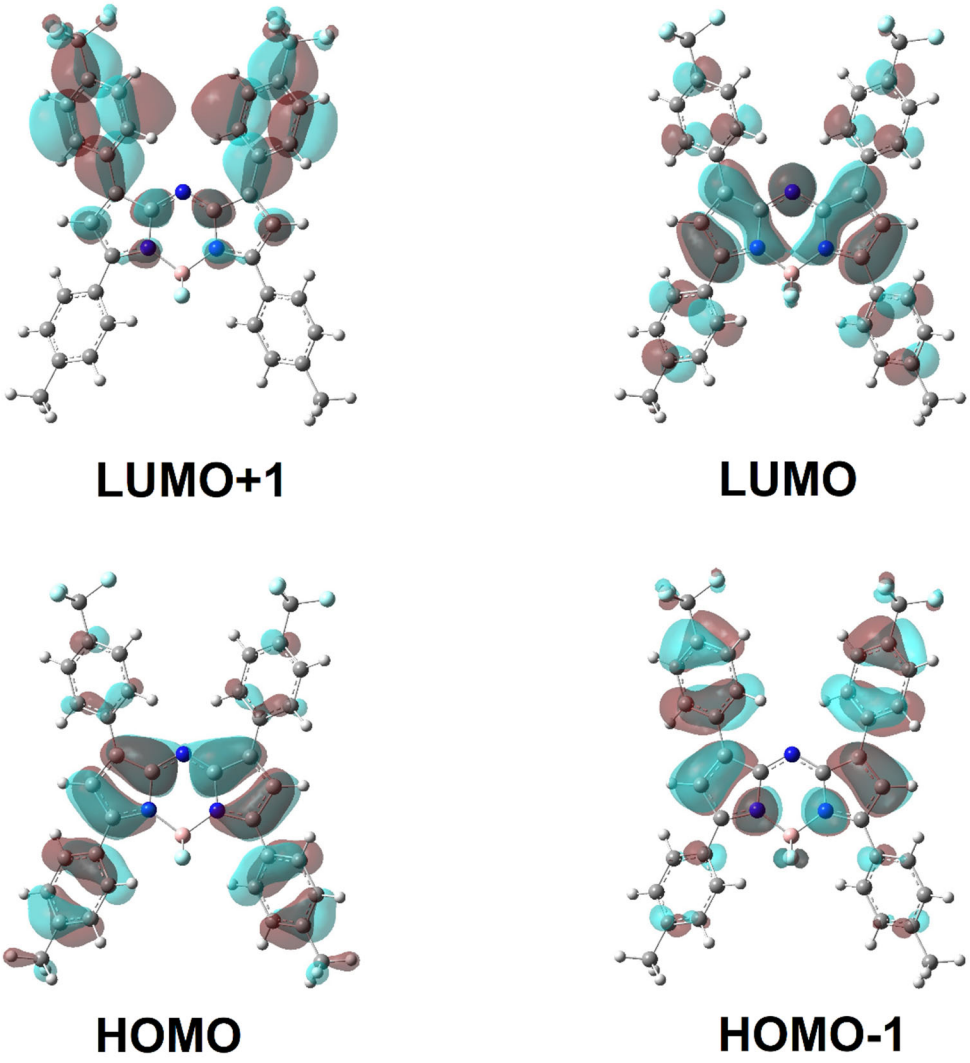


Figure S29. Frontier Molecular Oribtal Plots of **5f**.

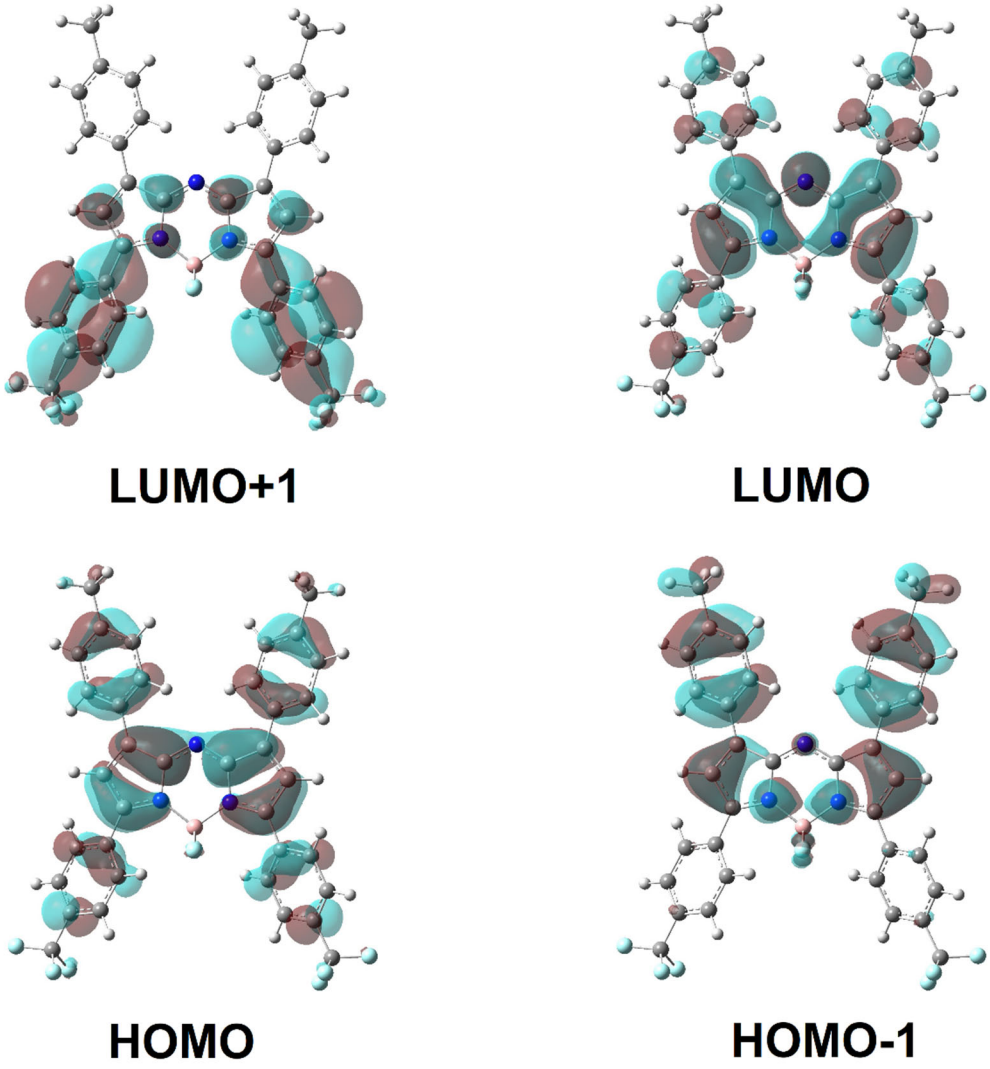
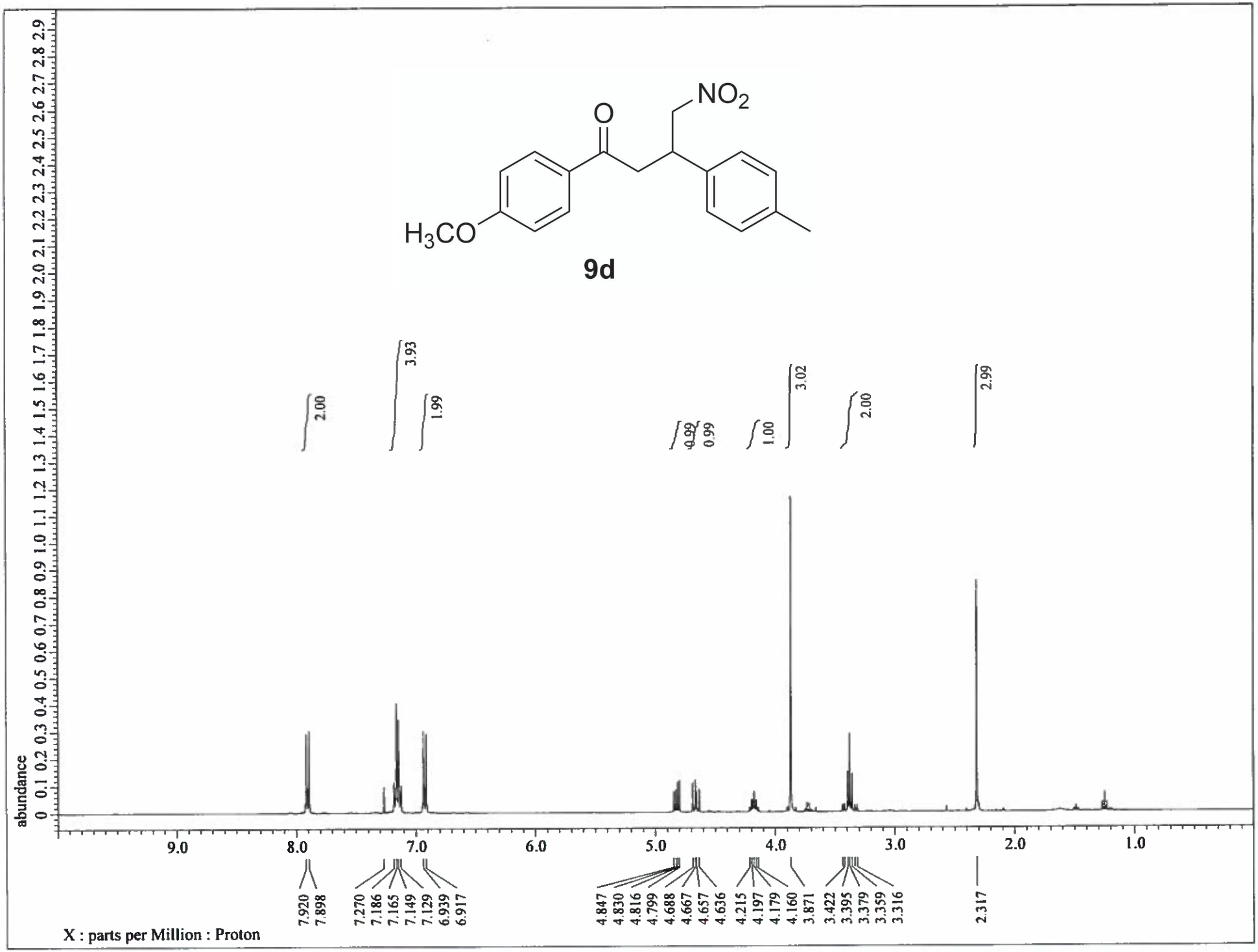
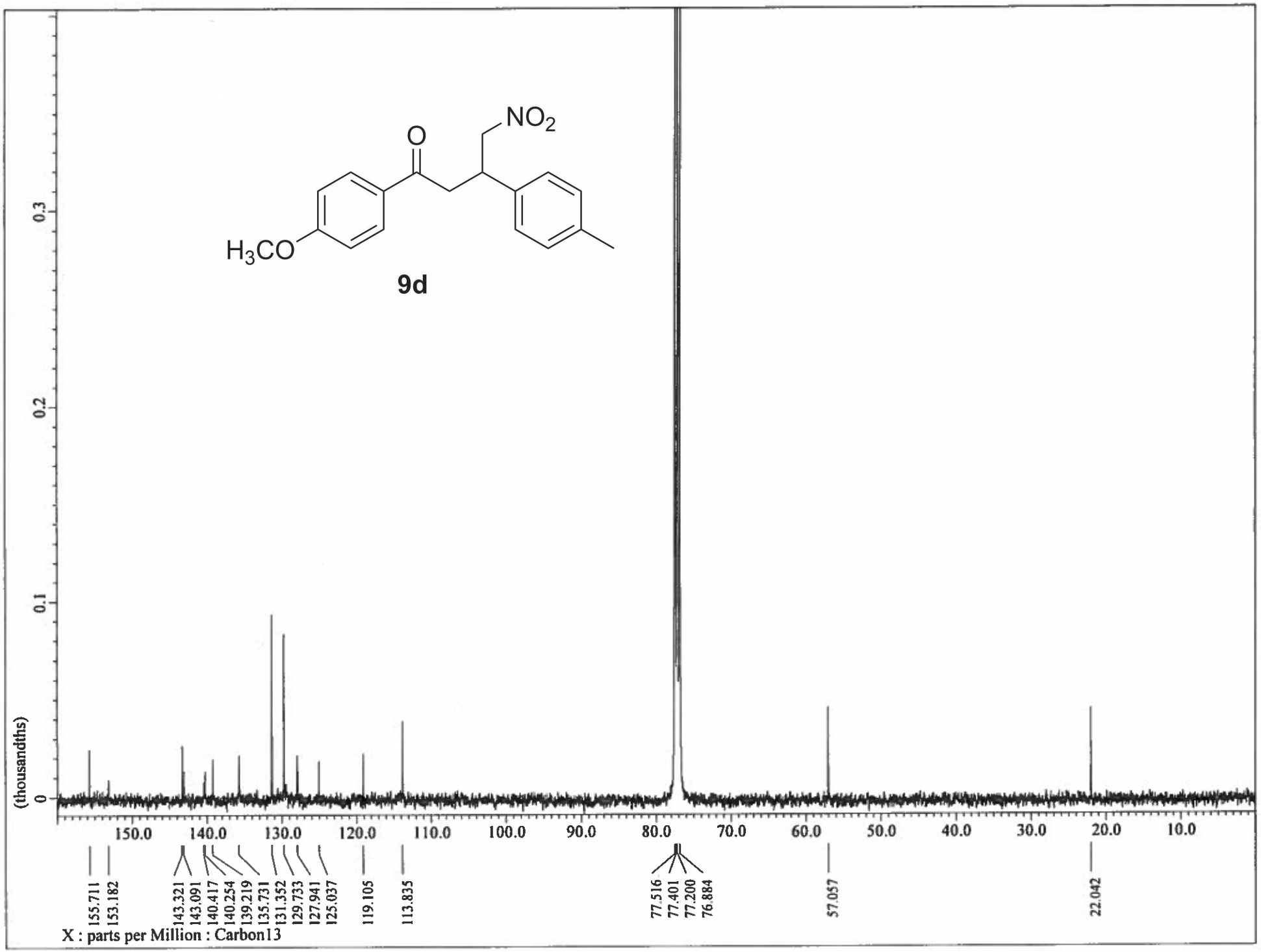


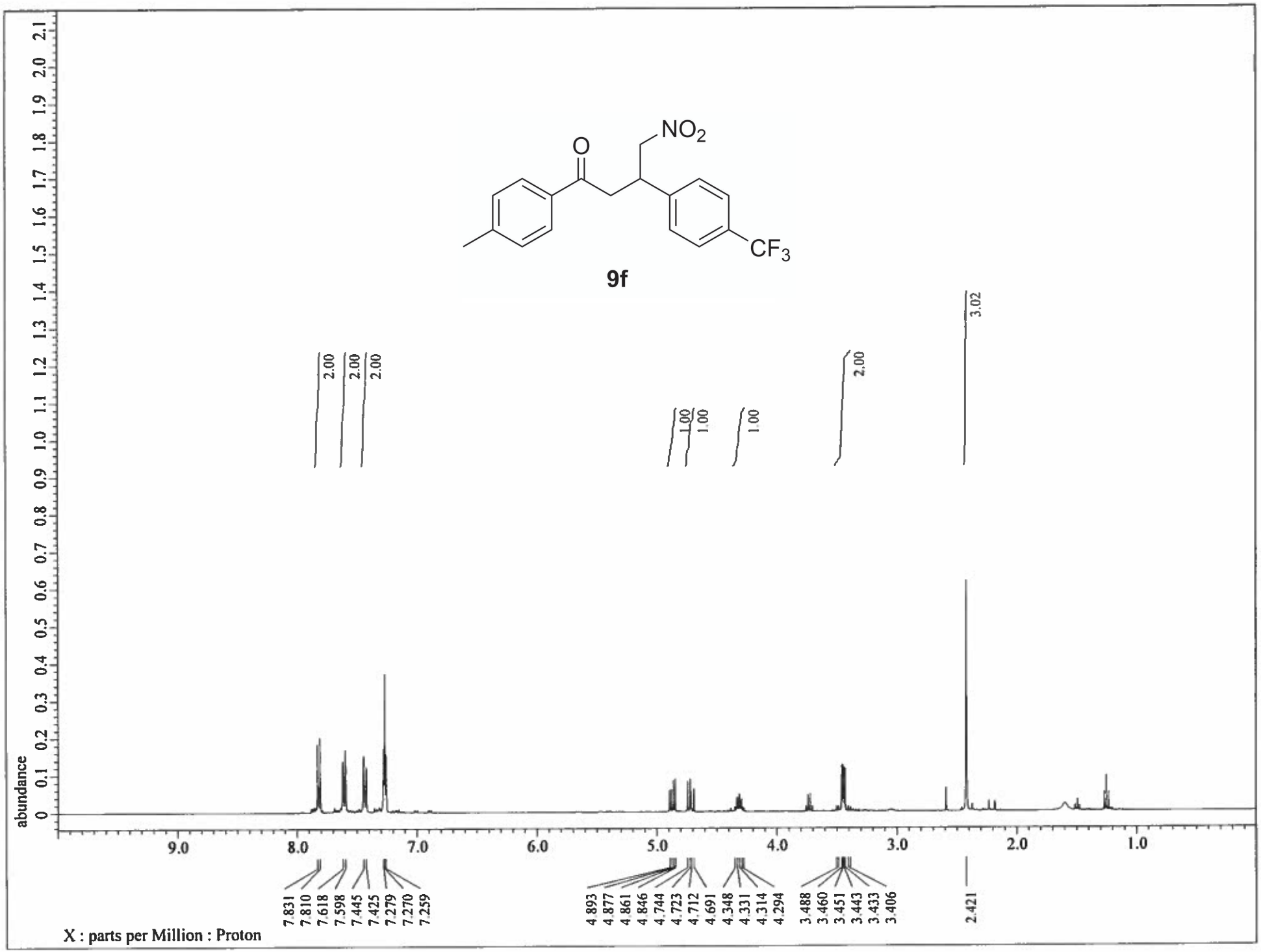
Figure S30. Frontier Molecular Oribtal Plots of **5g**.

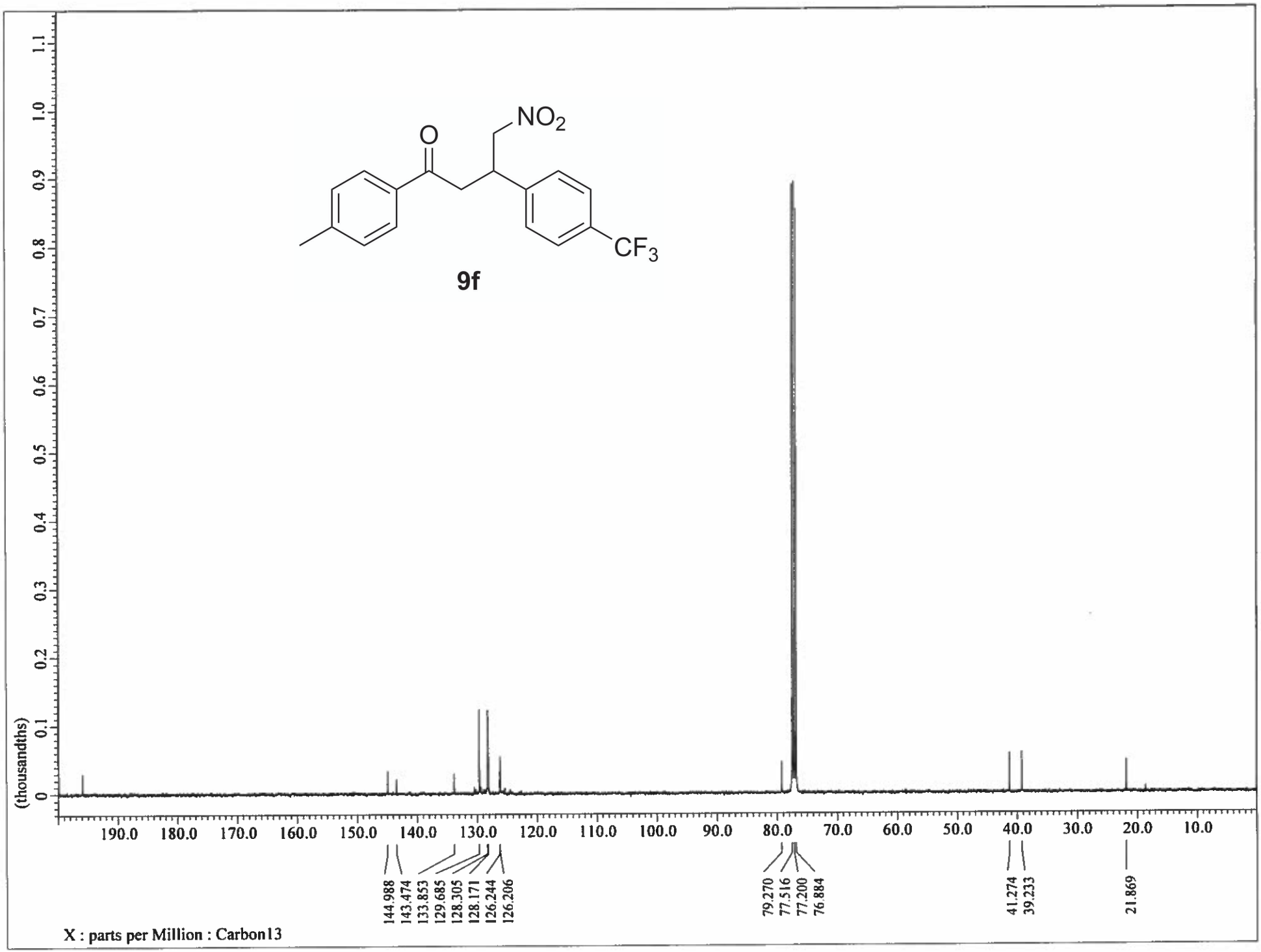
References

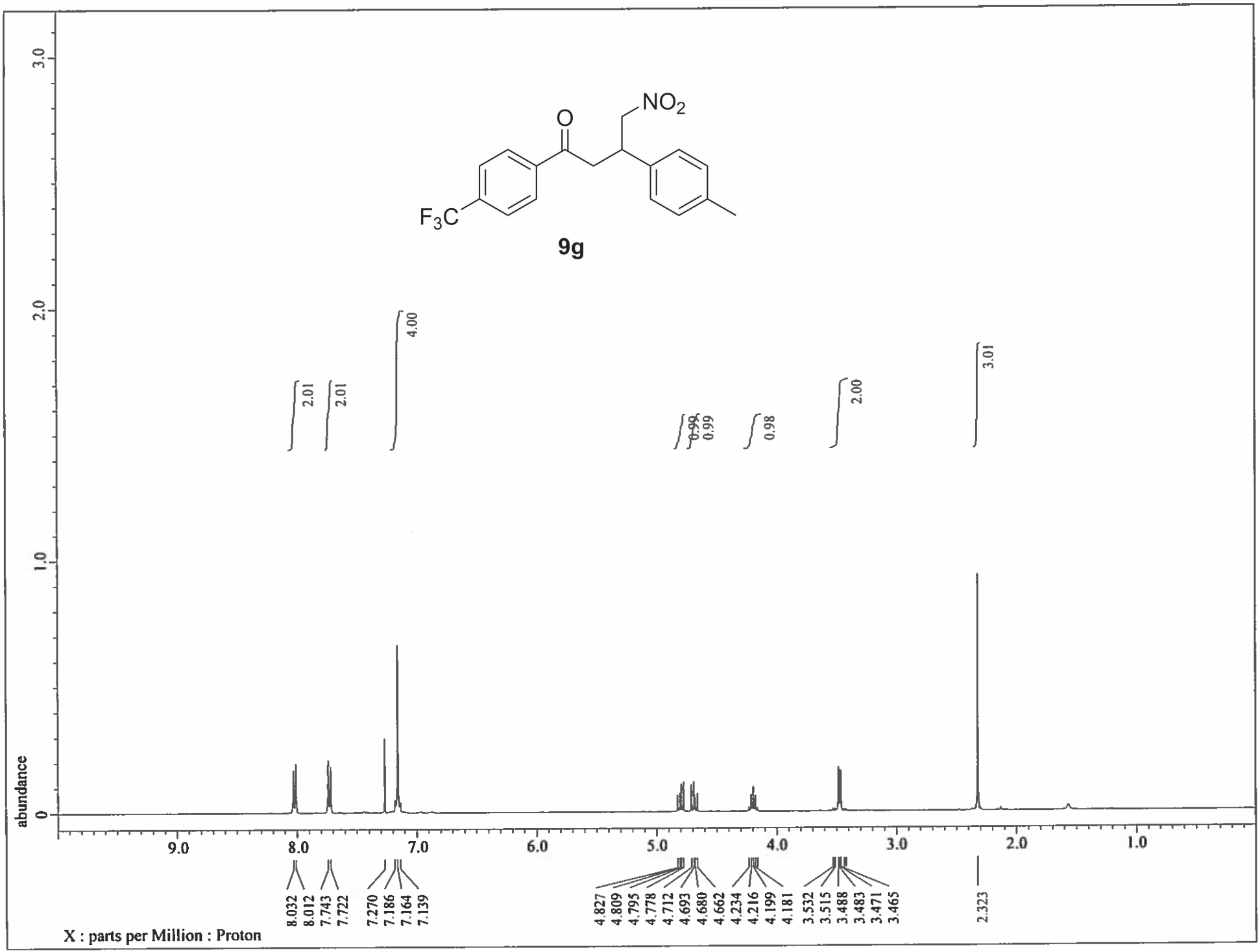
1. Zhang, G.; Musgrave, C. B. *J. Phys. Chem. A* **2007**, *111*, 1554-1561.


NO2
O
H3CO
9d
abundance
X : parts per Million : Proton
2.00
3.93
1.99
0.99
0.99
1.00
3.02
2.00
2.99
7.920
7.898
7.270
7.186
7.165
7.149
7.129
6.939
6.917
4.847
4.830
4.816
4.799
4.688
4.667
4.657
4.636
4.215
4.197
4.179
4.160
3.871
3.422
3.395
3.379
3.359
3.316
2.317


O
NO2
H3CO
9d
(thousandths)
0
0.1
0.2
0.3
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
155.711
153.182
143.321
143.091
140.417
140.254
139.219
135.731
131.352
129.733
127.941
125.037
119.105
113.835
77.516
77.401
77.200
76.884
57.057
22.042
X : parts per Million : Carbon13


NO2
O
CF3
9f
2.00
2.00
2.00
1.00
1.00
1.00
2.00
3.02
abundance
X : parts per Million : Proton
7.831
7.810
7.618
7.598
7.445
7.425
7.279
7.270
7.259
4.893
4.877
4.861
4.846
4.744
4.723
4.712
4.691
4.348
4.331
4.314
4.294
3.488
3.460
3.451
3.443
3.433
3.406
2.421


O
NO2
CF3
9f
(thousandths)
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
144.988
143.474
133.853
129.685
128.305
128.171
126.244
126.206
79.270
77.516
77.200
76.884
41.274
39.233
21.869
X : parts per Million : Carbon13


NO2
O
F3C
9g
abundance
X : parts per Million : Proton
2.01
2.01
4.00
0.99
0.99
0.98
2.00
3.01
8.032
8.012
7.743
7.722
7.270
7.186
7.164
7.139
4.827
4.809
4.795
4.778
4.712
4.693
4.680
4.662
4.234
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4.199
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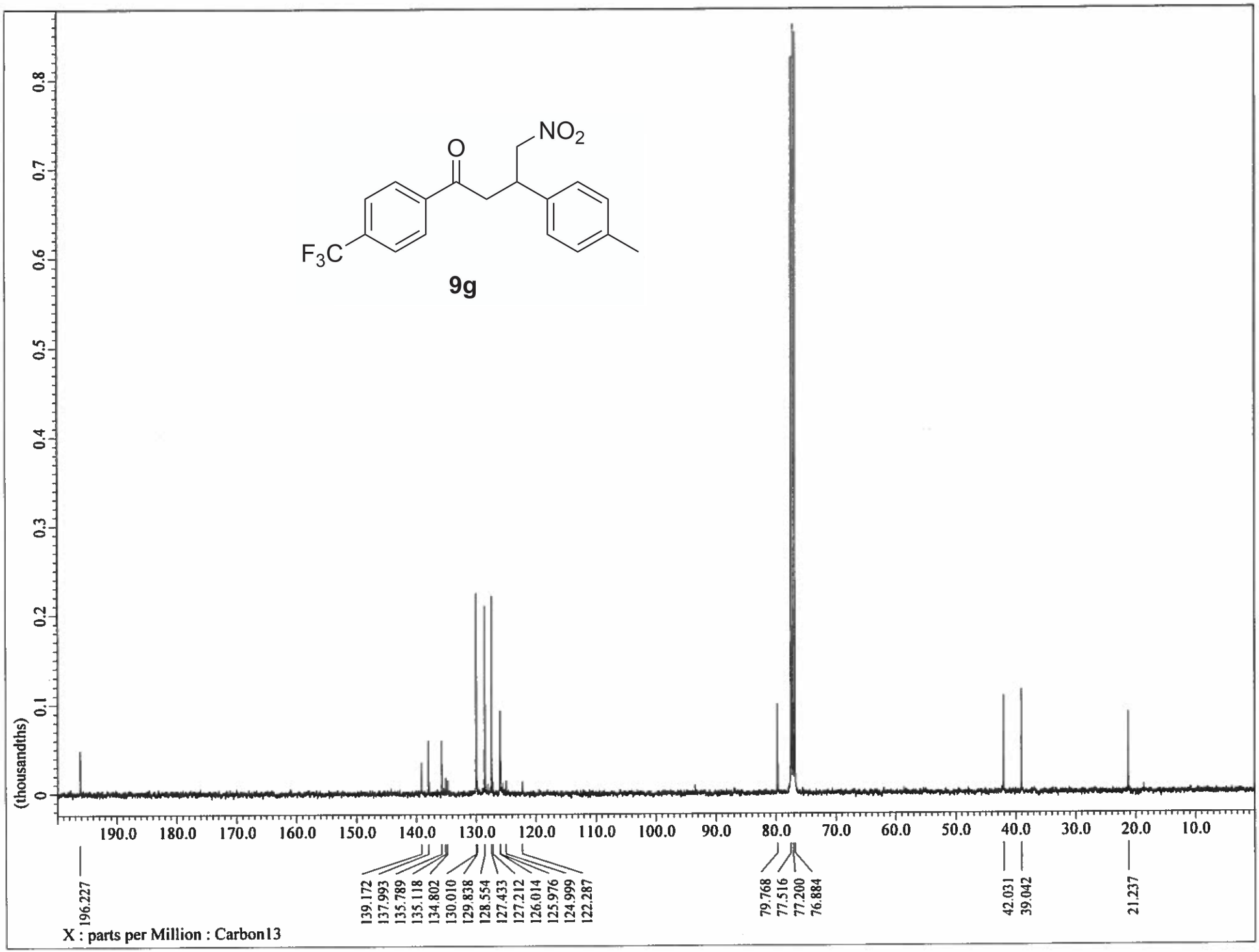
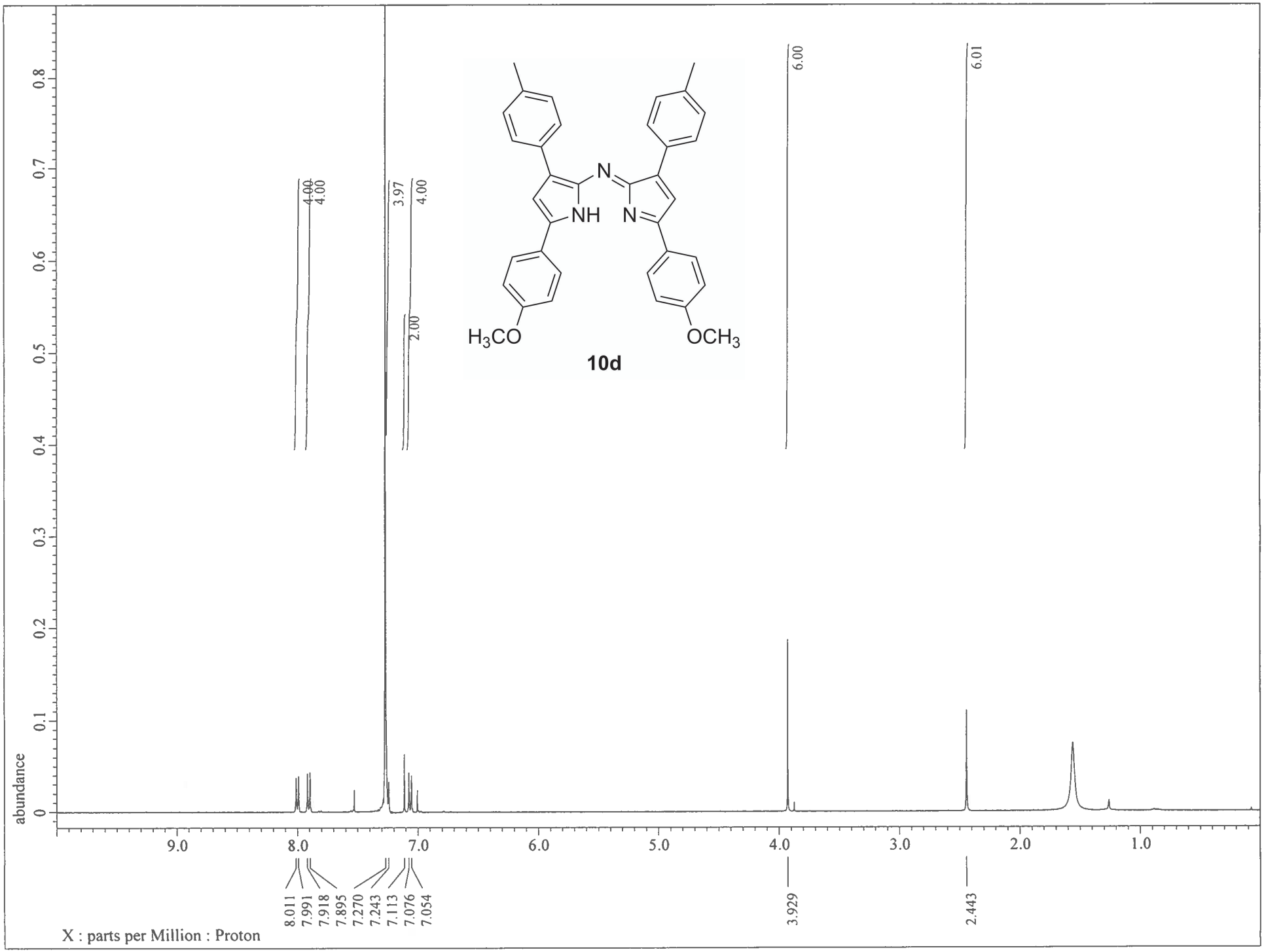
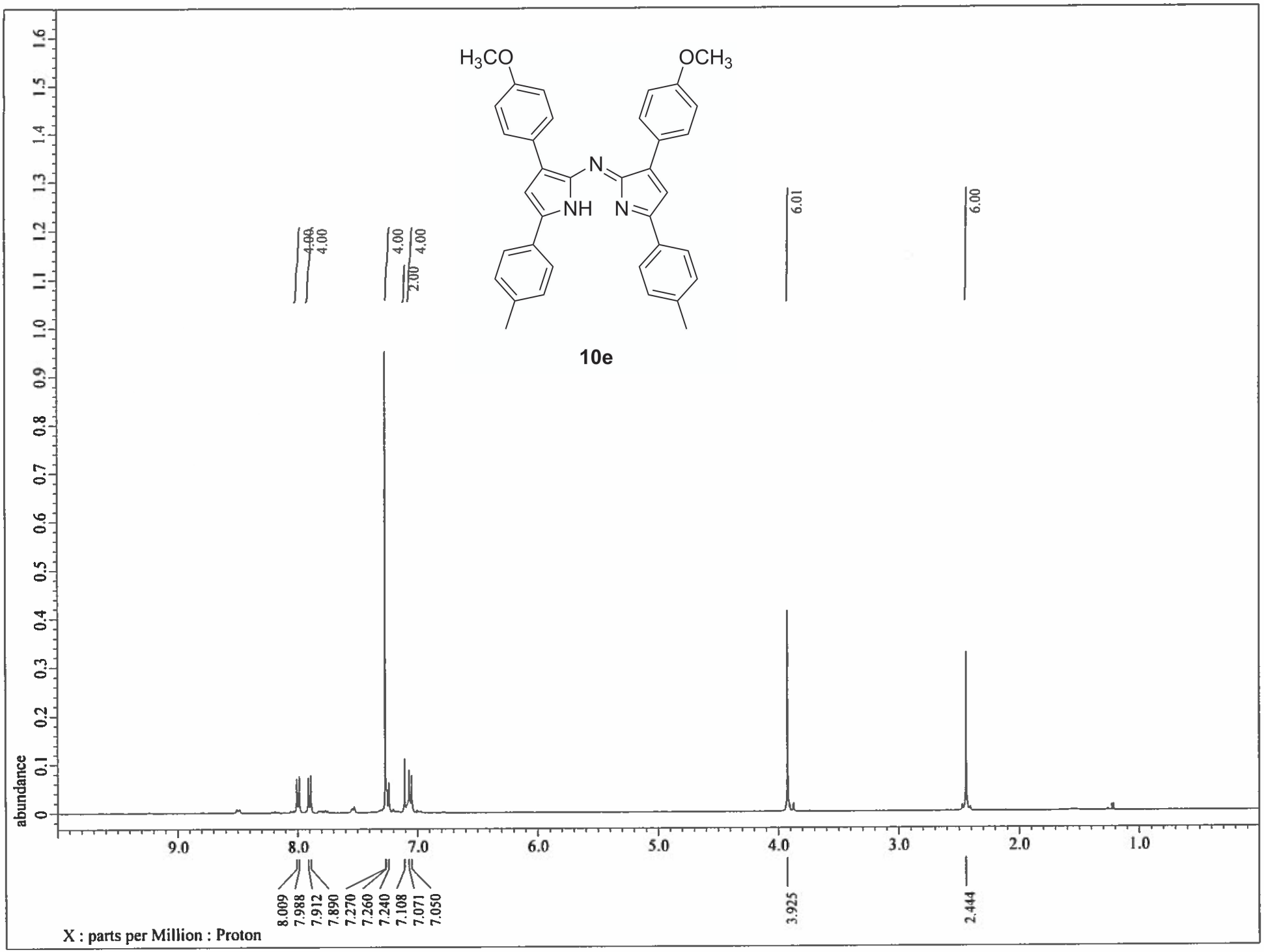
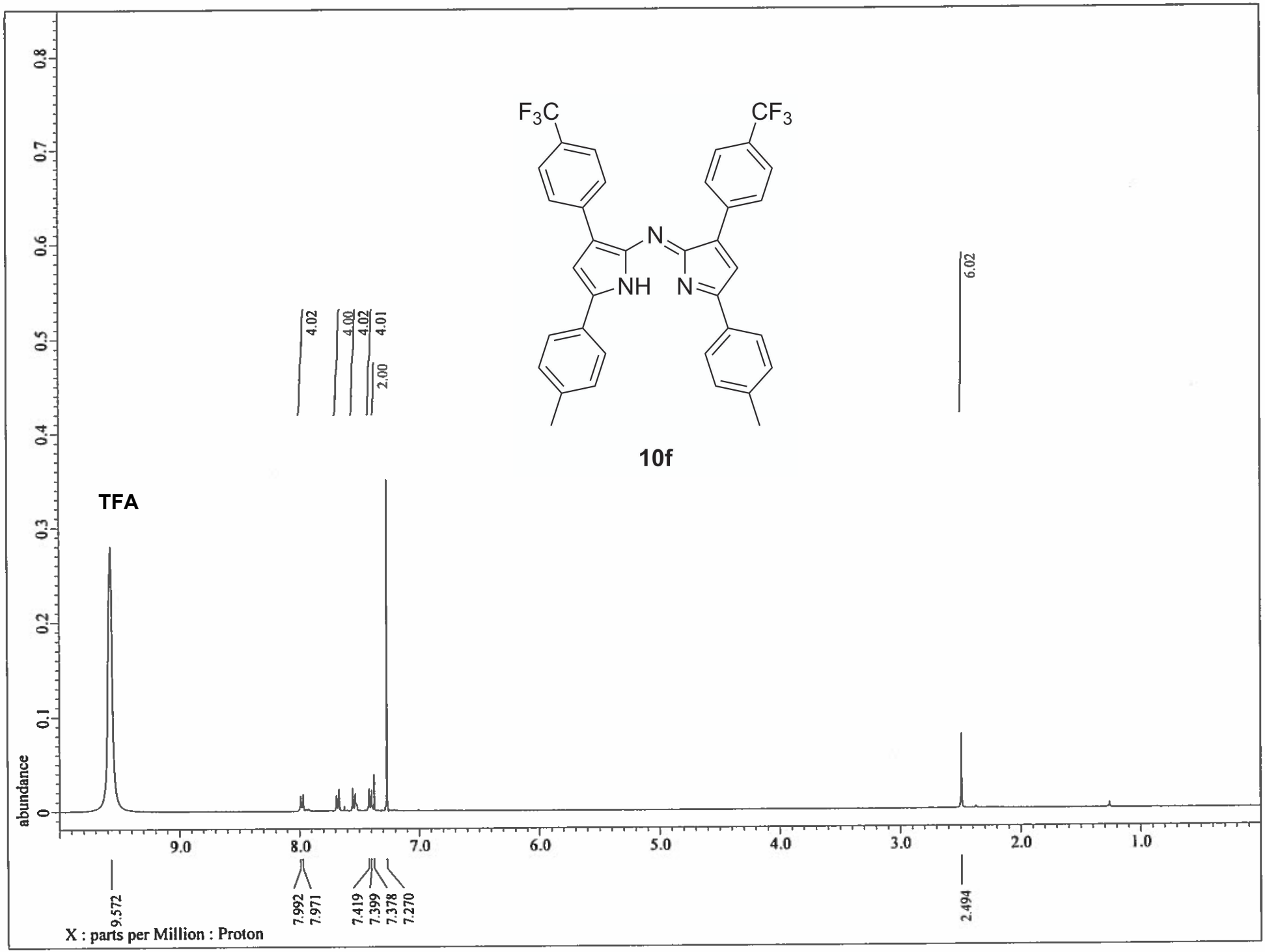
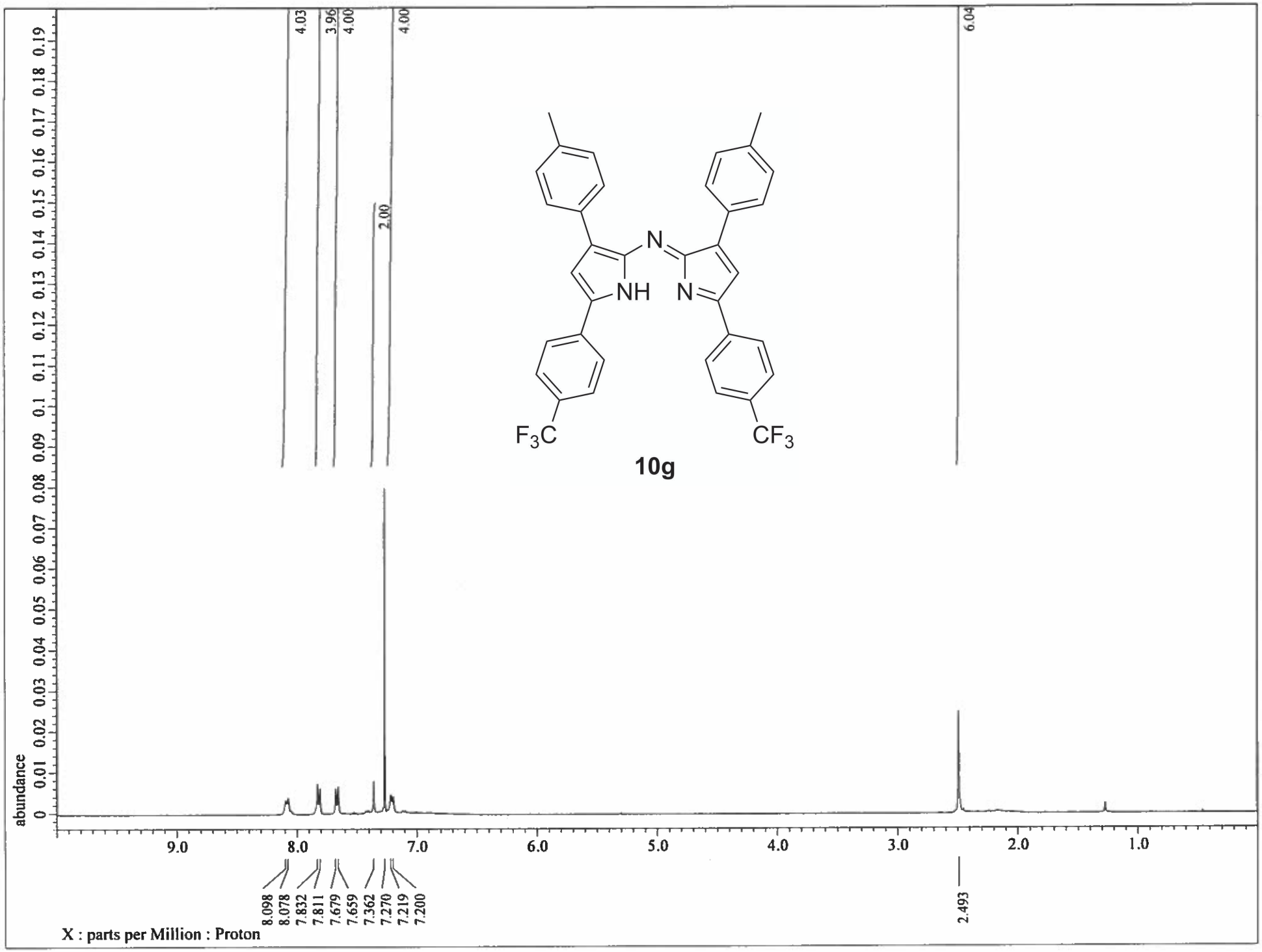
3.532
3.515
3.488
3.483
3.471
3.465
2.323

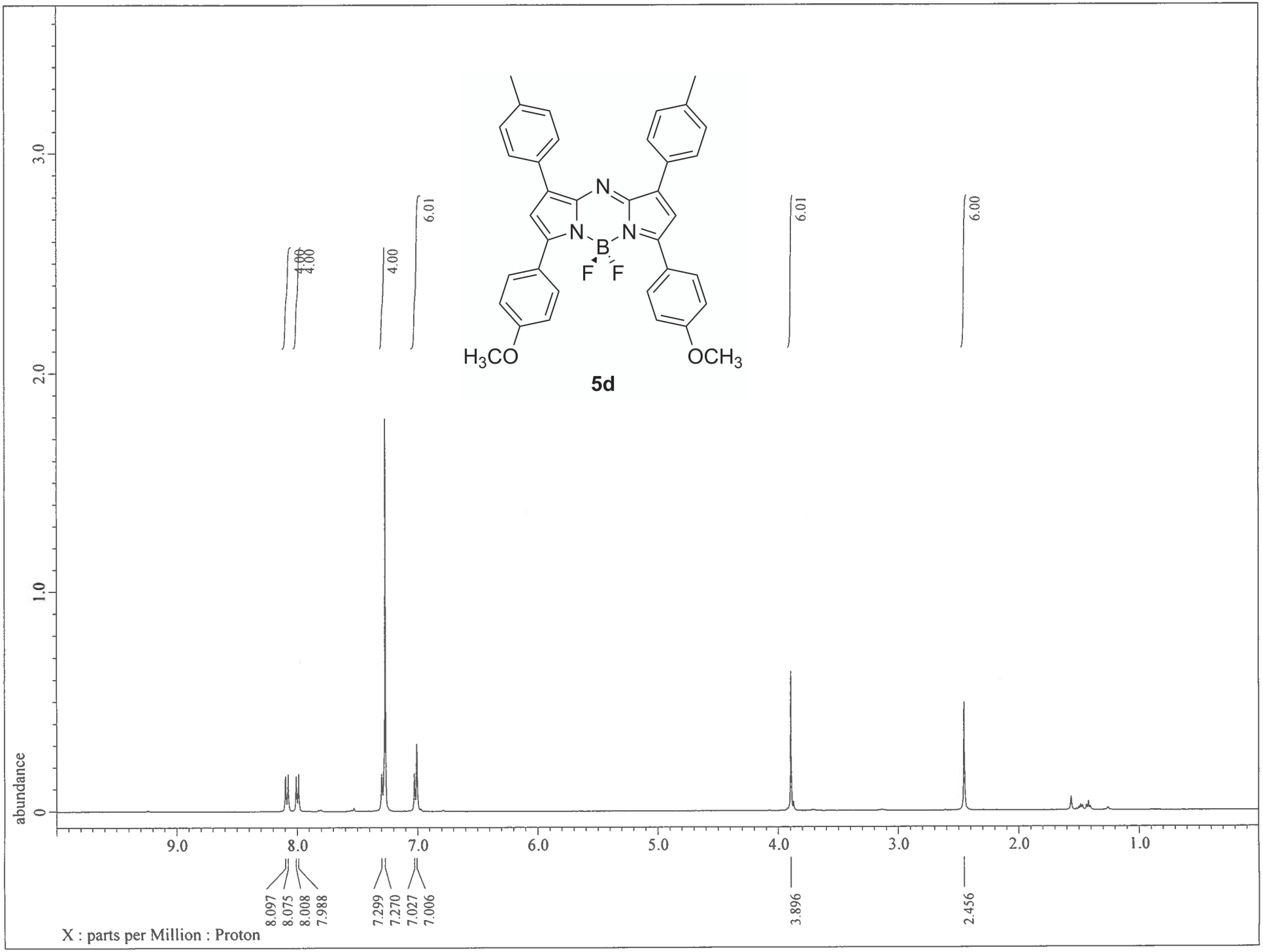

O
NO2
F3C
9g
(thousandths)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
196.227
139.172
137.993
135.789
135.118
134.802
130.010
129.838
128.554
127.433
127.212
126.014
125.976
124.999
122.287
79.768
77.516
77.200
76.884
42.031
39.042
21.237
X : parts per Million : Carbon13

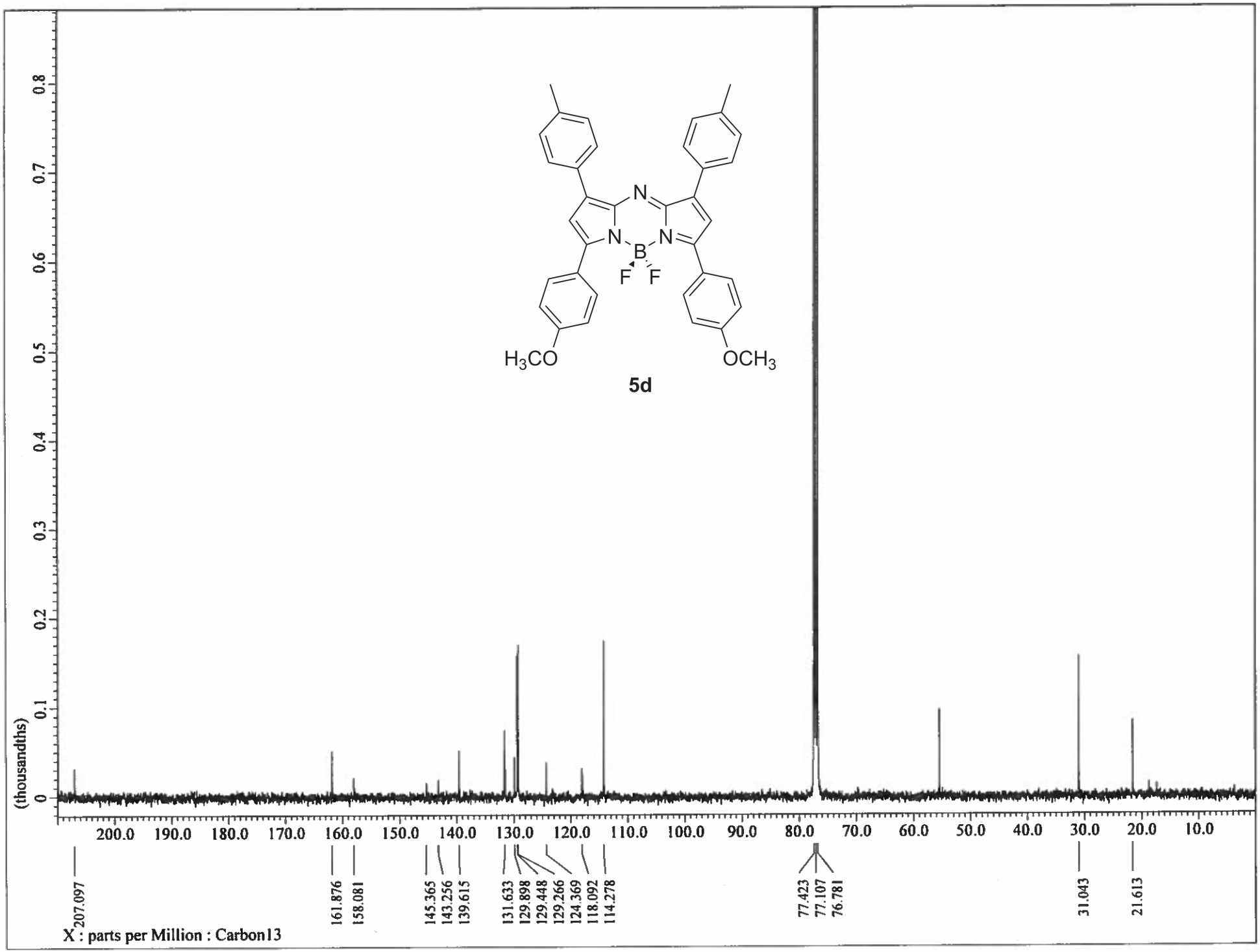

abundance
X : parts per Million : Proton
4.00
4.00
3.97
4.00
2.00
6.00
6.01
8.011
7.991
7.918
7.895
7.270
7.243
7.113
7.076
7.054
3.929
2.443
NH
N
N
H3CO
OCH3
10d


H3CO
OCH3
N
NH
N
10e
4.00
4.00
4.00
4.00
2.00
6.01
6.00
abundance
X : parts per Million : Proton
8.009
7.988
7.912
7.890
7.270
7.260
7.240
7.108
7.071
7.050
3.925
2.444

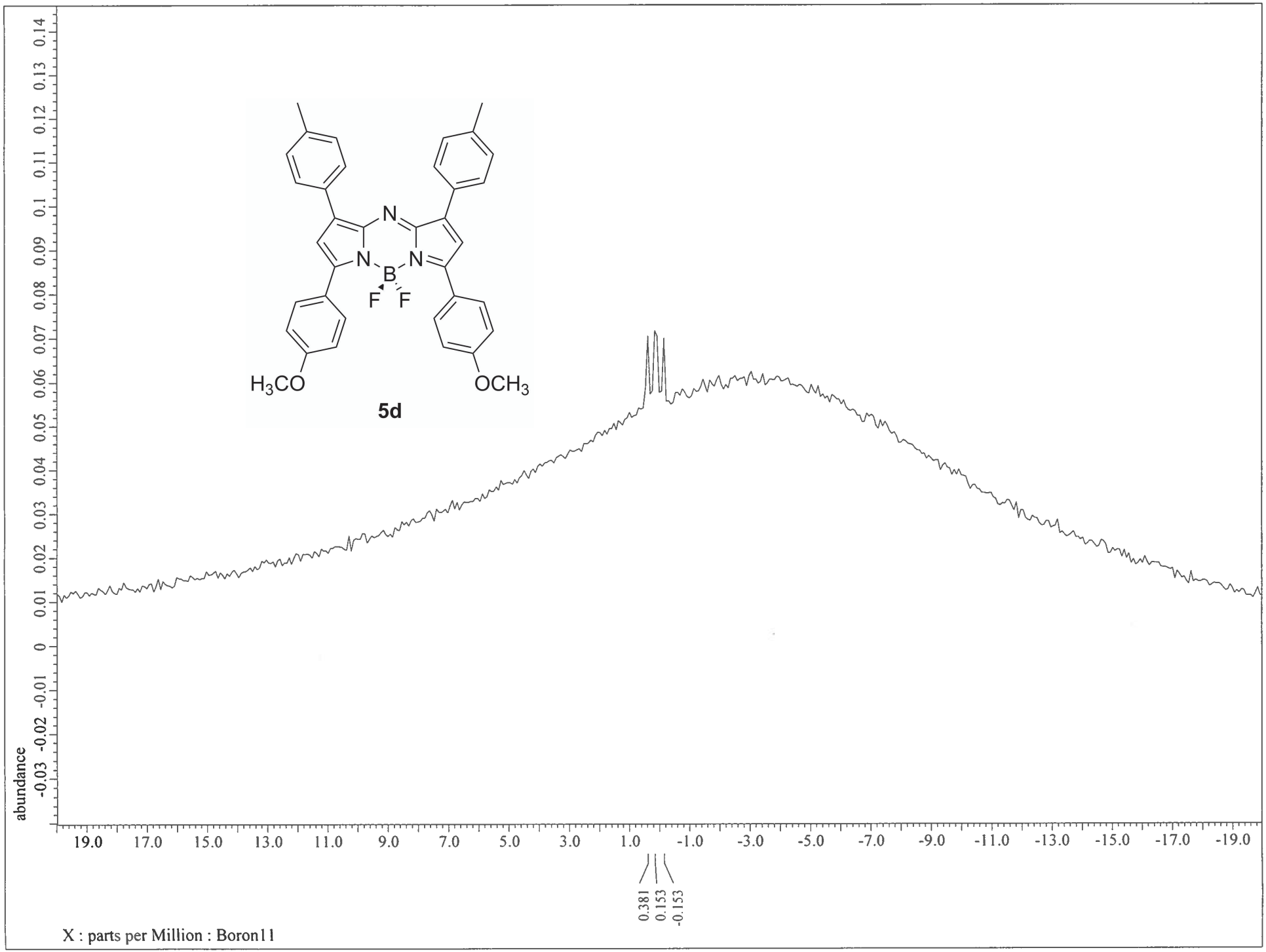

F3C
CF3
N
NH
N
10f
TFA
4.02
4.00
4.02
4.01
2.00
6.02
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
9.572
7.992
7.971
7.419
7.399
7.378
7.270
2.494
X : parts per Million : Proton


4.03
3.96
4.00
2.00
4.00
6.04
N
NH
N
F3C
CF3
10g
abundance
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18 0.19
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.098
8.078
7.832
7.811
7.679
7.659
7.362
7.270
7.219
7.200
2.493
X : parts per Million : Proton


N
N
B
N
F
F
H3CO
OCH3
5d
4.00
4.00
4.00
6.01
6.01
6.00
abundance
0
1.0
2.0
3.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.097
8.075
8.008
7.988
7.299
7.270
7.027
7.006
3.896
2.456
X : parts per Million : Proton

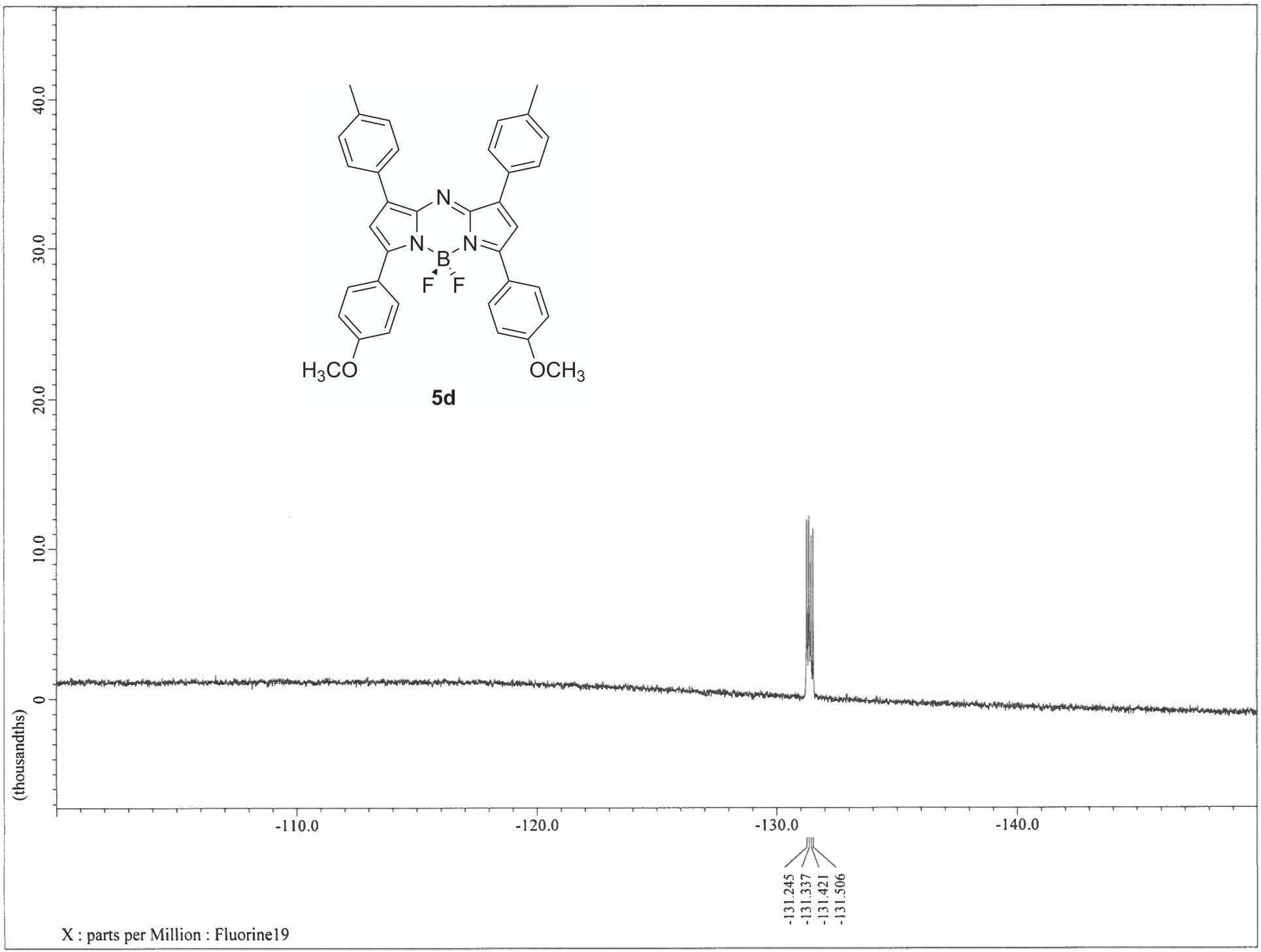

(thousandths)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
207.097
161.876
158.081
145.365
143.256
139.615
131.633
129.898
129.448
129.266
124.369
118.092
114.278
77.423
77.107
76.781
31.043
21.613
X : parts per Million : Carbon13
N
N
B
N
F
F
H3CO
OCH3

5d


abundance
0.14
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
0.381
0.153
-0.153
X : parts per Million : Boron11

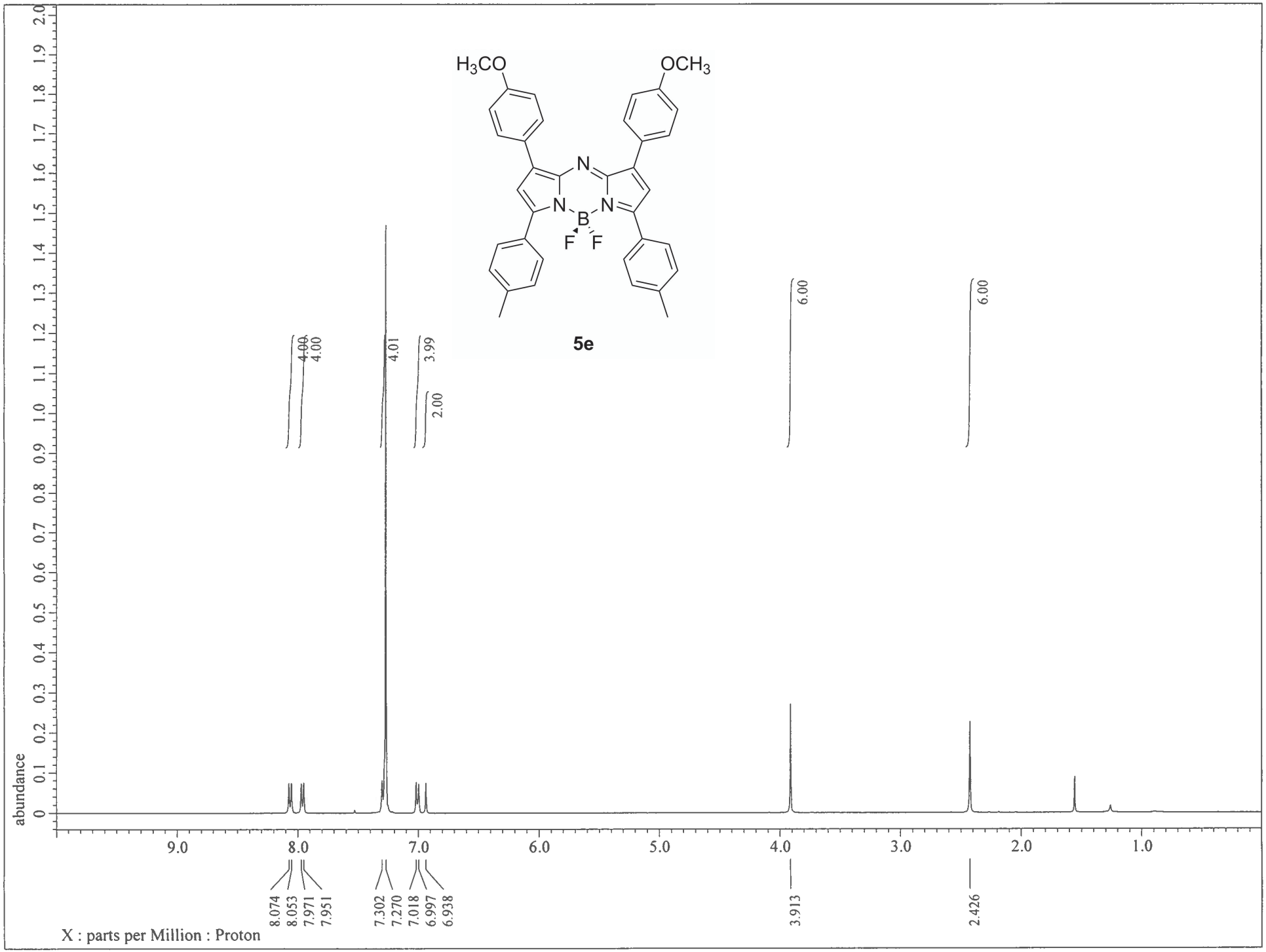
N
N
B
N
F
F
H3CO
OCH3

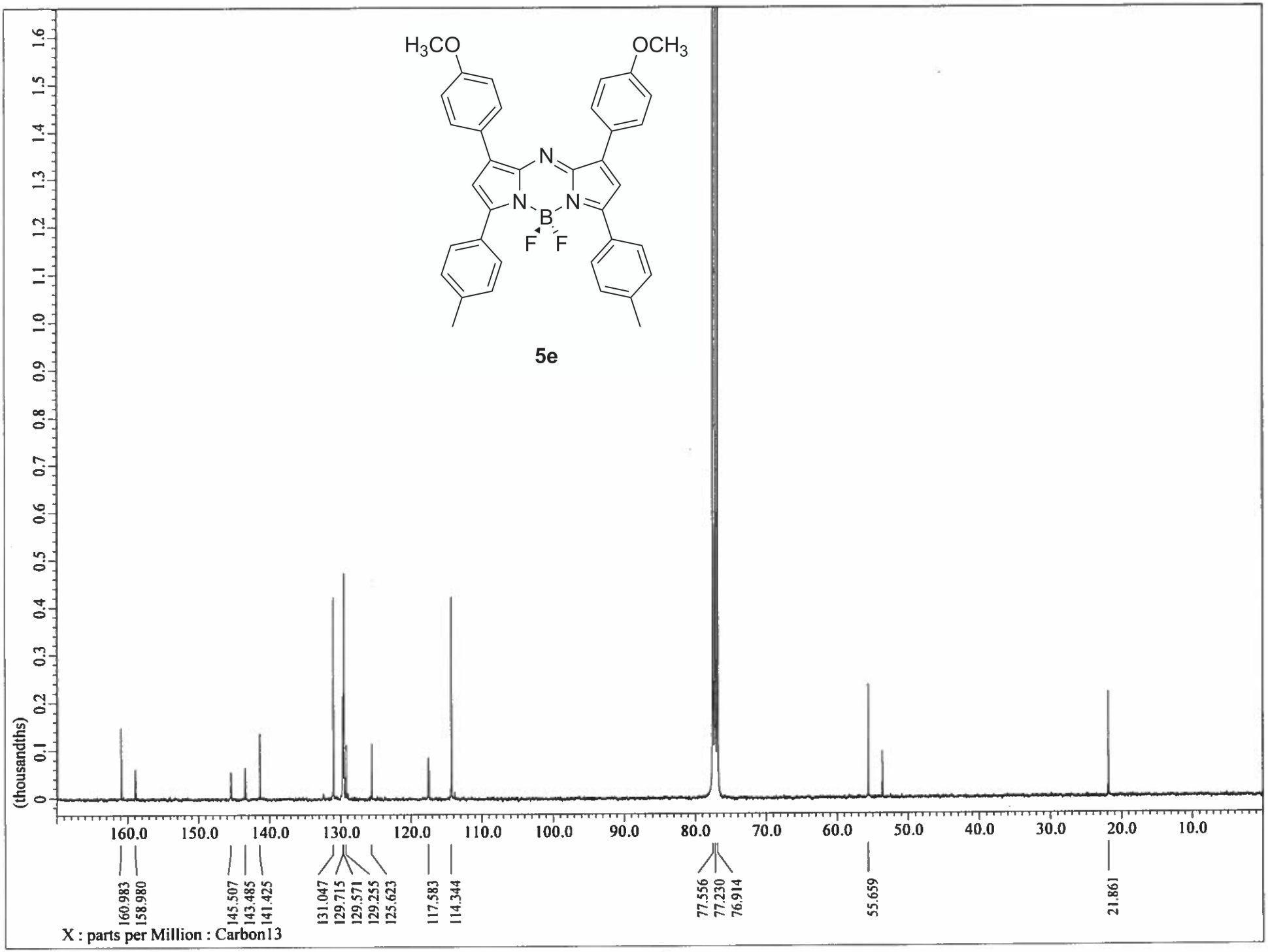
5d

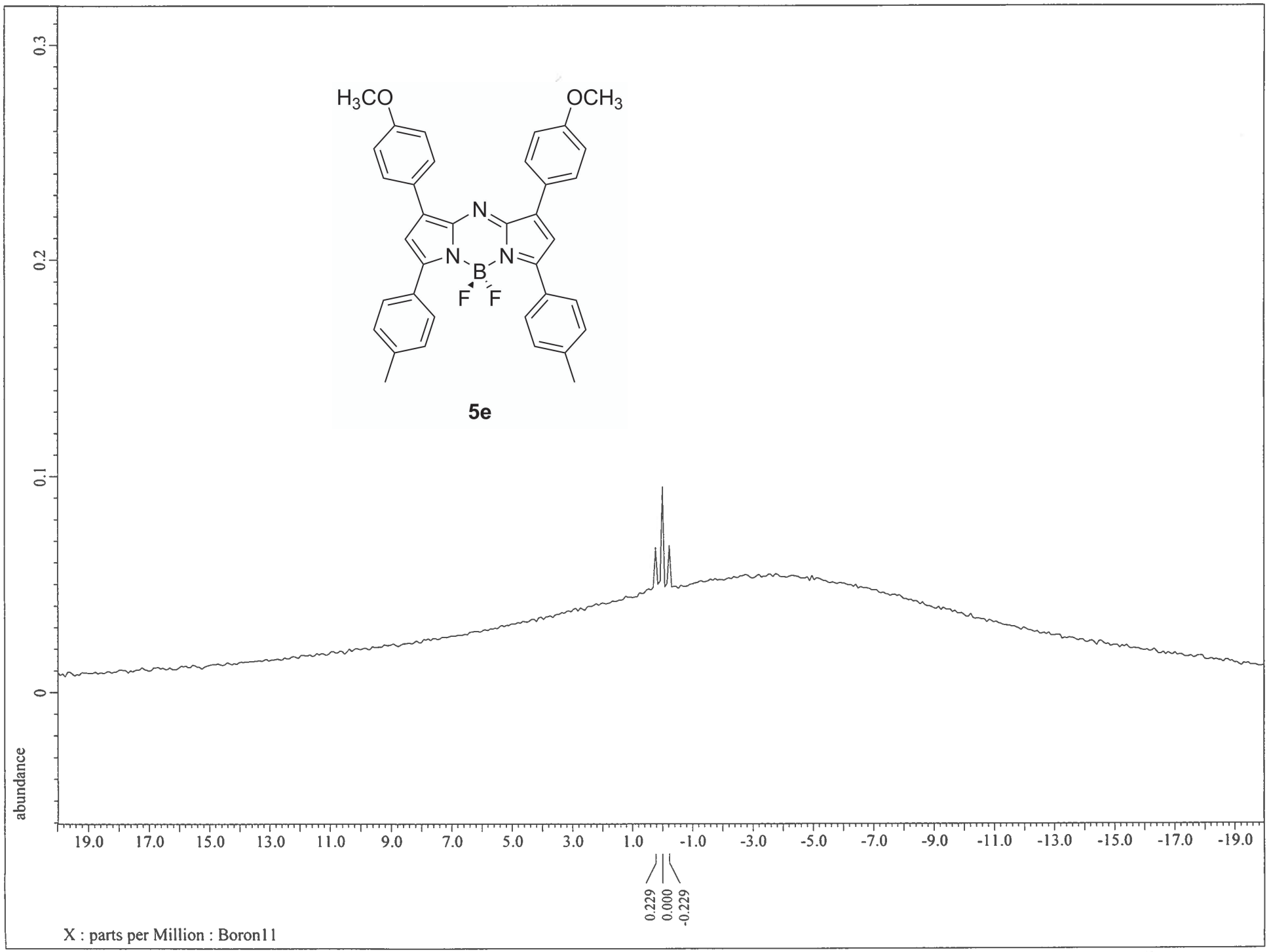

40.0
30.0
20.0
10.0
0
(thousandths)
-110.0
-120.0
-130.0
-140.0
-131.245
-131.337
-131.421
-131.506
X : parts per Million : Fluorine19

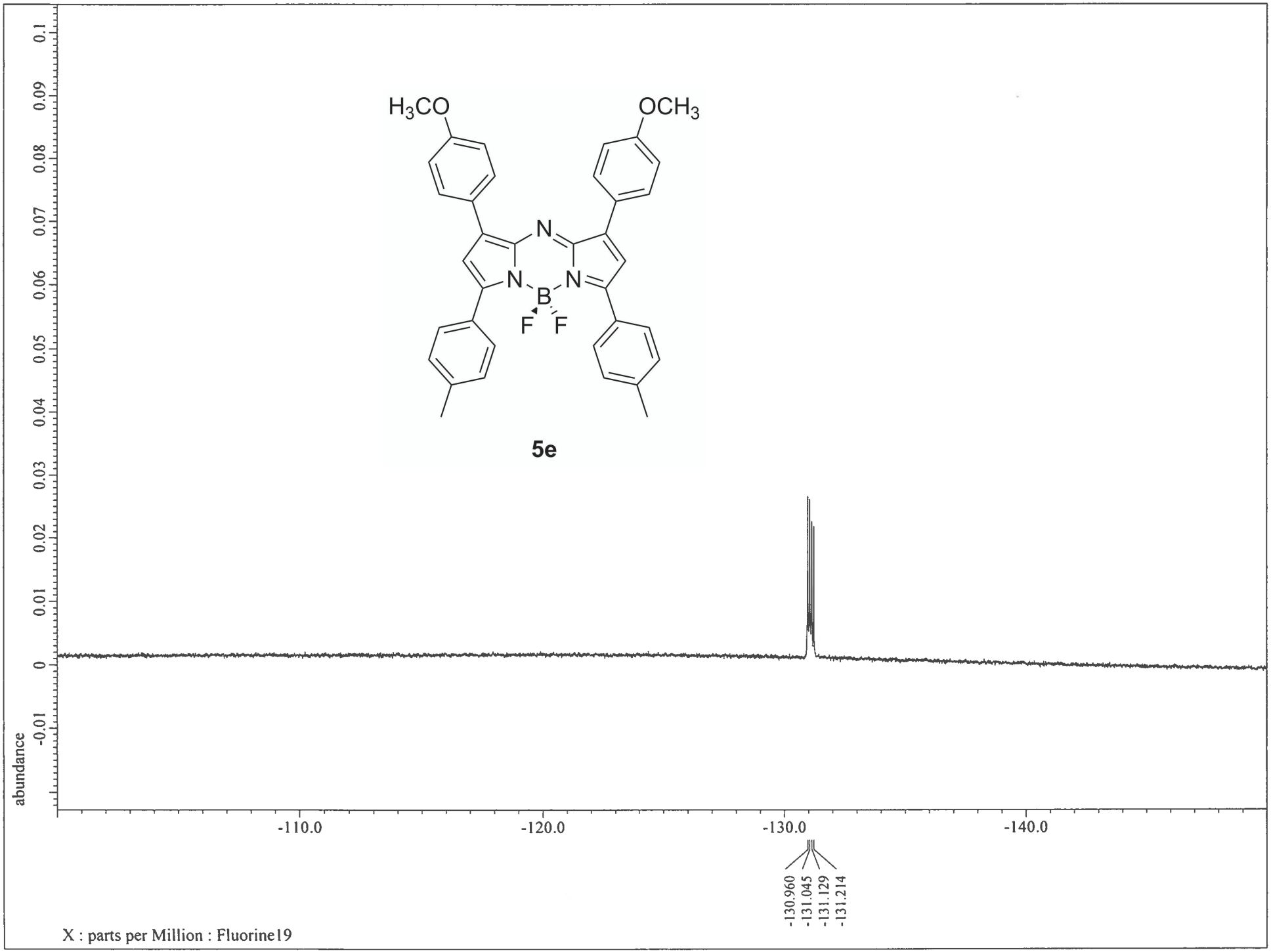
N
N
B
N
F
F
H3CO
OCH3

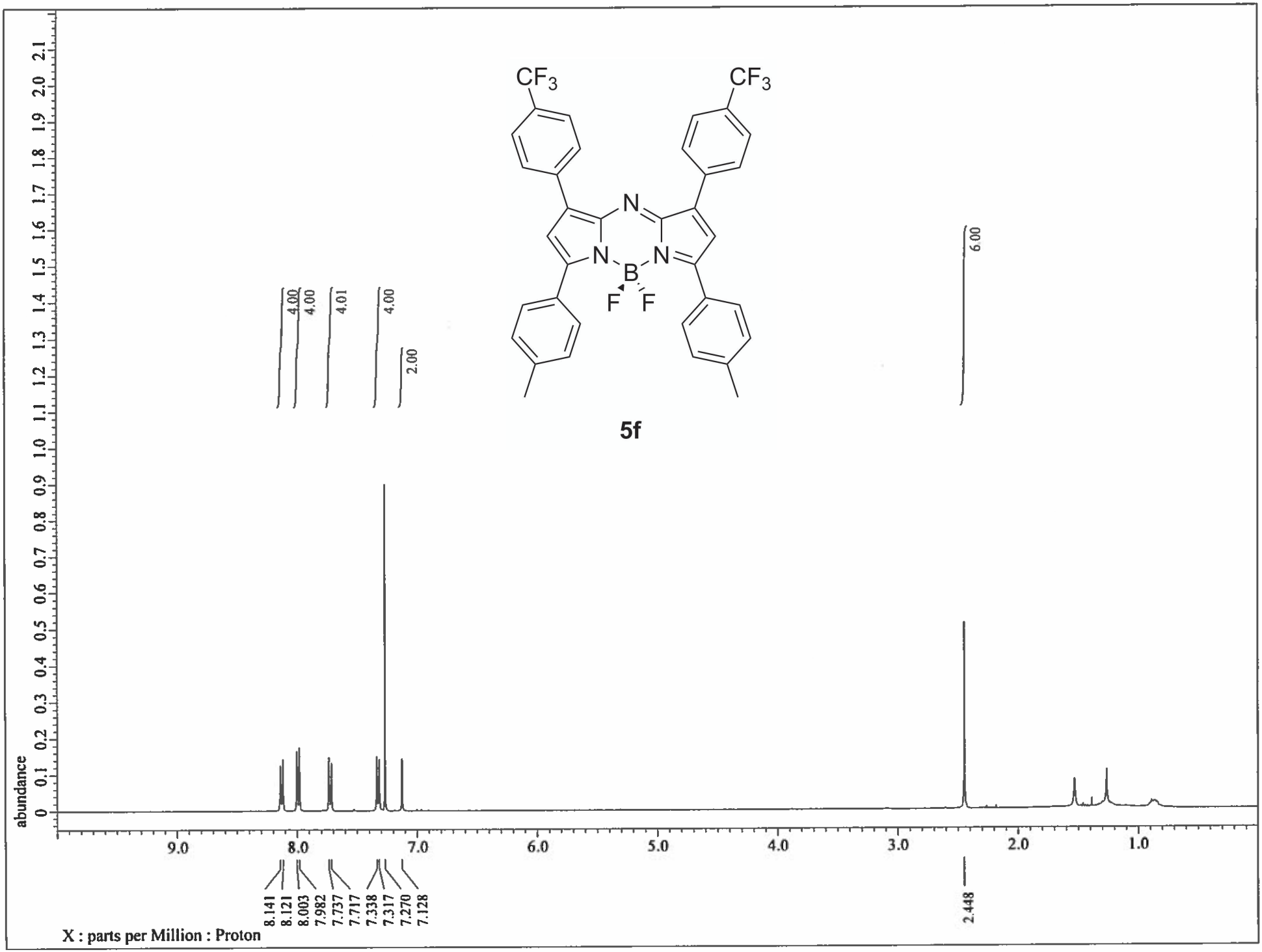
5d

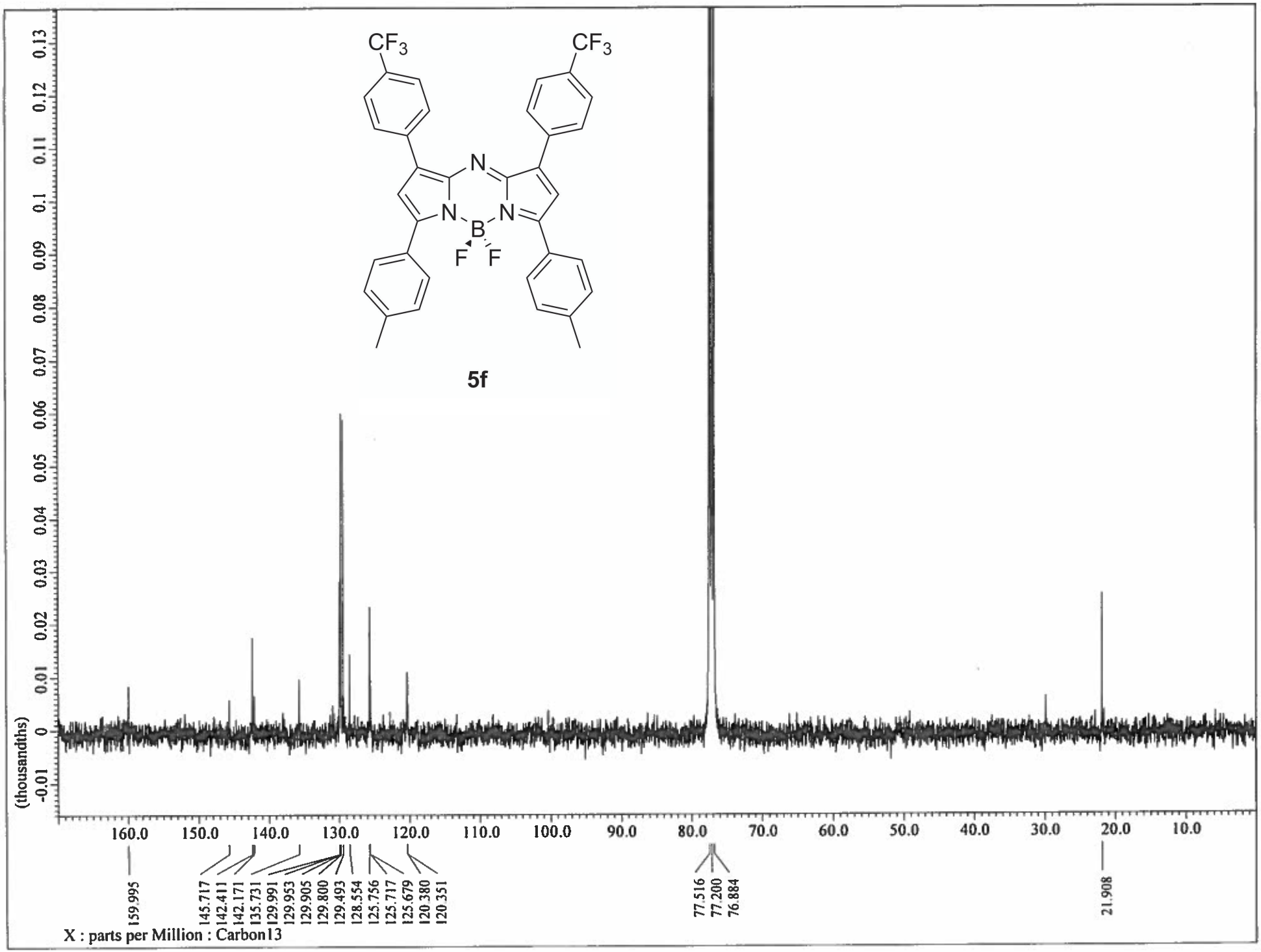

H3CO
OCH3
N
N
B
N
F
F
5e
4.00
4.00
4.01
3.99
2.00
6.00
6.00
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.074
8.053
7.971
7.951
7.302
7.270
7.018
6.997
6.938
3.913
2.426
X : parts per Million : Proton

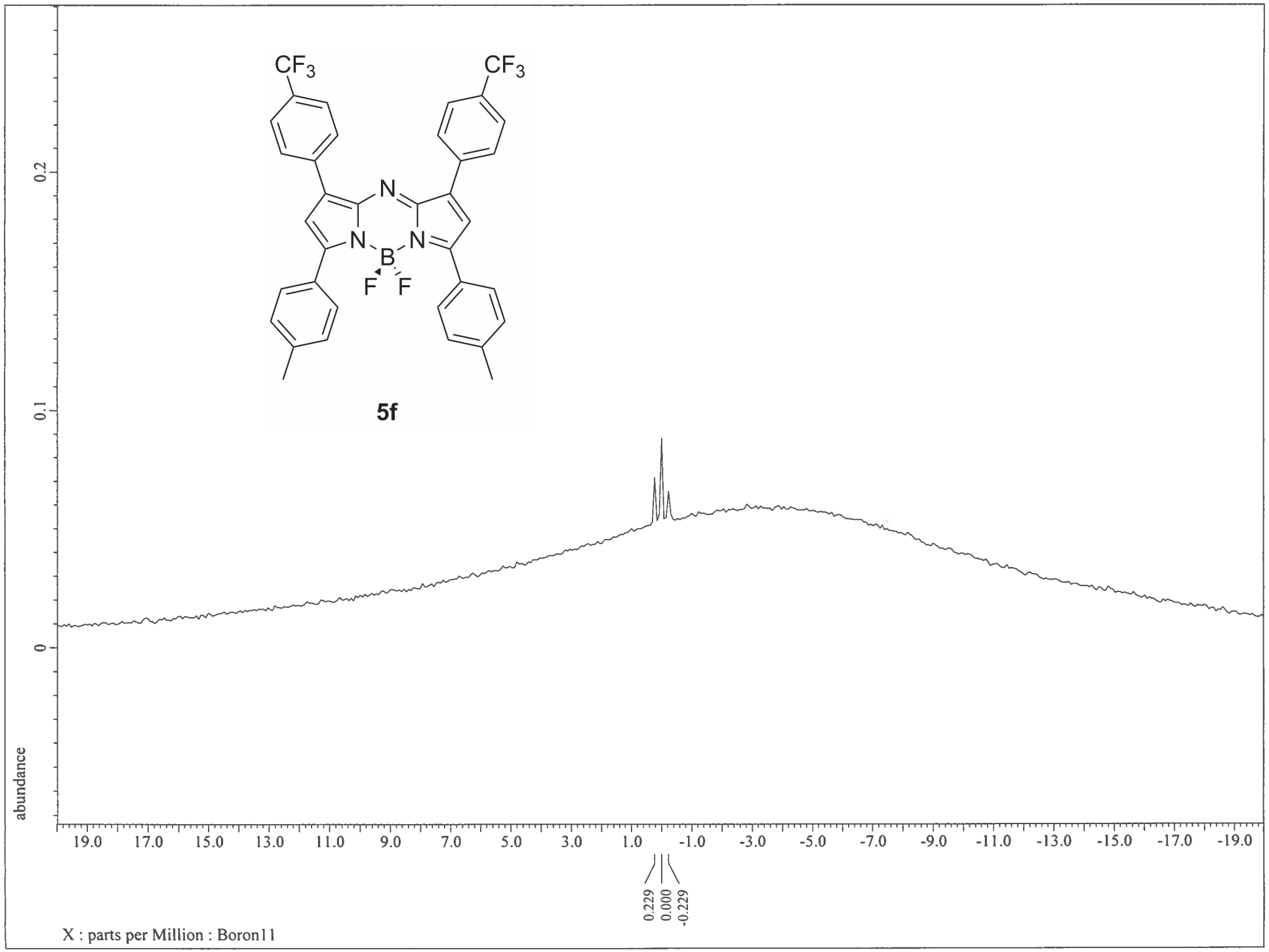

H3CO
OCH3
N
N
B
N
F
F
5e
(thousandths)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
160.983
158.980
145.507
143.485
141.425
131.047
129.715
129.571
129.255
125.623
117.583
114.344
77.556
77.230
76.914
55.659
21.861
X : parts per Million : Carbon13

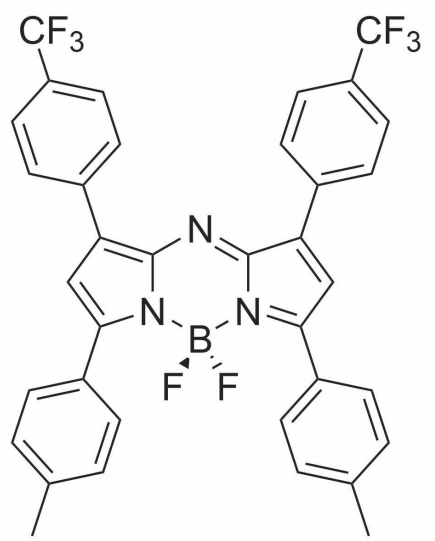

H3CO
OCH3
N
N
B
N
F
F
5e
0.3
0.2
0.1
0
abundance
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
0.229
0.000
-0.229
X : parts per Million : Boron11


H3CO
OCH3
N
N
B
N
F
F
5e
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
abundance
-110.0
-120.0
-130.0
-140.0
-130.960
-131.045
-131.129
-131.214
X : parts per Million : Fluorine19


CF3
CF3
N
N
B
N
F
F
4.00
4.00
4.01
4.00
2.00
6.00
5f
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.141
8.121
8.003
7.982
7.737
7.717
7.338
7.317
7.270
7.128
2.448
X : parts per Million : Proton

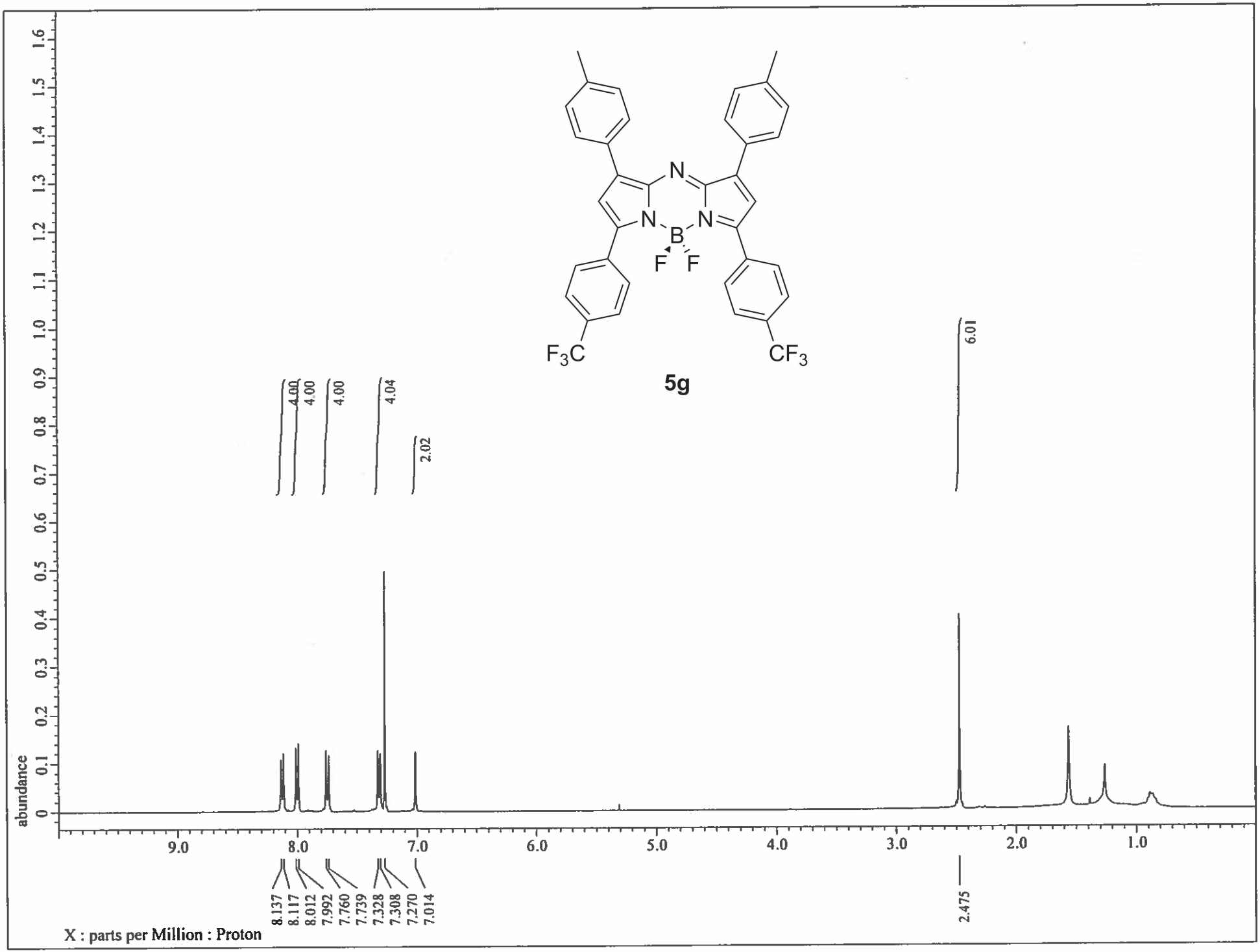

CF3
CF3
N
N
B
N
F
F
5f
(thousandths)
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
159.995
145.717
142.411
142.171
135.731
129.991
129.953
129.905
129.800
129.493
128.554
125.756
125.717
125.679
120.380
120.351
77.516
77.200
76.884
21.908
X : parts per Million : Carbon13

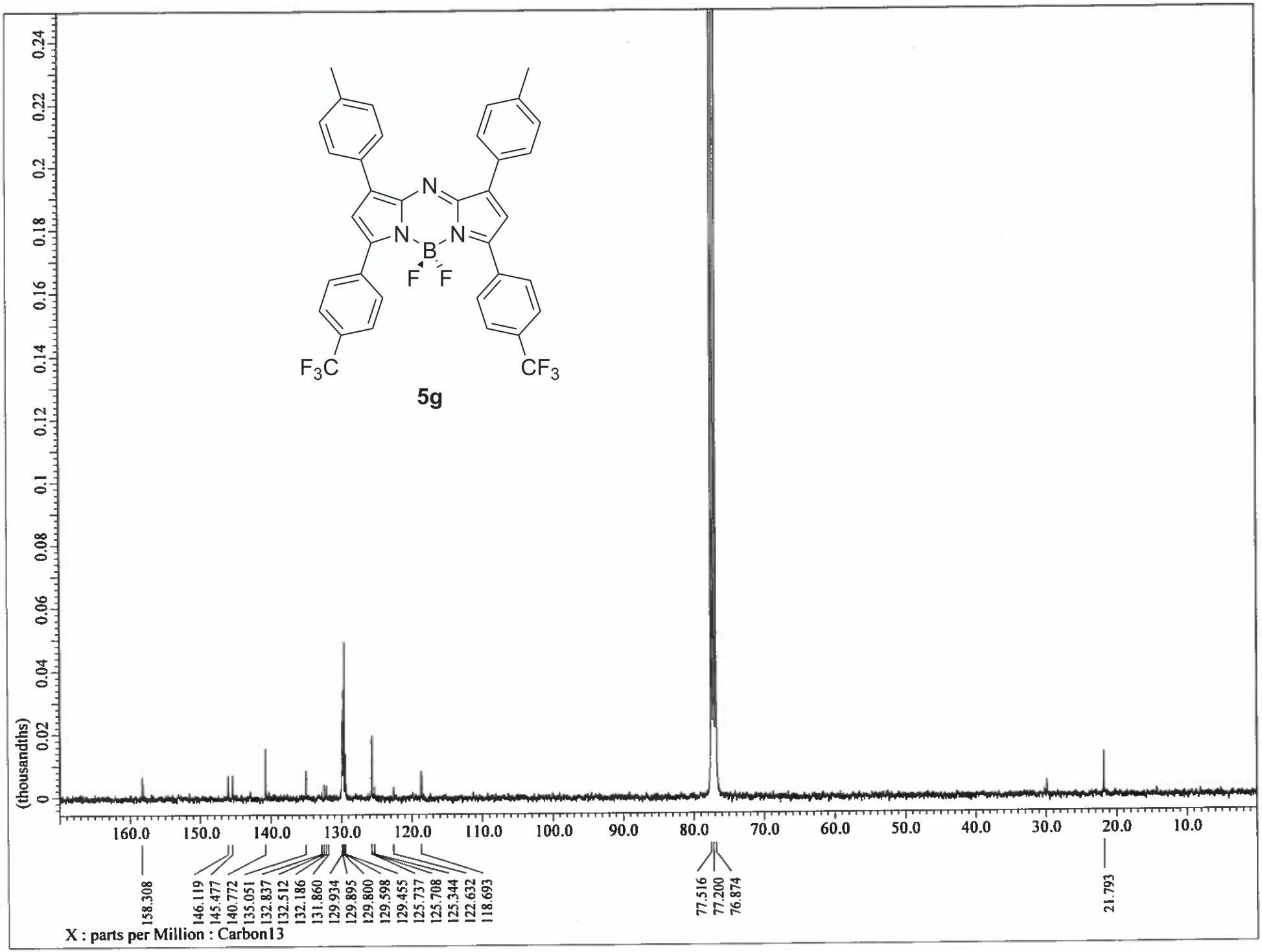

CF3
CF3
N
N
B
N
F
F
5f
0.2
0.1
0
abundance
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
0.229
0.000
-0.229
X : parts per Million : Boron11


CF3
CF3
N
N
B
N
F
F

5f

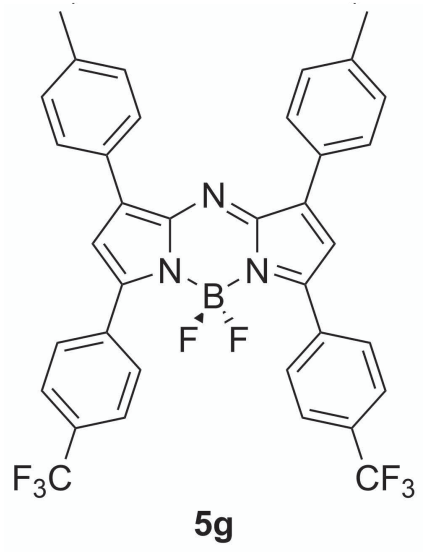
6.00
2.00
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-62.510
-131.729
-131.813
-131.898
-131.982
X : parts per Million : Fluorine19


N
N
B
N
F
F
F3C
CF3
5g
4.00
4.00
4.00
4.04
2.02
6.01
abundance
X : parts per Million : Proton
8.137
8.117
8.012
7.992
7.760
7.739
7.328
7.308
7.270
7.014
2.475


(thousandths)
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
158.308
146.119
145.477
140.772
135.051
132.837
132.512
132.186
131.860
129.934
129.895
129.800
129.598
129.455
125.737
125.708
125.344
122.632
118.693
77.516
77.200
76.874
21.793
X : parts per Million : Carbon13

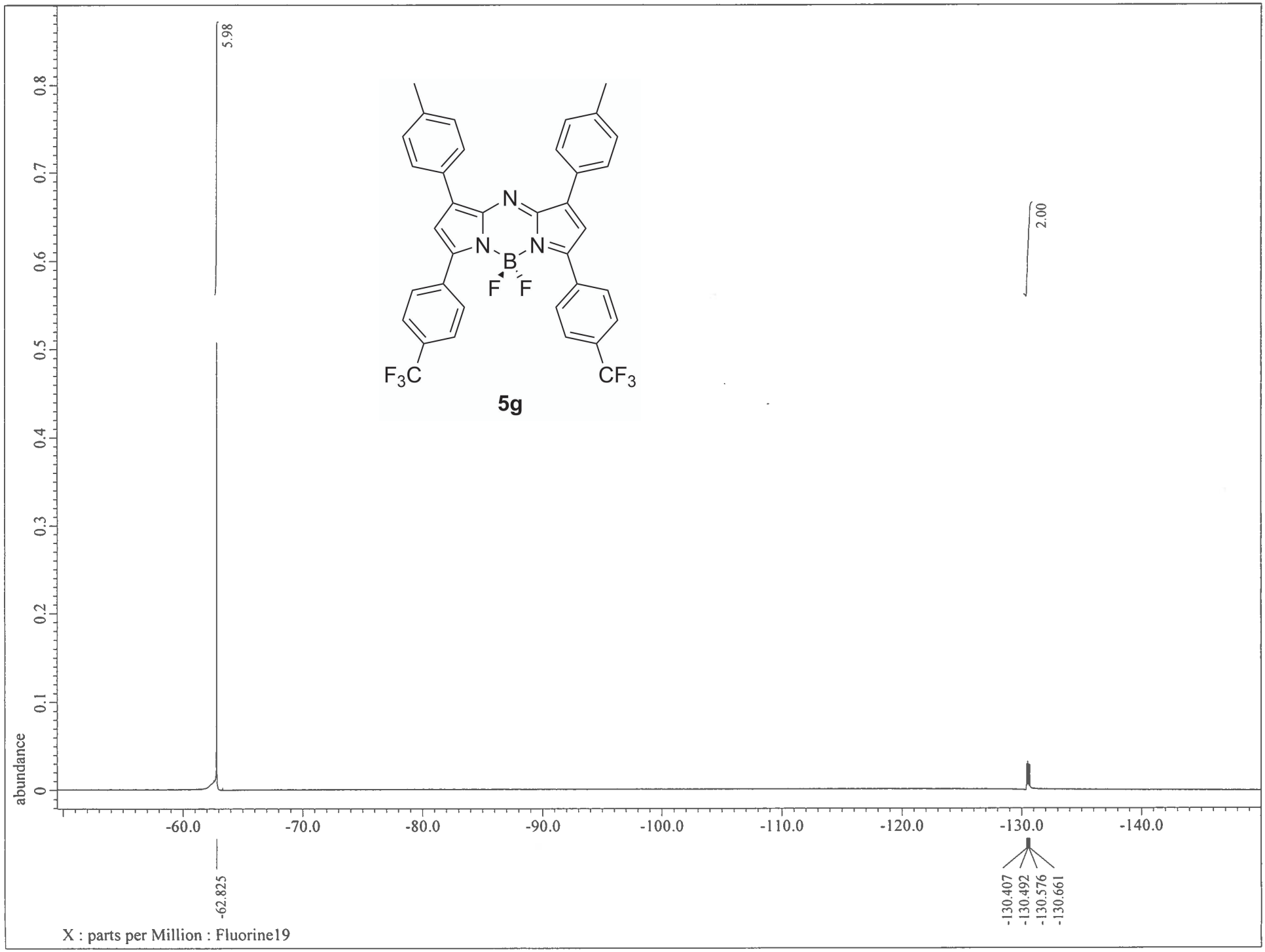
N
N
B
N
F
F
F3C
CF3

5g


N
N
B
N
F
F
F3C
CF3

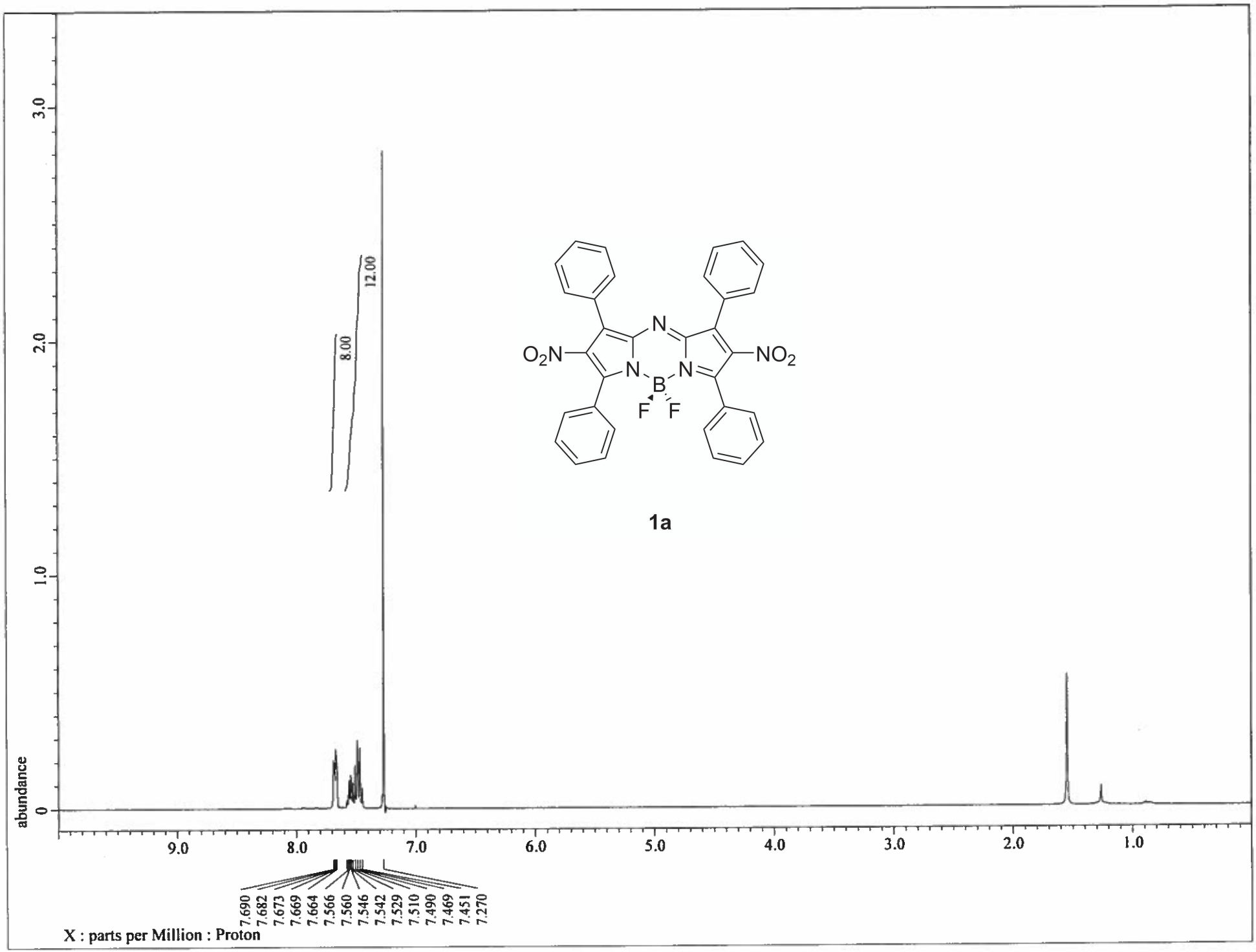
5g

0.3
0.2
0.1
0
abundance
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
0.076
-0.153
-0.381
X : parts per Million : Boron11

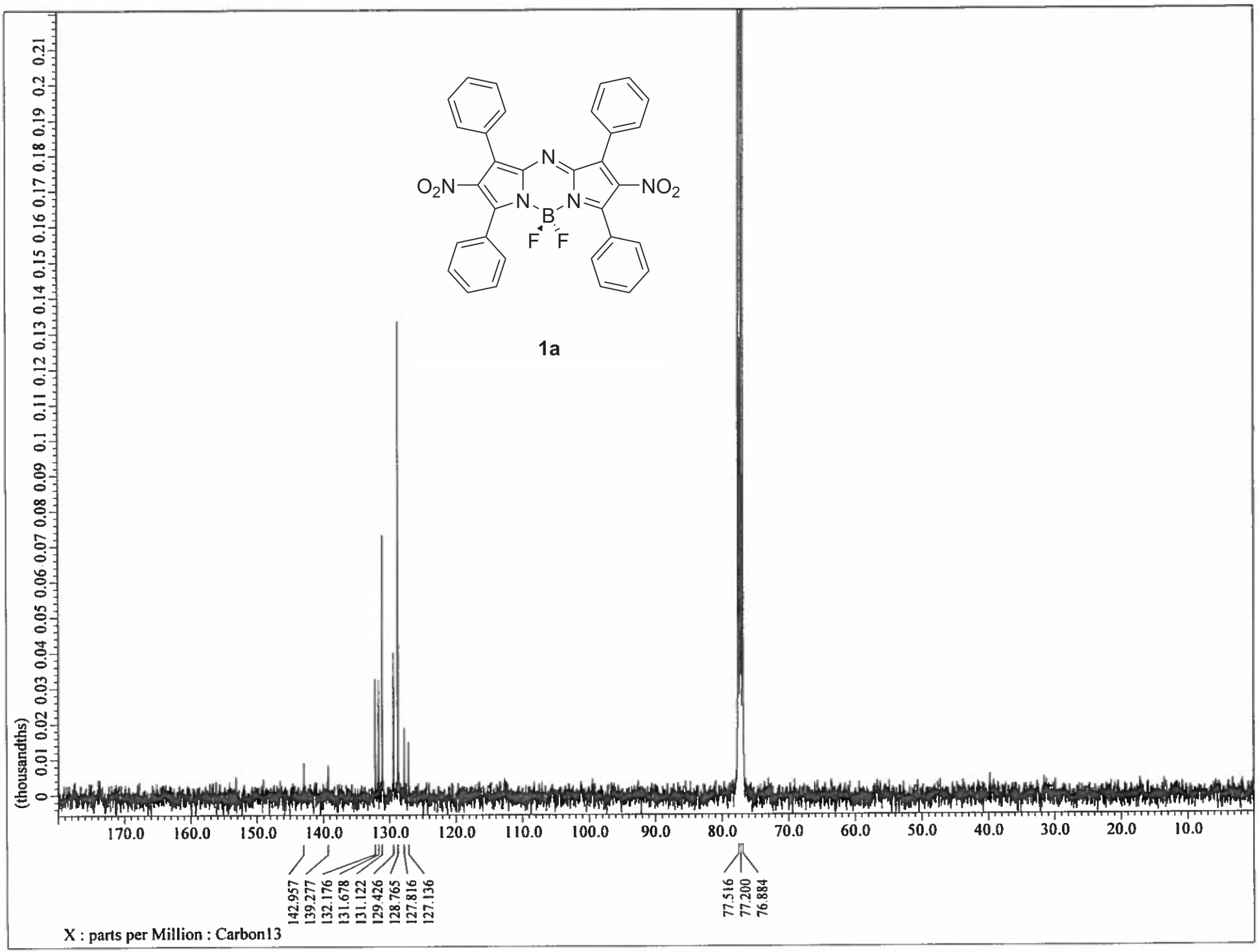

5.98
2.00
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-62.825
-130.407
-130.492
-130.576
-130.661
X : parts per Million : Fluorine19

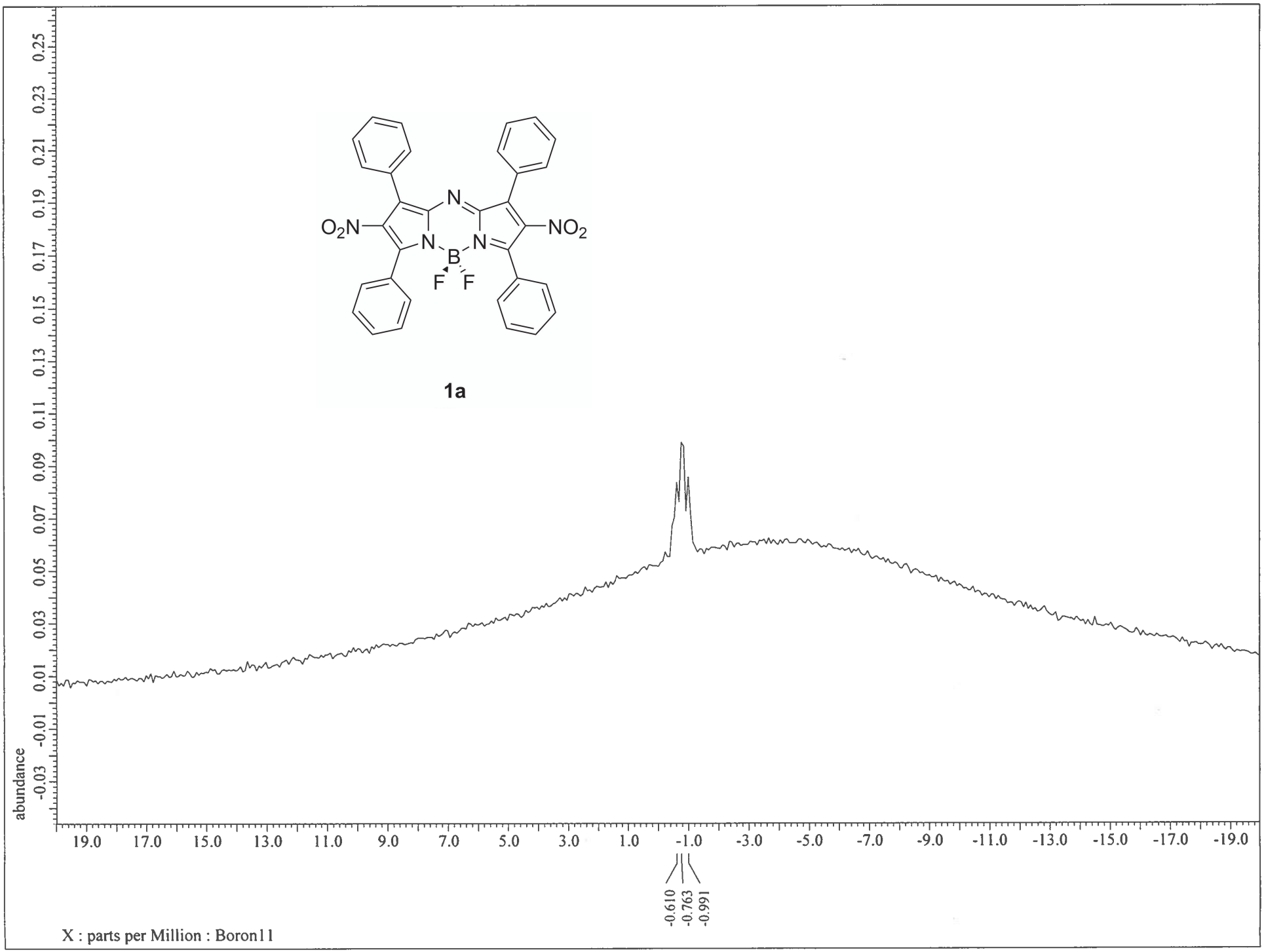
N
N
B
N
F
F
F3C
CF3

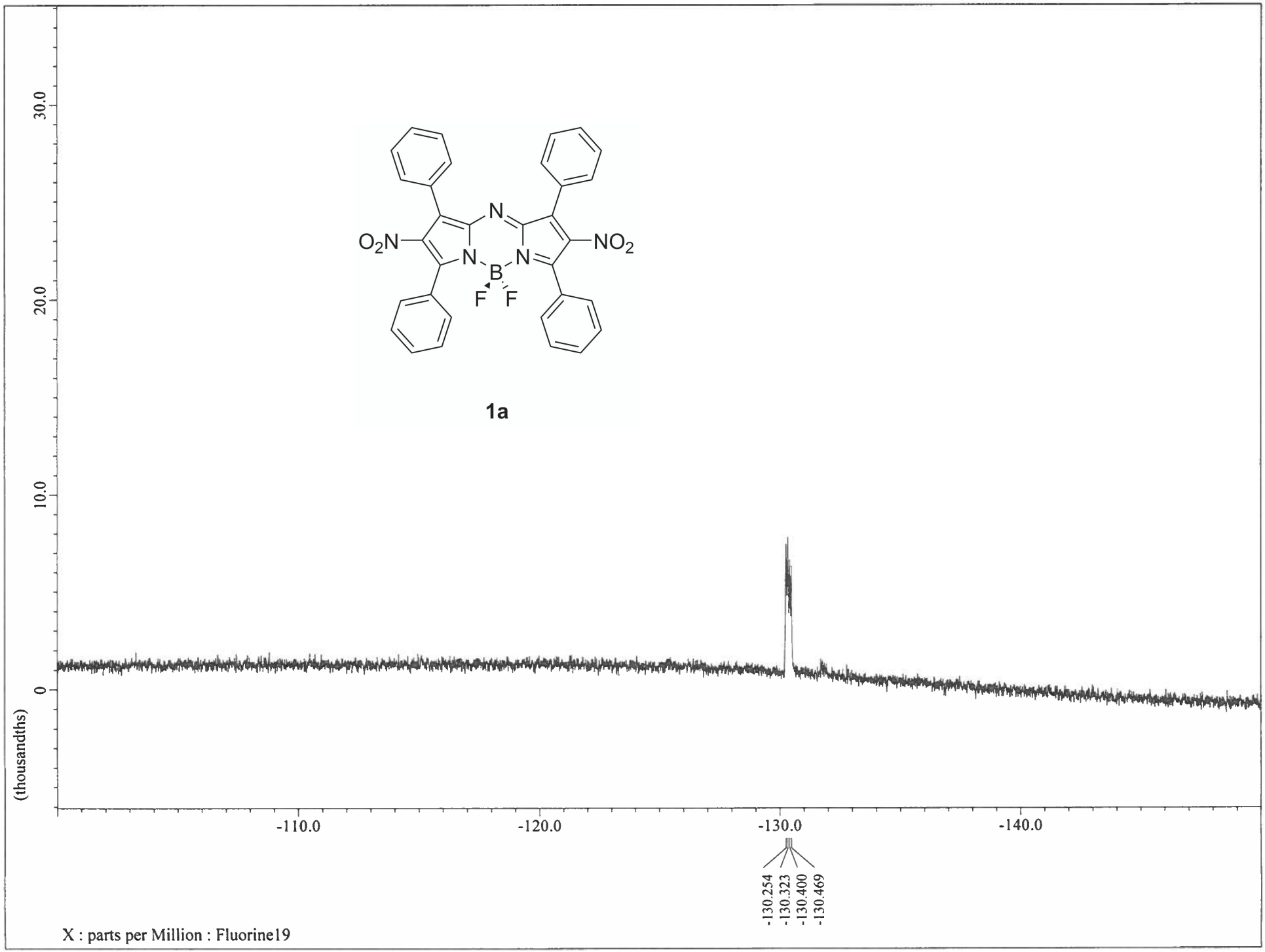
5g


3.0
2.0
1.0
0
abundance
8.00
12.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.690
7.682
7.673
7.669
7.664
7.566
7.560
7.546
7.542
7.529
7.510
7.490
7.469
7.451
7.270
X : parts per Million : Proton
O2N
NO2
N
N
B
N
F
F

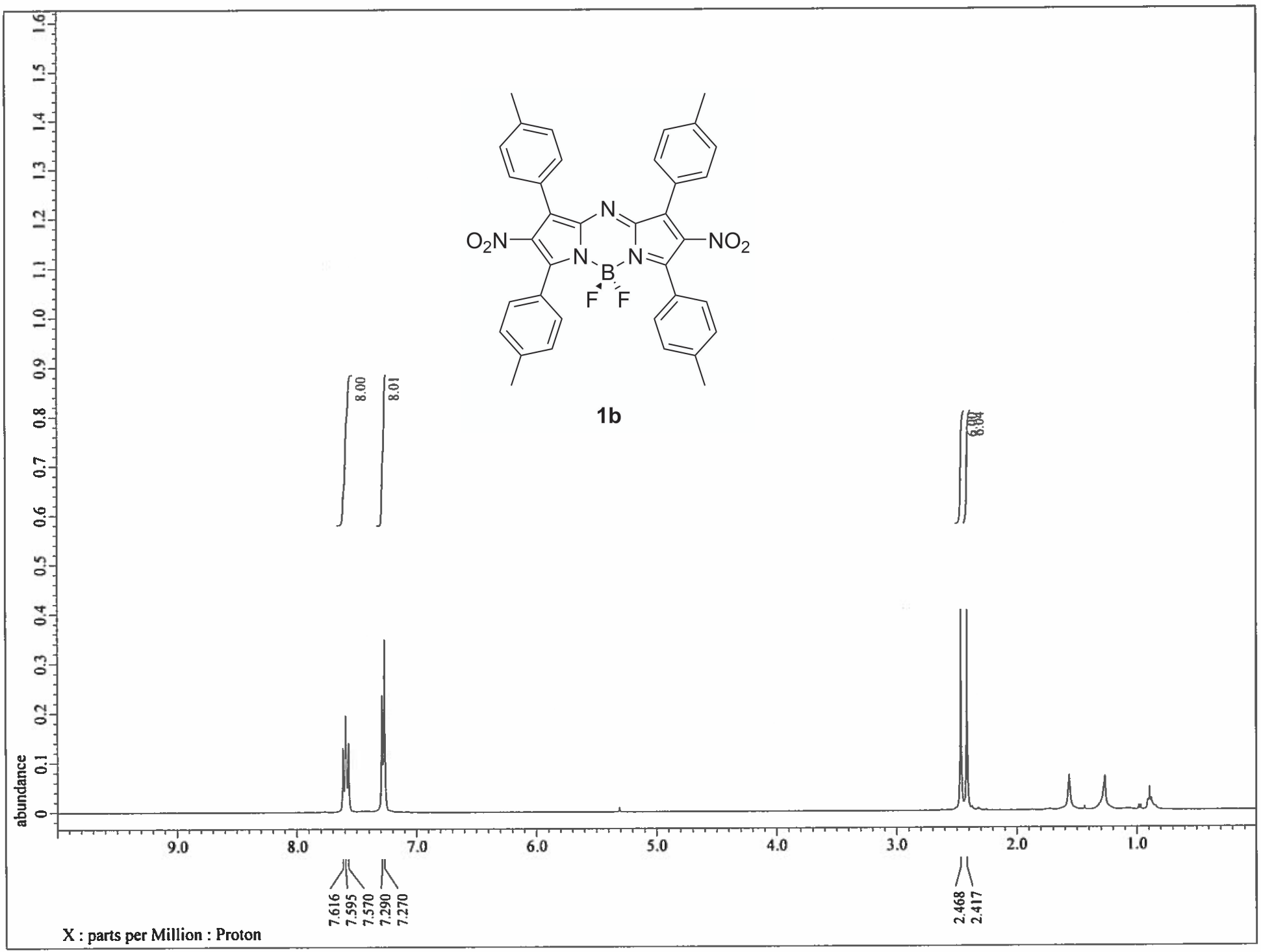
1a

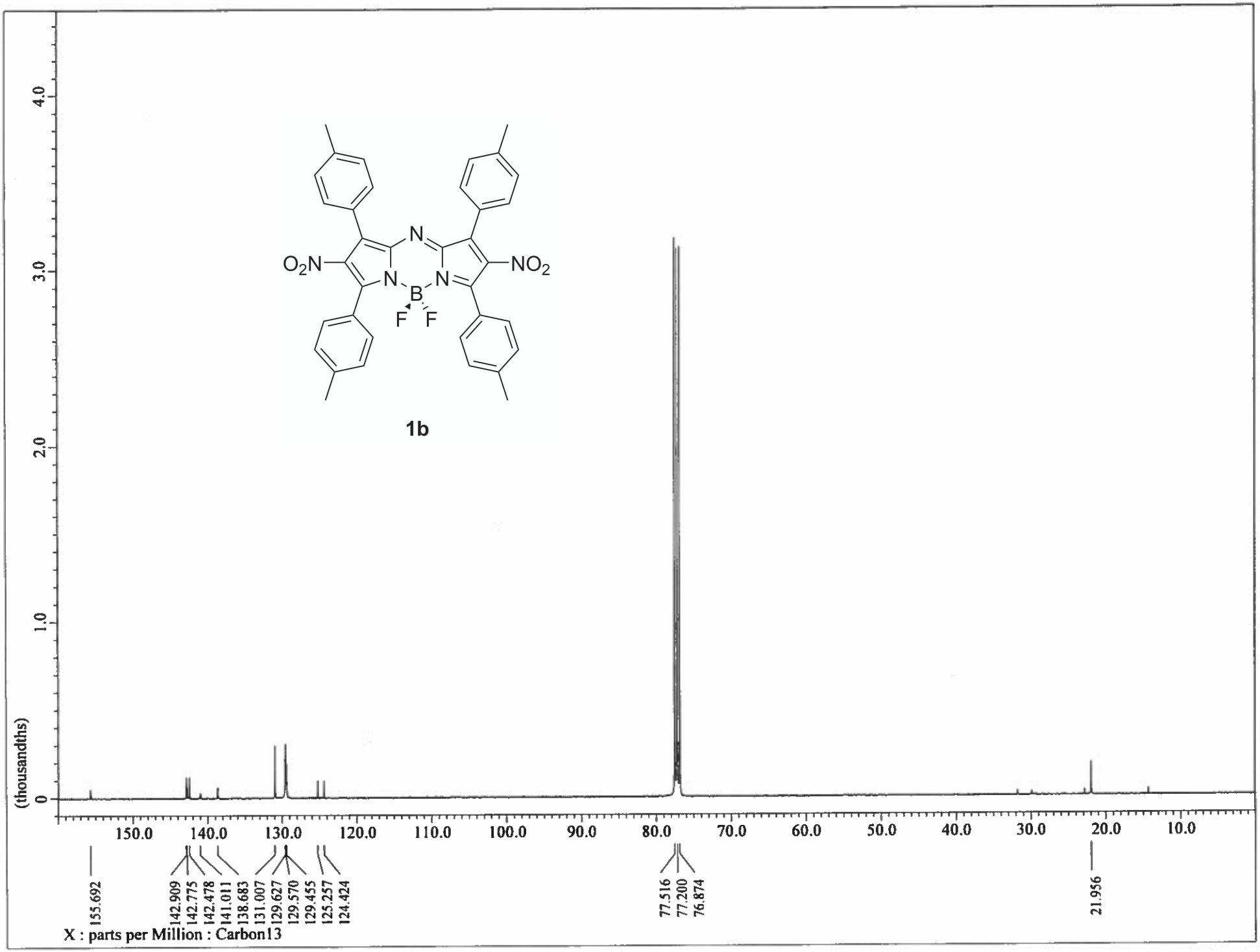

O2N
NO2
N
B
F
F
1a
(thousandths)
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18 0.19 0.2 0.21
170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
142.957
139.277
132.176
131.678
131.122
129.426
128.765
127.816
127.136
77.516
77.200
76.884
X : parts per Million : Carbon13

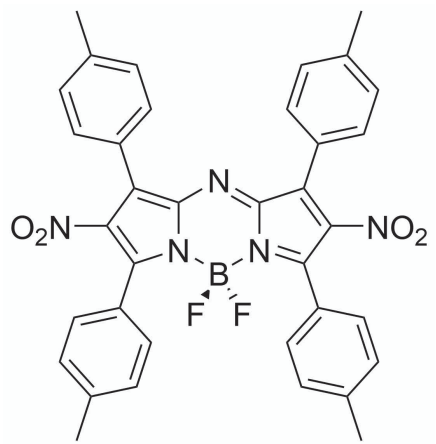

O2N
NO2
N
N
B
N
F
F
1a
abundance
-0.03
-0.01
0.01
0.03
0.05
0.07
0.09
0.11
0.13
0.15
0.17
0.19
0.21
0.23
0.25
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
-0.610
-0.763
-0.991
X : parts per Million : Boron11


30.0
20.0
10.0
0
(thousandths)
-110.0
-120.0
-130.0
-140.0
-130.254
-130.323
-130.400
-130.469
X : parts per Million : Fluorine19

1a


O2N
NO2
N
N
B
N
F
F
1b
8.00
8.01
8.04
8.04
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.616
7.595
7.570
7.290
7.270
2.468
2.417
X : parts per Million : Proton


O2N
NO2
N
N
B
N
F
F
1b
(thousandths)
4.0
3.0
2.0
1.0
0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
155.692
142.909
142.775
142.478
141.011
138.683
131.007
129.627
129.570
129.455
125.257
124.424
77.516
77.200
76.874
21.956
X : parts per Million : Carbon13



1b

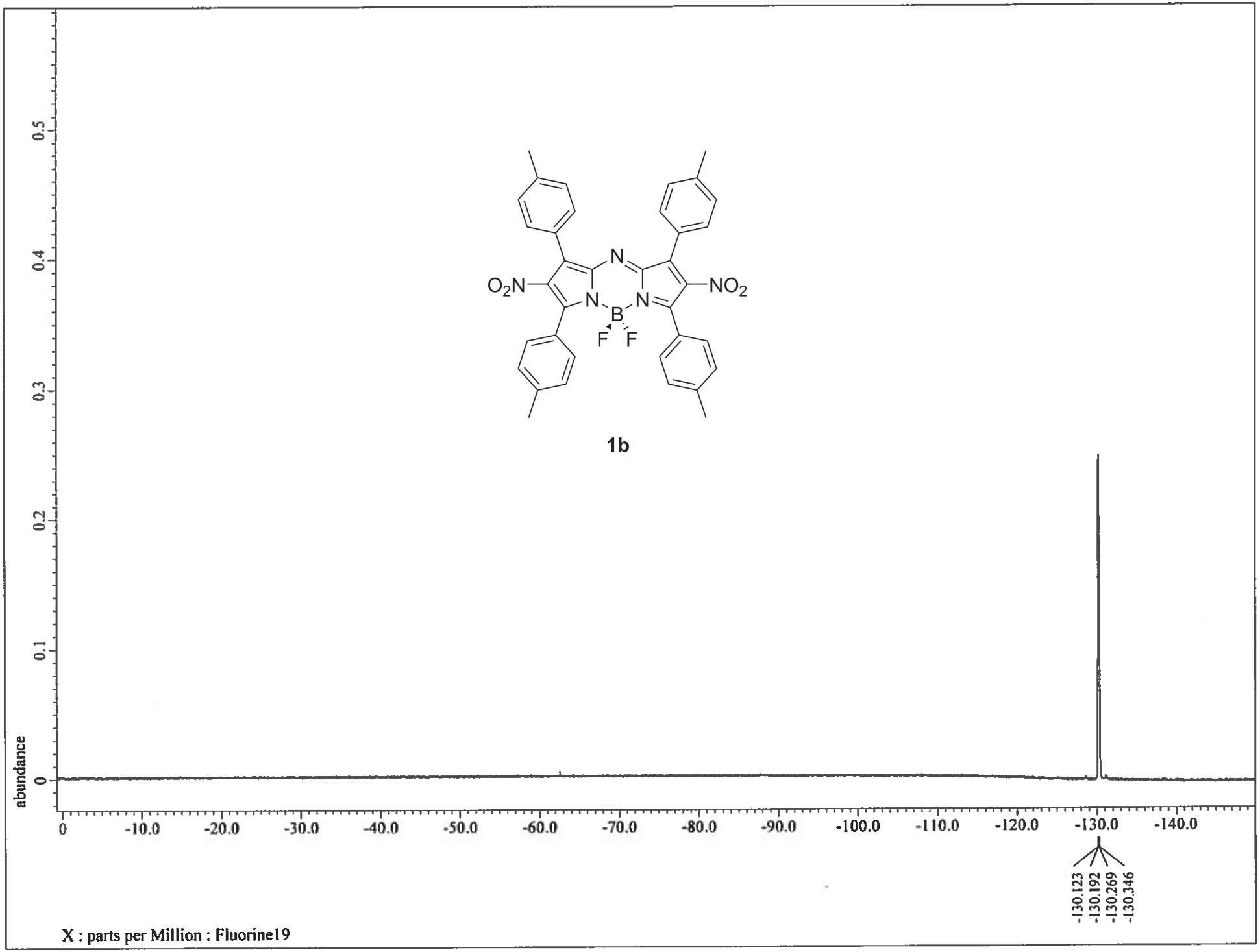
abundance

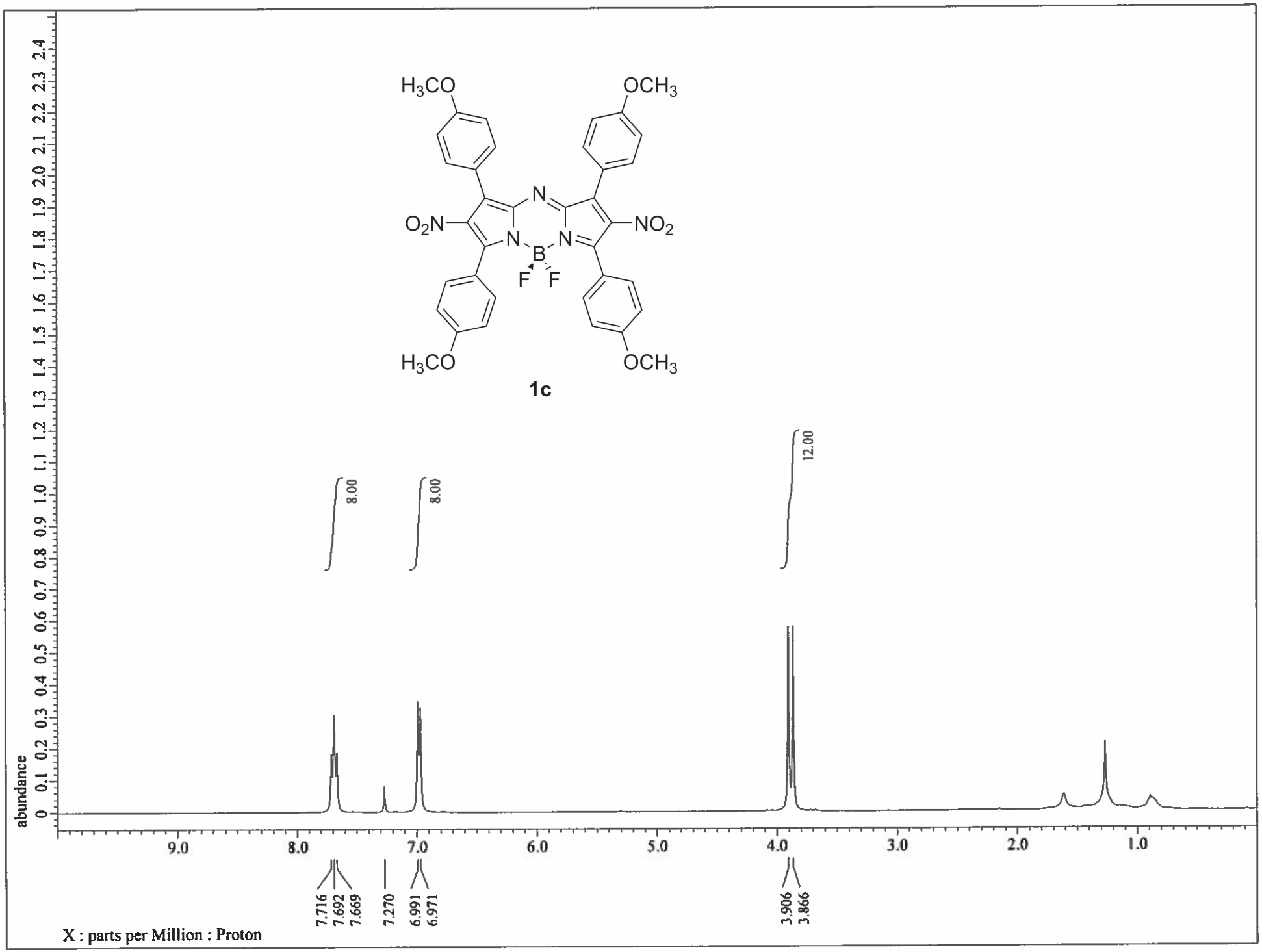
0.2 0.18 0.16 0.14 0.12 0.1 0.08 0.06 0.04 0.02 0 -0.02 -0.04

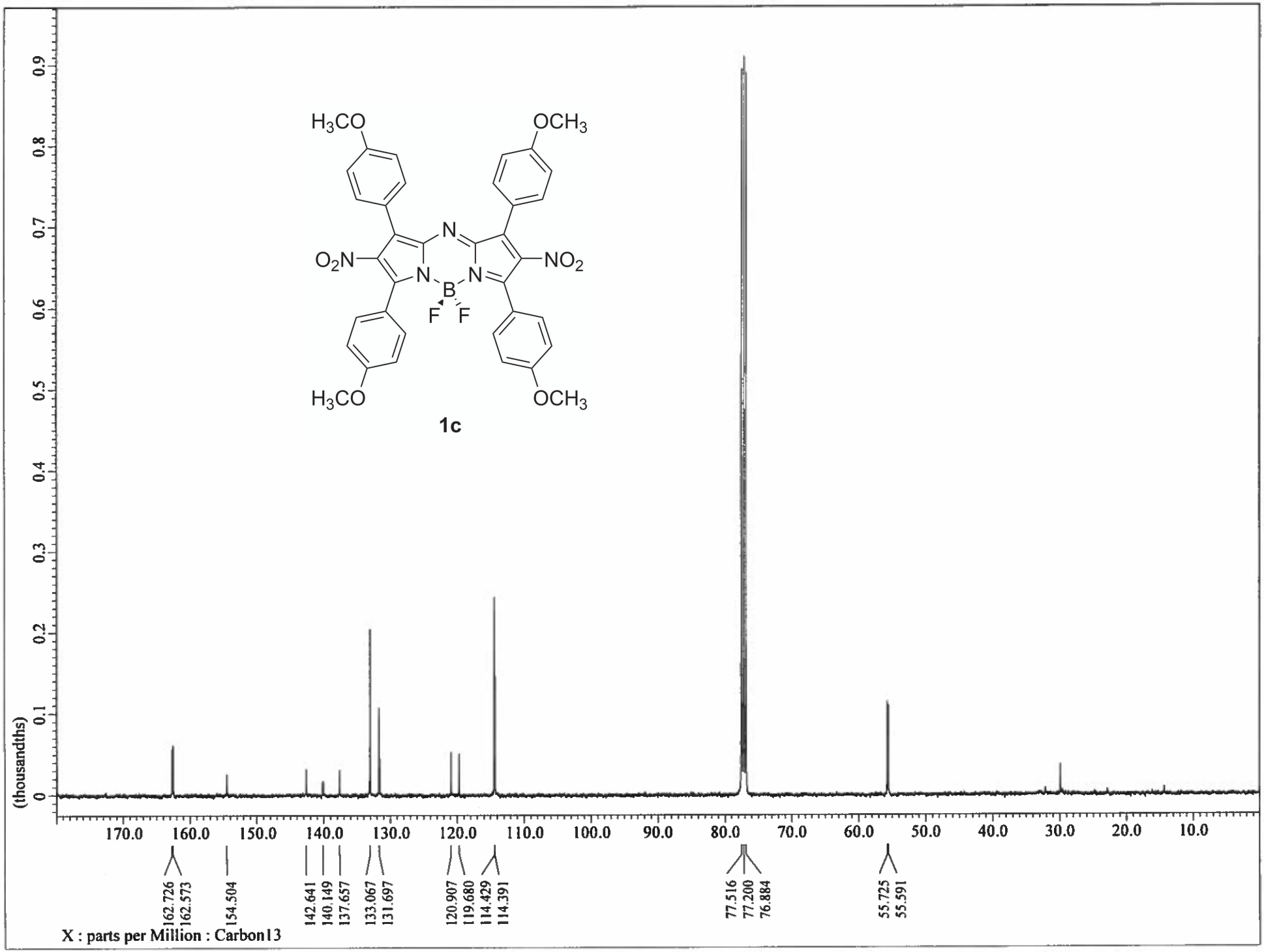
19.0 17.0 15.0 13.0 11.0 9.0 7.0 5.0 3.0 1.0 -1.0 -3.0 -5.0 -7.0 -9.0 -11.0 -13.0 -15.0 -17.0 -19.0

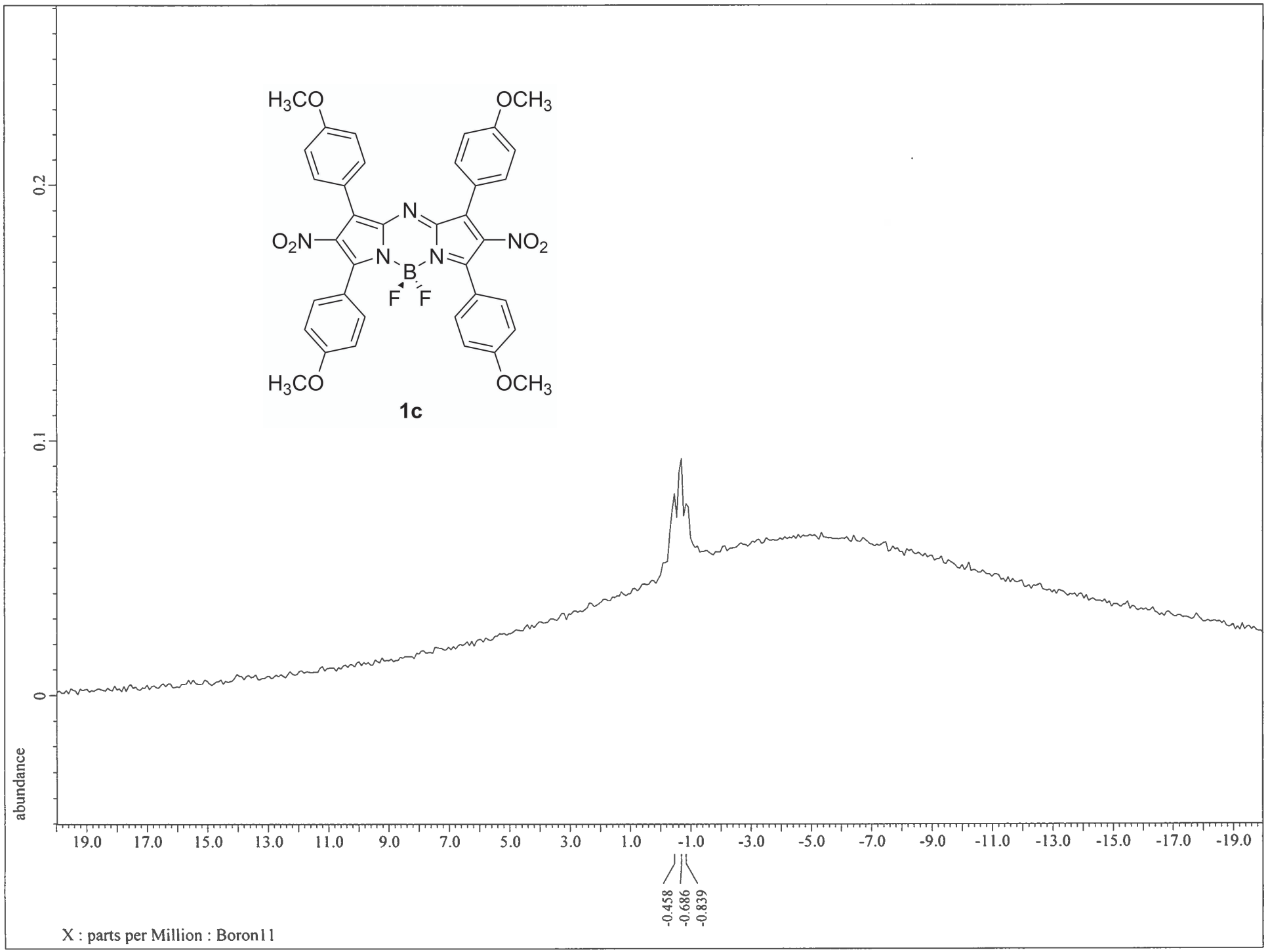
-0.534
-0.763
-0.991

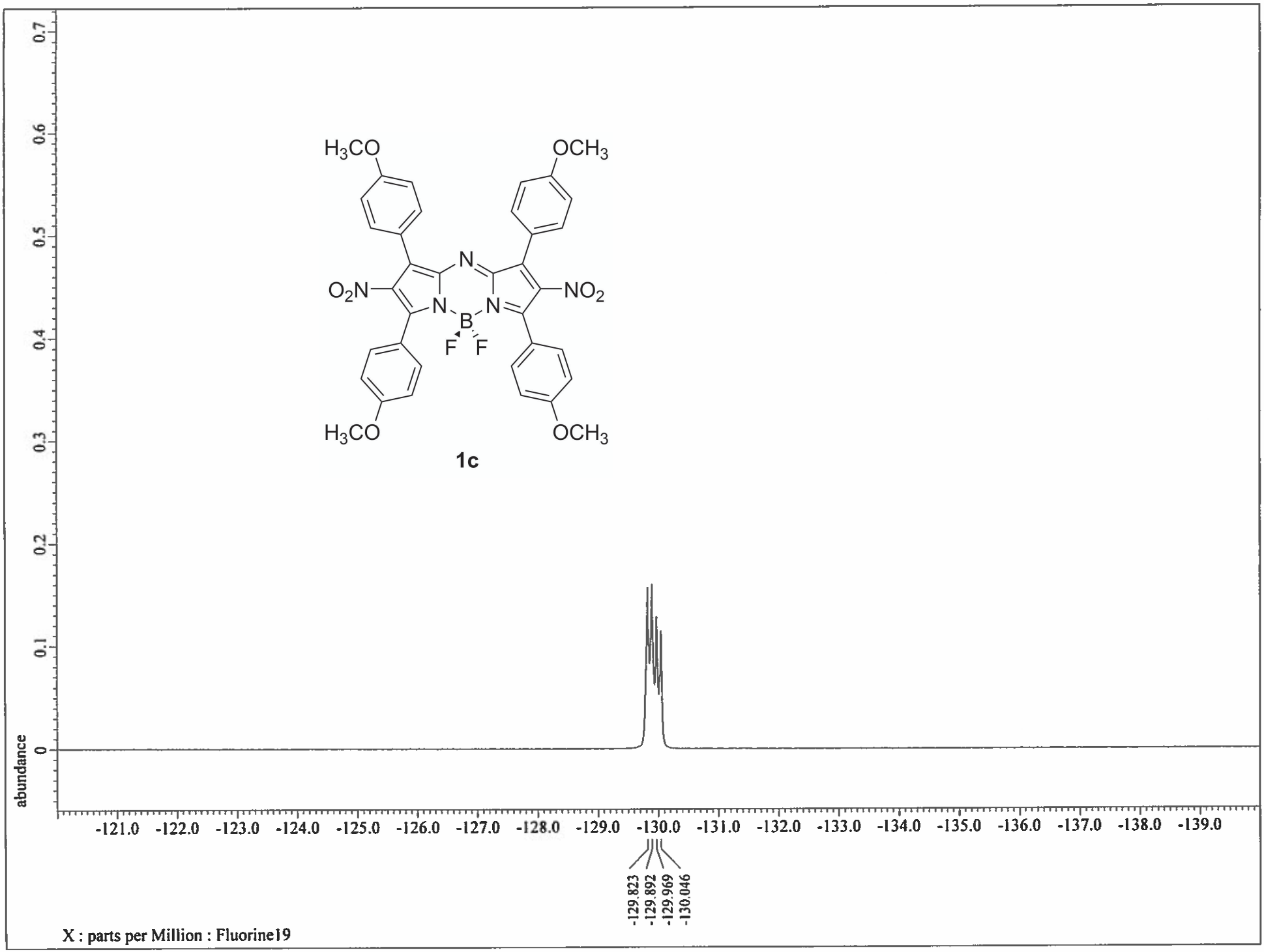
X : parts per Million : Boron11

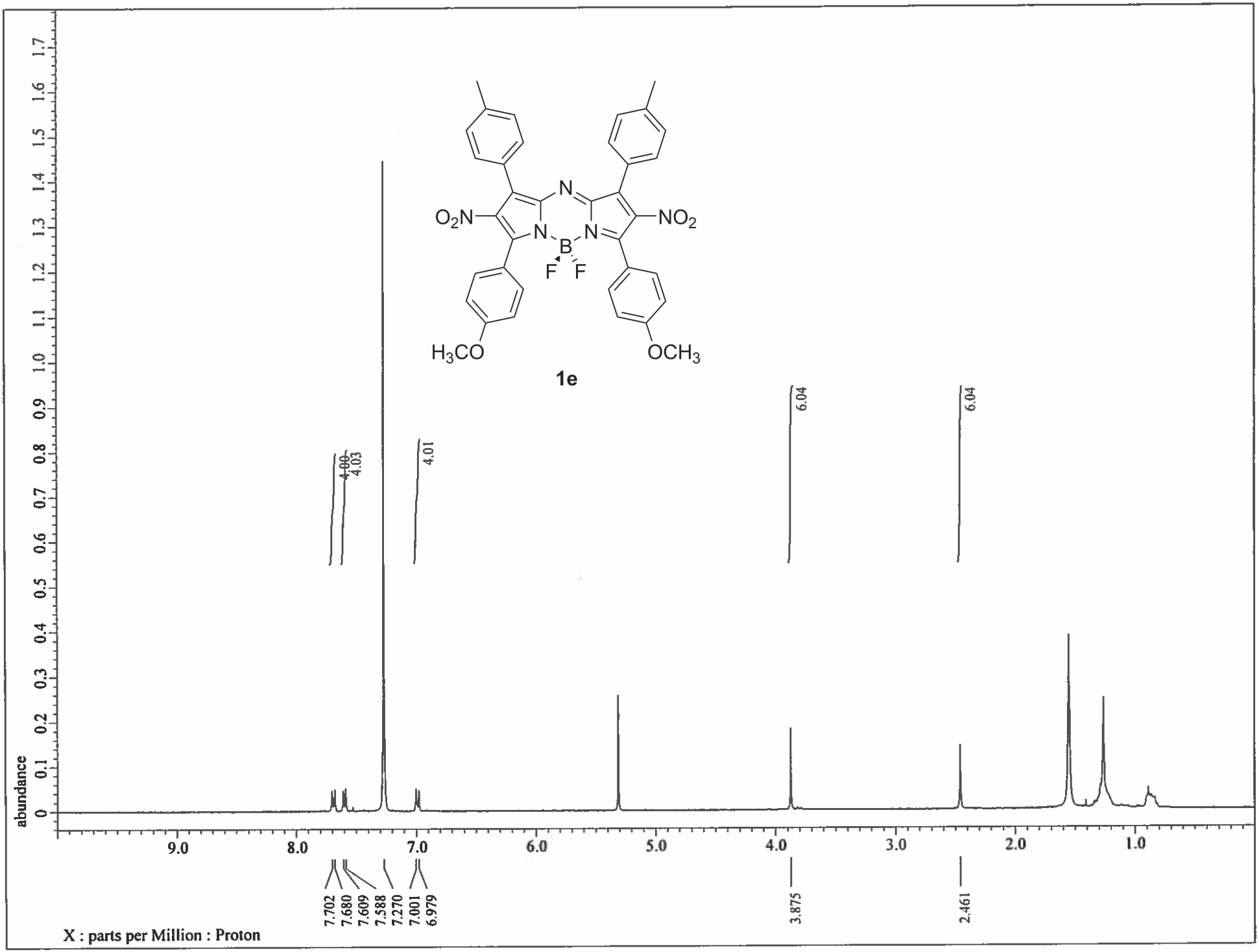

O2N
NO2
N
N
B
N
F
F
1b
abundance
0
0.1
0.2
0.3
0.4
0.5
0
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-130.123
-130.192
-130.269
-130.346
X : parts per Million : Fluorine19

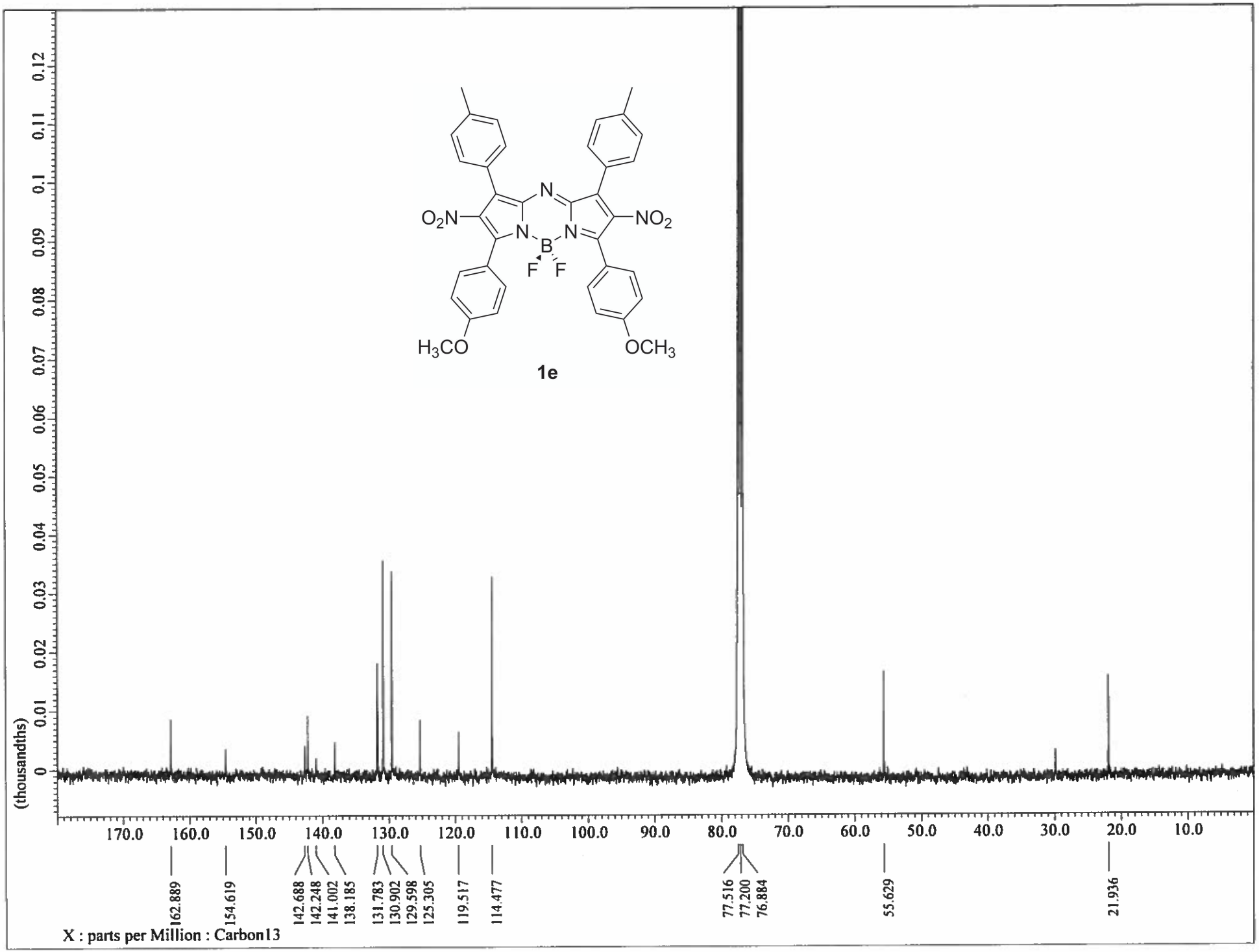

H3CO
OCH3
O2N
NO2
N
B
F
F
1c
8.00
8.00
12.00
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.716
7.692
7.669
7.270
6.991
6.971
3.906
3.866
X : parts per Million : Proton


H3CO
OCH3
O2N
NO2
N
B
F
F
H3CO
OCH3
1c
(thousandths)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
162.726
162.573
154.504
142.641
140.149
137.657
133.067
131.697
120.907
119.680
114.429
114.391
77.516
77.200
76.884
55.725
55.591
X : parts per Million : Carbon13


H3CO
OCH3
O2N
NO2
N
B
F
F
H3CO
OCH3
1c
0.2
0.1
0
abundance
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
-0.458
-0.686
-0.839
X : parts per Million : Boron11

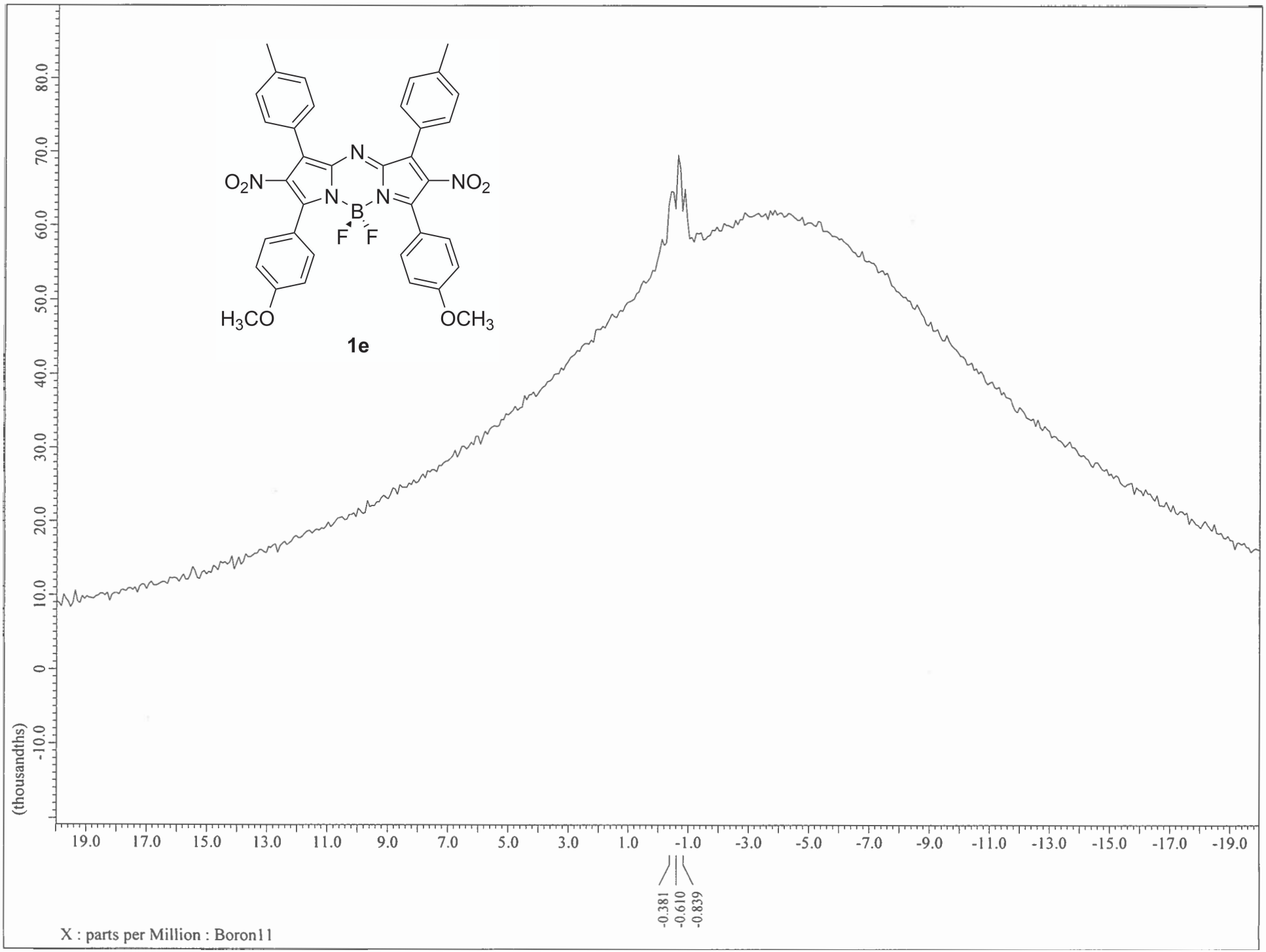

H3CO
OCH3
O2N
NO2
N
N
B
N
F
F
H3CO
OCH3
1c
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
-121.0
-122.0
-123.0
-124.0
-125.0
-126.0
-127.0
-128.0
-129.0
-130.0
-131.0
-132.0
-133.0
-134.0
-135.0
-136.0
-137.0
-138.0
-139.0
-129.823
-129.892
-129.969
-130.046
X : parts per Million : Fluorine19

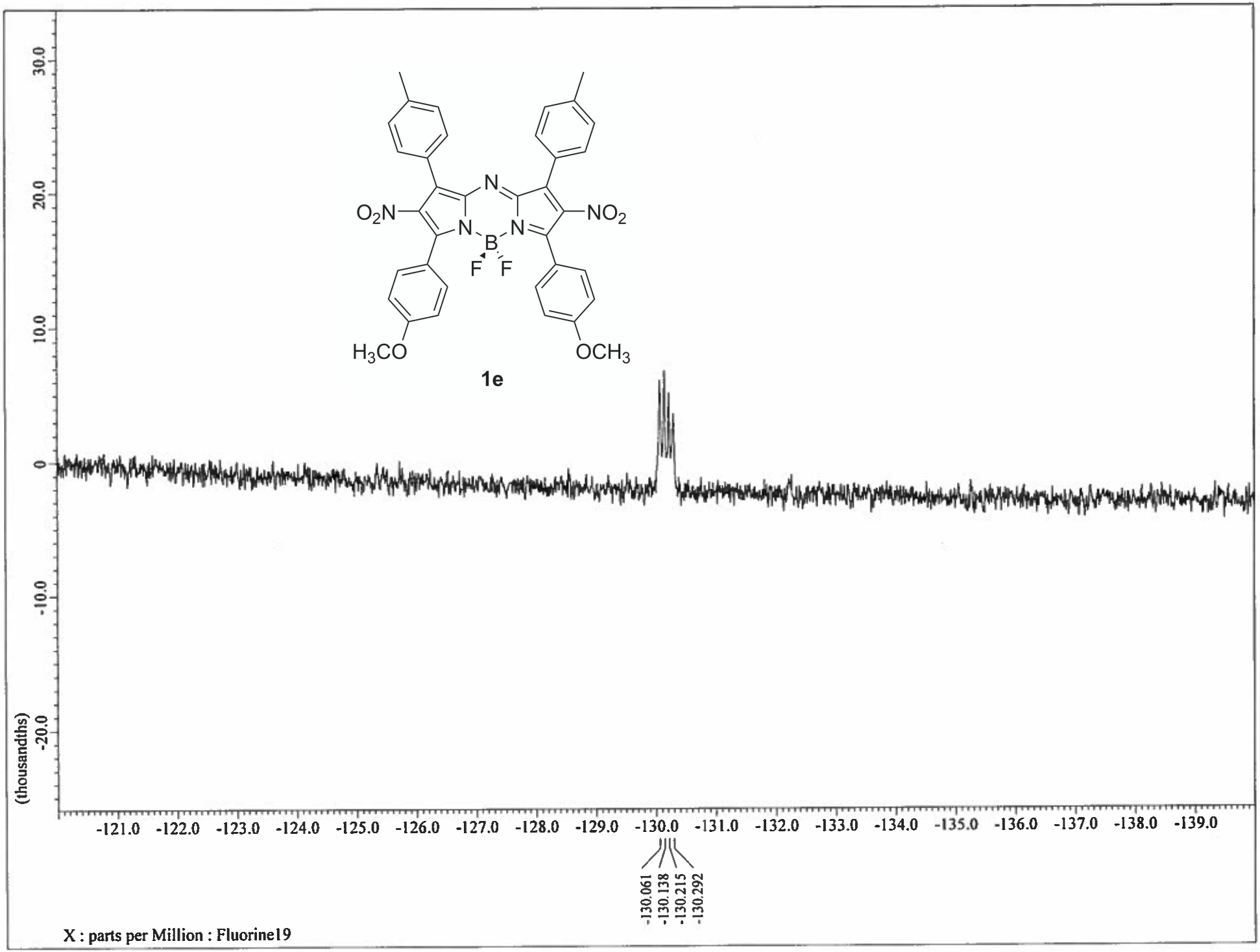

O2N
NO2
N
B
F
F
H3CO
OCH3
1e
abundance
X : parts per Million : Proton
7.702
7.680
7.609
7.588
7.270
7.001
6.979
4.03
4.00
4.01
6.04
6.04
3.875
2.461


(thousandths)
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
162.889
154.619
142.688
142.248
141.002
138.185
131.783
130.902
129.598
125.305
119.517
114.477
77.516
77.200
76.884
55.629
21.936
X : parts per Million : Carbon13

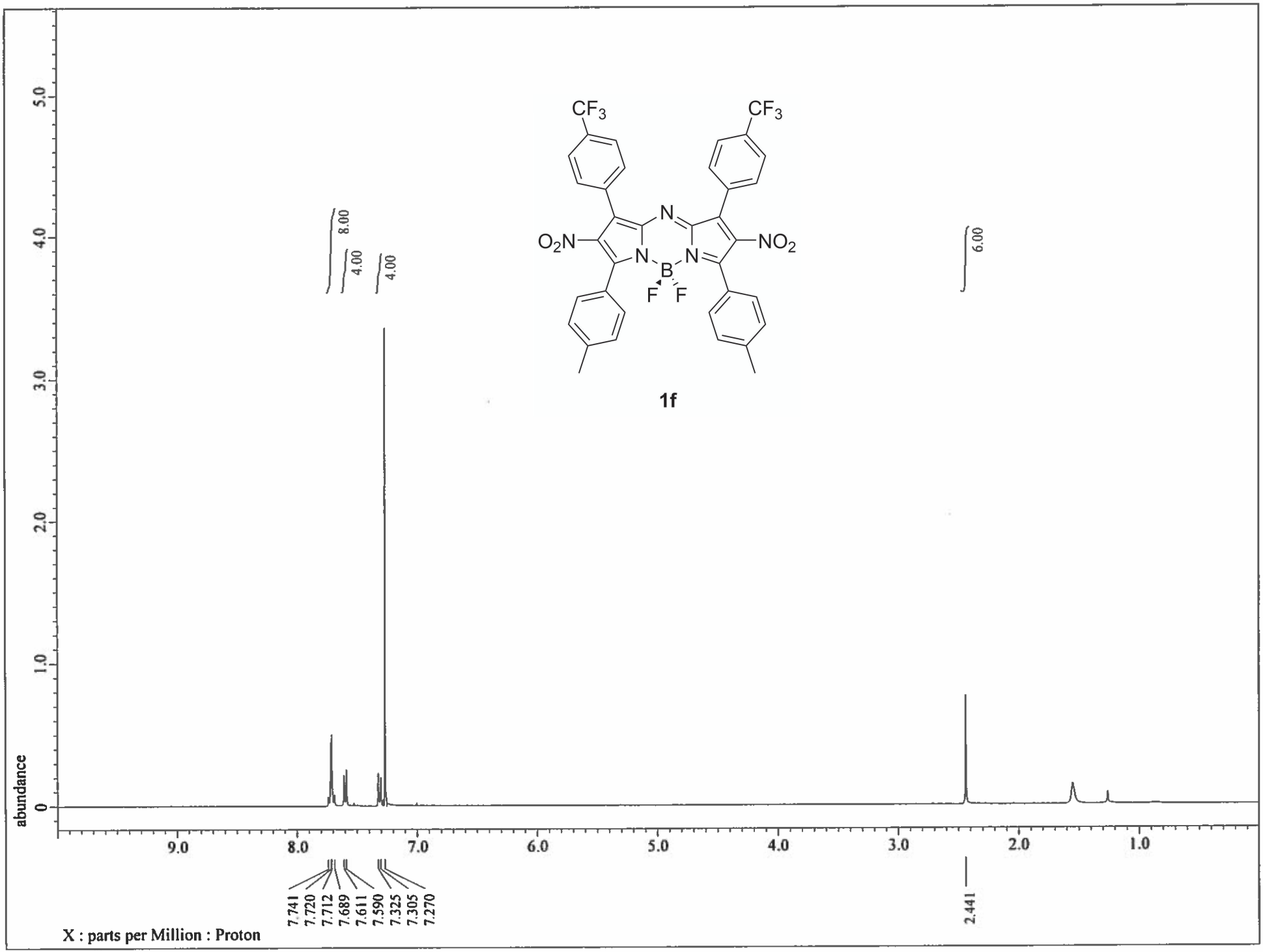
O2N
NO2
N
N
B
N
F
F
H3CO
OCH3

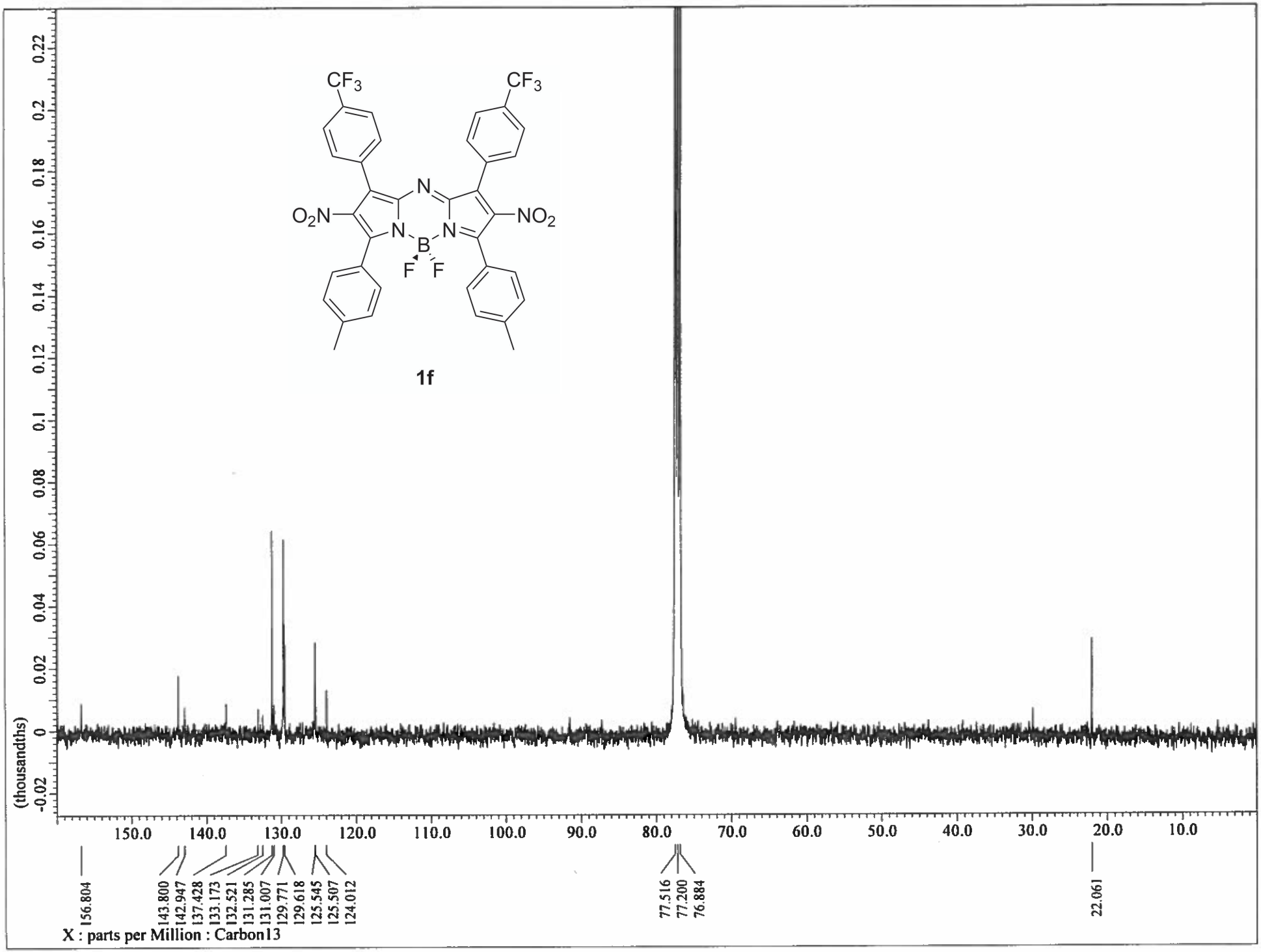
1e

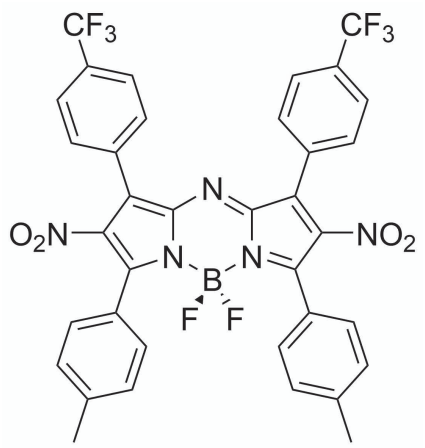

O2N
NO2
N
N
B
N
F
F
H3CO
OCH3
1e
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
(thousandths)
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
-0.381
-0.610
-0.839
X : parts per Million : Boron11


30.0
20.0
10.0
0
-10.0
-20.0
(thousandths)
-121.0 -122.0 -123.0 -124.0 -125.0 -126.0 -127.0 -128.0 -129.0 -130.0 -131.0 -132.0 -133.0 -134.0 -135.0 -136.0 -137.0 -138.0 -139.0
-130.061
-130.138
-130.215
-130.292
X : parts per Million : Fluorine19

1e

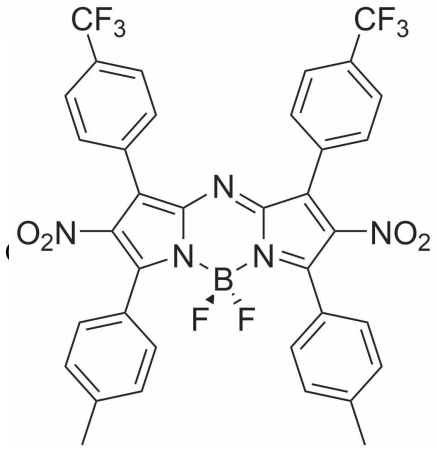

CF3
CF3
O2N
NO2
N
N
N
B
F
F
1f
8.00
4.00
4.00
6.00
abundance
0
1.0
2.0
3.0
4.0
5.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.741
7.720
7.712
7.689
7.611
7.590
7.325
7.305
7.270
2.441
X : parts per Million : Proton


CF3
CF3
O2N
NO2
N
N
B
N
F
F
1f
(thousandths)
0.22
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
-0.02
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
156.804
143.800
142.947
137.428
133.173
132.521
131.285
131.007
129.771
129.618
125.545
125.507
124.012
77.516
77.200
76.884
22.061
X : parts per Million : Carbon13


CF3
CF3
O2N
NO2
N
N
B
N
F
F

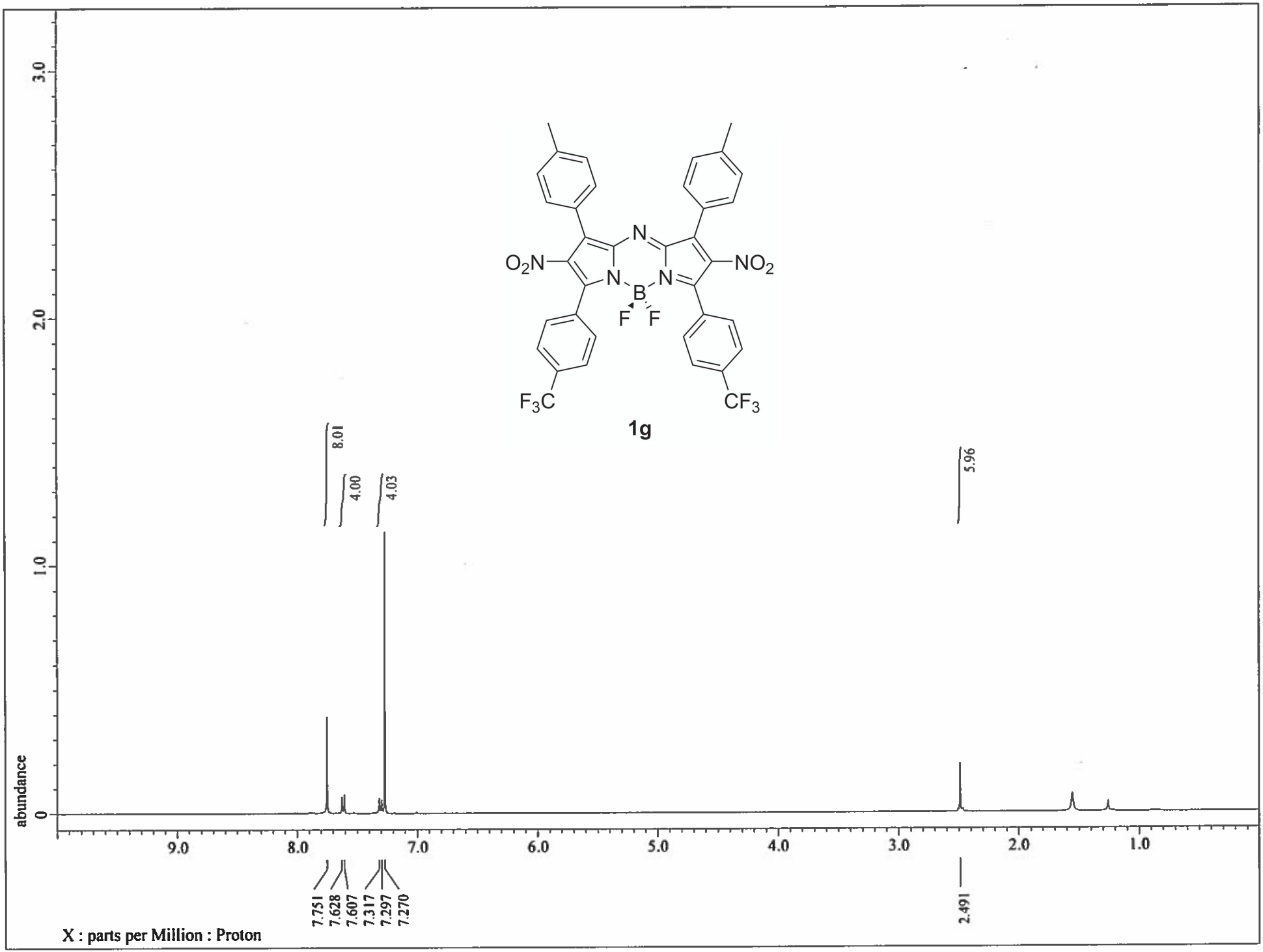
1f

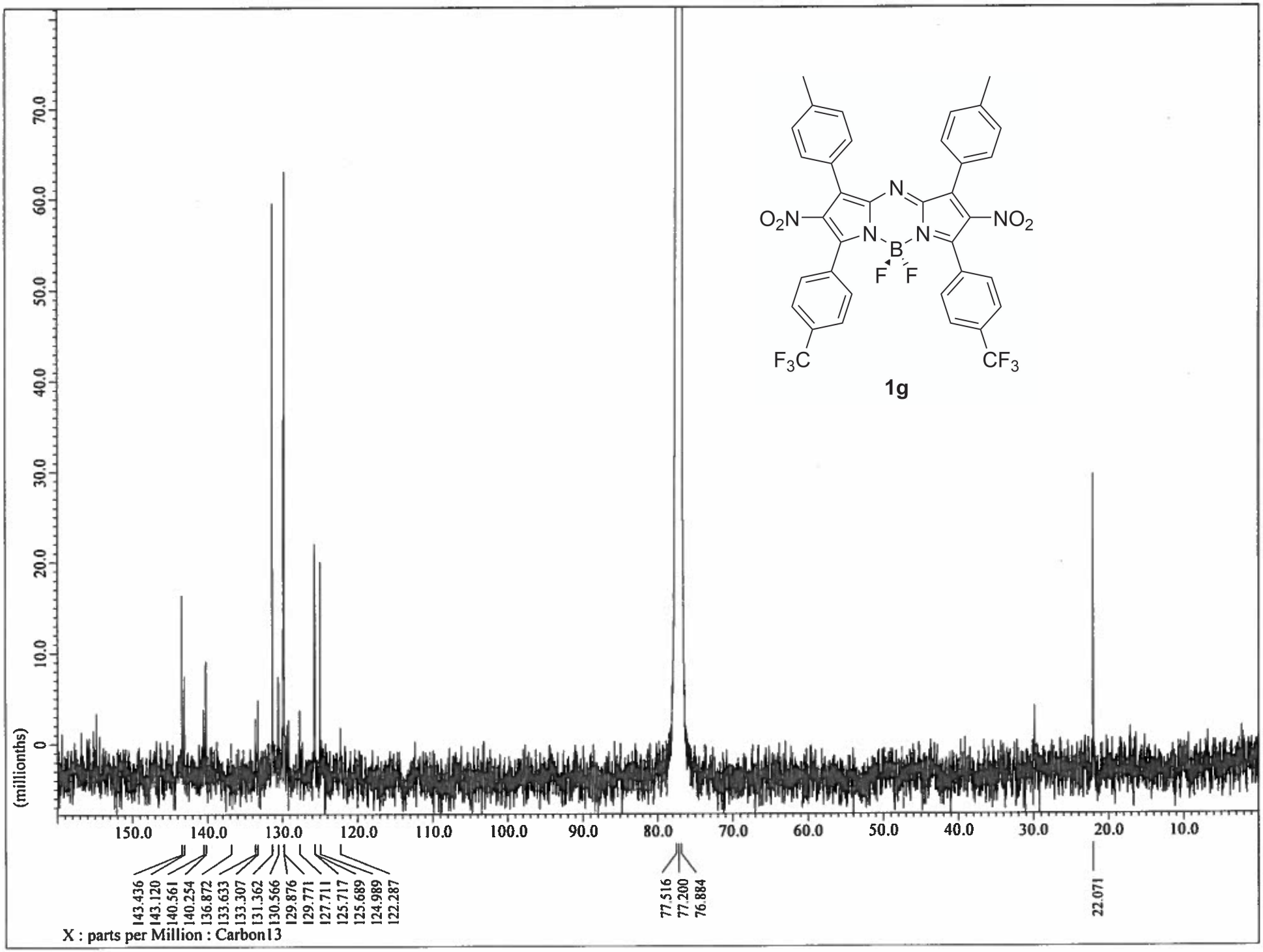
abundance
0.4
0.3
0.2
0.1
0
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
-0.534
-0.763
-0.915
X : parts per Million : Boron11


CF3
CF3
O2N
NO2
N
N
B
N
F
F

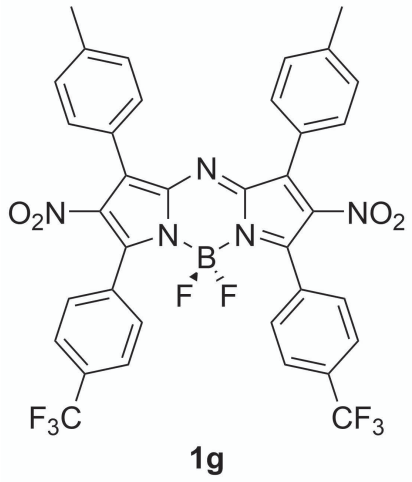
1f

6.00
2.04
abundance
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-63.063
-130.092
-130.161
-130.238
-130.307
X : parts per Million : Fluorine19


O2N
NO2
N
N
B
N
F
F
F3C
CF3
1g
8.01
4.00
4.03
5.96
abundance
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.751
7.628
7.607
7.317
7.297
7.270
2.491
X : parts per Million : Proton

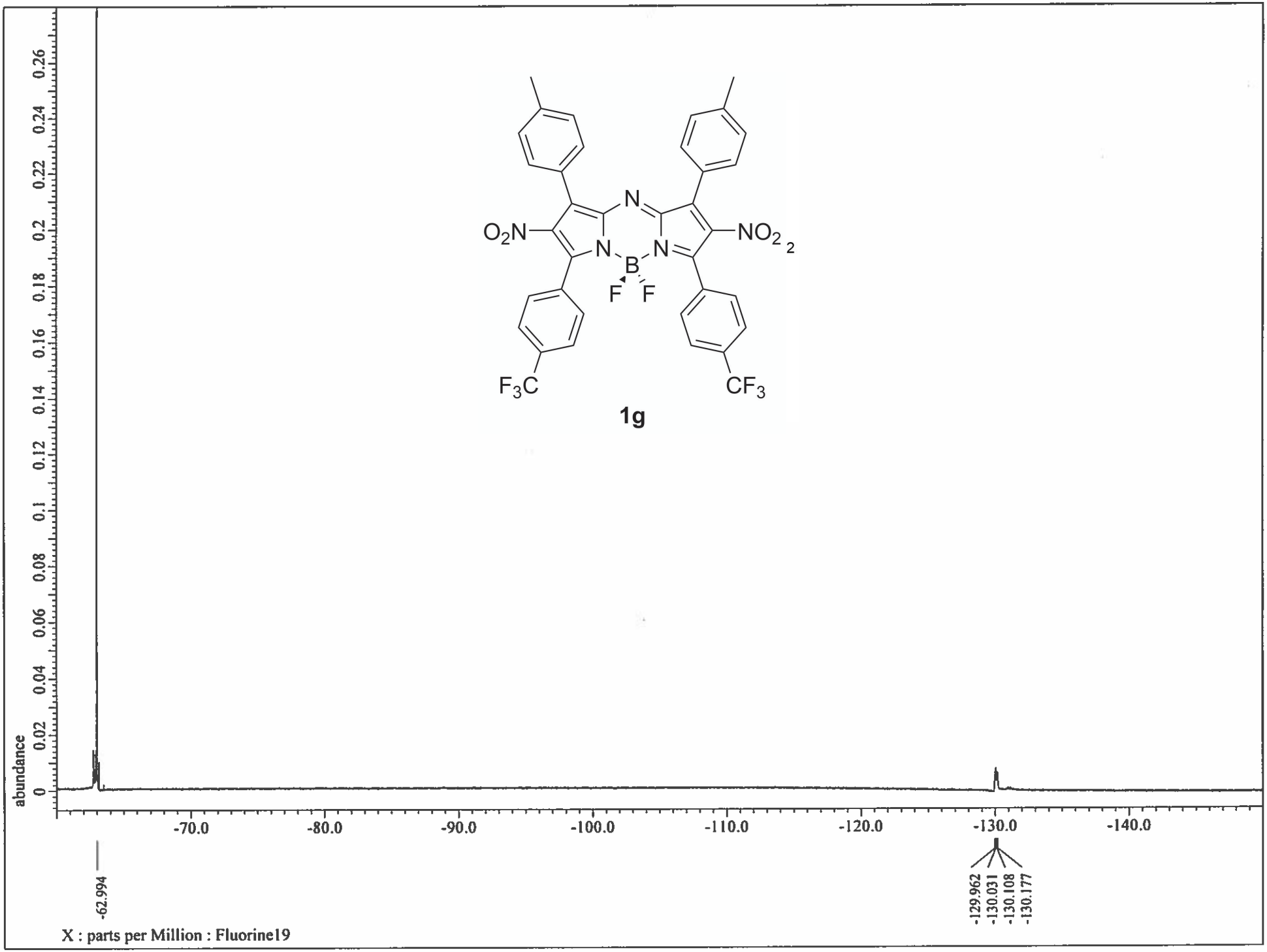

(millionths)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
143.436
143.120
140.561
140.254
136.872
133.633
133.307
131.362
130.566
129.876
129.771
127.711
125.717
125.689
124.989
122.287
77.516
77.200
76.884
22.071
X : parts per Million : Carbon13
O2N
NO2
N
N
B
N
F
F
F3C
CF3

1g


O2N
NO2
N
N
B
N
F
F
F3C
CF3

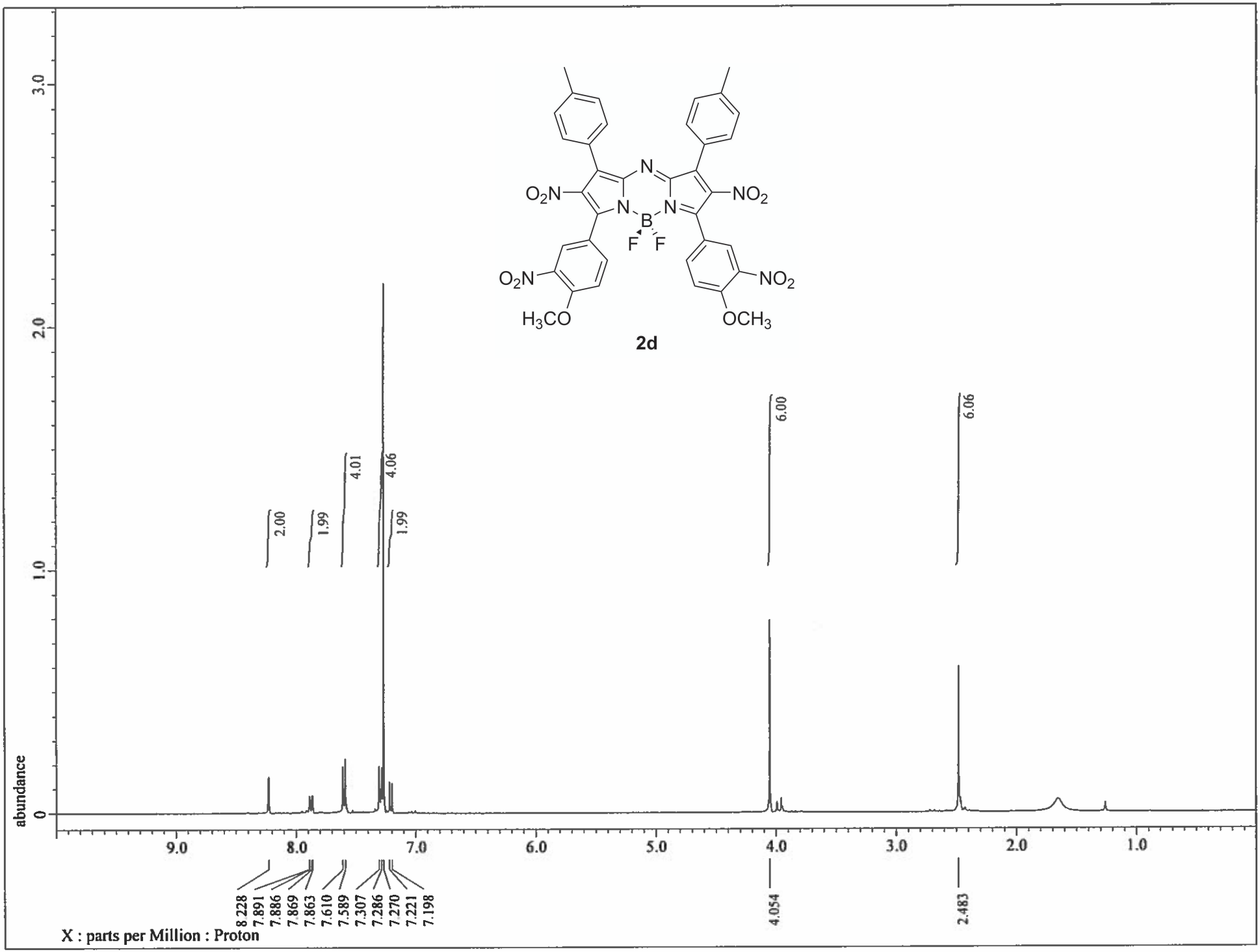
1g

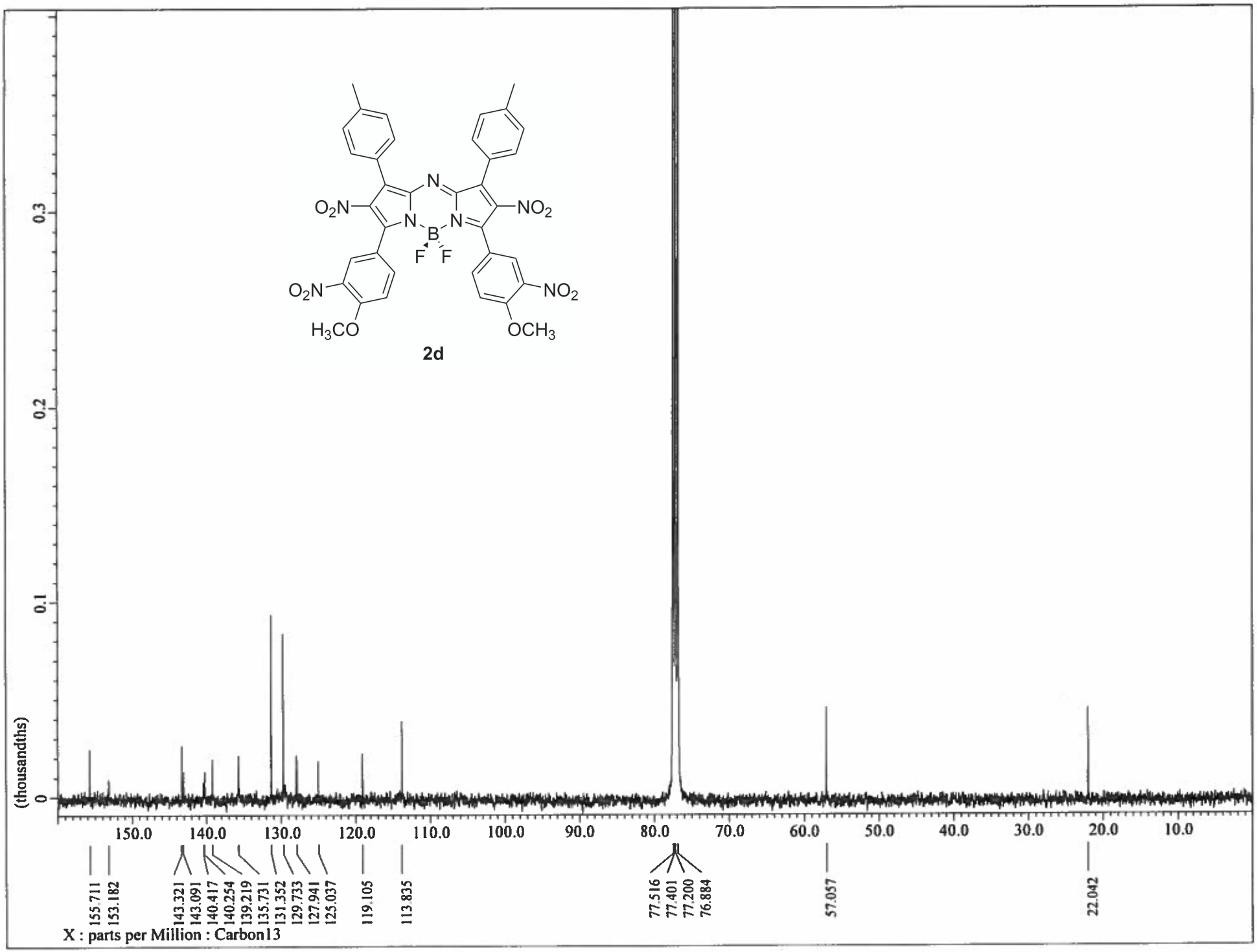
abundance
0.5
0.4
0.3
0.2
0.1
0
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
-0.381
-0.610
-0.839
X : parts per Million : Boron11

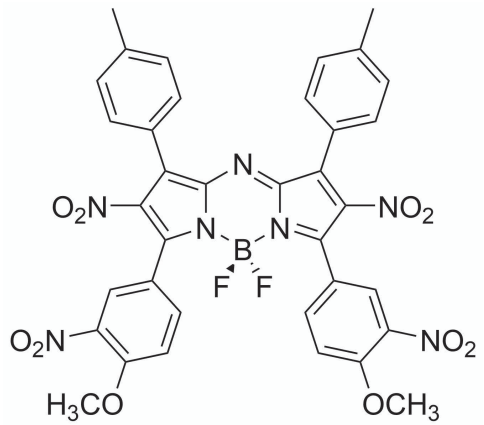

abundance
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-62.994
-129.962
-130.031
-130.108
-130.177
X : parts per Million : Fluorine19

O2N
NO2
N
N
B
N
F
F
F3C
CF3

1g


O2N
NO2
N
N
B
N
F
F
O2N
NO2
H3CO
OCH3
2d
abundance
X : parts per Million : Proton
2.00
1.99
4.01
4.06
1.99
6.00
6.06
8.228
7.891
7.886
7.869
7.863
7.610
7.589
7.307
7.286
7.270
7.221
7.198
4.054
2.483


O2N
NO2
N
B
N
N
F
F
O2N
NO2
H3CO
OCH3
2d
(thousandths)
0
0.1
0.2
0.3
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
155.711
153.182
143.321
143.091
140.417
140.254
139.219
135.731
131.352
129.733
127.941
125.037
119.105
113.835
77.516
77.401
77.200
76.884
57.057
22.042
X : parts per Million : Carbon13



2d

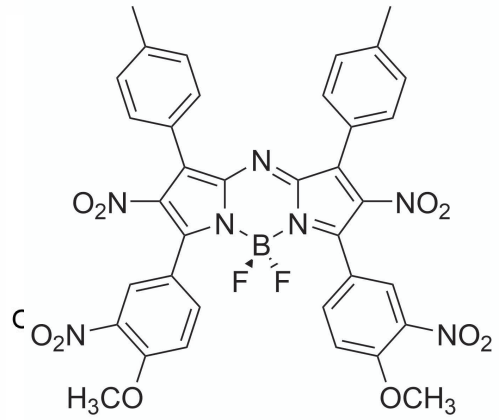
abundance

-0.04 -0.03 -0.02 -0.01 0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17

19.0 17.0 15.0 13.0 11.0 9.0 7.0 5.0 3.0 1.0 -1.0 -3.0 -5.0 -7.0 -9.0 -11.0 -13.0 -15.0 -17.0 -19.0

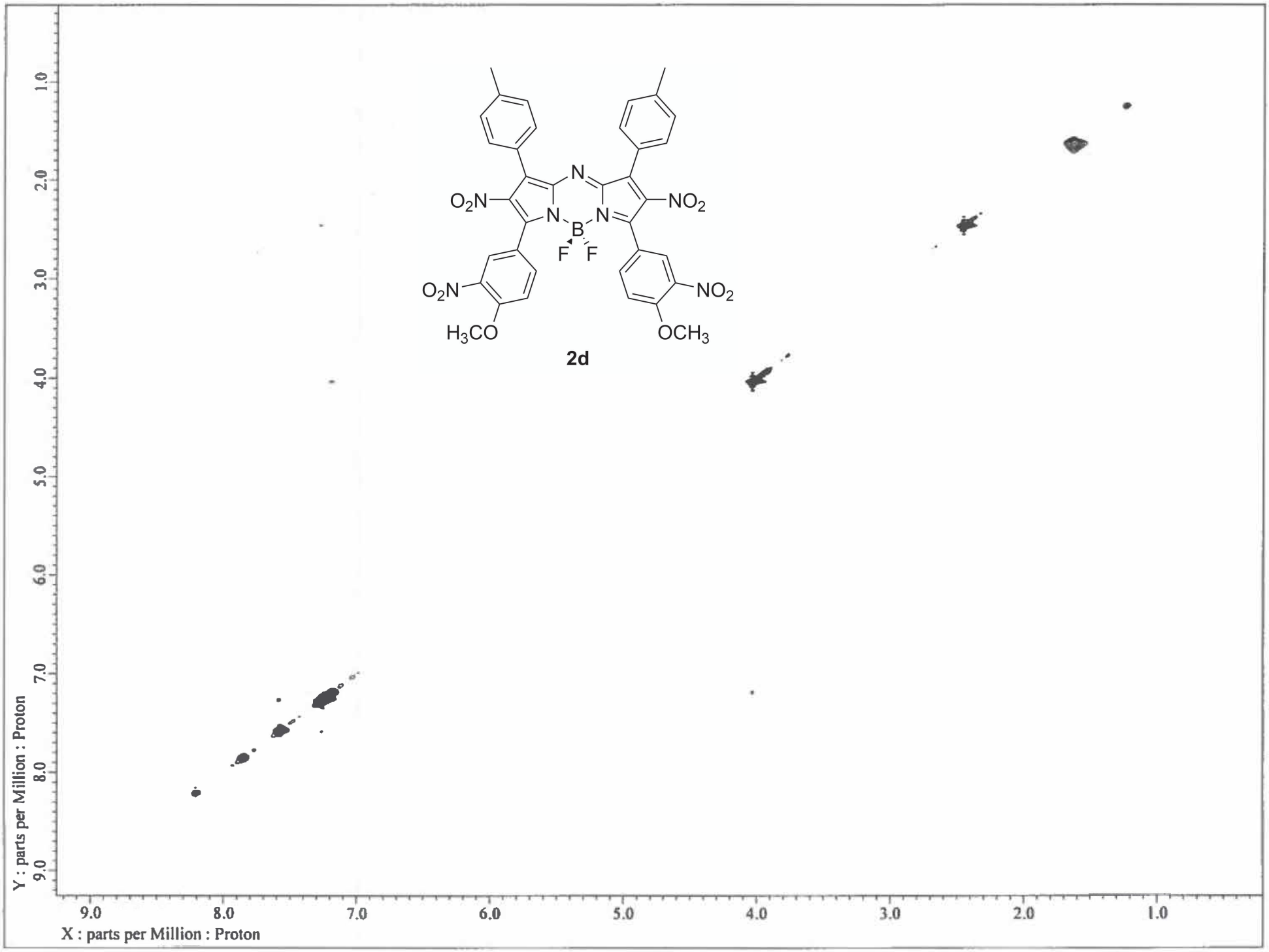
-0.686
-0.915
-1.144

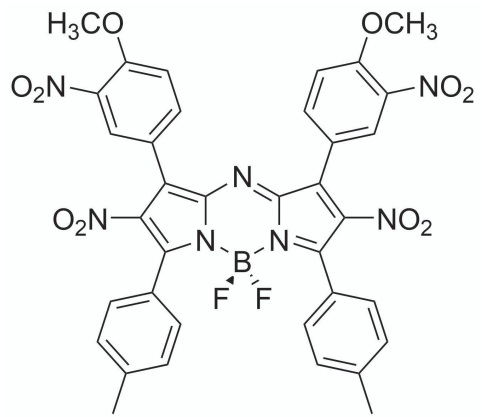
X : parts per Million : Boron11



2d

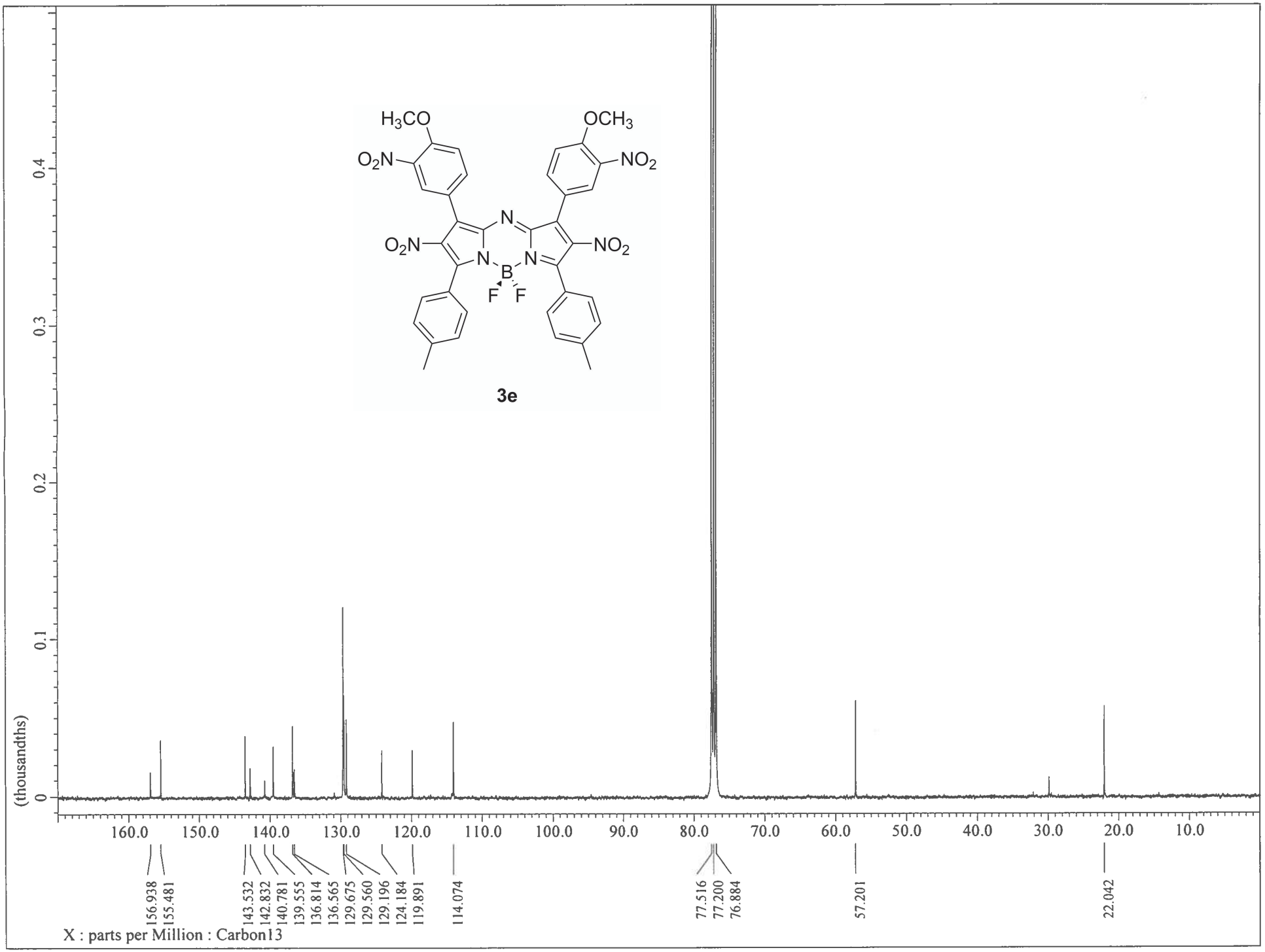
abundance
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
-0.02
0
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-129.539
-129.608
-129.693
-129.762
X : parts per Million : Fluorine19

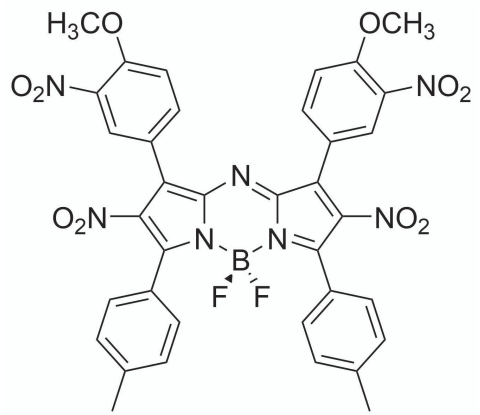

O2N
NO2
N
N
B
F
F
O2N
NO2
H3CO
OCH3
2d
Y : parts per Million : Proton
X : parts per Million : Proton
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0


H3CO
OCH3
O2N
NO2
O2N
NO2
N
N
N
B
F
F

3e

abundance
X : parts per Million : Proton
2.00
2.00
4.00
3.99
2.00
6.00
6.00
8.291
8.285
7.898
7.892
7.875
7.870
7.583
7.562
7.312
7.292
7.270
7.243
7.221
4.095
2.432


H3CO
OCH3
O2N
NO2
O2N
NO2
N
N
B
N
F
F
3e
(thousandths)
0
0.1
0.2
0.3
0.4
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
156.938
155.481
143.532
142.832
140.781
139.555
136.814
136.565
129.675
129.560
129.196
124.184
119.891
114.074
77.516
77.200
76.884
57.201
22.042
X : parts per Million : Carbon13



3e

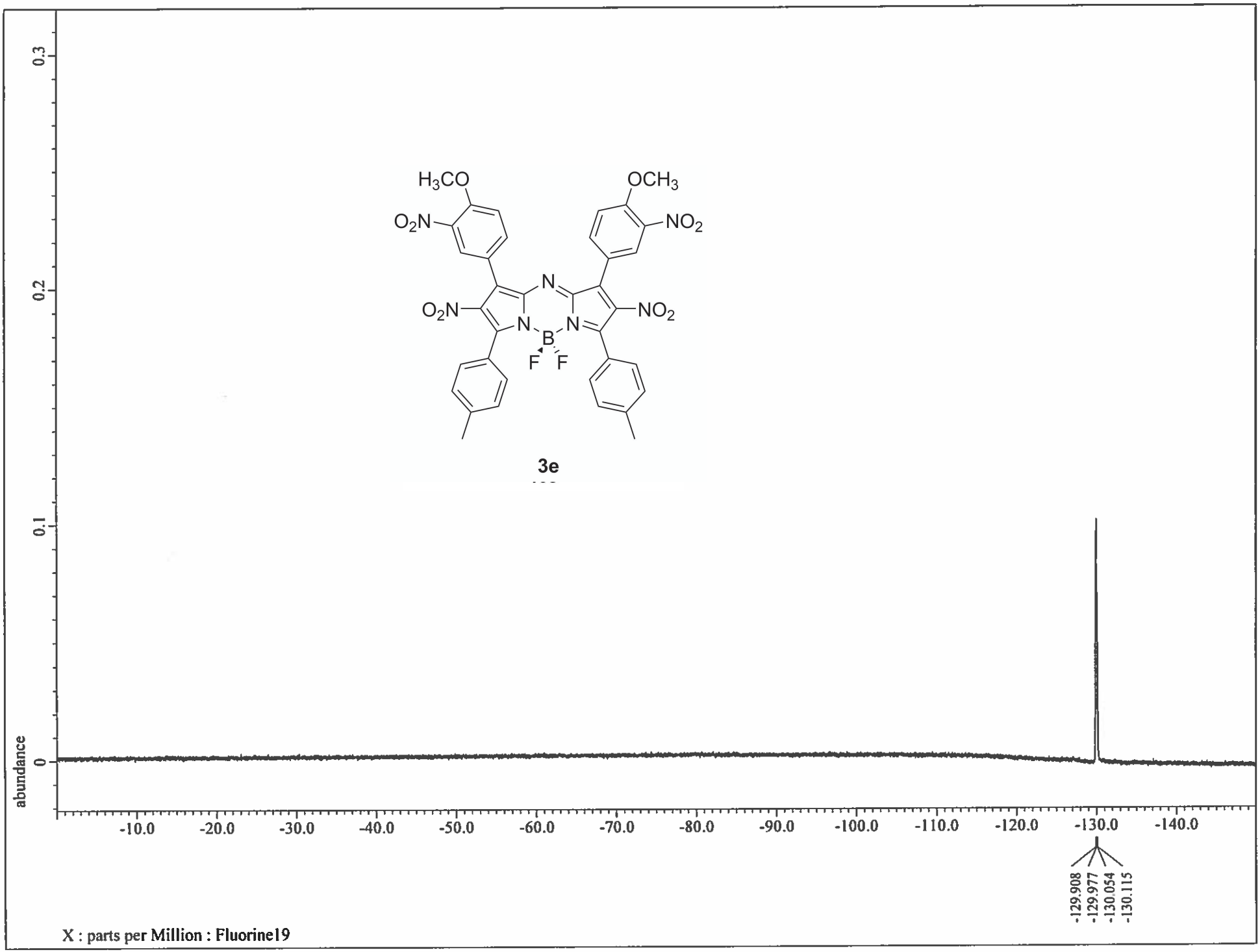
abundance

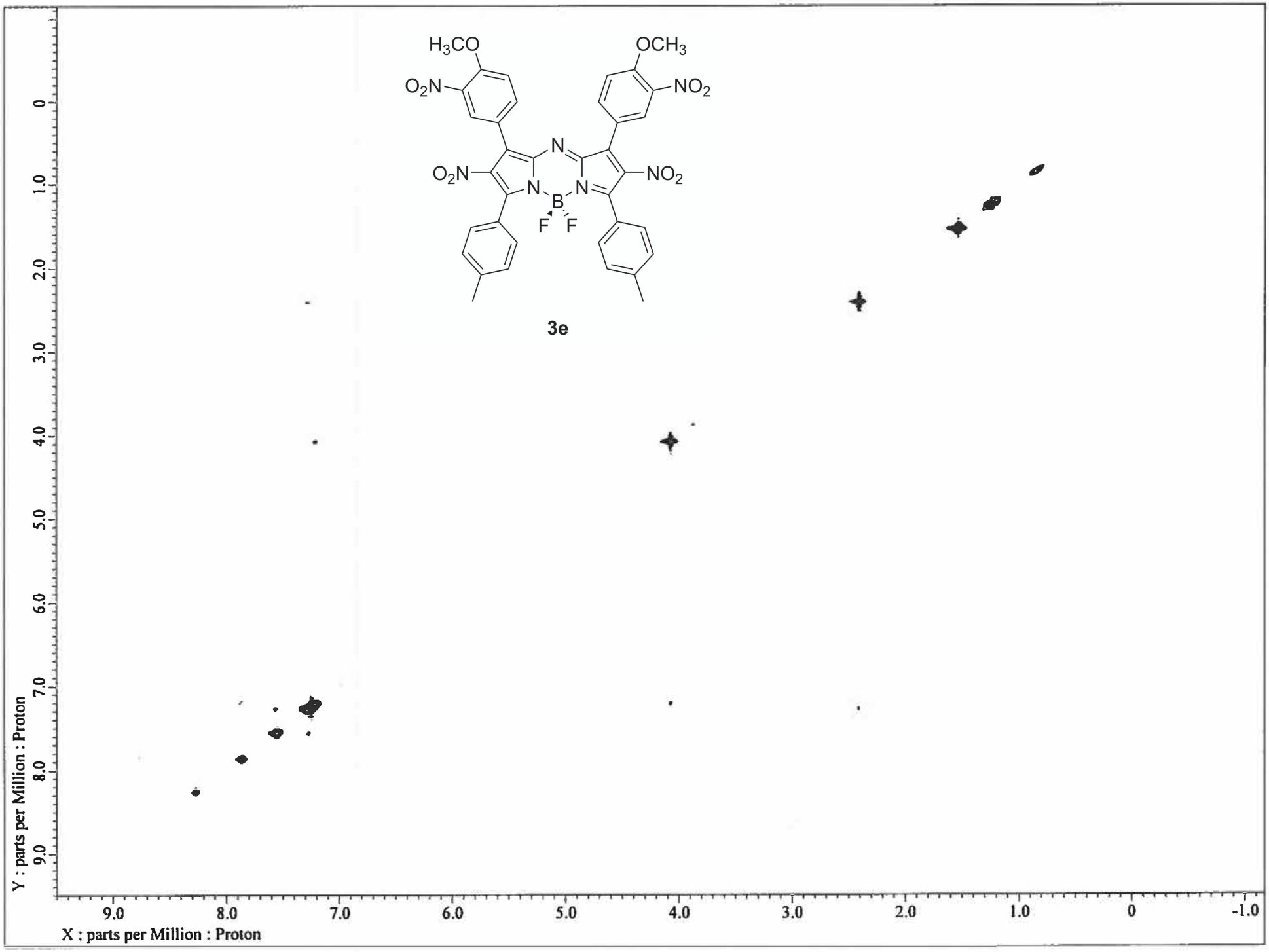
-0.03 -0.02 -0.01 0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16

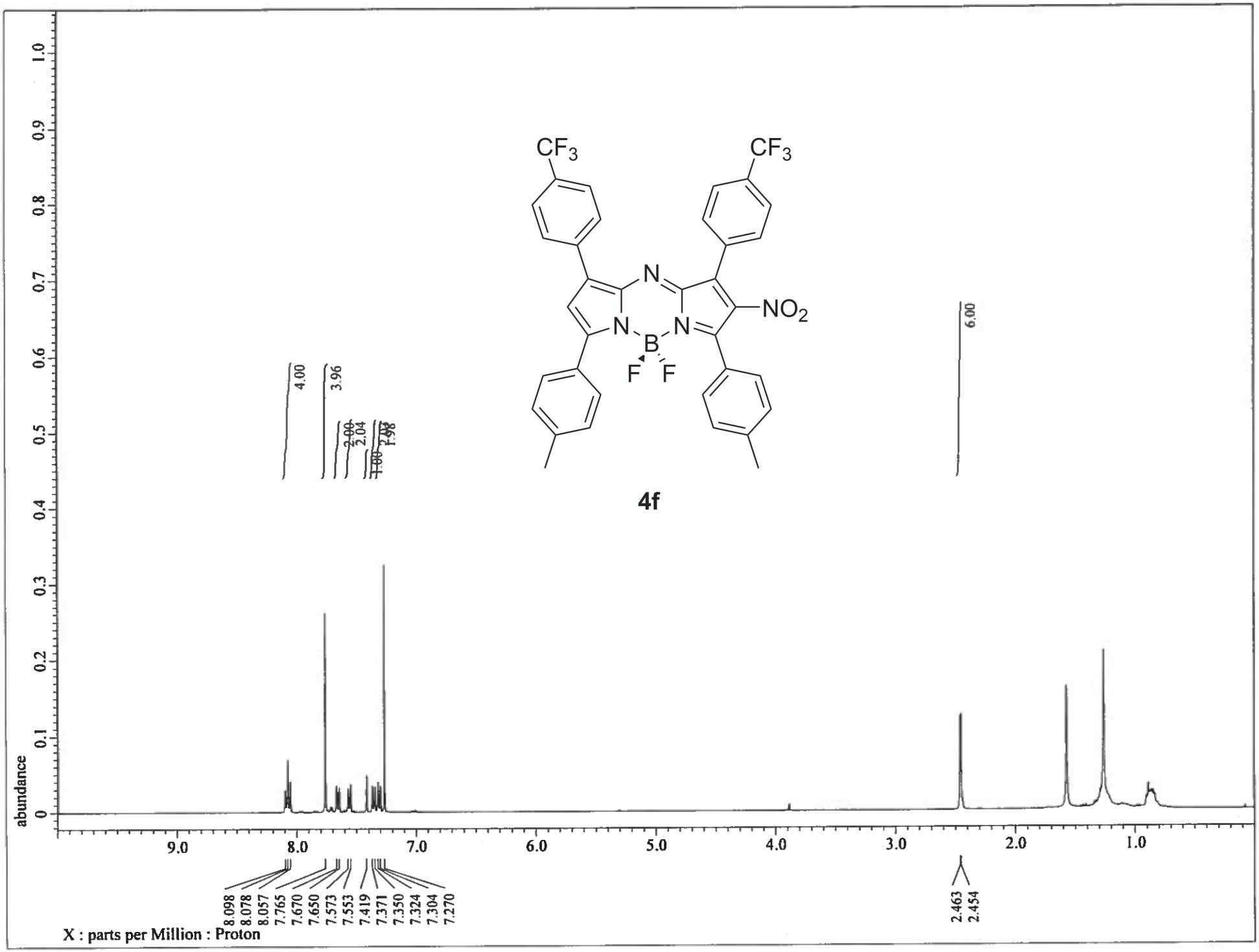
19.0 17.0 15.0 13.0 11.0 9.0 7.0 5.0 3.0 1.0 -1.0 -3.0 -5.0 -7.0 -9.0 -11.0 -13.0 -15.0 -17.0 -19.0

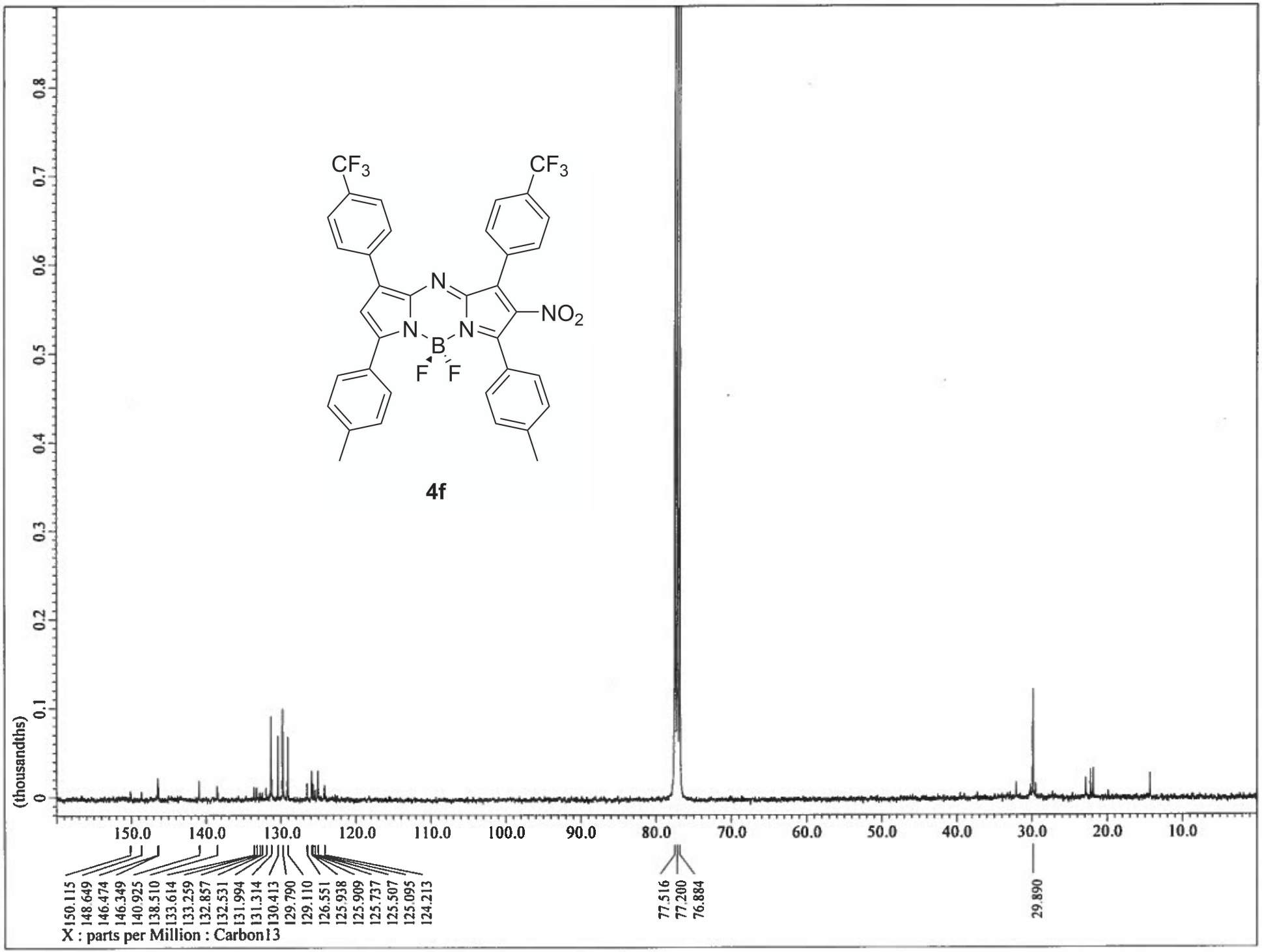
-0.610
-0.763
-0.991

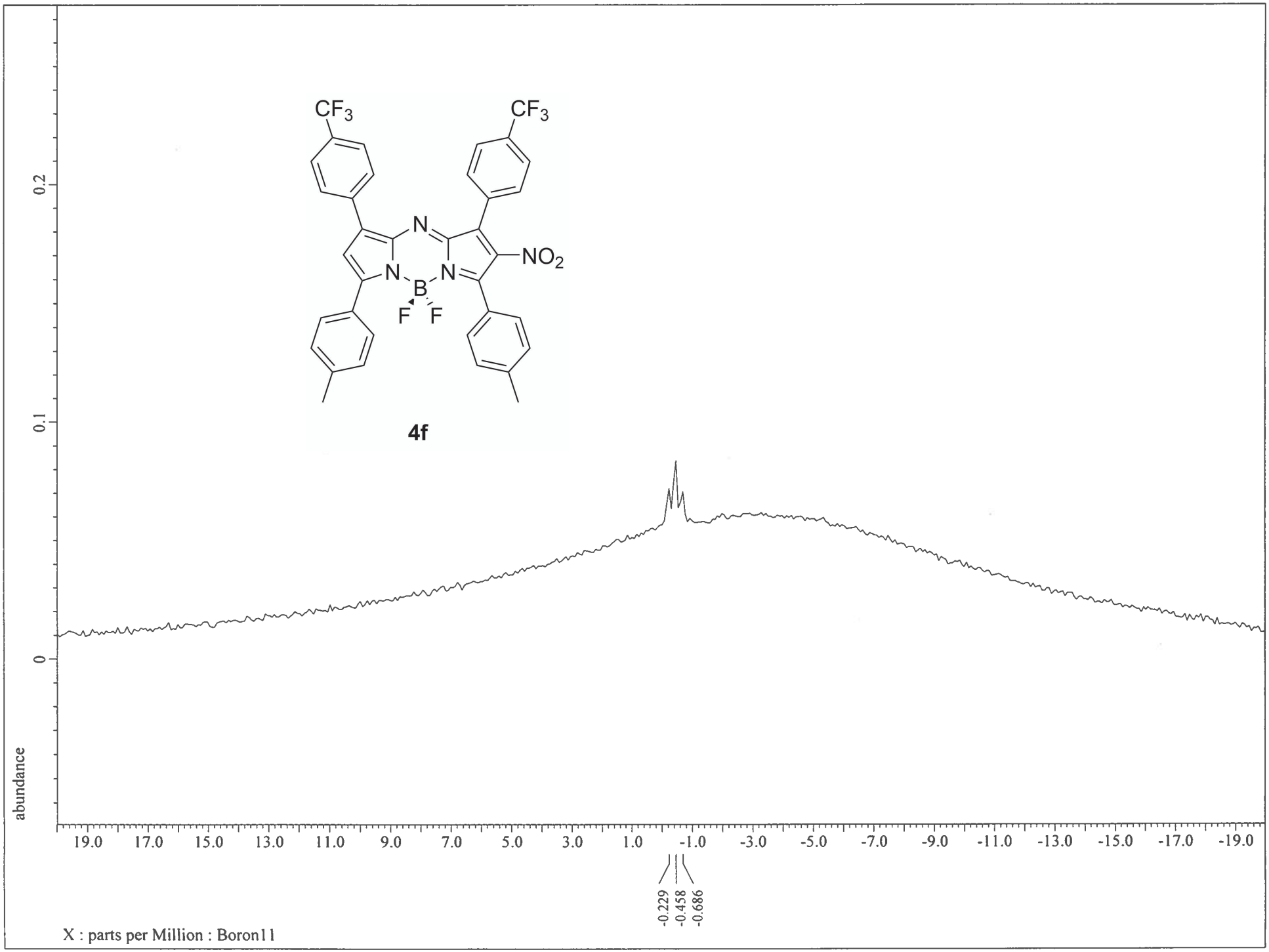
X : parts per Million : Boron11

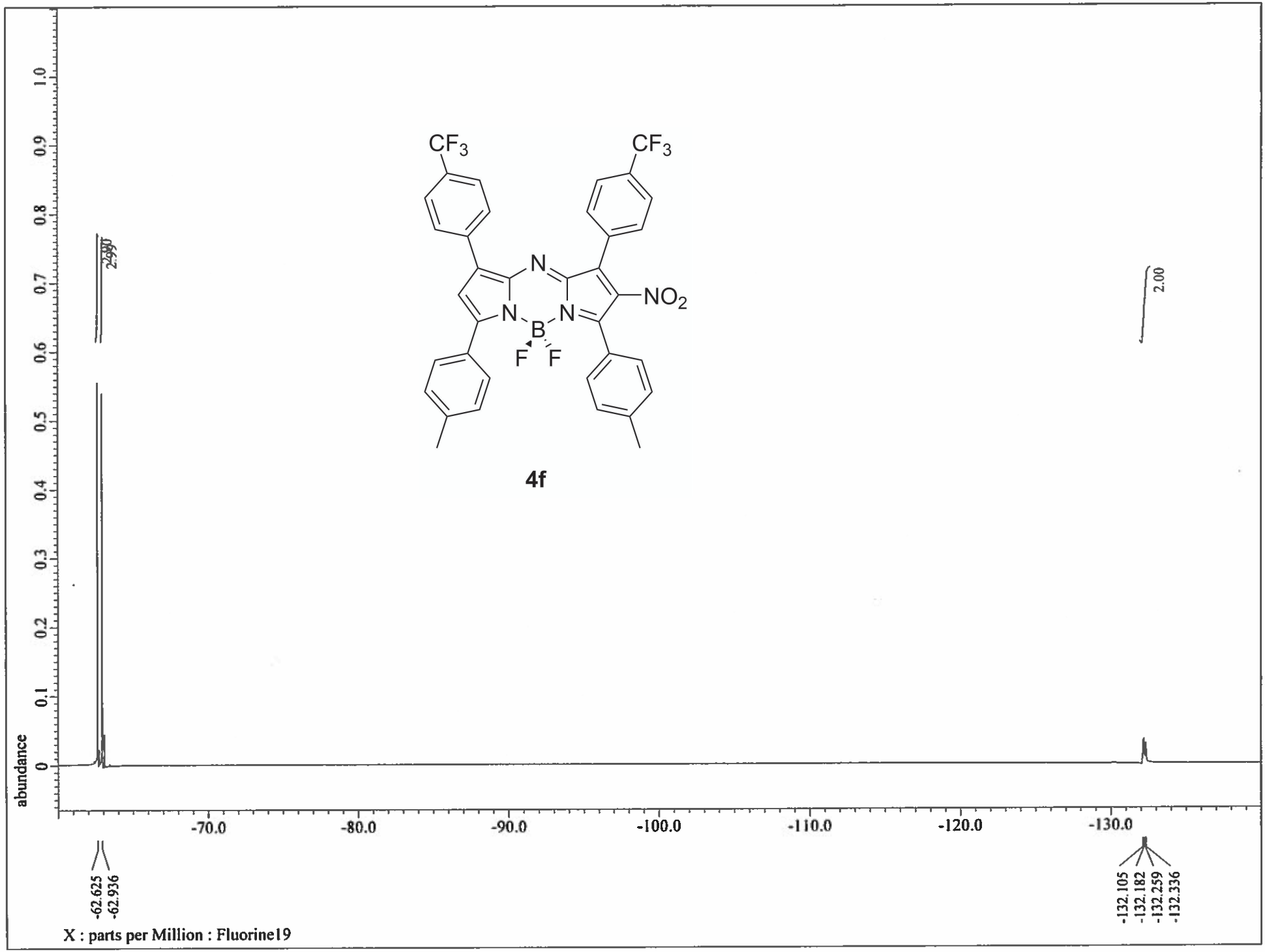

H3CO
OCH3
O2N
NO2
O2N
NO2
N
N
B
N
F
F
3e
abundance
0.3
0.2
0.1
0
-10.0
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-129.908
-129.977
-130.054
-130.115
X : parts per Million : Fluorine19

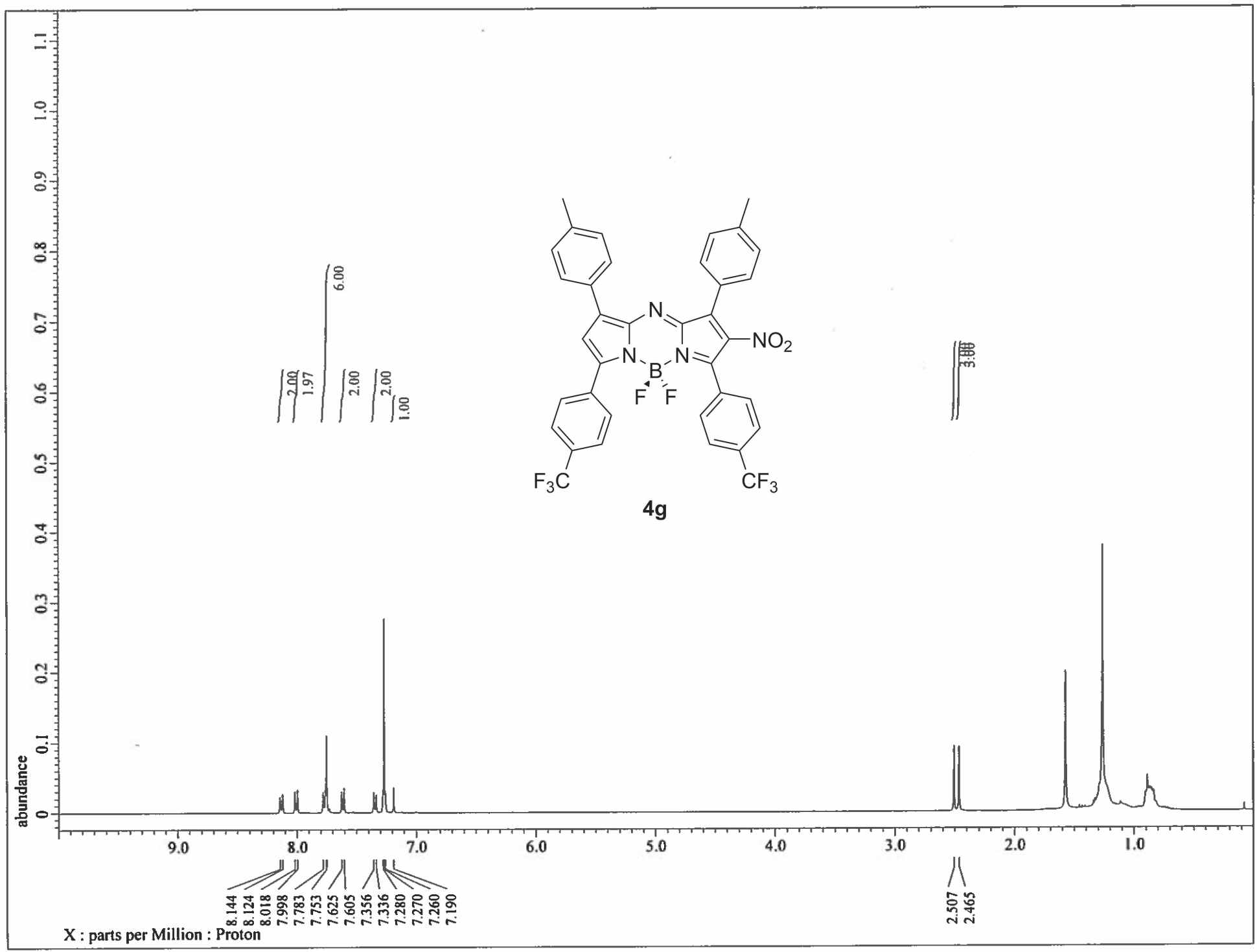

H3CO
OCH3
O2N
NO2
O2N
NO2
N
N
B
N
F
F
3e
Y : parts per Million : Proton
X : parts per Million : Proton
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
-1.0


CF3
CF3
N
NO2
N
B
N
F
F
4.00
3.96
2.00
2.04
1.00
1.98
6.00
4f
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
8.098
8.078
8.057
7.765
7.670
7.650
7.573
7.553
7.419
7.371
7.350
7.324
7.304
7.270
2.463
2.454
X : parts per Million : Proton

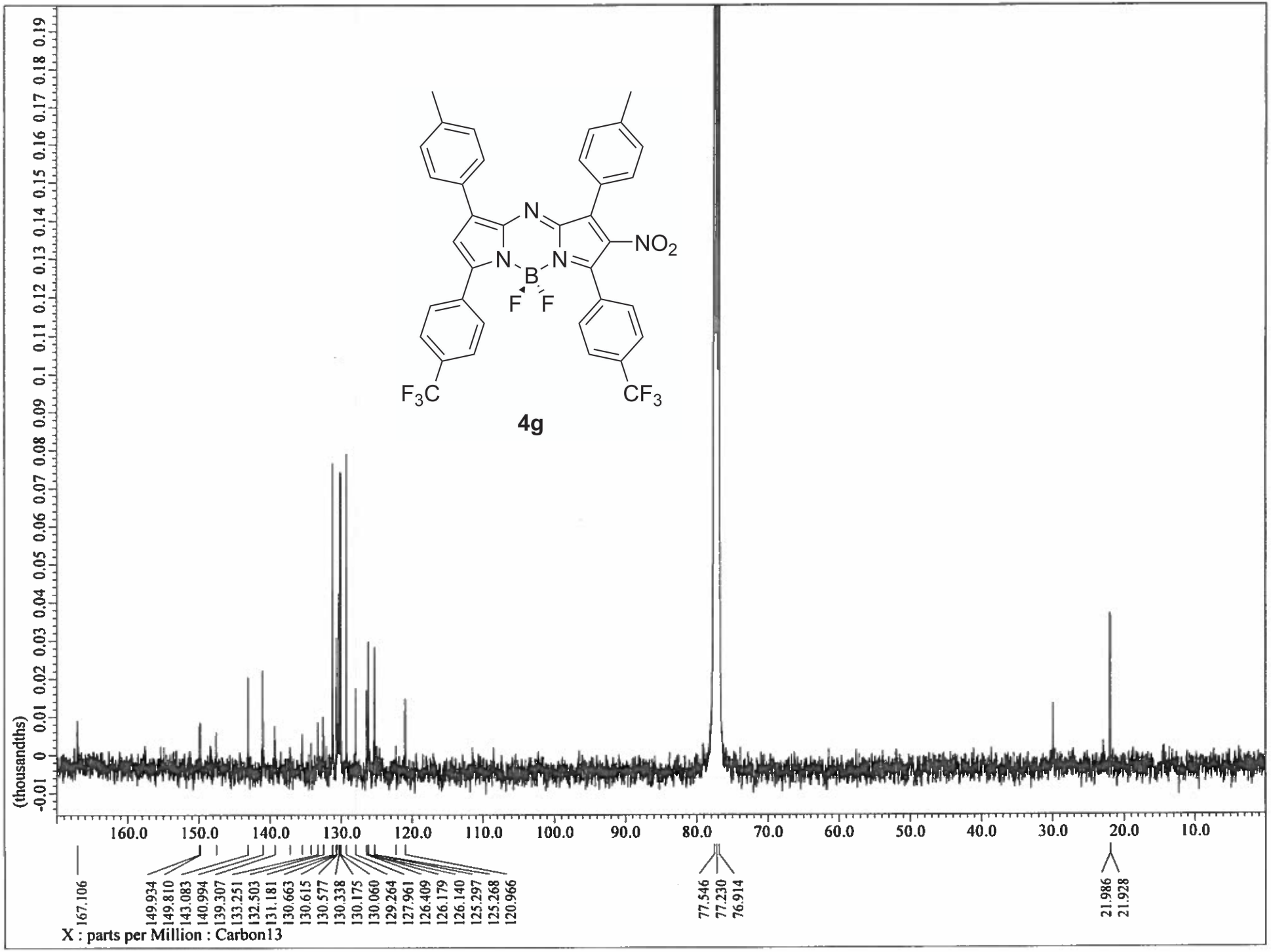

CF3
CF3
N
NO2
N
B
N
F
F
4f
(thousandths)
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
150.115
148.649
146.474
146.349
140.925
138.510
133.614
133.259
132.857
132.531
131.994
131.314
130.413
129.790
129.110
126.551
125.938
125.909
125.737
125.507
125.095
124.213
77.516
77.200
76.884
29.890
X : parts per Million : Carbon13

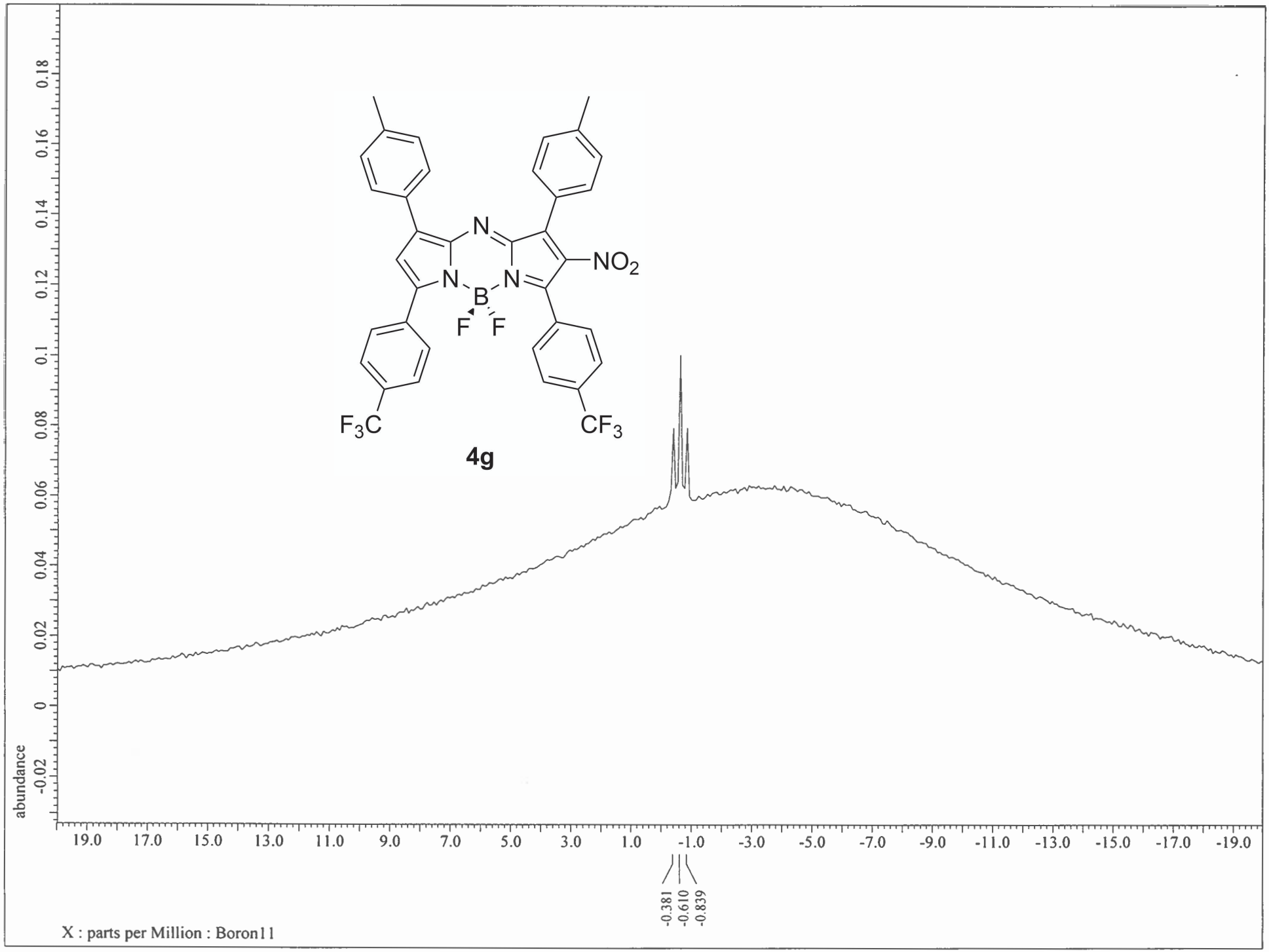

CF3
CF3
N
NO2
N
N
B
F
F
4f
0.2
0.1
0
abundance
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
-0.229
-0.458
-0.686
X : parts per Million : Boron11

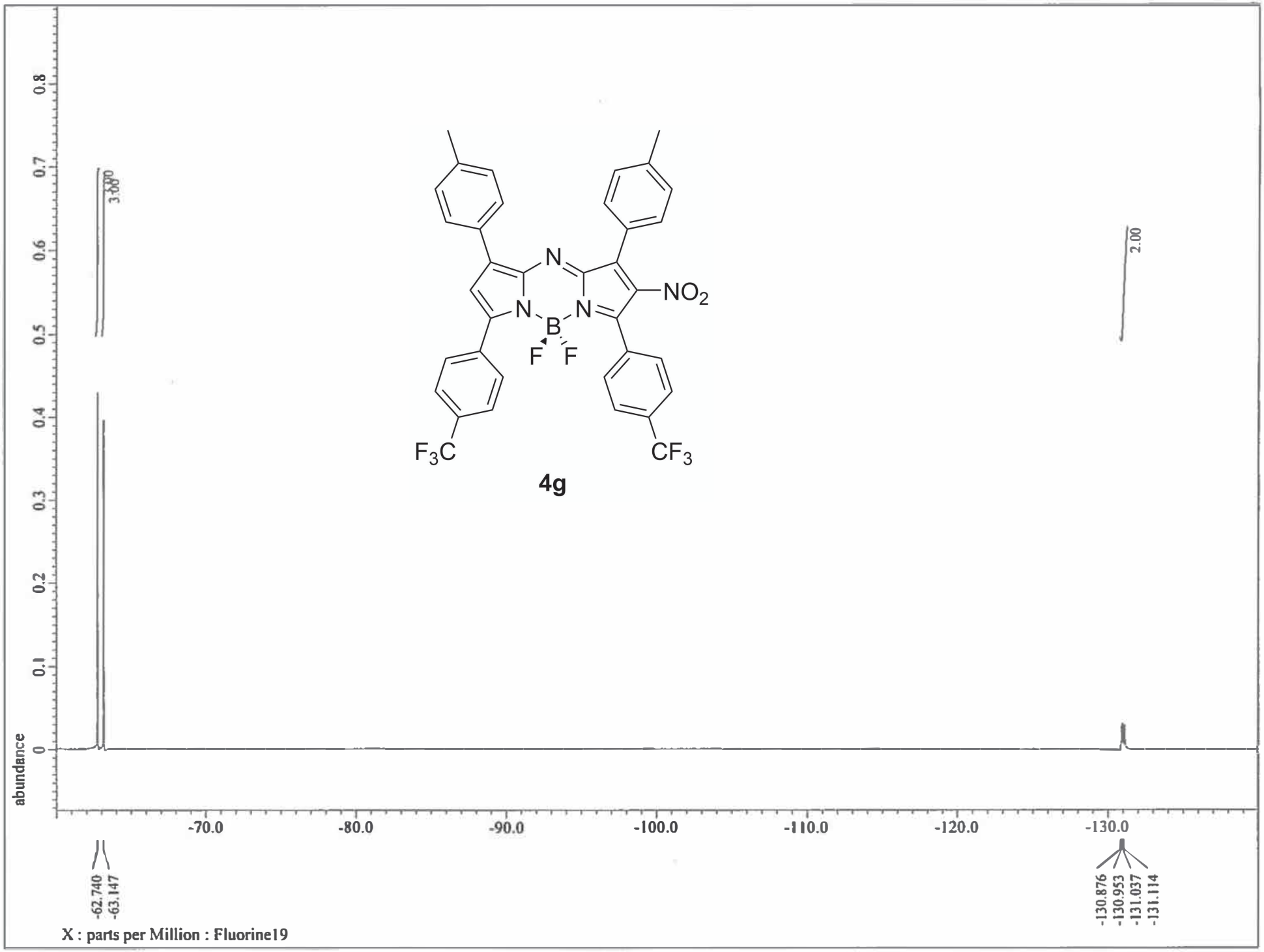

CF3
CF3
N
NO2
N
N
B
F
F
4f
2.00
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-62.625
-62.936
-132.105
-132.182
-132.259
-132.336
X : parts per Million : Fluorine19


abundance
X : parts per Million : Proton
8.144
8.124
8.018
7.998
7.783
7.753
7.625
7.605
7.356
7.336
7.280
7.270
7.260
7.190
2.507
2.465
2.00
1.97
6.00
2.00
2.00
1.00
3.00
N
N
B
N
F
F
NO2
F3C
CF3

4g


N
N
B
N
F
F
NO2
F3C
CF3
4g
(thousandths)
-0.01 0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18 0.19
160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
167.106
149.934
149.810
143.083
140.994
139.307
133.251
132.503
131.181
130.663
130.615
130.577
130.338
130.175
130.060
129.264
127.961
126.409
126.179
126.140
125.297
125.268
120.966
77.546
77.230
76.914
21.986
21.928
X : parts per Million : Carbon13


N
N
B
N
F
F
NO2
F3C
CF3
4g
abundance
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
-0.02
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-3.0
-5.0
-7.0
-9.0
-11.0
-13.0
-15.0
-17.0
-19.0
-0.381
-0.610
-0.839
X : parts per Million : Boron11


3.00
2.00
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-62.740
-63.147
-130.876
-130.953
-131.037
-131.114
X : parts per Million : Fluorine19

N
N
B
N
F
F
NO2
F3C
CF3

4g