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Anthracene-styrene-substituted *m*-carborane derivatives: Insights into the electronic and structural effects of substituents on photoluminescence.

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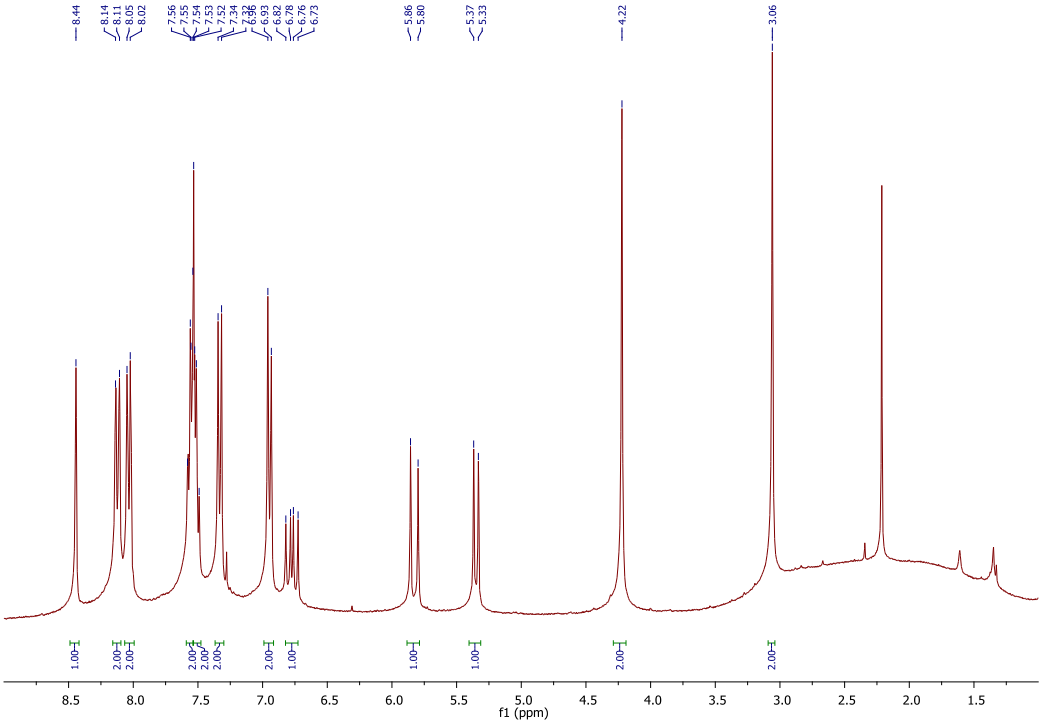
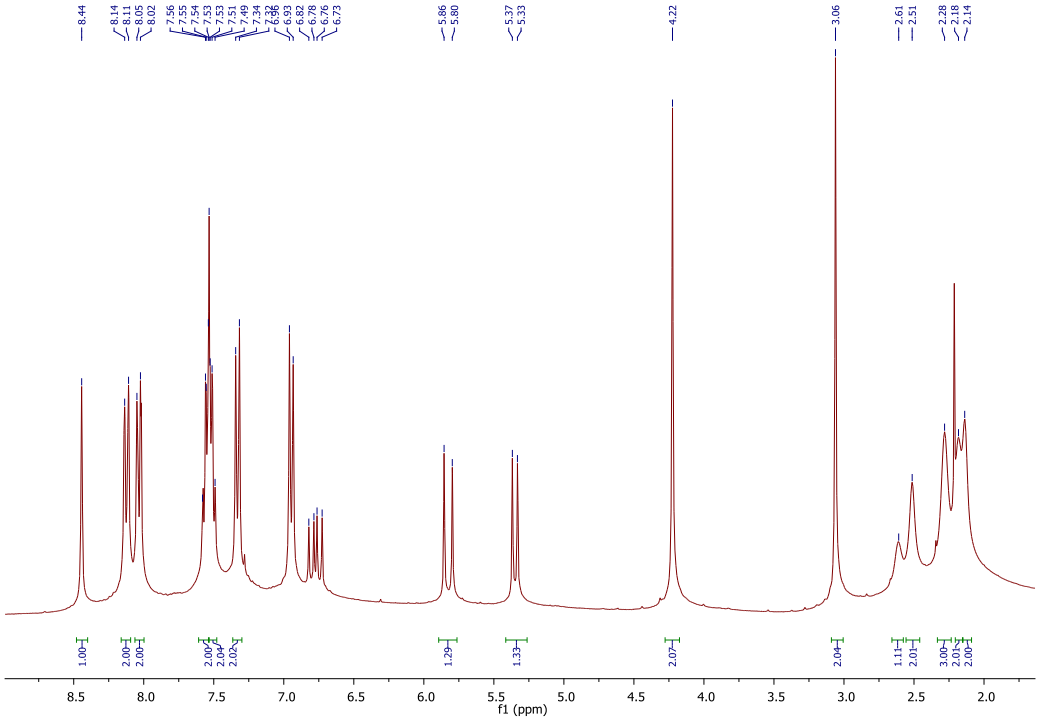
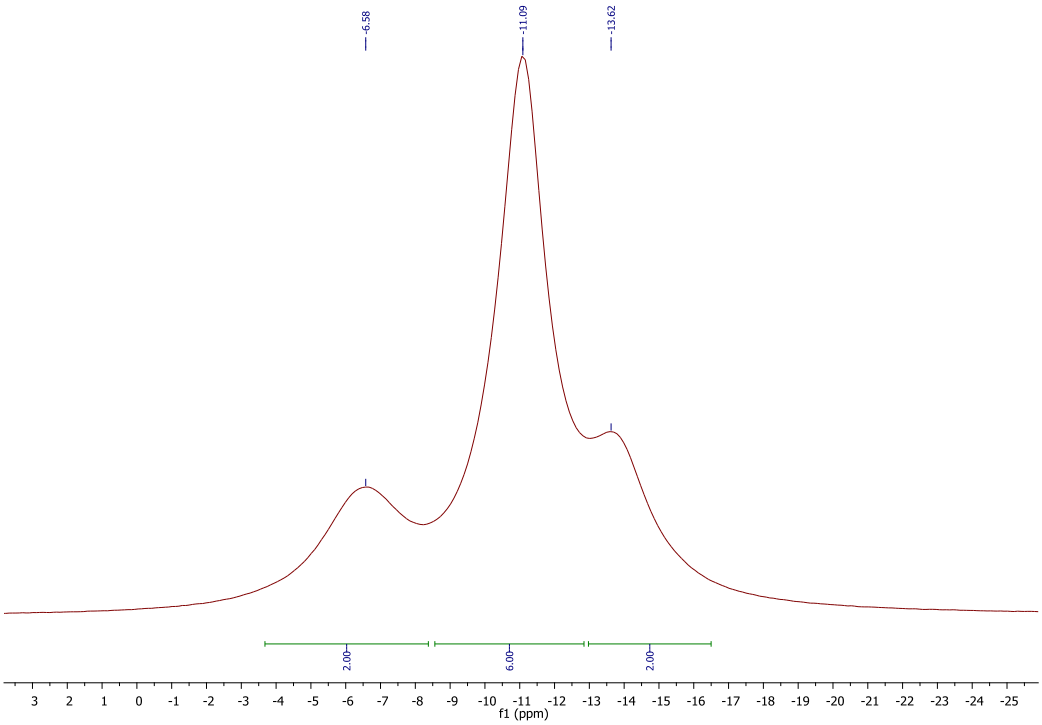
^{1}H, ^{11}B{^{1}H} and ^{13}C{^{1}H} NMR spectra of compounds.



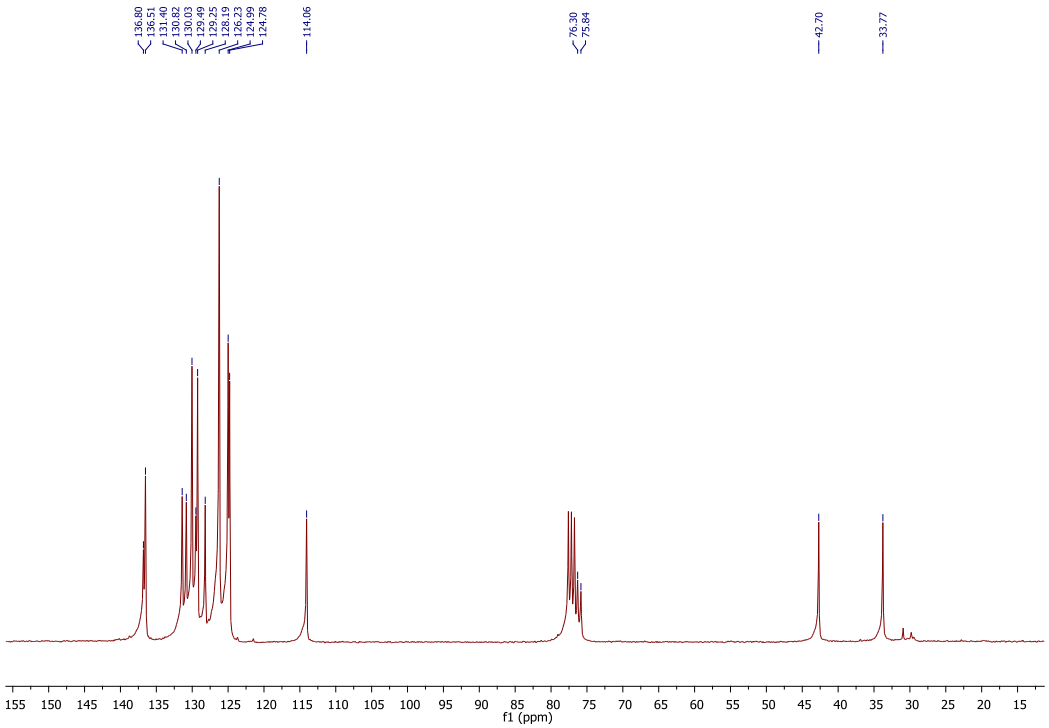
^{1}H NMR spectrum of **3**



^{1}H{^{11}B} NMR spectrum of **3**



$^{11}B\{^{1}H\}$ NMR spectrum of **3**



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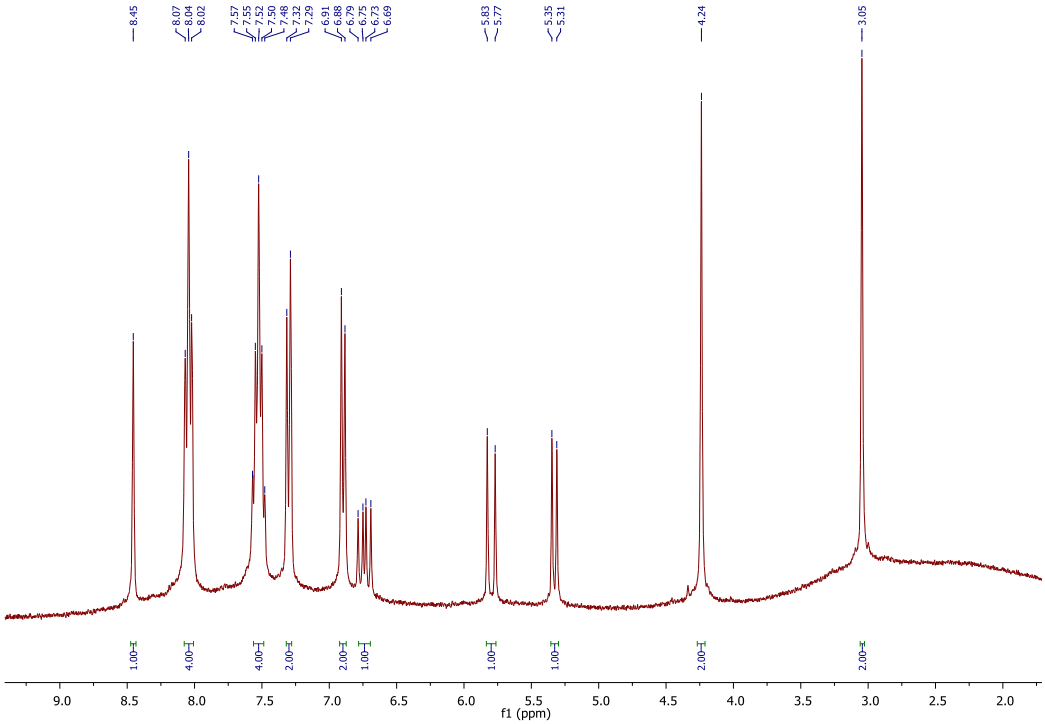

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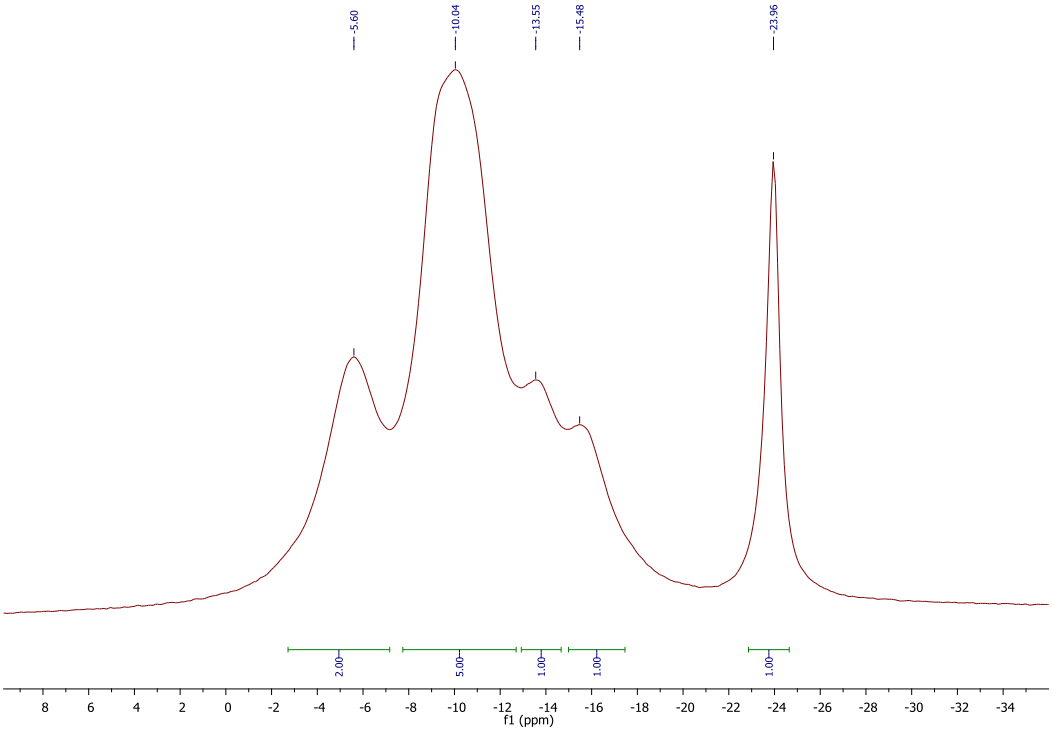

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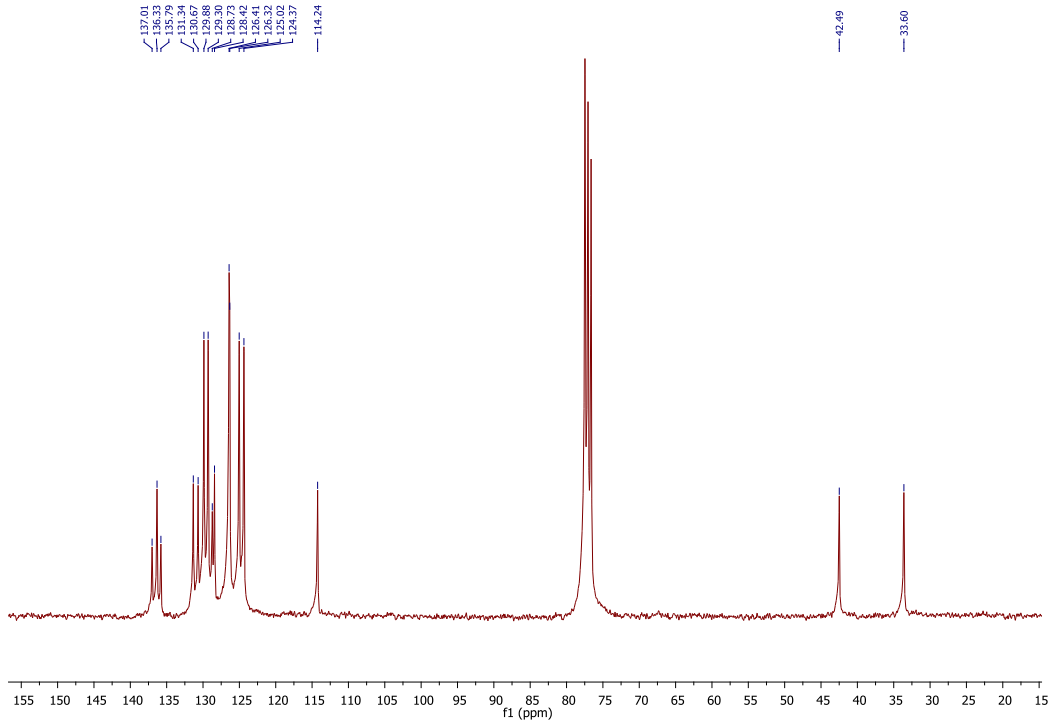

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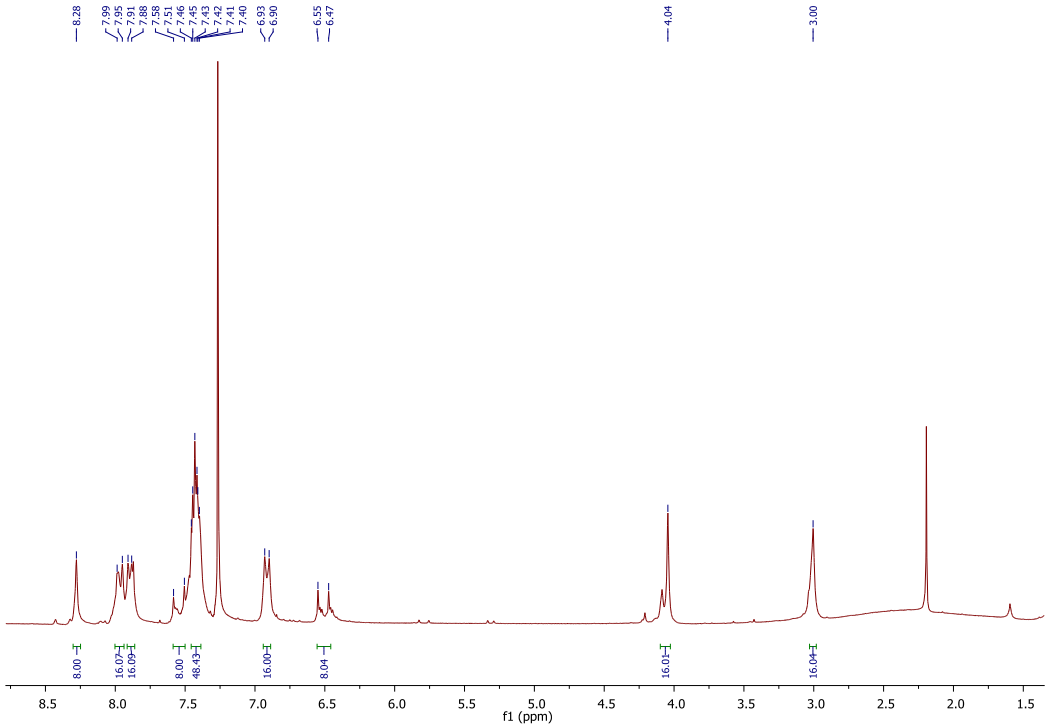

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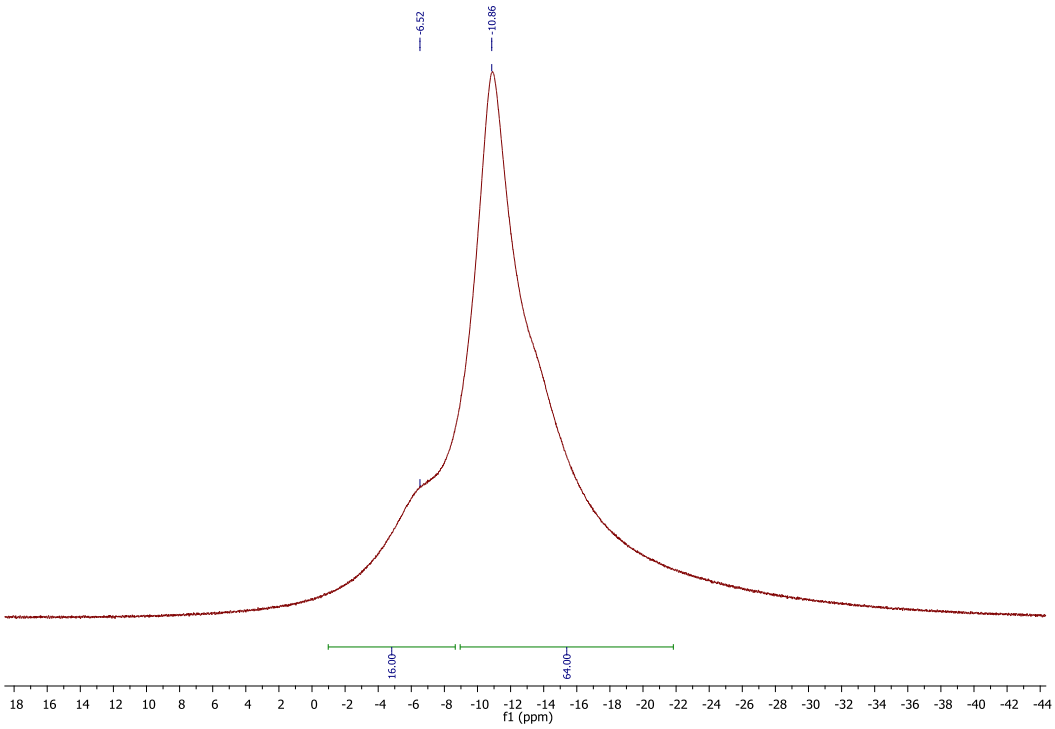

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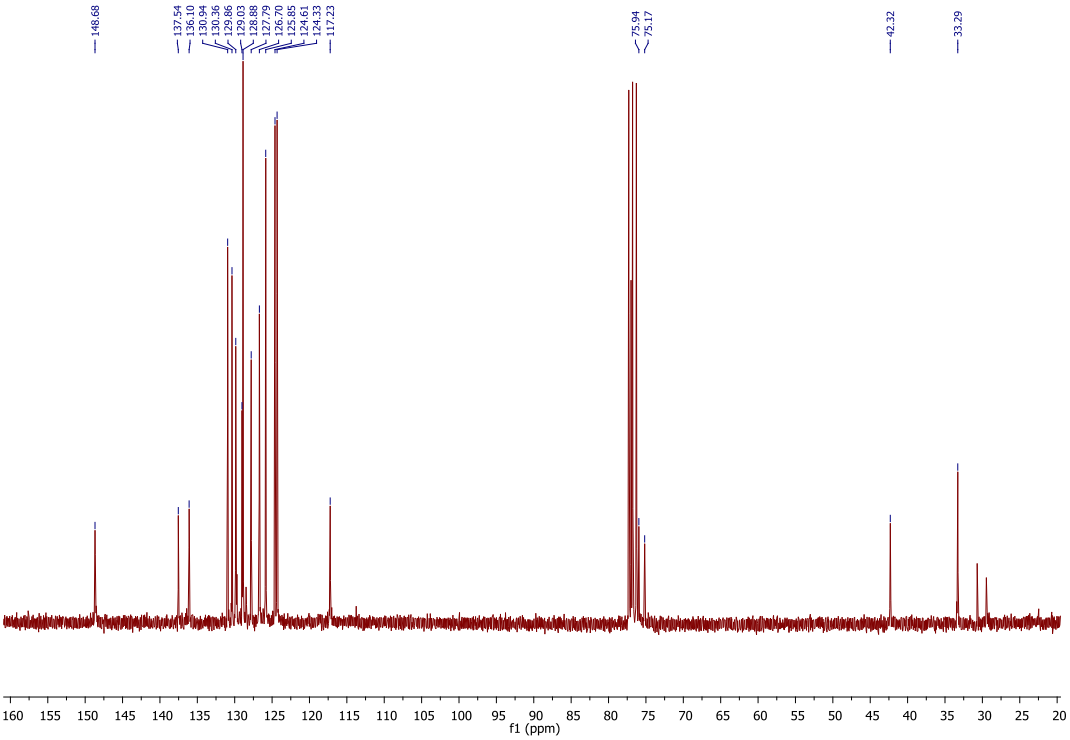

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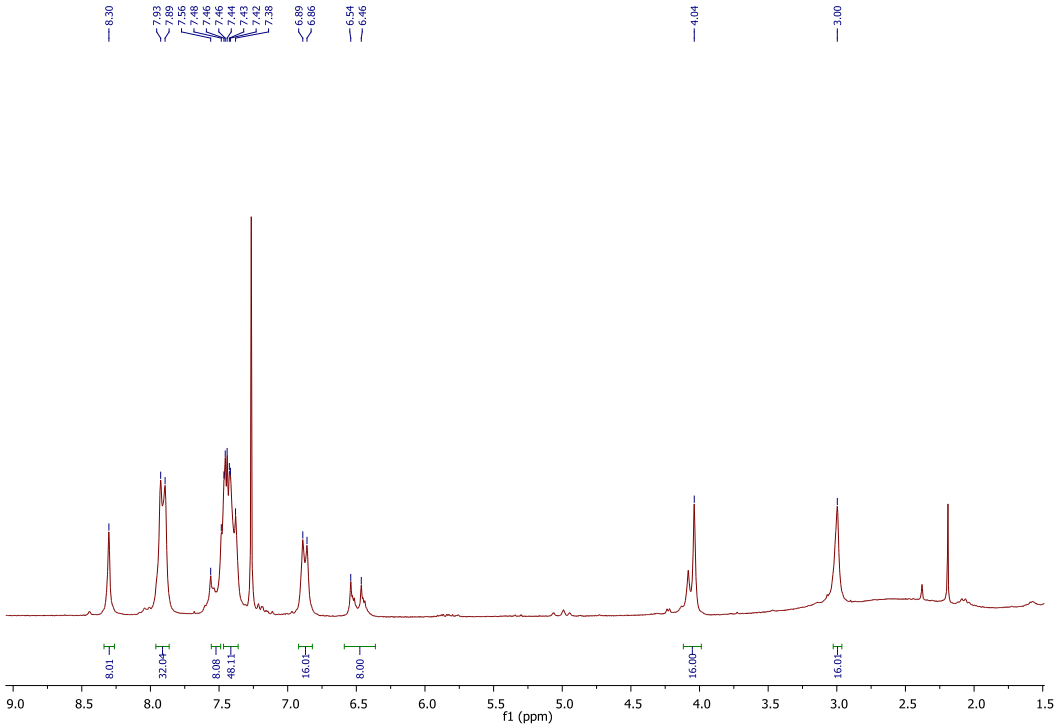
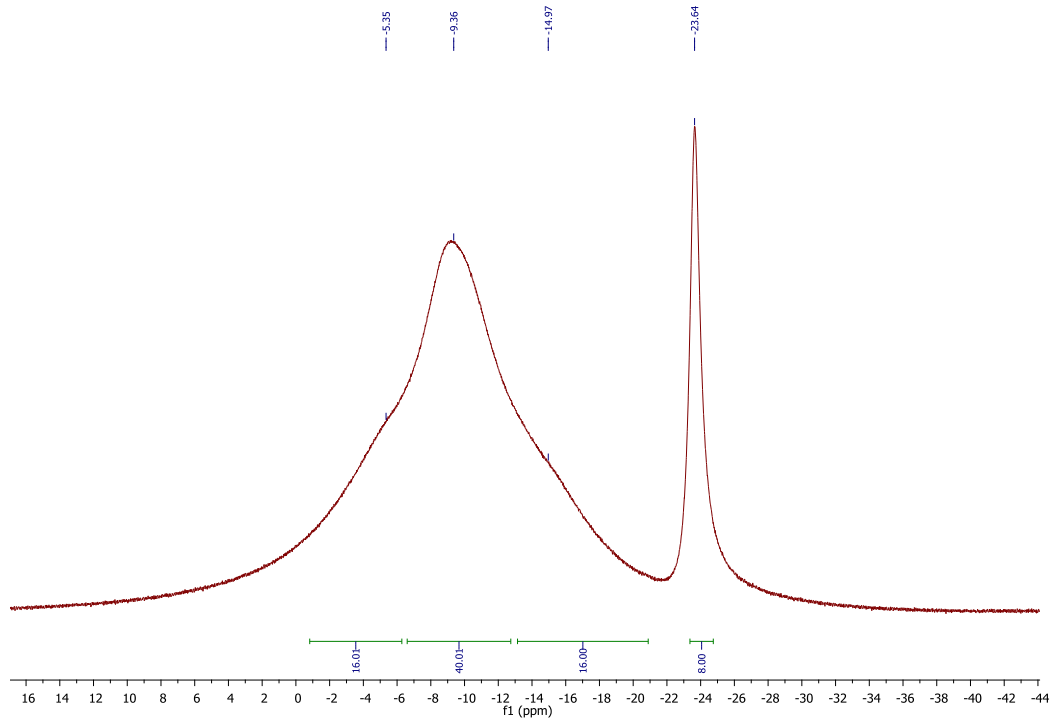
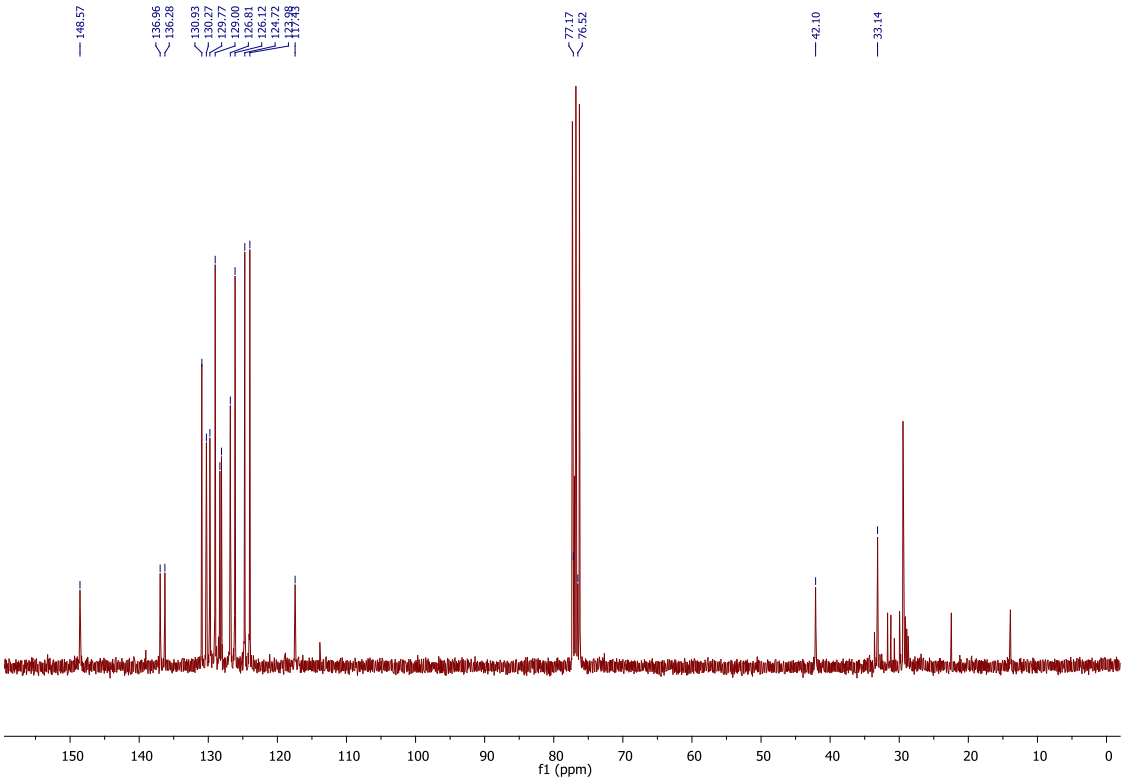


^{1}H NMR spectrum of **6**

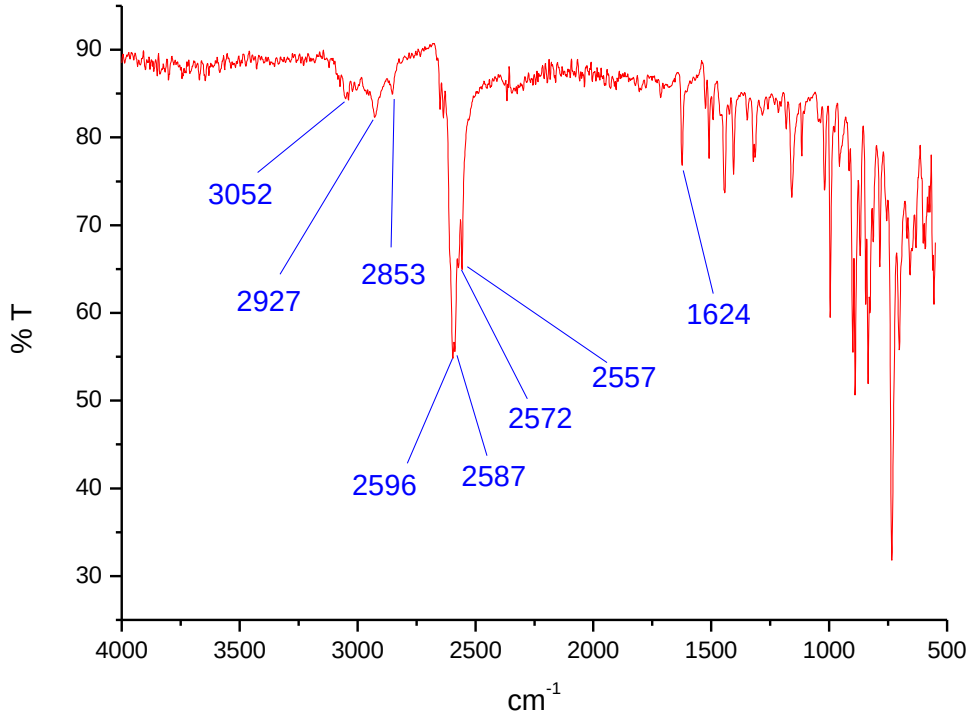


^{11}B{^{1}H} NMR spectrum of **6**

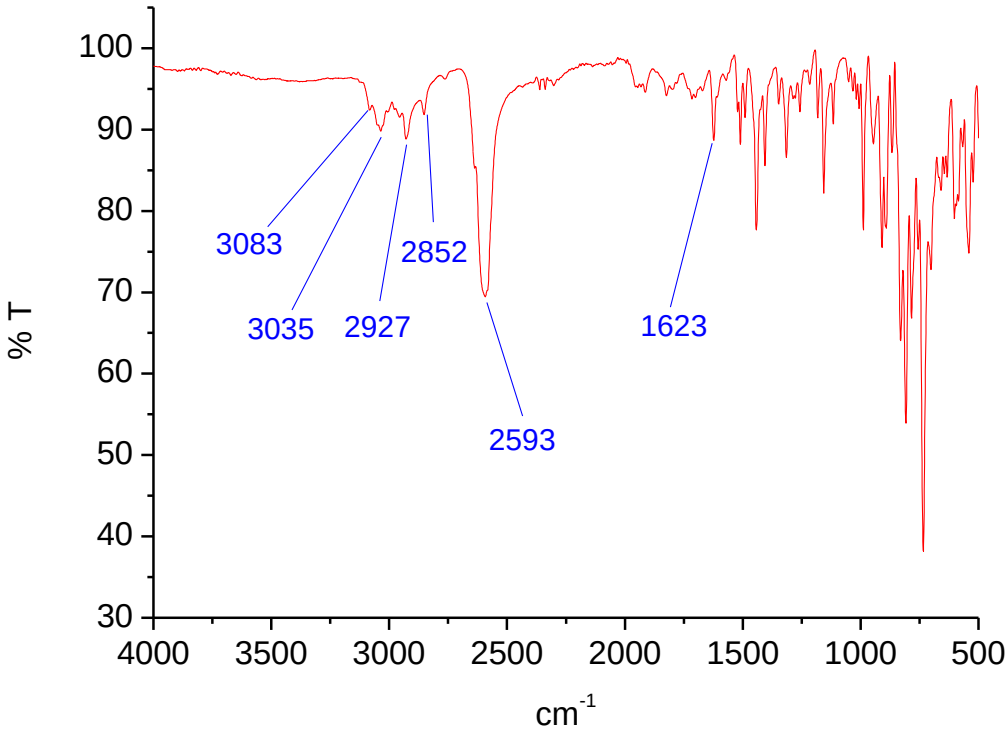


$^{13}C\{^{1}H\}$ NMR spectrum of **6**

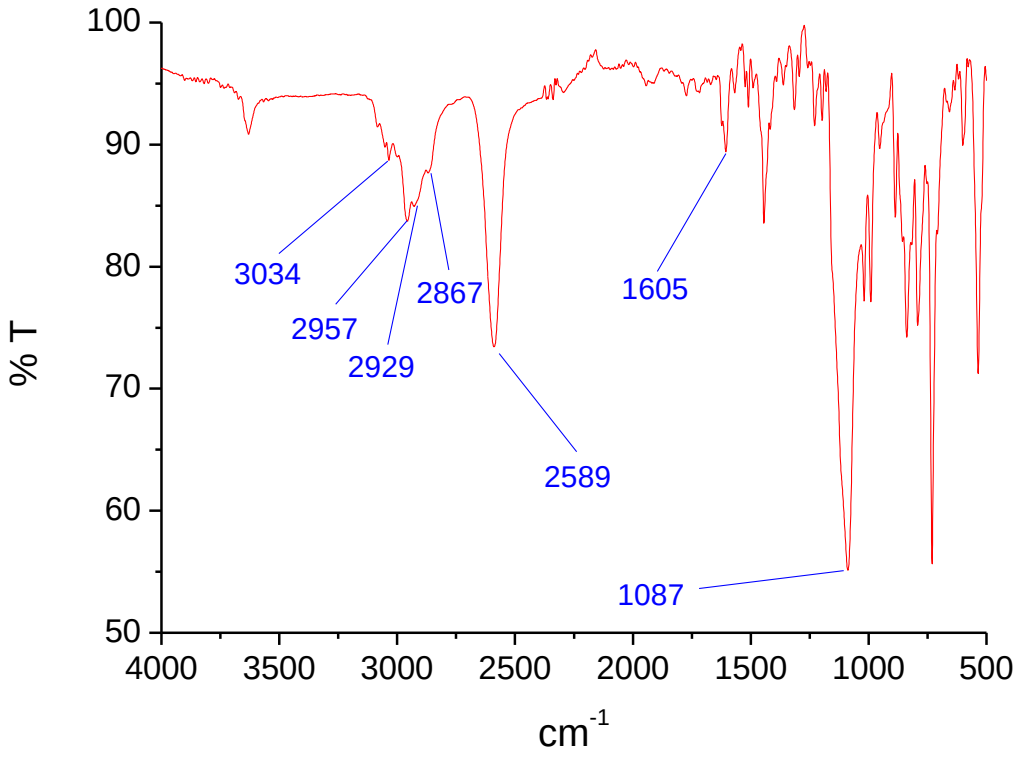
IR-ATR spectra of compounds.



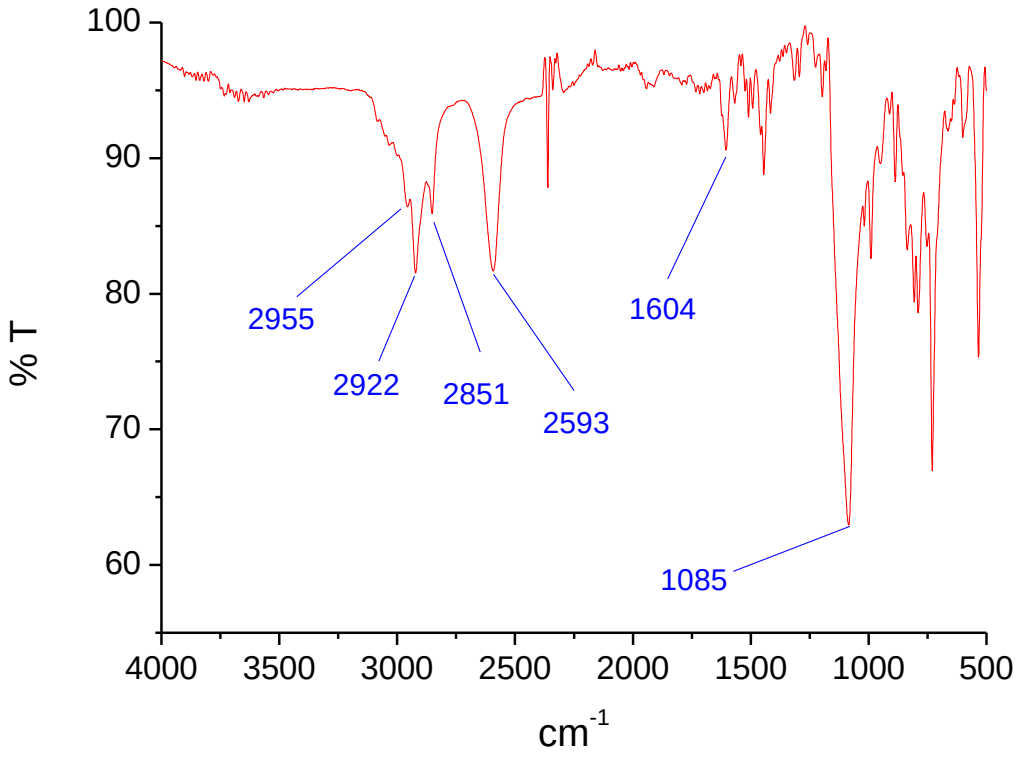
IR-ATR spectra of **3**



IR-ATR spectra of **4**



IR-ATR spectra of **5**



IR-ATR spectra of **6**

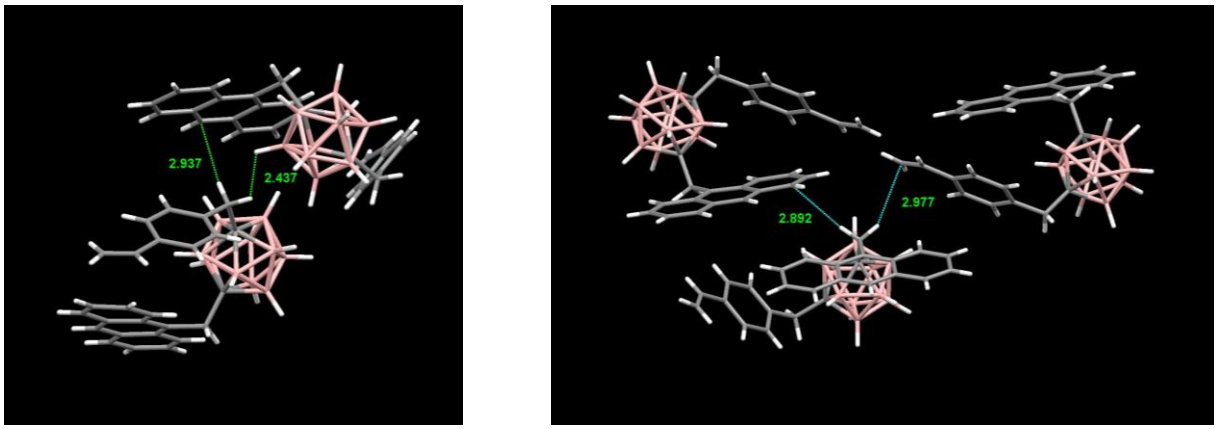
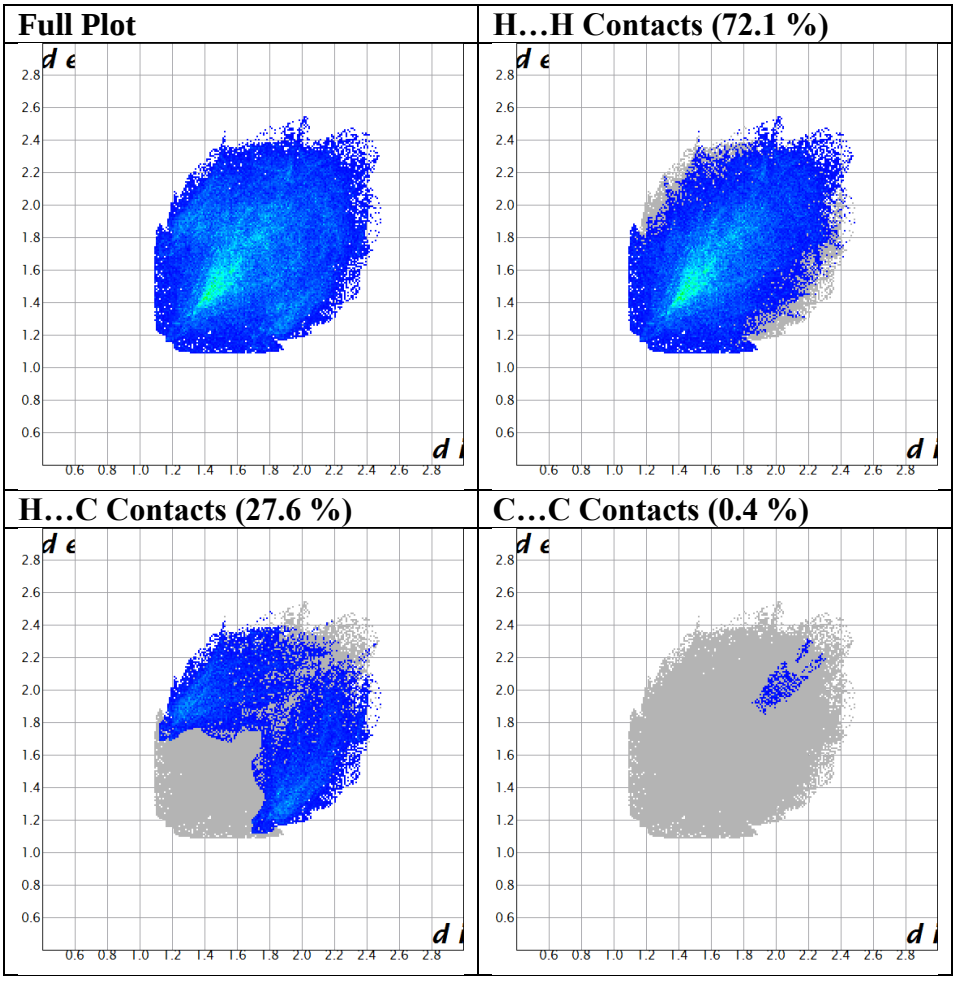


Figure S1. Picture indicating the intermolecular C–H···A interactions

Full and decomposed fingerprints for compound 3 were done by using CrystalExplorer17 (2017).[1] Legend: Close Contacts X···Y, where: X = atom inside the surface, Y = atom outside the surface.



Computational details.

All calculations were carried out with the Gaussian 09 program package.[2] Full geometry optimization calculations were performed and harmonic vibrational frequencies were calculated to establish the nature of the stationary points obtained, as characterized by none negative eigenvalue of the Hessian for minima structures. For the visualization of the molecules and orbitals the MOLDEN[3] and VMD program[4] were used.

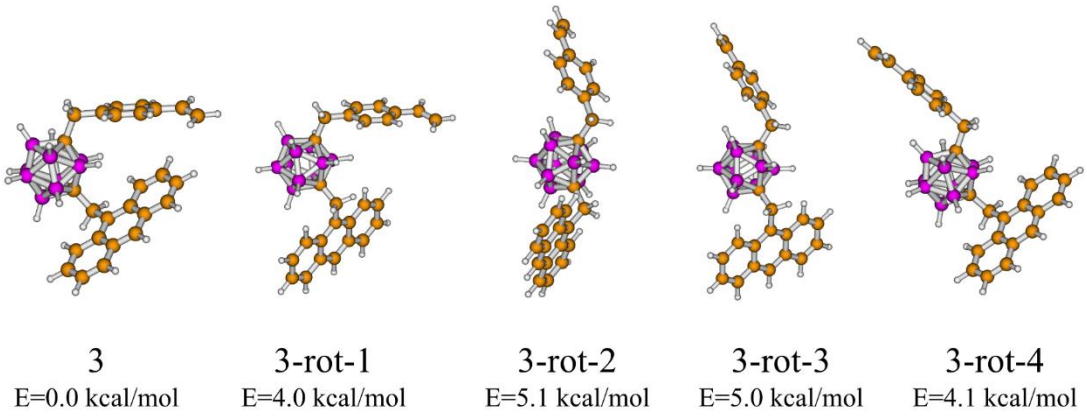


Figure S2. Different rotamers and their energies of **3** at ω-B97XD/6-31G* level of theory

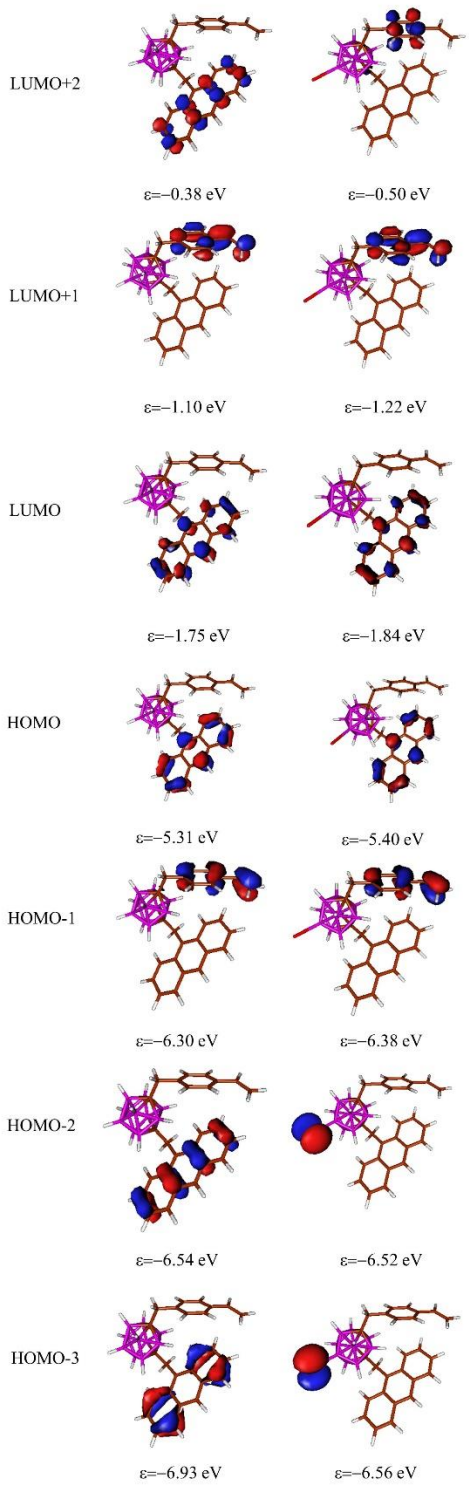


Figure S3. Kohn-Sahm molecular orbitals of **3** and **4** at B3LYP/6-31G*//ω-B97XD/6-31+G* level of theory

Table S1. The first excited state of **3** with different methods and basis sets

Method	**Absorption peak corresponds to the HOMO-LUMO transition (nm)**
B3LYP/cc-pVTZ	395
B3LYP/6-311+G**	394
B3LYP/6-31G*	384
B3LYP/6-31G* (PCM=THF)	387
cam-B3LYP/6-31G*	346
ω-B97XD/6-31G*	344
M06-2X/6-31G*	343
BP86/6-31G*	423

Table S2. TD-DFT results for **3** at B3LYP/6-31G*//ω-B97XD/6-31G* level of theory

Excited state	**λ_{abs} (nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
1	384	0.0882	HOMO → LUMO	100
2	332	0.0007	HOMO-2 → LUMO	2
			HOMO → LUMO+1	95
3	317	0.0038	HOMO-2 → LUMO	51
			HOMO → LUMO+1	4
			HOMO → LUMO+2	25
			HOMO → LUMO+3	18
4	304	0.0001	HOMO-1 → LUMO	100
5	278	0.0002	HOMO → LUMO+2	44
			HOMO → LUMO+3	52

Table S3. TD-DFT results for **4** at B3LYP/6-31G*//ω-B97XD/6-31G* level of theory

Excited state	**λ_{abs} (nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
1	385	0.0882	HOMO → LUMO	100
2	334	0.0000	HOMO → LUMO+1	100
3	317	0.0035	HOMO-4 → LUMO	51
			HOMO → LUMO+2	9
			HOMO → LUMO+3	34
4	306	0.0008	HOMO-1 → LUMO	100
5	287	0.0002	HOMO-2 → LUMO	100
6	284	0.0012	HOMO-2 → LUMO	100

Table S4. TD-DFT results for **5** at B3LYP/6-31G* level of theory (It should be noted that the anthracene units are not totally planar in the optimized geometry, which may lead controversial results.)

Excited state	**λ_{abs} (nm) Calculated**	**Intensity (*f*)**
1	416	0.0533
2	416	0.0793
3	416	0.1073
4	416	0.1131
5	415	0.0362
6	415	0.5343

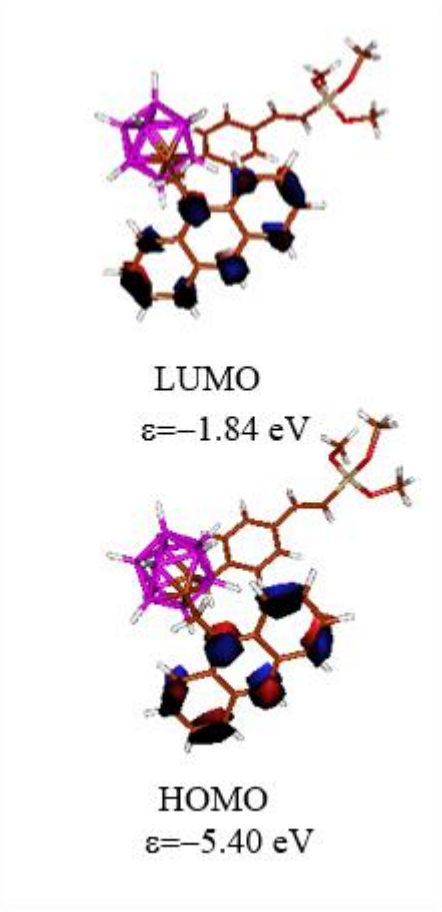


Figure S4. Kohn-Sahm molecular orbitals of trimethoxysilyl-substituted **3** at B3LYP/6-31G*//ω-B97XD/6-31+G* level of theory

XYZ coordinates and total energies in a.u. of the investigated systems

3

E(ω-B97XD/6-31+G*)= -1257.199037

C	0.065082	-3.996531	0.009613
C	-0.999491	-3.043292	-0.084117
C	-0.783373	-1.799735	-0.770659
C	0.521510	-1.582622	-1.329110
C	1.512527	-2.512881	-1.216955
C	1.285975	-3.744437	-0.539431
C	-1.832614	-0.859053	-0.860783
C	-3.085587	-1.142245	-0.274386
C	-3.288008	-2.390017	0.407129
C	-2.243257	-3.308216	0.484402
C	-4.558117	-2.673173	1.004272
C	-5.580239	-1.774480	0.944666
C	-5.387172	-0.530943	0.277727
C	-4.192311	-0.229317	-0.307888
C	-1.625337	0.443154	-1.606994
C	-1.109100	1.635037	-0.775846
B	0.028143	1.379826	0.459945
B	0.489855	2.146401	-1.073441
B	-0.873879	3.102234	-1.639816
B	-2.170017	2.948845	-0.444401
B	-1.614056	1.878060	0.851100
B	-0.238499	2.656471	1.636738
B	-1.608754	3.638431	1.085490
B	-1.153155	4.398781	-0.460810
B	0.496246	3.888459	-0.854380
B	0.050098	4.208954	0.828868
C	0.954322	2.813711	0.410832
C	2.437094	2.784678	0.828269
C	3.132397	1.462143	0.615787
C	3.822622	1.194510	-0.566376
C	4.440739	-0.036059	-0.765733
C	4.377119	-1.041798	0.204820
C	3.696027	-0.763606	1.397127
C	3.088517	0.467969	1.597413
C	5.018902	-2.343575	-0.058658
C	4.746810	-3.497796	0.557108
H	1.224545	1.547357	-1.782072
H	0.489397	0.321144	0.699552
H	-2.339636	1.095764	1.364702
H	-3.292979	2.875537	-0.826470
H	-1.113628	3.114396	-2.803658
H	0.123483	2.481586	2.755057
H	-2.347377	4.157245	1.860421
H	-1.567112	5.461940	-0.798091
H	1.345788	4.521111	-1.392900
H	0.605485	5.076806	1.421740
H	-2.557437	0.757682	-2.079582

H	-0.928071	0.291370	-2.433448
H	-4.080493	0.736879	-0.784496
H	-6.199505	0.189214	0.241331
H	-6.538476	-1.996289	1.405098
H	-4.686644	-3.626437	1.511326
H	-2.401415	-4.252642	1.001731
H	-0.126993	-4.931730	0.530330
H	2.089798	-4.470967	-0.465837
H	2.491884	-2.311101	-1.639051
H	0.746555	-0.651513	-1.834780
H	2.952990	3.571119	0.269855
H	2.486038	3.063356	1.884931
H	2.564722	0.661417	2.530826
H	3.654051	-1.510705	2.184111
H	5.767324	-2.340427	-0.851032
H	3.988656	-3.578915	1.332108
H	5.275082	-4.409179	0.293670
H	4.975305	-0.221469	-1.694864
H	3.878528	1.956578	-1.340349

E(ω-B97XD/6-31G*)= -1257.175101

C	-3.084317	0.461091	-1.596621
C	-3.135341	1.453362	-0.614771
C	-3.821467	1.180828	0.567828
C	-4.429760	-0.053011	0.767052
C	-4.359376	-1.056903	-0.203904
C	-3.682209	-0.773770	-1.396269
C	-2.447824	2.779714	-0.826231
C	-0.964829	2.813696	-0.410458
B	-0.064021	4.211012	-0.827971
B	-0.509383	3.888701	0.854833
B	1.138763	4.402726	0.461456
B	1.595643	3.644220	-1.085053
B	0.227525	2.659733	-1.636566
B	1.605038	1.883873	-0.851857
B	2.158438	2.954976	0.444164
B	0.862342	3.105022	1.639587
B	-0.499171	2.146430	1.072840
B	-0.035950	1.381396	-0.461020
C	1.100566	1.639102	0.774820
C	1.618701	0.447229	1.604398
C	1.829047	-0.853991	0.857836
C	0.781600	-1.795465	0.765961
C	1.002873	-3.040628	0.085036
C	2.248640	-3.304275	-0.477326
C	3.290080	-2.383683	-0.402069
C	3.082731	-1.134153	0.273537
C	-0.525043	-1.578695	1.317923
C	-1.512676	-2.510442	1.204005
C	-1.280820	-3.743205	0.532792
C	-0.058474	-3.995506	-0.009215

C	4.561270	-2.665102	-0.994845
C	5.578851	-1.763411	-0.937502
C	5.380761	-0.518208	-0.277605
C	4.185713	-0.217892	0.305104
C	-4.988525	-2.364352	0.058164
C	-4.693529	-3.514468	-0.550451
H	-1.233404	1.546389	1.781315
H	-0.496652	0.322494	-0.700893
H	2.333004	1.104303	-1.366016
H	3.281634	2.884783	0.825870
H	1.102228	3.117065	2.803138
H	-0.133998	2.485255	-2.754985
H	2.332749	4.165282	-1.859462
H	1.550358	5.466337	0.799091
H	-1.359904	4.519240	1.393863
H	-0.621083	5.077831	-1.420136
H	2.549830	0.763024	2.077442
H	0.920981	0.293014	2.429663
H	4.068532	0.749268	0.778208
H	6.190777	0.203970	-0.243561
H	6.538377	-1.983585	-1.395062
H	4.692741	-3.619940	-1.497247
H	2.410795	-4.250145	-0.989824
H	0.138358	-4.931309	-0.526133
H	-2.083524	-4.470290	0.458814
H	-2.493817	-2.310218	1.620965
H	-0.751960	-0.646342	1.820025
H	-2.498758	3.060439	-1.881980
H	-2.965823	3.562591	-0.265249
H	-2.563537	0.660212	-2.530001
H	-3.638628	-1.520691	-2.182754
H	-5.745534	-2.367213	0.841713
H	-3.923950	-3.585460	-1.314522
H	-5.211743	-4.433012	-0.293929
H	-4.962042	-0.243935	1.695792
H	-3.881982	1.943032	1.340655

Rotamer-1 of **3**

E(ω-B97XD/6-31G*)= -1257.168508

C	4.861326	0.934590	0.729145
C	3.867823	1.023733	-0.247786
C	4.224654	0.819894	-1.579749
C	5.536229	0.516043	-1.921956
C	6.531065	0.400847	-0.945328
C	6.171100	0.630076	0.388611
C	2.436254	1.303556	0.132662
C	1.600840	0.045416	0.436071
B	2.262343	-1.540700	0.300715
B	1.886373	-0.831274	1.879882

B	1.412059	-2.501962	1.520508
B	0.905049	-2.566132	-0.188882
B	1.070963	-0.934914	-0.864199
B	-0.522609	-1.530338	-0.378209
B	-0.308110	-2.488908	1.094573
B	0.293875	-1.424606	2.374278
B	0.463256	0.182054	1.686630
B	-0.046566	0.121594	-0.006527
C	-0.796371	-0.843229	1.176696
C	-2.219557	-0.517702	1.672527
C	-3.185707	0.033789	0.644558
C	-3.300491	1.427907	0.457634
C	-4.241194	1.943495	-0.497159
C	-5.032203	1.061315	-1.227954
C	-4.930841	-0.316664	-1.057329
C	-3.992675	-0.845830	-0.107850
C	-2.513107	2.386085	1.178531
C	-2.647896	3.726312	0.969186
C	-3.584362	4.226633	0.021611
C	-4.355147	3.356983	-0.686574
C	-5.747631	-1.210604	-1.819177
C	-5.647593	-2.558793	-1.663230
C	-4.716068	-3.093453	-0.729390
C	-3.923894	-2.273104	0.016987
C	7.905764	0.056562	-1.352736
C	8.880785	-0.390447	-0.560300
H	0.279633	1.195463	2.273968
H	-0.525756	1.100573	-0.466106
H	-1.435143	-1.710277	-1.111074
H	-1.106092	-3.324117	1.375182
H	-0.101897	-1.526440	3.489883
H	1.388495	-0.641209	-1.970332
H	1.052882	-3.533319	-0.864878
H	1.921120	-3.423517	2.073848
H	2.743393	-0.465950	2.616791
H	3.392133	-1.671703	-0.029723
H	-2.623034	-1.430722	2.112965
H	-2.127783	0.178744	2.508024
H	-3.211136	-2.720782	0.698836
H	-4.631430	-4.169767	-0.614792
H	-6.269467	-3.228917	-2.248621
H	-6.450585	-0.784393	-2.530218
H	-5.743814	1.456824	-1.949519
H	-5.076139	3.719739	-1.414485
H	-3.679281	5.297361	-0.129867
H	-2.033451	4.422216	1.532577
H	-1.780492	2.046707	1.900271
H	2.406444	1.947446	1.017002
H	1.936422	1.848021	-0.673886
H	4.604793	1.105564	1.771402
H	6.925819	0.586973	1.167929

H	8.111880	0.170868	-2.416401
H	8.738813	-0.560028	0.503546
H	9.863828	-0.616966	-0.960176
H	5.792621	0.356084	-2.966201

Rotamer-2 of **3**

E(ω-B97XD/6-31G*)= -1257.167031

C	5.252019	-0.416220	1.138755
C	4.443328	0.666098	0.785550
C	4.914057	1.563779	-0.170908
C	6.153865	1.375272	-0.768807
C	6.960280	0.282508	-0.433474
C	6.489278	-0.605806	0.541530
C	3.082409	0.844757	1.408773
C	1.938223	0.134561	0.661292
B	2.209413	-0.760359	-0.785221
B	1.815155	-1.573082	0.739874
B	1.002461	-2.055801	-0.760459
B	0.718540	-0.583021	-1.724144
B	1.360633	0.794893	-0.811664
B	-0.382084	0.466977	-0.814061
B	-0.601257	-1.292773	-0.777432
B	0.078939	-1.907117	0.738493
B	0.709357	-0.533186	1.630736
B	0.432653	0.925485	0.672230
C	-0.680262	-0.362548	0.664279
C	-1.996646	-0.173221	1.446226
C	-3.253771	0.035801	0.628606
C	-3.668329	1.342536	0.295103
C	-4.893668	1.538199	-0.426989
C	-5.656811	0.433786	-0.795675
C	-5.257524	-0.862629	-0.483143
C	-4.035026	-1.072862	0.240126
C	-2.920435	2.516405	0.641127
C	-3.353344	3.764757	0.306184
C	-4.574352	3.948454	-0.401397
C	-5.316865	2.864478	-0.756030
C	-6.052016	-1.987007	-0.871999
C	-5.667085	-3.257177	-0.572102
C	-4.453627	-3.476736	0.138572
C	-3.672736	-2.430384	0.529647
C	8.262880	0.115768	-1.103665
C	9.023038	-0.979955	-1.106106
H	0.685984	-0.409563	2.810092
H	0.256996	1.928982	1.279505
H	-1.212347	1.184041	-1.261090
H	-1.594382	-1.766322	-1.216352
H	-0.456068	-2.774619	1.349774
H	1.878869	1.772021	-1.244581

H	0.717037	-0.588450	-2.913113
H	1.201268	-3.117020	-1.259307
H	2.634241	-2.180772	1.348603
H	3.307135	-0.836725	-1.223786
H	-2.119184	-1.043577	2.093008
H	-1.858022	0.666382	2.130224
H	-2.745070	-2.641694	1.047674
H	-4.144854	-4.492554	0.365969
H	-6.275639	-4.104088	-0.873814
H	-6.974355	-1.799887	-1.415718
H	-6.586611	0.587264	-1.339160
H	-6.251248	2.984889	-1.298044
H	-4.903957	4.951041	-0.655896
H	-2.758990	4.631570	0.579370
H	-1.977129	2.418808	1.164369
H	3.094148	0.469015	2.436371
H	2.837550	1.909734	1.463219
H	4.905874	-1.120386	1.890845
H	7.103267	-1.446432	0.850434
H	8.607471	0.986917	-1.659867
H	8.732907	-1.896046	-0.598782
H	9.970866	-0.999821	-1.634114
H	6.502005	2.086237	-1.513836

Rotamer-3 of **3**

E(ω-B97XD/6-31G*)= -1257.167078

C	4.925607	1.353750	0.008474
C	4.450067	0.427551	-0.922178
C	5.252722	-0.665855	-1.241978
C	6.491352	-0.836061	-0.636031
C	6.963998	0.076799	0.312498
C	6.160825	1.183388	0.615711
C	3.089513	0.594859	-1.549406
C	1.935548	-0.042330	-0.752817
B	2.202950	-0.888114	0.723717
B	1.410311	0.696943	0.702204
B	0.738253	-0.618647	1.681825
B	0.950027	-2.138454	0.774554
B	1.750388	-1.746403	-0.759173
B	0.002465	-2.016322	-0.712001
B	-0.624597	-1.316792	0.789744
B	-0.342029	0.433223	0.749902
B	0.458967	0.801600	-0.768450
B	0.664644	-0.703533	-1.671370
C	-0.698590	-0.443237	-0.687584
C	-2.023067	-0.238765	-1.452306
C	-3.251893	0.056715	-0.618753
C	-4.068060	-1.001436	-0.166680
C	-5.260851	-0.710485	0.578077

C	-5.595273	0.613009	0.850973
C	-4.796894	1.668537	0.418997
C	-3.603391	1.391944	-0.329333
C	-3.770219	-2.383435	-0.410638
C	-4.585633	-3.379137	0.037958
C	-5.770057	-3.079917	0.768490
C	-6.092046	-1.783841	1.029318
C	-5.152215	3.023442	0.709664
C	-4.374886	4.059843	0.292958
C	-3.186806	3.796081	-0.444562
C	-2.818743	2.518350	-0.743951
C	8.277701	-0.150315	0.942293
C	8.737201	0.428836	2.052167
H	0.308275	1.785594	-1.413112
H	0.621978	-0.626347	-2.854141
H	-0.576279	-2.887037	-1.277276
H	-1.625321	-1.736226	1.265232
H	-1.137414	1.196790	1.183075
H	2.535641	-2.406233	-1.358409
H	1.120834	-3.185708	1.311776
H	0.760159	-0.574794	2.869835
H	1.970059	1.671624	1.085997
H	3.305502	-0.986639	1.145371
H	-1.866862	0.562121	-2.177894
H	-2.193100	-1.133257	-2.053629
H	-1.897981	2.360961	-1.292053
H	-2.564508	4.624664	-0.769131
H	-4.651631	5.084799	0.519503
H	-6.063215	3.204389	1.274197
H	-6.501108	0.827008	1.414166
H	-6.990643	-1.536567	1.588631
H	-6.407210	-3.887205	1.116174
H	-4.327356	-4.415395	-0.157856
H	-2.865021	-2.654244	-0.940838
H	2.866121	1.659114	-1.670359
H	3.087577	0.154229	-2.550774
H	4.318388	2.219251	0.260813
H	6.511817	1.930157	1.321431
H	8.908645	-0.882310	0.439231
H	8.151515	1.142851	2.624929
H	9.723619	0.193237	2.438227
H	7.101824	-1.696606	-0.898201

Rotamer-4 of **3**

E(ω-B97XD/6-31G*)= -1257.168775

C	-4.281007	-0.597816	1.278550
C	-4.091177	-1.058568	-0.026293
C	-4.501776	-0.246578	-1.082650
C	-5.065676	0.999563	-0.840341

C	-5.236335	1.476714	0.463858
C	-4.844288	0.646360	1.521538
C	-3.418612	-2.382468	-0.286767
C	-1.888586	-2.300123	-0.437801
B	-1.131240	-3.412908	-1.503217
B	-1.227071	-1.686949	-1.895422
B	0.295517	-2.569551	-2.126530
B	0.458185	-3.740741	-0.793211
B	-0.963267	-3.574306	0.250487
B	0.564071	-2.827050	0.717539
B	1.343869	-2.203095	-0.745651
B	0.307388	-0.937847	-1.431227
B	-1.102647	-0.785742	-0.394545
B	-0.948072	-1.951100	0.931280
C	0.415199	-1.172770	0.270234
C	1.070632	-0.118407	1.186862
C	2.256259	0.627517	0.612573
C	3.560584	0.119561	0.787568
C	4.683017	0.845607	0.263446
C	4.470812	2.045878	-0.408827
C	3.190456	2.562461	-0.588367
C	2.058738	1.845110	-0.072520
C	3.839290	-1.111891	1.468278
C	5.112553	-1.575795	1.612617
C	6.218770	-0.847922	1.090525
C	6.004838	0.326310	0.437110
C	2.989273	3.798535	-1.279626
C	1.740523	4.308066	-1.461349
C	0.611560	3.601493	-0.959566
C	0.764181	2.421459	-0.294604
C	-5.824760	2.812772	0.670689
C	-5.832454	3.513048	1.805687
H	-1.659937	0.227525	-0.146965
H	-1.413144	-1.640990	1.976861
H	1.194189	-3.100422	1.687253
H	2.520632	-2.074287	-0.781557
H	0.770312	0.036138	-1.920645
H	-1.533681	-4.429785	0.845437
H	1.009263	-4.786641	-0.924081
H	0.730122	-2.775117	-3.214260
H	-1.967490	-1.295890	-2.737962
H	-1.823605	-4.176258	-2.094696
H	0.294208	0.589089	1.483115
H	1.360757	-0.621826	2.110611
H	-0.122765	1.907727	0.055622
H	-0.383820	4.007711	-1.112008
H	1.598576	5.247543	-1.986493
H	3.863340	4.321283	-1.659250
H	5.324767	2.591321	-0.804685
H	6.836852	0.894249	0.029004
H	7.225023	-1.236136	1.214431

H	5.286322	-2.516892	2.125462
H	3.023776	-1.708104	1.859559
H	-3.812512	-2.829573	-1.203687
H	-3.637955	-3.080963	0.525847
H	-3.984634	-1.225108	2.115562
H	-4.996305	0.966649	2.547826
H	-6.279754	3.255510	-0.214603
H	-5.376690	3.148865	2.722428
H	-6.295902	4.492998	1.853557
H	-5.376052	1.618315	-1.678640

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E(ω-B97XD/6-31G*)= -1268.008355

C	3.753336	2.978715	-0.703938
C	2.387532	3.077946	-0.283709
C	1.860192	2.122372	0.650910
C	2.757305	1.103205	1.117842
C	4.053001	1.040026	0.695464
C	4.565592	1.991399	-0.231965
C	0.509770	2.211632	1.054196
C	-0.311864	3.243639	0.550733
C	0.230275	4.196096	-0.377981
C	1.562526	4.089048	-0.772771
C	-0.606277	5.237850	-0.893443
C	-1.913876	5.338779	-0.523374
C	-2.462694	4.394703	0.391382
C	-1.694518	3.391457	0.906324
C	-0.059100	1.204697	2.032209
C	-0.677454	-0.062914	1.406727
B	0.014412	-0.748944	0.014611
B	0.176914	-1.525270	1.601305
B	-1.296502	-1.222905	2.512264
B	-2.382680	-0.278616	1.484288
B	-1.565913	0.020633	-0.062261
B	-1.297611	-1.543199	-0.838638
B	-2.790437	-1.255104	0.070493
B	-2.632601	-2.025294	1.667165
B	-1.036512	-2.786414	1.738929
B	-1.952558	-2.806995	0.224501
C	-0.283858	-2.414327	0.235925
C	0.680883	-3.453923	-0.366631
C	2.126600	-3.024467	-0.425706
C	3.007830	-3.326702	0.612534
C	4.336100	-2.914833	0.559710
C	4.821976	-2.178613	-0.527064
C	3.935999	-1.887289	-1.573110
C	2.613824	-2.306544	-1.522147
C	6.230867	-1.741075	-0.528471
C	6.767141	-0.789585	-1.299111

H	1.256875	-1.572858	2.080421
H	0.990413	-0.328780	-0.495556
H	-1.685827	1.048970	-0.634027
H	-3.047840	0.576908	1.968419
H	-1.209672	-0.996401	3.674855
H	-1.196291	-1.734353	-2.005396
I	-4.713526	-1.064763	-0.951772
H	-3.567423	-2.473179	2.247643
H	-0.743460	-3.800125	2.283520
H	-2.289888	-3.840468	-0.252320
H	-0.828814	1.669441	2.650553
H	0.711939	0.884315	2.735859
H	-2.159034	2.681941	1.580459
H	-3.508492	4.470655	0.674649
H	-2.541665	6.129662	-0.923030
H	-0.172331	5.947152	-1.594182
H	1.966216	4.809578	-1.481708
H	4.127327	3.715155	-1.411379
H	5.601005	1.921809	-0.552536
H	4.702006	0.249881	1.059808
H	2.406178	0.346812	1.809227
H	0.588372	-4.370356	0.223321
H	0.321733	-3.688672	-1.372891
H	1.944554	-2.069370	-2.346162
H	4.284211	-1.340956	-2.444553
H	6.872473	-2.246421	0.193374
H	6.182901	-0.225273	-2.021656
H	7.821432	-0.541326	-1.222880
H	5.007461	-3.167038	1.377595

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E(B3LYP/6-31G*)= -12957.425947

C	10.997391	-8.675706	9.935420
C	11.304010	-8.231542	8.669913
C	12.030023	-9.036658	7.724786
C	12.507913	-10.312740	8.231019
C	12.122879	-10.763896	9.535870
C	11.374806	-9.976125	10.371077
C	12.354136	-8.643690	6.379730
C	13.426491	-9.338192	5.719428
C	13.889554	-10.608696	6.253534
C	13.362229	-11.093480	7.451179
C	14.900266	-11.358123	5.566808
C	15.514370	-10.865015	4.445682
C	15.149781	-9.574086	3.972242
C	14.147594	-8.849969	4.575225
C	11.489260	-7.616848	5.622756
B	9.887916	-7.244835	6.221627
B	11.164505	-5.997146	6.229749
B	12.141987	-6.234517	4.755130

B	10.899753	-4.955724	4.806699
B	9.507177	-5.586971	5.724574
B	9.468475	-5.549675	3.933719
B	11.093315	-5.966865	3.332911
B	11.458055	-7.632146	3.841959
B	10.095418	-8.256350	4.765338
B	9.810982	-7.209676	3.355102
C	8.945645	-6.961107	4.822363
C	7.456945	-7.378276	4.915383
C	6.468167	-6.466864	4.214664
C	6.112518	-6.684091	2.874147
C	5.206334	-5.839114	2.231623
C	4.618112	-4.750622	2.906950
C	4.967630	-4.545850	4.257379
C	5.873102	-5.389759	4.897013
C	3.679022	-3.885819	2.175392
C	3.016223	-2.806889	2.641692
Si	1.873736	-1.804002	1.572011
O	0.244520	-2.173746	1.845349
Si	-1.397468	-2.008696	1.480696
C	-2.418961	-3.139825	2.542015
C	-3.623455	-2.788279	3.037908
C	-4.525648	-3.627788	3.843091
C	-5.869178	-3.234756	3.998750
C	-6.772157	-4.022194	4.715605
C	-6.359797	-5.222869	5.313918
C	-5.009191	-5.599754	5.192886
C	-4.109448	-4.822029	4.467417
C	-7.340703	-6.083382	6.086333
C	-8.001369	-7.237362	5.289908
B	-8.587575	-8.536342	6.233207
C	-9.985182	-9.134488	5.364315
C	-11.187444	-9.678425	6.160377
C	-12.500833	-9.726354	5.576280
C	-13.667075	-9.754249	6.444185
C	-13.503242	-9.835692	7.827544
C	-12.244679	-10.044684	8.393112
C	-11.060169	-10.024398	7.550645
C	-14.986735	-9.718269	5.885535
C	-15.187687	-9.743750	4.530540
C	-14.059180	-9.828059	3.668623
C	-12.777403	-9.810854	4.167675
C	-9.838949	-10.426302	8.195425
C	-9.774749	-10.716536	9.538765
C	-10.924685	-10.616474	10.369966
C	-12.129223	-10.299179	9.798987
O	2.209588	-2.103715	-0.056773
Si	1.965053	-1.885908	-1.716085
C	3.161585	-2.948460	-2.661677
C	4.259155	-3.477388	-2.081417
C	5.279288	-4.340185	-2.697195

C	6.350724	-4.794289	-1.902390
C	7.342818	-5.621481	-2.431159
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B	8.947296	-9.383652	-5.444196
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C	11.110061	-12.625555	-4.037328
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Si	1.788508	1.386206	-1.765678
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Si	-1.477285	1.210416	-1.872321
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H	12.298465	15.088571	2.068737
H	8.451667	13.308895	2.639540
H	9.972083	14.598388	1.289725
H	-14.760031	11.955184	6.192373
H	-16.171023	10.749685	4.540230
H	-13.655223	7.306445	4.870165
H	-15.612470	8.379230	3.966671
H	-11.364052	12.017401	9.534249
H	-9.677687	10.864557	10.948338
H	-10.001734	7.362132	8.515728
H	-9.086408	8.487587	10.436832
H	-13.778344	11.072788	-7.748299
H	-13.242371	10.153410	-9.889508
H	-11.587331	9.278976	-11.523183
H	-8.473689	9.689017	-8.620389
H	-9.180044	9.139565	-10.855136
H	-14.316345	12.334322	-5.791723
H	-13.645586	13.446208	-3.673407
H	-9.642147	12.024827	-4.168100
H	-11.256796	13.321343	-2.940066
H	12.444704	13.382643	-6.899008
H	13.818154	13.686075	-4.968433
H	14.947037	12.789523	-2.944395
H	13.182977	8.954261	-3.631667
H	14.652078	10.375062	-2.358699
H	11.399095	13.068598	-9.025844

H	10.328085	11.603145	-10.722521
H	10.598782	8.275938	-8.049540
H	10.020751	9.173933	-10.206736
H	14.398425	-12.592420	-5.083995
H	14.653090	-11.500418	-7.196760
H	13.684851	-10.363920	-9.182453
H	9.785397	-10.599669	-7.441656
H	11.210754	-10.006039	-9.289496
H	14.175182	-14.009111	-3.172117
H	12.772398	-15.152792	-1.469978
H	9.271602	-13.285262	-3.067601
H	10.294206	-14.811319	-1.510163
H	-11.970209	-13.032090	-8.813013
H	-13.434891	-13.779791	-7.078918
H	-14.650781	-13.391884	-4.946958
H	-12.833938	-9.536660	-4.585811
H	-14.369142	-11.202374	-3.769433
H	-10.827654	-12.218571	-10.749019
H	-9.675010	-10.395773	-11.982716
H	-10.049772	-7.829094	-8.582476
H	-9.380319	-8.174516	-10.868878
H	-14.378049	-9.800858	8.471128
H	-15.827037	-9.702427	6.573561
H	-16.190051	-9.732661	4.115806
H	-11.966336	-9.925118	3.470825
H	-14.209841	-9.922736	2.598034
H	-13.036448	-10.264778	10.395234
H	-10.849037	-10.824562	11.431957
H	-8.833250	-11.046684	9.966244
H	-8.949286	-10.574468	7.608614
H	13.673208	-12.069107	7.814703
H	15.188163	-12.319016	5.983406
H	16.290370	-11.430851	3.941153
H	13.948676	-7.861146	4.202557
H	15.681398	-9.143933	3.129502
H	12.471767	-11.741232	9.856509
H	11.102064	-10.318553	11.363639
H	11.041189	-7.219109	8.417338
H	10.475600	-8.013358	10.618872

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