Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Photoluminescence in *m*-carborane-anthracene triads: a combined experimental and computational study

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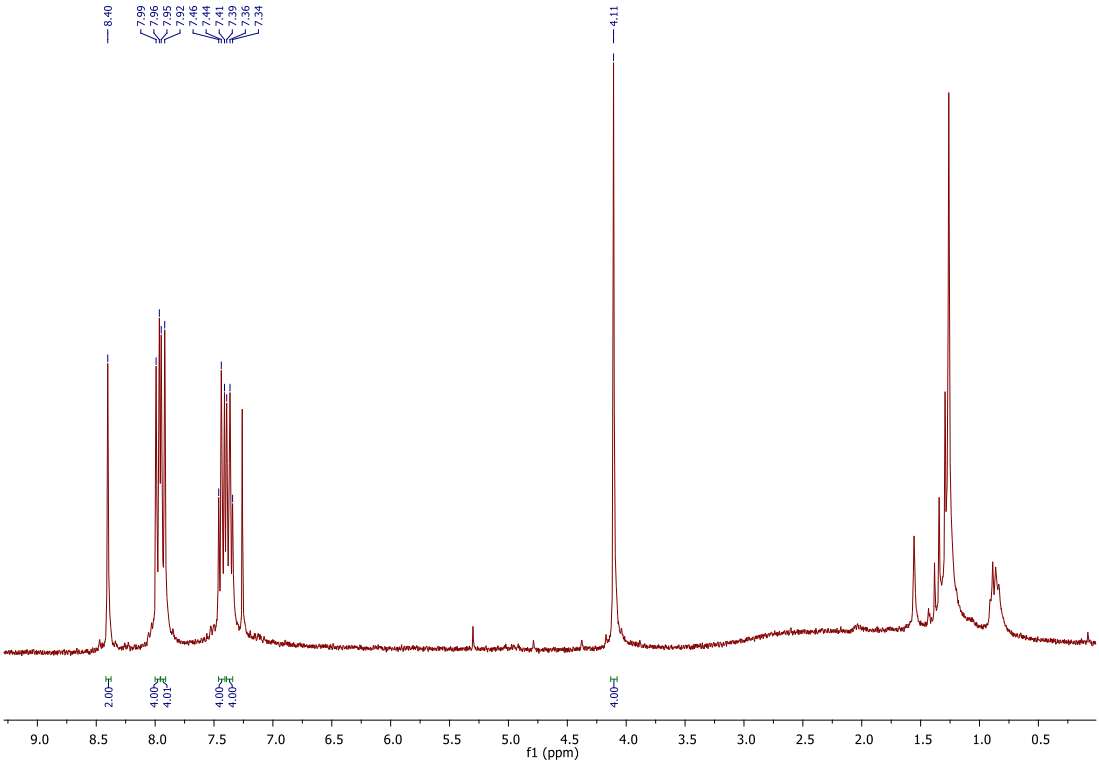
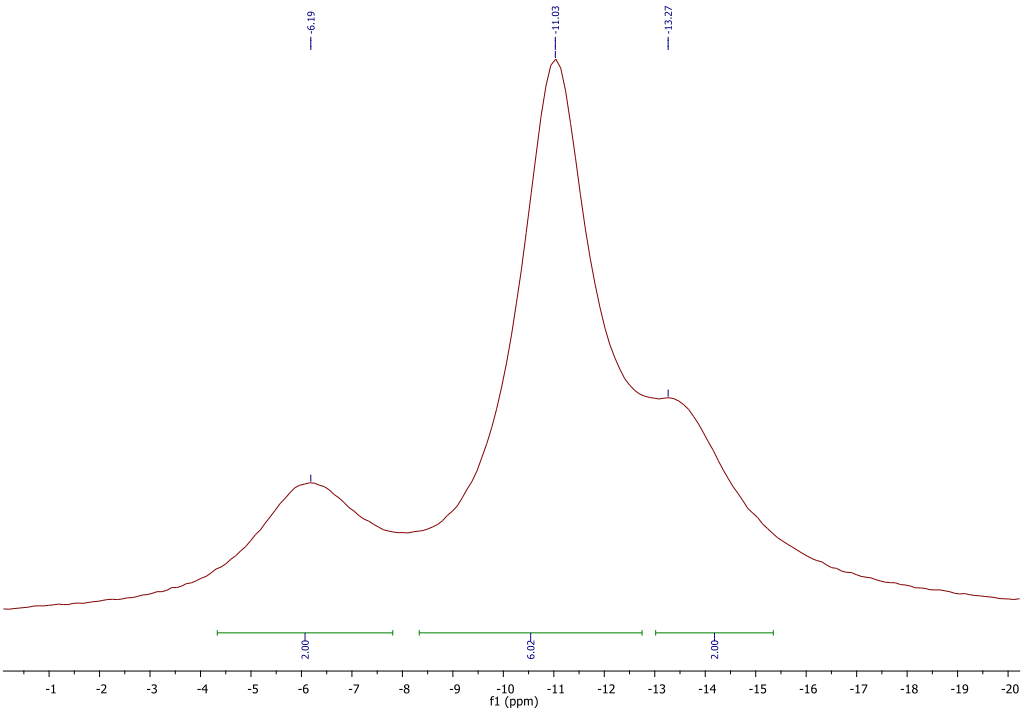
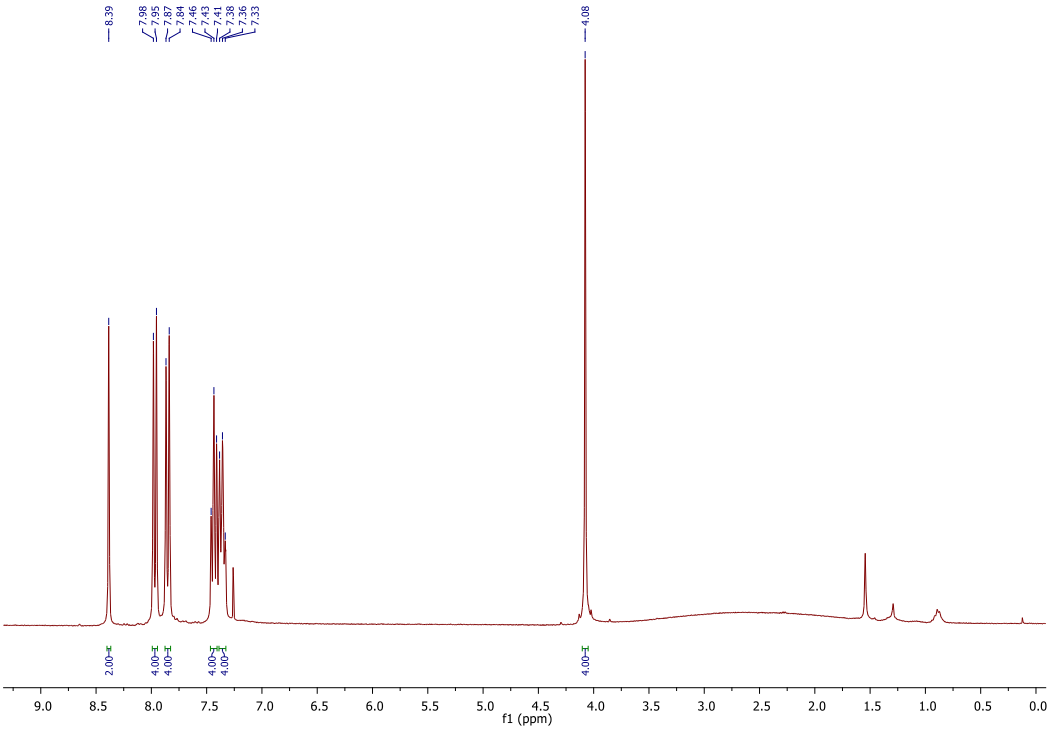
NMR spectra



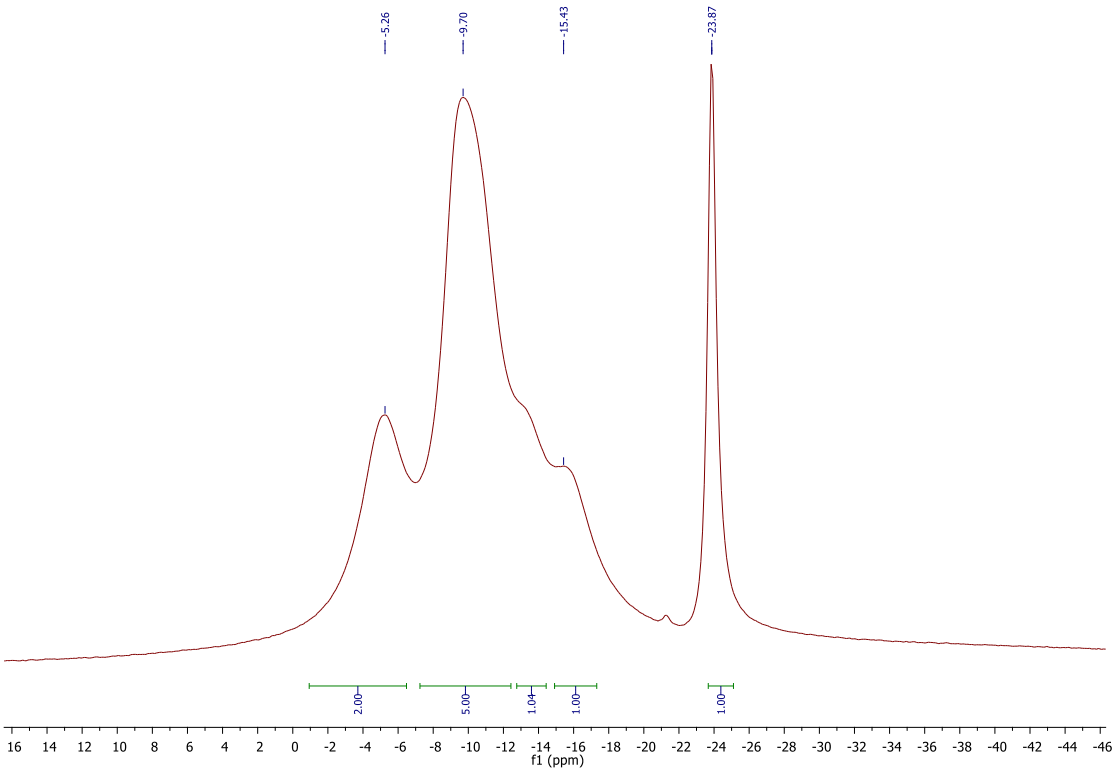
^{1}H NMR spectrum of **4**.



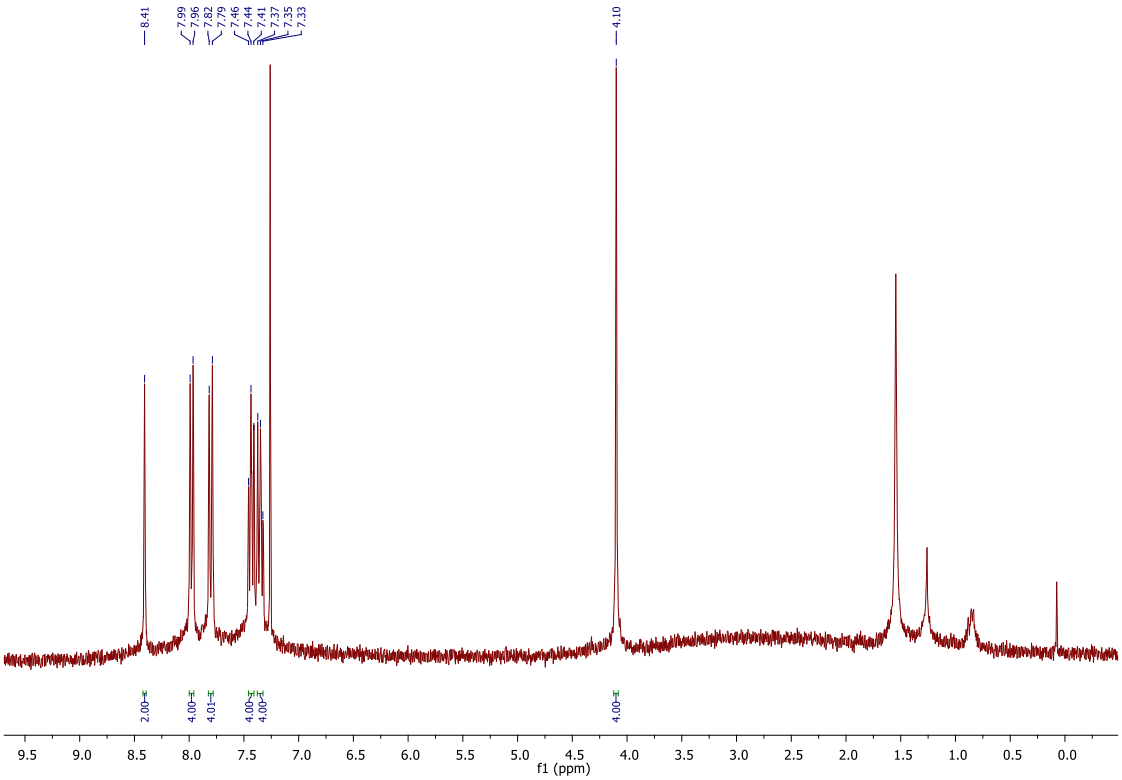
^{11}B{^{1}H} NMR spectrum of **4**.



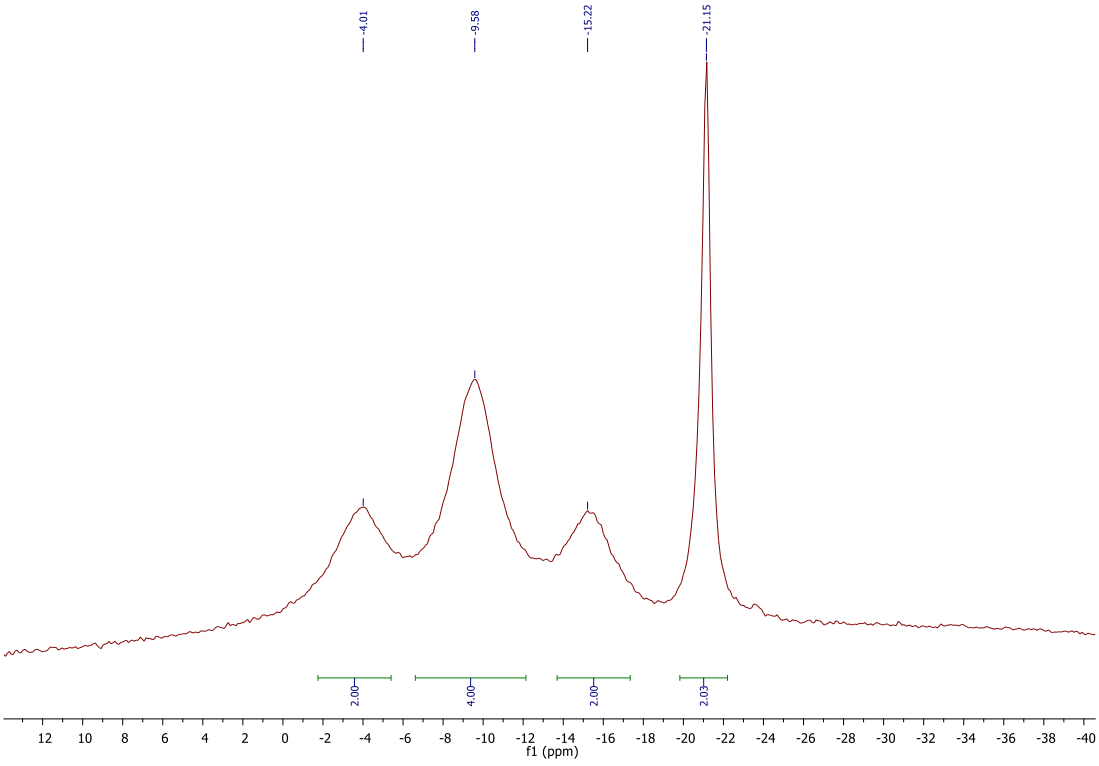
^{1}H NMR spectrum of **5**.



^{11}B{^{1}H} NMR spectrum of **5**.



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



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

Computational details

All calculations were carried out with the Gaussian 09 program package[1] at B3LYP/6-31G* level of theory as it was implemented in G09. Single point energy calculations at B3LYP/6-311+G** level of theory were also carried out. Our present study verified the earlier wisdom since using larger basis set does not improve the TD-DFT results, therefore this basis set was used for H, B, C atoms, and for the iodine atoms LANL2DZ basis was applied. 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[2] and VMD program[3] were used. The charge density difference maps were calculated with Multiwfn program.[4]

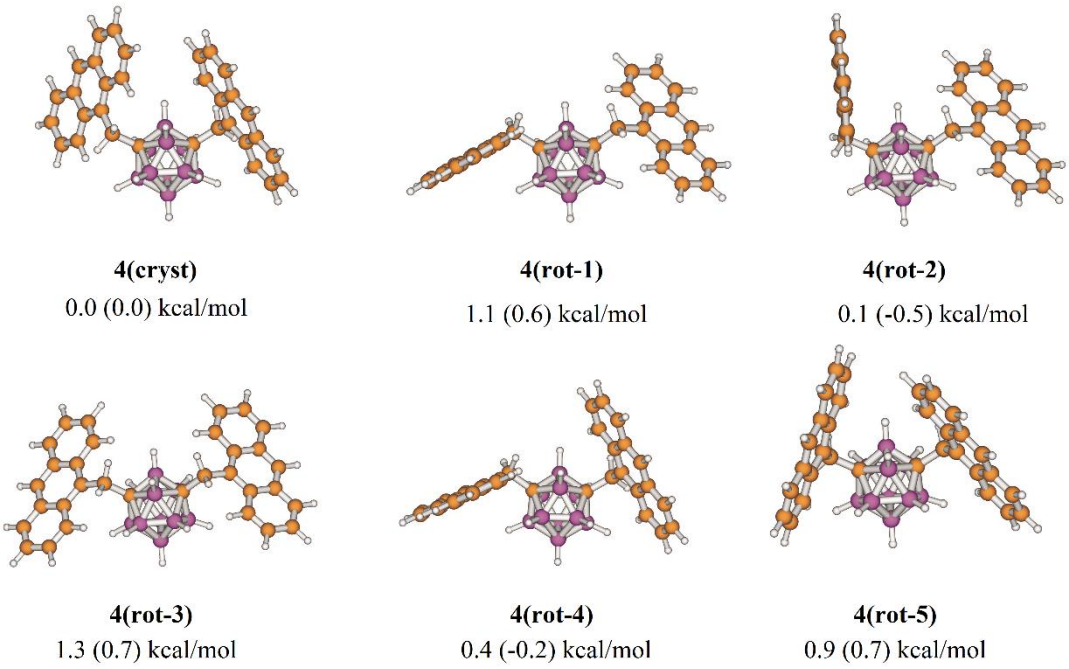


Figure S1 The investigated rotamers of **4** and their relative energies in kcal/mol unit at B3LYP/6-31G* and B3LYP/6-311+G**//B3LYP/6-31G* (in bracket) level of theory

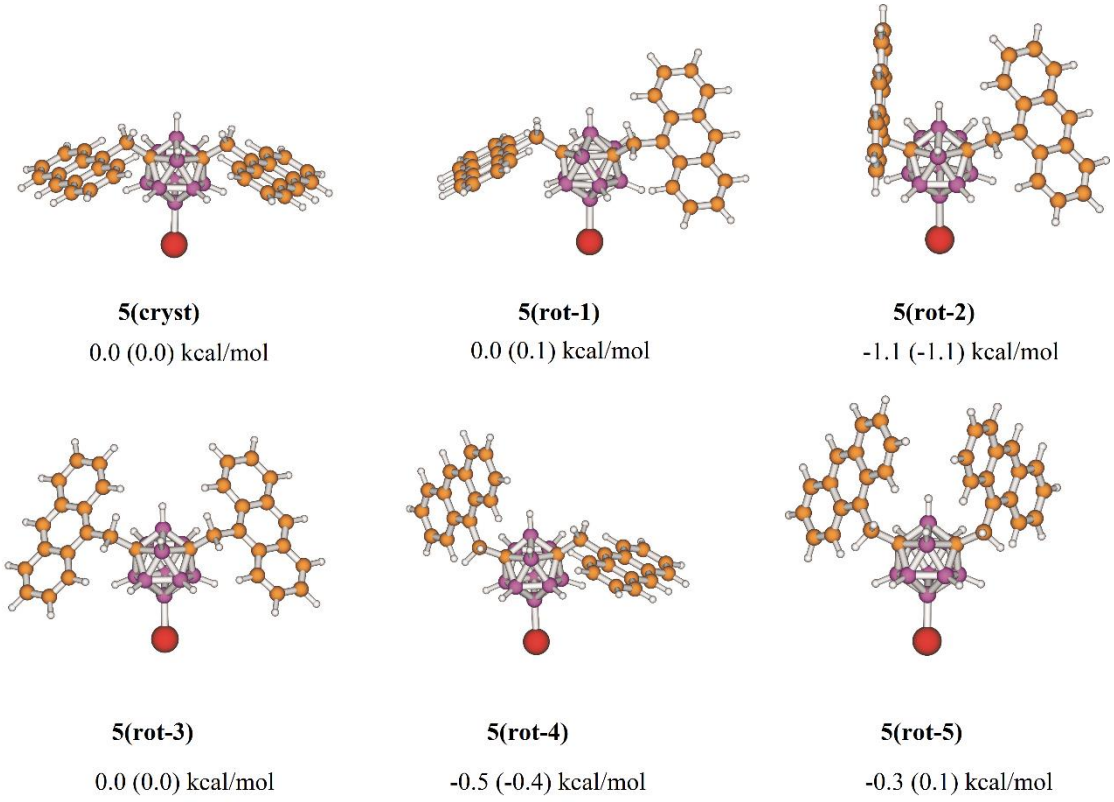


Figure S2 The investigated rotamers of **5** and their relative energies in kcal/mol unit at B3LYP/6-31G* and B3LYP/6-311+G**//B3LYP/6-31G* (in bracket) level of theory (for iodine LANL2DZ basis set was applied).

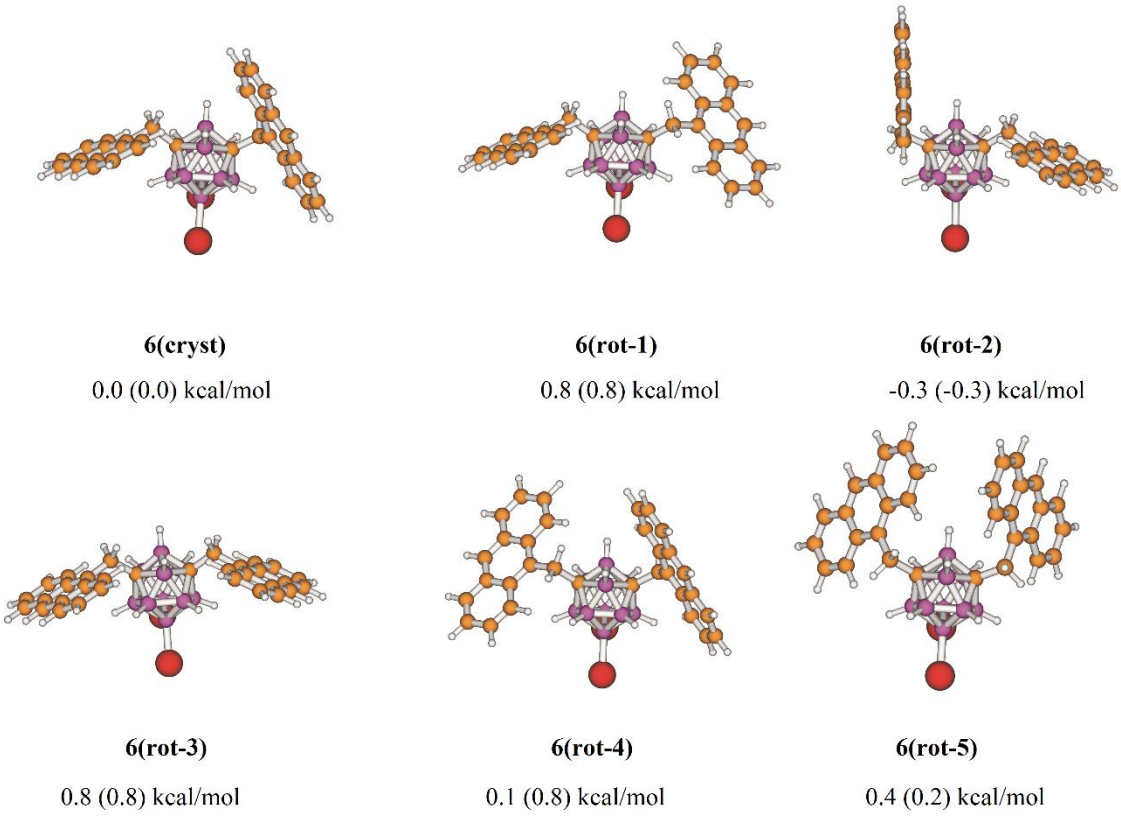


Figure S3 The investigated rotamers of **6** and their relative energies in kcal/mol unit at B3LYP/6-31G* and B3LYP/6-311+G**//B3LYP/6-31G* (in bracket) level of theory (for iodine LANL2DZ basis set was applied)

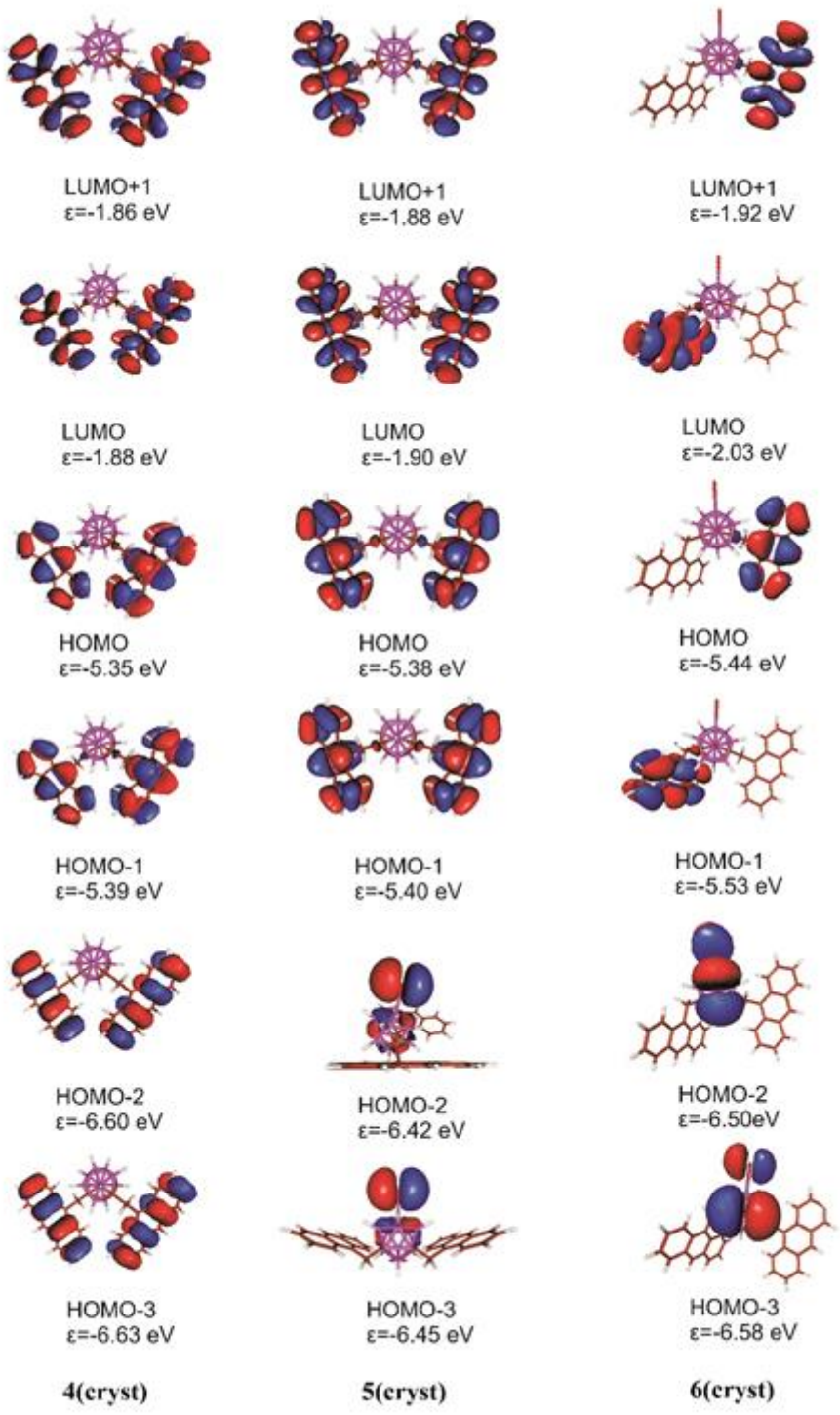


Figure S4 The Kohn-Sahm orbitals (and their energies in eV unit) of **4, 5** and **6** at B3LYP/6-31G* level of theory. The structures (**4(cryst)**, **5(cryst)**, **6(cryst)**) correspond to the crystal structures (the geometry optimization was started from the crystal structure)

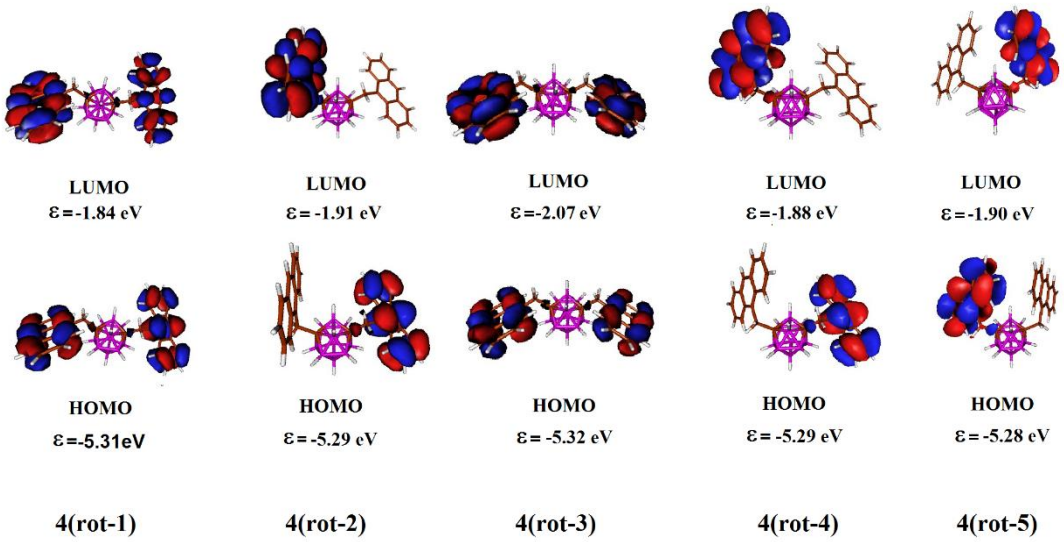


Figure S5 The Kohn-Sahm frontier orbitals (and their energies in eV unit) of the investigated rotamers of **4** at B3LYP/6-31G* level of theory.

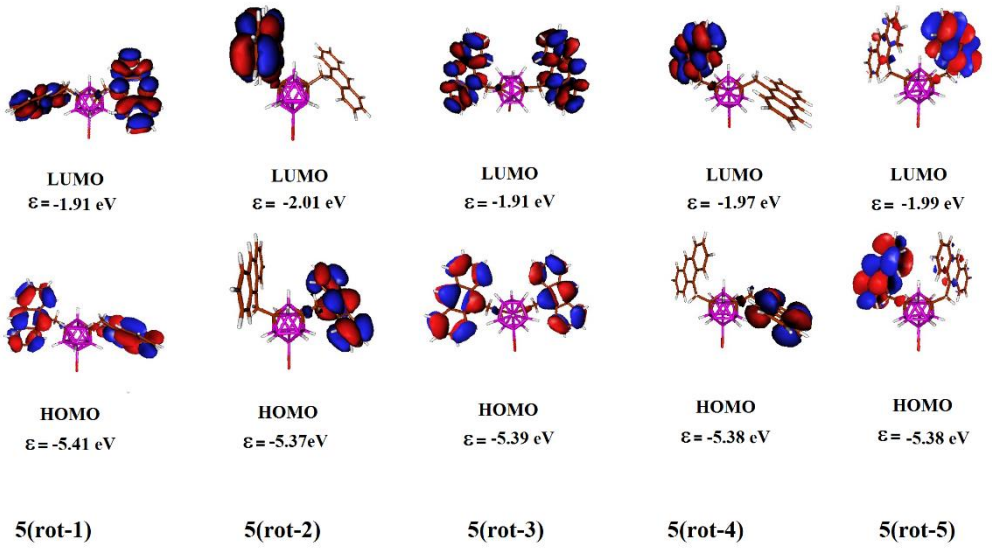


Figure S6 The Kohn-Sahm frontier orbitals (and their energies in eV unit) of the investigated rotamers of **5** at B3LYP/6-31G* level of theory.

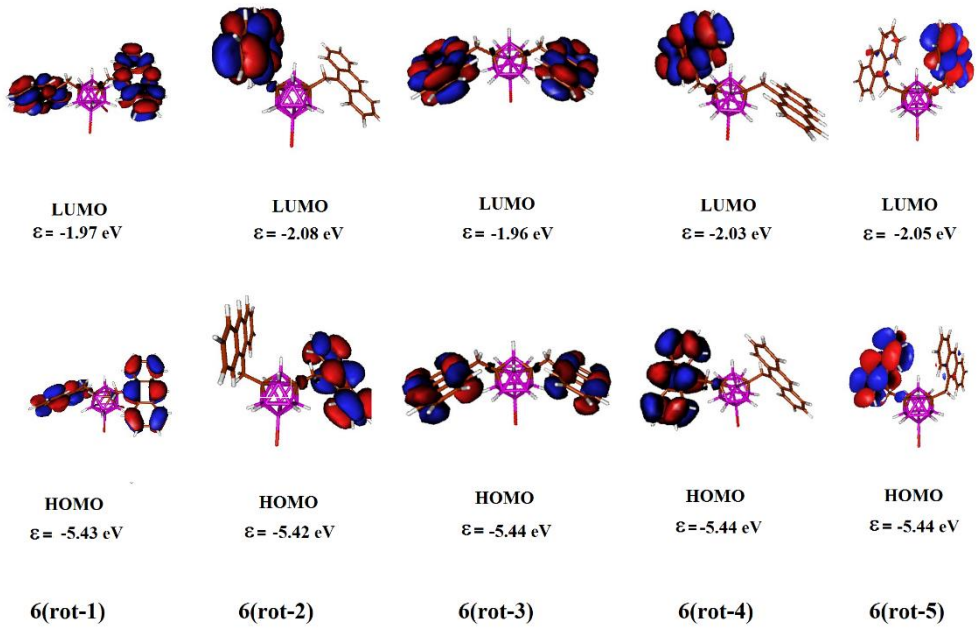


Figure S7 The Kohn-Sahm frontier orbitals (and their energies in eV unit) of the investigated rotamers of **6** at B3LYP/6-31G* level of theory.

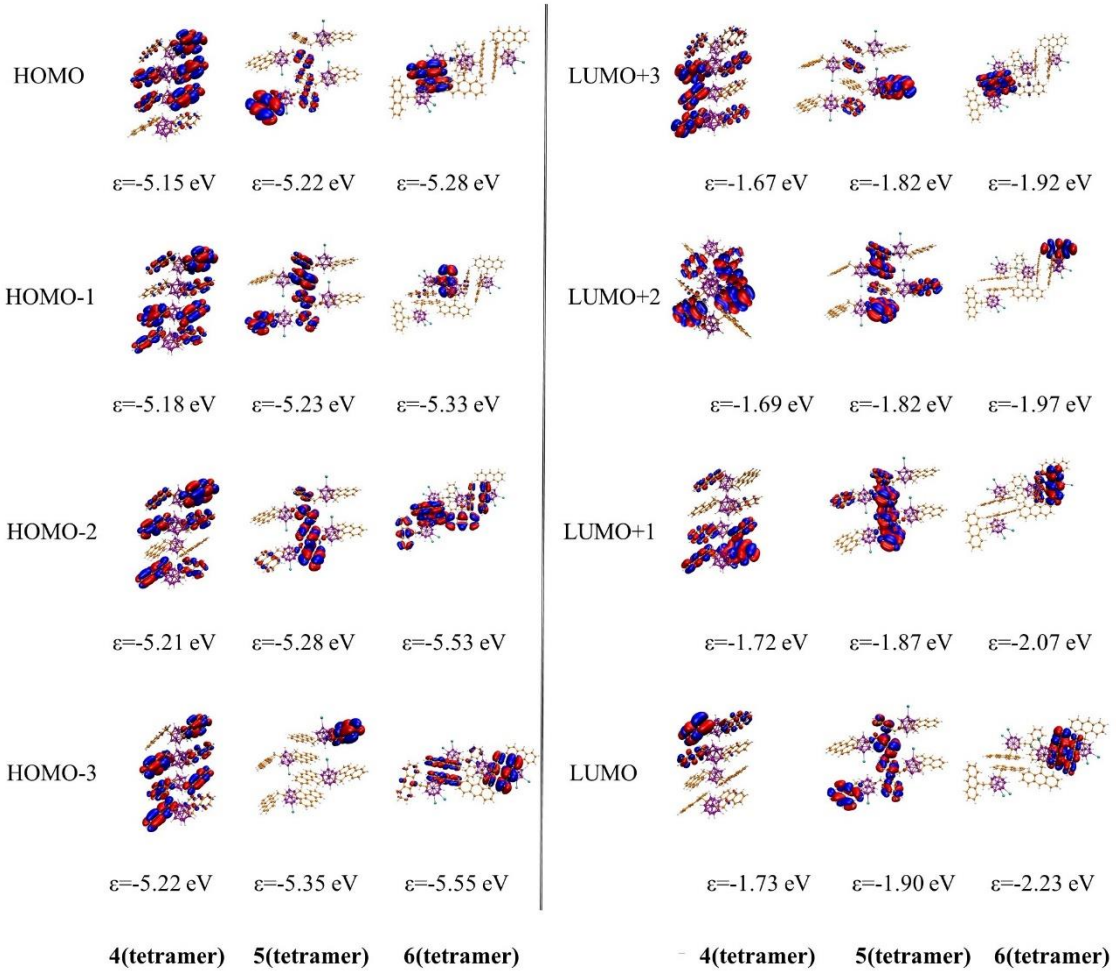


Figure S8. Kohn-Sahm orbitals of the tetrameric structures of **4-6**. The geometries were taken from the X-ray structures and used without further optimization.

Table S1 TD-DFT results of **4(cryst)**

	λ_{abs} (nm) Calculated	Intensity (*f*)	Transition	%
4(cryst)	397	0.0570	HOMO→LUMO	98.00
	394	0.032	HOMO-1→LUMO HOMO→LUMO+1	27.38 72.00
	388	0.0932	HOMO-1→LUMO HOMO→LUMO+1	72.00 25.92
	388	0.0492	HOMO-1→LUMO	98.00

Table S2 TD-DFT results of **4(rot-1)**

	λ_{abs} (nm) Calculated	Intensity (*f*)	Transition	%
4(rot-1)	392	0.2113	HOMO→LUMO HOMO-1→LUMO+1	84.50 13.52
	388	0.0029	HOMO→LUMO+1 HOMO-1→LUMO	42.32 56.18
	383	0.0000	HOMO→LUMO+1 HOMO-1→LUMO	56.18 42.32
	382	0.0225	HOMO→LUMO HOMO-1→LUMO+1	13.52 87.12

Table S3 TD-DFT results of **4(rot-2)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
4(rot-2)	406	0.0027	HOMO→LUMO	99.97
	391	0.1452	HOMO-1→LUMO+1 HOMO→LUMO+1	56.18 40.50
	388	0.0645	HOMO→LUMO+1 HOMO-1→LUMO	56.18 42.32
	375	0.0005	HOMO-1→LUMO+1	100

Table S4 TD-DFT results of **4(rot-3)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
4(rot-3)	392	0.1819	HOMO→LUMO HOMO-1→LUMO+1	20.48 79.38
	388	0.0345	HOMO→LUMO+1 HOMO-1→LUMO	44.18 54.08
	385	0.0000	HOMO→LUMO+1 HOMO-1→LUMO	54.08 44.18
	384	0.0128	HOMO→LUMO HOMO-1→LUMO+1	20.48 79.38

Table S5 TD-DFT results of **4(rot-4)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
4(rot-4)	401	0.0008	HOMO→LUMO	99.97
	391	0.1356	HOMO-1→LUMO HOMO→LUMO+1	54.08 46.08
	388	0.0741	HOMO-1→LUMO HOMO→LUMO+1	44.18 52.02
	377	0.0001	HOMO-1→LUMO	99.97

Table S6 TD-DFT results of **4(rot-5)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
4(rot-5)	414	0.0017	HOMO→LUMO	100
	393	0.0468	HOMO-1→LUMO HOMO→LUMO+1	62.72 35.28
	388	0.1355	HOMO-1→LUMO HOMO→LUMO+1	35.28 62.72
	384	0.0018	HOMO-1→LUMO	98.00

Table S7 TD-DFT results of **5(cryst)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
5(cryst)	392	0.1815	HOMO→LUMO HOMO-1→LUMO+1	79.13 19.34
	388	0.0298	HOMO→LUMO+1 HOMO-1→LUMO	45.13 53.05
	385	0.0000	HOMO→LUMO+1 HOMO-1→LUMO	46.08 54.08
	384	0.0135	HOMO→LUMO HOMO-1→LUMO+1	79.63 20.10

Table S8 TD-DFT results of **5(rot-1)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
5(rot-1)	403	0.2080	HOMO→LUMO	76.88
			HOMO-1→LUMO+1	18.00
	399	0.0018	HOMO→LUMO+1	44.18
			HOMO-1→LUMO	54.08
	391	0.0022	HOMO-1→LUMO	38.72
			HOMO-1→LUMO+1	5.12
			HOMO→LUMO	6.48
			HOMO→LUMO+1	48.02
	389	0.0091	HOMO-1→LUMO	5.12
			HOMO-1→LUMO+1	74.42
			HOMO→LUMO	14.58
			HOMO→LUMO+1	5.12

Table S9 TD-DFT results of **5(rot-2)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
5(rot-2)	416	0.0033	HOMO→LUMO	99.97
	401	0.1348	HOMO-1→LUMO HOMO→LUMO+1	58.32 38.72
	399	0.0674	HOMO-1→LUMO HOMO→LUMO+1	38.72 58.32
	379	0.0003	HOMO-1→LUMO+1	99.97

Table S10 TD-DFT results of **5(rot-3)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
5(rot-3)	403	0.1644	HOMO→LUMO HOMO-1→LUMO+1	24.50 74.42
	399	0.0427	HOMO→LUMO+1 HOMO-1→LUMO	48.02 50.00
	392	0.0000	HOMO→LUMO+1 HOMO-1→LUMO	50.00 48.02
	391	0.069	HOMO→LUMO HOMO-1→LUMO+1	24.50 74.42

Table S11 TD-DFT results of **5(rot-4)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
5(rot-4)	398	0.0005	HOMO→LUMO	99.97
	391	0.2072	HOMO-1→LUMO HOMO→LUMO+1	52.02 44.18
	388	0.0249	HOMO-1→LUMO HOMO→LUMO+1	44.18 52.02
	376	0.0001	HOMO-1→LUMO+1	99.97

Table S12 TD-DFT results of **5(rot-5)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
5(rot-5)	418	0.0066	HOMO→LUMO	99.97
	404	0.0394	HOMO-1→LUMO HOMO→LUMO+1	62.72 35.28
	399	0.1354	HOMO-1→LUMO HOMO→LUMO+1	35.28 62.72
	392	0.0051	HOMO-1→LUMO+1	99.97

Table S13 TD-DFT results of **6(cryst)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
6(cryst)	404	0.0010	HOMO→LUMO	99.97
	392	0.1363	HOMO-1→LUMO HOMO→LUMO+1	57.25 41.22
	389	0.1363	HOMO-1→LUMO HOMO→LUMO+1	41.04 57.03
	376	0.001	HOMO-1→LUMO+1	99.97

Table S14 TD-DFT results of **6(rot-1)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
6(rot-1)	394	0.2089	HOMO→LUMO HOMO-1→LUMO+1	11.52 87.12
	389	0.0007	HOMO→LUMO+1 HOMO-1→LUMO	36.98 60.50
	384	0.0000	HOMO→LUMO+1 HOMO-1→LUMO	62.72 36.98
	382	0.0252	HOMO→LUMO HOMO-1→LUMO+1	11.52 87.12

Table S15 TD-DFT results of **6(rot-2)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
6(rot-2)	412	0.0024	HOMO→LUMO	99.97
	392	0.1546	HOMO-1→LUMO HOMO→LUMO+1	60.50 36.98
	389	0.0770	HOMO-1→LUMO HOMO→LUMO+1	36.98 60.50
	371	0.0003	HOMO-1→LUMO+1	99.97

Table S16 TD-DFT results of **6(rot-3)**

	λ_{abs} (nm) Calculated	Intensity (*f*)	Transition	%
6(rot-3)	392	0.1812	HOMO→LUMO HOMO-1→LUMO+1	79.38 19.22
	388	0.0328	HOMO→LUMO+1 HOMO-1→LUMO	44.18 54.08
	386	0.0000	HOMO→LUMO+1 HOMO-1→LUMO	54.08 44.18
	385	0.0137	HOMO→LUMO HOMO-1→LUMO+1	20.48 79.38

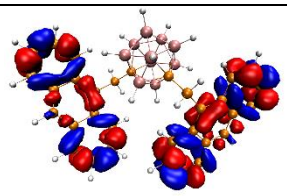
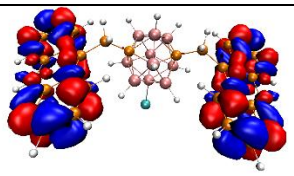
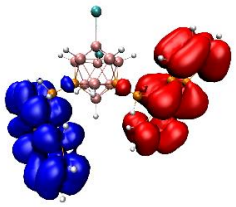
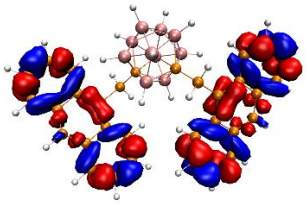
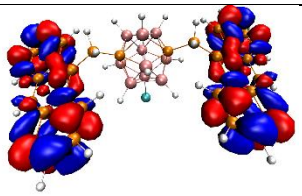
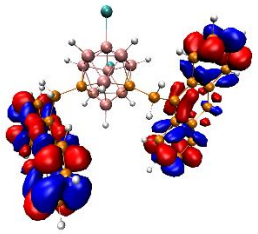
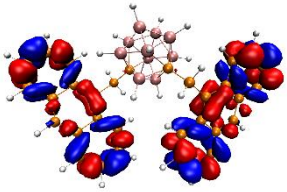
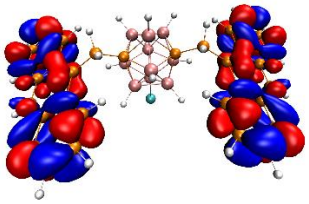
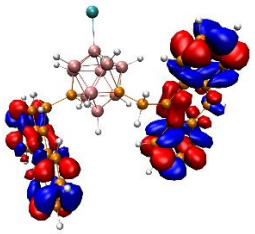
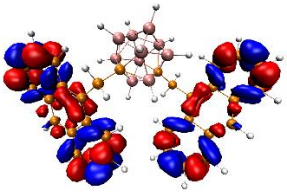
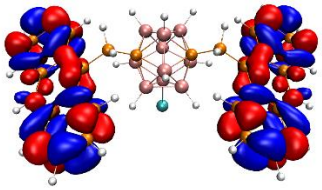
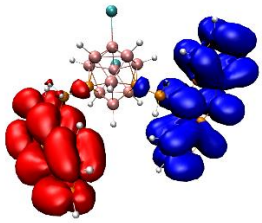
Table S17 TD-DFT results of **6(rot-4)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
6(rot-4)	398	0.0005	HOMO→LUMO	99.97
	392	0.2073	HOMO-1→LUMO HOMO→LUMO+1	54.08 44.18
	389	0.0284	HOMO-1→LUMO HOMO→LUMO+1	44.18 54.08
	377	0.0001	HOMO-1→LUMO+1	99.97

Table S18 TD-DFT results of **6(rot-5)**

	λ_{abs} **(nm) Calculated**	**Intensity (*f*)**	**Transition**	**%**
6(rot-5)	413	0.0038	HOMO→LUMO	98.00
	394	0.0485	HOMO-1→LUMO HOMO→LUMO+1	62.72 33.62
	389	0.1446	HOMO-1→LUMO HOMO→LUMO+1	35.28 62.72
	384	0.0053	HOMO-1→LUMO+1	98.00

Table S19 The charge density difference maps of the first 4 transitions of 4(cryst), 5(cryst) and 6(cryst). (The blue and red parts correspond to the region where electron density is increased and decreased after electron excitation, respectively. Isosurface value: 0.0005). The first 4 lowest transitions of 4(cryst) and 5(cryst) exhibit local transition mode, there is no charge transfer between the different parts of the molecules. In case of 6(cryst) the first and the fourth lowest transitions have charge transfer character, the charge transfer occurs between the two anthracene unit, but as it was stated above the oscillator strength of these transitions are significantly lower (0.001) than the local excitations in case of Type I rotamers of 6 (compare the f values in Table S13-S18). The carborane cage was not involved in the transitions.

	4(cryst)	**5(cryst)**	**6(cryst)**
S0→S1			
S0→S2			
S0→S3			
S0→S4			

XYZ coordinates and total energies of the investigated systems

4(cryst)
E(B3LYP/6-31G*)= -1487.396234
E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1487.72031

C	3.917633	3.677656	0.439407
C	4.102732	2.281408	0.192812
C	3.065732	1.526707	-0.478417
C	1.887856	2.249069	-0.862524
C	1.755046	3.592939	-0.623522
C	2.780205	4.323511	0.039236
C	3.260395	0.146588	-0.744094
C	4.478435	-0.478222	-0.370979
C	5.499863	0.287527	0.309640
C	5.281339	1.639916	0.577375
C	6.725802	-0.344438	0.687304
C	6.958682	-1.662731	0.406920
C	5.966007	-2.422807	-0.272100
C	4.775301	-1.854323	-0.643845
C	2.205668	-0.638917	-1.510639
C	1.134166	-1.432209	-0.711158
B	0.482048	-0.848922	0.745080
B	-0.482042	-0.848922	-0.745080
B	-0.022961	-2.267834	-1.682813
B	1.203095	-3.159286	-0.759690
B	1.519690	-2.272875	0.745337
B	0.022961	-2.267828	1.682819
B	0.478258	-3.714789	0.756019
B	-0.478261	-3.714789	-0.756008
B	-1.519690	-2.272871	-0.745329
B	-1.203096	-3.159282	0.759699
C	-1.134162	-1.432204	0.711164
C	-2.205662	-0.638907	1.510641
C	-3.260392	0.146591	0.744093
C	-3.065737	1.526711	0.478417
C	-4.102740	2.281405	-0.192816
C	-5.281342	1.639906	-0.577381
C	-5.499859	0.287516	-0.309646
C	-4.478428	-0.478226	0.370976
C	-3.917649	3.677654	-0.439411
C	-2.780227	4.323517	-0.039237
C	-1.755065	3.592952	0.623526
C	-1.887867	2.249081	0.862528
C	-6.725793	-0.344457	-0.687311
C	-6.958667	-1.662751	-0.406927
C	-5.965988	-2.422820	0.272096
C	-4.775286	-1.854329	0.643844
H	-0.765109	0.196104	-1.215883
H	0.765117	0.196106	1.215881
H	2.604989	-2.186723	1.204453
H	2.101670	-3.664618	-1.345891
H	0.057500	-2.168615	-2.861750
H	-0.057499	-2.168610	2.861756
H	0.819328	-4.712902	1.301510
H	-0.819332	-4.712902	-1.301497
H	-2.604987	-2.186717	-1.204448
H	-2.101675	-3.664607	1.345899
H	2.699360	-1.360106	-2.165067

H	1.672033	0.032203	-2.185886
H	4.041409	-2.473164	-1.144620
H	6.153237	-3.469523	-0.495586
H	7.894706	-2.131972	0.696574
H	7.473194	0.254743	1.201958
H	6.055131	2.212021	1.085282
H	4.713466	4.217156	0.947468
H	2.655495	5.387205	0.222220
H	0.851906	4.104103	-0.943698
H	1.072567	1.732637	-1.354283
H	-2.699352	-1.360092	2.165075
H	-1.672026	0.032218	2.185883
H	-4.041391	-2.473165	1.144621
H	-6.153212	-3.469537	0.495583
H	-7.894687	-2.131997	-0.696582
H	-7.473188	0.254719	-1.201967
H	-6.055136	2.212006	-1.085291
H	-4.713484	4.217149	-0.947474
H	-2.655523	5.387212	-0.222221
H	-0.851930	4.104121	0.943704
H	-1.072577	1.732655	1.354290

4(rot-1)

E(B3LYP/6-31G*)= -1487.394409

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1487.7193733

C	4.229396	-2.451415	-0.698985
C	4.686877	-1.176130	-0.229005
C	6.034085	-0.791939	-0.590565
C	6.833700	-1.673451	-1.383291
C	6.350623	-2.881413	-1.805332
C	5.028089	-3.270818	-1.453855
C	3.895429	-0.304031	0.561250
C	4.433396	0.931033	1.005270
C	5.781546	1.301352	0.633299
C	6.540095	0.434019	-0.154840
C	6.323824	2.546096	1.082250
C	5.592786	3.396979	1.864858
C	4.267694	3.041253	2.241322
C	3.711890	1.858507	1.827387
C	2.500233	-0.726927	0.996691
C	1.296898	-0.346137	0.087871
B	0.476370	-1.617110	-0.752824
B	1.383610	-0.372679	-1.635632
B	-0.235677	-0.862433	-2.188050
B	0.235635	0.862068	-2.188158
B	-0.476370	1.616921	-0.753004
B	1.233239	1.160804	-0.748809
B	0.227327	0.855722	0.662964
B	-0.227307	-0.855771	0.663077
B	-1.233239	-1.161003	-0.748644
B	-1.383635	0.372383	-1.635636
C	-1.296884	0.346033	0.087859
C	-2.500202	0.726911	0.996665
C	-3.895416	0.304065	0.561232
C	-4.686829	1.176181	-0.229039
C	-6.034050	0.792033	-0.590598
C	-6.540105	-0.433902	-0.154860
C	-5.781590	-1.301251	0.633296
C	-4.433431	-0.930972	1.005272
C	-4.229302	2.451442	-0.699036

C	-5.027965	3.270864	-1.453917
C	-6.350511	2.881503	-1.805391
C	-6.833632	1.673563	-1.383337
C	-6.323913	-2.545971	1.082257
C	-5.592911	-3.396868	1.864884
C	-4.267813	-3.041179	2.241358
C	-3.711965	-1.858457	1.827412
H	-0.400153	-1.477857	-3.190025
H	0.353739	1.368039	1.722821
H	-2.294321	0.321901	1.989694
H	-2.475651	1.810981	1.123226
H	-0.353698	-1.367948	1.723004
H	-2.136823	-1.917619	-0.661963
H	-2.408995	0.648035	-2.155398
H	-2.695118	-1.634261	2.125502
H	-3.688059	-3.718815	2.862297
H	0.400086	1.477370	-3.190212
H	-6.015635	-4.339774	2.200238
H	2.136815	1.917440	-0.662215
H	-7.338735	-2.798906	0.784530
H	-7.553488	-0.717845	-0.431253
H	-7.841414	1.357159	-1.641606
H	-6.967227	3.543638	-2.406613
H	-4.644227	4.228972	-1.793724
H	-3.222461	2.779573	-0.471511
H	2.475733	-1.810993	1.123283
H	2.294331	-0.321896	1.989707
H	0.888320	-2.724220	-0.649410
H	2.408952	-0.648420	-2.155383
H	3.222565	-2.779577	-0.471461
H	4.644386	-4.228942	-1.793652
H	6.967363	-3.543534	-2.406545
H	-0.888308	2.724043	-0.649694
H	7.841471	-1.357015	-1.641562
H	7.553471	0.717992	-0.431230
H	7.338640	2.799061	0.784531
H	6.015475	4.339903	2.200206
H	3.687911	3.718879	2.862243
H	2.695046	1.634281	2.125466

4(rot-2)

E(B3LYP/6-31G*)= -1487.396013

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1487.7210933

C	4.056107	-2.406472	-0.674380
C	4.156787	-0.977207	-0.611123
C	4.825328	-0.320176	-1.713458
C	5.341634	-1.100285	-2.795070
C	5.219371	-2.462613	-2.807882
C	4.566542	-3.119795	-1.727990
C	3.647603	-0.204916	0.464381
C	3.806495	1.204826	0.457985
C	4.478062	1.846613	-0.651413
C	4.963874	1.069000	-1.704257
C	4.642082	3.267257	-0.654062
C	4.177395	4.036414	0.377290
C	3.516997	3.416168	1.474304
C	3.338732	2.057328	1.512172
C	2.998160	-0.893569	1.656227
C	1.461761	-1.125081	1.632321
B	0.485824	-0.193324	2.714898

B	0.789768	-1.913665	3.015202
B	-0.849701	-1.255087	3.196816
B	-0.599434	-2.841582	2.415081
B	-0.680592	-2.598563	0.661630
B	0.887414	-2.746147	1.452457
B	0.648508	-1.539844	0.191911
B	0.404723	0.036712	0.975506
B	-1.083790	-0.041791	1.918508
B	-1.755907	-1.676135	1.729973
C	-0.918386	-0.901036	0.433248
C	-1.635485	-0.437733	-0.867079
C	-3.032655	0.152950	-0.749919
C	-4.170542	-0.685866	-0.866404
C	-5.496047	-0.108630	-0.807671
C	-5.639229	1.269553	-0.638055
C	-4.532364	2.114042	-0.535839
C	-3.200055	1.553100	-0.596178
C	-4.091165	-2.105391	-1.054276
C	-5.214729	-2.881538	-1.174114
C	-6.513103	-2.303126	-1.111468
C	-6.643106	-0.953527	-0.931550
C	-4.700724	3.525632	-0.381202
C	-3.622607	4.363033	-0.295687
C	-2.307632	3.823792	-0.360894
C	-2.105722	2.475419	-0.503632
H	-1.371365	-1.140605	4.257288
H	1.162742	-1.541230	-0.870789
H	-0.977908	0.283446	-1.356900
H	-1.661401	-1.296586	-1.540161
H	0.782599	0.986631	0.386127
H	-1.783899	0.908932	1.971005
H	-2.926701	-1.820563	1.654439
H	-1.087543	2.107748	-0.535176
H	-1.451812	4.489999	-0.293481
H	-0.944887	-3.861917	2.914858
H	-3.762831	5.434112	-0.179791
H	1.675073	-3.614295	1.276301
H	-5.713905	3.918019	-0.336130
H	-6.638724	1.697328	-0.592644
H	-7.626393	-0.491868	-0.881319
H	-7.391720	-2.935063	-1.206061
H	-5.113094	-3.954265	-1.314361
H	-3.123507	-2.590393	-1.091326
H	3.463110	-1.868983	1.809983
H	3.217940	-0.331181	2.565502
H	1.007513	0.635583	3.382945
H	1.529232	-2.227841	3.888062
H	3.555260	-2.946058	0.119873
H	4.469651	-4.202006	-1.740167
H	5.616883	-3.045038	-3.634302
H	-1.110914	-3.347647	-0.150150
H	5.838340	-0.579412	-3.610219
H	5.468299	1.557328	-2.535585
H	5.150404	3.722129	-1.500935
H	4.309475	5.114694	0.365203
H	3.147528	4.028487	2.292424
H	2.818218	1.628660	2.359621

4(rot-3)

E(B3LYP/6-31G*)= -1487.394220

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1487.7191252

C	3.153403	2.471785	0.674909
C	4.077399	1.430545	0.329944
C	5.298056	1.835730	-0.332880
C	5.524710	3.218730	-0.617199
C	4.609767	4.173672	-0.268375
C	3.408601	3.788058	0.389440
C	3.852803	0.058876	0.612567
C	4.832486	-0.904514	0.260307
C	6.049559	-0.482472	-0.398180
C	6.245050	0.870697	-0.680215
C	7.040258	-1.453306	-0.745817
C	6.862161	-2.779719	-0.463392
C	5.669747	-3.206144	0.185025
C	4.695162	-2.306108	0.530234
C	2.600782	-0.368723	1.363750
C	1.342002	-0.760139	0.538927
B	1.433746	-1.598377	-0.967094
B	0.887680	0.091061	-0.891646
B	-0.000348	0.291961	0.609724
B	0.000119	-1.254863	1.473448
B	-0.881765	-2.427410	0.502667
B	0.881740	-2.427259	0.502369
B	-0.000331	-2.649526	-1.016632
B	-0.000393	-1.086822	-1.882775
B	-1.434373	-1.598354	-0.966468
B	-0.888246	0.091102	-0.891534
C	-1.342234	-0.760045	0.539242
C	-2.600886	-0.368989	1.364365
C	-3.852909	0.058761	0.613274
C	-4.077473	1.430488	0.330880
C	-5.297926	1.835792	-0.332231
C	-6.244778	0.870815	-0.680119
C	-6.049280	-0.482424	-0.398456
C	-4.832398	-0.904595	0.260334
C	-5.524537	3.218843	-0.616351
C	-4.609700	4.173738	-0.267104
C	-3.408698	3.787986	0.390930
C	-3.153556	2.471655	0.676205
C	-7.039752	-1.453223	-0.746846
C	-6.861613	-2.779733	-0.464928
C	-5.669344	-3.206311	0.183655
C	-4.694972	-2.306322	0.529568
H	-0.000598	-1.014923	-3.067754
H	0.000288	-1.209328	2.656809
H	2.301913	0.427343	2.049045
H	2.838607	-1.218400	2.006499
H	-0.000101	1.263927	1.285403
H	1.564870	0.974817	-1.288163
H	2.495151	-1.849614	-1.423240
H	2.220054	2.221797	1.164475
H	2.682365	4.547931	0.665200
H	-0.000694	-3.692956	-1.583552
H	4.793053	5.221435	-0.489278
H	-1.563004	-3.218751	1.064359
H	6.449466	3.492802	-1.119362
H	7.161478	1.181902	-1.177485
H	7.944043	-1.107216	-1.241652
H	7.622155	-3.508384	-0.731151
H	5.528010	-4.260836	0.404691

H	3.795314	-2.676570	1.005283
H	-2.301978	0.426841	2.049908
H	-2.838641	-1.218838	2.006917
H	-1.565375	0.974938	-1.288042
H	-2.495888	-1.849661	-1.422377
H	-2.220336	2.221599	1.165974
H	-2.682520	4.547797	0.667017
H	-4.792928	5.221547	-0.487829
H	1.562623	-3.218822	1.064191
H	-6.449161	3.492958	-1.118731
H	-7.161005	1.182093	-1.177712
H	-7.943415	-1.107037	-1.242838
H	-7.621418	-3.508366	-0.733312
H	-5.527583	-4.261078	0.402938
H	-3.795234	-2.676935	1.004711

4(rot-4)

E(B3LYP/6-31G*)= -1487.395601

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1487.7206834

C	-3.670324	3.226007	2.776018
C	-4.442597	3.090290	1.655181
C	-4.458284	1.870867	0.908218
C	-3.638125	0.757964	1.335303
C	-2.851556	0.952168	2.518724
C	-2.867026	2.135361	3.211218
C	-5.262524	1.737311	-0.225005
C	-5.303657	0.550044	-0.958289
C	-6.148910	0.426963	-2.105137
C	-6.202063	-0.735372	-2.824121
C	-5.401138	-1.843326	-2.430047
C	-4.575325	-1.762937	-1.338850
C	-4.484791	-0.569889	-0.548146
C	-3.650995	-0.451184	0.593260
C	-2.828665	-1.642972	1.061644
C	-1.383283	-1.804711	0.515337
B	-1.040550	-3.127546	-0.545633
B	0.604687	-3.654716	-0.147519
H	0.451318	-2.967523	-2.676416
B	0.311942	-2.595619	-1.557503
B	-0.981596	-1.452155	-1.127038
H	-0.252413	-1.036886	2.669845
B	-0.397549	-0.452908	0.196495
B	-0.092660	-1.501858	1.593586
H	1.967441	-2.926422	2.021652
B	1.183096	-2.637648	1.180294
B	1.689924	-2.284721	-0.482710
C	1.177555	-1.017384	0.570350
B	0.710119	-0.928725	-1.087276
C	2.168273	0.003600	1.199061
C	3.329319	0.505022	0.353355
C	4.577202	-0.167868	0.392883
C	4.808606	-1.359318	1.156584
C	6.032667	-1.975940	1.178571
C	7.127639	-1.453718	0.435219
C	6.957939	-0.320508	-0.311647
C	5.698001	0.354361	-0.358199
C	5.536897	1.516349	-1.114823
C	4.319458	2.198103	-1.160676
C	3.189645	1.690681	-0.412660
C	1.972122	2.444652	-0.489461

C	1.877942	3.590058	-1.236746
C	2.994438	4.076759	-1.972019
C	4.179392	3.394765	-1.930826
B	-0.504805	-3.152669	1.145055
H	-0.734691	0.654991	0.423738
H	-1.807714	-1.018192	-1.852221
H	-1.939405	-3.829637	-0.871646
H	-1.036592	-3.843762	1.949069
H	1.179692	-0.096465	-1.782367
H	0.953830	-4.784454	-0.256471
H	2.831646	-2.358362	-0.780645
H	-3.358085	-2.566895	0.822306
H	-2.762238	-1.632794	2.151526
H	-3.967892	-2.623287	-1.086251
H	-5.441198	-2.764015	-3.005656
H	-6.848783	-0.818093	-3.693108
H	-6.752570	1.285153	-2.390727
H	-5.878438	2.577119	-0.540251
H	-5.066993	3.910397	1.308626
H	-3.668418	4.156655	3.336459
H	-2.257945	2.242666	4.104797
H	-2.219912	0.150418	2.880615
H	1.576895	0.856264	1.539520
H	2.558390	-0.451453	2.111489
H	1.092687	2.103693	0.042820
H	0.936587	4.131679	-1.271672
H	2.899945	4.985029	-2.560565
H	5.044713	3.750682	-2.484961
H	6.383183	1.903738	-1.678543
H	7.782004	0.093870	-0.887620
H	8.089693	-1.957612	0.463532
H	6.167863	-2.879138	1.767351
H	3.997371	-1.801730	1.721392

4(rot-5)

E(B3LYP/6-31G*)= -1487.394783

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1487.7192602

C	1.334386	4.362123	-0.209573
C	2.352044	3.994353	0.626630
C	2.933631	2.689971	0.556333
C	2.440998	1.735117	-0.413440
C	1.374475	2.173774	-1.265749
C	0.842585	3.433290	-1.168049
C	3.978202	2.328628	1.408378
C	4.570512	1.066220	1.346474
C	5.650438	0.721860	2.218042
C	6.245599	-0.508189	2.157306
C	5.783287	-1.465571	1.212246
C	4.748241	-1.173466	0.362040
C	4.089781	0.099886	0.382908
C	3.021527	0.442778	-0.486114
C	2.559055	-0.541923	-1.551614
C	1.416618	-1.539319	-1.208158
B	1.822310	-3.191223	-0.893482
B	0.497482	-4.156419	-1.566368
H	0.767621	-4.634905	1.003949
B	0.560308	-3.800100	0.185316
B	1.179189	-2.142512	0.387697
H	-0.234691	-0.498851	-2.832470
B	0.021595	-1.032073	-0.353337

B	-0.034876	-1.396837	-2.089879
H	-1.389431	-3.242617	-3.213172
B	-0.656150	-3.030053	-2.305635
B	-0.972949	-3.691955	-0.690580
C	-1.213177	-2.011882	-1.024227
B	-0.555832	-2.453455	0.510985
C	-2.682383	-1.522913	-1.174540
C	-3.165042	-0.365984	-0.313462
C	-3.728089	-0.619828	0.964020
C	-3.887034	-1.936356	1.511023
C	-4.441246	-2.141821	2.747708
C	-4.876700	-1.046677	3.544944
C	-4.756654	0.228321	3.065055
C	-4.198041	0.483650	1.773471
C	-4.116234	1.785108	1.275895
C	-3.614702	2.051429	0.000510
C	-3.128034	0.960769	-0.816883
C	-2.657805	1.299530	-2.128870
C	-2.674763	2.589948	-2.593508
C	-3.145732	3.654894	-1.775779
C	-3.596610	3.385846	-0.512511
B	1.077658	-2.716270	-2.428712
H	-0.159312	0.081450	-0.014945
H	1.863554	-1.750024	1.267695
H	2.966334	-3.499772	-0.884352
H	1.706222	-2.683363	-3.433855
H	-1.195330	-2.303993	1.492481
H	0.663425	-5.246315	-2.007691
H	-1.936155	-4.364555	-0.521903
H	3.408635	-1.144070	-1.878757
H	2.248631	0.010038	-2.441279
H	4.417314	-1.937874	-0.328996
H	6.254820	-2.443469	1.166506
H	7.066130	-0.758478	2.823905
H	5.988842	1.468380	2.932703
H	4.344286	3.051394	2.134756
H	2.742755	4.689168	1.366312
H	0.898462	5.355248	-0.146136
H	0.024400	3.720007	-1.821529
H	0.957014	1.495242	-1.999789
H	-3.314961	-2.394902	-0.998552
H	-2.832089	-1.281217	-2.227984
H	-2.286551	0.522687	-2.785233
H	-2.327734	2.801762	-3.601546
H	-3.151078	4.671209	-2.159935
H	-3.965466	4.184307	0.126863
H	-4.471384	2.610774	1.889062
H	-5.091279	1.078243	3.655009
H	-5.305958	-1.229477	4.526028
H	-4.546718	-3.154691	3.126518
H	-3.558781	-2.798261	0.943284

5(cryst)

E(B3LYP/6-31G*)= -1498.218939

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1498.5307122

C	4.708369	-1.705443	-1.763974
C	4.836687	-0.445014	-1.089940
C	6.047868	-0.233548	-0.325774
C	7.041270	-1.263014	-0.270613
C	6.871667	-2.449538	-0.934156

C	5.685441	-2.667182	-1.692009
C	3.852231	0.576414	-1.145498
C	4.070162	1.805617	-0.469861
C	5.286018	2.000850	0.291187
C	6.236034	0.977468	0.345949
C	5.504919	3.240408	0.973401
C	4.586089	4.254968	0.916273
C	3.388553	4.076296	0.165968
C	3.141601	2.899682	-0.496829
C	2.604626	0.385747	-1.995935
C	1.342781	-0.232276	-1.327549
B	1.436505	-1.481137	-0.140580
B	0.889016	0.157834	0.289779
B	-0.000018	-1.262299	0.879498
B	-0.000014	-2.501550	-0.406873
B	-0.881665	-1.834670	-1.788812
B	0.881639	-1.834674	-1.788809
B	-0.000010	-0.426893	-2.366567
B	-0.000014	0.793505	-1.083959
B	-0.889040	0.157828	0.289785
B	-1.436522	-1.481144	-0.140581
C	-1.342790	-0.232281	-1.327548
C	-2.604637	0.385743	-1.995945
C	-3.852237	0.576422	-1.145506
C	-4.070157	1.805624	-0.469860
C	-5.286005	2.000861	0.291196
C	-6.236026	0.977478	0.345960
C	-6.047863	-0.233541	-0.325763
C	-4.836688	-0.445007	-1.089936
C	-5.504895	3.240417	0.973417
C	-4.586061	4.254973	0.916290
C	-3.388529	4.076296	0.165980
C	-3.141591	2.899684	-0.496828
C	-4.708374	-1.705434	-1.763977
C	-5.685450	-2.667172	-1.692021
C	-6.871672	-2.449531	-0.934158
C	-7.041266	-1.263011	-0.270605
I	0.000004	-1.788290	3.015508
H	-0.000014	-0.033705	-3.482942
H	-2.304671	1.346636	-2.420728
H	-2.846618	-0.239733	-2.858047
H	-0.000016	1.923184	-1.435766
H	-1.564707	0.875356	0.938875
H	-2.494295	-1.854107	0.228120
H	-2.210695	2.802804	-1.042012
H	-2.658818	4.880839	0.122269
H	-0.000008	-3.662725	-0.166075
H	-4.763456	5.191468	1.438132
H	1.564278	-2.425252	-2.556393
H	-6.425268	3.357839	1.541138
H	-7.147022	1.129312	0.921917
H	-7.939483	-1.078207	0.314406
H	-7.632427	-3.223913	-0.885081
H	-5.549474	-3.610210	-2.215227
H	-3.815428	-1.922367	-2.337156
H	2.304661	1.346643	-2.420715
H	2.846603	-0.239726	-2.858040
H	1.564678	0.875364	0.938871
H	2.494270	-1.854102	0.228137
H	2.210702	2.802806	-1.042008

H	2.658846	4.880843	0.122259
H	4.763493	5.191465	1.438110
H	-1.564296	-2.425253	-2.556398
H	6.425297	3.357830	1.541112
H	7.147037	1.129298	0.921898
H	7.939487	-1.078210	0.314397
H	7.632419	-3.223924	-0.885075
H	5.549457	-3.610224	-2.215204
H	3.815419	-1.922386	-2.337139

5(rot-1)

E(B3LYP/6-31G*)= -1498.176015

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1498.5306274

C	4.700948	-1.705864	-1.763583
C	4.834451	-0.445893	-1.091871
C	6.049901	-0.234651	-0.335756
C	7.041975	-1.263624	-0.286404
C	6.866689	-2.449180	-0.946336
C	5.676400	-2.667112	-1.695026
C	3.852840	0.577089	-1.144279
C	4.072857	1.804221	-0.467578
C	5.292991	1.998750	0.285507
C	6.242303	0.975984	0.332894
C	5.516018	3.236658	0.966235
C	4.597264	4.249136	0.916339
C	3.395693	4.071121	0.175067
C	3.144598	2.897383	-0.487820
C	2.603755	0.389507	-1.992396
C	1.342478	-0.228976	-1.324385
B	1.436554	-1.478337	-0.138629
B	0.889293	0.160525	0.292764
B	-0.000029	-1.259712	0.879844
B	-0.000036	-2.498465	-0.405718
B	-0.881698	-1.830193	-1.786678
B	0.881656	-1.830212	-1.786668
B	-0.000001	-0.422535	-2.362912
B	0.000004	0.796581	-1.080304
B	-0.889314	0.160547	0.292754
B	-1.436606	-1.478305	-0.138643
C	-1.342488	-0.228946	-1.324400
C	-2.603747	0.389564	-1.992414
C	-3.852832	0.577150	-1.144301
C	-4.072787	1.804238	-0.467501
C	-5.292910	1.998766	0.285603
C	-6.242267	0.976040	0.332917
C	-6.049918	-0.234559	-0.335814
C	-4.834480	-0.445800	-1.091949
C	-5.515874	3.236630	0.966432
C	-4.597067	4.249064	0.916621
C	-3.395502	4.071046	0.175340
C	-3.144465	2.897349	-0.487642
C	-4.701023	-1.705739	-1.763731
C	-5.676512	-2.666953	-1.695230
C	-6.866792	-2.449020	-0.946526
C	-7.042031	-1.263497	-0.286522
I	-0.000042	-1.787923	3.023182
H	0.000009	-0.028319	-3.478964
H	-2.304066	1.351698	-2.413679
H	-2.844034	-0.233978	-2.856000
H	0.000019	1.926283	-1.432411

H	-1.564015	0.878609	0.942518
H	-2.494364	-1.852547	0.228930
H	-2.211043	2.799713	-1.028267
H	-2.666028	4.875579	0.138176
H	-0.000049	-3.659784	-0.166611
H	-4.777128	5.184959	1.437872
H	1.562985	-2.420522	-2.555765
H	-6.440159	3.352835	1.527239
H	-7.157362	1.128227	0.901498
H	-7.943709	-1.077581	0.292030
H	-7.626880	-3.223828	-0.902045
H	-5.537210	-3.610580	-2.215625
H	-3.804031	-1.920817	-2.331079
H	2.304095	1.351638	-2.413681
H	2.844039	-0.234054	-2.855969
H	1.564002	0.878569	0.942539
H	2.494297	-1.852605	0.228961
H	2.211174	2.799753	-1.028443
H	2.666263	4.875689	0.137833
H	4.777373	5.185064	1.437514
H	-1.563031	-2.420488	-2.555782
H	6.440310	3.352862	1.527031
H	7.157408	1.128174	0.901458
H	7.943663	-1.077706	0.292132
H	7.626748	-3.224014	-0.901810
H	5.537061	-3.610764	-2.215365
H	3.803947	-1.920942	-2.330918

5(rot-2)

E(B3LYP/6-31G*)= -1498.177797

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1498.5325353

C	1.173238	3.711630	-0.273282
C	2.406301	3.136620	0.180923
C	3.612066	3.895605	-0.071768
C	3.529882	5.150792	-0.752487
C	2.327730	5.655127	-1.167768
C	1.134652	4.920573	-0.919519
C	2.488846	1.892180	0.857362
C	3.747553	1.407651	1.297216
C	4.943267	2.180096	1.038573
C	4.842679	3.396044	0.359535
C	6.211758	1.693723	1.485849
C	6.318034	0.508207	2.160417
C	5.148460	-0.258775	2.422956
C	3.915223	0.172991	2.007602
C	1.221412	1.116022	1.181916
C	0.724944	0.052238	0.160668
B	1.811883	-0.997646	-0.673160
B	0.912002	0.263800	-1.540373
B	-0.663058	0.427090	-0.765626
B	-0.739007	-0.720477	0.587394
B	-0.645893	-2.349808	-0.071187
B	0.783788	-1.604242	0.644687
B	0.932283	-2.529727	-0.857640
B	1.016269	-1.375896	-2.216598
B	-0.509776	-2.207584	-1.837696
B	-0.516448	-0.486563	-2.257397
C	-1.445223	-1.079051	-0.922831
C	-2.987874	-1.172498	-1.092268
C	-3.860152	-0.235264	-0.269872

C	-4.343034	-0.646132	0.999793
C	-5.210870	0.231396	1.755506
C	-5.566490	1.472285	1.222986
C	-5.112845	1.889677	-0.030101
C	-4.243902	1.024211	-0.798389
C	-5.699074	-0.183900	3.034223
C	-5.364722	-1.402416	3.559054
C	-4.515990	-2.275576	2.822846
C	-4.025294	-1.911576	1.595130
C	-5.501715	3.158111	-0.564383
C	-5.070723	3.571134	-1.795562
C	-4.219080	2.726845	-2.561895
C	-3.821540	1.505050	-2.082417
H	1.628516	-1.604325	-3.205859
H	-1.357089	-0.398548	1.539639
H	0.397830	1.814810	1.342286
H	1.346693	0.603463	2.137733
H	-1.248312	1.442330	-0.634322
H	1.456478	1.227161	-1.953880
H	2.975150	-0.887352	-0.506295
H	0.241011	3.183294	-0.115312
H	0.180212	5.322317	-1.248764
I	1.961637	-4.483112	-0.888737
H	2.277615	6.610045	-1.683325
H	-1.288015	-3.217375	0.413993
H	4.452791	5.697483	-0.930834
H	5.745529	3.971850	0.166506
H	7.093454	2.294274	1.275226
H	7.286678	0.148102	2.495294
H	5.235325	-1.202245	2.954678
H	3.054317	-0.451360	2.212261
H	-3.266628	-2.207409	-0.886035
H	-3.198163	-1.030228	-2.153722
H	-1.086827	-0.109678	-3.225350
H	-1.081736	-2.984525	-2.525247
H	-3.374262	-2.602790	1.074785
H	-4.252156	-3.243421	3.240230
H	-5.742834	-1.707934	4.530514
H	1.241048	-1.879546	1.701815
H	-6.348355	0.496608	3.579904
H	-6.219342	2.127604	1.795927
H	-6.154640	3.787644	0.035410
H	-5.374548	4.535755	-2.192227
H	-3.878523	3.055881	-3.539886
H	-3.163260	0.900176	-2.694170

5(rot-3)

E(B3LYP/6-31G*)= -1498.176043

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1498.5306664

C	-4.750928	-1.341983	1.007086
C	-4.821466	-0.000033	0.505378
C	-5.993767	0.346902	-0.268715
C	-7.006564	-0.636028	-0.500619
C	-6.891804	-1.903453	0.001341
C	-5.744891	-2.255325	0.766768
C	-3.819215	0.976826	0.737709
C	-3.979840	2.291193	0.228274
C	-5.156622	2.620635	-0.546382
C	-6.124847	1.641049	-0.776156
C	-5.319132	3.945080	-1.060996

C	-4.383506	4.916120	-0.829436
C	-3.225643	4.605973	-0.063039
C	-3.032131	3.346047	0.442521
C	-2.610152	0.634672	1.595282
C	-1.342154	0.074765	0.887919
B	-0.886813	0.571675	-0.701787
B	-1.435521	-1.087660	-0.382759
B	-0.000006	-0.802742	-1.392885
B	-0.000037	-2.114689	-0.182167
B	0.884053	-1.551336	1.243734
B	-0.884032	-1.551312	1.243804
B	0.000084	-0.185912	1.911196
B	0.000034	1.115860	0.711436
B	0.886907	0.571625	-0.701741
B	1.435506	-1.087781	-0.382802
C	1.342224	0.074772	0.887872
C	2.610252	0.634469	1.595290
C	3.819329	0.976712	0.737750
C	3.979915	2.291103	0.228341
C	5.156740	2.620611	-0.546222
C	6.125014	1.641071	-0.775976
C	5.993914	0.346874	-0.268669
C	4.821583	-0.000124	0.505350
C	5.319232	3.945076	-1.060791
C	4.383522	4.916058	-0.829320
C	3.225570	4.605822	-0.063099
C	3.032083	3.345877	0.442430
C	7.006688	-0.636057	-0.500651
C	6.891860	-1.903541	0.001144
C	5.744904	-2.255486	0.766473
C	4.750967	-1.342143	1.006877
H	-0.000012	-1.017954	-2.558708
H	0.000027	0.130939	3.051636
H	2.300836	1.518091	2.157515
H	2.900232	-0.095909	2.353103
H	0.000078	2.216700	1.142425
H	1.565272	1.336190	-1.294182
H	2.492651	-1.445606	-0.767186
H	2.130404	3.152552	1.010375
H	2.483496	5.378011	0.121085
I	-0.000157	-4.250510	-0.746473
H	4.518325	5.919047	-1.224150
H	-1.566398	-2.197910	1.963908
H	6.212256	4.161958	-1.642029
H	7.007585	1.894764	-1.359568
H	7.874897	-0.347508	-1.088277
H	7.667081	-2.642281	-0.181455
H	5.652965	-3.264001	1.159941
H	3.887128	-1.659473	1.578122
H	-2.300615	1.518375	2.157297
H	-2.900130	-0.095560	2.353238
H	-1.565168	1.336328	-1.294129
H	-2.492679	-1.445497	-0.767109
H	-2.130544	3.152816	1.010653
H	-2.483667	5.378225	0.121276
H	-4.518324	5.919093	-1.224303
H	1.566311	-2.197987	1.963901
H	-6.212112	4.161902	-1.642323
H	-7.007370	1.894665	-1.359852
H	-7.874742	-0.347505	-1.088305

H	-7.667038	-2.642193	-0.181192
H	-5.652996	-3.263778	1.160402
H	-3.887129	-1.659284	1.578407

5(rot-4)

E(B3LYP/6-31G*)= -1498.176798

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1498.5314

C	-7.067568	0.458859	1.515355
C	-6.094952	-0.322327	0.815741
C	-5.001557	0.336071	0.133882
C	-4.964770	1.768336	0.202069
C	-5.918886	2.482834	0.879799
C	-6.987964	1.824194	1.549381
C	-4.038575	-0.439097	-0.562798
C	-4.164899	-1.851766	-0.605553
C	-5.262316	-2.494755	0.084956
C	-6.190369	-1.714841	0.777856
C	-5.389180	-3.918758	0.043702
C	-4.494824	-4.691355	-0.645534
C	-3.417568	-4.069857	-1.337056
C	-3.259261	-2.707776	-1.315921
C	-2.912632	0.249864	-1.319987
C	-1.580020	0.522246	-0.567202
B	-1.160071	2.160298	-0.203599
B	0.602987	2.242166	-0.361893
I	1.627124	4.086024	-1.014291
B	1.304318	1.140480	0.837201
B	-0.148803	2.084283	1.249914
B	-1.555709	1.008724	1.087382
B	-0.968704	-0.574979	0.584446
B	-0.216433	-0.404293	-1.011072
B	-0.344258	1.273184	-1.509066
B	1.186689	0.644441	-0.869106
C	0.730641	-0.426834	0.401742
B	-0.033604	0.382815	1.725830
C	1.535849	-1.722103	0.709908
C	3.048376	-1.679192	0.554062
C	3.866697	-1.342516	1.662884
C	5.306486	-1.349738	1.519031
C	5.873230	-1.690214	0.289196
C	5.085636	-2.038222	-0.810001
C	3.644432	-2.039462	-0.681885
C	3.346932	-0.994337	2.953489
C	4.171873	-0.682502	4.003401
C	5.586459	-0.688987	3.849042
C	6.132281	-1.013643	2.637316
C	5.687012	-2.398882	-2.056487
C	4.924590	-2.753985	-3.135566
C	3.506510	-2.766588	-3.019372
C	2.893248	-2.422399	-1.842189
H	-0.124302	2.958143	2.051071
H	-0.293116	-1.327900	-1.745231
H	2.149261	0.424592	-1.516075
H	-1.476806	-1.609313	0.838559
H	-2.567025	1.080414	1.693385
H	-1.924021	3.018475	-0.491076
H	-0.566085	1.524863	-2.644896
H	0.125478	-0.042157	2.820595
H	2.366678	1.254206	1.339463
H	-3.260705	1.213744	-1.695462

H	-2.666999	-0.326370	-2.214453
H	-4.159695	2.310631	-0.278161
H	-5.855862	3.567084	0.909820
H	-7.732883	2.407852	2.082772
H	-7.876789	-0.063523	2.019971
H	-7.013096	-2.204288	1.294981
H	-6.221909	-4.373612	0.574753
H	-4.602600	-5.771978	-0.671507
H	-2.711469	-4.684167	-1.889341
H	-2.421659	-2.277689	-1.851166
H	1.127361	-2.512528	0.076684
H	1.282945	-2.017938	1.729674
H	2.276022	-0.960638	3.111956
H	3.739968	-0.421824	4.965744
H	6.223373	-0.435600	4.691774
H	7.210682	-1.023956	2.498546
H	6.956387	-1.689840	0.186335
H	6.772166	-2.384575	-2.123997
H	5.392484	-3.025989	-4.077434
H	2.902235	-3.049519	-3.877076
H	1.810892	-2.435085	-1.802551

5(rot-5)

E(B3LYP/6-31G*)= -1498.176529

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1498,5305723

C	-5.607082	-1.023781	-1.044372
C	-4.571271	-1.701476	-0.328342
C	-3.255417	-1.829184	-0.917638
C	-3.075373	-1.259855	-2.222048
C	-4.100133	-0.634937	-2.886296
C	-5.386770	-0.507122	-2.291991
C	-2.235557	-2.521793	-0.214284
C	-2.523091	-3.121519	1.039251
C	-3.840427	-2.974318	1.619220
C	-4.820637	-2.261085	0.926582
C	-4.128770	-3.574569	2.885171
C	-3.184580	-4.304026	3.554411
C	-1.891227	-4.471634	2.984765
C	-1.573254	-3.901649	1.779003
C	-0.862798	-2.700742	-0.843076
C	0.261561	-1.684174	-0.492370
B	0.573134	-1.187962	1.131632
B	1.669836	-2.304322	0.292371
B	1.698722	-1.863392	-1.429561
B	2.377559	-0.235048	-1.558707
B	0.637948	-0.474402	-1.633140
B	-0.065998	-0.059192	-0.058839
B	1.252596	0.437820	1.004291
B	2.333721	-0.956504	1.231653
B	3.025541	-1.373841	-0.361065
B	2.766329	0.319615	0.082729
C	1.288205	0.782997	-0.684547
C	1.154564	2.235011	-1.228421
C	0.357012	3.245578	-0.414982
C	-1.025387	3.433768	-0.672879
C	-1.764777	4.431061	0.071849
C	-1.106765	5.200230	1.032918
C	0.256803	5.044253	1.288698
C	1.011237	4.052897	0.552337
C	-1.758199	2.689442	-1.655596

C	-3.093195	2.907052	-1.879879
C	-3.809982	3.886519	-1.137743
C	-3.157569	4.624424	-0.188713
C	2.410323	3.955034	0.850166
C	3.007592	4.757134	1.788552
C	2.253888	5.723580	2.511036
C	0.915120	5.858004	2.263107
H	2.925272	-1.123134	2.245619
H	-0.015640	-0.270166	-2.597007
H	1.727643	-2.694160	-2.273095
H	-1.154635	0.389132	-0.043946
H	1.071096	1.313291	1.776161
H	3.618522	1.128284	0.221548
H	2.940934	0.207074	-2.502037
H	-0.128520	-1.558169	2.005647
I	5.046351	-2.234148	-0.590911
H	1.688109	-3.451070	0.589592
H	2.170780	2.606724	-1.372192
H	0.735645	2.165697	-2.234625
H	3.020235	3.224068	0.335608
H	4.070818	4.650934	1.985558
H	2.744068	6.348153	3.252474
H	0.320938	6.592074	2.802091
H	-1.668964	5.946423	1.590609
H	-3.685909	5.378722	0.389459
H	-4.868329	4.041300	-1.327647
H	-3.613661	2.313364	-2.625015
H	-1.257979	1.922779	-2.235202
H	-0.473623	-3.688534	-0.589189
H	-0.956828	-2.710776	-1.930209
H	-2.111507	-1.326110	-2.711609
H	-3.928611	-0.235745	-3.882705
H	-6.185693	-0.006981	-2.832205
H	-6.583789	-0.940872	-0.573780
H	-5.809958	-2.155527	1.366911
H	-5.124788	-3.440745	3.300324
H	-3.415487	-4.758600	4.513632
H	-1.144808	-5.056979	3.514542
H	-0.573110	-4.045210	1.388818

6(cryst)

E(B3LYP/6-31G*)= -1508.985457

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1509.3410073

C	5.650896	3.529576	-1.036449
C	5.349585	2.190333	-0.634937
C	4.326922	1.443950	-1.336128
C	3.673685	2.110844	-2.425372
C	3.994215	3.395231	-2.783953
C	4.994841	4.122454	-2.080521
C	4.027530	0.116186	-0.935449
C	4.746404	-0.480740	0.132442
C	5.768192	0.278524	0.820696
C	6.035583	1.590007	0.422810
C	6.494743	-0.322555	1.895964
C	6.244980	-1.609566	2.287006
C	5.244880	-2.366887	1.615399
C	4.525176	-1.824486	0.581981
C	2.985151	-0.691839	-1.693937
C	1.513405	-0.642507	-1.194911
B	0.394632	-1.575144	-2.117919

B	0.374852	0.182108	-2.165156
B	0.836723	0.789121	-0.566838
B	-0.408602	0.297607	0.575939
B	-0.406486	-1.477351	0.646089
I	-0.881609	-2.513154	2.527017
B	0.841354	-2.063350	-0.468837
B	1.126280	-0.589086	0.482365
B	-0.860573	-2.094916	-0.975987
I	-1.960971	-3.968253	-1.318513
B	-1.637374	-0.632519	-0.317686
B	-1.138312	-0.696632	-2.023180
C	-0.805726	0.692597	-1.051633
C	-1.527490	2.022065	-1.417119
C	-2.578003	2.559549	-0.457665
C	-3.940239	2.200760	-0.625272
C	-4.941621	2.762745	0.255117
C	-4.554005	3.654655	1.257057
C	-3.220162	4.029891	1.429894
C	-2.206109	3.477870	0.557792
C	-6.315752	2.404254	0.085889
C	-6.706251	1.539481	-0.899647
C	-5.730782	0.983677	-1.773954
C	-4.403355	1.300694	-1.641239
C	-2.847533	4.957401	2.452738
C	-1.545124	5.340576	2.622366
C	-0.539836	4.808260	1.767621
C	-0.857514	3.913664	0.778035
H	0.682036	0.827292	-3.107192
H	1.419360	1.813332	-0.526682
H	1.984971	-0.541483	1.290590
H	1.533671	-3.009680	-0.313752
H	0.791278	-2.175562	-3.058133
H	-0.719013	1.021977	1.453813
H	-1.930840	-0.614016	-2.898479
H	-2.777050	-0.526134	-0.033774
H	3.275204	-1.743899	-1.707386
H	2.978252	-0.389067	-2.742978
H	3.763363	-2.433126	0.110845
H	5.045478	-3.387599	1.929401
H	6.802686	-2.056392	3.105068
H	7.255045	0.272734	2.395802
H	6.802953	2.156627	0.946159
H	6.421922	4.066336	-0.488981
H	5.233895	5.139525	-2.377825
H	3.478222	3.864602	-3.617250
H	2.901763	1.597578	-2.985921
H	-0.750648	2.775432	-1.564358
H	-1.975261	1.879845	-2.402713
H	-0.057051	3.526147	0.159761
H	0.494428	5.112284	1.903737
H	-1.273613	6.045894	3.402623
H	-3.630977	5.352722	3.094779
H	-5.311719	4.072068	1.916926
H	-7.045472	2.839396	0.764425
H	-7.752646	1.273302	-1.018554
H	-6.042005	0.294013	-2.553643
H	-3.694100	0.841214	-2.318713

6(rot-1)

E(B3LYP/6-31G*)= -1508.984251

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1509.3397492

C	3.756321	-2.968483	1.715427
C	4.448353	-2.124924	0.784589
C	5.800168	-1.743541	1.131461
C	6.373445	-2.201736	2.358996
C	5.669079	-3.003367	3.215241
C	4.341510	-3.391313	2.881289
C	3.880193	-1.667669	-0.432391
C	4.644970	-0.859754	-1.312682
C	5.996582	-0.489975	-0.951551
C	6.531920	-0.935986	0.258477
C	6.770485	0.322579	-1.838195
C	6.258515	0.756196	-3.030379
C	4.931950	0.395763	-3.397914
C	4.157401	-0.378445	-2.572759
C	2.477279	-2.103260	-0.826771
C	1.282507	-1.203634	-0.395749
B	1.372402	0.521682	-0.426707
B	1.279122	-0.370903	1.111176
B	0.260286	-1.779927	0.844884
B	-0.260276	-1.779866	-0.845016
B	-1.279122	-0.370829	-1.111204
B	0.415844	-0.367124	-1.632909
B	-0.269361	1.067580	-0.855487
B	0.269352	1.067519	0.855565
B	-1.372408	0.521642	0.426744
B	-0.415844	-0.367248	1.632881
C	-1.282501	-1.203672	0.395660
C	-2.477268	-2.103337	0.826614
C	-3.880183	-1.667718	0.432270
C	-4.644973	-0.859900	1.312639
C	-5.996583	-0.490090	0.951535
C	-6.531908	-0.935978	-0.258544
C	-5.800144	-1.743438	-1.131606
C	-4.448330	-2.124850	-0.784763
C	-6.770499	0.322367	1.838257
C	-6.258542	0.755861	3.030491
C	-4.931978	0.395396	3.398001
C	-4.157417	-0.378721	2.572771
C	-6.373407	-2.201507	-2.359195
C	-5.669028	-3.003042	-3.215518
C	-4.341460	-3.391014	-2.881597
C	-3.756283	-2.968303	-1.715685
I	0.628035	2.893090	2.028243
H	-0.406451	-2.835490	-1.357769
H	2.282556	-3.103425	-0.433637
H	2.421140	-2.208653	-1.911913
H	0.406468	-2.835589	1.357558
H	2.209094	-0.444911	1.833229
H	2.378557	1.050946	-0.740867
H	2.739932	-3.279805	1.507398
H	3.783552	-4.028981	3.561622
I	-0.628057	2.893237	-2.028030
H	6.114649	-3.345182	4.145068
H	-2.209094	-0.444792	-1.833263
H	7.389671	-1.895208	2.594738
H	7.547458	-0.651279	0.525607
H	7.781531	0.587297	-1.538364
H	6.854852	1.373484	-3.696141
H	4.525262	0.744368	-4.343144

H	3.147656	-0.613319	-2.886887
H	-2.421127	-2.208815	1.911748
H	-2.282542	-3.103469	0.433400
H	-0.781816	-0.457273	2.754858
H	-2.378566	1.050875	0.740944
H	-3.147675	-0.613623	2.886884
H	-4.525301	0.743904	4.343272
H	-6.854888	1.373076	3.696312
H	0.781817	-0.457064	-2.754893
H	-7.781544	0.587111	1.538445
H	-7.547445	-0.651249	-0.525654
H	-7.389633	-1.894960	-2.594913
H	-6.114588	-3.344762	-4.145386
H	-3.783491	-4.028606	-3.561993
H	-2.739893	-3.279640	-1.507681

6(rot-2)
E(B3LYP/6-31G*)= -1508.985907
E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1509.341499

C	-0.259181	4.003731	0.417341
C	-1.488737	3.735656	-0.270571
C	-2.601413	4.614996	0.016261
C	-2.438700	5.681001	0.955614
C	-1.244081	5.892928	1.588053
C	-0.140611	5.039352	1.308363
C	-1.652166	2.677625	-1.201592
C	-2.894517	2.501036	-1.863336
C	-3.996443	3.390610	-1.566092
C	-3.820994	4.415097	-0.633770
C	-5.249585	3.214779	-2.232586
C	-5.428098	2.220471	-3.155076
C	-4.350080	1.343075	-3.459654
C	-3.134879	1.477420	-2.838887
C	-0.474555	1.778355	-1.544060
C	-0.277567	0.477138	-0.712160
B	-1.613422	-0.511149	-0.232207
B	-0.666720	0.408533	0.963000
B	1.007661	0.440857	0.412910
B	1.105017	-0.438672	-1.124744
B	0.690144	-2.121242	-0.820768
B	-0.505720	-1.028652	-1.522827
B	-0.994001	-2.180992	-0.270305
B	-1.094906	-1.287179	1.280740
B	0.330552	-2.285351	0.911093
B	0.529589	-0.690626	1.666352
C	1.535097	-1.177611	0.350126
C	3.009410	-1.560512	0.664214
C	4.109353	-0.623294	0.188653
C	4.711675	-0.822440	-1.080472
C	5.787329	0.046377	-1.507548
C	6.222854	1.068343	-0.661374
C	5.652291	1.272353	0.596830
C	4.574902	0.413051	1.038734
C	6.394724	-0.153850	-2.786879
C	5.981099	-1.158419	-3.618632
C	4.928092	-2.022444	-3.207059
C	4.318786	-1.860347	-1.989231
C	6.123243	2.316058	1.453929
C	5.576040	2.517985	2.691672
C	4.518541	1.676959	3.138311

C	4.037924	0.667362	2.344286
I	-2.495058	-1.791805	2.898729
H	1.889093	-0.060169	-1.920496
H	0.454319	2.347427	-1.469237
H	-0.538992	1.477951	-2.591577
H	1.743565	1.350221	0.557792
H	-1.123615	1.350954	1.506579
H	-2.714455	-0.179121	-0.493921
H	0.604596	3.373823	0.243635
H	0.808331	5.209357	1.809686
I	-2.263517	-3.902841	-0.782257
H	-1.132004	6.706527	2.299067
H	1.263471	-2.981257	-1.396666
H	-3.293426	6.323292	1.153619
H	-4.654349	5.078626	-0.412353
H	-6.060285	3.896031	-1.985811
H	-6.384432	2.095385	-3.654783
H	-4.494068	0.552180	-4.190516
H	-2.348531	0.776533	-3.091815
H	3.172036	-2.557290	0.250701
H	3.078638	-1.690298	1.745669
H	0.996627	-0.601102	2.749795
H	0.679438	-3.256482	1.490301
H	3.515780	-2.536368	-1.722043
H	4.602120	-2.821222	-3.867554
H	6.450727	-1.302089	-4.587540
H	-0.848553	-1.030290	-2.655559
H	7.199610	0.515152	-3.081628
H	7.031678	1.718539	-0.988249
H	6.933496	2.946311	1.095300
H	5.943489	3.312389	3.335062
H	4.085854	1.837612	4.121945
H	3.224867	0.058908	2.720915

6(rot-3)

E(B3LYP/6-31G*)= -1508.984236

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1509.3397516

C	4.705907	-1.084897	-1.723685
C	4.832098	0.185785	-1.071087
C	6.040973	0.410841	-0.308413
C	7.033847	-0.615804	-0.234050
C	6.865190	-1.812268	-0.875709
C	5.681598	-2.043867	-1.630756
C	3.849742	1.206694	-1.146507
C	4.062148	2.444851	-0.487666
C	5.275921	2.652851	0.271883
C	6.226084	1.632150	0.342662
C	5.491807	3.901369	0.935168
C	4.572081	4.911652	0.862464
C	3.376891	4.720458	0.114370
C	3.132740	3.536205	-0.532350
C	2.607081	1.003275	-1.999966
C	1.342439	0.393312	-1.329554
B	0.889538	0.790645	0.284997
B	1.438272	-0.850003	-0.133447
B	-0.000041	-0.622931	0.889440
B	-0.000019	-1.867691	-0.402060
B	-0.883817	-1.206416	-1.784852
B	0.883815	-1.206405	-1.784862

B	-0.000021	0.196362	-2.366579
B	-0.000003	1.420439	-1.090025
B	-0.889608	0.790641	0.284945
B	-1.438321	-0.850041	-0.133480
C	-1.342449	0.393351	-1.329564
C	-2.607033	1.003346	-2.000031
C	-3.849709	1.206761	-1.146581
C	-4.062050	2.444888	-0.487662
C	-5.275814	2.652908	0.271893
C	-6.226009	1.632236	0.342653
C	-6.040945	0.410942	-0.308461
C	-4.832103	0.185888	-1.071192
C	-5.491654	3.901414	0.935218
C	-4.571881	4.911657	0.862560
C	-3.376676	4.720426	0.114500
C	-3.132571	3.536185	-0.532261
C	-7.033823	-0.615698	-0.234072
C	-6.865206	-1.812148	-0.875766
C	-5.681666	-2.043731	-1.630899
C	-4.705972	-1.084768	-1.723853
I	-0.000096	-1.089565	3.037499
H	0.000056	0.579566	-3.485992
H	-2.306644	1.957521	-2.438418
H	-2.853469	0.366026	-2.851708
H	-0.000027	2.548442	-1.444995
H	-1.564957	1.510091	0.931905
H	-2.492584	-1.230328	0.234417
H	-2.204153	3.429724	-1.079916
H	-2.646752	5.523449	0.058444
I	-0.000012	-4.035803	-0.028749
H	-4.746596	5.855804	1.370502
H	1.561893	-1.808928	-2.544865
H	-6.411321	4.027718	1.501354
H	-7.136128	1.794480	0.916356
H	-7.930319	-0.419307	0.348987
H	-7.625207	-2.585571	-0.811608
H	-5.547008	-2.996218	-2.135899
H	-3.814717	-1.311112	-2.296006
H	2.306717	1.957430	-2.438416
H	2.853544	0.365892	-2.851588
H	1.564880	1.510140	0.931915
H	2.492491	-1.230369	0.234490
H	2.204347	3.429794	-1.080059
H	2.647019	5.523524	0.058251
H	4.746826	5.855801	1.370390
H	-1.561818	-1.808940	-2.544925
H	6.411476	4.027654	1.501305
H	7.136223	1.794389	0.916334
H	7.930376	-0.419400	0.348954
H	7.625200	-2.585686	-0.811597
H	5.546886	-2.996378	-2.135697
H	3.814600	-1.311272	-2.295746

6(rot-4)

E(B3LYP/6-31G*)= -1508.985268

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1509.3397492

C	7.057895	-0.160560	1.101480
C	6.065878	0.764611	0.648307
C	4.979832	0.299563	-0.187214

C	4.970022	-1.095633	-0.519797
C	5.941810	-1.951202	-0.068276
C	7.003358	-1.483086	0.755654
C	3.998148	1.219180	-0.638585
C	4.097656	2.590607	-0.288034
C	5.188067	3.038133	0.551365
C	6.135291	2.114635	0.998279
C	5.288343	4.419936	0.906583
C	4.374867	5.335645	0.460319
C	3.304165	4.909316	-0.374217
C	3.171189	3.591898	-0.731356
C	2.880647	0.747250	-1.557013
C	1.556168	0.253470	-0.909052
B	1.154711	-1.424914	-1.039742
B	-0.613288	-1.478431	-1.211759
I	-1.633205	-3.023394	-2.397710
B	-1.314539	-0.782291	0.266706
B	0.155274	-1.783173	0.380180
B	1.551562	-0.691166	0.530226
B	0.943289	0.960616	0.515073
B	0.179657	1.253928	-1.055960
B	0.319564	-0.203171	-2.021399
B	-1.212340	0.193313	-1.218231
C	-0.755562	0.852289	0.308022
B	0.025142	-0.296575	1.331925
C	-1.569048	1.987094	0.995027
C	-3.079486	1.997873	0.818323
C	-3.907288	1.334563	1.760211
C	-5.345752	1.392911	1.615058
C	-5.901213	2.103971	0.549427
C	-5.103767	2.773886	-0.380700
C	-3.663708	2.728314	-0.248417
C	-3.399039	0.596484	2.880037
C	-4.233492	-0.026300	3.772165
C	-5.646689	0.035124	3.617270
C	-6.181791	0.726848	2.565228
C	-5.694097	3.508205	-1.456643
C	-4.921988	4.177969	-2.366159
C	-3.504977	4.146633	-2.241900
C	-2.902199	3.450033	-1.225992
I	0.177116	-3.741233	1.381915
H	0.242018	2.350704	-1.490839
H	-2.184681	0.578910	-1.764790
H	1.444586	1.878154	1.061645
H	2.563722	-0.934892	1.085540
H	1.923042	-2.157282	-1.562532
H	0.534517	-0.112610	-3.182107
H	-0.129170	-0.223273	2.503025
H	-2.367458	-1.054446	0.723551
H	3.242450	-0.067847	-2.186360
H	2.618558	1.544896	-2.255086
H	4.172622	-1.499478	-1.131627
H	5.898351	-3.002296	-0.339493
H	7.762390	-2.177196	1.104921
H	7.861211	0.217044	1.729468
H	6.952841	2.457322	1.629182
H	6.116451	4.726173	1.541253
H	4.462702	6.383000	0.734735
H	2.583071	5.638739	-0.733297
H	2.338069	3.310580	-1.363587

H	-1.153100	2.934474	0.645762
H	-1.327638	1.948423	2.058895
H	-2.329618	0.508743	3.028004
H	-3.810186	-0.579542	4.605897
H	-6.290860	-0.467928	4.332760
H	-7.258913	0.785171	2.428802
H	-6.983444	2.141110	0.443844
H	-6.778682	3.521113	-1.532715
H	-5.381438	4.732313	-3.179521
H	-2.893015	4.680126	-2.964197
H	-1.820260	3.446424	-1.175464

6(rot-5)

E(B3LYP/6-31G*)= -1508.984825

E(B3LYP/6-311+G**//B3LYP/6-31G*)= -1509.340728

C	-5.993056	-1.889802	-0.607028
C	-4.756099	-2.396716	-0.099446
C	-3.549356	-2.268803	-0.888190
C	-3.679638	-1.631859	-2.166919
C	-4.888468	-1.175691	-2.628337
C	-6.066336	-1.299305	-1.839262
C	-2.327284	-2.791578	-0.390507
C	-2.302987	-3.473691	0.853612
C	-3.516314	-3.582365	1.634405
C	-4.701922	-3.033089	1.142519
C	-3.491419	-4.263750	2.891816
C	-2.341226	-4.832557	3.366134
C	-1.146062	-4.748264	2.598219
C	-1.127512	-4.093985	1.393488
C	-1.062029	-2.698816	-1.227961
C	-0.094858	-1.503288	-0.989383
B	0.369921	-1.014736	0.596305
B	1.509078	-1.879319	-0.463123
B	1.184487	-1.380691	-2.137601
B	1.532877	0.349564	-2.263988
B	-0.125149	-0.207416	-2.095920
B	-0.636724	0.015725	-0.413375
B	0.719379	0.716932	0.469935
B	2.053468	-0.461194	0.449041
B	2.560924	-0.690756	-1.257577
B	2.073025	0.911758	-0.668756
C	0.430665	1.116440	-1.177980
C	-0.048339	2.535136	-1.605494
C	-0.822763	3.370322	-0.595558
C	-2.239653	3.304960	-0.557188
C	-2.969432	4.124394	0.387062
C	-2.269629	4.974896	1.244530
C	-0.877513	5.072616	1.205736
C	-0.131889	4.262655	0.266284
C	-3.020782	2.466927	-1.420287
C	-4.389881	2.435165	-1.352287
C	-5.094811	3.238913	-0.413765
C	-4.397398	4.059421	0.429632
C	1.292350	4.427595	0.262199
C	1.921920	5.300976	1.111610
C	1.178923	6.082529	2.039307
C	-0.183734	5.967308	2.079296
I	3.419793	-0.615908	2.165799
H	-0.945195	-0.095624	-2.939471
H	1.232911	-2.163717	-3.024244

H	-1.769760	0.252376	-0.201563
H	0.514848	1.512878	1.316723
H	2.778528	1.856271	-0.596872
H	1.855251	0.920307	-3.249953
H	-0.099285	-1.538024	1.543156
I	4.618733	-1.148387	-1.882422
H	1.781559	-3.008478	-0.236587
H	0.841961	3.080240	-1.924013
H	-0.643492	2.412586	-2.513011
H	1.900724	3.848149	-0.419773
H	3.003755	5.394814	1.077806
H	1.695771	6.765652	2.707257
H	-0.771185	6.558255	2.777875
H	-2.823911	5.583617	1.955915
H	-4.916105	4.683778	1.153161
H	-6.179502	3.196420	-0.372436
H	-4.942762	1.777025	-2.015526
H	-2.528525	1.827860	-2.143734
H	-0.469123	-3.605520	-1.093849
H	-1.322221	-2.690695	-2.287736
H	-2.809739	-1.510450	-2.800736
H	-4.948861	-0.717518	-3.612176
H	-7.014717	-0.931072	-2.220327
H	-6.881625	-1.998195	0.010183
H	-5.611116	-3.119530	1.733805
H	-4.416198	-4.323083	3.460570
H	-2.334060	-5.350122	4.321118
H	-0.234894	-5.205276	2.973866
H	-0.192182	-4.044794	0.849345

Powder X-ray Diffraction

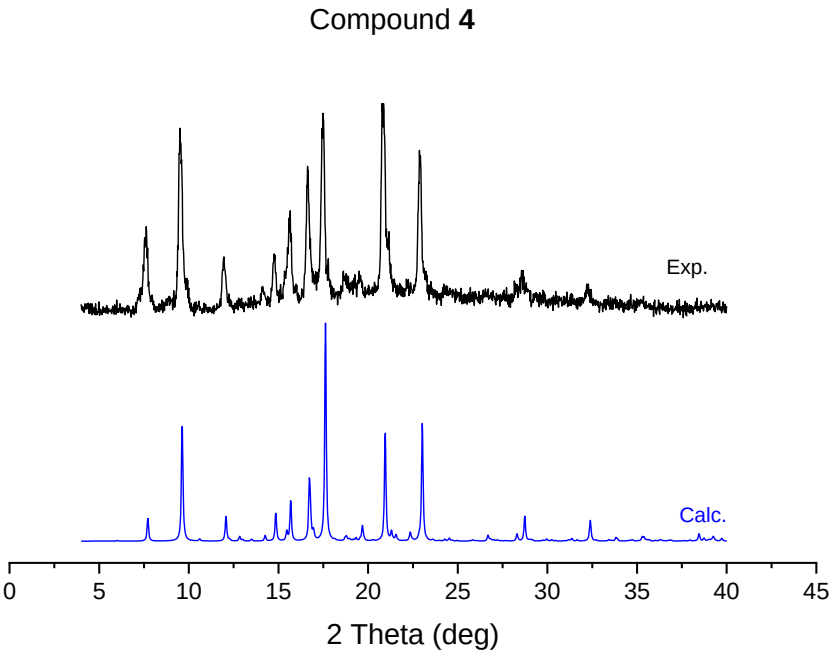


Figure S9. Simulated (blue) and experimental (black) PXRD patterns of **4**.

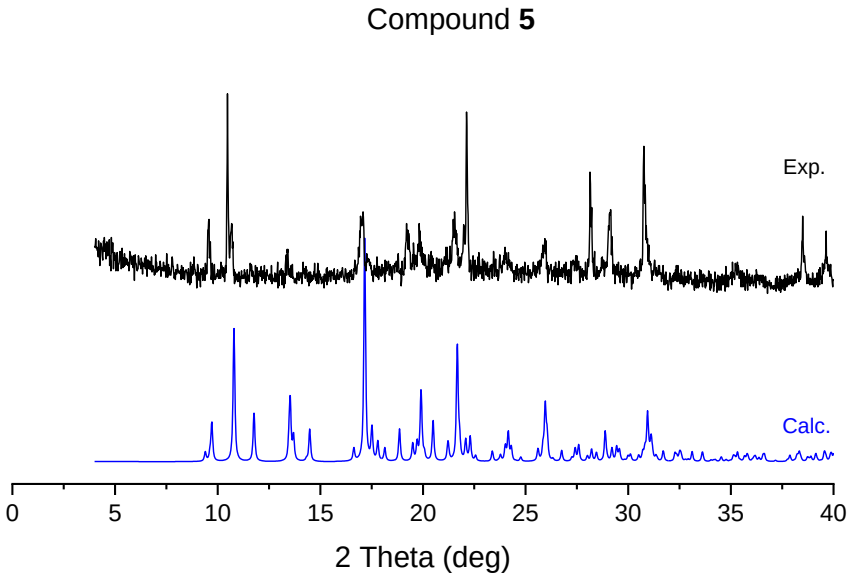


Figure S10. Simulated (blue) and experimental (black) PXRD patterns of **5**.

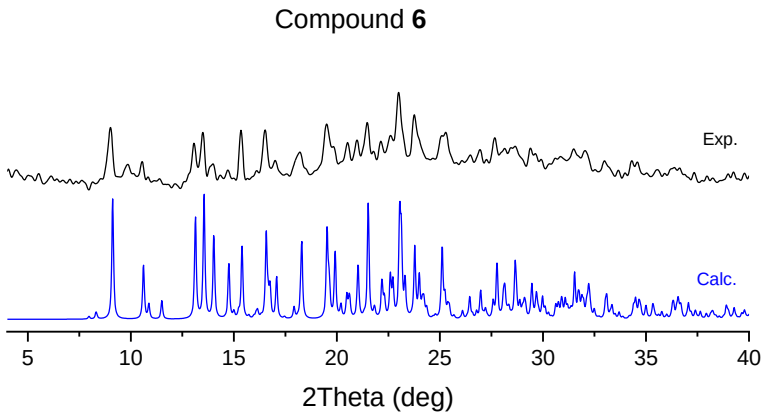
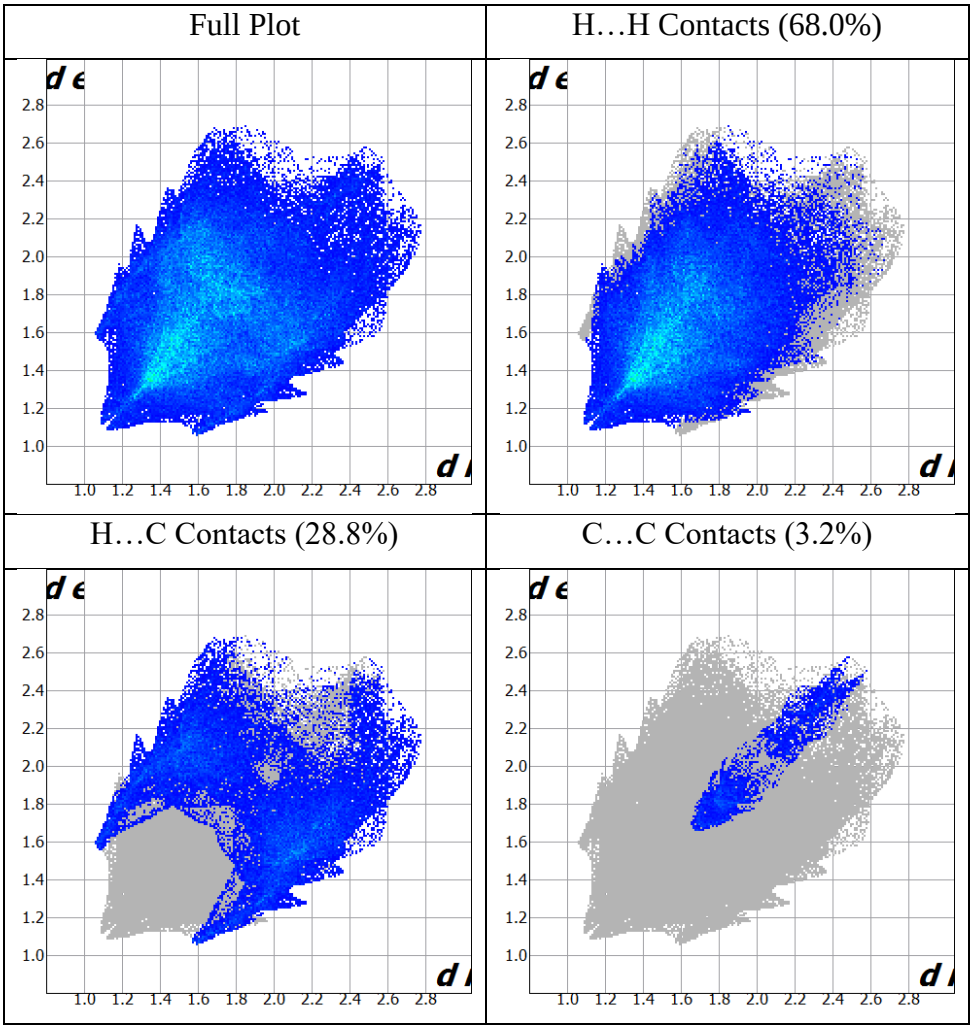


Figure S11. Simulated (blue) and experimental (black) PXRD patterns of **6**.

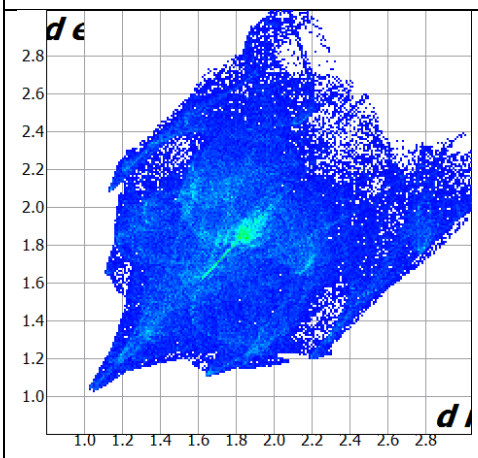
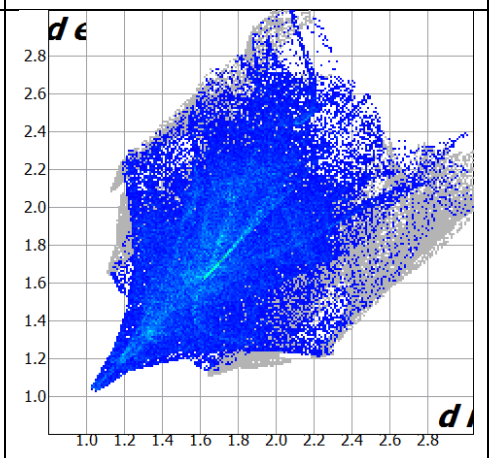
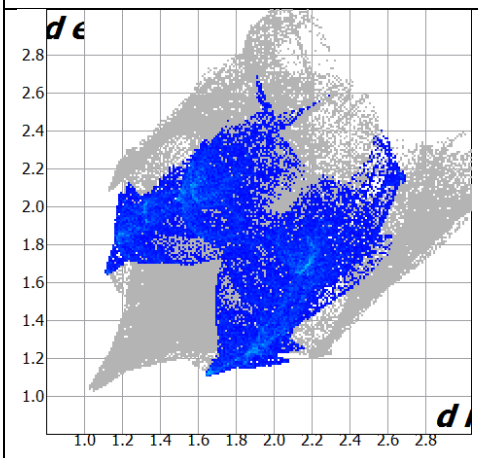
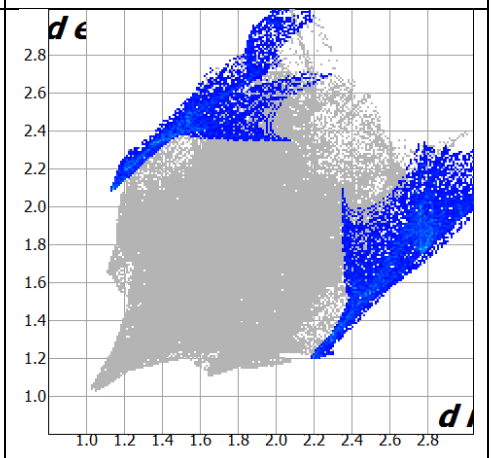
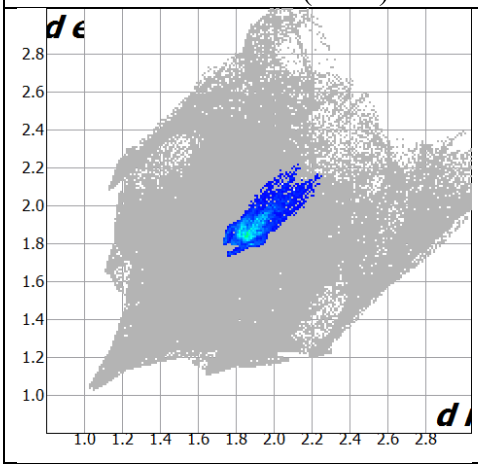
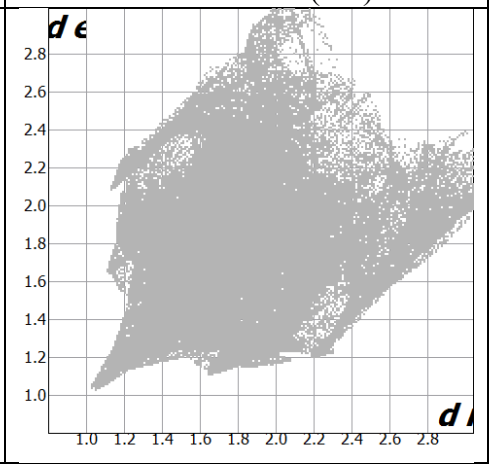
Hirshfeld Surface Analyses

Full and decomposed fingerprints for each compound were done by using CrystalExplorer17 (2017).[5] Legend: Close Contacts X···Y, where: X = atom inside the surface, Y = atom outside the surface.

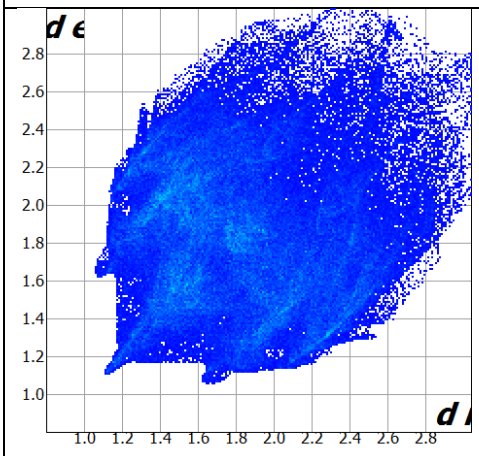
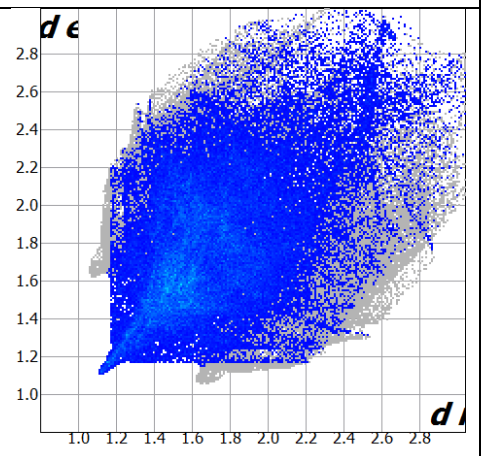
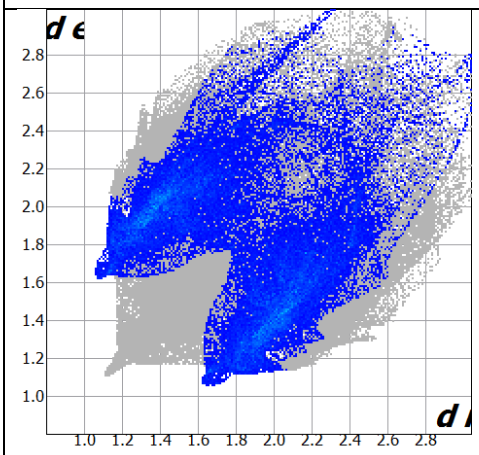
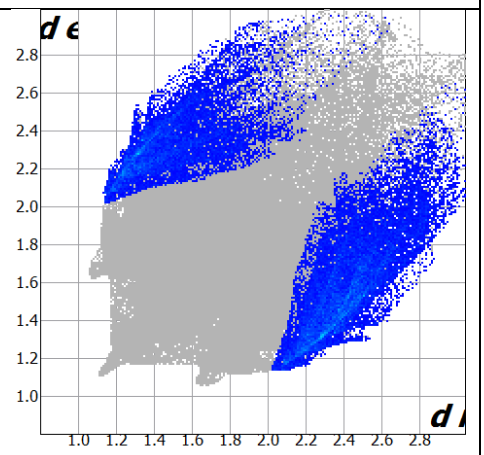
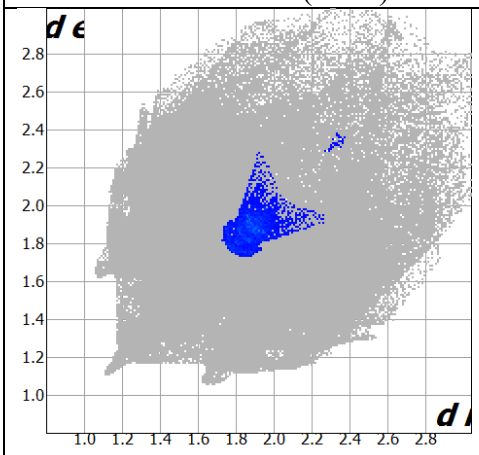
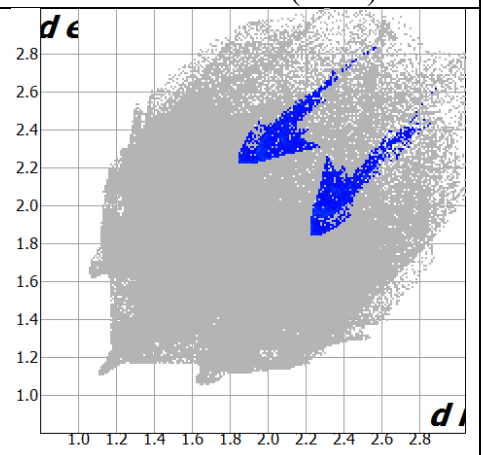
Compound (4)



Compound (5)

Full Plot	H…H Contacts (55.8%)
	
H…C Contacts (25.4%)	H…I Contacts (13.5%)
	
C…C Contacts (5.2%)	C…I Contacts (0%)
	

Compound (6)

Full Plot	H…H Contacts (46.6%)
	
H…C Contacts (28.9%)	H…I Contacts (20.4%)
	
C…C Contacts (1.9%)	C…I Contacts (2.2%)
	

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