Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information (ESI)

Columnar self-assembly of N,N',N''-trihexylbenzene-1,3,5-tricarboxamides investigated by means of NMR spectroscopy and computational methods in solution and solid state

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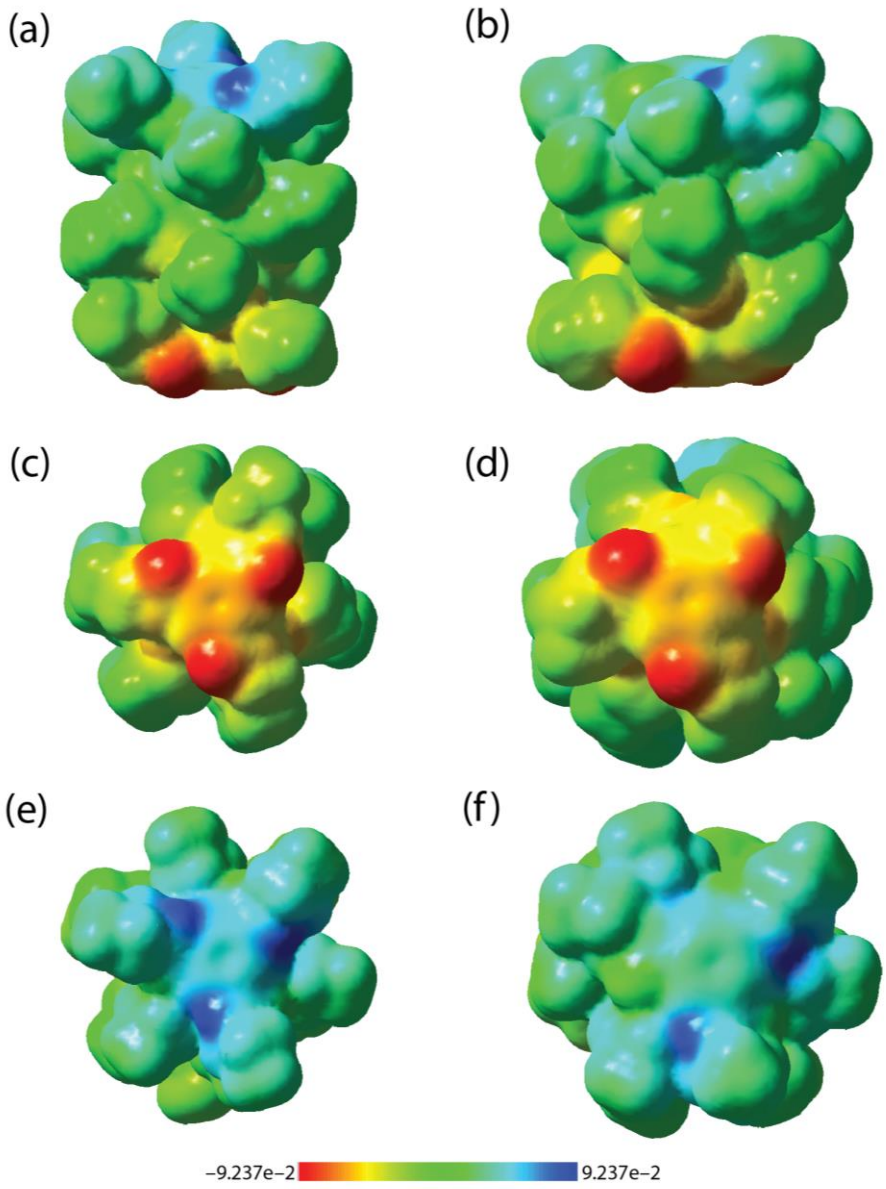

Figure ESI2 (a) Electron density isosurface at 0.004 e bohr^{-3} color-coded with electrostatic potential in the range ± 0.0924 V for pentameric BTA assembly as calculated at the B3LYP/6-31+G(d,p) level. (b) Analogous structure as produced by the B97D functional. (c,d) Bottom view down the column axis of the same structures of (a) and (b), respectively. (e,f) Top view down the column axis of the same structure of (a) and (b), respectively. One amide function of the top BTA unit in (f) is discordantly oriented with respect to the other two, as indicated by the only two positively charged regions (blue spots on the isosurface) due to the amide protons.

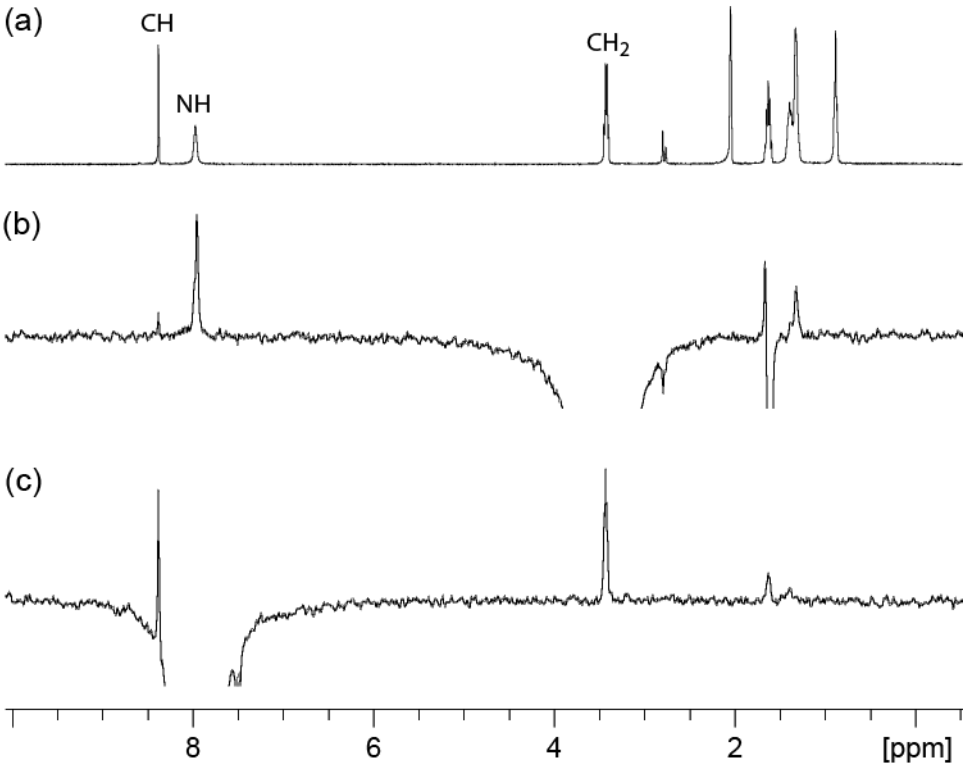

Figure ESI2 (a) Proton NMR spectrum of a 5 mM solution of BTA in acetone-d_6 at 9.4 T (400 MHz). (b, c) ROE spectra on the same sample of (a) where the irradiated peaks were the CH_2 at 3.42 ppm and the NH at 7.97 ppm, respectively. The number of scans was 4 in (a) and 6144 in (b, c). A recycling delay of 2 s was used in all cases. A spin locking time of 50 ms was used for the ROE spectra of (b, c).

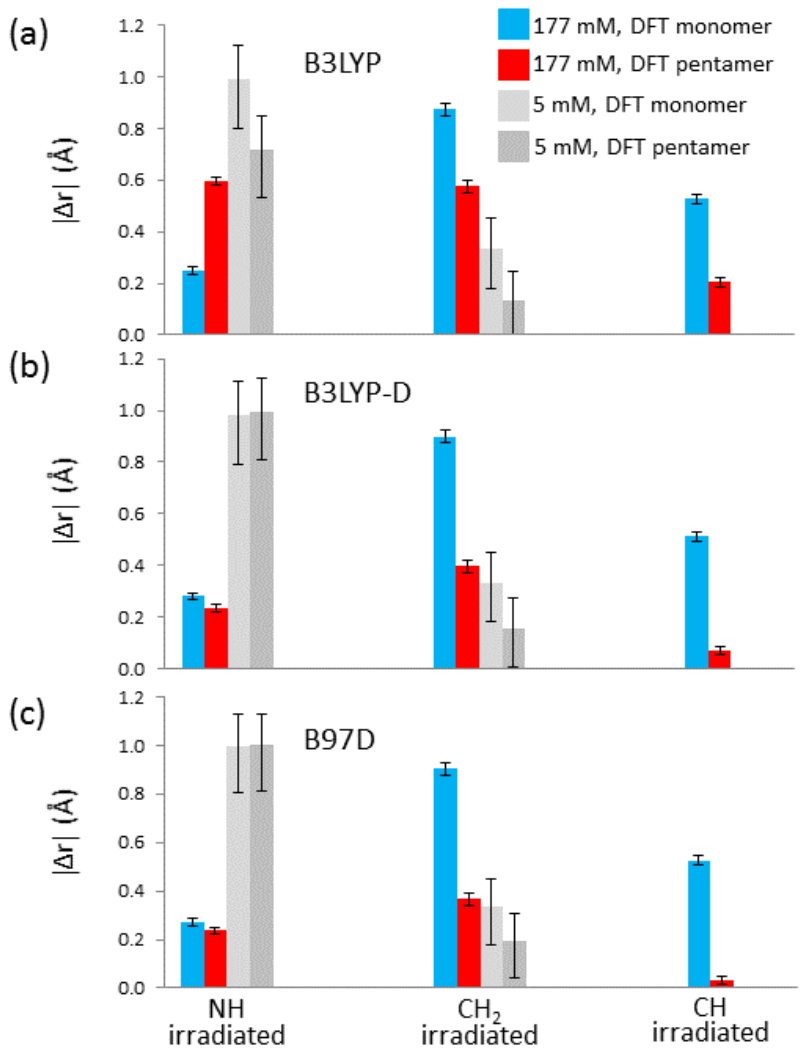

Figure ESI3 (a) Histogram of differences $|\Delta r| = |r_{ROE} - r_{DFT}|$ between interatomic distances as calculated with B3LYP and those measured from the experiments of Figure 1. Data for both 177 and 5 mM are shown with the color code indicated in the caption. (b,c) Histograms analogous to that of (a) for distances taken from structures optimized with the B3LYP-D and B97D functionals. The diluted sample results in much larger error bars that prevent the identification of a preferred structure. The overall inaccuracy of the ROE measurements in the more diluted case may be ascribed to i) much lower S/N in the 1D ROE spectra, ii) much longer spin locking pulse (50 ms vs 5 ms used in the 177 mM sample) in the attempt to gain sensitivity. This latter feature results in a less accurate measurement of distances due to a less strict fulfillment of the condition of linear growth of the ROE enhancement. Finally, iii) chemical exchange of the NH protons with the residual water of the solvent introduces leakage of the ROE enhancement towards the water proton bath.

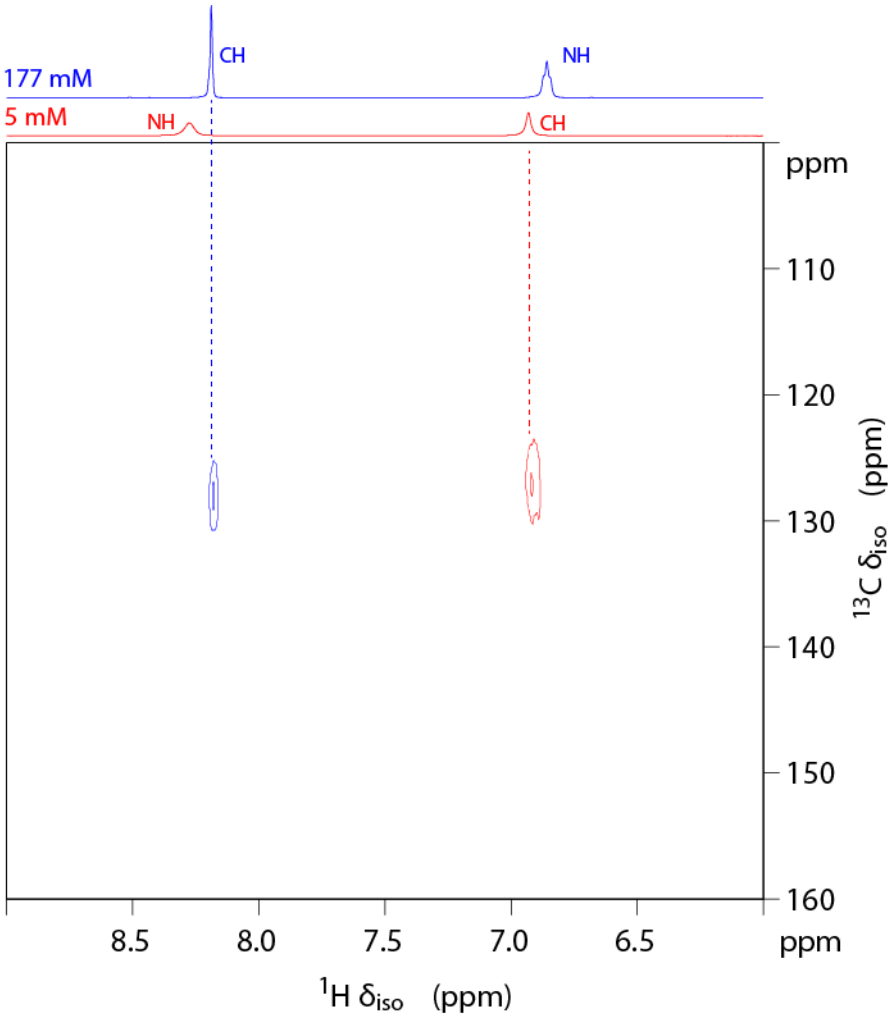

Figure ESI4 ^{1}H-^{13}C HSQC spectra of a 177 mM (blue) and 5 mM (red) solution of BTA in $CDCl_2$ at 9.4 T. The NH signals do not show correlations. The CH and NH signals invert their order from high to low concentration.

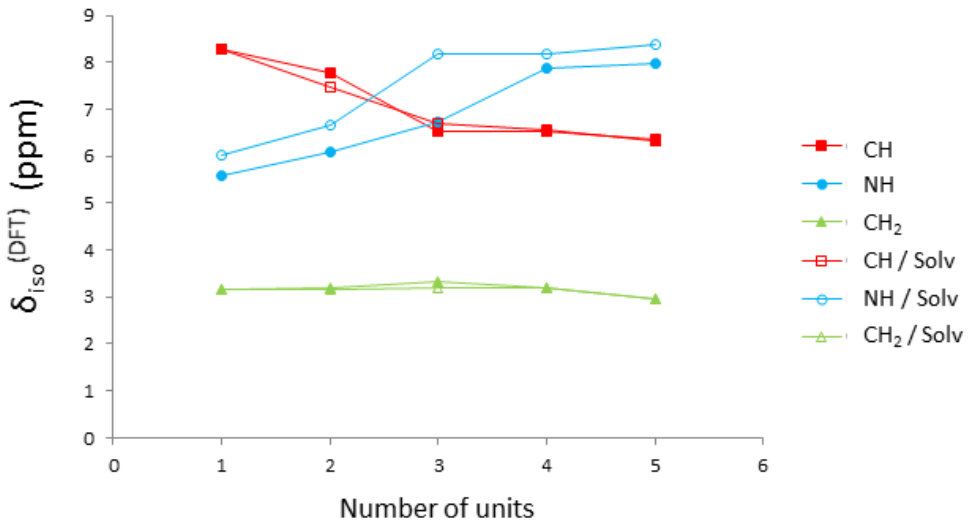

Figure ESI5 Calculated isotropic chemical shifts of the relevant proton sites as a function of the number of BTA units constituting the columnar assembly increases. Each structure was optimized with B3LYP/6-31G(d,p) and magnetic sheldings were calculated on these optimized structures with the GIAO method at the B3LYP/6-31+G(d,p) level. Empty and full data point indicate calculations where solvent effects (dichloromethane) were, and were not included, respectively.

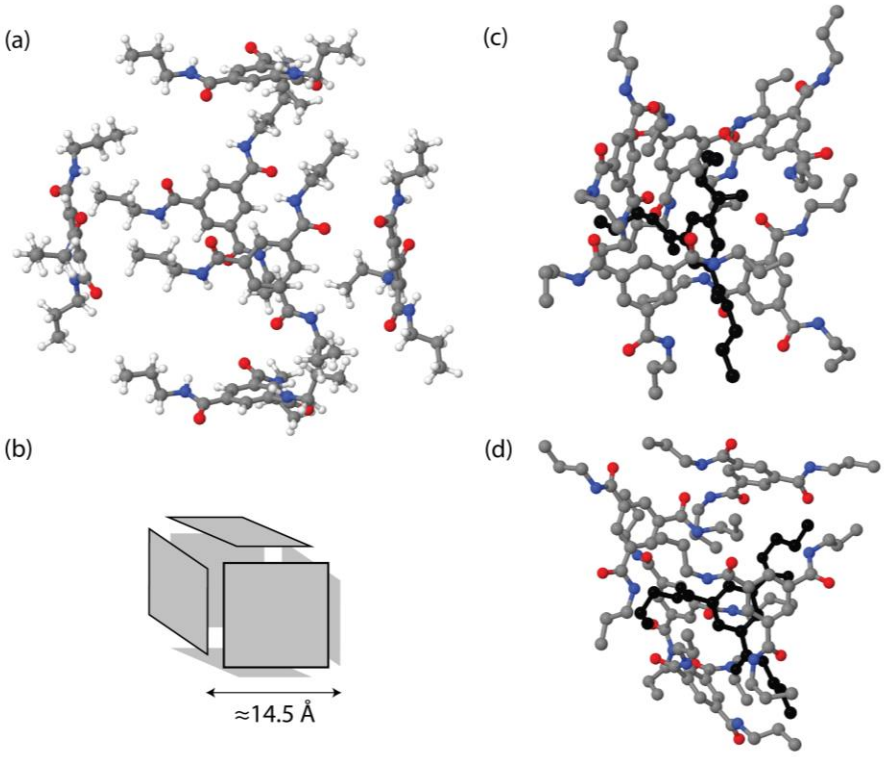

Figure ESI6 Hexameric face-centered cubic arrangement of BTA units utilized as initial geometry for optimization so as to produce a structure that mimics disorder in the solid state. (b) Schematic representation of the cubic arrangement of monomers shown in (a). (c, d) Resulting optimized structures with B3LYP and B97D functionals, respectively. Hydrogen atoms are omitted in (c) and (d) for clarity. Only the most inner molecule of the aggregates, shown in black, was considered for calculations of the chemical shifts.

The effect of truncation of the aliphatic chains was further investigated with a series of calculations performed with the B3LYP method. Within one monomeric BTA unit, the aliphatic chain of one amide substituent was varied across the alkyl series, from methyl to hexyl group. Both isotropic and anisotropic carbon chemical shifts were examined. The corresponding plots are given in ESI7. No substantial influence on both δ_{iso} and Δ_{CS} was observed for the CH, C and CO sites of interest.

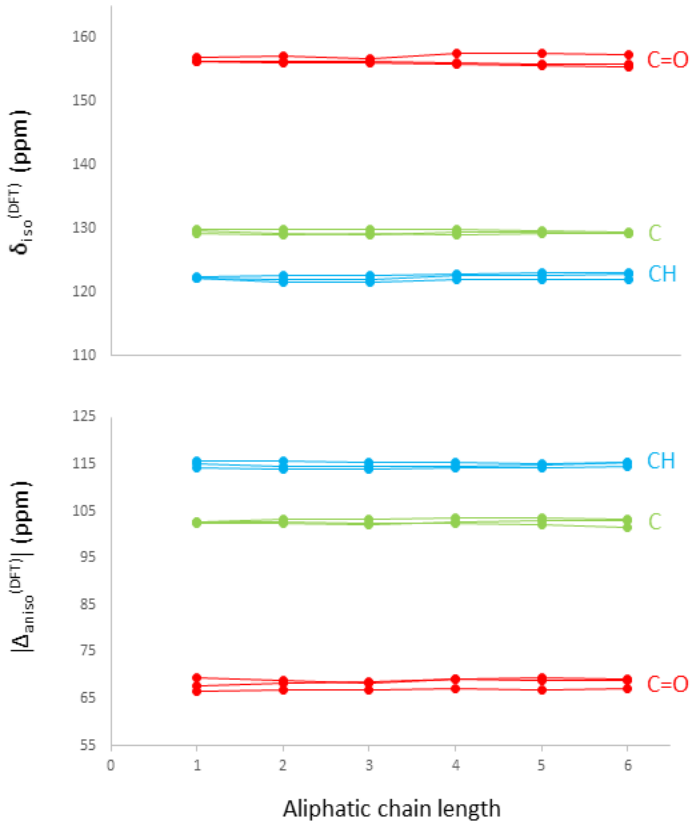

Figure ESI7 Calculated isotropic (top) and anisotropic (bottom) parts of the shift interactions for the relevant carbon sites of a single BTA unit as the aliphatic chain on one amide substituent is varied from methyl, ethyl, propyl, butyl, pentyl and hexyl groups. Each structure was optimized with B3LYP/6-31G(d,p) while freezing the dihedral angle at the desired value. Magnetic shieldings were calculated on these optimized structures with the GIAO method at the B3LYP/6-31+G(d,p) level.

The influence of the orientation of the amide functions with respect to the aromatic cores on the chemical shift parameters was specifically addressed by a series of calculations performed on a monomeric BTA where one of the three dihedral angles HCCCO was varied in five steps of 60°, from its equilibrium value. Each structure was optimized with B3LYP/6-31G(d,p) while freezing the dihedral angle at the desired value. Magnetic shieldings were calculated on these optimized structures with the GIAO method at the B3LYP/6-31+G(d,p) level. The corresponding profiles are shown in Figure ESI8(a) and (b), for δ_{iso} and Δ_{CS}, respectively. No averaging of values over equivalent sites was performed in this case. The vertical dashed line indicates the equilibrium angle as found in the pentameric self-assembly at the same level of theory of the optimization. The carbon environment mostly affected, both in δ_{iso} and Δ_{CS} parameters, is the CH, with the other C and CO sites being much less influenced. However, in proximity of the value of dihedral angle as found in the self-assembly, all carbon sites are characterized by relatively small variations (less than ca. 3 ppm), for both δ_{iso} and Δ_{CS}.

A series of calculations was performed with the B3LYP-D functional in order to highlight the influence of non-covalent and dispersive contributions on chemical shift parameters in a self-assembly. For this purpose, the optimized structure of columnar trimer of BTA units was progressively 'expanded' by moving the first and third outermost units away from the central one, along the column axis, 2 Å away from the equilibrium interplane distance, in four steps of 0.5 Å. The four structures thus generated were not subject to further geometry optimization and used as is for the calculation of the NMR parameters. The corresponding profiles are shown in Figure ESI8(c) and (d), for δ_{iso} and Δ_{CS}, respectively. As found for the orientation of the amide functions, the carbon site most affected by the 'loosing' of π-π stacking effects is the CH of the aromatic core, with an overall average shielding of 13.5 and 7.6 ppm, for anisotropic and isotropic parameters, respectively. These values, calculated for these trimeric structures in this set of data, are consistent with the values calculated for monomeric and pentameric structures as used in Figure 8, for which CH experiences an average deshielding upon packing of 12.5 and 3.3 ppm, for anisotropic and isotropic parameters, respectively. The other relevant carbon environments, CO and C, are less affected by the columnar packing, with variations of $\Delta_{CS} < 5$ ppm and $\delta_{iso} < 2$ ppm.

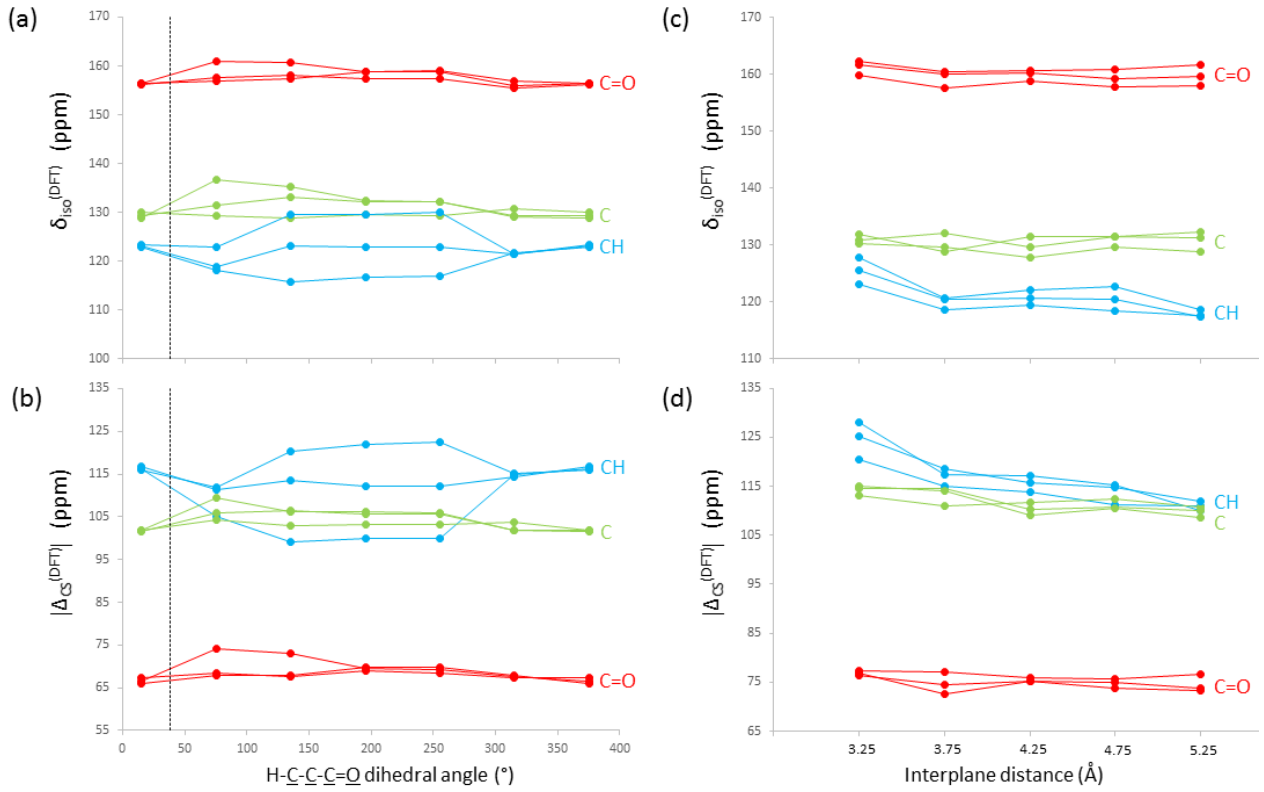

Figure ESI8 Calculated isotropic (a) and anisotropic (b) parts of the shift interactions for the relevant carbon sites of a single BTA unit as a function of one dihedral angle H-C-C-C=O determining the orientation of one of the three amide functions. The vertical dashed line indicates the angle as found in the pentameric self-assembly at the same level of theory of the optimization. Calculated isotropic (c) and anisotropic (d) shift parameters for the relevant carbon sites of the central BTA unit within a trimeric column as the top and bottom units are progressively moved apart along the column axis, from their equilibrium interplane distance in steps of 0.5 Å. The equilibrium trimeric structure was optimized at the B3LYP-D/6-31G(d,p) level. The other structures were not subject to geometry optimization. Magnetic shieldings were calculated on all structures with the GIAO method at the B3LYP-D/6-31+G(d,p) level.

Table ESI1 Differences $\Delta r = \left| r_{ROE} - r_{DFT} \right|$ as calculated with the B3LYP functional and 6-31+G(d,p) basis set and used in the histogram of Fig. 4(a).

	177 mM		5 mM	
Irradiated site	monomer	pentamer	monomer	pentamer
NH	0.25	0.60	0.99	0.72
CH_2	0.87	0.58	0.33	0.13
CH	0.53	0.20	-	-

Table ESI2 Differences $\Delta r = \left| r_{ROE} - r_{DFT} \right|$ as calculated with the B3LYP-D functional and 6-31G(d,p) basis set and used in the histogram of Fig. 4(a).

	177 mM		5 mM	
Irradiated site	monomer	pentamer	monomer	pentamer
NH	0.28	0.24	0.98	1.00
CH_2	0.90	0.40	0.33	0.16
CH	0.51	0.07	-	-

Table ESI3 Differences $\Delta r = \left| r_{ROE} - r_{DFT} \right|$ as calculated with the B97D functional and 6-31G(d,p) basis set and used in the histogram of Fig. 4(b).

	177 mM		5 mM	
Irradiated site	monomer	pentamer	monomer	pentamer
NH	0.27	0.24	1.00	1.00
CH_2	0.90	0.37	0.33	0.19
CH	0.53	0.03	-	-

Table ESI4 Proton chemical shifts (ppm) calculated with the B3LYP functional and 6-31+G(d,p) basis set, as used in the plot in Fig. 5(a) and (c).

	$\delta_{iso}(^1H)$				
	monomer	dimer	trimer	tetramer	pentamer
CH	8.29	7.76	6.54	6.53	6.36
NH	5.57	6.10	6.72	7.88	7.96
CH_2	3.16	3.18	3.34	3.21	2.96

Table ESI5 Proton chemical shifts (ppm) calculated with the B3LYP-D functional and 6-31+G(d,p) basis set, as used in the plot in Fig. 5(a) and (c).

	$\delta_{iso}(^1H)$				
	monomer	dimer	trimer	tetramer	pentamer
CH	8.30	7.61	6.90	6.99	7.08
NH	5.60	6.01	8.04	8.28	8.77
CH_2	3.09	3.30	3.43	3.32	3.19

Table ESI6 Proton chemical shifts (ppm) calculated with the B97D functional and 6-31+G(d,p) basis set, as used in the plot in Fig. 5(b) and (d).

	$\delta_{iso}(^1H)$				
	monomer	dimer	trimer	tetramer	pentamer
CH	8.06	7.45	6.79	7.03	7.00
NH	5.63	7.04	7.85	8.90	8.57
CH_2	3.14	3.36	3.58	3.46	3.36

Table ESI7 Experimental proton chemical shifts (ppm) of BTA as used in Fig. 5(d-f).

	$\delta_{iso}(^1H)$	
	177 mM	5 mM
CH	6.88	8.30
NH	8.22	6.42
CH_2	3.24	3.43
CH_3	0.89	0.89

Table ESI8 Calculated carbon chemical shift parameters (ppm) of BTA at the B3LYP/6-31+G(d,p) level, as used in Fig. 8(a) and (d).

	B3LYP					
	monomer		pentamer		disordered	
	δ_{iso}	Δ_{CS}	δ_{iso}	Δ_{CS}	δ_{iso}	Δ_{CS}
C=O	156.3	67	161.6	77	162.5	77
C	129.4	102	130.5	114	131.6	110
CH	123.2	116	121.9	117	123.2	112
CH_2	42.0	24	42.5	27	42.6	24

Table ESI9 Calculated carbon chemical shift parameters (ppm) of BTA at the B3LYP-D/6-31+G(d,p) level, as used in Fig. 8(b) and (d).

	B3LYP-D					
	monomer		pentamer		disordered	
	δ_{iso}	Δ_{CS}	δ_{iso}	Δ_{CS}	δ_{iso}	Δ_{CS}
C=O	156.8	68	162.1	80	153.5	71
C	129.4	103	133.9	121	126.8	102
CH	121.6	112	124.9	127	119.6	108
CH_2	36.6	22	41.0	26	45.2	22

Table ESI10 Calculated carbon chemical shift parameters (ppm) of BTA at the B97D/6-31+G(d,p) level, as used in Fig. 8(c) and (d).

	B97D					
	monomer		pentamer		disordered	
	δ_{iso}	Δ_{CS}	δ_{iso}	Δ_{CS}	δ_{iso}	Δ_{CS}
C=O	152.4	61	157.7	75	153.5	71
C	126.8	97	129.7	113	126.8	102
CH	116.0	106	119.6	118	119.6	108
CH_2	45.9	28	43.8	27	45.2	22

Table ESI11 Correlation coefficients R^2 as used in Fig. 8(d).

	Δ_{CS}			δ_{iso}		
	B3LYP	B3LYP-D	B97D	B3LYP	B3LYP-D	B97D
monomer	0.9708	0.9837	0.9750	0.9980	0.9982	0.9996
disordered	0.9969	0.9936	0.9936	0.9999	0.9996	0.9996
pentamer	0.9985	0.9950	0.9960	0.9999	0.9992	0.9999

Cartesian coordinates of the BTA monomeric structure used in this study and optimized at the B3LYP/6-31G(d,p) level.

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   51
Monomer B3LYP
 H     0.656757    -2.132294     0.840490
 C     0.335817    -1.159939     0.481663
 C    -1.001132    -0.861436     0.212936
 C    -2.132940    -1.849804     0.338894
 C    -1.346210     0.439350    -0.175295
 H    -2.395328     0.625344    -0.378985
 C    -0.370926     1.429717    -0.301513
 C    -0.659040     2.854235    -0.703876
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C	0.969526	1.103929	-0.058881
H	1.691179	1.906995	-0.164532
C	1.332077	-0.186950	0.329858
C	2.745558	-0.616023	0.635629
O	2.970529	-1.671720	1.225727
N	3.740980	0.224202	0.229146
O	0.241025	3.593328	-1.101343
O	-3.302683	-1.469023	0.362261
N	-1.788223	-3.165986	0.435571
N	-1.955393	3.266078	-0.607136
C	-2.795587	-4.215828	0.523777
C	-2.347230	4.634585	-0.930217
C	5.147465	-0.110778	0.415363
H	-1.735343	4.948173	-1.778992
C	-2.168595	5.626534	0.229607
H	-3.393810	4.612191	-1.255323
C	5.750836	-0.899890	-0.754657
H	5.212700	-0.699681	1.333399
H	5.701917	0.822054	0.572642
H	-3.643172	-3.796098	1.071130
H	-2.380412	-5.035417	1.121962
C	-3.264788	-4.735605	-0.842116
H	-3.672220	-3.891634	-1.409608
C	-4.318434	-5.838181	-0.707975
H	-2.400338	-5.111797	-1.405190
H	5.172628	-1.821940	-0.881667
C	7.228065	-1.231378	-0.526997
H	5.636653	-0.321387	-1.681073
C	-3.028371	5.308724	1.455839
H	-2.415346	6.628153	-0.145437
H	-1.108191	5.644856	0.504069
H	-0.835315	-3.434546	0.244447
H	3.512358	0.983351	-0.394366
H	-2.618263	2.676996	-0.128430
H	7.828909	-0.322303	-0.408013
H	7.641347	-1.793166	-1.369920
H	7.362689	-1.838231	0.374995
H	-2.875869	6.048856	2.247159
H	-2.779723	4.327965	1.875281
H	-4.096339	5.306070	1.206673
H	-4.644591	-6.194850	-1.689478
H	-5.204151	-5.475806	-0.174862
H	-3.927792	-6.700148	-0.154832

Cartesian coordinates of the BTA monomeric structure used in this study and optimized at the B97D/6-31G(d,p) level.

51
Monomer B97D

H	-2.335020	-0.059487	-0.885021
C	-1.299048	-0.062080	-0.546645
C	-0.596770	-1.255390	-0.310491
C	-1.209645	-2.632627	-0.443165
C	0.764007	-1.191296	0.044289
H	1.278593	-2.133754	0.229338
C	1.417089	0.045338	0.171008
C	2.876242	0.188056	0.544254
C	0.688631	1.231667	-0.038378
H	1.229147	2.172888	0.056686
C	-0.669937	1.187938	-0.393039
C	-1.512249	2.418257	-0.656245
O	-2.587278	2.346442	-1.263837
N	-1.006701	3.606731	-0.187436
O	3.324347	1.246599	1.002005
O	-0.505152	-3.641870	-0.570109
N	-2.581607	-2.686324	-0.431959
N	3.655090	-0.927610	0.356648
C	-3.288333	-3.966773	-0.468846

C	5.100717	-0.883700	0.578956
C	-1.784345	4.843306	-0.273893
H	5.270193	-0.300116	1.493854
C	5.872386	-0.243615	-0.589352
H	5.447290	-1.913632	0.754669
C	-2.841447	4.969719	0.837770
H	-2.279055	4.847634	-1.254363
H	-1.080486	5.689051	-0.237110
H	-2.763998	-4.606615	-1.191556
H	-4.305662	-3.780198	-0.845434
C	-3.337360	-4.672578	0.898840
H	-2.301865	-4.818193	1.238991
C	-4.068462	-6.021062	0.808057
H	-3.837482	-4.015888	1.630313
H	-3.510593	4.099692	0.767550
C	-3.642453	6.274853	0.707474
H	-2.343117	4.925085	1.820669
H	5.671675	-0.811650	-1.513115
C	7.382870	-0.199982	-0.309692
H	5.479160	0.773026	-0.734825
H	-3.095599	-1.874884	-0.114199
H	-0.253955	3.578374	0.488499
H	3.294215	-1.672003	-0.226857
H	-4.152470	6.322367	-0.267198
H	-2.982392	7.153707	0.784206
H	-4.406001	6.354504	1.494684
H	-3.564996	-6.688711	0.091710
H	-5.107734	-5.886022	0.467714
H	-4.093843	-6.527126	1.783914
H	7.929170	0.262089	-1.144612
H	7.787454	-1.213641	-0.158664
H	7.593196	0.384368	0.599497

Cartesian coordinates of the BTA pentameric self-assembly used in this study and optimized at the B3LYP/6-31G(d,p) level.

255
Pentamer B3LYP

H	4.265765	-2.064366	-1.669505
C	4.239884	-1.192629	-1.024735
C	4.261122	0.083044	-1.604392
C	4.363582	0.195248	-3.100503
C	4.288512	1.212175	-0.783699
H	4.350083	2.205906	-1.213025
C	4.285665	1.076417	0.610310
C	4.391068	2.318654	1.449792
C	4.267547	-0.198421	1.178422
H	4.314734	-0.323892	2.254400
C	4.236725	-1.337890	0.364352
C	4.294093	-2.687415	1.025052
O	4.984920	-2.874432	2.038199
N	3.563075	-3.667955	0.446187
O	5.082734	3.280637	1.082190
O	5.073460	-0.586280	-3.751498
N	3.663337	1.200366	-3.676715
N	3.702577	2.311973	2.614707
C	3.774646	1.469935	-5.107020
C	3.743079	3.446243	3.528243
C	3.548136	-5.021758	0.984684
H	3.631037	3.059171	4.547268
C	2.660337	4.495727	3.240916
H	4.733773	3.900470	3.445097
C	2.471090	-5.237400	2.057319
H	4.537585	-5.220703	1.404419
H	3.388062	-5.711776	0.148635
H	4.794348	1.212367	-5.401924
H	3.639258	2.547801	-5.252898
C	2.774794	0.687940	-5.973054

H	2.878907	-0.376680	-5.735281
H	3.074184	0.802798	-7.023111
C	1.321763	1.140826	-5.803540
H	2.650810	-4.527828	2.873205
C	2.467565	-6.670457	2.596424
H	1.490623	-4.994959	1.627557
H	2.789187	4.850203	2.211931
C	2.720782	5.674713	4.216000
H	1.675631	4.013781	3.295022
H	2.952222	1.694715	-3.139058
H	2.840229	-3.431997	-0.233871
H	2.990451	1.601057	2.783273
H	6.366743	5.014886	-1.784297
H	7.317154	-3.216883	-4.937377
H	8.109940	4.945654	-2.046250
H	8.006251	-4.238743	-3.662240
H	8.115428	0.169179	-2.625430
C	7.333708	4.855282	-1.282196
C	7.195491	-3.544464	-3.896985
C	7.392120	7.334613	-0.708057
O	8.479303	-3.552295	-1.408716
N	7.411369	3.502145	-0.757349
O	8.704517	2.688946	-2.462744
N	7.356766	-2.389679	-3.027757
C	5.677123	-5.442229	-4.668362
C	7.512811	5.902959	-0.178570
H	6.732971	3.253661	-0.039298
C	7.978363	-2.503417	-1.817314
C	8.099361	2.517383	-1.403611
C	8.064455	0.030909	-1.550838
H	6.728949	-1.605228	-3.192891
C	5.838246	-4.243098	-3.729965
H	6.761769	5.728634	0.602317
H	5.041835	-3.511493	-3.915385
C	8.011664	-1.246628	-0.988104
H	8.492152	5.755099	0.292185
C	8.065176	1.168493	-0.733357
H	5.741765	-4.565916	-2.686378
C	7.996105	-1.385888	0.406055
C	8.045258	1.016966	0.654774
H	7.992548	-2.388037	0.820632
H	8.076726	1.878139	1.313321
C	7.998687	-0.259133	1.231511
C	7.963275	-0.346335	2.734559
H	6.656726	-1.944188	2.655367
O	8.494810	0.514995	3.437240
N	7.306796	-1.429000	3.246122
H	5.001696	-1.481051	4.707858
H	5.815856	0.060872	4.975872
C	7.153612	-1.595727	4.682284
C	5.844172	-1.006005	5.226930
H	7.202238	-2.667211	4.913967
H	8.008220	-1.106212	5.156371
C	5.702359	-1.194768	6.739746
C	-5.158554	-6.276019	3.428043
C	-5.149599	-4.909541	2.737396
H	-6.098851	-4.750557	2.208821
H	-5.057272	-4.109950	3.482495
H	-4.072878	-5.549574	0.965680
H	-3.037304	-4.892320	2.243620
C	-3.996117	-4.772182	1.734253
H	0.939701	-3.093985	4.878948
C	1.077093	-2.280705	6.885455
H	2.006181	-1.699904	5.017080
C	1.054273	-2.116545	5.363595
C	-1.407650	-5.974297	-4.112006
N	-3.971627	-3.476255	1.064803
H	-1.208394	-5.056232	-2.158105
O	-2.473983	-2.545703	2.509171
H	0.667737	-4.197225	-3.554348
H	-4.689273	-3.300542	0.363840

C	-1.395605	-4.749428	-3.193460
O	1.176532	-3.465765	-1.252208
C	-3.204112	-2.456037	1.510490
C	-0.077364	-1.190821	4.897372
H	-0.843641	-1.560813	2.941111
H	-1.047762	-1.586492	5.215319
C	-0.320131	-3.731339	-3.597304
H	0.500316	-2.251694	1.035653
H	-2.376169	-4.256113	-3.211393
H	0.050712	-0.199571	5.344487
N	-0.131524	-1.034971	3.447015
H	-0.491086	-3.390534	-4.624465
C	0.476137	-2.511341	-1.624580
N	-0.287260	-2.553217	-2.739124
C	-3.269539	-1.179012	0.719139
C	0.480065	-1.281886	0.550078
H	-3.121915	0.016551	2.495870
H	-3.307402	-2.104826	-1.232481
C	0.638955	-0.131929	2.803859
C	0.449624	-1.223568	-0.849501
C	-3.203573	0.035802	1.414435
C	-3.307693	-1.173588	-0.676333
H	-0.992793	-1.834915	-2.902829
C	0.527488	-0.108116	1.304656
O	1.398096	0.648543	3.399860
H	-4.413302	2.016514	2.851824
C	0.481705	0.016786	-1.489012
C	-3.188515	1.247031	0.720388
C	-3.294279	0.036971	-1.381660
C	0.559308	1.131648	0.653461
H	0.500228	0.075175	-2.571651
O	-2.605762	-0.884707	-3.474756
N	-3.706303	2.701906	2.592004
H	-3.597592	3.631311	4.447530
C	-3.227168	1.241968	-0.680142
C	-3.259898	-0.012132	-2.884363
C	0.530180	1.199372	-0.740425
C	-3.038562	2.567993	1.423668
H	0.642524	2.035556	1.246926
H	-5.748391	4.335700	3.356401
C	-3.633482	3.920187	3.390818
H	-5.294548	-0.657732	-5.301807
C	-4.812972	4.871657	3.147762
O	-2.331367	3.465525	0.941439
H	-3.162239	2.186738	-1.209025
H	-2.691790	4.414946	3.142754
N	-3.968342	0.942962	-3.528451
H	-4.627657	1.519821	-3.009373
C	0.636141	2.510237	-1.468239
H	-3.107169	0.537362	-5.360613
C	-4.729060	6.131741	4.013369
H	-4.826651	5.142738	2.084973
H	-0.766361	3.365770	-0.223819
C	-5.261001	0.398779	-5.594961
C	-4.004368	1.033364	-4.983922
O	1.335018	2.623225	-2.487371
N	-0.061419	3.540660	-0.940284
H	-6.147123	0.881535	-5.162207
C	-5.290436	0.523980	-7.120693
H	-3.948329	2.092523	-5.260650
H	-0.906357	4.332030	-3.415097
H	-2.069910	4.889814	-2.211609
C	-0.022262	4.872018	-1.533482
C	-1.073807	5.080189	-2.632211
H	0.979019	5.021183	-1.945900
H	-0.169480	5.599149	-0.727398
C	-1.017247	6.489025	-3.229030
H	-6.352467	5.018522	-2.148427
H	-8.599298	4.576916	-3.121226
C	-8.481525	5.366969	-2.370739
C	-7.245359	5.048963	-1.520282

H	-9.376995	5.337110	-1.736000
H	-7.094307	5.821928	-0.758389
C	-8.372520	6.732932	-3.053932
N	-7.326300	3.757238	-0.839962
H	-7.910642	3.683802	-0.020124
O	-6.234481	2.591939	-2.460167
C	-6.815869	2.618966	-1.368416
C	-6.969539	1.367853	-0.547642
H	-6.785312	2.299707	1.398952
H	-6.993791	0.160143	-2.312886
C	-6.918887	1.375260	0.846936
C	-7.036383	0.145350	-1.228914
H	-8.205426	-1.736451	-2.706726
C	-6.942465	0.172666	1.566009
O	-6.066492	1.141826	3.563915
C	-7.059282	-1.058317	-0.523641
C	-6.748557	0.242993	3.056030
N	-7.604964	-2.492625	-2.412828
C	-7.009060	-1.038836	0.876532
H	-8.352985	0.980545	5.671626
H	-7.567730	-3.440327	-4.261519
C	-6.989977	-2.395103	-1.209783
H	-9.728145	-4.080326	-3.110708
C	-7.598097	-3.722668	-3.203327
N	-7.336625	-0.731107	3.791055
C	-8.356737	-0.070713	5.981254
H	-6.948409	-1.987011	1.400426
H	-7.995167	-1.344278	3.333634
H	-9.320834	-0.491111	5.666175
C	-8.799232	-4.635242	-2.924654
H	-6.259211	-0.352118	5.508945
H	-6.667170	-4.243947	-2.969091
C	-7.222084	-0.796646	5.247376
O	-6.379030	-3.339945	-0.695098
C	-8.214658	-0.174026	7.502323
C	-8.767310	-5.902498	-3.783307
H	-8.794744	-4.898457	-1.860863
H	-7.193438	-1.853665	5.534240
H	-8.788986	-5.662054	-4.852030
H	-9.628006	-6.542496	-3.569933
H	-7.861758	-6.488093	-3.592284
H	-9.260239	6.941487	-3.657621
H	-7.501750	6.776467	-3.716743
H	-8.272815	7.540352	-2.320050
H	-7.273057	0.269112	7.843648
H	-8.231544	-1.217607	7.835723
H	-9.030674	0.348926	8.008928
H	-5.261725	-7.089126	2.700882
H	-5.988923	-6.358122	4.136036
H	-4.230052	-6.444371	3.984091
H	0.639858	0.517148	-6.391411
H	1.193450	2.178572	-6.133449
H	1.006267	1.097096	-4.756704
H	-6.194461	0.071198	-7.539250
H	-4.427860	0.025660	-7.575987
H	-5.270187	1.573713	-7.434087
H	-5.577925	6.797390	3.829592
H	-3.813532	6.695644	3.804776
H	-4.728640	5.881789	5.080143
H	-1.606565	-5.691783	-5.152226
H	-2.178159	-6.690467	-3.809614
H	-0.444126	-6.494907	-4.089223
H	0.142300	-2.718103	7.255956
H	1.213496	-1.315830	7.386789
H	1.896359	-2.934384	7.198718
H	-1.772180	6.620417	-4.010606
H	-0.038195	6.689678	-3.677570
H	-1.193754	7.254406	-2.464477
H	1.942249	6.412685	3.997468
H	3.688006	6.186097	4.158877
H	2.582951	5.343276	5.251835

H	2.279461	-7.396754	1.797094
H	1.693350	-6.807855	3.358191
H	3.430744	-6.923995	3.052960
H	5.757770	-5.139141	-5.719056
H	4.702793	-5.924603	-4.537114
H	6.448968	-6.197965	-4.483053
H	6.410845	7.508637	-1.165149
H	8.151693	7.542212	-1.470450
H	7.518259	8.068154	0.094771
H	5.720055	-2.256832	7.012390
H	4.761443	-0.773634	7.109270
H	6.520282	-0.702945	7.278400

Cartesian coordinates of the BTA pentameric self-assembly used in this study and optimized at the B97D/6-31G(d,p) level.

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Pentamer B97D

H	3.428934	-2.373535	-1.330449
C	3.562396	-1.389267	-0.894593
C	3.580984	-0.273952	-1.745685
C	3.341611	-0.515777	-3.209123
C	3.757526	1.006870	-1.206359
H	3.779341	1.885845	-1.846978
C	3.909480	1.172032	0.179695
C	4.013914	2.575940	0.705715
C	3.891323	0.051927	1.021358
H	4.011197	0.166801	2.094049
C	3.703946	-1.233197	0.489963
C	3.595022	-2.382516	1.454090
O	4.162086	-2.357341	2.566767
N	2.799161	-3.410897	1.052479
O	4.555025	3.481984	0.040190
O	3.713611	-1.569375	-3.763317
N	2.655234	0.469526	-3.855744
N	3.426822	2.781161	1.917619
C	2.130673	0.301654	-5.208834
C	3.192496	4.114076	2.464018
C	2.441211	-4.532626	1.916385
H	3.433826	4.105276	3.538925
C	1.723962	4.535831	2.254878
H	3.874553	4.810032	1.959017
C	0.934999	-4.515043	2.238852
H	3.040711	-4.451833	2.831921
H	2.707222	-5.476604	1.412311
H	2.715883	-0.487495	-5.697933
H	2.277280	1.241708	-5.764169
C	0.634259	-0.066467	-5.176468
H	0.522477	-0.997205	-4.599286
C	0.028877	-0.236147	-6.577469
H	0.092193	0.721638	-4.630861
H	0.690988	-3.559702	2.724268
C	0.518133	-5.675996	3.152909
H	0.372494	-4.545123	1.293273
H	1.507858	4.510124	1.174888
C	1.418329	5.928747	2.825226
H	1.072947	3.786158	2.733550
H	2.222740	1.220201	-3.311921
H	2.230019	-3.318173	0.205845
H	2.871503	2.030047	2.341803
H	5.222466	4.242430	-2.992106
H	5.118327	-4.801350	-3.857732
H	6.472685	3.536843	-4.063213
H	5.741039	-5.488100	-2.329544
H	6.788640	-1.017994	-2.918516
C	6.268637	3.896680	-3.045992
C	5.113691	-4.696998	-2.760990
H	7.122425	5.834973	-3.463553

O	6.692500	-4.200457	-0.485386
N	6.416375	2.759644	-2.143606
O	7.483350	1.389658	-3.657404
N	5.723917	-3.413788	-2.417584
C	3.013295	-6.157106	-2.554265
C	7.216711	5.057586	-2.685671
H	5.918902	2.824937	-1.253585
C	6.418347	-3.256521	-1.239933
C	7.028542	1.592498	-2.523467
C	6.884324	-0.808793	-1.853923
H	5.278923	-2.602301	-2.848219
C	3.672980	-4.809431	-2.227370
C	6.922799	5.660561	-1.301710
H	3.075098	-3.992698	-2.658010
C	6.790402	-1.832256	-0.897243
H	8.251019	4.680878	-2.725608
C	7.060701	0.527510	-1.453368
H	3.703285	-4.659809	-1.137697
C	6.936856	-1.517020	0.467063
C	7.189669	0.829988	-0.089991
H	6.861647	-2.329184	1.188618
H	7.314679	1.857806	0.248717
C	7.117594	-0.187193	0.879828
C	7.107139	0.249255	2.327766
H	5.800262	-1.290883	2.791182
O	7.628045	1.313597	2.690127
N	6.438236	-0.594206	3.182626
H	3.979691	-0.133687	4.235578
H	4.793687	1.413602	3.958342
C	6.120541	-0.178919	4.546465
C	4.759168	0.537357	4.624060
H	6.112224	-1.074004	5.189460
H	6.921736	0.490396	4.886937
C	4.396097	0.974042	6.050437
C	-3.773438	-6.443445	2.904522
C	-3.931969	-5.002803	2.394057
H	-4.977420	-4.816745	2.091404
H	-3.675551	-4.283459	3.184108
H	-3.241617	-5.392696	0.357639
H	-1.962929	-4.895503	1.496096
C	-3.005861	-4.723143	1.196435
H	1.215786	-3.131120	4.802993
C	2.053664	-2.272302	6.619013
H	2.494805	-1.948557	4.510355
C	1.625577	-2.168244	5.146695
C	-2.335905	-5.730417	-3.389230
N	-3.115248	-3.352042	0.700146
H	-1.648164	-4.691651	-1.600387
O	-1.917159	-2.460277	2.429768
H	0.044350	-4.263740	-3.365158
H	-3.756885	-3.176940	-0.078751
C	-1.988980	-4.448567	-2.617203
O	0.739277	-3.477961	-1.015951
C	-2.532142	-2.315823	1.351265
C	0.563113	-1.068957	4.948042
H	-0.425872	-1.438195	3.075457
H	-0.374072	-1.344896	5.456320
C	-0.865293	-3.650483	-3.306454
H	0.538539	-2.060198	1.165422
H	-2.884531	-3.814988	-2.520341
H	0.922757	-0.122020	5.372357
N	0.262270	-0.834456	3.534723
H	-1.161062	-3.365065	-4.326598
C	0.213002	-2.434018	-1.459257
N	-0.543654	-2.419879	-2.586447
C	-2.652169	-0.970017	0.691805
C	0.519167	-1.113615	0.636297
H	-2.428028	0.056931	2.566773
H	-2.810530	-1.702943	-1.337801
C	0.901600	0.121975	2.813721
C	0.367076	-1.117193	-0.757953

C	-2.561620	0.176068	1.494353
C	-2.777846	-0.828466	-0.695140
H	-1.100271	-1.592913	-2.825699
C	0.663938	0.093422	1.331685
O	1.647472	0.979966	3.331999
H	-3.719989	1.791681	3.191691
C	0.366961	0.096339	-1.454746
C	-2.617383	1.450974	0.915880
C	-2.815692	0.444122	-1.286896
C	0.657191	1.306948	0.626911
H	0.272541	0.113578	-2.536306
O	-2.435577	-0.395800	-3.502812
N	-3.178300	2.627551	2.948887
H	-3.347866	3.318298	4.901549
C	-2.722626	1.584607	-0.478176
C	-2.896445	0.517489	-2.783607
C	0.499739	1.311327	-0.765375
C	-2.529292	2.688879	1.755310
H	0.795139	2.238441	1.169437
H	-5.135354	4.447548	3.527586
C	-3.125603	3.732853	3.908508
H	-4.773895	-0.064725	-4.945691
C	-4.111635	4.860269	3.556438
O	-1.922549	3.711384	1.367830
H	-2.705526	2.578890	-0.917566
H	-2.101563	4.133451	3.915540
N	-3.489101	1.624902	-3.301869
H	-4.059133	2.219955	-2.698551
C	0.461917	2.576732	-1.570904
H	-2.787160	1.409962	-5.250432
C	-4.037899	6.024869	4.555329
H	-3.864502	5.217344	2.547229
H	-0.610519	3.519762	-0.071416
C	-4.918689	0.985740	-5.237324
C	-3.691070	1.772837	-4.743191
O	0.895711	2.619140	-2.740629
N	-0.100700	3.649953	-0.950154
H	-5.813857	1.365196	-4.715340
C	-5.095681	1.099119	-6.759226
H	-3.806654	2.845369	-4.954876
H	-1.653001	3.991969	-3.147866
H	-2.510671	4.592234	-1.715605
C	-0.371927	4.892896	-1.668395
C	-1.708495	4.826576	-2.432649
H	0.454973	5.069707	-2.368662
H	-0.391055	5.709657	-0.931582
C	-2.032779	6.141783	-3.156618
C	-5.321297	-2.328141	7.324642
H	-4.989703	-3.371701	4.758522
C	-5.931706	-1.841664	6.000506
H	-6.951271	-2.241987	5.877550
C	-5.068984	-2.276858	4.804218
H	-4.054179	-1.866261	4.902086
H	-6.003166	-0.744819	5.988654
N	-5.599979	-1.829510	3.510982
H	-6.132604	-2.484904	2.955325
C	-5.424400	-0.562369	3.058664
O	-4.875420	0.313747	3.758705
H	-5.728214	-2.315742	0.887518
C	-5.884338	-1.266198	0.645245
O	-5.119564	-3.051527	-1.406147
C	-5.827920	-0.272120	1.633824
H	-6.326602	-4.496090	-3.233884
C	-6.503071	-3.946288	-4.168675
C	-5.711980	-2.000770	-1.730581
C	-5.970852	-0.918093	-0.714262
H	-6.101413	-4.560809	-4.990259
C	-5.871468	1.081244	1.251390
C	-8.004441	-3.694642	-4.376624
H	-5.773555	1.816358	2.047581
H	-4.612363	-2.869064	-4.002742

C	-5.681691	-2.645828	-4.119879
N	-6.071348	-1.755531	-3.014640
C	-5.997452	0.437022	-1.074888
C	-5.918272	1.450075	-0.100743
H	-6.618668	-0.932172	-3.225373
H	-5.815095	-2.069434	-5.045989
H	-5.122698	3.520588	1.271528
H	-5.940993	0.746150	-2.116790
C	-5.622054	2.845371	-0.613106
N	-5.244654	3.780648	0.300364
O	-5.640070	3.081200	-1.838462
C	-4.727137	5.102835	-0.066946
H	-3.705034	5.182684	0.335778
H	-5.743182	6.139848	1.543123
C	-5.604007	6.251437	0.455895
H	-4.669155	5.136433	-1.161284
H	-6.599919	6.179318	-0.007972
C	-4.955949	7.611051	0.147426
H	-4.809548	7.739169	-0.936267
H	-3.970295	7.691514	0.631964
H	-5.581633	8.439990	0.507004
H	-5.245049	-3.426677	7.345964
H	-5.934284	-2.013999	8.181078
H	-4.309087	-1.917613	7.462291
H	-8.187998	-3.155078	-5.319706
H	-8.416353	-3.090780	-3.553594
H	-8.563199	-4.640452	-4.412997
H	-4.740819	6.825373	4.283131
H	-3.024313	6.453482	4.574187
H	-4.282496	5.688155	5.574521
H	-4.022263	-7.171229	2.116528
H	-4.429156	-6.637945	3.765753
H	-2.735108	-6.629671	3.218404
H	-4.208718	0.708829	-7.281550
H	-5.232664	2.148348	-7.063226
H	-5.971785	0.530461	-7.104375
H	-2.990356	6.074063	-3.694735
H	-1.248645	6.390655	-3.887885
H	-2.103143	6.977004	-2.441480
H	2.799348	-3.068576	6.755485
H	1.193548	-2.495126	7.271438
H	2.501538	-1.326145	6.958969
H	-2.675560	-5.496004	-4.411195
H	-3.138349	-6.291579	-2.887657
H	-1.457560	-6.389050	-3.470834
H	0.126969	0.691174	-7.164441
H	-1.040607	-0.487608	-6.508399
H	0.536070	-1.039990	-7.133564
H	0.359915	6.190709	2.673126
H	2.036179	6.698398	2.336855
H	1.628233	5.966703	3.906064
H	0.727582	-6.649166	2.681726
H	-0.557704	-5.627456	3.380575
H	1.067527	-5.640519	4.106886
H	2.974212	-6.324974	-3.643100
H	1.983696	-6.185820	-2.166352
H	3.575090	-6.992398	-2.106825
H	5.909665	6.091822	-1.271337
H	7.644815	6.452753	-1.051447
H	6.970535	4.889665	-0.519798
H	3.407470	1.457005	6.068213
H	5.135969	1.686810	6.447916
H	4.366189	0.108374	6.732341

Cartesian coordinates of the BTA pentameric self-assembly used in this study and optimized at the B3LYP-D/6-31G(d,p) level.

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Pentamer B3LYP-D

H	3.617595	-1.750789	-1.688078
C	3.660962	-0.866621	-1.069030
C	3.612110	0.385512	-1.686102
C	3.471945	0.407362	-3.173920
C	3.674688	1.543063	-0.912525
H	3.632949	2.524664	-1.370610
C	3.789322	1.444768	0.477642
C	3.740929	2.716498	1.267486
C	3.854761	0.190975	1.084663
H	3.951391	0.102402	2.157828
C	3.770457	-0.971836	0.315213
C	3.738765	-2.288834	1.031421
O	4.256083	-2.423401	2.153170
N	3.069028	-3.285453	0.409784
O	4.203940	3.771968	0.810552
O	3.987827	-0.479810	-3.872899
N	2.734075	1.416106	-3.695280
N	3.098198	2.623822	2.456261
C	2.470656	1.465190	-5.129412
C	2.658279	3.789574	3.209340
C	2.802283	-4.574551	1.033718
H	2.923979	3.660277	4.266152
C	1.139694	3.962501	3.062180
H	3.195239	4.659944	2.823830
C	1.314233	-4.714639	1.379152
H	3.420483	-4.642760	1.931948
H	3.106729	-5.372589	0.344969
H	3.354410	1.067794	-5.632874
H	2.346009	2.515646	-5.415901
C	1.225184	0.651011	-5.519101
H	1.284534	-0.316689	-5.006257
H	1.260248	0.441972	-6.596129
C	-0.086162	1.370686	-5.177741
H	1.037897	-3.898367	2.052933
C	0.981047	-6.051748	2.041098
H	0.728197	-4.586269	0.461310
H	0.911067	4.107317	1.998952
C	0.577593	5.125715	3.879844
H	0.652597	3.028007	3.367994
H	2.167529	2.004013	-3.084090
H	2.522947	-3.094717	-0.429030
H	2.632907	1.747301	2.700367
H	4.892463	4.622163	-2.560282
H	5.475596	-3.600666	-4.539474
H	6.605076	4.862515	-2.904357
H	6.036655	-4.525024	-3.127288
H	6.815387	0.013139	-2.846748
C	5.883377	4.743602	-2.091372
C	5.408025	-3.690179	-3.448186
C	5.440907	7.227178	-1.938378
O	6.857793	-3.562237	-1.058569
N	6.243531	3.544803	-1.351403
O	7.173098	2.494073	-3.154960
N	5.944685	-2.475318	-2.850441
C	3.340699	-5.187024	-3.649656
C	5.866687	5.968669	-1.177221
H	5.746643	3.416696	-0.472997
C	6.581553	-2.512260	-1.641501
C	6.831121	2.481610	-1.971520
C	6.907308	0.014807	-1.766177
H	5.489233	-1.616659	-3.152589
C	3.951844	-3.930018	-3.030402
H	5.181653	5.778413	-0.343203
H	3.357772	-3.054971	-3.318551
C	6.882347	-1.170298	-1.027492
H	6.867416	6.102812	-0.748098
C	6.992185	1.252812	-1.120123
H	3.923771	-4.001750	-1.937722
C	6.999063	-1.113736	0.367643
C	7.101379	1.297716	0.270443

H	6.962628	-2.046494	0.920156
H	7.154760	2.242601	0.800862
C	7.092569	0.117079	1.022424
C	7.022131	0.273430	2.518876
H	5.806495	-1.386323	2.650637
O	7.461809	1.278109	3.080745
N	6.385961	-0.737441	3.180589
H	3.874522	-0.610531	4.177695
H	4.585858	1.002366	4.191602
C	5.993738	-0.576117	4.573361
C	4.590507	0.031393	4.701850
H	6.019172	-1.559277	5.060054
H	6.732277	0.069568	5.055896
C	4.153466	0.200087	6.157604
C	-3.047917	-7.333877	1.596321
C	-3.373814	-5.842992	1.477729
H	-4.455490	-5.696116	1.344628
H	-3.070339	-5.313134	2.386191
H	-2.913769	-5.680592	-0.642871
H	-1.552621	-5.338346	0.441708
C	-2.630733	-5.203654	0.300498
H	1.549065	-3.907241	4.153302
C	2.284878	-3.262963	6.088296
H	2.685963	-2.568155	4.070220
C	1.850310	-2.976017	4.649043
C	-1.915652	-5.454925	-4.070700
N	-2.897394	-3.776228	0.160883
H	-1.345374	-4.456323	-2.234679
O	-1.668511	-3.208249	1.989407
H	0.283243	-3.807724	-4.017312
H	-3.523880	-3.458466	-0.577326
C	-1.700166	-4.190144	-3.236842
O	1.031357	-3.273623	-1.668814
C	-2.333135	-2.874382	0.993089
C	0.681415	-1.982857	4.610428
H	-0.278224	-2.146827	2.704740
H	-0.215950	-2.431120	5.053098
C	-0.653163	-3.261937	-3.869022
H	0.643833	-2.313286	0.692967
H	-2.647391	-3.648827	-3.115526
H	0.937808	-1.087287	5.183193
N	0.354648	-1.562113	3.251873
H	-0.997182	-2.893842	-4.841532
C	0.409485	-2.229833	-1.934161
N	-0.376434	-2.105776	-3.025282
C	-2.535660	-1.438256	0.632474
C	0.586176	-1.292020	0.347752
H	-2.395202	-0.767796	2.669018
H	-2.591575	-1.784028	-1.496933
C	0.883889	-0.445442	2.712308
C	0.466479	-1.047850	-1.022336
C	-2.530331	-0.466752	1.636921
C	-2.643193	-1.052130	-0.702749
H	-1.011299	-1.309120	-3.102639
C	0.651618	-0.232376	1.249049
O	1.538525	0.379063	3.373985
H	-3.826421	0.894637	3.552796
C	0.395374	0.262306	-1.490912
C	-2.655891	0.880006	1.296448
C	-2.788992	0.291015	-1.047045
C	0.572751	1.077874	0.775784
H	0.318704	0.465824	-2.551470
O	-2.457632	-0.131876	-3.375153
N	-3.247475	1.732208	3.472348
H	-3.629481	2.281403	5.435225
C	-2.784281	1.256079	-0.042118
C	-2.887720	0.639949	-2.499421
C	0.427109	1.328197	-0.587208
C	-2.609191	1.976215	2.311539
H	0.641271	1.894970	1.481654
H	-5.363817	3.379193	4.003221

C	-3.353408	2.766490	4.494010
H	-4.970163	0.822203	-4.798887
C	-4.375035	3.847252	4.116686
O	-2.033034	3.051205	2.064722
H	-2.848976	2.308472	-0.282832
H	-2.368816	3.228677	4.618110
N	-3.457615	1.828568	-2.784208
H	-4.012333	2.303764	-2.071761
C	0.274116	2.718077	-1.119439
H	-2.761205	1.935444	-4.734391
C	-4.431236	4.963876	5.160970
H	-4.085140	4.250344	3.141164
H	-0.830802	3.219342	0.545266
C	-4.930448	1.917030	-4.779819
C	-3.595838	2.323477	-4.146246
O	0.700516	3.030745	-2.242444
N	-0.394198	3.570730	-0.308024
H	-5.748861	2.274309	-4.139545
C	-5.079728	2.475351	-6.196713
H	-3.514261	3.415591	-4.113366
H	-2.602910	4.113647	-1.737546
H	-2.845794	4.487525	-0.031707
C	-0.860887	4.880502	-0.741806
C	-2.379950	4.850370	-0.956683
H	-0.334304	5.135916	-1.664422
H	-0.602529	5.624331	0.021927
C	-2.965463	6.211024	-1.334682
H	-4.902471	5.031709	0.583423
H	-6.905852	5.320521	-0.847140
C	-6.915380	5.698788	0.180269
C	-5.906199	4.885149	0.994130
H	-7.923171	5.536270	0.583251
H	-5.894867	5.209775	2.038707
C	-6.561504	7.188374	0.207740
N	-6.181263	3.447855	0.990593
H	-6.658376	3.042820	1.780802
O	-5.400470	3.148197	-1.111119
C	-5.873584	2.669247	-0.067360
C	-6.032495	1.183337	0.091315
H	-5.814051	1.159318	2.246466
H	-5.969561	0.911455	-2.019119
C	-5.917735	0.572460	1.341104
C	-6.000340	0.395217	-1.066488
H	-6.170091	-0.512767	-3.504465
C	-5.756689	-0.813371	1.448804
O	-4.991992	-0.577931	3.698890
C	-5.836755	-0.989180	-0.976842
C	-5.324721	-1.351561	2.786639
N	-5.656173	-1.371663	-3.388102
C	-5.730677	-1.582497	0.286150
H	-5.821570	-2.248864	5.545215
H	-5.098028	-1.238025	-5.375608
C	-5.427161	-1.843299	-2.147752
H	-6.686525	-3.167256	-5.201657
C	-5.012381	-1.966040	-4.563273
N	-5.220901	-2.688698	2.926102
C	-5.546767	-3.286775	5.332218
H	-5.485940	-2.637651	0.308526
H	-5.556369	-3.300479	2.199563
H	-6.468507	-3.829651	5.086694
C	-5.619464	-3.305078	-4.986038
H	-3.699299	-2.745703	4.340365
H	-3.947260	-2.080921	-4.335527
C	-4.619201	-3.294424	4.114743
O	-4.816856	-2.908940	-1.957713
C	-4.861458	-3.920801	6.545546
C	-4.892503	-3.860023	-6.213720
H	-5.538831	-4.000632	-4.145522
H	-4.340449	-4.316473	3.844879
H	-4.976753	-3.175536	-7.066727
H	-5.306087	-4.827716	-6.514511

H	-3.826737	-4.000594	-6.000154
H	-7.276712	7.775009	-0.377282
H	-5.562107	7.356402	-0.209711
H	-6.566427	7.575270	1.234128
H	-3.946519	-3.374966	6.804732
H	-4.583935	-4.962424	6.342787
H	-5.519418	-3.910962	7.420194
H	-3.337163	-7.873756	0.686595
H	-3.571387	-7.791054	2.442309
H	-1.971620	-7.479086	1.745150
H	-0.949139	0.704840	-5.279395
H	-0.228580	2.233691	-5.841087
H	-0.076736	1.756521	-4.152910
H	-6.032433	2.177300	-6.646847
H	-4.270371	2.113734	-6.841442
H	-5.037942	3.570755	-6.189156
H	-5.156867	5.735937	4.882672
H	-3.450952	5.443787	5.262411
H	-4.716818	4.571375	6.144235
H	-2.242093	-5.207818	-5.088262
H	-2.679078	-6.101556	-3.623871
H	-0.986217	-6.030744	-4.150546
H	1.460887	-3.686996	6.676782
H	2.611743	-2.340415	6.581678
H	3.118001	-3.972881	6.113126
H	-4.048202	6.134476	-1.483372
H	-2.520627	6.589512	-2.262519
H	-2.778135	6.952466	-0.548182
H	-0.507758	5.195055	3.743710
H	1.024337	6.078737	3.571630
H	0.783160	4.991173	4.949068
H	1.231981	-6.894349	1.385146
H	-0.087548	-6.106268	2.279732
H	1.542454	-6.176846	2.975150
H	3.348392	-5.130816	-4.745861
H	2.303059	-5.304679	-3.317143
H	3.900311	-6.084501	-3.358048
H	4.436287	7.104273	-2.362519
H	6.128373	7.436320	-2.767395
H	5.425277	8.104562	-1.282301
H	4.188294	-0.759931	6.688590
H	3.127839	0.582323	6.212760
H	4.810528	0.898185	6.690607

Cartesian coordinates of the BTA pentameric self-assembly used in this study and optimized at the B3LYP-D/6-31G(d,p) level with inclusion of solvent effects with the PCM method.

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Pentamer B3LYP/Solvent CH2Cl2

H	4.07411	-2.04322	-1.53874
C	4.0603	-1.16613	-0.90194
C	4.08863	0.10321	-1.4924
C	4.16821	0.19714	-2.9896
C	4.11528	1.23925	-0.68268
H	4.17063	2.22874	-1.12203
C	4.10008	1.11586	0.71198
C	4.19289	2.36443	1.54132
C	4.07109	-0.15333	1.29183
H	4.09256	-0.26769	2.36953
C	4.04415	-1.29936	0.48752
C	4.08006	-2.64438	1.15715
O	4.75803	-2.81898	2.18802
N	3.35299	-3.61859	0.57641
O	4.90602	3.31733	1.1705
O	4.86838	-0.60491	-3.63738
N	3.45386	1.18481	-3.56265
N	3.47719	2.38079	2.68159
C	3.43143	1.3973	-5.00771
C	3.47427	3.53304	3.57985

C	3.28058	-4.9743	1.11513
H	3.34385	3.15484	4.59822
C	2.3808	4.55098	3.24545
H	4.46026	3.99896	3.51897
C	1.99788	-5.22483	1.91146
H	4.16169	-5.12075	1.74247
H	3.34564	-5.67371	0.27499
H	4.36823	1.00474	-5.40805
H	3.41594	2.47741	-5.18473
C	2.23386	0.7319	-5.69055
H	2.25316	-0.35155	-5.53978
H	2.25513	0.93005	-6.76692
H	1.29191	1.12002	-5.29104
H	1.93678	-4.5522	2.77254
H	1.97505	-6.2562	2.2774
H	1.11538	-5.0642	1.2847
H	2.51349	4.93991	2.23168
H	2.4201	5.39174	3.9454
H	1.38788	4.09582	3.31467
H	2.75573	1.68814	-3.01059
H	2.6699	-3.37609	-0.14456
H	2.76427	1.66518	2.84115
H	6.29527	4.9206	-1.92408
H	7.05207	-3.24313	-4.76124
H	8.049	5.03474	-1.82234
H	7.75948	-4.26056	-3.50092
H	7.91518	0.17437	-2.49153
C	7.14624	4.86806	-1.23041
C	6.94514	-3.56737	-3.72067
H	6.89717	6.91719	-0.58724
O	8.27815	-3.53506	-1.24446
N	7.24278	3.52877	-0.65743
O	8.51773	2.6821	-2.35406
N	7.13097	-2.40024	-2.86325
H	5.49353	-5.11417	-4.17889
C	6.99848	5.92487	-0.13788
H	6.55345	3.29337	0.05795
C	7.77295	-2.48745	-1.6724
C	7.91629	2.53284	-1.28053
C	7.86967	0.04598	-1.41582
H	6.50838	-1.6111	-3.03799
C	5.58871	-4.24738	-3.51678
H	6.11058	5.73468	0.47286
H	4.77165	-3.55448	-3.73935
C	7.80812	-1.22819	-0.8476
H	7.87206	5.93207	0.52118
C	7.87547	1.18786	-0.60487
H	5.47932	-4.58998	-2.48331
C	7.78839	-1.35895	0.54707
C	7.85169	1.04374	0.78381
H	7.77051	-2.35609	0.97222
H	7.88003	1.91167	1.43295
C	7.79401	-0.2286	1.36753
C	7.75307	-0.31161	2.8707
H	6.41747	-1.87434	2.7958
O	8.30729	0.55307	3.56431
N	7.0639	-1.35637	3.39136
H	4.70999	-1.41384	4.85306
H	5.50782	0.14961	5.11657
C	6.88181	-1.51149	4.83119
C	5.56119	-0.92164	5.33357
H	6.93101	-2.58022	5.06523
H	7.72918	-1.02368	5.31693
H	5.46994	-1.05915	6.41592
H	-5.17995	-6.04592	2.95302
C	-5.20741	-5.03931	2.52401
H	-6.16748	-4.91232	2.01429
H	-5.1502	-4.31433	3.34147
H	-4.0986	-5.59101	0.7448
H	-3.08755	-4.98012	2.06041
C	-4.04307	-4.85036	1.54872

H	0.70387	-3.15605	4.86902
H	0.78835	-2.28928	6.4144
H	1.80549	-1.77675	5.05508
C	0.82131	-2.16905	5.32683
H	-1.57006	-5.44316	-4.01525
N	-4.02876	-3.52641	0.92988
H	-1.49301	-4.9727	-2.30591
O	-2.55323	-2.6126	2.41316
H	0.54296	-4.16777	-3.54195
H	-4.74819	-3.33613	0.2307
C	-1.57426	-4.59116	-3.32799
O	1.06811	-3.39591	-1.26119
C	-3.28589	-2.51024	1.41061
C	-0.28371	-1.21548	4.86616
H	-0.98828	-1.57244	2.88338
H	-1.26616	-1.59964	5.15284
C	-0.41163	-3.64838	-3.64804
H	0.35007	-2.20467	1.01198
H	-2.53406	-4.0754	-3.42994
H	-0.15627	-0.23504	5.33307
N	-0.3042	-1.03089	3.4159
H	-0.48722	-3.28947	-4.67915
C	0.3661	-2.44173	-1.64937
N	-0.3703	-2.47633	-2.77632
C	-3.36884	-1.21296	0.65546
C	0.3338	-1.23166	0.53383
H	-3.25182	-0.05875	2.46247
H	-3.39743	-2.09212	-1.31708
C	0.45125	-0.10534	2.7983
C	0.31782	-1.16142	-0.86498
C	-3.31997	-0.01536	1.38112
C	-3.40237	-1.17424	-0.73993
H	-1.07175	-1.75104	-2.94254
C	0.36074	-0.06459	1.29929
O	1.18959	0.68938	3.41307
H	-4.53571	1.903	2.86992
C	0.34183	0.08449	-1.49358
C	-3.31647	1.21293	0.71642
C	-3.40102	0.05339	-1.41482
C	0.38407	1.18122	0.66013
H	0.36649	0.15547	-2.57511
O	-2.67882	-0.8029	-3.52601
N	-3.83621	2.60656	2.62805
H	-3.77906	3.47299	4.51026
C	-3.35186	1.24203	-0.68391
C	-3.35757	0.04622	-2.91761
C	0.36769	1.25996	-0.73331
C	-3.18004	2.5157	1.45456
H	0.44017	2.08189	1.26111
H	-5.90608	4.27081	3.41278
C	-3.78169	3.80219	3.4665
H	-5.49339	-0.49339	-5.39696
C	-4.94777	4.76158	3.2166
O	-2.48355	3.43738	0.98796
H	-3.30725	2.20002	-1.19001
H	-2.82879	4.29631	3.26702
N	-4.07601	1.00504	-3.53458
H	-4.74421	1.55719	-2.99497
C	0.46048	2.5769	-1.44949
H	-3.24716	0.63783	-5.3908
H	-4.8684	5.63091	3.87695
H	-4.94491	5.11432	2.18098
H	-0.94538	3.39632	-0.19697
C	-5.40971	0.57958	-5.5947
C	-4.1245	1.14695	-4.98817
O	1.1664	2.69637	-2.46983
N	-0.24699	3.59178	-0.9183
H	-6.2899	1.07779	-5.17659
H	-5.41427	0.73194	-6.67854
H	-4.03423	2.21248	-5.22415
H	-1.17846	4.44414	-3.39591

H	-2.32102	4.96868	-2.14148
C	-0.24096	4.93335	-1.49788
C	-1.32391	5.13538	-2.56084
H	0.74895	5.10147	-1.92799
H	-0.37595	5.64374	-0.67691
H	-1.28406	6.15793	-2.94956
H	-6.49814	5.02597	-2.01994
H	-8.74861	4.64098	-3.05787
C	-8.63245	5.35189	-2.23471
C	-7.39545	5.01681	-1.39855
H	-9.54061	5.32583	-1.62452
H	-7.26131	5.75356	-0.60098
H	-8.53624	6.35644	-2.6582
N	-7.46667	3.69767	-0.77271
H	-8.06292	3.59277	0.03585
O	-6.34616	2.59829	-2.42164
C	-6.93533	2.58766	-1.32707
C	-7.0748	1.31031	-0.54263
H	-6.90767	2.19642	1.42619
H	-7.10625	0.14505	-2.33869
C	-7.02019	1.28276	0.85316
C	-7.13194	0.10495	-1.2553
H	-8.33713	-1.76527	-2.74462
C	-7.02942	0.06173	1.54116
O	-6.14618	0.98109	3.56522
C	-7.14135	-1.11754	-0.57975
C	-6.83046	0.09011	3.03325
N	-7.70488	-2.51065	-2.49022
C	-7.08579	-1.1335	0.82033
H	-8.44072	0.7407	5.7425
H	-7.71755	-3.38967	-4.36624
C	-7.06417	-2.4344	-1.30482
H	-9.83317	-4.14408	-3.18961
C	-7.70077	-3.71318	-3.32152
N	-7.41513	-0.90112	3.73922
C	-8.43385	-0.33356	5.9482
H	-7.02717	-2.09233	1.32325
H	-8.08244	-1.49711	3.27005
H	-9.40643	-0.74685	5.66319
C	-8.87566	-4.64983	-3.03044
H	-6.3336	-0.59159	5.47042
H	-6.75193	-4.22258	-3.14258
C	-7.29659	-1.02335	5.19138
O	-6.42433	-3.3863	-0.82521
H	-8.30603	-0.47693	7.02563
H	-8.83493	-5.51858	-3.69482
H	-8.83976	-5.00525	-1.99666
H	-7.2695	-2.09062	5.42978