Supporting information for

Understanding Cooperativity in Hydrogen Bond Induced Supramolecular Polymerization: A Density Functional Theory Study

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Geometries

Please note that the following format is used:

[Atom type] [coordinate in x direction] [coordinate in y direction] [coordinate in z direction]

The dimension of all coordinates is **angstrom**.

All VASP calculations, unless stated otherwise, were performed using the following set of parameters and conditions:

- Perdew-Becke-Ernzerhof (PBE) functional with plane augmented waves (PAW)
- Kpoints: 1x1x1 (gamma point)
- Cutoff: 400eV
- Gaussian smearing with sigma = 0.0002 eV
- Conjugate-gradient algorithm
- Kosugi algorithm as integer selecting algorithm
- Energetic threshold of 10^{-5} eV for the energetic SC-loop and a threshold of 0.005 eV/Å for the ionic loop

All Gaussian calculations, unless stated otherwise, were performed using the following set of parameters and conditions:

- Perdew-Becke-Ernzerhof (PBE) functional
- A 6-31g(d,p) basisset
- Modified gdiis algorithm (opt=gdiis)
- Ultrafine numerical integration grid (int=grid=ultrafine)

BTA monomer, relaxed geometry using VASP

C	8.631644	10.22072	10.11856
C	14.80796	8.08476	10.03354
C	5.93004	6.811794	9.854289
C	10.88614	11.07192	10.00569
C	9.108537	8.909553	10.03719
C	8.232536	7.682678	10.04699
C	9.251788	15.11692	10.03887
C	10.49053	8.691869	9.957252
C	9.512066	11.3114	10.09601
C	8.886269	12.68125	10.18503
C	11.38687	9.764339	9.943672
C	12.88583	9.621226	9.857101
H	10.68804	13.57099	9.753388
H	10.80922	7.648913	9.891163
H	6.573444	8.833616	9.671719
H	11.63302	11.86919	9.993403
H	12.74952	7.62886	10.33705
H	7.571873	10.46423	10.22581
H	5.133354	6.997185	10.59091
H	6.459756	5.888356	10.11823
H	5.471679	6.6874	8.860265
H	9.893426	15.72414	10.69417
H	8.228463	15.11022	10.43371
H	9.23896	15.57081	9.034715
H	15.2028	7.890086	11.04379
H	15.31682	8.964437	9.621038
H	15.01415	7.210725	9.398251
N	13.38687	8.369539	10.06291
N	6.897872	7.890416	9.857714
N	9.71847	13.74491	9.996541
O	8.71889	6.55416	10.2142
O	7.675094	12.81449	10.41544
O	13.60808	10.59892	9.611398

BTA dimer, relaxed geometry using VASP

C	10.35583	11.35589	8.236392
C	11.35174	10.37704	8.23922
C	12.79812	10.68307	8.520732
C	14.50138	12.44572	8.766796
C	8.647653	9.651555	8.222258
C	8.999136	11.00391	8.241761
C	8.014902	12.10978	8.522659
C	5.643123	12.73571	8.734845
C	10.97828	9.02613	8.221288
C	9.632088	8.652679	8.221163
C	9.178414	7.240652	8.477277
C	9.834494	4.871395	8.613874
C	9.445983	8.711794	11.78731
C	8.612131	9.83404	11.77864
C	7.111566	9.743434	11.69346
C	5.201983	8.396257	10.92805
C	11.39568	10.13902	11.8103
C	10.84071	8.856198	11.78267
C	11.65957	7.595891	11.69158
C	13.75143	6.581058	10.89892
C	9.183192	11.11489	11.80793
C	10.57251	11.27525	11.80694
C	11.24858	12.61977	11.76282
C	11.05716	14.96712	11.05623
H	10.58253	12.41785	8.349529
H	12.54222	12.6284	7.951999
H	7.612699	9.318946	8.324597
H	6.450615	10.93593	7.92968
H	11.78296	8.295645	8.324261
H	10.96264	6.495307	7.815193
H	9.042302	7.697322	11.798
H	7.25808	8.001044	10.58126
H	12.47576	10.29545	11.83834
H	13.10574	8.578809	10.58046
H	8.507429	11.97213	11.835
H	9.683765	13.39775	10.64915
H	14.86347	13.22786	8.087053
H	15.21272	11.61108	8.774396
H	14.42651	12.85339	9.788311
H	4.77586	12.62999	8.070472
H	6.007314	13.76951	8.69893
H	5.341807	12.50368	9.76979
H	10.35358	4.192719	7.924949
H	8.757903	4.665036	8.58907
H	10.20086	4.702794	9.63962
H	4.912251	7.406159	11.31189
H	4.910116	8.449345	9.865386
H	4.666151	9.175004	11.48465

H	14.7872	6.837806	11.16521
H	13.74196	6.235436	9.850713
H	13.39767	5.764314	11.54034
H	10.33133	15.70498	11.42929
H	11.29221	15.2162	10.00764
H	11.97807	15.02751	11.64949
N	13.21383	11.95469	8.305377
N	6.706018	11.84935	8.290308
N	10.05666	6.246946	8.199058
N	6.623425	8.61561	11.09951
N	12.88211	7.723589	11.09747
N	10.52968	13.62332	11.1795
O	13.55232	9.803841	8.982095
O	8.403353	13.19709	8.993552
O	8.054636	7.015382	8.968691
O	6.384245	10.65985	12.11311
O	11.21679	6.509972	12.10277
O	12.39775	12.77898	12.20829

BTA trimer, relaxed geometry using VASP

C	10.62951	11.26628	10.07871
C	11.41524	10.11116	10.07047
C	12.91318	10.17003	10.16916
C	9.22971	11.17526	10.0728
C	8.622267	9.917241	10.07376
C	8.431928	12.44475	10.16764
C	9.401144	8.750453	10.069
C	10.79467	8.853485	10.07217
C	8.700108	7.42573	10.16657
C	9.407903	8.704794	6.403015
C	8.593874	9.839876	6.416242
C	7.104927	9.762532	6.603019
C	10.80513	8.827621	6.384897
C	9.339579	8.775217	13.772
C	8.584164	9.951283	13.77104
C	7.079436	9.952805	13.76002
C	10.74188	8.828684	13.77491
C	11.38178	10.09956	6.380928
C	11.62273	7.575456	6.537456
C	10.57632	11.24785	6.395317
C	11.38116	10.07171	13.8033
C	11.49574	7.527916	13.76797
C	10.63392	11.25884	13.8026
C	9.186536	11.11091	6.411586
C	11.25636	12.57726	6.556694
C	9.237858	11.19232	13.79741
C	11.38389	12.56249	13.82759
C	5.062314	8.428773	6.199182
C	13.79199	6.485558	6.076423
C	11.10667	15.01104	6.148063
C	14.94825	11.38496	9.516912
C	8.740992	5.049173	9.533831
C	6.358055	13.59721	9.521334
C	11.44063	14.87615	13.00282
C	13.50313	6.356018	12.97323
C	5.061521	8.818827	12.93718
H	11.08996	12.25434	10.13497
H	12.9709	11.6978	8.781981
H	7.536204	9.821405	10.1269
H	7.058292	11.71231	8.810287
H	11.42005	7.960327	10.12502
H	10.00993	6.595768	8.80118
H	8.984527	7.702114	6.491542
H	7.033112	8.068871	5.465851
H	8.860456	7.794248	13.78936
H	7.073437	8.357403	12.43249
H	12.46307	10.23366	6.45139

H	13.09427	8.374661	5.369607
H	12.46943	10.14662	13.84622
H	12.90077	8.329947	12.46794
H	8.531708	11.97986	6.508051
H	9.78679	13.4807	5.465003
H	8.627485	12.09686	13.8319
H	10.03941	13.37047	12.46787
H	4.898777	7.427805	6.624554
H	4.650753	9.182541	6.880537
H	4.541692	8.49661	5.232033
H	14.71518	6.826469	6.568722
H	13.32429	5.706487	6.68968
H	14.04502	6.066652	5.091579
H	10.36766	15.63615	6.671803
H	12.03366	14.98419	6.732492
H	11.31417	15.4519	5.161942
H	15.15969	12.41926	9.827589
H	15.37951	10.69192	10.24908
H	15.41905	11.21293	8.536226
H	9.527153	4.354557	9.86635
H	7.913222	5.028651	10.25269
H	8.3736	4.715145	8.550699
H	5.396776	13.29884	9.968782
H	6.811285	14.38152	10.13953
H	6.164549	13.9925	8.512413
H	10.79231	15.66057	13.42654
H	12.38415	14.8503	13.5632
H	11.64782	15.13205	11.95135
H	14.48767	6.515228	13.4429
H	12.99113	5.531189	13.48543
H	13.66496	6.086612	11.91746
H	4.720232	7.834902	13.29645
H	4.602587	9.607061	13.548
H	4.732942	8.936546	11.8914
N	13.51778	11.1531	9.458502
N	7.273269	12.4735	9.464717
N	9.253449	6.404257	9.467732
N	6.482297	8.692706	6.048213
N	6.499463	8.942839	13.05003
N	12.84391	7.577401	5.946756
N	12.67337	7.537979	13.07981
N	10.62472	13.64783	6.013993
N	10.8216	13.57098	13.10119
O	13.53652	9.353272	10.87813
O	8.834925	13.4003	10.86311
O	7.671678	7.300181	10.86297
O	6.498571	10.63503	7.253571
O	6.43376	10.83269	14.35394
O	11.18989	6.608635	7.19335
O	11.04823	6.523685	14.34732

O	12.33363	12.66954	7.175584
O	12.44736	12.67976	14.45956

BTA tetramer, relaxed geometry using VASP

C	10.56415	11.38167	7.362414
C	11.3945	10.25857	7.361804
C	12.8722	10.33358	7.628266
C	9.17109	11.24132	7.275383
C	10.60105	11.14776	14.58441
C	11.40078	10.00298	14.61202
C	12.89486	10.0899	14.70431
C	9.203951	11.03892	14.57709
C	8.613777	9.963551	7.195656
C	8.326303	12.47238	7.440824
C	9.435637	8.82759	7.190399
C	8.612168	9.773288	14.61038
C	8.391802	12.29922	14.61773
C	9.406206	8.61854	14.64426
C	10.82093	8.981637	7.268938
C	8.773053	7.482286	7.266945
C	10.79796	8.737583	14.6469
C	8.731204	7.287253	14.78934
C	9.325034	8.646842	10.92356
C	8.529196	9.795328	10.90305
C	7.031487	9.71739	10.97235
C	10.72306	8.753647	10.9589
C	9.435118	8.867624	18.39945
C	8.673994	10.03743	18.31975
C	7.170102	10.03318	18.28816
C	10.83683	8.930396	18.40078
C	11.31504	10.01869	10.98083
C	11.53632	7.496967	11.07766
C	10.52631	11.17821	10.9593
C	11.47088	10.17493	18.34555
C	11.59948	7.635888	18.46566
C	10.71737	11.35636	18.26536
C	9.134054	11.06063	10.92735
C	11.21452	12.50748	11.08105
C	9.321796	11.28133	18.26798
C	11.46065	12.66132	18.17361
C	14.9166	11.70943	7.49186
C	6.172178	13.55325	6.885862
C	8.911698	5.094006	6.64264
C	13.62501	6.36038	10.45045
C	5.017869	8.542161	10.19615
C	11.15793	14.89698	10.50927
C	14.92172	11.2643	14.02949
C	8.731424	4.918989	14.20252
C	6.370628	13.45902	13.90665
C	13.53321	6.385908	17.6133
C	11.46907	14.91443	17.19743
C	5.164052	8.86225	17.49018

H	10.96621	12.38555	7.515969
H	12.98065	12.15649	6.711158
H	11.05051	12.14177	14.61025
H	12.94216	11.59079	13.27842
H	7.532198	9.815371	7.217171
H	6.944396	11.70645	6.149352
H	7.526598	9.666055	14.65768
H	7.034269	11.54089	13.2429
H	11.48288	8.116364	7.345858
H	10.21617	6.682349	6.065355
H	11.43048	7.851216	14.72394
H	9.965658	6.451644	13.35603
H	8.87139	7.654325	10.95587
H	7.017698	8.264636	9.506127
H	8.960305	7.887313	18.47425
H	7.18053	8.349	17.06932
H	12.39843	10.12492	11.06023
H	12.91245	8.239778	9.732661
H	12.55957	10.25561	18.37223
H	12.92431	8.336702	17.02673
H	8.498729	11.94761	10.96592
H	9.879256	13.36771	9.756437
H	8.705101	12.18193	18.23873
H	10.04954	13.3756	16.82661
H	15.03991	12.41943	8.325035
H	15.38756	10.75871	7.767297
H	15.40828	12.11545	6.597892
H	5.200301	13.16749	7.227113
H	6.549757	14.27828	7.616553
H	6.037738	14.05641	5.91696
H	9.652103	4.422109	7.102194
H	7.990446	5.071535	7.235676
H	8.693633	4.742619	5.623546
H	14.56638	6.655998	10.93995
H	13.15821	5.55705	11.03353
H	13.85792	5.992518	9.439926
H	4.780788	7.551119	10.61383
H	4.540118	9.311526	10.81511
H	4.616741	8.592362	9.172935
H	10.5306	15.51263	11.17399
H	12.17492	14.86617	10.91961
H	11.1719	15.36164	9.513508
H	15.17376	12.14527	13.42657
H	15.24139	11.42912	15.0689
H	15.47373	10.38942	13.64867
H	9.401818	4.227392	13.6776
H	8.667205	4.630579	15.26145
H	7.718525	4.836709	13.77477
H	5.485342	13.2293	13.30144
H	6.058797	13.70459	14.93218

H	6.876868	14.34623	13.49225
H	14.51128	6.517954	18.10542
H	12.99377	5.570132	18.11205
H	13.71104	6.121872	16.5597
H	10.84057	15.72337	17.60563
H	12.43988	14.9219	17.71084
H	11.62305	15.10509	16.12318
H	4.775098	7.978576	18.02257
H	4.702831	9.765199	17.91119
H	4.888815	8.772405	16.42785
N	13.51232	11.45587	7.21849
N	13.487	11.05688	13.96749
N	7.141086	12.47716	6.781367
N	7.242561	12.2998	13.9043
N	9.396031	6.46369	6.623691
N	9.262253	6.26367	14.08173
N	6.44907	8.777533	10.19104
N	6.600342	8.978785	17.63572
N	12.7008	7.476755	10.38599
N	12.72599	7.585877	17.69986
N	10.64915	13.54118	10.41372
N	10.86025	13.61777	17.40815
O	13.45824	9.401953	8.21385
O	13.54595	9.311243	15.43344
O	8.705296	13.41341	8.164785
O	8.766462	13.28921	15.28165
O	7.714334	7.333477	7.907339
O	7.743876	7.145024	15.54155
O	6.390069	10.48504	11.72102
O	6.515157	10.9512	18.811
O	11.13956	6.544746	11.78211
O	11.19653	6.684907	19.15728
O	12.25061	12.62756	11.7703
O	12.5523	12.82626	18.74482

BTA pentamer, relaxed geometry using VASP

C	10.63606	11.24814	9.109465
C	11.41169	10.08624	9.108762
C	12.9067	10.13459	9.226719
C	9.2361	11.16681	9.104087
C	10.54332	11.25952	16.53515
C	11.37138	10.13386	16.53543
C	12.86516	10.24127	16.60073
C	9.148669	11.11494	16.52805
C	8.617473	9.913894	9.101809
C	8.442586	12.43486	9.219423
C	9.387827	8.741868	9.098029
C	8.58758	9.835884	16.53146
C	8.299909	12.34915	16.60083
C	9.410373	8.700864	16.53844
C	10.78198	8.833513	9.106776
C	8.683344	7.420542	9.196099
C	10.79858	8.854542	16.54459
C	8.767496	7.349355	16.62174
C	9.378687	8.788424	5.353606
C	8.631577	9.968651	5.358922
C	7.137326	9.963413	5.500524
C	10.77961	8.834027	5.348032
C	9.396574	8.747799	12.81427
C	8.59782	9.893287	12.80561
C	7.102418	9.809823	12.87975
C	10.79381	8.857833	12.82597
C	9.412578	8.722162	20.30597
C	8.583692	9.84746	20.29122
C	7.08305	9.750079	20.26881
C	10.80811	8.865155	20.29869
C	11.42882	10.07051	5.350319
C	11.52595	7.540221	5.485846
C	10.6889	11.26113	5.357815
C	11.38695	10.12287	12.83452
C	11.60894	7.602624	12.92111
C	10.59355	11.27922	12.82371
C	11.36943	10.14574	20.30358
C	11.64456	7.615819	20.28532
C	10.54735	11.28176	20.29134
C	9.293251	11.20519	5.362747
C	11.43487	12.55431	5.504364
C	9.2015	11.15839	12.81385
C	11.27097	12.61536	12.91376
C	9.15794	11.12699	20.29604
C	11.20474	12.63374	20.27334
C	11.13601	14.91538	19.41122
C	14.87167	11.40942	15.86256
C	11.29982	14.94886	12.20332

C	14.97982	11.24611	8.576059
C	11.54328	14.94125	4.939323
C	13.55298	6.271074	4.933313
C	8.617025	5.076713	8.512726
C	13.6285	6.415392	12.24473
C	8.790596	5.025072	15.89372
C	13.64252	6.512646	19.43072
C	5.131655	8.567275	19.41457
C	5.078814	8.650428	12.1652
C	5.026236	8.839825	4.94919
C	6.429909	13.65904	8.576246
C	6.283607	13.4944	15.85026
H	11.10762	12.23086	9.16718
H	13.02681	11.61394	7.785229
H	10.96915	12.2639	16.57346
H	12.87702	11.746	15.17172
H	7.530231	9.830702	9.150765
H	7.105814	11.79445	7.778353
H	7.504839	9.703229	16.56841
H	7.024771	11.62277	15.13369
H	11.39881	7.934328	9.16062
H	9.9158	6.595737	7.753091
H	11.45376	7.982465	16.59118
H	10.04726	6.597927	15.17351
H	8.894066	7.812307	5.426274
H	6.98586	8.3676	4.229555
H	8.944827	7.754509	12.84891
H	7.063091	8.317404	11.44134
H	8.994708	7.713625	20.33039
H	7.159749	8.186484	18.89451
H	12.51666	10.1355	5.41957
H	12.99144	8.21101	4.227652
H	12.47229	10.22602	12.88691
H	12.9436	8.300194	11.499
H	12.4516	10.28767	20.32888
H	12.94338	8.445876	18.88266
H	8.693556	12.11492	5.437395
H	10.14767	13.48824	4.21832
H	8.566237	12.04554	12.8476
H	10.02257	13.40168	11.45893
H	8.49528	11.99442	20.31611
H	9.816245	13.33245	18.88713
H	10.52528	15.48437	18.69906
H	11.14335	15.43741	20.38098
H	12.17815	14.87591	19.05362
H	15.11158	12.2481	15.19798
H	15.23387	11.63261	16.87722
H	15.39723	10.50528	15.51418
H	10.69395	15.59466	11.55626
H	11.28131	15.34095	13.23055

H	12.34674	14.96731	11.86054
H	15.26886	12.08438	7.931389
H	15.28751	11.45843	9.610095
H	15.50851	10.33582	8.251414
H	10.93554	15.65399	4.369734
H	11.6033	15.27174	5.985349
H	12.56322	14.92354	4.527177
H	14.47621	6.449376	4.370006
H	13.80332	6.048728	5.980041
H	13.03489	5.397026	4.511432
H	9.185977	4.423684	7.840632
H	8.663058	4.674621	9.535517
H	7.559452	5.085067	8.206271
H	14.48326	6.60202	11.58405
H	13.99135	6.242742	13.26871
H	13.10728	5.501345	11.91801
H	9.405167	4.395537	15.23949
H	8.805994	4.613927	16.91362
H	7.746067	5.006149	15.5431
H	14.46645	6.753799	18.74756
H	14.05392	6.227898	20.41151
H	13.08796	5.641335	19.04398
H	4.930597	7.74272	18.7192
H	4.670928	8.338919	20.38851
H	4.659749	9.490181	19.03871
H	4.832851	7.783526	11.54066
H	4.734511	8.468204	13.19356
H	4.542381	9.535962	11.7877
H	4.718498	7.950115	4.388458
H	4.714951	8.735342	5.997932
H	4.523535	9.724293	4.530348
H	5.551845	13.4758	7.946022
H	6.106564	13.82834	9.613164
H	6.941639	14.57234	8.233412
H	5.444182	13.27773	15.17854
H	5.901117	13.67568	16.86502
H	6.791008	14.41389	15.5163
N	13.5391	11.07901	8.497124
N	13.43327	11.21808	15.85883
N	7.302794	12.50095	8.497726
N	7.184625	12.35681	15.83752
N	9.19381	6.408806	8.459695
N	9.329284	6.371983	15.87549
N	6.471929	8.97192	4.862698
N	6.516483	8.84591	12.13537
N	6.56763	8.720647	19.54306
N	12.72017	7.459507	4.85393
N	12.74957	7.569834	12.19767
N	12.78663	7.676951	19.54664
N	10.92294	13.62833	4.858747

N	10.74854	13.60675	12.15953
N	10.57025	13.58693	19.5375
O	13.52066	9.342414	9.974305
O	13.53858	9.457743	17.30566
O	8.820801	13.3673	9.961699
O	8.615884	13.31158	17.33333
O	7.683508	7.276567	9.932862
O	7.768554	7.148388	17.34621
O	6.546655	10.8202	6.186781
O	6.446648	10.59201	13.60253
O	6.365422	10.57383	20.86323
O	11.06986	6.59879	6.16424
O	11.24325	6.64832	13.64183
O	11.29962	6.590663	20.8992
O	12.46497	12.63102	6.202212
O	12.26219	12.78954	13.65702
O	12.26688	12.85194	20.88222

BTA hexamer, relaxed geometry using VASP

C	8.608476	9.918938	8.482978
C	9.214085	11.16704	12.23726
C	10.61109	11.25408	15.96264
C	11.39891	10.12697	19.66715
C	10.80807	8.841749	23.39919
C	9.419655	8.738473	27.15966
C	9.232482	11.16806	8.478405
C	10.60712	11.27548	12.23319
C	11.40579	10.10576	15.95072
C	10.80563	8.862587	19.65868
C	9.418566	8.702269	23.39617
C	8.59227	9.864955	27.14505
C	8.456447	12.44482	8.611416
C	11.29701	12.60335	12.33581
C	12.9003	10.1813	16.03463
C	11.62285	7.607802	19.72816
C	8.75994	7.356446	23.44885
C	7.09275	9.765447	27.13068
C	9.370934	8.741841	8.489209
C	8.598964	9.907243	12.23934
C	9.213529	11.14848	15.96914
C	10.60461	11.28176	19.67324
C	11.39341	10.11554	23.40095
C	10.81506	8.879512	27.16755
C	10.76534	8.826774	8.490789
C	9.3894	8.755693	12.24221
C	8.615364	9.88638	15.97423
C	9.212791	11.16169	19.6775
C	10.57874	11.25011	23.40867
C	11.37741	10.15901	27.1805
C	8.648707	7.434323	8.640768
C	7.105248	9.835139	12.35717
C	8.402495	12.40433	16.07094
C	11.281	12.61641	19.7635
C	12.88752	10.2115	23.46726
C	11.6498	7.629362	27.17911
C	11.40136	10.07668	8.486429
C	10.78801	8.853912	12.23988
C	9.405002	8.728507	15.96318
C	8.608696	9.896643	19.66956
C	9.183331	11.11938	23.40439
C	10.55753	11.29689	27.16537
C	10.63243	11.2422	8.482626
C	11.392	10.11361	12.23883
C	10.79699	8.843412	15.95436
C	9.408484	8.751681	19.6669
C	8.608166	9.846112	23.40477
C	9.167872	11.14372	27.15863

C	12.89424	10.11506	8.632002
C	11.59139	7.591976	12.35046
C	8.722	7.397387	16.05316
C	7.114182	9.814011	19.75023
C	8.352229	12.36497	23.46969
C	11.21669	12.64819	27.17156
C	14.98379	11.26972	8.059823
C	13.6093	6.381509	11.69848
C	8.695865	5.060391	15.35182
C	5.085853	8.650808	19.05411
C	6.340892	13.52958	22.73924
C	11.17817	14.93373	26.32806
C	8.59323	5.040268	8.097875
C	5.05568	8.664468	11.72936
C	6.371149	13.58908	15.42329
C	11.29372	14.95453	19.06823
C	14.90472	11.36808	22.74401
C	13.6496	6.50532	26.36012
C	6.424907	13.68386	8.004331
C	11.3383	14.94733	11.64829
C	14.93257	11.33988	15.33754
C	13.63335	6.434012	18.99041
C	8.769498	5.044898	22.66871
C	5.136308	8.575406	26.29822
H	11.38557	7.931105	8.568115
H	8.929774	7.767013	12.29466
H	7.529764	9.785002	16.02387
H	8.578506	12.04879	19.7199
H	11.01565	12.24953	23.44922
H	12.45972	10.2981	27.21692
H	7.521947	9.832633	8.554622
H	8.586907	12.05963	12.28457
H	11.06601	12.24543	16.00214
H	12.48503	10.2306	19.70176
H	11.4547	7.962799	23.43188
H	9.000661	7.730592	27.18232
H	7.042589	11.75862	7.302668
H	10.06297	13.41022	10.88409
H	12.9508	11.6793	14.6056
H	12.92901	8.323853	18.28544
H	10.03984	6.622464	21.9895
H	7.158923	8.209812	25.74439
H	11.10009	12.2266	8.556259
H	12.47847	10.20965	12.28687
H	11.42805	7.953152	15.98568
H	8.95806	7.757928	19.70111
H	7.523762	9.726952	23.44145
H	8.504918	12.01093	27.17753
H	9.964817	6.516758	7.371834
H	7.01085	8.348833	10.92082

H	7.06344	11.71524	14.64993
H	10.023	13.40403	18.31698
H	12.91573	11.70763	22.02887
H	12.95514	8.427068	25.7652
H	8.600477	4.691725	9.140739
H	4.765284	8.438986	12.76588
H	6.019151	13.74295	16.45414
H	11.27547	15.33981	20.09827
H	15.24929	11.56871	23.76915
H	14.03773	6.232094	27.35338
H	13.01731	11.68575	7.325907
H	12.92677	8.251069	10.91328
H	9.974619	6.606426	14.60586
H	7.067866	8.314758	18.31928
H	7.055119	11.64822	22.01699
H	9.87818	13.35315	25.73948
H	15.27239	12.14793	7.471111
H	14.49279	6.575836	11.07868
H	9.315638	4.406556	14.72645
H	4.835521	7.781456	18.43408
H	5.46479	13.30274	22.11972
H	10.54012	15.54255	25.67525
H	15.28683	11.41772	9.10621
H	13.92409	6.205706	12.73713
H	8.692558	4.680301	16.38376
H	4.750746	8.471977	20.08614
H	6.015427	13.74607	23.76722
H	11.23598	15.40328	27.32126
H	15.51067	10.38402	7.674566
H	13.10916	5.466562	11.34329
H	7.656541	5.037298	14.98637
H	4.546379	9.535333	18.67882
H	6.838667	14.43313	22.35145
H	12.20158	14.90844	25.91791
H	9.178322	4.349348	7.47996
H	4.782956	7.820973	11.08416
H	5.510292	13.40557	14.76957
H	10.68304	15.60153	18.427
H	15.15458	12.22056	22.10097
H	14.48967	6.738046	25.6939
H	7.550431	5.048543	7.748243
H	4.496833	9.559899	11.41463
H	6.882678	14.51164	15.10606
H	12.33931	14.98066	18.72199
H	15.43482	10.47085	22.38588
H	13.10365	5.629359	25.9718
H	5.515804	13.48816	7.424089
H	10.73626	15.60119	11.00602
H	15.18281	12.21231	14.72243
H	14.50536	6.661031	18.36571

H	9.403642	4.418903	22.02903
H	4.930624	7.716997	25.64713
H	6.153192	13.90249	9.046453
H	11.31688	15.33005	12.67896
H	15.2696	11.5127	16.3699
H	13.96556	6.213304	20.0152
H	8.749641	4.627374	23.68612
H	4.692559	8.395513	27.28919
H	6.934168	14.56782	7.592809
H	12.38586	14.96527	11.3082
H	15.47087	10.45725	14.95594
H	13.13131	5.532674	18.60286
H	7.736777	5.030719	22.28357
H	4.65335	9.475318	25.88236
N	7.28202	12.51071	7.941167
N	10.78228	13.6069	11.59102
N	13.49478	11.14481	15.29619
N	12.7476	7.583871	18.97799
N	9.313753	6.390071	22.68062
N	6.572869	8.741298	26.40024
N	9.181508	6.367365	8.000126
N	6.489819	8.872737	11.63475
N	7.258783	12.44205	15.35149
N	10.7499	13.60974	19.01626
N	13.46558	11.17884	22.7197
N	12.79467	7.673044	26.44521
N	13.54241	11.10106	7.968724
N	12.72798	7.533785	11.6219
N	9.247871	6.401953	15.30524
N	6.523938	8.846884	19.01217
N	7.227672	12.38095	22.71919
N	10.60708	13.60461	26.42001
O	8.871372	13.38645	9.31525
O	12.28859	12.75792	13.08183
O	13.54543	9.394524	16.76229
O	11.27229	6.648238	20.44989
O	7.756245	7.151664	24.16542
O	6.37905	10.57877	27.74449
O	7.618019	7.342426	9.336026
O	6.481504	10.62017	13.10423
O	8.770842	13.35281	16.79879
O	12.27588	12.78861	20.50176
O	13.5542	9.431601	24.18205
O	11.30047	6.619176	27.81512
O	13.49734	9.288928	9.34462
O	11.22021	6.656453	13.09259
O	7.725877	7.23155	16.79146
O	6.462358	10.59959	20.47319
O	8.69165	13.33136	24.1869
O	12.2562	12.86438	27.81932

BTA heptamer, relaxed geometry using VASP

C	8.576659	9.924651	9.213118
C	9.213884	11.19135	12.94338
C	10.60437	11.27598	16.62638
C	11.39848	10.11979	20.29964
C	10.8239	8.837352	23.98729
C	9.459889	8.722726	27.69709
C	8.612835	9.823641	31.48739
C	9.216755	11.1655	9.199891
C	10.60823	11.28634	12.93029
C	11.39504	10.12378	16.60814
C	10.80666	8.854559	20.29076
C	9.433544	8.703327	23.995
C	8.629029	9.844992	27.69562
C	9.161579	11.1091	31.47875
C	8.459078	12.45518	9.324628
C	11.30953	12.60982	13.02555
C	12.89167	10.19234	16.67866
C	11.62101	7.598195	20.35878
C	8.771098	7.361171	24.07503
C	7.136299	9.721184	27.76964
C	8.315112	12.35196	31.46688
C	9.325344	8.739341	9.216925
C	8.587627	9.93658	12.9531
C	9.206573	11.1772	16.64399
C	10.60364	11.27395	20.31563
C	11.41504	10.1081	23.98339
C	10.85349	8.873097	27.69134
C	9.445547	8.695157	31.48033
C	10.72052	8.806117	9.208946
C	9.367689	8.777481	12.95535
C	8.604428	9.916749	16.65296
C	9.212369	11.153	20.32765
C	10.60478	11.24559	23.99353
C	11.41035	10.1542	27.69089
C	10.83358	8.860844	31.49092
C	8.589339	7.441562	9.364581
C	7.093511	9.876457	13.07659
C	8.401319	12.43776	16.74321
C	11.27874	12.60895	20.41378
C	12.90973	10.20131	24.05579
C	11.70661	7.642961	27.77066
C	8.797972	7.339145	31.46533
C	11.3732	10.04806	9.195688
C	10.76719	8.861546	12.9404
C	9.389314	8.755318	16.63605
C	8.610418	9.887249	20.32008
C	9.20886	11.12063	23.99946
C	10.58413	11.28695	27.69047

C	11.39553	10.14584	31.48421
C	10.61791	11.22258	9.193023
C	11.38216	10.11661	12.9314
C	10.78212	8.863278	16.61676
C	9.409672	8.742696	20.30524
C	8.628042	9.850081	24.00517
C	9.196216	11.12718	27.69842
C	10.55593	11.26348	31.48964
C	12.8692	10.06004	9.322863
C	11.55887	7.591761	13.04636
C	8.705984	7.425686	16.73625
C	7.118388	9.800954	20.4186
C	8.381906	12.36725	24.08374
C	11.22263	12.64251	27.76861
C	12.89352	10.26318	31.47534
C	14.975	11.18422	8.745583
C	13.54146	6.347624	12.3574
C	8.68251	5.081417	16.05772
C	5.085663	8.641086	19.72909
C	6.359456	13.53677	23.38793
C	11.17692	14.97122	27.06067
C	14.83454	11.47576	30.6407
C	8.499828	5.051952	8.812369
C	5.029973	8.729275	12.44165
C	6.390123	13.63731	16.0598
C	11.28882	14.95056	19.72589
C	14.92599	11.38087	23.36103
C	13.72778	6.503095	27.02221
C	8.87641	5.053971	30.62414
C	6.437392	13.71399	8.722132
C	11.38255	14.94744	12.32345
C	14.92315	11.3479	15.97435
C	13.62064	6.406911	19.63112
C	8.766596	5.034084	23.34762
C	5.133519	8.559584	27.01904
C	6.320308	13.45529	30.61167
H	11.32901	7.90252	9.284213
H	8.898023	7.79389	13.01387
H	7.51911	9.818978	16.70823
H	8.578806	12.04002	20.37884
H	11.04592	12.24317	24.02895
H	12.49285	10.28791	27.72743
H	11.50417	7.999603	31.51783
H	7.489078	9.85239	9.286708
H	8.597468	12.09148	12.98794
H	11.06533	12.26466	16.66276
H	12.48475	10.22463	20.32984
H	11.46732	7.956536	24.0187
H	9.034573	7.718207	27.73529
H	7.532111	9.67109	31.50709

H	7.036126	11.78465	8.019274
H	10.08337	13.42387	11.57187
H	12.9394	11.69683	15.25498
H	12.93517	8.304634	18.91938
H	10.03717	6.594063	22.62342
H	7.126659	8.245935	26.30703
H	7.029115	11.52648	30.04992
H	11.09692	12.20234	9.253847
H	12.46961	10.20187	12.97168
H	11.40975	7.970695	16.64609
H	8.960126	7.748653	20.33772
H	7.543514	9.734712	24.04777
H	8.53896	11.99794	27.73844
H	10.9649	12.27512	31.51386
H	9.883078	6.512526	8.08082
H	6.981947	8.392864	11.63768
H	7.071514	11.74887	15.3141
H	10.01806	13.40278	18.97239
H	12.93882	11.71311	22.63671
H	12.9728	8.362683	26.291
H	10.18192	6.64383	30.07213
H	8.452898	4.724482	9.860452
H	4.735959	8.516775	13.47919
H	6.038485	13.81271	17.08702
H	11.24516	15.34423	20.75215
H	15.26357	11.57782	24.38927
H	14.08617	6.316533	28.04536
H	8.829571	4.569051	31.61117
H	13.00864	11.63677	8.0275
H	12.87933	8.226912	11.58293
H	9.959714	6.621432	15.29743
H	7.06102	8.320413	18.96942
H	7.061223	11.65381	22.65169
H	9.948205	13.38606	26.3091
H	12.80934	11.81039	30.08349
H	15.27386	12.07954	8.188011
H	14.39439	6.510443	11.68772
H	9.279972	4.432206	15.4062
H	4.831355	7.783742	19.09398
H	5.488252	13.32282	22.75702
H	10.54494	15.60417	26.42572
H	15.02908	12.3335	29.98538
H	15.28609	11.28687	9.794242
H	13.9076	6.185643	13.38194
H	8.7164	4.693194	17.08639
H	4.761647	8.439734	20.76083
H	6.026349	13.73253	24.4175
H	11.15883	15.3536	28.09202
H	15.27815	11.66588	31.62952
H	15.4842	10.30609	8.321581

H	13.0026	5.437626	12.04926
H	7.630852	5.060875	15.72946
H	4.538936	9.531158	19.37759
H	6.86071	14.4476	23.02281
H	12.21887	15.02205	26.70566
H	15.32852	10.57964	30.22921
H	9.105388	4.342413	8.237316
H	4.753222	7.880256	11.8057
H	5.528576	13.44699	15.40852
H	10.69283	15.59136	19.06499
H	15.1737	12.2401	22.7259
H	14.58011	6.733335	26.37158
H	9.515517	4.460066	29.95892
H	7.475685	5.06185	8.410613
H	4.478921	9.625581	12.11706
H	6.907858	14.55005	15.72425
H	12.34248	14.97434	19.40516
H	15.46656	10.49104	22.99993
H	13.238	5.580733	26.66958
H	7.849205	5.076544	30.22232
H	5.491639	13.50116	8.20985
H	10.78368	15.60901	11.68675
H	15.17145	12.22163	15.36035
H	14.50433	6.62778	19.02139
H	9.408005	4.385139	22.73924
H	4.896908	7.688952	26.39571
H	5.477591	13.20497	29.95493
H	6.233003	13.97987	9.767767
H	11.38105	15.33347	13.35278
H	15.26752	11.51653	17.005
H	13.93331	6.17632	20.65932
H	8.728599	4.649589	24.37666
H	4.779321	8.384388	28.04523
H	5.937922	13.74834	31.60087
H	6.922895	14.57493	8.237936
H	12.42614	14.9461	11.97111
H	15.4565	10.46506	15.58614
H	13.11423	5.514205	19.22982
H	7.740161	5.010458	22.94628
H	4.598377	9.441503	26.62972
H	6.859159	14.32441	30.19975
N	7.280052	12.53103	8.663082
N	10.8046	13.61601	12.27844
N	13.48445	11.1583	15.9432
N	12.74785	7.566677	19.61286
N	9.316686	6.376883	23.32614
N	6.570564	8.762152	27.00315
N	7.182232	12.29428	30.71649
N	9.107566	6.369816	8.720153
N	6.466553	8.925441	12.3497

N	7.268983	12.48303	16.00891
N	10.74869	13.60429	19.67005
N	13.4892	11.17876	23.3247
N	12.81572	7.631039	26.99814
N	9.435581	6.386991	30.73086
N	13.52971	11.04127	8.663757
N	12.68146	7.516234	12.29917
N	9.231391	6.423847	15.99806
N	6.522132	8.844053	19.6743
N	7.248121	12.3895	23.34903
N	10.66346	13.61471	27.01447
N	13.40088	11.29358	30.74626
O	8.893671	13.39732	10.01602
O	12.30398	12.75894	13.76923
O	13.53823	9.396206	17.3957
O	11.26344	6.640108	21.08019
O	7.770741	7.175149	24.80315
O	6.460269	10.47324	28.50585
O	8.646346	13.3711	32.09836
O	7.559634	7.359223	10.06294
O	6.477806	10.6627	13.82944
O	8.768025	13.3842	17.47565
O	12.27118	12.77936	21.15719
O	13.57088	9.412968	24.76835
O	11.39966	6.688896	28.51836
O	7.74019	7.114597	32.07911
O	13.46452	9.21344	10.01828
O	11.19084	6.664139	13.80044
O	7.708993	7.266083	17.47545
O	6.473895	10.57397	21.16286
O	8.733464	13.32821	24.80427
O	12.2115	12.84963	28.50605
O	13.61601	9.456651	32.08761

BTA periodic chain, relaxed geometry using VASP

C	9.253005	11.17176	2.166032
C	10.64229	11.24475	4.750319
C	10.64727	11.23784	0
C	11.39737	10.07117	0.232704
C	11.37139	12.54479	0.24142
C	12.89096	10.10409	0.235397
C	8.603872	9.930372	0.232874
C	9.2428	11.18532	0.2419
C	9.357573	8.755798	0.236033
C	8.604806	9.943853	0.233684
C	7.111112	9.898491	0.244515
C	8.465093	12.46021	0.236936
C	10.75656	8.813852	0.232168
C	9.355766	8.76161	0.244358
C	11.39632	10.05427	0.235751
C	10.74975	8.829167	0.231522
C	11.53289	7.537789	0.24182
C	8.636971	7.452735	0.235306
C	13.50269	6.291086	0.163632
C	8.53419	5.122936	0.21603
C	5.038673	8.820091	0.171558
C	6.47991	13.70069	0.147447
C	11.48037	14.87506	0.146603
C	14.95863	11.19159	0.150624
H	8.865549	7.781977	0.212214
H	7.516165	9.880448	0.165315
H	8.655382	12.08442	0.211084
H	11.1334	12.21929	0.236474
H	10.15103	13.36754	0.08522
H	12.99326	11.55253	0.179991
H	12.4856	10.11453	0.234533
H	11.34963	7.91781	0.084848
H	7.002983	8.439409	0.065664
H	7.146724	11.81603	0.17956
H	4.708168	8.678218	0.281485
H	6.198979	13.91192	0.093048
H	12.83822	8.183299	0.063699
H	9.854044	6.635024	0.214762
H	14.41143	6.509676	0.110107
H	9.170226	4.441494	0.065928
H	13.77113	6.055683	0.211066
H	8.46206	4.770551	0.109398
H	13.01042	5.402662	0.093636
H	7.518057	5.116661	0.226262
H	4.760639	7.943336	0.111983
H	5.578679	13.4924	0.094157
H	4.520248	9.707564	0.103389
H	6.974774	14.59986	0.086882

H	10.82353	15.56698	0.084634
H	15.21933	12.11978	0.101187
H	11.59798	15.21317	0.229386
H	15.29528	11.24753	0.11349
H	12.47726	14.88434	0.09113
H	15.48755	10.35078	0.223696
N	10.88391	13.55171	0.171988
N	13.51815	11.02149	0.100277
N	6.480998	8.975593	0.132109
N	7.349007	12.53954	0.142743
N	12.63862	7.456448	0.140534
N	9.122933	6.449095	0.144442
O	12.36365	12.67707	0.287409
O	13.49804	9.32684	0.182512
O	6.501154	10.68325	0.289635
O	8.836326	13.38121	0.371642
O	11.16835	6.61753	0.372729
O	7.650886	7.315996	0.374919

BTA monomer, relaxed geometry using Gaussian

C	-1.256904000	0.603083000	-0.089479000
H	-2.268458000	1.008858000	-0.194701000
C	-0.108899000	1.405819000	-0.016619000
C	-0.112945000	2.916500000	-0.018495000
O	0.936827000	3.556737000	-0.182658000
N	-1.328644000	3.519219000	0.173037000
H	-2.135494000	2.942192000	0.390496000
C	-1.474362000	4.962887000	0.202094000
C	0.109064000	-1.395212000	0.001050000
H	0.265134000	-2.478779000	0.000325000
C	-1.159466000	-0.800116000	-0.064028000
C	-2.464325000	-1.558455000	-0.137739000
O	-3.524242000	-0.978088000	-0.418067000
N	-2.400386000	-2.901367000	0.127390000
H	-1.519747000	-3.301360000	0.436880000
C	-3.581208000	-3.745090000	0.108980000
C	1.154357000	0.789736000	0.044399000
H	2.014497000	1.464106000	0.105955000
C	1.273940000	-0.607727000	0.042295000
C	2.584021000	-1.357356000	0.099197000
O	2.614658000	-2.570721000	0.355219000
N	3.712467000	-0.620722000	-0.150695000
H	3.612277000	0.342320000	-0.457537000
C	5.035355000	-1.217920000	-0.147580000
H	-2.215475000	5.303348000	-0.540666000
H	-0.491259000	5.389445000	-0.041440000
H	-1.782785000	5.319647000	1.200206000
H	-3.459507000	-4.585924000	-0.594733000
H	-4.420381000	-3.115240000	-0.217854000
H	-3.804831000	-4.150777000	1.110889000
H	5.488995000	-1.204387000	-1.153847000
H	4.915490000	-2.261274000	0.176118000
H	5.707759000	-0.692401000	0.551382000

BTA dimer, relaxed geometry using Gaussian <u>without</u> CP correction

C	0.035797000	1.399020000	-1.785190000
H	0.003215000	2.485532000	-1.661944000
C	1.238531000	0.677734000	-1.778178000
C	2.574408000	1.305200000	-1.461529000
O	3.507934000	0.612609000	-1.004568000
N	2.688274000	2.649002000	-1.638880000
H	1.879946000	3.161531000	-1.979957000
C	3.784142000	3.410761000	-1.052554000
C	-1.228325000	-0.665846000	-1.786502000
H	-2.153024000	-1.237564000	-1.664678000
C	-1.205093000	0.736388000	-1.778055000
C	-2.416733000	1.579118000	-1.461473000
O	-2.284238000	2.733503000	-1.003414000
N	-3.637214000	1.005797000	-1.640240000
H	-3.676639000	0.049884000	-1.982406000
C	-4.845613000	1.573939000	-1.055530000
C	1.191922000	-0.728213000	-1.786446000
H	2.149377000	-1.243144000	-1.664209000
C	-0.034051000	-1.409209000	-1.779280000
C	-0.158597000	-2.880084000	-1.463797000
O	-1.225552000	-3.342735000	-1.008266000
N	0.948623000	-3.650214000	-1.640314000
H	1.797022000	-3.206086000	-1.979978000
C	1.059846000	-4.980701000	-1.055158000
C	-0.286530000	-1.373209000	1.714282000
H	-0.467036000	-2.451858000	1.726238000
C	-1.338539000	-0.443361000	1.697655000
C	-2.792935000	-0.829568000	1.583250000
O	-3.699145000	-0.053693000	1.937377000
N	-3.032361000	-2.063195000	1.033456000
H	-2.283007000	-2.548206000	0.527133000
C	-4.387768000	-2.545082000	0.841289000
C	1.331849000	0.435628000	1.714251000
H	2.356213000	0.818665000	1.726199000
C	1.052555000	-0.940353000	1.696588000
C	2.114246000	-2.006605000	1.580863000
O	1.895466000	-3.179928000	1.933188000
N	3.302337000	-1.596336000	1.031799000
H	3.347860000	-0.704026000	0.526940000
C	4.397628000	-2.528763000	0.839006000
C	-1.043852000	0.932748000	1.715447000
H	-1.887721000	1.628396000	1.728370000
C	0.287432000	1.378865000	1.697524000
C	0.679977000	2.831537000	1.582686000

O	1.805828000	3.228386000	1.934325000
N	-0.269907000	3.655869000	1.035350000
H	-1.065062000	3.249485000	0.529594000
C	-0.009687000	5.070618000	0.842880000
H	4.057354000	4.247505000	-1.712671000
H	4.641394000	2.733558000	-0.942250000
H	3.497329000	3.791720000	-0.055869000
H	-5.705906000	1.392538000	-1.716992000
H	-4.687772000	2.654884000	-0.944612000
H	-5.033897000	1.134850000	-0.059284000
H	1.648862000	-5.634908000	-1.715169000
H	0.044682000	-5.384813000	-0.946585000
H	1.531961000	-4.923727000	-0.057840000
H	-4.487673000	-3.581047000	1.204693000
H	-4.686511000	-2.525454000	-0.223476000
H	-5.059810000	-1.887065000	1.409885000
H	5.344656000	-2.097008000	1.202293000
H	4.529909000	-2.797004000	-0.225859000
H	4.164275000	-3.440069000	1.407331000
H	-0.858630000	5.674622000	1.202959000
H	0.160185000	5.319097000	-0.221485000
H	0.894171000	5.324755000	1.414157000

BTA dimer, relaxed geometry using Gaussian with CP correction on the PES

C	0.408163000	1.341401000	-1.881430000
H	0.679439000	2.397563000	-1.788081000
C	1.374222000	0.325058000	-1.883959000
C	2.850577000	0.588637000	-1.735262000
O	3.599286000	-0.250681000	-1.202018000
N	3.298931000	1.787285000	-2.210258000
H	2.642199000	2.395091000	-2.691690000
C	4.681408000	2.213296000	-2.072436000
C	-1.360558000	-0.316748000	-1.878390000
H	-2.410549000	-0.610155000	-1.782455000
C	-0.963590000	1.028043000	-1.883260000
C	-1.929690000	2.174978000	-1.733789000
O	-1.575735000	3.244327000	-1.203996000
N	-3.193545000	1.962528000	-2.203818000
H	-3.392844000	1.089479000	-2.683945000
C	-4.253379000	2.946793000	-2.063929000
C	0.959983000	-1.019585000	-1.878554000
H	1.739169000	-1.782073000	-1.782482000
C	-0.403280000	-1.348044000	-1.880879000
C	-0.913759000	-2.757878000	-1.729219000
O	-2.017162000	-2.984928000	-1.199615000
N	-0.098416000	-3.747436000	-2.197467000
H	0.758063000	-3.485084000	-2.677096000
C	-0.421905000	-5.157039000	-2.055107000
H	5.146157000	2.383265000	-3.058027000
H	5.217884000	1.406615000	-1.554479000
H	4.754011000	3.138088000	-1.476119000
H	-4.632849000	3.267114000	-3.048688000
H	-3.822529000	3.813214000	-1.543904000
H	-5.090599000	2.545909000	-1.468656000
H	-0.502798000	-5.648603000	-3.038999000
H	-1.391162000	-5.215557000	-1.541391000
H	0.339693000	-5.679916000	-1.452919000
C	-0.484816000	-1.318337000	1.842336000
H	-0.825691000	-2.357084000	1.882320000
C	-1.391362000	-0.247422000	1.832283000
C	-2.888213000	-0.431775000	1.826086000
O	-3.644131000	0.412191000	2.333178000
N	-3.335636000	-1.578411000	1.216750000
H	-2.704661000	-2.099159000	0.601651000
C	-4.754396000	-1.866971000	1.121547000
C	1.376983000	0.238695000	1.846654000
H	2.446952000	0.462247000	1.891014000
C	0.902886000	-1.081779000	1.831594000

C	1.811685000	-2.285380000	1.822109000
O	1.459024000	-3.364381000	2.324290000
N	3.028825000	-2.096141000	1.214639000
H	3.164595000	-1.286436000	0.603589000
C	3.989384000	-3.179031000	1.115874000
C	-0.902178000	1.072482000	1.846603000
H	-1.631396000	1.886760000	1.890932000
C	0.478505000	1.322359000	1.835812000
C	1.067740000	2.710540000	1.831465000
O	2.176787000	2.941910000	2.338676000
N	0.299422000	3.672440000	1.222563000
H	-0.467863000	3.387525000	0.608124000
C	0.761156000	5.044583000	1.126246000
H	-4.977106000	-2.882525000	1.490348000
H	-5.118787000	-1.789664000	0.081137000
H	-5.281461000	-1.127071000	1.740819000
H	4.978748000	-2.866032000	1.490323000
H	4.108776000	-3.526069000	0.073513000
H	3.610551000	-4.009838000	1.728262000
H	-0.002483000	5.746836000	1.501420000
H	1.003328000	5.322021000	0.084358000
H	1.670001000	5.127960000	1.739293000

Example of convergence with respect to box size and cutoff energies

BTA dimer
Cutoff=400eV
Kpoints=Gamma point (1x1x1)

Box size [Å^3]	**Electronic Energy [eV]**
20x20x20	-419.569222 eV
40x40x40	-419.583352 eV

BTA dimer
Box size: 20x20x20 Å^3
Kpoints=Gamma point (1x1x1)

Cutoff energy	**Electronic Energy [eV]**
400eV	-419.569222
500eV	-419.583352
600eV	-419.501457

Calculation of cooperativity as a result of pairwise dipole-dipole interactions

To calculate the additional energy gain as a result of pairwise dipole-dipole interactions the following assumptions are made:

- Each monomer contains one dipole which is the resultant of all the individual dipoles of the monomer.
- All the individual dipoles within an oligomer are aligned (i.e. the angle between the dipole vectors equals 0°), see Figure S1.
- The magnitude of each of the individual dipoles is constant.
- The distance between adjacent monomers within an oligomer is assumed constant (see Figure S1).

Under these conditions, the pairwise dipole-dipole electrostatic energy of a dimer is proportional to:

$$E_2 \propto \frac{1}{R_{1-2}^{\ 3}} \tag{1.1}$$

Where E is the energy and R is the distance between adjacent dipoles.

For a trimer the pairwise dipole-dipole electrostatic energy is proportional to:

$$E_3 \propto \frac{2}{R_{1-2}^{\ 3}} + \frac{1}{R_{1-3}^{\ 3}} = \frac{2}{R_{1-2}^{\ 3}} + \frac{1}{8 \cdot R_{1-2}^{\ 3}} \tag{1.2}$$

Note that $\frac{1}{R_{1-3}^{\ 3}} = \frac{1}{8 \cdot R_{1-2}^{\ 3}}$, since the 1-3 distance is twice the 1-2 distance (Figure S1).

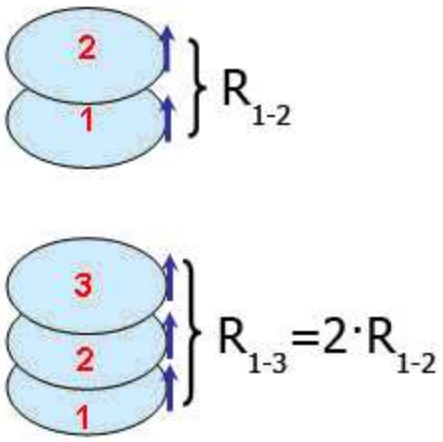

Figure S1: Schematic representation of a dimer and a trimer showing the orientation of the dipoles and the

Likewise for the tetramer and the pentamer the energy is proportional to:

$$E_4 \propto \frac{3}{R_{1-2}^{\ 3}} + \frac{2}{R_{1-3}^{\ 3}} + \frac{1}{R_{1-4}^{\ 3}} = \frac{3}{R_{1-2}^{\ 3}} + \frac{2}{8R_{1-2}^{\ 3}} + \frac{1}{27R_{1-2}^{\ 3}} \tag{1.3}$$

$$E_5 \propto \frac{4}{R_{1-2}^{\ 3}} + \frac{3}{R_{1-3}^{\ 3}} + \frac{2}{R_{1-4}^{\ 3}} + \frac{1}{R_{1-5}^{\ 3}} = \frac{4}{R_{1-2}^{\ 3}} + \frac{3}{8\cdot R_{1-2}^{\ 3}} + \frac{2}{27\cdot R_{1-2}^{\ 3}} + \frac{1}{64\cdot R_{1-2}^{\ 3}} \tag{1.4}$$

Since the strength of each dipole is the same, we can assume that the proportionality constant is the same for each polymer.

For an oligomer composed of *n* monomers the total energy as a result of pairwise dipole-dipole interactions is proportional to:

$$E_n \propto \sum_{k=1}^{n-1} \frac{k}{(n-k)^3 \cdot R_{1-2}^{\ 3}} \tag{1.5}$$

For example, to calculate the additional stabilization of a heptamer due to pairwise dipole-dipole interactions as compared to a dimer, we calculate the pairwise dipole-dipole energy of the heptamer and subtract the energy of a trimer and a tetramer and divide this number by the energy of a dimer:

$$\eta = \frac{\sum_{k=1}^{7-1} \frac{k}{(7-k)^3 \cdot R_{1-2}{}^3} - \sum_{k=1}^{4-1} \frac{k}{(4-k)^3 \cdot R_{1-2}{}^3} - \sum_{k=1}^{3-1} \frac{k}{(3-k)^3 \cdot R_{1-2}{}^3}}{\frac{1}{R_{1-2}{}^3}} \approx 1.43 \qquad (1.6)$$

resulting in an energetic enhancement (cooperativity) of 43%.

Average interaction energies using ZPE and finite temperature corrections

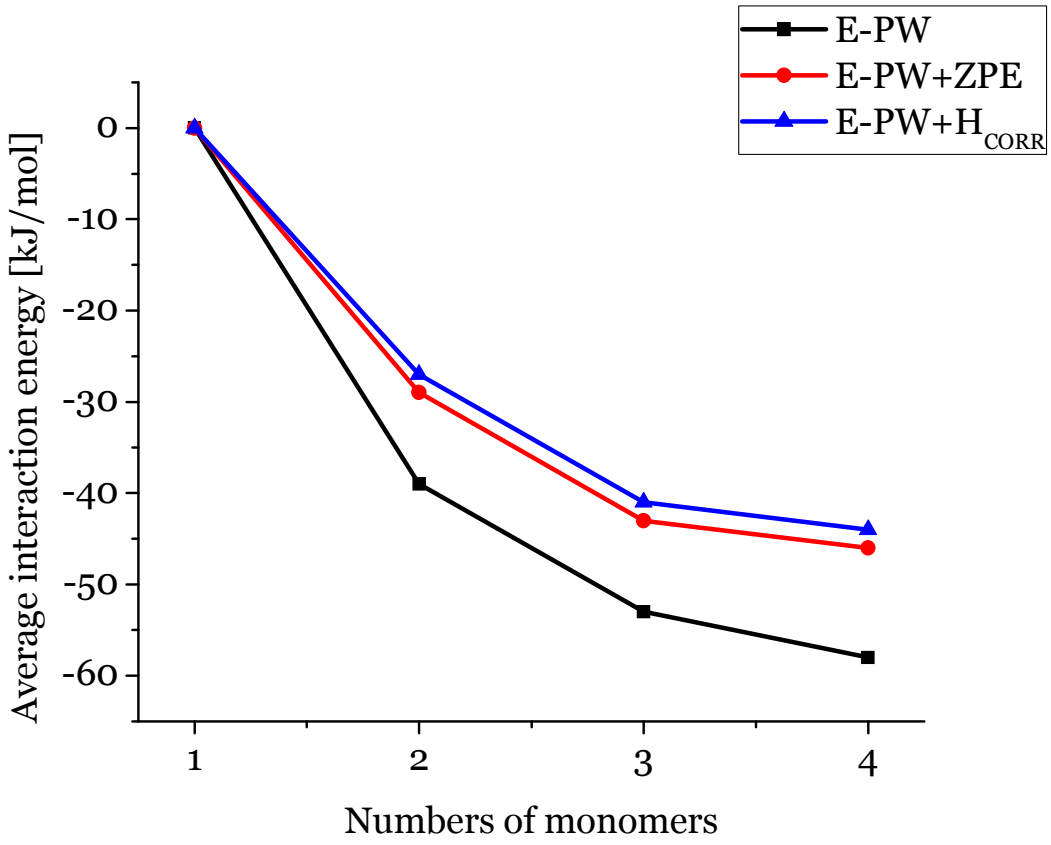

Figure S2: Average interaction energies of 1-4 BTA, as calculated in VASP. The ZPE and finite temperature (H_{CORR}) corrections are uniform and do not change the observed trend. Zero point (E_{ZPE}) and finite temperature (H_{CORR}) corrections were computed using the results of the normal-mode analysis within the ideal gas approximation at a pressure of 1 atm and temperatures of 298 K.