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

Supporting Information

Computational study of bulk porous two-dimensional polymers related to graphyne

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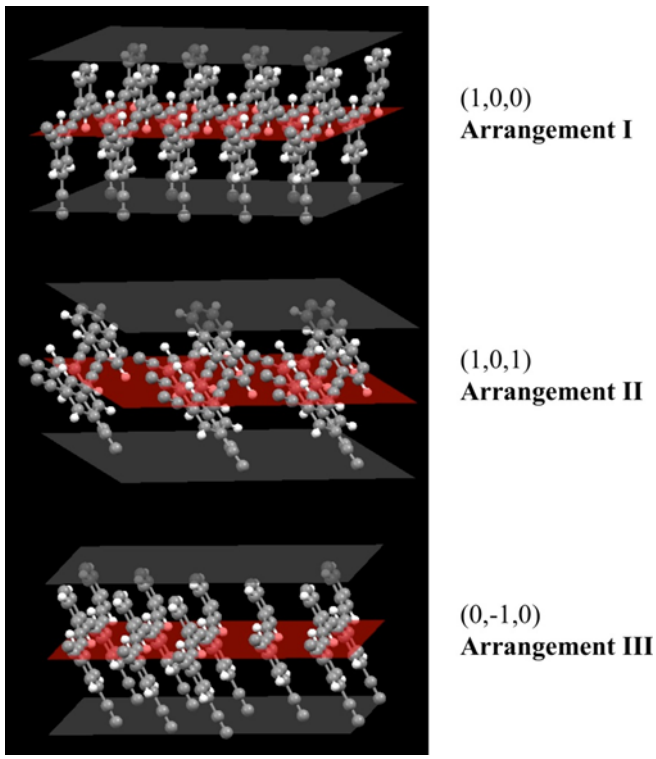

Figure S1. Diffraction planes and their Miller index corresponding to the main diffraction peak at lower θ of the different stacking structures of compound **A**.

Cartesian coordinates for the building blocks with the respective unit cell parameters, for compounds A, B and C

A – arrangement I

length_a 11.896305
length_b 11.894936
length_c 4.150357
angle_alpha 90.002768
angle_beta 90.012049
angle_gamma 59.995113

C	5.730383	-0.742833	-0.000558
C	4.679224	-0.134479	-0.000076
C	3.448741	0.577704	0.000110
C	3.443679	1.978770	0.000015
C	2.231257	-0.115652	0.000108
C	2.234472	2.686463	-0.000100
H	4.383378	2.519822	0.000019
C	1.015372	0.580485	-0.000002
H	2.230003	-1.199982	0.000176
C	1.023654	1.981551	-0.000111
H	0.085219	2.524793	-0.000203
C	-0.216772	-0.128826	-0.000015
C	-1.269915	-0.733740	-0.000070
C	2.236157	4.108189	0.000019
C	2.238279	5.322690	0.000331
C	-2.501975	-1.443184	0.000135
C	-3.717957	-0.747231	-0.000277
C	-2.510029	-2.844249	0.000526
C	-4.935333	-1.440778	0.000037
H	-3.716859	0.337098	-0.001762
C	-3.720725	-3.549356	0.000239
H	-1.571499	-3.387323	0.000217
C	-4.930040	-2.841842	0.000088
H	-5.869655	-3.383038	-0.000902

A - arrangement II

length_a 11.892917
length_b 11.893369
length_c 7.804510
angle_alpha 90.016757
angle_beta 40.354012
angle_gamma 60.000164

C	5.727356	-0.742269	0.039220
C	4.676211	-0.133446	0.047238
C	3.445719	0.579170	0.046349
C	3.442126	1.980101	0.017415
C	2.228725	-0.115312	0.055449
C	2.232159	2.686376	-0.007451
H	4.381857	2.520908	-0.002880
C	1.013455	0.581801	0.030587
H	2.227516	-1.199694	0.064548
C	1.020442	1.982735	0.002169
H	0.082183	2.525498	-0.030476
C	-0.218491	-0.128147	0.014282
C	-1.270619	-0.734935	-0.007489
C	2.234093	4.107277	-0.062431
C	2.235771	5.320812	-0.116892
C	-2.502553	-1.444895	-0.023190
C	-3.717836	-0.747826	-0.048303
C	-2.509519	-2.845821	0.005525
C	-4.934804	-1.442339	-0.039035
H	-3.716714	0.336559	-0.057104
C	-3.721214	-3.549498	0.014837
H	-1.571251	-3.388575	0.038104
C	-4.931200	-2.843263	-0.010129
H	-5.870922	-3.384082	0.010337

A - arrangement III

length_a 11.894972
length_b 11.894848
length_c 5.014155
angle_alpha 53.036667
angle_beta 53.022098
angle_gamma 59.991635

C	3.440481	1.977920	0.048329
C	3.444581	0.576805	0.030476
C	2.227735	-0.117187	-0.001967
C	1.012230	0.580053	-0.010676
C	1.019690	1.981337	-0.002190
C	2.230926	2.685089	0.030147
H	4.379622	2.518554	0.086684
H	2.226335	-1.201304	-0.019746
H	0.081467	2.524542	-0.020151
C	-0.219711	-0.129113	-0.012969
C	-1.272124	-0.734808	-0.000462
C	4.675371	-0.135309	0.057175
C	5.726883	-0.743275	0.085801
C	2.233231	4.107048	0.056563
C	2.235531	5.321671	0.084804
C	-2.504033	-1.443999	-0.002832
C	-2.511520	-2.845254	-0.011445
C	-3.719575	-0.746885	-0.011536
C	-3.722712	-3.549057	-0.044039
H	-1.573215	-3.388280	0.006678
C	-4.936398	-1.440897	-0.044216
H	-3.718058	0.337213	0.006490
C	-4.932359	-2.842021	-0.062328
H	-5.871468	-3.382683	-0.101121

B - arrangement I

length_a 6.870813
length_b 6.870836
length_c 4.095603
angle_alpha 90.000002
angle_beta 90.000002
angle_gamma 59.997629

C	2.727617	0.756963	-0.000003
C	2.019854	1.982892	-0.000003
C	2.021745	-0.466143	-0.000003
C	1.413797	-1.518363	-0.000002
C	0.707710	-2.741345	-0.000003
C	-0.707885	-2.741432	-0.000002
C	0.607665	1.983196	-0.000002
C	-0.607563	1.982754	-0.000001
C	-2.019753	1.982818	-0.000002
C	-2.727583	0.756933	-0.000001
C	-2.021652	-0.466113	0.000011
C	-1.414176	-1.518594	0.000010

B - arrangement II

length_a 6.863697
length_b 6.863677
length_c 5.693813
angle_alpha 52.934404
angle_beta 52.934329
angle_gamma 60.000718

C	2.017834	1.981374	0.000240
C	2.724827	0.756846	0.000235
C	0.606597	1.981817	-0.000480
C	-0.606647	1.981570	-0.000726
C	-2.017892	1.981336	-0.000126
C	-2.724825	0.756741	0.000524
C	2.019602	-0.465528	-0.000469
C	1.412900	-1.516170	-0.000734
C	0.707084	-2.738211	-0.000125
C	-0.706935	-2.738200	0.000540
C	-1.413012	-1.516329	0.000570
C	-2.019568	-0.465604	0.000584

B - arrangement III

length_a 6.872451
length_b 6.872377
length_c 5.058864
angle_alpha 110.014392
angle_beta 69.757918
angle_gamma 60.002565

C	2.019772	1.983428	0.000599
C	2.727733	0.757393	-0.000568
C	2.022373	-0.465549	-0.001106
C	1.414077	-1.519057	-0.000785
C	0.708632	-2.741958	-0.000627
C	-0.707167	-2.742900	0.000148
C	0.607972	1.983800	0.001134
C	-0.608580	1.983345	0.000756
C	-2.020390	1.983614	0.000590
C	-2.728885	0.757889	-0.000126
C	-1.413711	-1.519265	0.000422
C	-2.022131	-0.465625	-0.000398

C - arrangement I

length_a 11.537746
length_b 11.537930
length_c 4.137744
angle_alpha 90.000000
angle_beta 90.000000
angle_gamma 59.997966

C	3.039616	0.469358	0.000000
C	1.918505	-0.374613	0.000000
C	0.617389	0.130498	0.000000
C	0.446852	1.523554	0.000000
C	1.534982	2.397766	0.000000
C	2.826488	1.848623	0.000000
H	2.054224	-1.453049	0.000000
H	-0.555090	1.945044	0.000000
H	3.692470	2.505529	0.000000
C	-0.497914	-0.813640	0.000000
C	-1.809754	-0.518759	0.000000
H	-0.196160	-1.860590	0.000000
H	-2.111426	0.528207	0.000000
C	4.414816	-0.024423	0.000000
C	4.815483	-1.307818	0.000000
H	5.170609	0.760267	0.000000
H	4.059628	-2.092434	0.000000
C	1.275050	3.835670	0.000000
C	2.186562	4.824141	0.000000
H	0.217600	4.098144	0.000000
H	3.243985	4.561579	0.000000
C	-2.925009	-1.462848	0.000000
C	-4.226039	-0.957750	0.000000
C	-2.754584	-2.855831	0.000000
C	-5.347146	-1.801594	0.000000
H	-4.361724	0.120654	0.000000
C	-3.842664	-3.729969	0.000000
H	-1.752688	-3.277330	0.000000
C	-5.134045	-3.180769	0.000000
H	-6.000007	-3.837629	0.000000

C - arrangement II

length_a 11.526385
length_b 11.510203
length_c 5.126447
angle_alpha 51.814354
angle_beta 51.405336
angle_gamma 60.095307

C	3.035738	0.471852	-0.031903
C	1.916869	-0.376069	-0.059844
C	0.614873	0.127175	-0.102390
C	0.441457	1.519522	-0.145427
C	1.529271	2.395727	-0.108249
C	2.821987	1.852072	-0.055540
H	2.052514	-1.454050	-0.039334
H	-0.559997	1.935690	-0.214431
H	3.685557	2.511323	-0.038068
C	-0.501882	-0.816060	-0.092800
C	-1.799480	-0.515853	0.087980
H	-0.215435	-1.855621	-0.242954
H	-2.085933	0.523715	0.238062
C	4.411776	-0.018557	0.032571
C	4.813102	-1.303436	0.023399
H	5.162674	0.767085	0.105004
H	4.062196	-2.089058	-0.049108
C	1.268957	3.835248	-0.126050
C	2.159669	4.815376	0.114652
H	0.238470	4.105016	-0.355129
H	3.190128	4.545603	0.343847
C	-2.916269	-1.459042	0.097537
C	-4.218215	-0.955736	0.054202
C	-2.742942	-2.851376	0.141290
C	-5.337118	-1.803599	0.026105
H	-4.353784	0.122244	0.033164
C	-3.830798	-3.727534	0.103975
H	-1.741535	-3.267553	0.210979
C	-5.123453	-3.183821	0.050412
H	-5.987059	-3.843021	0.032776

C - arrangement III

length_a 11.492519
length_b 11.520725
length_c 7.051687
angle_alpha 48.137996
angle_beta 32.937636
angle_gamma 60.078838

C	3.035127	0.472366	-0.137809
C	1.915552	-0.373638	-0.161191
C	0.613930	0.132856	-0.139693
C	0.441241	1.525403	-0.123586
C	1.531551	2.399406	-0.107795
C	2.824390	1.853071	-0.124440
H	2.051825	-1.451251	-0.192601
H	-0.561669	1.944357	-0.127162
H	3.691549	2.508360	-0.119841
C	-0.502205	-0.811234	-0.127183
C	-1.791473	-0.520640	0.127213
H	-0.224249	-1.842866	-0.338518
H	-2.069415	0.510993	0.338565
C	4.408457	-0.027658	-0.114458
C	4.790364	-1.299403	0.106649
H	5.171767	0.731160	-0.280455
H	4.027051	-2.058215	0.272657
C	1.270834	3.837574	-0.068821
C	2.177947	4.818060	0.095600
H	0.220317	4.106602	-0.176985
H	3.228462	4.549018	0.203734
C	-2.907623	-1.464709	0.139686
C	-4.209233	-0.958187	0.161302
C	-2.734971	-2.857257	0.123388
C	-5.328831	-1.804161	0.137873
H	-4.345483	0.119426	0.192842
C	-3.825303	-3.731231	0.107534
H	-1.732073	-3.276239	0.126836
C	-5.118130	-3.184872	0.124328
H	-5.985302	-3.840144	0.119692