Supplementary Material For Modelling the Solid State, Surface and Morphological Properties of Para Amino Benzoic Acid in terms of the Strength and Directionality of its Intermolecular Synthons

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Abstract

Additional details are provided to supplement the data presented in the publication including:

A1. Full intermolecular interaction list for α-PABA showing where the intermolecular interactions contributing to the growth of the α-PABA (1 0 1) surface rank compared to the strongest intermolecular interactions.

A2. The five strongest intermolecular interactions from the α-PABA AMBNAC 06 crystal structure with the planar amino group, highlighting their similarity to the interactions calculated for the AMBNAC 01 structure.

A1. Full Intermolecular Interaction List for α-PABA AMBNAC 01 Structure

Table A1 and A2 shows the all the intermolecular interactions calculated for the α-PABA AMBNAC 01 crystal structure. This aids in highlighting how far down the total list the intermolecular interactions that contribute to the α-PABA (1 0 1) surface, J, M and O (figure 16 and table 6 in paper),

compared to the bulk strongest interactions. This reveals how weak the interactions contributing to this face are compared to the (1 0 -1) and (0 1 -1) surfaces of α-PABA.

Table A1: Total intermolecular interactions of α-PABA molecule 1

Bond	Multiplicity	Distance (Å)	Intermolecular Energy (kcal/mol)	Percentage Contribution to Lattice Energy	Dominating Interatomic Interaction Type
Aα1	1	8.23	-5.67	23.10	H-Bond
Cα1	2	3.86	-5.36	21.84	π-π Stacking
Dα1	1	7.90	-2.27	9.25	H-Bond
Eα1	1	7.75	-2.00	8.15	H-Bond
Fα1	2	7.96	-2.26	9.21	vdW
Gα1	1	6.39	-0.89	3.60	vdW
Hα1	2	6.96	-0.85	6.94	vdW
Iα1	1	8.80	-0.77	3.14	vdW
Jα1	1	6.86	-0.72	2.94	vdW
Kα1	1	8.40	-0.60	2.45	vdW
Lα1	1	6.91	-0.50	2.04	vdW
Mα1	1	6.68	-0.40	1.63	vdW
Nα1	1	7.99	-0.19	0.78	vdW
Oα1	1	8.91	-0.16	0.65	vdW
Pα1	1	8.84	-0.15	0.61	vdW
Qα1	1	9.17	-0.15	0.61	vdW
Rα1	1	8.48	-0.11	0.45	vdW
Sα1	1	9.42	-0.11	0.45	vdW
Tα1	1	8.51	-0.11	0.45	vdW
Uα1	1	11.17	-0.11	0.45	vdW

Table A2: Total intermolecular interactions of α-PABA molecule 2

Bond	Multiplicity	Distance (Å)	Intermolecular Energy (kcal/mol)	Percentage Contribution to Lattice Energy	Dominating Interatomic Interaction Type
Bα2	1	8.34	-5.63	22.94	H-Bond
Cα2	2	3.86	-5.32	21.68	π-π Stacking
Dα2	1	7.90	-2.27	9.25	H-Bond
Eα2	1	7.76	-1.21	4.93	H-Bond
Fα2	2	6.94	-1.9	7.74	vdW
Gα2	1	6.39	-0.89	3.63	vdW
Hα2	1	8.80	-0.77	3.14	vdW
Iα2	1	6.86	-0.72	2.94	vdW
Jα2	1	8.40	-0.60	2.45	vdW
Kα2	1	6.91	-0.50	2.04	vdW
Lα2	1	6.68	-0.40	1.63	vdW
Mα2	1	7.99	-0.19	0.78	vdW
Nα2	1	8.91	-0.16	0.65	vdW
Oα2	1	9.17	-0.15	0.61	vdW
Pα2	1	10.42	-0.14	0.57	vdW
Qα2	2	8.83	-0.14	1.14	vdW
Rα2	1	8.98	-0.12	0.49	vdW
Sα2	1	8.48	-0.11	0.44	vdW
Tα2	1	8.51	-0.11	0.44	vdW
Uα2	1	11.17	-0.11	0.44	vdW

A2: Strongest Intermolecular Interactions Calculated from α-PABA AMBNAC 06 Crystal Structure

Table A3 and A4 shows the top 5 bulk intermolecular interactions in the AMBNAC 06 structure for α-PABA. These pairwise interactions are the same in nature as the interactions found in the AMBNAC 01 crystal structure (table 3 in paper), highlighting that the slight pyrimadilisation of the amino group makes little difference in the ranking of the strength of the intermolecular interactions, and therefore little difference in the morphological prediction regardless of the geometry of the amino group.

Table A3: Bulk intermolecular interactions from α-PABA AMBNAC 06 crystal structure for molecule one. Intermolecular interaction strength ranking for the top 5 same as AMBNAC 01

Bond	Multiplicity	Distance (Å)	Intermolecular Energy (kcal/mol)	Percentage Contribution to Lattice Energy
Aα1	1	8.07	-7.10	29.04
Cα1	2	3.84	-2.58	21.10
Dα1	1	7.91	-1.90	7.77
Eα1	1	7.82	-1.28	5.24
Gα1	2	6.98	-0.97	7.93
Total			-17.38	71.08

Table A4: Bulk intermolecular interactions from α-PABA AMBNAC 06 crystal structure for molecule two. Intermolecular interaction strength ranking for the top 5 same as AMBNAC 01

Bond	Multiplicity	Distance (Å)	Intermolecular Energy (kcal/mol)	Percentage Contribution to Lattice Energy
Bα2	1	8.03	-6.94	28.38
Cα2	2	3.84	-2.68	21.92
Dα2	1	7.91	-1.90	7.77
Eα2	1	7.82	-1.28	5.23
Fα2	2	6.99	-1.01	8.26
Total			-17.50	71.56