The phase behavior of heptanamide adsorbed on a graphite substrate

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Supporting Information Table. Coordinates for the single repeating motif in the asymmetric unit for the *pgg* phase of heptanamide. X and Y coordinates are fractional (w.r.t the unit cell lengths) and the Z coordinate is the absolute distance (Å) of the atom above the C-C-C plane of the molecule (which is parallel to the graphite plane).

Atom	*pgg* phase			*p2* phase		
	X_{frac}	Y_{frac}	Z_{abs} (Å)	X_{frac}	Y_{frac}	Z_{abs} (Å)
O	-0.0228	-0.1205	0.0000	-0.0503	-0.1284	0.0000
N	-0.0142	0.3027	0.0000	-0.0158	0.3093	0.0000
C	-0.0037	0.0705	0.0000	-0.0045	0.0720	0.0000
C	0.0300	0.0239	0.0000	0.0607	0.0302	0.0000
H	0.0360	-0.0883	0.8950	0.0678	-0.0844	0.8950
H	0.0360	-0.0883	-0.8950	0.0678	-0.0844	-0.8950
C	0.0489	0.2594	0.0000	0.1080	0.2764	0.0000
H	0.0430	0.3717	0.8950	0.1009	0.3910	0.8950
H	0.0430	0.3717	-0.8950	0.1009	0.3910	-0.8950
C	0.0827	0.2128	0.0000	0.1731	0.2346	0.0000
H	0.0886	0.1005	0.8950	0.1802	0.1200	0.8950
H	0.0886	0.1005	-0.8950	0.1802	0.1200	-0.8950
C	0.1016	0.4483	0.0000	0.2204	0.4808	0.0000
H	0.0957	0.5606	0.8950	0.2133	0.5954	0.8950
H	0.0957	0.5606	-0.8950	0.2133	0.5954	-0.8950
C	0.1354	0.4017	0.0000	0.2856	0.4390	0.0000
H	0.1413	0.2894	0.8950	0.2927	0.3244	0.8950
H	0.1413	0.2894	-0.8950	0.2927	0.3244	-0.8950
C	0.1543	0.6372	0.0000	0.3329	0.6851	0.0000
H	0.1483	0.7494	0.8950	0.3257	0.7997	0.8950
H	0.1483	0.7494	-0.8950	0.3257	0.7997	-0.8950
H	-0.0379	0.3354	0.0000	-0.0614	0.3386	0.0000
H	0.1793	0.5933	0.0000	0.3807	0.6446	0.0000
H	-0.0010	0.4676	0.0000	0.0173	0.4816	0.0000