The hcp structure is fully specified by two numbers, e.g. c and a. d-spacings can be directly calculated from the c/a ratio and the volume per molecule ($\sqrt{3}ca^2/4$) in the tables below. The observed d-spacings are: (100)=$\sqrt{3}a/2$, (101)=$\sqrt{(3a^2/4+c^2)}$ and (002) =$c/2$

BLYP					
Pressure	Volume	c/a	$< cos\theta >$	initiated	Phase
10	11.9804	1.6247	0.506480	P63m	I
20	9.1007	1.619415	0.4962698	P63m	I
30	7.8787	1.620801	0.508926	P63m	I
40	7.0702	1.609334	0.4996069	P63m	I
50	6.4600	1.599574	0.5051744	P63m	I
75	5.5644	1.597964	0.5018897	P63m	I
100	4.9660	1.591320	0.4865163	P63m	I
125	4.5356	1.585926	0.4764345	P63m	I
150	4.2018	1.577247	0.4698209	P63m	I
175	3.9393	1.571384	0.4662826	P63m	I
190	3.8078	1.566554	0.4507833	P63m	I
200	3.7320	1.562305	0.4266832	P63m	I
210	3.6532	1.558341	0.4177813	P63m	I
225	3.5491	1.553017	0.4081023	P63m	I
250	3.3899	1.552009	0.4016243	P63m	I
275	3.2574	1.547899	0.41143	P63m	I
300	3.1358	1.54326	0.4024638	P63m	I
400	2.7490	1.517	0.3613476	P63m	Cmca
410	2.6943	1.508	0.442654	P63m	Cmca

TABLE I: Summary of the 300K simulations using BLYP functional, showing average volume, c/a and $\langle \cos\theta \rangle$ Simulations were initiated in P63m using a 4-layer 128 atom supercell based on a Phase II candidate. This supercell is incompatible with the G'B and BG'BG" structures, which means it represents the continuation of Phase I to high pressures. The hcp structure is fully specified by two numbers, here we give volume in Å^3/atom and c/a.

BLYP					
Pressure	Volume	c/a	$< cos\theta >$	initiated	Phase
100	4.9604	1.5883	0.4439265	$P6_122$	I
120	4.6034	1.579752	0.4185463	$P6_122$	I
130	4.4539	1.576561	0.4116525	$P6_122$	I
140	4.3176	1.573193	0.397990	$P6_122$	I
150	4.1895	1.571013	0.402121	$P6_122$	I
160	4.0992	1.568875	0.3899782	$P6_122$	I
170	3.9935	1.562581	0.3584516	$P6_122$	I
180	3.8947	1.556153	0.3523557	$P6_122$	III*
190	3.7827	1.536208	0.295101	$P6_122$	IV
200	3.7258	1.534587	0.3058081	$P6_122$	III*
210	3.6255	1.518815	0.2798709	$P6_122$	III*
220	3.5560	1.516970	0.2702824	$P6_122$	III*
250	3.3657	1.512323	0.267668	$P6_122$	III*
180a	3.8671	1.543891	0.3188191	648 $P6_122$	I
180	3.8718	1.54544	0.324068	648 $P6_122$	I
200	3.6988	1.529433	0.2883576	648 $P6_122$	IV GxGyGz
220	3.5607	1.514826	0.271664	648 $P6_122$	IV GxGyGz
220a	3.5611	1.51676	0.2756257	648 $P6_122$	IV GxGyGz

TABLE II: Data for BLYP runs initiated using $P6_122$ is a candidate for Phase III, upper section is from 324 atom supercells with 6-layers, making its Phase IV compatible with BGxBGyBGz but incompatible with BG'BG". The 648 atom cell is compatible with either Phase IV candidate. The runs marked * undergo a transition some time after equilibration. The structure remains in the same phase, but the stacking goes from BGBG to GBGB, possibly via Phase I. This can only be detected by careful analysis of the trajectory. The barrier to such a transition scales with the system size, so it is a finite size effect. That such transformations do occur, but rarely, suggests that our simulations are on the edge of an acceptable size.

BLYP					
Pressure	Volume	c/a	$< cos\theta >$	initiated	Phase
075	5.5675	1.596835	0.4742624	Pbcn	I
100	4.9652	1.589387	0.4523625	Pbcn	I
120	4.6145	1.582851	0.4385514	Pbcn	I
140	4.3276	1.576478	0.418559	Pbcn	I
160	4.0724	1.561678	0.3615409	Pbcn	I
170	3.9885	1.556033	0.3630052	Pbcn	I
180	3.8619	1.535091	0.302474	Pbcn	I
200	3.6941	1.529361	0.264194	Pbcn	IV
210	3.6246	1.522132	0.2599856	Pbcn	IV
220	3.5605	1.519139	0.257028	Pbcn	IV BG"BG"
230	3.4960	1.516730	0.2434004	Pbcn	IV
240	3.4382	1.515042	0.2521973	Pbcn	IV
260	3.3116	1.509366	0.2279203	Pbcn	IV
280	3.2103	1.506743	0.2278928	Pbcn	IV
300	3.1251	1.504065	0.2176326	Pbcn	IV

TABLE III: Data for BLYP initiated in Pbcn, a 288 atom, 4-layer supercell which is compatible with high temperature Phase IV BG'BG" and with the C2c Phase III candidate.

PBE					
30	7.5415	1.606	0.4999189	P63m	I
50	6.2177	1.604116	0.5058818	P63m	I
75	5.3597	1.584457	0.4855751	P63m	I
100	4.7469	1.581542	0.4859878	P63m	I
100	4.7592	1.578000	0.4859255	P63m	I
125	4.3423	1.576183	0.4816306	P63m	I
150	4.0264	1.576154	0.4699437	P63m	I
175	3.7825	1.558993	0.4494359	P63m	I
190	3.6545	1.554261	0.4195735	P63m	I
200	3.5765	1.552071	0.4066827	P63m	I
210	3.5031	1.55059	0.3973104	P63m	I
225	3.3991	1.555776	0.40315	P63m	I
250	3.1821	1.598206	0.4765108	P63m	Cmca
275	3.0503	1.415706	0.3946689	P63m	Cmca
100	4.7506	1.569458	0.4194362	$P6_122$	I
120	4.4120	1.568748	0.3881728	$P6_122$	I
140	4.112	1.529070	0.302	$P6_122$	III
160	3.8982	1.527	0.289	$P6_122$	III
180	3.7112	1.5293	0.274	$P6_122$	III
200	3.5575	1.532584	0.2660064	$P6_122$	III
220	3.410	1.533	0.260	$P6_122$	III
240	3.281	1.537366	0.257	$P6_122$	III
300	2.9781	1.500390		$P6_122$	Cmca

TABLE IV: Same as Table I,II except using the PBE functional

PBE					
100	4.7771	1.588260	0.4276767	Pbcn	I
120	4.4714	1.582647	0.4137635	Pbcn	I
140	4.0992	1.5369	0.2987385	Pbcn	IV*
160	3.8973	1.5303	0.2844748	Pbcn	IV
180	3.7157	1.5294	0.2696992	Pbcn	IV
200	3.5624	1.5290	0.2621374	Pbcn	IV
210	3.4930	1.5297	0.2641268	Pbcn	IV
220	3.4271	1.5317	0.2584371	Pbcn	IV
230	3.3666	1.5297	0.2496307	Pbcn	IV
240	3.3092	1.5310	0.2520884	Pbcn	IV
250	3.2552	1.5240	0.2303325	Pbcn	IV
260	3.2039	1.5240	0.2247819	Pbcn	IV

TABLE V: Same as Table II, except using the PBE functional

Heating	BLYP				
P/GPa (T/K)	volume	c/a	$\langle\cos\theta\rangle$	initial	Phase
190(10K)	3.7437	1.519093	0.08143561	$P6_122$	III
190(100K)	3.7530	1.520747	0.1543091	$P6_122$	III
190 (200K)	3.7678	1.525460	0.2234783	$P6_122$	III
190(300K)	3.7827	1.536208	0.295101	$P6_122$	IV
200(10K)	3.6668	1.516609	0.1087127	$P6_122$	III
200(100K)	3.6730	1.513000	0.1558589	$P6_122$	III
200(200K)	3.6861	1.520019	0.2210022	$P6_122$	III
200(225K)	3.6907	1.52181	0.251898	$P6_122$	III
200(250K)	3.6873	1.523928	0.2542677	$P6_122$	III
200(275K)	3.6965	1.524237	0.2772103	$P6_122$	III
200(300K)	3.7258	1.534587	0.3058081	$P6_122$	I
200(325K)	3.7312	1.5559256	0.3753127	$P6_122$	I
200(350K)	3.7310	1.555410	0.3574772	$P6_122$	I
200(375K)	3.7303	1.560755	0.3820667	$P6_122$	I
200(390K)	3.7363	1.560824	0.3850054	$P6_122$	I
200(400K)	3.7195	1.557527	0.3714859	$P6_122$	I
200(410K)	3.7393	1.561903	0.3942159	$P6_122$	I
200(425K)	3.7419	1.565146	0.3973676	$P6_122$	I
200(450K)	3.7444	1.567228	0.4036871	$P6_122$	I
200(500K)	3.7474	1.569	0.4135272	$P6_122$	I
200(550K)	3.7523	1.5681	0.4204169	$P6_122$	I

TABLE VI: Same as Table III, except with variable temperature.