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

Supporting Information:

Is Pbam-32 thermodynamic stable comparing with diamond and graphite under variable P-T conditions?

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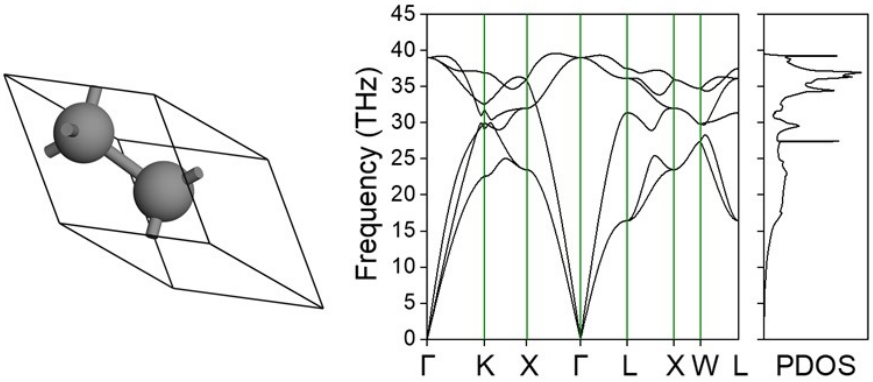

Fig. S1 Structures and phonon dispersion of diamond. High symmetric points in the first Brillouin Zone: Γ(0, 0, 0), K(0.375, 0.375, 0.75), X(0.5, 0, 0.5), Γ(0, 0, 0), L(0.5, 0.5, 0.5), X(0.5, 0, 0.5), W(0.5, 0.25, 0.75), L(0.5, 0.5, 0.5).

Fig. S2 Structures and phonon dispersion of graphite. High symmetric points in the first Brillouin Zone: Γ(0, 0, 0), K(-0.333, 0.667, 0), M(0, 0.5, 0), Γ(0, 0, 0).

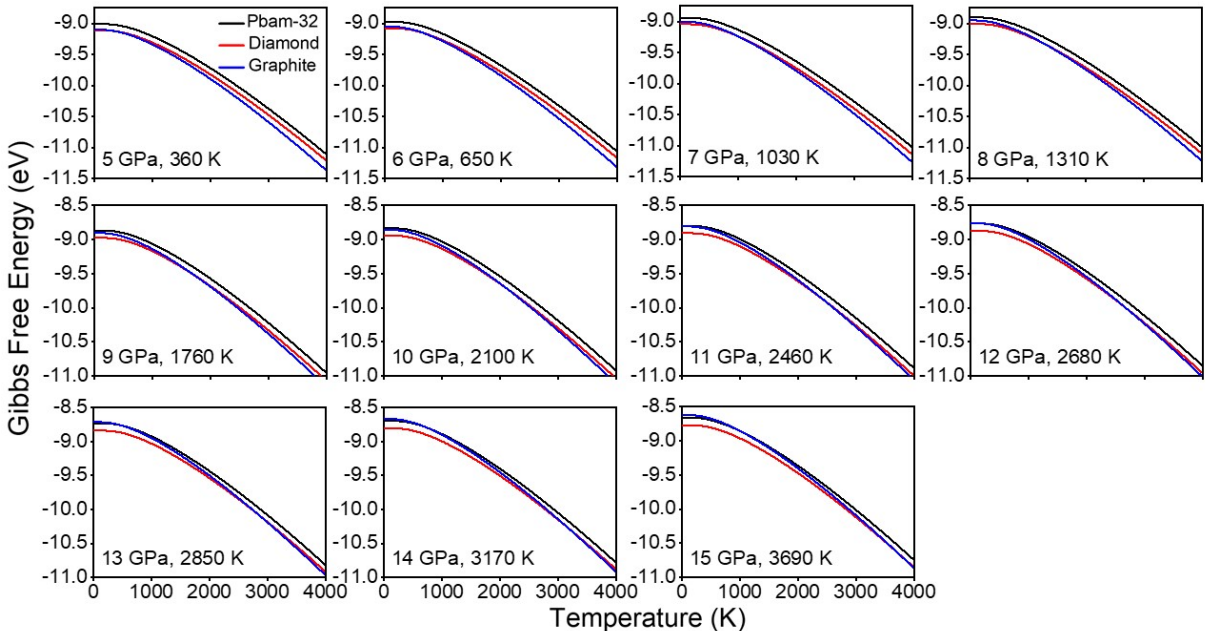

Fig. S3 Gibbs free energies of Pbam-32, diamond and graphite under 5 ~ 15 GPa pressure.

Table S1. Lattice parameters of Pbam-32, diamond and graphite.

Configuration	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
Pbam-32	8.303	8.865	2.511	90	90	90
Diamond	2.515	2.515	2.515	60	60	60
Graphite	2.467	2.467	6.709	90	90	120

Table S2. Bonds and their fractions in Pbam-32.

Bond	Length (Å)	Fraction
C_1-C_1	1.580	2/64
C_1-C_2	1.528	8/64
C_1-C_8	1.559	4/64
C_2-C_3	1.541	4/64
C_2-C_6	1.574	4/64
C_3-C_4	1.524	8/64
C_3-C_5	1.545	4/64
C_4-C_4	1.456	2/64
C_4-C_7	1.543	4/64
C_5-C_6	1.503	4/64
C_5-C_8	1.554	8/64
C_6-C_7	1.541	8/64
C_7-C_8	1.566	4/64

Table S3. Angles and their fractions in Pbam-32.

Angle	Degree (°)	Fraction
C_2-C_1-C_2	110.235	4/144
C_2-C_1-C_8	110.054	8/144
C_1-C_1-C_8	111.267	4/144
C_1-C_1-C_2	107.586	8/144
C_1-C_2-C_3	116.126	4/144
C_1-C_2-C_6	109.902	4/144
C_3-C_2-C_6	93.120	4/144
C_2-C_3-C_4	99.260	4/144
C_2-C_3-C_5	129.683	4/144

C_4-C_3-C_5	108.481	4/144
C_3-C_4-C_4	110.017	8/144
C_3-C_4-C_3	110.689	4/144
C_3-C_4-C_7	106.583	8/144
C_4-C_4-C_7	112.863	4/144
C_3-C_5-C_6	108.243	4/144
C_3-C_5-C_8	110.789	4/144
C_6-C_5-C_8	109.752	4/144
C_5-C_6-C_2	111.609	4/144
C_5-C_6-C_7	114.927	4/144
C_2-C_6-C_7	102.556	4/144
C_6-C_7-C_8	118.173	8/144
C_6-C_7-C_4	100.560	8/144
C_6-C_7-C_6	108.875	4/144
C_4-C_7-C_8	107.361	4/144
C_1-C_8-C_7	114.168	4/144
C_1-C_8-C_5	109.221	8/144
C_5-C_8-C_7	108.254	8/144
C_5-C_8-C_5	107.516	4/144