Supporting Information

Piezochromism, Structural and Electronic Properties of Benz[a]anthracene under Pressure

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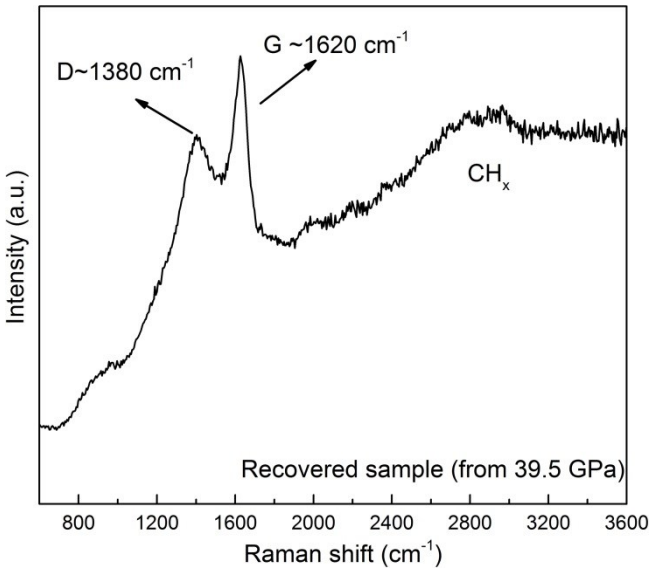

Fig. S1. Raman spectrum of recovered BaA sample from 39.5 GPa at RT.

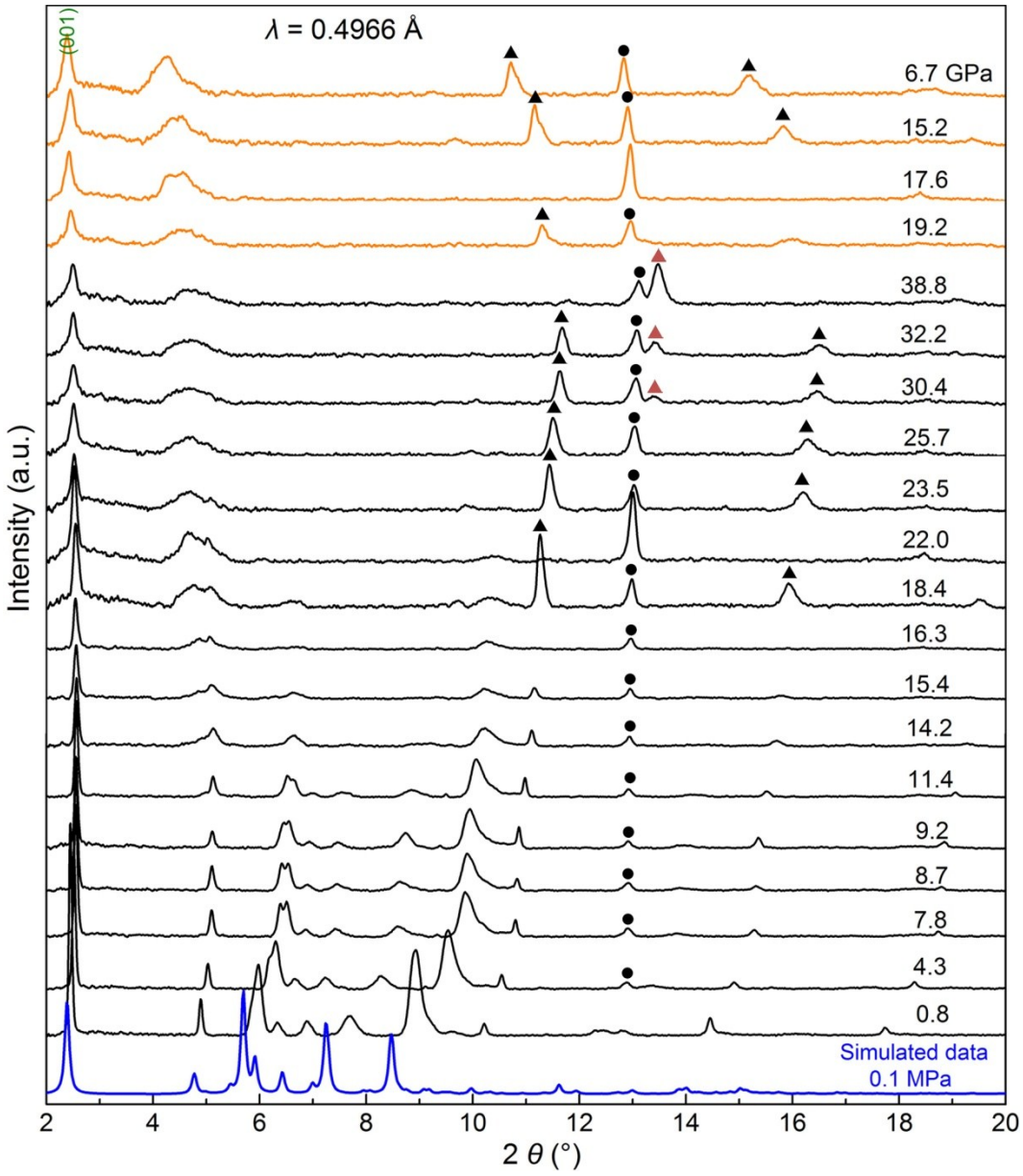

Fig. S2. Integrated XRD patterns of BaA upon compression up to 38.8 GPa (black) and released to 6.7 GPa (orange) measured at room temperature (λ = 0.4966 Å). The diffraction peaks marked with triangles and circles indicate peaks from NaCl and Re gasket, respectively.

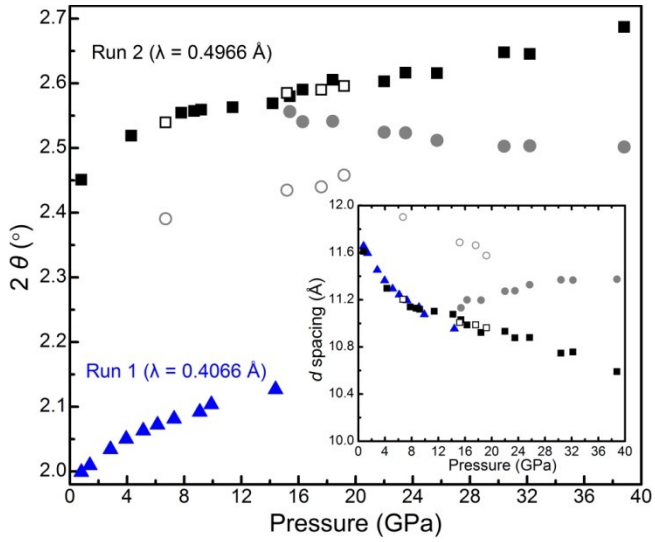

Fig. S3. Changes of 2θ angles of (001) peak as a function of pressure in BaA. The inset indicates the *d* spacing of (001) peak as a function of pressure. The cycles indicate reflections from newly formed polymers. The decompression data are illustrated as unfilled symbols.

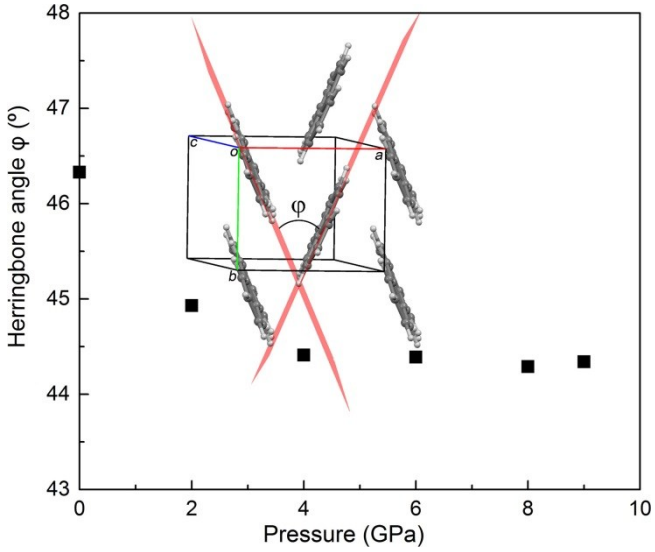

Fig. S4. Changes of herringbone angle φ as a function of pressure. The inset shows the definition of angle φ.

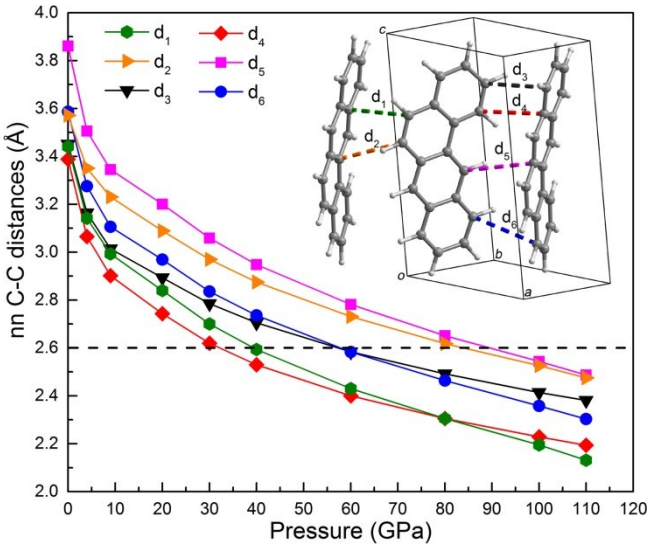

Fig. S5. Pressure dependence of nearest neighbor (nn) C-C distances in the molecular phase.

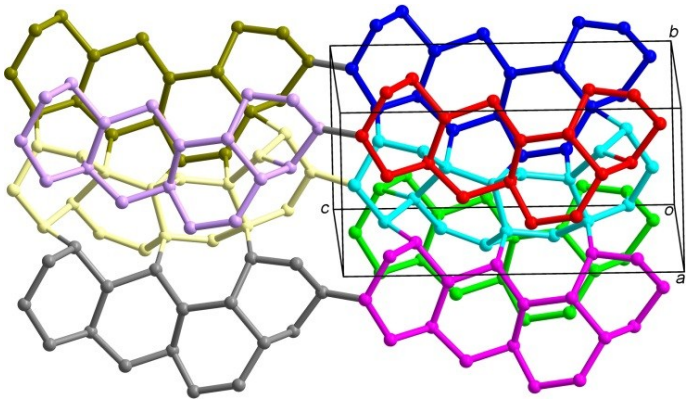

Fig. S6. Structure of polymer I (at 100 GPa) with different numbered carbon rings. The H atoms are omitted for clarity.

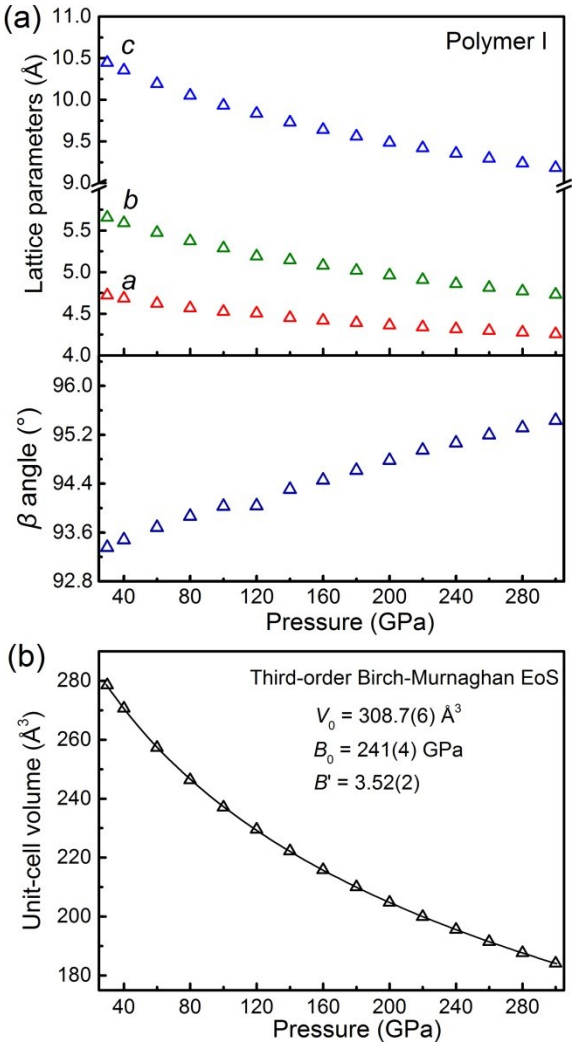

Fig. S7. Pressure dependence of lattice parameters of BaA polymer I obtained from DFT calculations. (b) Third-order Birch–Murnaghan EoS fits to the unit-cell volume data.

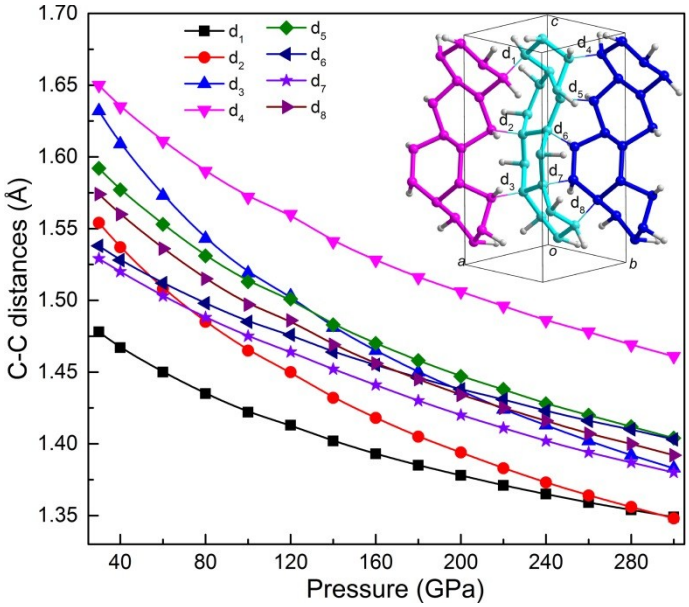

Fig. S8. The interatomic C-C distances among the adjacent molecules as a function of pressure in polymer I.

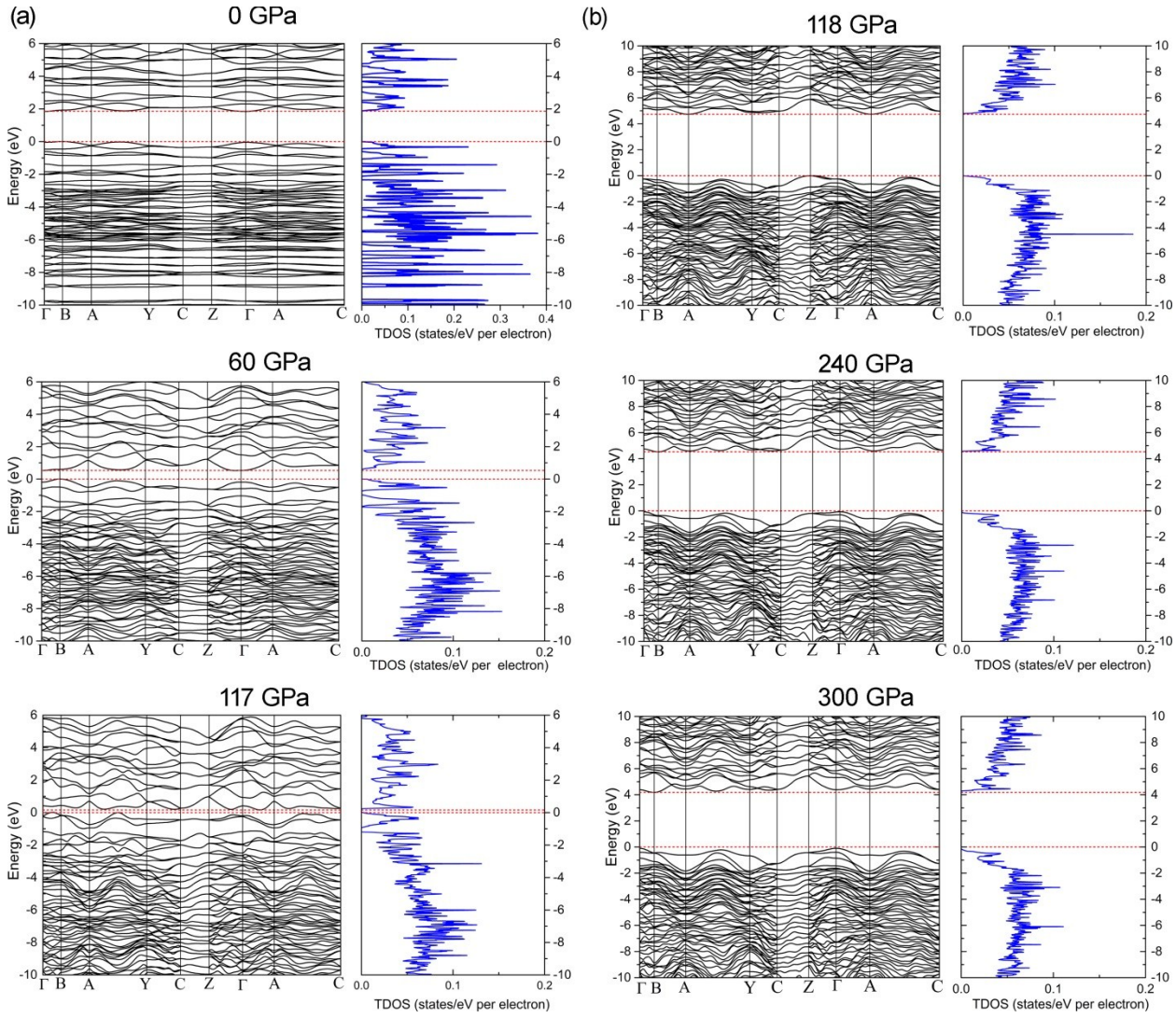

Fig. S9. Calculated band structures and total density of states (TDOS) of (a) molecular phase at 0, 60 and 117 GPa and (b) polymer I at 118, 240 and 300 GPa.