Hydrogen Bond-Modulated Negative Linear Compressibility in a V-shaped Molecular Crystal

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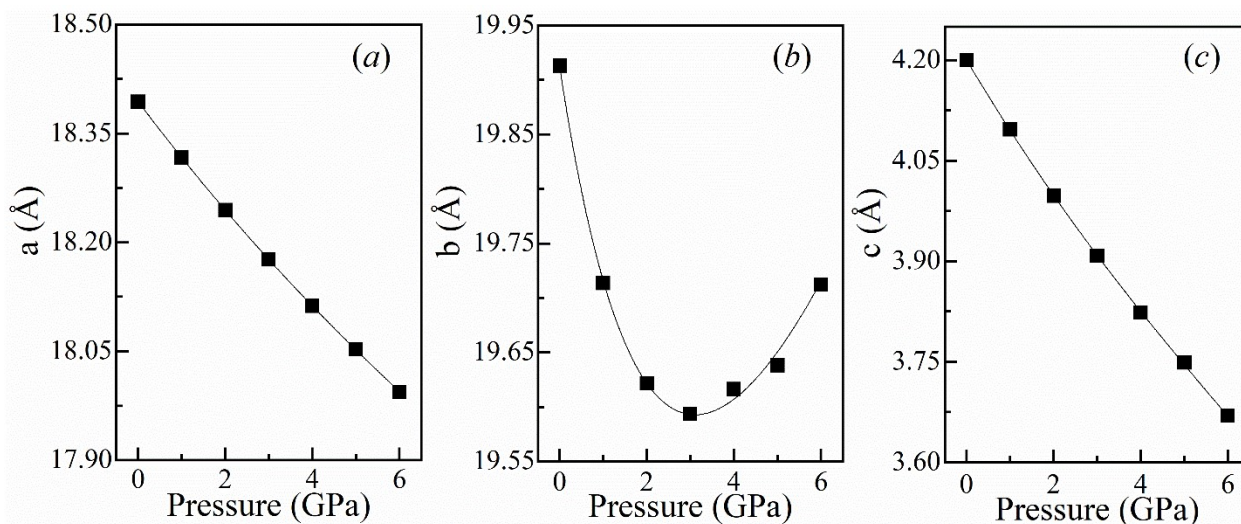
Fig. S1. Lattice parameters as a function of pressure from 0 to 6 GPa. The scatter solid points are computational data and the curves in solid line are fitting of the scatter points using fifth-order polynomial function $l = a_0 + a_1p + a_2p^2 + \cdots$ to get a highly smooth l-p curve.
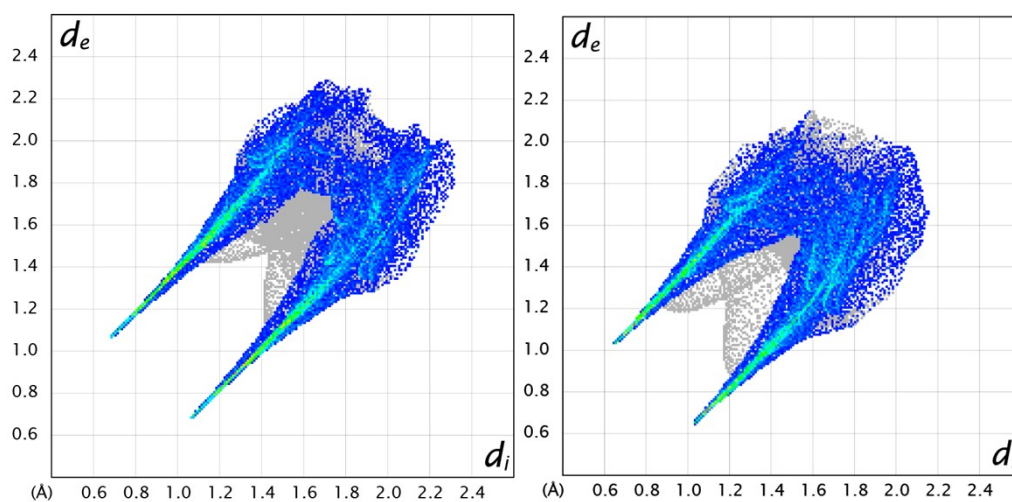

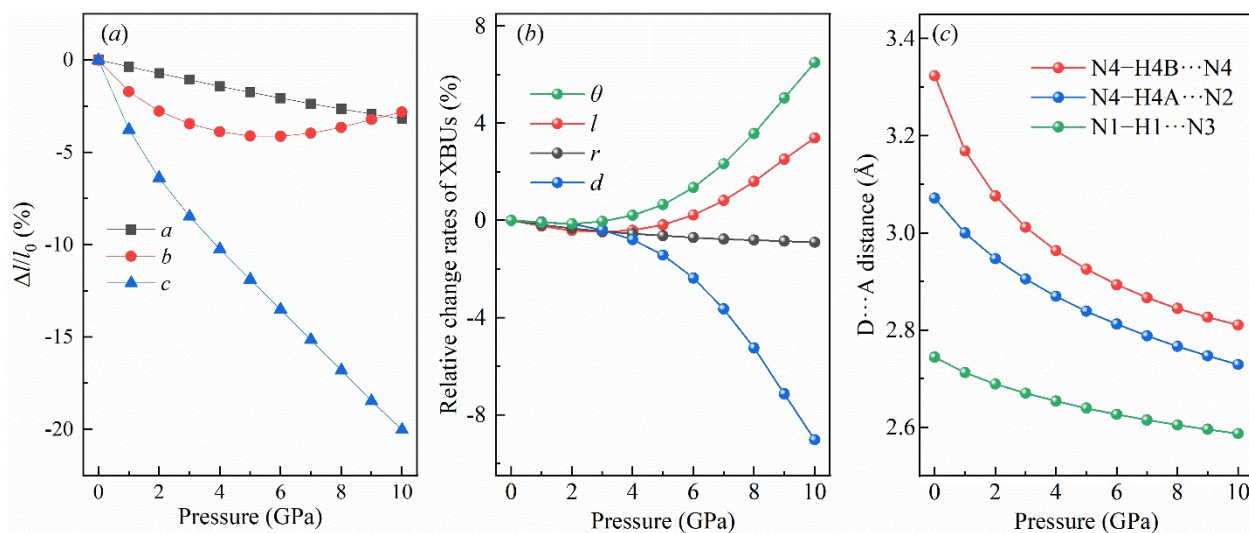Fig. S2. The 2D fingerprint of N-H distance in BATZM at 0 (left) and 6 GPa (right).

Fig. S3. Evolution of the relative change rate of (a) lattice parameters, (b) BBU parameters as a function of pressure. (c) Evolution of (b) D···A distance of hydrogen bonds as a function of pressure. All data are calculated by DFT-GGA without dispersion corrections.