Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Pressure-induced phase transition of 4-aminobenzonitrile: the formation and enhancement of N-H···N weak hydrogen bonds

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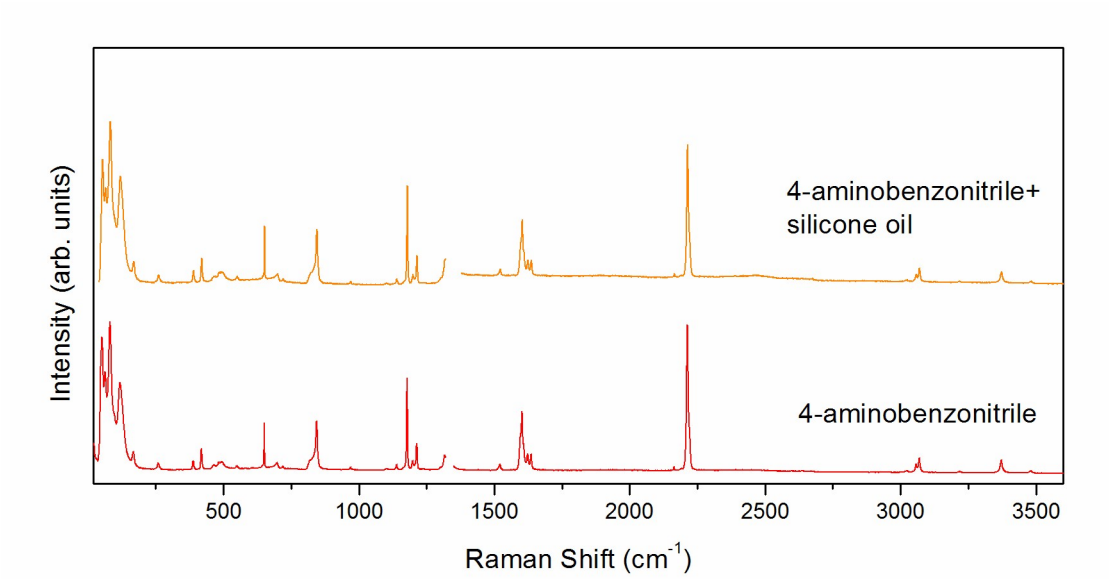

Fig. S1. The Raman spectra of 4-aminobenzonitrile and 4-aminobenzonitrile + silicone oil at 1 atm are same.

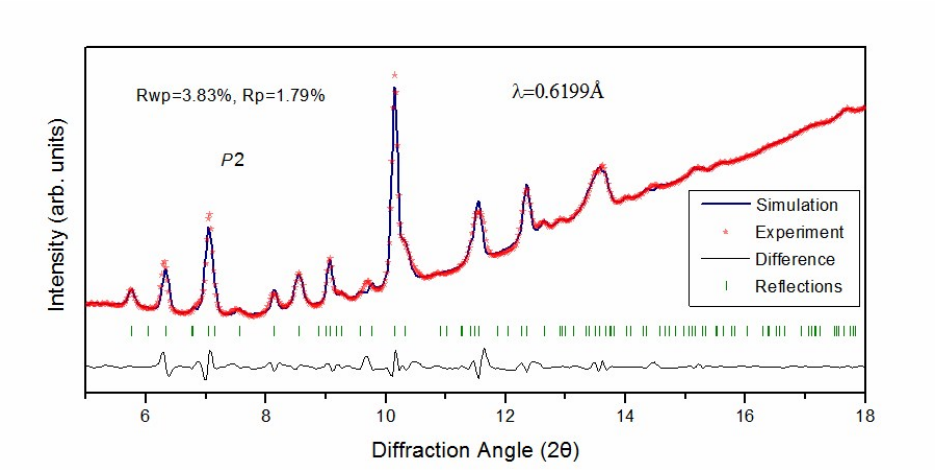

Fig. S2. Pawley refinements of the diffraction patterns collected at 1.6 GPa. Solid lines and asterisks represent the simulated and observed profiles, respectively.

Table S1 Lattice Parameters of 4-aminobenzonitrile at 1.6 GPa

symmetry	pressure (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	*β* (deg)
monoclinic	1.6	6.50(6)	12.30(9)	5.91(1)	107.90(9)

Table S2 Assignment of the Major Raman Bands of 4-Aminobenzonitrile

Frequency (cm^{-1})	Assignment
3480	$NH_2\nu_{as}$
3373	$NH_2\nu_s$
3070	CH stretching
3058	CH stretching
2211	C≡N stretching
1622	NH_2 scissoring
1601	ring C=C stretching
1519	ring C=C stretching
1436	ring C=C stretching
1334	ring C=C stretching
1314	ν_s(ph−N)
1299	ring CH in-plane bending
1212	ν_s(ph−CN)
1176	ring CH in-plane bending
1138	ring CH in-plane bending
965	ring CH out-plane bending
841	ring breathing
819	ring CH out-plane bending
718	ring CH out-plane def.
696	ring CCin-plane def.
650	ring CCin-plane def.
547	NH_2 wagging
481	NH_2 wagging
418	ring CC in-plane def.
387	ph−N in-plane bending

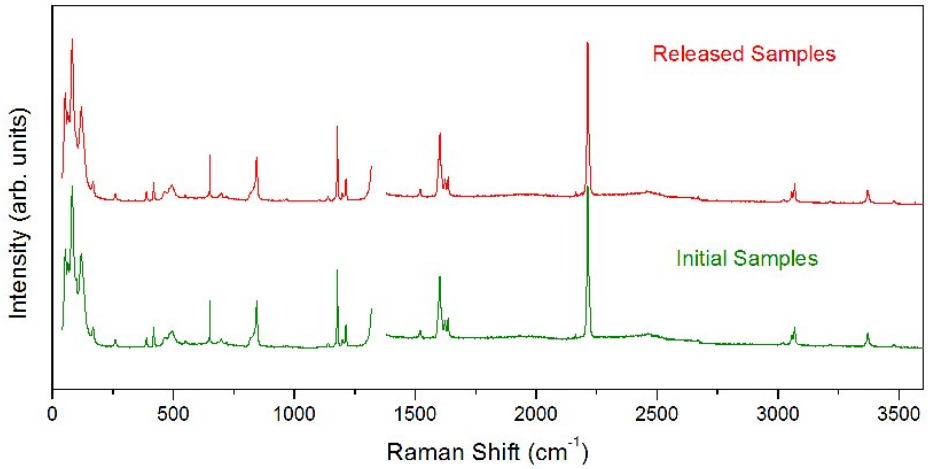

Fig. S3. Raman spectra of 4-aminobenzonitrile at 1 atm and the released samples.

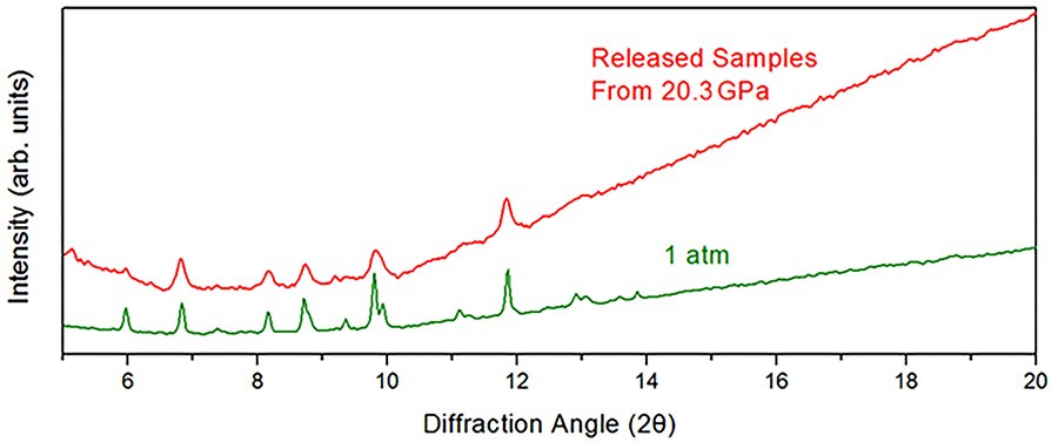

Fig. S4. Representative synchrotron XRD patterns of 4-aminobenzonitrile at 1 atm and the released samples from 20.3 GPa.

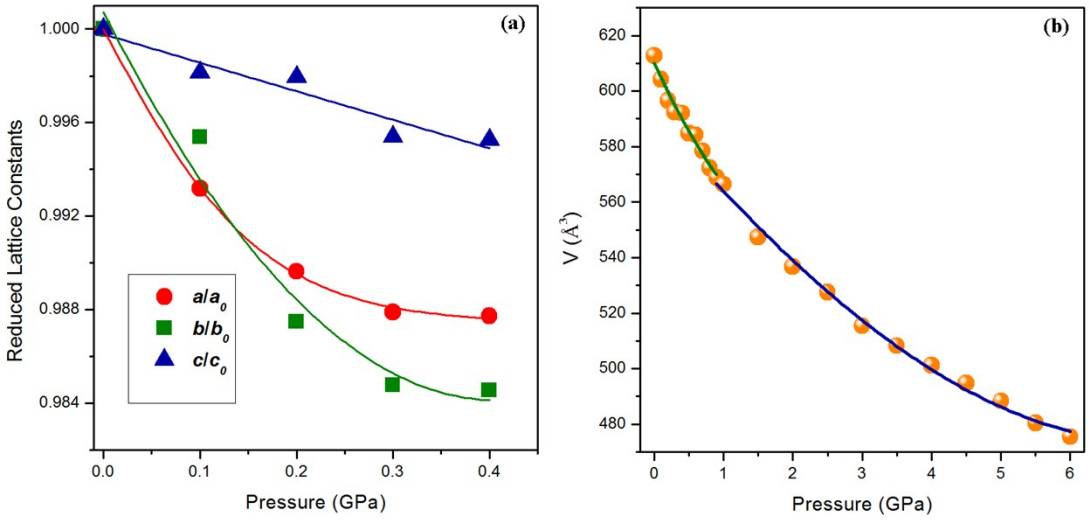

Fig. S5. (a) Reduced lattice constants of calculated results, (b) calculated unit cell volume as a function of pressure: The results of the second-order Birch-Murnaghan equation fitting on the calculated unit cell volume by the free online program PASCal from http://pascal.chem.ox.ac.uk/: V_0 = 610.33(3) Å^3, B_0 =11.18(1) GPa, B_0'= 4 (fixed) (0-0.9 GPa); V_0 = 590.43(8) Å^3, B_0 = 17.70(7) GPa, B_0'= 4 (fixed) (1.0-6.0 GPa).