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

Supplementary Information for

Phase transition and chemical reactivity of 1H-tetrazole under high pressure up to 100 GPa

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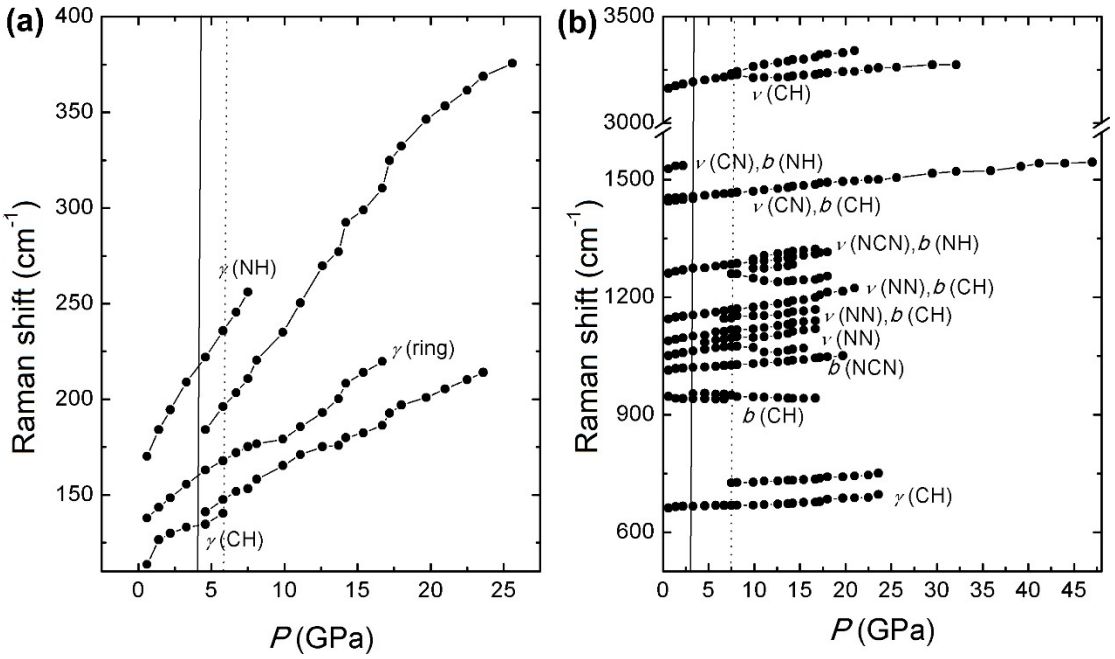

Figure S1. Raman frequency shifts of 1H-tetrazole as a function of pressure in the range of (a) 50-400 cm^{-1}and (b) 600-3500 cm^{-1}. Vertical solid line represents the beginning of phase transition and vertical dotted line represents the end of phase transition.

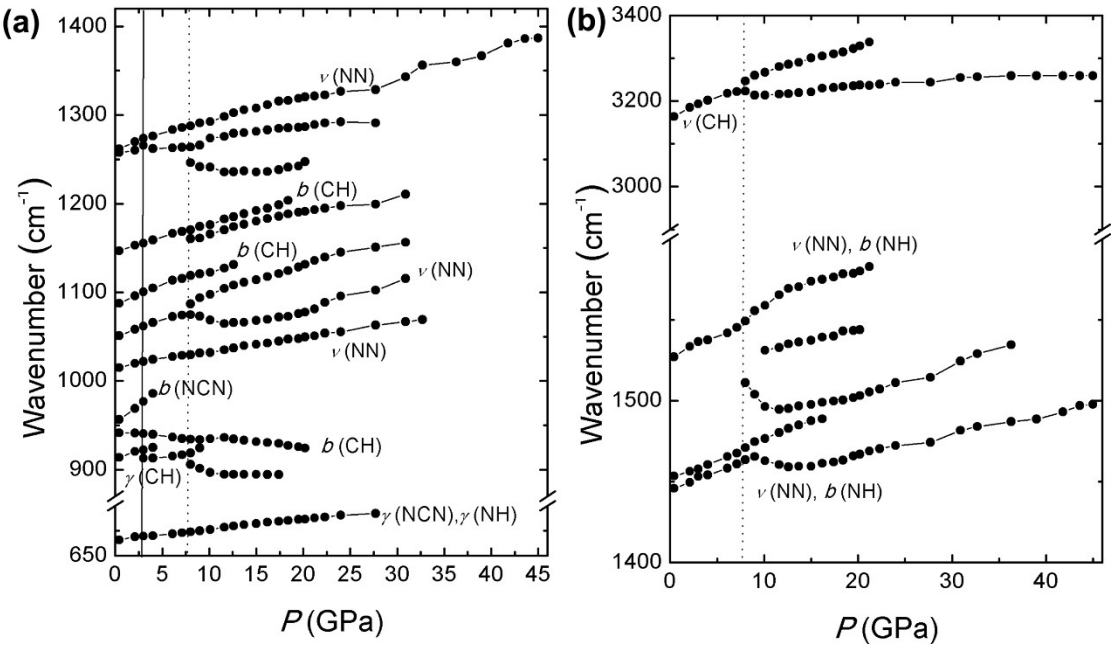

Figure S2. IR frequency shifts of 1H-tetrazole as a function of pressure in the range of (a) 600-1400 cm^{-1}and (b) 1400-3400 cm^{-1}. Vertical solid line represents the beginning of phase transition and vertical dotted line represents the end of phase transition.

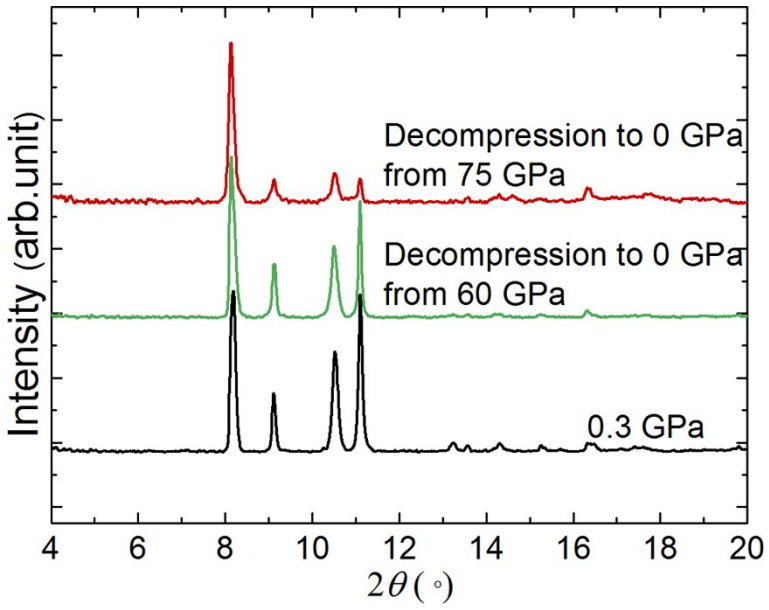

Figure S3. XRD patterns of the 1H-tetrazole recovered from high pressure. 1H-tetrazole undergoes a reversible phase transition process in compression-decompression cycle up to 60.0 and 75.0 GPa. The sample decompression from 75.0 GPa has strong orientation.

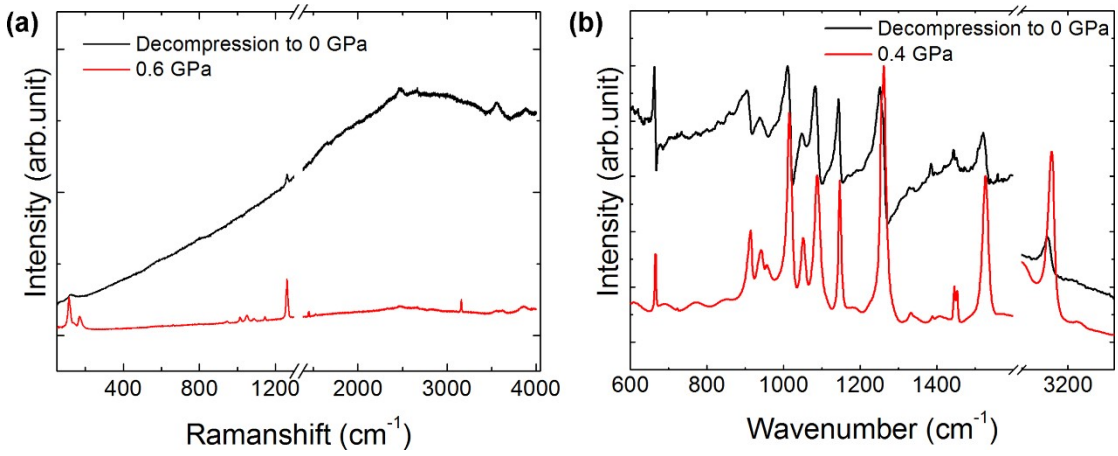

Figure S4. a) Raman and b) IR spectra of the 1H-tetrazole recovered from 100.3 GPa. As show in the IR spectra, the products after decompressing to ambient pressure from 100.3 GPa are still the 1H-tetrazole while strong background exists in Raman spectra.

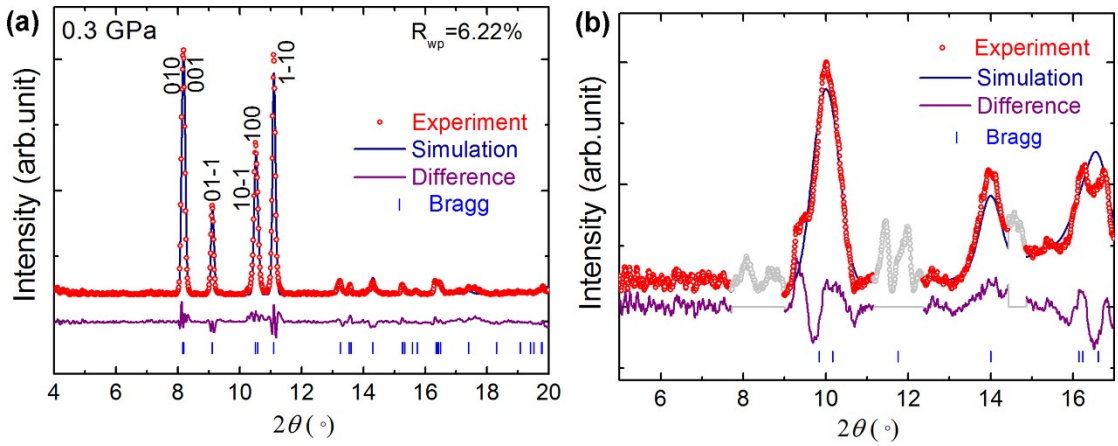

Figure S5. The Rietveld refinement results of the XRD patterns of phase I at 0.3 GPa and phase II at 100.3 GPa.

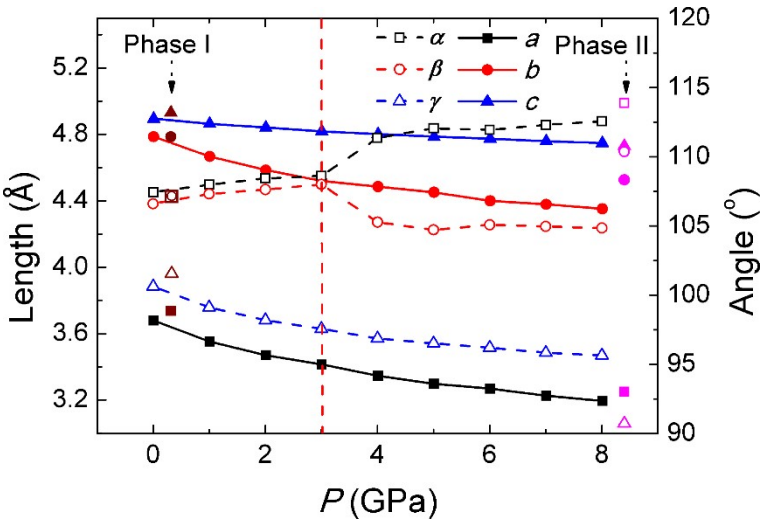

Figure S6. Optimized lattice parameters of phase I under high pressure. Above 4 GPa, the lattice parameters obviously change. The experimental data of phase I (0.3 GPa) and phase II (8.4 GPa) are also shown for comparison.

Table S1. Atomic coordinates in phase II at 10 GPa

Label	x	y	z
N1	0.1426	0.1672	0.8605
N2	0.3064	0.4268	0.8357

N3	0.3116	0.3460	0.5544
N4	0.1541	0.0383	0.3982
C5	0.0520	-0.0660	0.5963
D1	0.0942	0.1628	0.0124
H5	-0.0732	-0.2588	0.5479

Note: The uncertainty of the atomic coordinates is not provided by the software under the rigid body restrictions.

Table S2. Lattice parameters of phase II at 100.3 GPa and polymers obtained from XRD and simulation results, respectively

	100.3 GPa	Polymer 1	Polymer 2
a (Å)	2.567 (2)	2.591	2.361
b (Å)	3.691 (8)	3.355	3.673
c (Å)	3.825 (9)	4.577	4.038
α (°)	107.7 (4)	109.83	114.50
β (°)	95.67 (17)	117.91	89.84
γ (°)	92.95 (10)	94.76	93.89