Supplementary information

Crystal structure of anhydrous 5-aminotetrazole and its high-pressure behavior

Hiroshi Fujihisa,*[a] Kazumasa Honda,[a] Shigeaki Obata,[a] Hiroshi Yamawaki,[a]

Satoshi Takeya,[a] Yoshito Gotoh,[a] Takehiro Matsunaga [b]

[a] *Research Institute of Instrumentation Frontier (RIIF), National Institute of Advanced Industrial Science and Technology (AIST), AIST Tsukuba Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki, 305-8565, Japan*

[b] *Research Institute of Science for Safety and Sustainability (RISS), National Institute of Advanced Industrial Science and Technology (AIST), AIST Tsukuba Central 5, 1-1-1 Higashi, Tsukuba, Ibaraki, 305-8565, Japan*

Table S1. Numerical data for Fig. 4 (a-d).

(a) Lattice parameters and cell volume

P (GPa)	a (Å)	b (Å)	c (Å)	V (Å^3)
0.0	5.0900	3.6660	18.0740	337.3
0.6	5.0638	3.5549	17.9439	323.0
0.6	5.0641	3.5526	17.9409	322.8
1.5	5.0375	3.4607	17.8132	310.5
2.8	4.9963	3.3703	17.6909	297.9
3.7	4.9784	3.3181	17.6457	291.5
4.8	4.9624	3.2575	17.5375	283.5
6.3	4.9379	3.2054	17.4874	276.8
8.0	4.9040	3.1405	17.4292	268.4
11.6	4.8629	3.0809	17.2703	258.7

(b) Intramolecular distances (N-H)

P (GPa)	N6H8	N6H9	N1H7
0.0	1.0346	1.0404	1.0454
0.6	1.0353	1.0405	1.0460
0.6	1.0352	1.0406	1.0459
1.5	1.0358	1.0408	1.0466
2.8	1.0370	1.0407	1.0481
3.7	1.0373	1.0411	1.0488
4.8	1.0372	1.0418	1.0494
6.3	1.0377	1.0420	1.0504
8.0	1.0386	1.0417	1.0522
11.6	1.0391	1.0422	1.0548

(c) Intramolecular distances (N-N, C-N)

P (GPa)	N2N3	C5N6	C5N1	C5N4	N1N2	N3N4
0.0	1.3132	1.3379	1.3562	1.3566	1.3656	1.3710
0.6	1.3130	1.3372	1.3557	1.3561	1.3651	1.3706
0.6	1.3131	1.3372	1.3557	1.3561	1.3652	1.3706
1.5	1.3128	1.3364	1.3548	1.3555	1.3642	1.3700
2.8	1.3125	1.3352	1.3540	1.3545	1.3630	1.3696
3.7	1.3121	1.3343	1.3534	1.3541	1.3621	1.3690
4.8	1.3118	1.3330	1.3525	1.3537	1.3611	1.3681
6.3	1.3114	1.3318	1.3517	1.3530	1.3599	1.3675
8.0	1.3109	1.3304	1.3508	1.3519	1.3585	1.3667
11.6	1.3100	1.3280	1.3491	1.3504	1.3561	1.3651

(d) Hydrogen bond distances (H...N)

P (GPa)	H9...N4	H8...N4	H7...N2	H7...N3
0.0	1.9226	2.0033	2.0522	2.1916
0.6	1.9262	2.0007	2.0774	2.1760
0.6	1.9150	1.9769	2.0847	2.1316
1.5	1.9134	1.9789	2.0907	2.1297
2.8	1.8977	1.9542	2.0815	2.0923
3.7	1.8789	1.9215	2.1099	2.0220
4.8	1.8629	1.9078	2.0981	1.9991
6.3	1.8394	1.8971	2.0741	1.9830
8.0	1.8234	1.8776	2.0708	1.9488
11.6	1.8071	1.8513	2.1022	1.8929