

Supplementary Material to the article
“First principles calculations of phase stability in the N-H system at
pressures to 1.5 TPa”

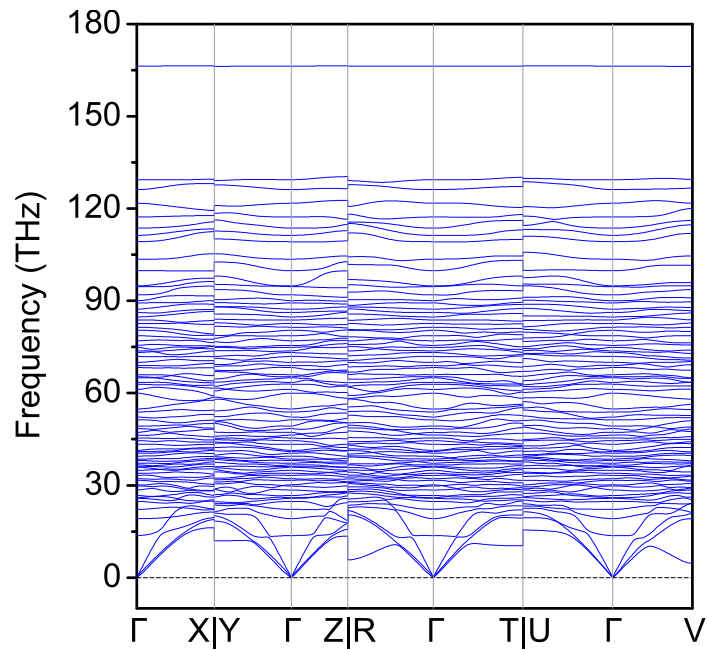


Fig. S1. Phonon spectrum of N_3H_{10} - $P1$ at 800 GPa.

Table S1. Crystal structure data for new NH phases at 1 TPa.

| Space group | Unit cell parameters (Å, degree) | | | Atom | Coordinates | | |
|-------------------|----------------------------------|--------------|---------------|------|-------------|--------|--------|
| | | | | | x | y | z |
| $P4_122$ (#91) | $a = 2.0273$ | $b = 2.0273$ | $c = 3.5145$ | N | 0.5 | 0.7998 | 0 |
| | $\alpha = 90$ | $\beta = 90$ | $\gamma = 90$ | H | 0.8534 | 0.8534 | 0.3750 |
| $P4_322$ (#95) | $a = 2.0273$ | $b = 2.0273$ | $c = 3.5145$ | N | 0.5 | 0.7998 | 0 |
| | $\alpha = 90$ | $\beta = 90$ | $\gamma = 90$ | H | 0.8534 | 0.8534 | 0.6250 |

Table S2. Crystal structure data for new N₃H₁₀ phase at 1 TPa.

| Space group | Unit cell parameters (Å, degree) | | | Atom | Coordinates | | |
|----------------|----------------------------------|-------------------|-------------------|------|-------------|----------|----------|
| | | | | | <i>x</i> | <i>y</i> | <i>z</i> |
| <i>P1</i> (#1) | <i>a</i> = 3.2090 | <i>b</i> = 3.2220 | <i>c</i> = 3.9039 | N | 0.84231 | 0.47315 | 0.85333 |
| | <i>α</i> = 77.80 | <i>β</i> = 77.97 | <i>γ</i> = 60.56 | N | 0.59506 | 0.22781 | 0.31639 |
| | | | | N | 0.2152 | 0.85728 | 0.5746 |
| | | | | N | 0.5082 | 0.15002 | 0.82024 |
| | | | | N | 0.88981 | 0.52157 | 0.54281 |
| | | | | N | 0.13614 | 0.76788 | 0.08179 |
| | | | | H | 0.49328 | 0.64114 | -0.09371 |
| | | | | H | 0.21701 | 0.72621 | 0.31762 |
| | | | | H | 0.64405 | 0.16974 | 0.07575 |
| | | | | H | 0.67746 | 0.42108 | 0.49267 |
| | | | | H | 0.82925 | 0.74735 | 0.17502 |
| | | | | H | -0.07909 | 0.06049 | 0.4107 |
| | | | | H | 0.67925 | 0.49846 | 0.18974 |
| | | | | H | 0.24851 | 0.37928 | 0.47142 |
| | | | | H | 0.56511 | 0.77099 | 0.23102 |
| | | | | H | 0.09118 | 0.34589 | 0.23771 |
| | | | | H | 0.11494 | 0.16982 | 0.15874 |
| | | | | H | 0.45792 | -0.05408 | 0.03349 |
| | | | | H | 0.36721 | 0.02537 | 0.38028 |
| | | | | H | 0.29816 | 0.4356 | -0.00789 |
| | | | | H | 0.35047 | 0.01589 | 0.70227 |
| | | | | H | 0.85454 | 0.02484 | 0.71339 |
| | | | | H | 0.01236 | 0.11227 | -0.0723 |
| | | | | H | 0.34617 | 0.51628 | 0.68565 |
| | | | | H | -0.04697 | 0.67998 | 0.89364 |
| | | | | H | 0.72996 | 0.8619 | 0.48833 |