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


# Supplementary Information for

# Prediction of a reservoir of N-rich high-energy density material at the Earth's mantle

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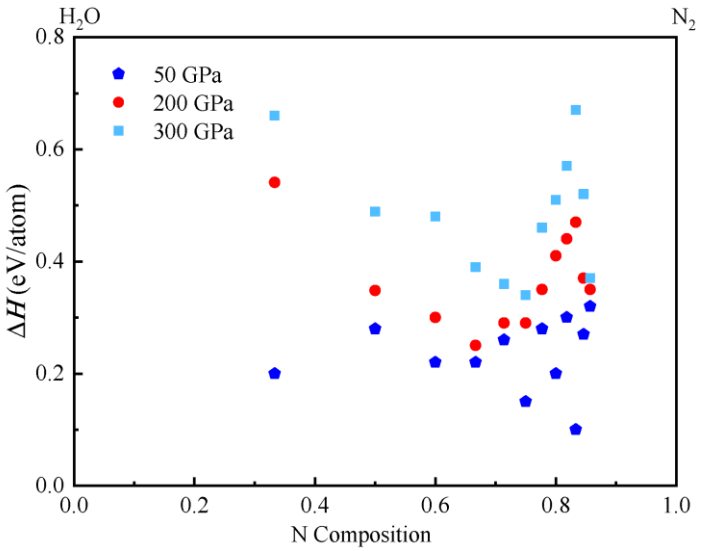


Fig. S1. Calculated formation enthalpies of $H_2O(N_2)_x$ ($x$=0.25, 0.5, and 1-6) compounds relative to solid $H_2O$ and $N_2$ at 50, 200 and 300 GPa. Calculations considered all ground states of solid $H_2O$ and $N_2$ at different pressures: X phase of $H_2O$ at 0-280 GPa; *Pbcm* phase of $H_2O$ at 280-300 GPa; ε phase of $N_2$ at 0-120 GPa; $I2_13$ phase of $N_2$ at 120-195 GPa; *Pba*2 phase of $N_2$ at 195-275 GPa; $I\bar{4}3m$ phase of $N_2$ at 275-300 GPa.

Table S1. **Structure Parameters.** The structural parameters of $H_2ON_{10}$ and $H_2ON_6$.

| Crystal structure | Pressure | Space group | Lattice parameters | Wyckoff position |
|---|---|---|---|---|
| $H_2ON_{10}$ | 100 GPa | *P*1 | *a* = 3.7886 Å | N1:1*a* (0.40887, 0.15619, 0.20540) |
| | | | *b* = 4.0792 Å | N2:1*a* (0.93521, 0.94154, 0.88580) |
| | | | *c* = 4.8578 Å | N3:1*a* (0.46401, 0.83800, 0.69493) |
| | | | *α* = 112.336 ° | N4:1*a* (0.02805, 0.65341, 0.89542) |
| | | | *β* = 84.263 ° | N5:1*a* (0.19834, 0.05252, 0.75844) |
| | | | *γ* = 90.803 ° | N6:1*a* (0.85065, 0.24075, 0.44572) |
| | | | | N7:1*a* (0.57505, 0.41544, 0.16805) |
| | | | | N8:1*a* (0.36736, 0.60072, 0.79273) |
| | | | | N9:1*a* (0.58857, 0.03928, 0.35350) |
| | | | | N10:1*a* (0.84562, 0.47137, 0.32123) |
| | | | | H1:1*a* (0.09829, 0.17171, 0.61388) |
| | | | | H2:1*a* (0.53743, 0.49813, 0.98033) |
| | | | | O1:1*a* (0.06923, 0.68770, 0.33573) |
| $H_2ON_6$ | 100 GPa | *P*1 | *a* = 2.65446 Å | N1:4*a* (0.87185, 0.29186, 0.45009) |
| | | | *b* = 4.06144 Å | N2:4*a* (0.41866, 0.72248, 0.21343) |
| | | | *c* = 4.34679 Å | N3:4*a* (0.67294, 0.55060, 0.47271) |
| | | | *α* = 81.35 ° | N4:4*a* (0.48144, 0.68209, 0.93653) |
| | | | *γ* = 108.57 ° | N5:4*a* (0.10706, 0.13318, 0.73883) |
| | | | *β* = 95.95 ° | N6:4*a* (0.30332,0.88765, 0.68785) |
| | | | | H1:4*a* (0.63266, 0.46131, 0.92706) |
| | | | | H2:4*a* (0.22967, 0.93517, 0.23339) |
| | | | | O1:4*a* (0.93014, 0.20588, 0.18895) |

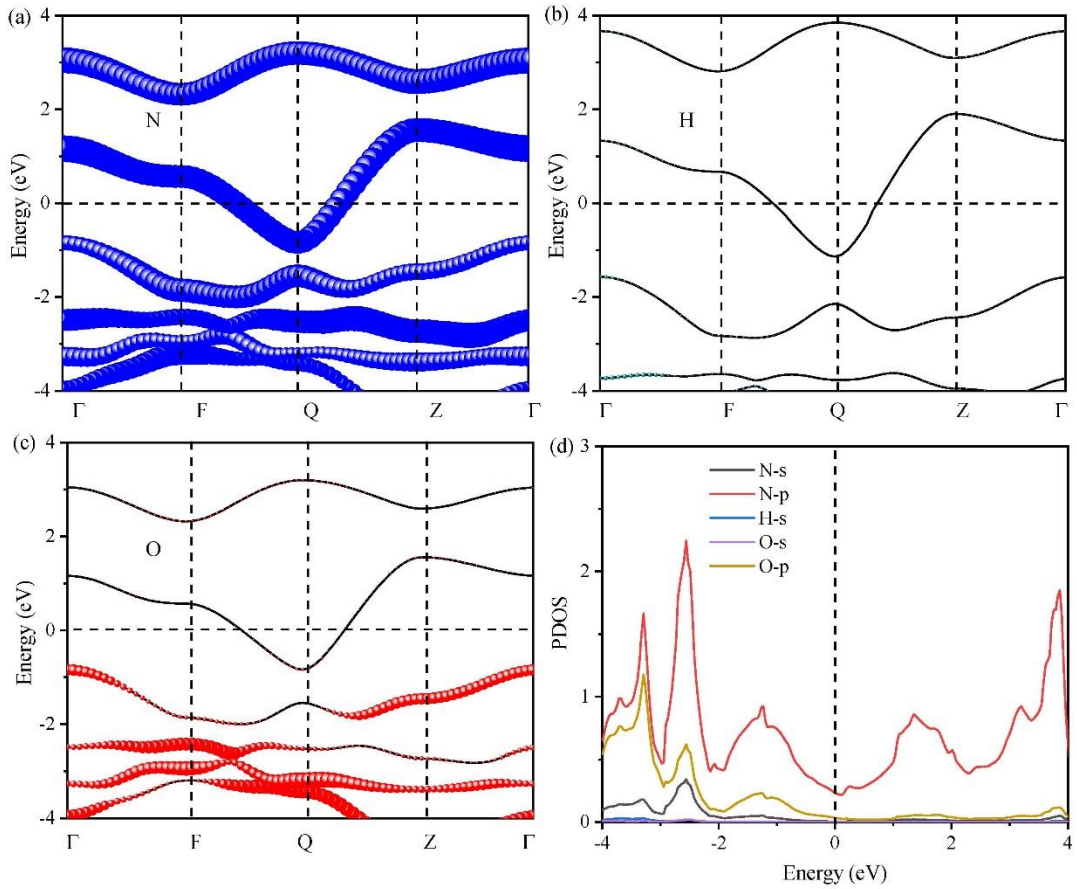


Fig. S2. The band structures of $H_2ON_6$ projected onto different atomic orbitals (a) N, (b) H and (c) O atoms, respectively, at 100 GPa. (d) Projected density of states (PDOS) of $H_2ON_6$ at 100 GPa.

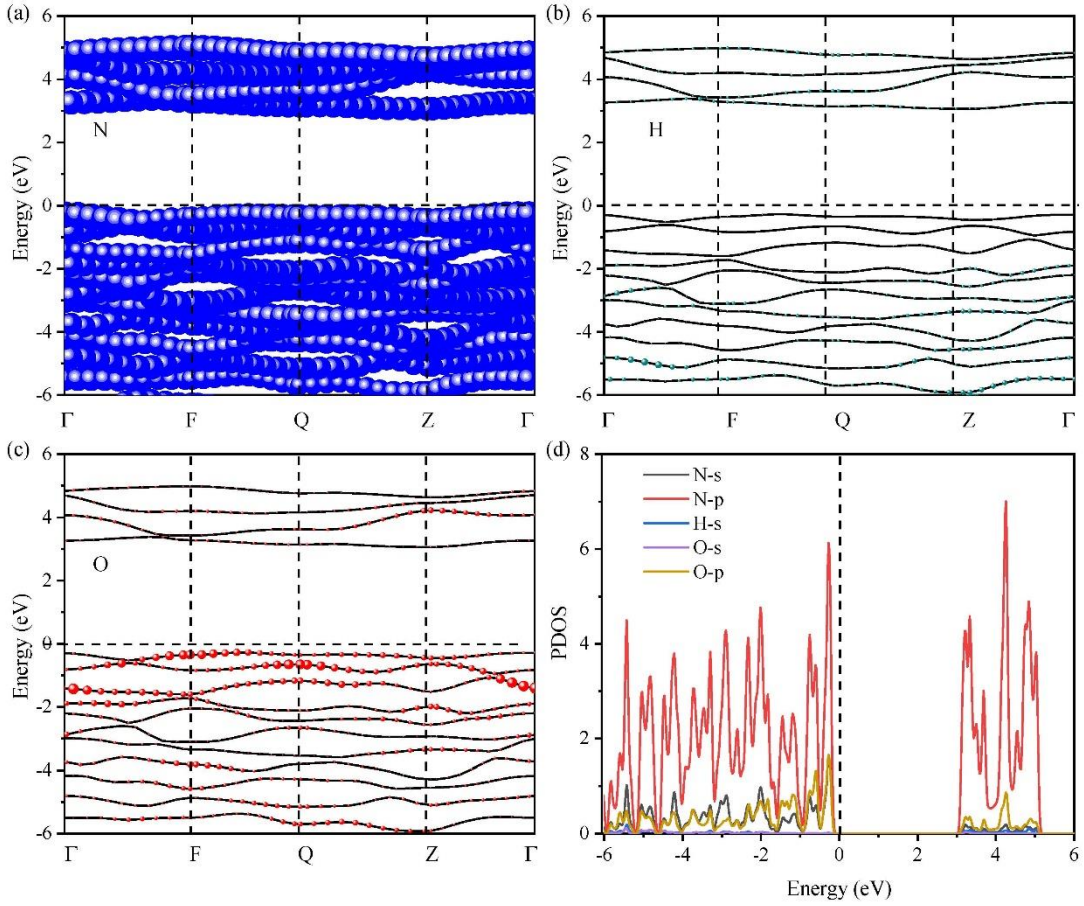


Fig. S3. The band structures of $H_2ON_{10}$ projected onto different atomic orbitals (a) N, (b) H and (c) O atoms, respectively, at 100 GPa. (d) Projected density of states (PDOS) of $H_2ON_{10}$ at 100 GPa.

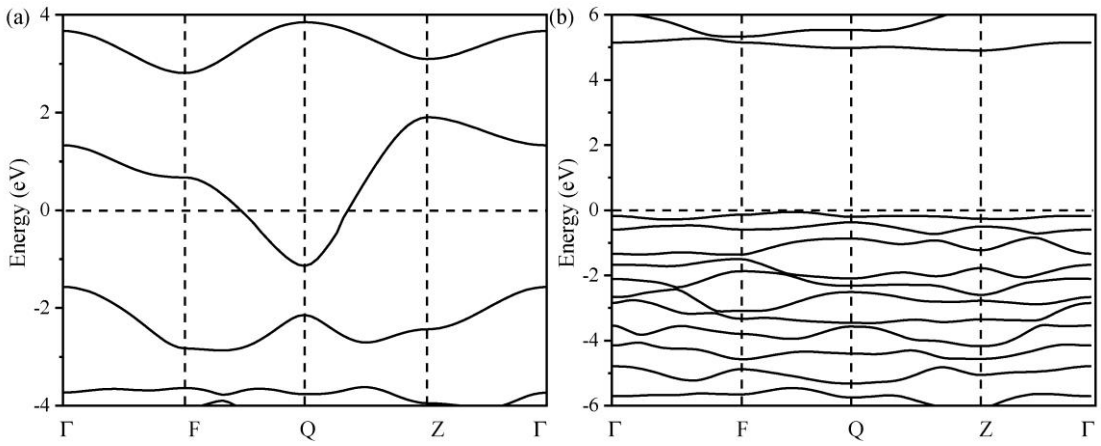


Fig. S4. Electronic band structures (HSE06) of (a) $H_2ON_6$ and (b) $H_2ON_{10}$ at 100 GPa.

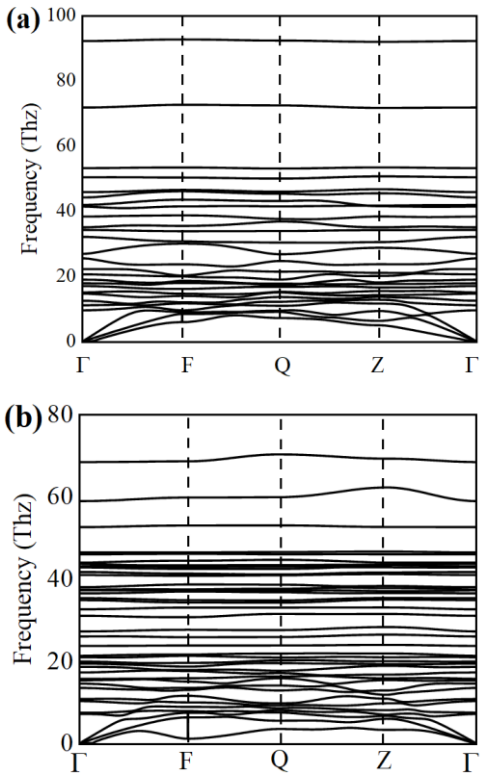


Fig. S5. Calculated phonon dispersions for (a) $H_2ON_6$ and (b) $H_2ON_{10}$ at 100 GPa.

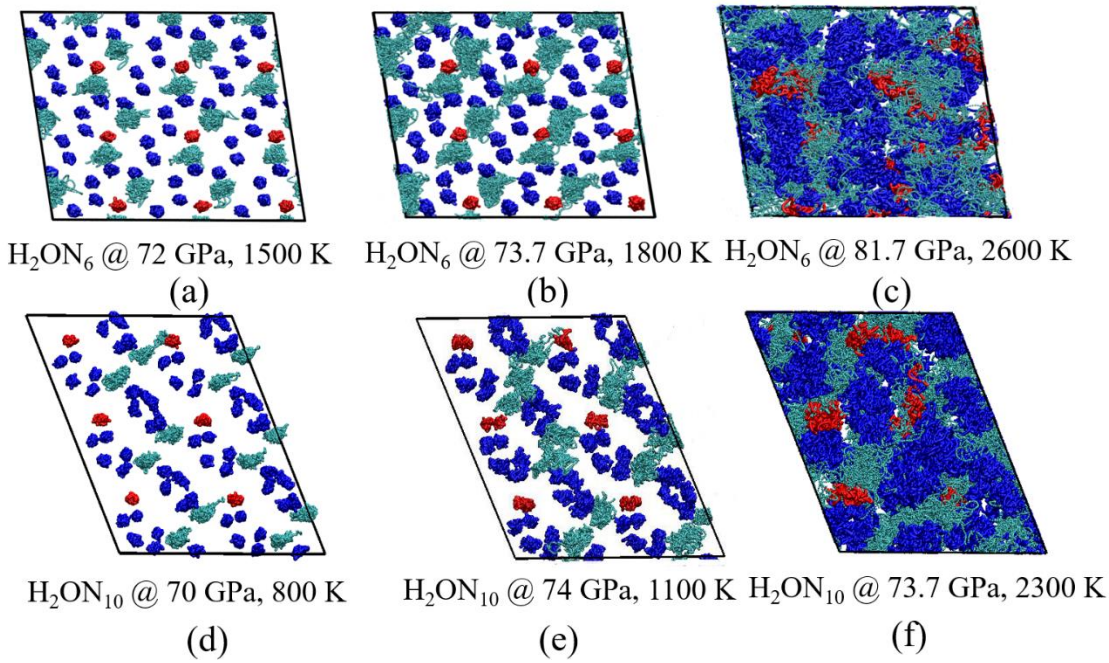


Fig. S6. The atomic trajectories of the atomic positions of $H_2ON_6$ (upper panel) at (a) 72 GPa and 1500 K, (b) 73.7 GPa and 1800 K, (c) 81.7 GPa and 2600 K and $H_2ON_{10}$ (lower panel) at (d) 70 GPa and 800 K, (e) 74 GPa and 1100 K and (f) 73.7 GPa and 2300 K.

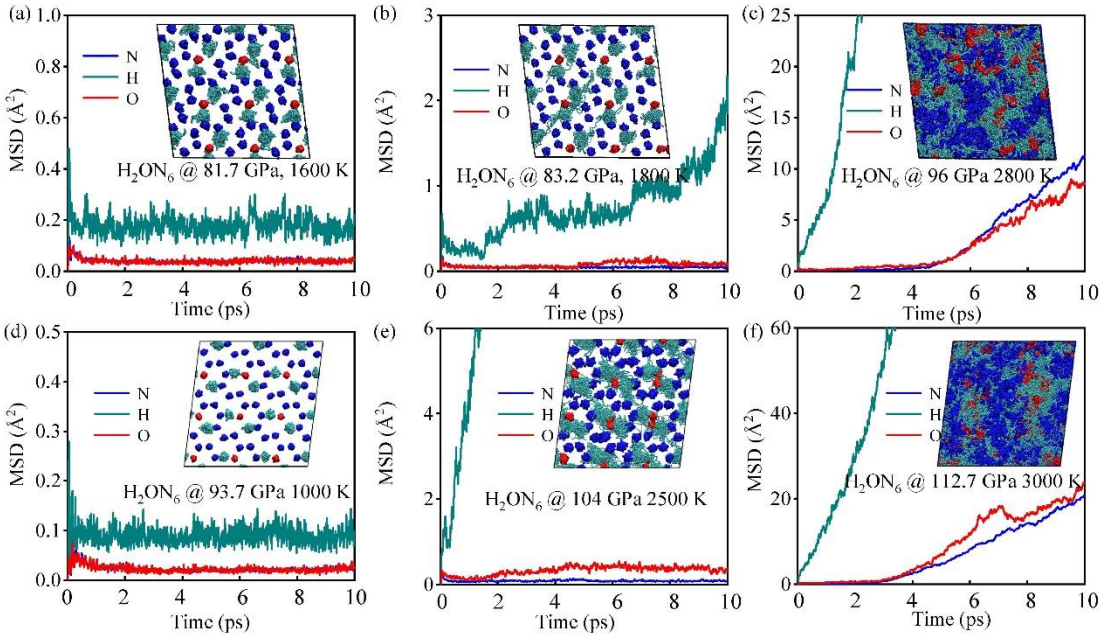


Fig. S7. The calculated mean squared displacement (MSD) and atomic trajectories (inset) of the atomic positions of $H_2ON_6$ phase. (a)-(f) represent MSD at 81.7 GPa, 83.2 GPa, 96 GPa, 93.7 GPa, 104 GPa and 112.7 GPa and different temperatures.

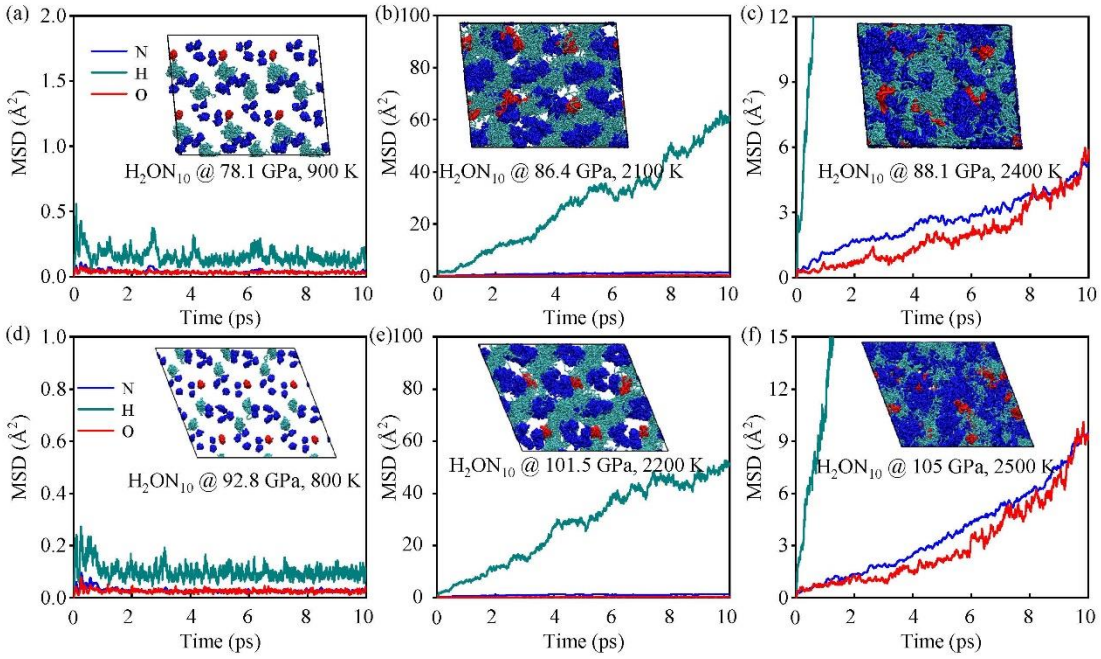


Fig. S8. The calculated MSD and atomic trajectories (inset) of the atomic positions of $H_2ON_{10}$ phase (a)-(f) represent MSD at 78.1 GPa, 86.4 GPa, 88.1 GPa, 92.8 GPa, 101.5 GPa and 105 GPa and different temperature.

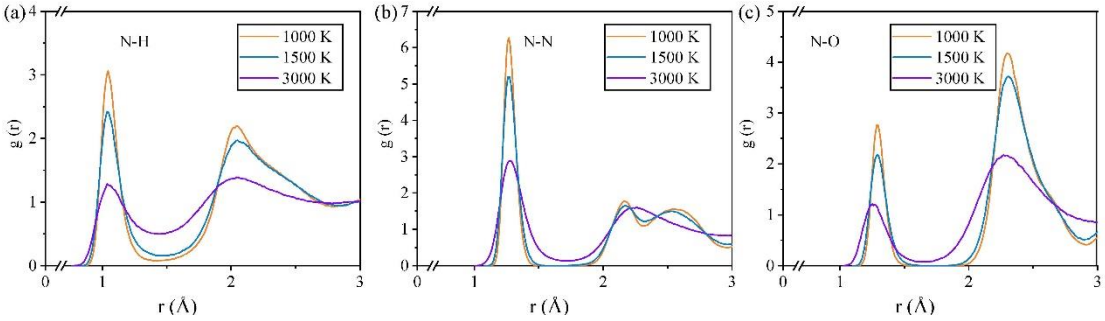


Fig. S9. The radial distribution functions (RDFs) for a N-H, (b) N-N and (c) N-O of $H_2ON_6$ at different temperatures at 100 GP

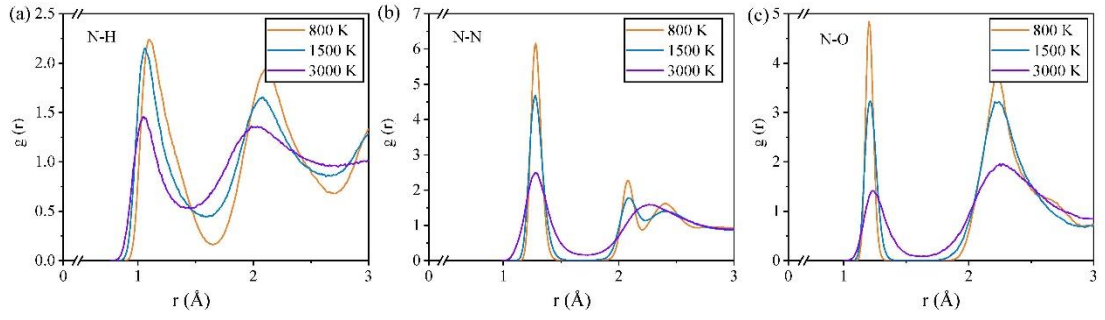


Fig. S10. The RDFs for a N-H, (b) N-N and (c) N-O of $H_2ON_{10}$ at different temperatures at 100 GPa.

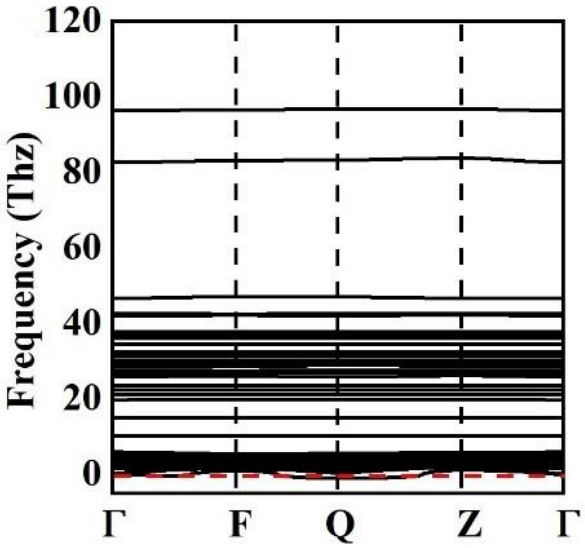


Fig. S11. Phonon dispersion of structure of $H_2ON_{10}$ at 0 GPa.