# Pressure Effects on the Thermal Decomposition of LLM-105 Crystal

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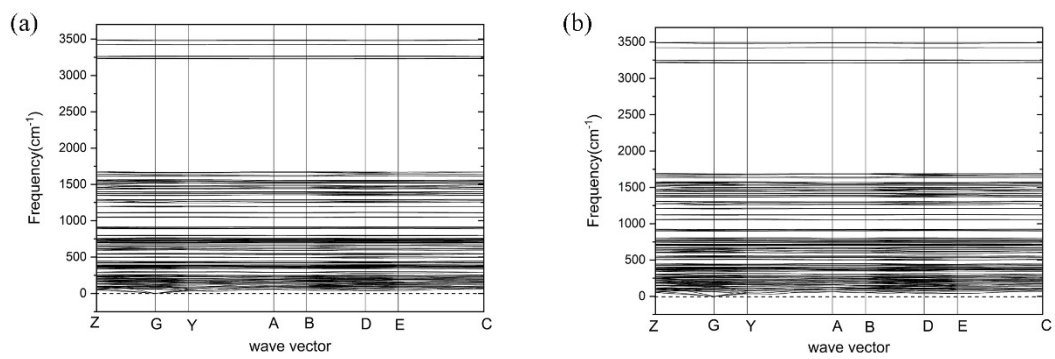
Figure S1. Phonon spectra of LLM-105 at high pressures of (a) 6.0GPa (b) 10.2GPa. There is no imaginary phonon mode in the whole Brillouin zone so it is dynamically stable for the initial high pressure structure
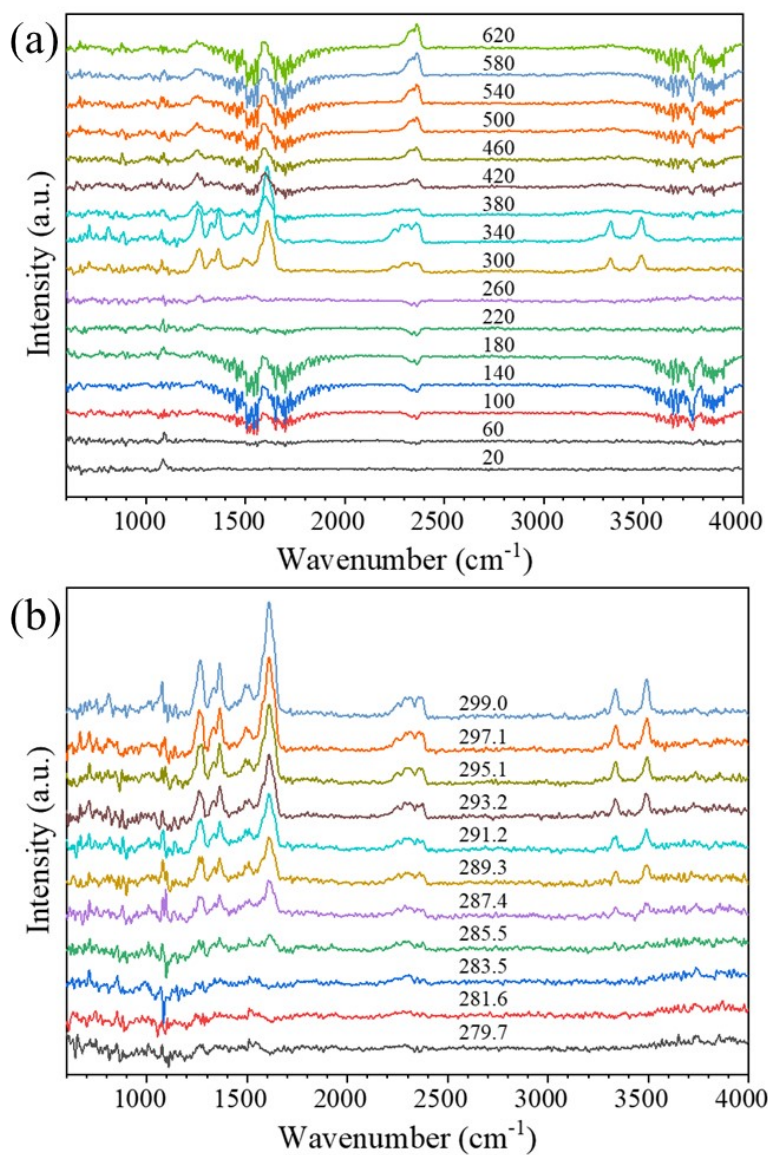
Figure S2. The IR spectra of LLM-105 decomposition products at ambient pressure. IR spectra from (a) 20°C to 600°C (b) 279°C to 300°C. IR absorptions for the decomposition products occur around 300 °C
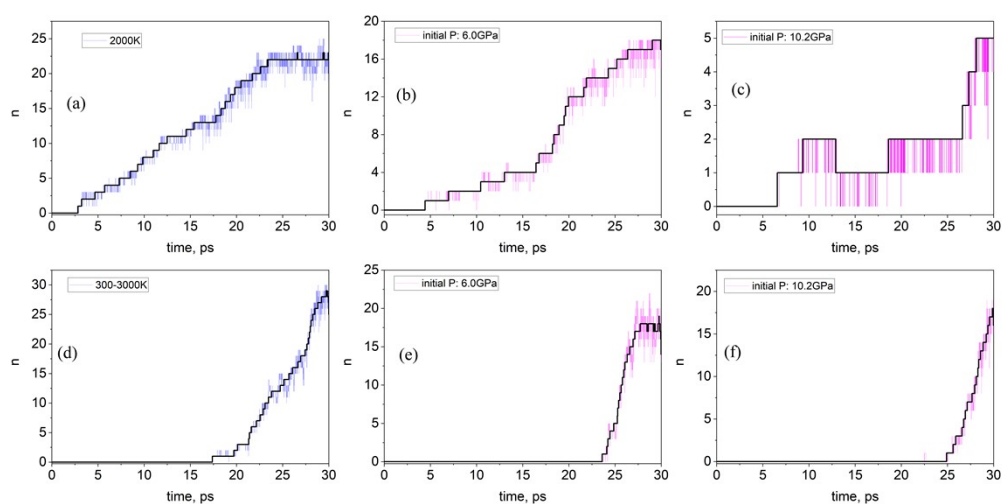
Figure S3. Evolution of the number of intermediate NO molecules under various conditions. (a-c) Constant temperature of 2000 K at different initial pressures, 0 GPa, 6.0 GPa and 10.2 GPa; (d-f) Program heating of 300-3000 K at different initial pressures, 0 GPa, 6.0 GPa and 10.2 GPa. The tendency of NO under HP-HT is the same as H_2O as a final product. High pressure impedes the production of NO at high temperatures.
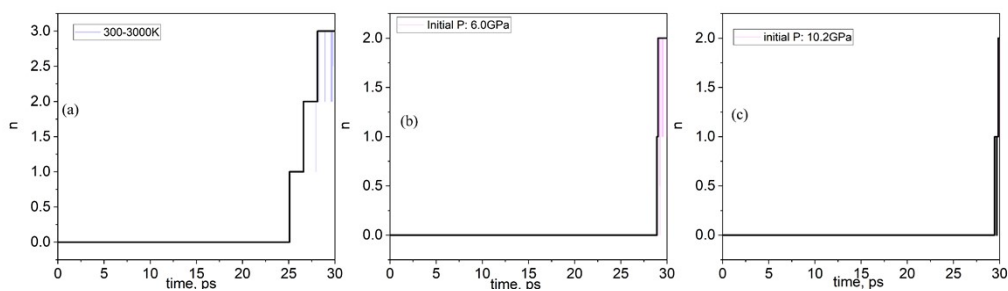
Figure S4. Evolution of the number of intermediate N_2 molecules under various conditions. (a-c) Program heating of 300-3000 K at different initial pressures, 0 GPa, 6.0 GPa and 10.2 GPa. N_2 occurs at relatively high temperature, so there is no N_2 at 2000K of different initial pressures. High pressure also impedes the final production of N_2.
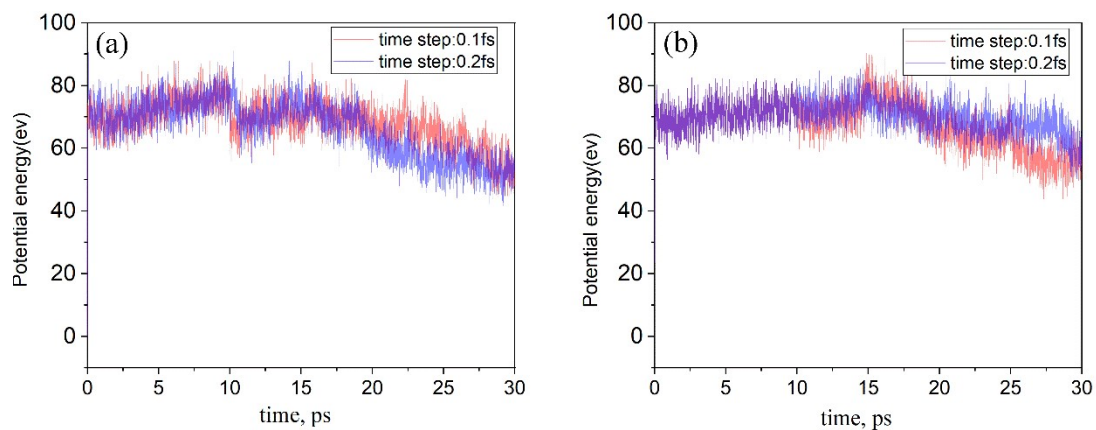
Figure S5. Evolution of potential energy at different time step (a-b) constant temperature of 2000 K at different initial pressures of 6.0 GPa, 10.2 GPa. As shown in the figure, the potential energy at time step of 0.1fs is the same as that at the time step of 0.2fs. Although at the end of the simulation time, there exists minor accumulation of numerical errors, the tendency of two curves always keep the same. Except for the potential energy, the 0.1 fs time step calculations show the initial decomposition mechanisms and the evolution of major chemical species were almost the same as we discussed with the step time of 0.2 fs. Considering the computational cost, we choose 0.2 fs as the time step.
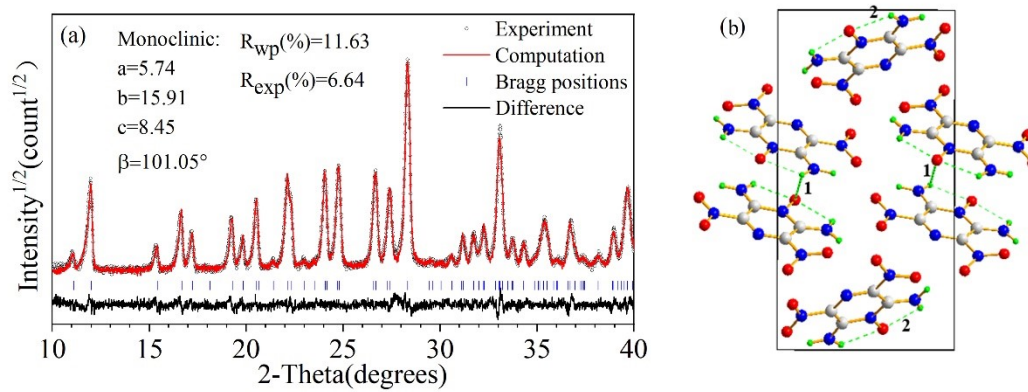
Figure S6. Results of refined XRD patterns of LLM-105 crystal at ambient pressure.
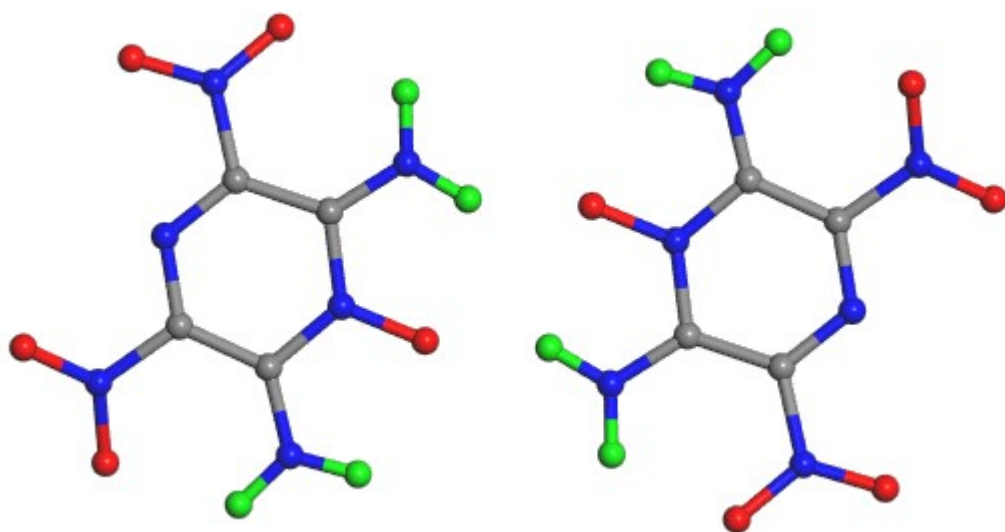
(see more in attached file SV1.gif)

Figure S7. The sketch map of intermolecular hydrogen transfer process under HP-HT.