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High Pressure Synchrotron X-ray diffraction and Raman Scattering Studies of Ammonium Azide HONGYANG ZHU, XIAOXIN WU, HANG CUI, JIAN ZHANG, RIDONG CONG, QILIANG CUI, Jilin University — Highpressure in situ X-ray powder diffraction and Raman scattering studies on NH₄N₃ have been conducted up to 50.5 GPa and 48 GPa, respectively. The compressibility of orthorhombic phase is isotropic due to the orientation of azide anions. The hydrogen bonding weaken with increasing pressure due to the bending of N-H···N bonding, leading to the increase of N-H stretch frequency and rotation of azide anions at 2b and 4h Wyckoff positions up to 2.9 GPa. The rotation of azide anions obviously influences the intermolecular interactions along c axis in orthorhombic phase. The pressure induced phase transition involves a proximity of a and c, temporally assigned as a reversible second-order orthorhombic-to-tetragonal transition. The bulk modulus of the orthorhombic phases are determined to be $K_{OT} = 24.5\pm3.5$ GPa with $K'_{OT} = 3.4\pm3.2$.

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