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Pressure-Induced Irreversible Phase Transition in the Energetic Material Urea Nitrate[1] SHOURUI LI, BO ZOU, State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China — The behavior of energetic material Urea Nitrate ($(NH_2)_2COH^+ \cdot NO_3^-$, UN) has been investigated up to the pressure of ∼26 GPa. UN exhibits the typical supramolecular structure with uronium cation and nitrate anion held together by multiple hydrogen bonds in the layer. Both Raman and XRD data provide obvious evidence for the distorted phase transition in the pressure range ∼9–15 GPa. Further analysis indicates phase II has Pc symmetry. The mechanism for the phase transition involves collapse of the initial 2D supramolecular structure to 3D hydrogen-bonded networks in phase Pc. Importantly, the transition is irreversible and leads to a large reduction in volume on release of pressure. The density in phase Pc has been increased by ∼11.8% compared to the phase $P2_1/c$ under ambient conditions and therefore phase Pc is expected to have much higher detonation power. This study opens new opportunities for preparing energetic materials with high density combining supramolecular chemistry with high-pressure techniques. Corresponding author. E-mail: zoubo@jlu.edu.cn Reference: JPCC. 2013, 117, 152.

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