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Near-Equivalency of Inter and Intramolecular Hydrogen Bonding Under High-Pressure M. RIAD MANAA, LAURENCE FRIED, Lawrence Livermore National Laboratory — Triamino-trinitro-benzene (TATB, $C_6H_6N_6O_6$) exhibits unusually strong intramolecular hydrogen bonding as evidenced by the high rotational energy barrier of the nitro and amino groups. In the condensed phase, the competing intermolecular hydrogen bonding becomes pronounced at high-pressure in its graphitic-like crystal structure. We report density functional theoretical calculations of the equation of state of TATB under hydrostatic compression of up to 250 GPa. Our results show Our results show increasing bond equivalency between the intramolecular and intermolecular hydrogen bonds of the amino and nitro groups in the region 30<P<70 GPa, beyond which the difference between the two bond distances remains constant. This approximate bond equivalency is manifested by a rapid decrease of the intermolecular -NO—HN- distance along the b lattice direction from 2.6 Å at the zero pressure equilibrium geometry to 1.72 Å at 67 GPa, and by a decrease of the intramolecular -NO—HN- bond from 1.65 Å to 1.57 Å for the same pressure region. It is expected that vibrational motions involving the NO—HN modes are sensitive to the nearly equivalent hydrogen bonding, as recent spectroscopic IR analysis of the NH_2 stretches revealed.

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