

# High-pressure crystal structure of *n*-hexylamine

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*n*-Hexylamine (HA), a primary aliphatic amine, was studied under high-pressure conditions using single-crystal X-ray diffraction. A single crystal was grown at ambient temperature in a diamond-anvil cell, and the crystal structure of HA was determined from its freezing pressure up to 1.40 GPa. The structure remains orthorhombic (space group  $Pca2_1$ ), identical to that reported at low temperature and ambient pressure [1], making HA the first *n*-amine in which the crystal symmetry remains unchanged between low-temperature and high-pressure conditions. The HA crystal structure is dominated by infinite chains of NH $\cdots$ N hydrogen bonds; however, no CH $\cdots$ N hydrogen bonds were observed, even at 1.40 GPa. This behavior differs from that of other *n*-amines (from methylamine to *n*-pentylamine) [2, 3], where high pressure favors such interactions. Only at 1.40 GPa does the first intermolecular H $\cdots$ H distance become shorter than the sum of the van der Waals radii of two hydrogen atoms. This observation correlates with the presence of crystal voids around the methyl groups at the ends of the aliphatic chains.

[1] Maloney, A. G. P., Wood, P. A. & Parsons, S. (2014). *CrystEngComm.*, **16**, 3867.

[2] Podsiadło, M., Olejniczak, A. & Katrusiak, A. (2017). *Cryst. Growth Des.*, **17**, 2218.

[3] Sacharczuk, N., Olejniczak, A., Bujak, M. & Podsiadło, M. (2023). *Cryst. Growth Des.*, **23**, 7119.

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