

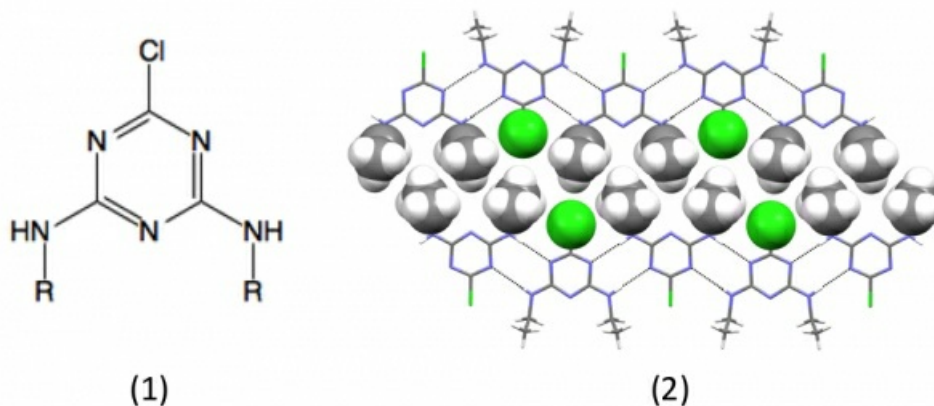
*Crystal engineering of self-complementary NH...N chloro-triazine tapes*

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Self-complementary hydrogen-bonded systems such as the O-H...O carboxylic acid dimer are well known supramolecular synthons for crystal engineering [1]. Here we explore a self-complementary system using N-H...N hydrogen-bonds formed by the chloro-s-triazine (1), a heterocyclic system that includes the ubiquitous herbicides atrazine and simazine. These compounds have emerged as robust supramolecular components that form NH...N hydrogen-bonded tapes such as (2) in the solid state. A search of the CCDC reveals numerous examples of (1) assembling into variants of the tape where morphology is dependent on the size and shape of the nitrogen R-groups [2]. Based on this behaviour, we proposed that simple N-alkyl derivatives of (1) would be promising tools to explore the potential for crystal engineering in this system. Indeed, a series of increasing chain length derivatives of (1), where R = ethyl, propyl, and butyl, drives the tapes apart in the expected way. However, this predictability is limited to structures measured at low temperatures. At room temperature each compound forms a new crystal structure where the tape persists, but disorder in the N-alkyl chains produces an unpredictable spacing between the tapes. Variable temperature Raman spectroscopy was performed to complement the X-ray diffraction studies, and may offer new insights into the structural transitions occurring as each derivative warms to room temperature.

[1] Aakeröy, C.B. et al (2001). Aust. J. Chem. 54(7), 409-421.

[2] Le, T. et al. (2016). CrystEngComm. 18(6), 962-970.



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