Poster Presentation

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Temperature dependent conformational switching of alkyl chains in N-propyl-triazines

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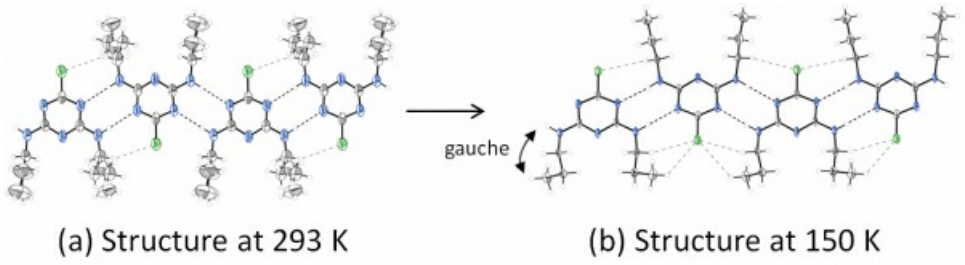
Single-crystal analysis of the herbicide Atrazine revealed packing as tapes comprising self-complementary N-H…N hydrogen bonds with an extensive conformational disorder in the alkyl side chains [1]. Synthesis and single-crystal analysis of related bis-N-alkyl-s-triazines showed that these compounds all form a tape with an orientational disorder in the alkyl chains, with a notable exception of the n-propyl derivative. The X-ray structure determined at room temperature (293 K) exhibited an extensive disorder in the alkyl chains (fig. 1a), but the structure determined at 150 K showed a perfect ordering of alkyl chains (fig1b). The low-temperature phase showed doubling of the unit cell volume with two independent molecules having different conformations of the alkyl groups. This transition from the disordered to ordered phase was accompanied by the formation of a third C-H…Cl interaction that compensates for the less favourable gauche conformation required to bend the methyl group towards the chlorine atom.

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



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