

Poster Presentation

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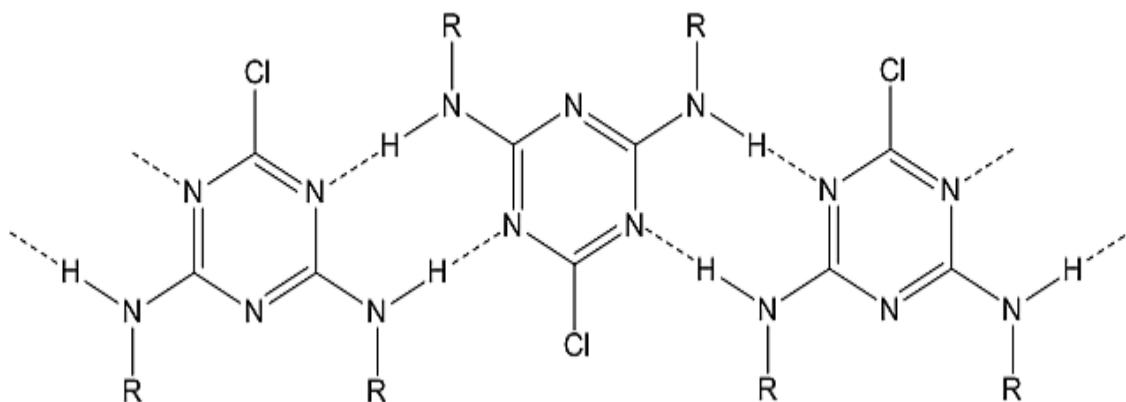
A Persistent N-H...N Ribbon Motif in the Crystal Structures of Triazine Herbicides

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Triazines have been used for many years as herbicides, but we now report for the first time the crystal structures of two ubiquitous exemplars, Simazine 1 (R = ethyl) and Atrazine 2 (R = i-propyl, 2 polymorphs), which were possible only with the Synchrotron diffraction measurements. Analysis of the crystal structures reveals infinite molecular ribbons (I) comprising centrosymmetric N-H...N hydrogen bonds, with weaker secondary C-H...Cl interactions. The hydrogen bonding constrains each molecule into a very specific conformation, yet the ribbon is conserved across 1 and both polymorphs of 2. Accommodation of the ribbon in each of the crystal structures results in changes in space group and some out-of-plane buckling in the ribbon. A search through the Cambridge Crystallographic Data showed N-H...N synthon is present in other members of the chlorotriazine family, forming a ribbon whenever the alkyl/aryl R groups can "solve" the packing problem to produce a hydrophobic domain parallel to the hydrogen bonds¹. Such is the dominance of this ribbon motif that it may persist across a large range of chlorotriazines yet to be analyzed or synthesized.

[1] Mei-Xiang Wang, Hai-Bo Yang, *J. Am. Chem. Soc.*, 2004, 126, 15412-15422, [2] A. Quesada, M. A. Fontecha, M. V. Lopez, et al., *Acta Crystallogr., Sect.C*, 2008, 64, o463-o466



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