

Extended Hydrogen Bond Patterns in Small Molecule Crystal Structures: A CSD Study

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A search algorithm, 3DSEARCH¹, is used to identify extended hydrogen bond patterns in a set of small molecule crystal structures obtained from the Cambridge Structural Database. Searches are performed to identify the frequency of occurrence of various classes of 1-D tape and 2-D sheet motif that are composed of arrangements of strong inter-molecular hydrogen bonds. The 'R2 tape', 'R4 sheet' and the 'R2R6 sheet' patterns are found to be the most common out of the types considered (see Figure 1). An R4 sheet, for example, is composed of hydrogen bond ring motifs that span 4 molecules. Analysis of polymorphic systems shows that extended patterns are conserved between polymorphic forms for 75% of cases studied.

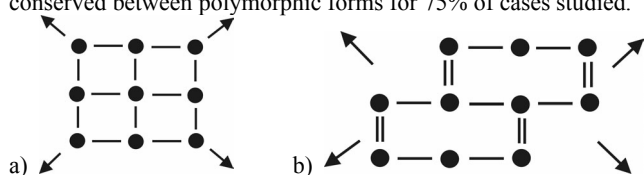


Figure 1. a) An 'R4 sheet' motif. b) An R2R6 sheet motif. Dots represent molecules, lines represent inter-molecular hydrogen bonds. The arrows indicate that these patterns are infinitely repeating in 2D.

[1] Chisholm J. A., Motherwell S., *J. Appl. Cryst.*, 2004, **37**, 311.

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