Hydrogen Bond Capacity of Organic Functional Groups: a CSD Derived Database

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The H-bonding behaviour of organic functional groups is of general interest. We have devised new methodology[1] to build a specialized database of non-bonded contacts extracted from the Cambridge Structural Database (CSD), using the Microsoft Access database program. We extracted 35,056 crystal structures where all hydrogen atoms had 3D-coordinates present, no metal atoms, OH, NH, or SH present, giving the possibility of at least one strong H-bond. The data were processed by the Pluto program, calculating the number of non-bonded contacts for 108 chemical groups, (distance < sum of van der Waals radii + 0.1 Å). Contacts are classified as D (donor bond), A (acceptor bond), X (not H-bond), and U (uncertain). Contacts are both inter- and intra-molecular. The accessible surface area of atoms was also calculated.

This database, CSDContact, can be used to derive average values for H-bond behaviour of functional groups (e.g. OH in COOH D=99% A=4% X=21%; in OH-CH_2-R D=94% A=63% X=19%). We present average figures for the number of donor/acceptor bonds per group, the dependency on available steric surface, total donor/acceptor atom ratio, and some examples of competition effects between groups in specific ratios. More practically, CSDContact can be used to answer questions where we limit the number and ratio of the chemical groups[2], e.g. What happens if the crystals contain just one alcohol OH and one cyano group?

OH-R-CN molecule → crystal OH…OH or OH…NC ? [92%, 4%]

[1] Infantes L., Motherwell W.D.S., *Chem. Commun*, 2004, 1166-1167. [2] Infantes L., Motherwell W.D.S., *Z. Kristallogr*., 2005, **220**, 1-8.

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