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Area correction of multi-atom-acceptor hydrogen bond frequency distributions.

Autorzy

Zbigniew Ciunik

G. R. Desiraju

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Streszczenie

Frequency distributions of hydrogen bond trajectories for X–H···Ph interactions (X = O, N, C) need to be corrected for the finite area of the acceptor moiety and once this correction has been performed, it is seen that the donor groups have a distinct tendency to interact with the centroid of the aromatic ring. Statistical analysis of experimental and theoretical data is very important for a correct interpretation of several chemical phenomena. Hydrogen bonds are typically described in terms of various parameters (lengths, angles) obtained from crystal structure determinations. These parameters are most simply depicted as histograms. However, such simple methods of analysis can be sometimes misleading.[1] For example, it was found that a distribution of hydrogen bond angles, θ, in O–H···O hydrogen bonds is in the range 120–180° with a maximum at around 160°. Such an observation suggests that hydrogen bonds in crystals are non-linear.[2] This is, however, inconsistent with theoretical predictions in the gas phase, say for the water–water dimer. The reason for this seeming contradiction is the failure to take into account a geometrical factor that seriously influences the crystal statistics. The number of hydrogen bonds with angle θ is proportional to sinθ for purely geometrical reasons, there being a greater probability of finding such interactions on the rims of cones of increasing solid angles. A simple procedure, namely the use of N/sinθ instead of N (where N is the number of hydrogen bonds in the interval $\theta$to $\theta + \Delta\theta$) in the histograms, effectively resolves this contradiction. This is known today as the *cone correction* and is illustrated in Fig. 1(a). This correction is used widely in the interpretation of hydrogen bonds and occurs as a standard procedure in the program VISTA that is a part of the Cambridge Structural Database (CSD).[3]

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