Topological information of the electron density distribution in hydrogen bonded systems.

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Using the topological properties of the experimental electron density distribution $\rho(\mathbf{r})$ observed in 83 hydrogen bonds [X-H···O (X=C,N,O)], we have related the total energy density observed at the bond critical point (H^{CP}) to the H…O interaction potential (U) by means of a proportional relationship $U \propto \cdot H^{CP}$.[1] This function has been successfully checked against several physical and chemical properties and compared to Morse and Buckingham type potentials. Recently,[2] we have undertaken the theoretical study of $\rho(\mathbf{r})$ calculated for the isolated H···F interaction and for 79 X-H···F-Y complexes. The analysis of all these systems lead to three characteristic $\rho(\mathbf{r})$ regions for distances H···F ranging from weak van der Waals to strong covalent interactions. While the extreme regions are respectively associated to *pure* CS and SS interactions, the middle region is associated to the redistribution of $\rho(\mathbf{r})$ between those electronic states. The analysis carried out with the isolated H···F interaction has permitted to associate this transit region to internuclear geometries involved in the building of the H-F bonding molecular orbital. The interaction energies of X-H···F-Y *pure* CS interactions have been estimated by using the bond degree parameter (B.D. = H^{CP}/ρ^{CP}) and the $[F\cdots H\cdots F]^-$ proton transfer geometry has been associated to the local maximum of the electron kinetic energy density $(G^{CP})_{max}$.

References

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