**[MS25 - 05] Crystallographic Evidences of the Nature of Homopolar H···H Interactions.**

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Weak intermolecular forces are responsible for the aggregation of organic molecules in condensed phases. Among them, homopolar H···H interactions are thought to be responsible for the relatively low boiling point of hydrocarbons or the relatively high crystal lattice energy of organic crystals. Understanding those forces has both theoretical and practical implications and deserves chemical and physical investigation. Crystallography is a powerful discipline to explore how atoms and molecules interact and – indirectly – to retrieve information about the forces that hold them together. The very origin of modern crystallography 100 years ago coincided with the elucidation of the ionic bond in sodium chloride. In the following decades the rapid development of diffraction techniques resulted in a vast database of structures that provided with the necessary information to answer a number of questions. Unfortunately most of the entries in the database are structures determined by x-ray radiation, which is not suitable for the accurate localization of hydrogen atoms. Neutron-radiation data are needed to give an insight on the forces acting on hydrogen atoms. In order to understand how hydrogen atoms interact, crystals with short H···H distances have been designed, synthesized and analyzed by neutron diffraction and quantum mechanics (QM) calculations. Other data have been retrieved by the Cambridge Structural Database (CSD). This study reveals that the atoms are somewhat closer than predicted on the bases of geometrical optimization and neutron normalization. This could be explained by the existence of an attractive interaction between hydrogen atoms. In conclusion this work highlights the limits of neutron normalization and QM calculation and reports the first crystallographic evidence of the interactions between homopolar hydrogen atoms.