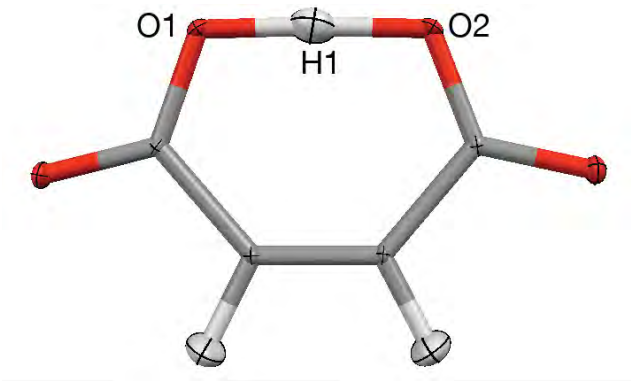

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Keywords: Experimental electron density, electric field, crystalline environment

MS21-O5

Quantum crystallography towards "quantitative crystal engineering"

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Understanding solid-state supramolecular chemistry requires quantitative insights into the nature and strength of intermolecular interactions. Over the past few decades, charge density multipole modelling (CDMM) formalism has contributed significantly to the understanding of chemical bonding in crystals [1]. However, the applicability and accuracy of CDMM in the intermolecular regime is a grey area. This is owing to the issues related to the partitioning of electron density in the intermolecular space using CDMM. Recent developments in the high resolution X-ray quantum crystallography offer significant prospects in this context. I will discuss recent results on the studies of intermolecular interactions, their strength and nature in terms of bond orders, electron density and interaction energies derived from both experiment and theory. Especially the applications of such quantitative descriptors will be discussed in the context of crystal engineering of molecular solids, their relative stabilities and intriguing mechanical properties[2,3].

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