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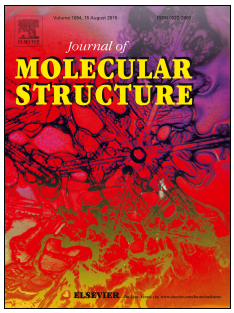

Investigation of non-covalent and hydrogen bonding interactions on the formation of crystalline networks and supramolecular synthons of a series of α-aminophosphonates: Crystallography and DFT studies

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Investigation of non-covalent and hydrogen bonding interactions on the formation of crystalline networks and supramolecular synthons of a series of α-aminophosphonates: Crystallography and DFT studies

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ABSTRACT

α-Aminophosphonates have been rarely explored in the field of crystal engineering. These organic molecules are capable of forming reliable and reproducible supramolecular synthons through non-covalent interactions that can be employed for designing high dimensional supramolecular architectures. Here, we systematically study the influence of conventional and unconventional hydrogen bonding interactions on the formation of these synthons and stability of the crystal packing. The theoretical studies were employed to further confirm the presence of these synthons by comparing the stabilization energies of the dimers and monomers. The dependence of the stability of NH…O hydrogen bonds to the aromatic substituents were investigated using NBO analysis. The most stable compound was determined by comparing the HOMO-LUMO energy gap of all compounds and compared with NBO analysis.

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