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Molecular crystals of o-phenylenediamine with organic dicarboxylic acids

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Molecular recognition, is a process where we can design and build supramolecular assemblies of different chemical species with the help of specific non-covalent interactions, like hydrogen bonding, aromatic $\pi \cdots \pi$ stacking, steric repulsion and van der Waals forces.1

Protonation of o-Phenylenediamine (OPDA) with simple organic dicarboxylic acids resulted to produce the molecular crystals of different architectures. The single crystal X-ray diffraction study confirmed the formation of salts of OPDA-Fumarate (OPDFA), [C6H9N2].[C4H4O4] (1), OPDA-malate (OPDMA), [C6H9N2].[C4H5O5] (2) and OPDA-Succinate [C7H4N2O6]·[C3H7NO] (3). All these structures adopted the hetero supramolecular synthons.2 Interestingly, both the protons of fumaric acid is transferred to OPDA to form 1:2 product but one proton each in the cases of malic acid and succinic acid transferred to OPDA to 1:1 product. Compound 1 crystallized in orthorhombic body centred non-centrosymmetric Iba2 space group, Compound 2 crystallised monoclinic centrosymmetric P21/c space group and Compound 3 crystallized in triclinic centrosymmetric P-1 space group with Z' 2.3 The resultant products are also prepared using mechanochemical experimental techniques i.e. liquid assisted grinding / dry co-grinding and the confirmed products are analysed using powder x-ray diffraction and thermal studies.

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