

Poster Presentation

MS35.P03

Molecular complexes of cyclohexanehexacarboxylic acid with aza-donors

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Hydrogen bond mediated molecular complexes of cyclohexane-1,2,3,4,5,6-hexacarboxylic acid (1) with aza-donors distinguished by positional isomerism like 4,4'-bipyridine (a), 2,2'-bipyridine (b), trans-1,2-bis(4-pyridyl)ethylene (c), trans-1,2-bis(2-pyridyl)ethylene (d), 4,7-phenanthroline (e) and 1,10-phenanthroline (f) have been prepared either from a solvent mixture of methanol-water or from DMSO by solvent evaporation method. All the complexes crystallized as hydrates with different molecular ratios of 1, aza-donor and water. Detailed structural analyses of these molecular complexes have been investigated by single crystal X-ray diffraction. Structural diversity was found in the landscape of these molecular complexes depending upon the flexibility and positional isomerism of organic spacers (aza-donors) as well. Both intra and inter molecular hydrogen bonds played an important role in the formation of supramolecular architectures. Intramolecular O-H...O hydrogen bonds are present in the acid molecule due to the favourable orientation of -COOH groups in the chair form of the cyclohexane ring. In basic recognition pattern of each complex, it has been noted that acid molecules interact with aza-donors as well as water molecules through O-H...N and O-H...O hydrogen bonds, respectively. Different topological patterns like sheets, tapes, ribbons and host-guest networks have been observed in three dimensional arrangements. Inclusion of water molecules in each molecular adduct indicates the importance of water molecules to stabilise the molecular ensembles of 1 and the corresponding aza-donors. Presence of water molecules in the crystal lattices was also supported by thermogravimetric analysis (TGA).

Keywords: cyclohexanehexacarboxylic acid, aza-donors, molecular complexes