A CRYSTALLISATION / CRYSTAL ENGINEERING APPROACH TO AID SALT SELECTION - ANIONS

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Salt selection is critical in the drug development process as selection of an appropriate form can reduce significantly the time to market of a new pharmaceutical entity. Salt formation is often employed to modify the final drug product. It is a simple chemical modification that can change to advantage the physiochemical, formulation, biochemical and therapeutic properties of a drug without varying the basic chemical structure. Crystal engineering is the understanding of intermolecular interactions in the context of crystal packing and in the utilisation of such understanding in the design of new solids with desirable physical and chemical properties. The aim being to establish reliable connections between molecular and supramolecular structure on the basis of intermolecular interactions. Taking the known synthesis and structure of diiodotetrafluorobenzene (2), and Br...N in trans-1,2-(4-pyridyl)ethylene 1,4-dicarboxylic acid (3),7 the hydrogen bonding networks have been described and the relationship between structure and crystal morphology evaluated.

References

Keywords: SALTS, CRYSTAL ENGINEERING, HYDROGEN BONDING

THE HALOGEN BOND \(\Gamma^\circ\), I-N, Br-N AS A TEMPERATURE FUNCTION

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The X-B interaction, or halogen bond, between a halogen atom (X = I, Br) in perfluoro derivatives and a neutral or charged base (B = amines, pyridines, N-oxides, iodide etc.), is a useful synthons we have extensively used to produce a variety of supra-molecular structures. The goal of the present study is to determine the chemical and thermal stability as well as the colour and spectral features of the metallophthalocyaninato (MPc) complexes. The metallophthalocyaninato (MPc) complexes are an important class of compounds extensively used in the industry of colorants and high technologies, including among others, display devices, sensing elements, photochemical redox agents and markers in photodynamic therapy of cancer. The oxidation state of the metal cation and its location relative to the phthalocyaninato ring determine the chemical and thermal stability as well as the colour and spectral features of the complexes. The new complex, which is stable up to about 483 K, was obtained as a result of intermolecular reaction of the triple decker indium phthalocyanine with 4 methylpyridine (4-Mepy). The crystal is triclinic, space group P1, with one molecule per asymmetric unit. Differential Scanning Calorimetry (DSC) has been employed to investigate the thermodynamic properties of rac-CMA and (S)-CMA. Though their hydrogen bonding patterns display some similarities to the ones observed in the related tartaric and malic acids, they also reveal some distinct differences. Attempts are made to rationalize these differences in crystal packing in terms of differences in the thermodynamic properties. A binary phase diagram for (R)-CMA and (S)-CMA was constructed from thermodynamic data. To examine the many ways enigmatic melting behavior observed for a racemate that is made as a mechanical mixture of the two enantiomers, we performed DSC experiments to elucidate how the variation in crystal size influences the melting curves.

Keywords: CRYSTAL PACKING, PHYSICO CHEMICAL PROPERTIES, CRYSTAL SIZE

SYNTHESIS AND CRYSTAL STRUCTURE OF THE COMPLEX OF AZA-BRIDGED INDIUM(III) PHTHALOCYANINE AND 4-METHYLPSYRIDINE

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The metallophthalocyaninato (MPc) complexes are an important class of compounds extensively used in the industry of colorants and high technologies, including among others, display devices, sensing elements, photochemical redox agents and markers in photodynamic therapy of cancer. The oxidation state of the metal cation and its location relative to the phthalocyaninato ring determine the chemical and thermal stability as well as the colour and spectral features of the complexes. The new complex, which is stable up to about 483 K, was obtained as a result of intermolecular reaction of the triple decker indium phthalocyanine with 4 methylpyridine (4-Mepy). The crystal is triclinic, space group P1, with two independent formula units in the elementary cell. Each molecule consists of dimeric indium phthalocyanine (PcIn) bridged by a pair of the In-N-In bonds and one molecule of non bonded 4-Mepy, trapped into the area between two Pc rings of the dimer. The In ions are coordinated by four isodole N atoms and two bridging nitrogens. The averaged distance between the In ions and the plane passing the isodole N atoms is 0.8 Å. The In-N-In units are bent, forming the angles ranging from 105.3 to 112°. This type of double linked Pcm[III][N,N[MIII][Pc moiety, has been observed for the first time among the phthalocyaninato complexes.

Keywords: PHTHALOCYANINE, DIMER, N BRIDGED

Keywords: HALOGEN BOND, INTERMOLECULAR INTERACTIONS, THERMAL EXPANSION


