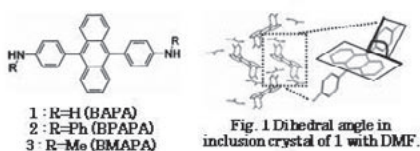


P06.09.35

Acta Cryst. (2008). A64, C393**Guest-dependent luminescence modulation in inclusion crystals of anthracene derivatives**

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Luminescent modulations in solid state are attracting attention in material investigation because of their potential applications in optical device. Much scholarly research has been conducted on luminescent modulations in solution. On the other hand there has been little research on luminescent modulations in solid state. In this work, modulation factors in solid-state luminescence are developed from analyses of crystal structures and emission properties of organic crystals. To provide further insight into luminescence modulations depending on guests, many inclusion crystals were prepared and compared with each other. Luminescence of inclusion crystals, which were formed on recrystallization of 1-3 from various solutions, successfully ranges in color from blue to green under UV light. In almost all crystals, hydrogen bonds formed between amine group of 1-3 and guests were confirmed by X-ray analysis. Additionally, inclusion crystals with polar guest and with much planar conformation of hosts (Fig. 1) show long wavelength emission. The polarity of guests and the planarity of host were found to have cooperative effect on luminescence wavelength of inclusion crystals of 1-3.



Keywords: organic crystal, luminescent modulation, inclusion

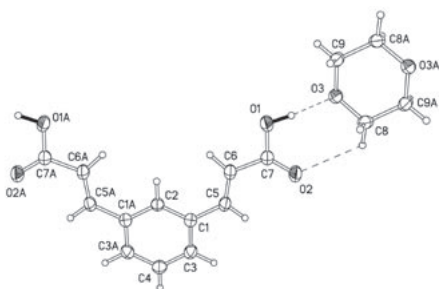
P06.07.36

Acta Cryst. (2008). A64, C393**Synthesis, structure and solid-state photochemistry of *m*-benzenediacyrylic acid and its complexes**

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Unlike bis(pyridyl)alkenes, which can be readily [2+2]-dimerized by exposure to UV light in the solid state, the solid-state photochemistry of alkene-substituted acids has not been investigated yet. Due to the photoreactivity of the double bonds and the versatile coordination ability of the carboxylate groups, these compounds can serve as convenient bridging units for construction of photochemically active metal coordination compounds. To explore



such potentials, *m*-benzenediacyrylic acid was synthesized, and the solid-state photochemistry of the pure ligand and some of its complexes was studied. The crystals of the dioxane solvate of *m*-benzenediacyrylic acid, C₆H₄(CHCHCOOH)₂·C₄H₈O₂, are monoclinic (space group *P*2₁/*m*), with cell dimensions: *a* = 4.0165(2), *b* = 29.8961(12), *c* = 6.2402(3) angstrom, beta = 90.084(4) degree. In the crystal structure, the molecules of *m*-benzenediacyrylic acid and dioxane interact with intermolecular interactions. The solid-state photochemistry of the compound and its metal compounds are currently being studied.

Keywords: crystal structure, photochemistry, complexes

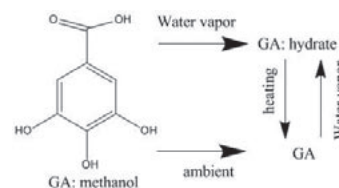
P06.07.37

Acta Cryst. (2008). A64, C393**Vapor induced reversible guest exchange of organic inclusion crystal**

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By using host-guest crystal, controlled release of guests such as pharmaceuticals or functional chemicals is realized. Moreover, it is also possible to exchange the guest with new molecule by simply applying gas or vapor molecule. In this study, some examples of the guest exchange phenomena by vapor application and their crystal structure changes are presented. The crystal structures after guest release were successfully determination by structure solution from powder diffraction data technique. By application of water vapor, gallic acid methanol solvates crystal lost methanol molecules and new hydrate crystal was grown as powder crystalline form. Also, the methanol and water guests were lost in ambient condition or by heating to form dehydrated powder crystal. In both methanol and hydrate structure, large solvent channels were observed. In dehydrate form; the channel was closed by small displacement of hosts and by hydrogen bonds formation, so the water absorption proceeds slowly. This kind of reversible guest exchange process was observed for pyromellitic acid solvates. Solvent channel and hydrogen bonding pattern similarity are the keys for these guest exchange phenomena.



Keywords: host-guest complexes, powder structure determination, polymorphic structures

P06.07.38

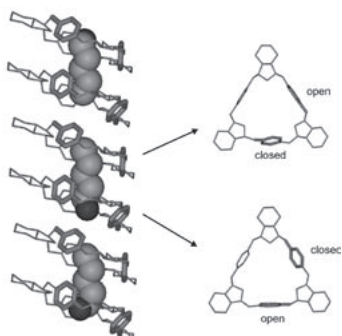
Acta Cryst. (2008). A64, C393-394**Inclusion properties of trianglamines**

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Trianglamine is a macrocycle obtained through [3+3] cyclocondensation between enantiomerically pure *trans*-1,2-diaminocyclohexane and terephthalic aldehyde, followed by the subsequent reduction of the imine bonds. This chiral hexamine displays considerable ring flexibility that allows both inter- and

intramolecular inclusion of simple solvent molecules. Bridging of the neighboring nitrogen atoms by the methylene groups gives rise to more rigid macrocycle with a well defined inner cavity. We shall demonstrate the ability of this molecule to include in its inner cavity simple alcohol molecules belonging to the homologous series (ethanol, 1-propanol, 1-pentanol and 1-hexanol). Of interest in the investigated crystal structures is a concerted host/guest disorder and the ability of the host molecules to switch in between the various conformations which either allow or prevent the solvent molecules to enter the intramolecular cavity. Our studies also demonstrate that the inner cavity of triangelamines is not large enough to accommodate any aromatic guest molecule.



Keywords: inclusion, macrocycles, triangelamines

P06.07.39

Acta Cryst. (2008). A64, C394

Molecular complexes of 4,4'-dinitrophenyl

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Complexes of para disubstituted and 4-monosubstituted biphenyl formed with 4,4'-dinitrophenyl (DNBP), demonstrate intense colours, from pale yellow to dark red, upon formation. These colours are dissimilar to the colour combination of the parent compounds. The focus of this study was to investigate the nature of these molecular donor-acceptor interactions in the solid state, using spectroscopic techniques such as IR, Raman, UV-Vis, NMR and X-ray crystallography. Typical interactions observed in such molecular complexes include pi-pi interactions, hydrogen bonding, charge transfer and van der Waals interactions. Complexes of DNBP, as acceptor, studied included a variety of mono- and disubstituted donors, such as dihalo, diamino, di- and monohydroxy groups. The crystal structures of these complexes showed retention of the non-planar conformation of DNBP with a dihedral angle of around 35 deg. This conformation for DNBP has also been confirmed using density functional theory (Guassian) calculations that showed good agreement between the theoretically calculated and experimentally observed IR and Raman spectra in the solid state. It appears as if the packing of the complexes in the solid state is directed mainly by the similar packing of DNBP units in these complexes. Some of the molecular ratios for these complexes that vary, depending on the electronic properties of the donor molecules, were determined using NMR spectroscopy.

Keywords: molecular complexes, molecular cocrystals, crystallographic analysis

P06.07.40

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(Z)-Ethyl 4-chloro-2-[(4-chlorophenyl)-hydrazino]-3-oxobutanoate

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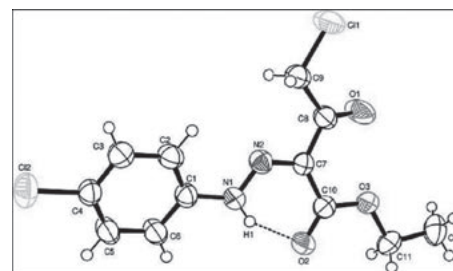
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The title compound, (Z)-Ethyl 4-chloro-2-[(4-chlorophenyl)-hydrazino]-3-oxobutanoate, crystallizes as a nonmerohedral twin with a twinning ratio of 0.51:0.49. The molecule adopts a keto-hydrazo tautomeric form stabilized by an intramolecular N-H...O hydrogen bond. The configuration around the N-N bond is trans. The overall view and atom-labelling of the molecule are displayed in Fig.1. The molecule is approximately planar with dihedral angle between the aromatic C1-C6 ring and the plane of the C7-C12/O1-O3/C11 aliphatic chain being 19.71(12) degrees. Intramolecular N-H...O hydrogen bond generate S(6) ring motif (Bernstein et al., 1995).

Reference:

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* 34, 1555 – 1573.

Fig.1.



Keywords: single-crystal structure determination, tautomerism, small organic molecules

P06.08.41

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Synthesis and structural characterization of 1,4-bis-(2-phenyl-4-oxo-1,3-thiazolidin-3-yl)butane

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Thiazolidinones are important heterocyclic compounds, which exhibit a broad range of biological activities, including interesting profile as fungicidal, pesticide, antibacterial, anticonvulsant, antihistaminic, antioxidant, anti-inflammatory and antinociceptive agents. As a consequence many different protocols allowing the synthesis of 4-thiazolidinone skeletons have been developed. However, few are known about a,w-bis-(2-hetaryl-4-oxothiazolidin-3-yl)alkanes. Even though, several studies have revealed their anti-