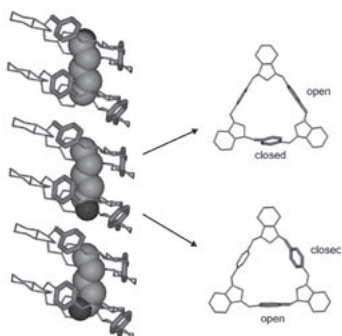


intramolecular inclusion of simple solvent molecules. Bridging of the neighboring nitrogen atoms by the methylene groups gives rise to more rigid macrocycle with a well defined inner cavity. We shall demonstrate the ability of this molecule to include in its inner cavity simple alcohol molecules belonging 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

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#### 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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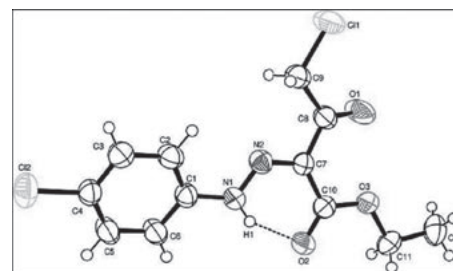
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The title compound, (Z)-Ethyl 4-chloro-2-[(4-chlorophenyl)-hydrazino]-3-oxobutanoate, crystallizes as a nonmerohedral twin with a twinning ratio of 0.51:0.49. The molecule adopts a keto-hydrazo tautomeric form stabilized by an intramolecular N-H...O 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-