

MS23-P2 High Pressure Studies of a Trio of Polymorphs with Conformational Variability. Alexander J. Blake, Jeremiah Tidey, Henry L.S. Wong, Martin Schröder, *School of Chemistry, The University of Nottingham, Nottingham NG7 2RD, UK*
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We are engaged in a search for new phenomena which can be induced by the effects of pressure on metal coordination complexes. Phenomena identified so far include dramatic and multiple colour changes, modifications to coordination geometry and catenation, and new conformations [1]; more recently we have identified unprecedented processes such as the induction of π - π interactions and the deformation of internal molecular geometry [2]. As an extension of this work we have investigated the mononuclear complex [PdCl₂(1-oxa-4,7-dithiacyclononane)], see Figure]. In the process we have discovered two new polymorphs of the complex which exhibit different conformations of the nine-membered 1-oxa-4,7-dithiacyclononane ring. In the known (α) phase [3], the O-donor atom is directed *endo*, *i.e.*, in the direction of the Pd(II) metal centre (see Figure). The β phase appears to be metastable, reverting readily to the α form, but we have determined that the O-donor atom is directed *exo*, *i.e.*, away from the metal centre. The γ form also features an *exo* O donor, but in this case the molecular packing is such that the O atom points towards the Pd(II) centre in a neighbouring molecule, raising the possibility of specific intermolecular interactions and extended structural motifs. We have explored these possibilities by compressing crystals of the α and γ phases within a diamond anvil cell.

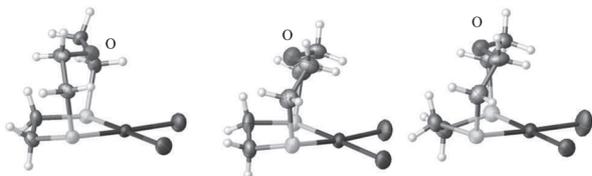


Figure. From left to right: views of the α (*endo*), β (*exo*) and γ (*exo*) conformations of the ligand in [PdCl₂(1-oxa-4,7-dithiacyclononane)].

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Keywords: coordination complex; high pressure; polymorph screening

MS23-P3 Charge density studies of halogen bond in crystals of chloro-nitrobenzene derivatives. Teresa Borowiak^a, Grzegorz Dutkiewicz^a, Bogusław Misterkiewicz^b
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The charge density distributions in 2-chloro-4-nitrobenzoic acid (2-Cl-4-NBA) and 2,5-dichloronitrobenzene (1,5-DCNB) have been determined by means of high resolution X-ray diffraction at 100 K. The supramolecular structure of both crystals is stabilized among others, by intermolecular halogen bonds C-Cl...O. In the current presentation the deformation density distribution of electron density and topological analysis of electron density for the title compounds are shown. The deformation density clearly indicates a significantly anisotropic distribution of electrons in the halogen atom with less of them in the direction of C-Cl bond and more in the other directions (see the deformation density, Fig. 1 below). The topological analysis confirms conclusions derived from the deformation density distribution.

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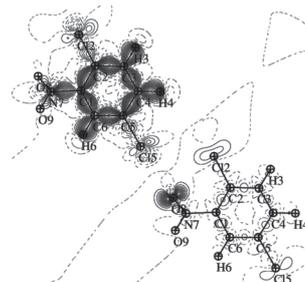


Fig. 1. Deformation density distribution in 2,5-DCNB (the electron density in the halogen bond is shown).

Keywords: halogen bond; charge density study of