[Mo(CO)3(NCMe)2(SnBuCl2)Cl], reacted with phosphanes (Ph2PCH2CH2PPh2, dppe; Ph2PCH2PPh2, dpmm; Ph2PNHPPh2, dpna) to afford complexes \([\text{Mo(CO)}_6(\text{NCMe})_2(\text{SnBuCl}_2)\text{Cl}]\) \((L=\text{dppe}, \text{dpmm}, \text{dpna})\). When these complexes reacted with \([\text{NH}_3][\text{S}_2\text{P} \{\text{OEt}\}_2]\), the nitrile and the chloride ligands were replaced by the \(\text{S}_2\text{P} \{\text{OEt}\}_2\) anionic ligand, yielding \([\text{Mo(CO)}_6(\text{S}_2\text{P} \{\text{OEt}\}_2)_2(\text{P-P})(\text{SnBuCl}_2)]\) \((L=\text{dppe}, \text{dpmm}, \text{dpna})\). Complexes 5, 6, and 7 could also be obtained from a ‘one pot’ reaction starting from \([\text{Mo(CO)}_6(\text{S}_2\text{P} \{\text{OEt}\}_2)_2(\text{P-P})(\text{Ph}_2\text{PCH}_2\text{CH}_2\text{PPh}_2)]\) and the appropriate phosphane. Similar reactions took place when \(\text{SnPhCl}_2\) was used instead of \(\text{SnBuCl}_2\) in the starting material, leading to the formation of complexes 8, 9, 10. The structure of complexes 2, 3, 5, 6, 8, 9, 10 were determined using single crystal X-ray diffraction. In these complexes, Mo(II) is heptacoordinate, with a Mo-Sn bond. The tin atom has a tetrahedral environment in all the complexes, except in \([\text{Mo(CO)}_6(\text{NCMe})_2(\text{NCMe})_2(\text{SnBuCl}_2)\text{Cl}]\) (2, figure), where the Cl ligand bridges Mo and Sn. DFT (Density Functional Theory) calculations were performed in order to discuss the nature of the Mo-Sn bond.

Keywords: Mo(II) complexes, Sn derivatives, crystal structures

**Poster Sessions**

**P08.12.78**

**Acta Cryst.** (2008). A64, C442

Guest-dependent high-pressure behavior in a nanoporous metal-organic framework material

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The structural and chemical versatility of metal-organic framework (MOF) materials underlie important technological, industrial, and environmental applications, including in strategic gas storage and separation. The extensive structural complexities now well-documented for these systems are likely to be associated with unprecedented pressure-induced behavior compared with the traditional solid state materials more commonly explored under high pressure conditions. Furthermore, the typically open (low density, often porous) nature of MOF materials is likely to induce such phenomena at more moderate pressures, such as may be routinely encountered in practical applications. For example, densification of powdered nanoporous MOF materials to optimize volumetric gas storage capacity through sample compression (up to several GPa) may distort the framework and pore structure, and accordingly may significantly alter the guest sorption properties (e.g., selectivity). Accordingly, understanding the impact of pressure on MOF systems is not only of considerable fundamental interest, but is relevant to the applications for which MOF materials are being considered. Here we report the structural investigation of a nanoporous MOF material at high pressures within a diamond anvil cell using synchrotron-based X-ray powder diffraction.

Keywords: high-pressure X-ray diffraction, microporous materials, coordination polymers

**P08.12.79**

Femtosecond to hours structural dynamics of self-assembling systems

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In the following we will present time-resolved small angle x-ray scattering studies on photoactive, self-organising systems like photo-sensitized liquid crystal systems and other reference systems of biological relevance. In the first system, we have studied the kinetics and dynamics of the photo-induced phase transition from a liquid crystal to a microemulsion system and vice versa. In the second system, we mainly concentrate on the structural response function upon photo-irradiation. In the millisecond time domain, the structural dynamics studies have been performed at home-based time-resolved photo small angle X-ray diffraction apparatus [1, 2], the nanosecond and picosecond time scale have been explored employing plasma based home laboratory sources and synchrotron based x-ray scattering sources (ID09B beamline / ESRF, France) [3] and the femtosecond time domain has been investigated employing the FLASH free electron laser facility at DESY, Germany. We will give an overview over the varying time-scales underlying the photo-activated structural transformation processes. We will also discuss the various x-ray sources and compare the different experimental approaches.


Keywords: time-resolved x-ray scattering, ultrafast processes, structural dynamics

**P08.13.80**

**Acta Cryst.** (2008). A64, C442–443

Dimers or not dimers in 1-arylanilinoethanones

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Few 1-arylaninoethanone derivatives have been structurally characterised up to date. However, these derivatives are important in synthesis and some of them possess interesting charge-transfer properties while also displaying rather unusual supramolecular arrangements. In the present study we present results from our structural characterisation of four derivatives, with substitutions (Cl-, MeO-, H-, Me-) in the 4-anilino position of the 1-arylaninoethanones. The Cl- and Me- derivatives form distant dimers while MeO- and H- derivatives are found as monomers. The formation of distant dimers has been found to be related to the planarity of the N atom in these structures, in agreement with the formation of similar dimers.