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Enhancing experimental exploration space with greater dimensions in modern printing

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Spin crossover is a phenomenon in which a metal ion undergoes a spin transition due to external stimuli such as temperature, pressure, photo-irradiation or electric currents.[1] $[Fe(Phen)_2(NCS)_2]$ (Phen =1,10 phenanthroline) is one of the archetype spin crossover systems which has been analysed by various methods including X-ray Diffraction (XRD) with known experimental values for transitions.[2] Being able to measure the changes in bond length to determine the spin state of the metal ion allows us to set a standard to work by. Light induced excited spin state trapping (LIESST) uses photo-irradiation to cause a spin transition at low temperatures,[3] this effect is usually measured by Mossbauer spectroscopy showing the ratio of high spin and low spin atoms in a sample based on magnetic susceptibility. XRD allows us to see the changes in bond length which can be used to determine roughly the spin state, to do this with photo-irradiation means a system has to be designed to allow us to illuminate the sample in the hutch.

Adaptation of this system allows for new spin crossover systems to be found and synthesised, to improve on current research and current properties of these systems.

The applications of these systems including high density memory and display devices, these can only be achieved with spin crossover properties being at relatively easy to obtain conditions. These include being close to room temperature and standard pressure for practical applications to be possible. The presented material will include the development and production of a new light irradiation source that can be mounted within the enclosure of a 3-circle diffractometer and the results of this equipment being used during the collection of data for a novel spin crossover system

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Keywords: Spin Crossover, 3D printing,

MS36-P31

A Systematic study of radiation damage in transition metal chloride complexes with 1,5-cyclooctadiene ligands using diffraction and spectroscopy.

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Transition metal chloride complexes with 1,5-cyclooctadiene ligands have a variety of applications as catalysts or precatalysts in e.g. hydrogenation and hydrogen-transfer reactions.(1) However, their interactions with X-rays has, to date, been assumed to be non-destructive with no reports in the literature of behaviours indicating radiation damage such as intensity loss in diffraction peaks or peak broadening. Interaction of X-rays with the crystal lattice is an effect that causes well-known problems in biological systems,(2) but this effect is only formally starting to be recognised in chemical crystallography. A survey of the effects of radiation damage to small molecule single crystals(3) demonstrated a relationship between the damage and the intensity of the source. The improving intensity of sources both at central facilities and for in-house instruments is increasing awareness of radiation damage, with a particular lack of understanding for small molecule crystallographers and spectroscopists currently complicating data collection. A series of compounds have been studied where M = Ir, Rh and Cu to, quite literally, shed light on the chemical changes resulting from X-ray exposure via structural and electronic insights. The combination of powder X-ray diffraction, single crystal X-ray diffraction, computational studies and X-ray photoemission spectroscopy reveal the impact of X-ray radiation on these materials in great detail and also provide insight into the importance of identifying appropriate data collection techniques for experiments.

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Keywords: X-rays, Catalysts, Synchrotron