

Exploiting this result, we carried out a fs XANES study of the ultrafast light-induced SCO in $[\text{FeII}(\text{bpy})_3]^{2+}$, which allowed us to unravel the detailed mechanism of the ultrafast spin conversion in FeII-complexes. This is the first femtosecond X-ray study of a molecule in solution ever to be carried out.

Keywords: molecular dynamics, femtosecond phenomena, X-ray absorption spectroscopy

MS.24.4

Acta Cryst. (2008). A64, C50

Photocrystallographic studies on metastable linkage isomers of transition metal complexes

Paul R Raithby¹, Teresa L Savarese¹, Stephanie Schiffrers¹, Mark R Warren¹, Simon J Teat², John E Warren³

¹University of Bath, Department of Chemistry, Department of Chemistry, University of Bath, Bath, Avon, BA2 7AY, UK, ²Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA94720, USA, ³STFC Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK, E-mail: p.r.raithby@bath.ac.uk

Photocrystallography is a technique that allows the structure of materials to be determined when the species are in an energetically activated state [1,2]. A proportion of the molecules within a crystal are activated by illumination with a light source and then the structure of the material, which contains percentages of both ground state and metastable structures, is determined using single crystal X-ray diffraction techniques. The technique has met with considerable success and the structures of a range of metastable linkage isomers have been determined [3, 4]. However, the technique remains challenging because of the relatively low levels of excitation that can be obtained. This is because the light penetrates only a few microns into the crystal which means that only surface molecules are excited. This introduces strain into the crystal causing fragmentation. Similarly, if the structural change caused by the change of the coordination mode of the ligands is large then strain is introduced into the crystal and fragmentation occurs. We now describe a systematic series of photocrystallographic studies using synchrotron X-ray radiation, small crystals, and a variety of light sources, on transition metal nitrosyl, nitrite and carbonyl complexes, with a range of ancillary ligands and counter ions that show how optimum activation may be achieved. The incorporation of the complexes to be activated into Metal Organic Frameworks prior to irradiation also shows high levels of excitation.

[1] P. Coppens, et. al., *Acta Crystallogr.*, Sect. A, 2005, 61, 162; [2] J. M. Cole, *Chem. Soc. Rev.*, 2004, 33, 501; [3] A. Yu. Kovalevsky, et. al., *Chem. Eur. J.*, 2005, 11, 7254; [4] K. F. Bowes, et. al., *Chem. Commun.*, 2006, 2448.

Keywords: photochemistry coordination compounds, metastable structure determination, isomers

MS.24.5

Acta Cryst. (2008). A64, C50

Metastable photoisomerism in materials targeted for optical data storage

Anthony E. Phillips, Jacqueline M. Cole

The University of Cambridge, Department of Physics, Cavendish Laboratory, University of Cambridge, J J Thomson Avenue, Cambridge, Cambridgeshire, CB3 0HE, UK, E-mail: aep40@cam.ac.uk

Recent developments in single-crystal X-ray diffraction have enabled light-induced electronic perturbations in chemical structures to be directly probed. Such structural information is key to understanding many photoactivated processes. Photoisomerism in the crystalline state is particularly noteworthy due to its potential applications in media for holographic data storage. Although holograms were first successfully used for this purpose over a decade ago, their widespread adoption has been heavily hampered by two factors: the high optical precision required for writing and reading data, and a dearth of suitable light-sensitive materials. We aim to overcome this materials supply bottleneck using photocrystallographic techniques. Our group's recent studies on the series $[(\text{SO}_2)\text{Ru}(\text{NH}_3)_4 \text{X}]\text{Y}$ are of particular interest in this regard as the SO_2 ligand undergoes photoinduced linkage isomerisation, providing a means by which one might encode binary information into these materials. The photorefractive properties observed in these compounds arise from the electric dipolar changes directly associated with photoisomerism, in contrast to the mechanistic origin of conventional photorefractive materials. Photocrystallographic results of these compounds and related materials will be presented, in tandem with complementary results from density-functional theory and optical measurements of their holographic characteristics. The paper will include a description of the key experimental parameters that are required for a successful photocrystallographic experiment, and will highlight the important interplay of the complementary theoretical and optical studies. We will conclude with an outlook on new X-ray facilities whose incipient operation will facilitate further work in this area.

Keywords: photochemistry, holography, optical materials

MS.25.1

Acta Cryst. (2008). A64, C50

Web assisted crystallography teaching and learning

Gervais Chapuis

EPFL, laboratoire de cristallographie, BSP/Cubotron, Lausanne, Vaud, 1015, Switzerland, E-mail: gervais.chapuis@epfl.ch

The part dedicated to crystallography teaching in the science curriculum is getting shorter and this tendency seems to continue. Under these conditions, crystallography teachers are thus under heavy pressure to improve their teaching in order to maintain the highest standards in the subject. Fortunately, the web can be of great help for this endeavour and many interesting tools are currently available. Presenting the three-dimensional characteristics of structures, the concept of symmetry and diffraction can take full advantage of applets, i.e. self-contained applications directly available on the web. Currently, many authors have created applets, which are useful for teaching every aspect of crystallography covering the representation of structures, point and space group symmetry, the diffraction phenomena and all its variants, the resolution of structures, databases and many others. The possibility to benefit from a web access in the classroom has greatly contributed to improve teaching. It should also be mentioned that the use of applets is not only limited to teachers. The advantage is that the students can also use them for reviewing lectures or preparing exams. In this presentation, we propose to explore and demonstrate the various possibilities available on open websites in order to facilitate the understanding of the many faces of crystallography.

Keywords: teaching aids in crystallography, web resources, simulation software