Exploiting this result, we carried out a fs XANES study of the ultrafast light-induced SCO in [FeII(bpy)]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

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Photocrystallographic studies on metastable linkage isomers of transition metal complexes
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Photocrystallography is a technique that allows the structure of materials to be determined when the molecules 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 techniques have 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.

Keywords: photochemistry, holography, optical materials

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Web assisted crystallography teaching and learning
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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