

MS13-2-6 Comparative photocrystallographic study using CW and pulsed laser irradiation on a photo-switchable ruthenium nitrosyl complex

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With the growing emphasis in solid state materials, Photoinduced linkage isomers (PLI) in nitrosyl complexes has been the subject of interest owing to its application as photoswitches. The generation of these PLI is induced by the photochromic and photorefractive response [1]. Potential applications of these materis are wide ranging, from data storage to smart window [2]. These applications are based on either CW or pulsed Laser irradiation. It is, therefore, important to understand the structural response of the material under these two excitation conditions. We present a photocrystallographic study of $[\text{Ru}(\text{NH}_3)_5(\text{NO})]\text{Cl}_3 \cdot \text{H}_2\text{O}$ [3] in order to compare the PLI induced by CW and Pulsed laser irradiation. Firstly, CW laser was used for the irradiation of the ground state (GS) at 100K generating two PLI as verified in infrared spectroscopy and absorption measurements of the crystal (Fig.1). The PLI1 was generated at 422nm and a transfer by subsequent irradiation at 1064nm yields PLI2 with significant populations of 45 and 10.6% respectively. The PLI configurations were first identified on photodifference maps. Interestingly, in photodifference maps of PLI2, two distinct positions of nitrogen were found evidencing two PLI2 positions. Subsequent refinement using isonitrosyl and side-on configuration of the NO ligand for PLI1 and PLI2 as PLI2A & PLI2B converged determining a structural model for these two states in *Pnma* space group. Secondly, the experiment was repeated by using pulse laser irradiation at 100K. We obtained same results of structural dynamics, types of PLI and population of PLI1 and PLI2 as with the CW laser irradiation, demonstrating the pulsed and CW Laser irradiation generating the same structural response. This complex is thus a suitable candidate for next step of our in-house time resolved photocrystallographic study in order to study the dynamics of photoswitching.

References

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Steady state photocrystallographic analysis

