

**MS40-2-2 Factors governing photoswitchability of selected nickel(II) nitro complexes**  
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**Abstract**

Development of effective photoswitchable compounds has gained great amount of interest in recent years due to their applicability in optoelectronics, photonics and photovoltaics <sup>[1]</sup>. The most desirable materials are characterised by high efficiency of the light-induced reaction in the solid, close to ambient working temperature and stability.

Amongst many types of structure-altering processes induced by external factors such as temperature, pressure and/or electromagnetic radiation, system undergoing linkage isomerism are suitable candidates for photoswitchable materials. Essential for this phenomenon to occur is the presence of ambidentate ligands such as NO, NO<sub>2</sub>, SO<sub>2</sub> that provide many different coordination modes.

Apart from external factors which may trigger linkage isomerism reactions, there are also internal factors which may facilitate or hamper this process, including crystal packing and intermolecular interactions. Especially important here are hydrogen bonds involving the ambidante groups which have decisive influence on their freedom of movement during linkage isomerism reaction <sup>[2]</sup>. Another important factor is the reaction cavity volume i.e. the amount of space available for the ambidentate ligand.

In order to find effective photoswitchable compounds there was prepared a series of nickel complexes with nitrite group serving as an ambidentate ligand that were thoroughly investigated crystallographically and spectroscopically. Three nickel complexes with various photoswitchable properties are presented here. Great amount of attention was paid to structural analysis that would contribute to design of this kind of compounds in the future. The examined compounds varied in amount of nitrite groups present in the structure and by the size and structure of ancillary ligands. Compounds with less favourable potential to undergo photoisomeration possessed two smaller ancillary ligands – derivatives of ethylenediamine. In comparison, it turned out that bulky (N,N,O) chelating ligand are much more beneficial. Structural investigations were supported by Hirshfeld surface analysis and computational modelling at the B3LYP/6-311++G\*\* level of theory.

**References**

[1] J. M. Cole, Zeitschrift Fur Kristallographie, 2008, 223, 4-5/2008.

[2] Hatcher, L. E., Bigos, E. J., Bryant, M. J., MacCready, E. M., Robinson, T. P., Saunders, L. K., ... Raithby, P. R., CrystEngComm, 2014, 16(35), 8263–8271.