

MS31-P05 | STRUCTURAL AND COMPUTATIONAL STUDIES OF A SERIES OF NEW PHOTOSWITCHABLE NICKEL NITRO COMPLEXES

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Transition-metal switchable complexes, thanks to the specific interactions and presence of molecular fragments that can exist in multiple isomeric forms, resulting in their interesting properties. Hence, the current study was devoted to a series of photoactive Ni(II) 8-aminoquinoline and pyridine complexes, which contain the NO₂ group bound to the nickel centre. The photoisomerisation reaction may undergo in the solid state under certain conditions. Understanding of the process' mechanism is a key step towards conscious development of photoswitchable materials.

The six presented complexes were examined crystallographically and computationally. They all crystallise in the centrosymmetric space groups belonging to the monoclinic and triclinic crystal systems. The crystals are stabilised majorly by π -stacking interactions and the C-H...O hydrogen-bond-like contacts involving the nitro species. The effect of small modifications of a molecular structure (e.g. introduction of the methyl substituent) on the crystal packing and intermolecular interactions was investigated. According to the Hirshfeld surface and reaction cavity analysis, there should be enough space in the crystal lattice to enable efficient switching between the NO₂ group coordination modes.

The intermolecular interactions were characterised energetically, especially these involving the nitro ligand. Additionally, the stability of different linkage isomers of the studied complexes was examined both for isolated molecule DFT calculations and employing the QM/MM approach. Both approaches prove that *endo*-nitrito isomer is more thermodynamically stable than the *exo*-analogue. The photoswitchable properties were confirmed by the photocrystallographic experiments.

Thanks the PRELUDIUM grant (2017/25/N/ST4/02440) of the NCN in Poland and The WCSS (grant No. 285)