MS33-P02

Applying fast, accurate lattice energies for molecular crystal structure prediction using CrystalExplorer model energies

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The interaction energy between two molecules can be understood as a sum of several discrete terms [1]: generally electrostatic, polarisation (or induction), dispersion and exchange-repulsion ($E_{tot} = E_{ele} + E_{pol} + E_{dis} + E_{rep}$). CrystalExplorer (CE) model energies [2], calibrated for use in intermolecular interactions, have been shown to estimate experimental crystal lattice energies [4] showing a favourable mean absolute deviation of only 6.6 kJ/mol from reference values in 110 crystal structures (the X23, G60, K7 and Z20 benchmark sets).

The relative energies of sets of crystal structures composed of the same molecular building blocks are of particular importance in crystal structure prediction (CSP), as lattice energy ranking is used as a primary predictor for the likelihood of a predicted structure being realized in the laboratory.

We investigate the potential use of CE lattice energies (and variations thereof) in CSP protocols – both in terms of relative energy ordering for different polymorphs and in terms of absolute energies – with reference to density functional and force-field based methods. Using CE lattice energies on the landscape of predicted crystal structures may constitute an accurate technique to improve predicted results, without the associated computational cost (and scaling) of periodic density functional calculations.

Keywords: Lattice Energies, CrystalExplorer, Polymorphism

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Synthesis, characterization and photochemical properties of a series of new Ni and Cu nitro complexes chelated by the (N,N,O)-type ligands

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Stimuli-responsive chemical systems in the solid state exhibiting specific photoactive properties have gained a lot of attention nowadays due to their potential technological applications (solar cells, LEDs, data storage assemblies, biological markers, etc.). It is, thus, of great importance to understand the phenomena behind the properties of interest, so as to design the desired materials and sensibly control their properties.

Hence here we present a detailed study of the photo-induced solid state linkage isomerism in a series of new Ni/Cu nitro complexes using spectroscopic methods (i.e., UV-vis, IR) physicochemical analyses (e.g., DSC), and advanced crystallographic approaches. The choice of these metals and substrates was dictated by their low price and abundance, which is in contrast to expensive literature-reported Rh or Pd complexes. [1,2] The desired photoswitchable materials should also be characterised by full conversions (100%), controllable reversibility, stability and preferably switching observable at temperatures closest to room temperature.

Our Ni complexes exhibit full conversion from the nitro to nitrito form when irradiated with the 590 nm or 660 nm LED light at 160 K, whereas the metastable state can be stable up to 240 K. To date, solely the Pd complex reported by Hatcher et al. [3] exhibited similar properties. In turn, the copper systems work best at 10 K, whereas the metastable form is usually stable up to 60 K, which makes them more difficult to be analysed and less applicable materials. It should be emphasized that the newly designed complexes can be relatively easily obtained and modified, and are fully air-stable.

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Figure 1.a) Molecular structure of the Ni^{II}–NO_2 complex based on the (N,N,O) chelating ligand at 100 K, **b)** Comparison of IR spectra for the ground and metastable state population at 10 K, for 590 nm LED.