

MS40-2-1 Photocrystallographic and spectroscopic studies of a simple photoswitchable $\text{Co}(\text{acac})_2(\text{imidazole})\text{NO}_2$ complex
#MS40-2-1

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Abstract

The importance of transition-metal photoswitchable complexes owing molecular fragments that can exist in multiple isomeric forms (e.g. NO_2 , NO or SO_2) is constantly increasing. Hence, in the current study new photoactive bis(acetyloacetato- O,O')(imidazole)nitrocobalt(III) complexes was designed and synthesized. Crystals of both cis and trans isomers of the studied compounds were obtained and structurally analysed. Multi-temperature X-ray diffraction and solid-state IR/UV-Vis spectroscopic experiments were conducted to determine optimal photoisomerisation reaction conditions. It occurred that almost full nitro-nitrito conversion was observed for the cis isomer after 365-405 nm LED irradiation in the 100 – 290 K temperature range, while for the trans isomer only small changes were observed in the solid-state IR spectra. The isomerization reaction progress was monitored using selected bands corresponding to the NO_2 vibrations, which were assigned based on normal-mode frequencies calculated at the DFT(B3LYP)/6-311++G** level of theory and literature contributions. Spectroscopic results were confirmed photocrystallographically using our homemade light-delivery device [1], which also enabled evaluation of the molecular structure of the metastable product – the exo-nitrito linkage isomer. The stability of the light-induced species was thoroughly examined.

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References

[1] Kamiński R. Jarzemska K.N. Kutyla S.E. Kamiński M. J.Appl.Cryst.2016, 49, 1383-1387

Figure 1: (a) Schematic representation of the cis isomer of title compound; (b) IR absorption spectra in the solid state after 405nm LED irradiation at room temperature; (c) schematic representation of the trans isomer of title compound.

