Title:	Solid-state photochromic arylazopyrazole-based transition metal complexes
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Abstract:	A new class of photoactive and chelating ligands L1–3 has been designed and synthesized by incorporating arylazo-3,5-dimethylpyrazole units in the ligand frameworks. Significantly, they are designed in such a way that azopyrazole units directly coordinate as neutral N-donor ligands. The resulting tri- and tetra-dentate chelating ligands have been complexed with a few transition metal ions (Ni2+, Cu2+, Co2+) to synthesize the complexes L1–Cu, L1–Ni, L2–Ni, L2–Co, L2–Cu, L3–Co and L3–Cu. The photoswitching properties of ligands and the complexes were explored using UV–vis and 1H NMR spectroscopy. The utility of azoheteroarene units provides remarkable advantages as the free ligands and their complexes show excellent forward and reverse photoisomerization in both the solid and the solution states, and considerably long thermal half-lives for the ZZ isomers, apart from intriguing photochromism. DFT calculations were performed on the ligands as well as on the metal complexes to estimate the difference in energy between the isomers and also to understand the nature of the metal–ligand bonding. Further TD-DFT calculations were performed to gain insights into the various UV–vis transitions observed.
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