Experimental charge and spin densities of the *p*-$O_2NC_6F_4CNSSN$ radical using joint refinement method

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The *p*- $O_2NC_6F_4CNSSN$ radical carries one unpaired electron delocalized on the thiazolyl ring and exhibits ferromagnetic order below 1.3 K (Luzon et al. (2010)). To investigate the magnetic interactions in the solid, high resolution X-ray and polarized neutron diffraction experiments have been carried out. The spin resolved electron density is modelled using the MOLLYNX program (Deutsch et al. (2012); Deutsch et al. (2014)), that allows simultaneous determination of both charge and spin densities.
This communication will detail the methodology used and the analysis of spin and charge densities and derived properties such as the electrostatic potential. Finally, the topology of the electron density will characterize intra and intermolecular interactions, especially those involved in magnetic pathways.

References

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