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Charge and spin density study of Ni(III) dithiolate complex

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In studied compound of (CH3P(Ph)3)[Ni(bdtCl2)2], the methyl triphenylphosphonium bis (3,6-dichlorobenzene-1,2-dithiolato) nickelate(1-) complex, the central atom coordination is square planar with nickel in oxidation state III [1]. A new method was recently developed for the combined refinement of a unique electron density model, based on the data provided by three complementary techniques: X-ray diffraction (XRD), polarized neutron diffraction (PND) and neutron diffraction (ND) [2]. Data collections for ND and PND were performed at 2 K on D19 and D3, respectively. X-ray diffractions experiments were performed by means of Stoe STADIVARI diffractometer equipped with a Dectris Pilatus 3R 300K and a Incoatec IμS Ag High Brilliance microfocus source (Ag-Kα, λ = 0.56083 Å) at 100 K using a nitrogen gas open-flow cooler Cobra Oxford Cryosystems. This method allows modeling both charge and spin densities from these three data sets and provides spin-resolved electron densities. Electronic structure and the results of AIM analysis together with the results of polarized neutron experiments will be discussed.

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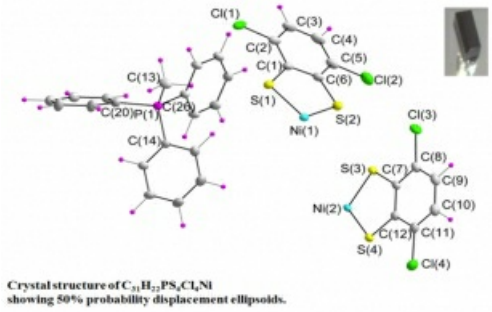
[2] M. Deutsch, N. Claiser, S. Pillet, Y. Chumakov, P. Becker, J.M. Gillet, B. Gillon, C. Lecomte & M. Souhassou, Acta Cryst. (2012) A68, 675-686; M. Deutsch, B. Gillon, N. Claiser, J.-M. Gillet, C. Lecomte, and M. Souhassou, IUCrJ (2014) 1, 194–199.



Crystal structure of $C_{38}H_{22}PS_4Cl_4Ni$ showing 50% probability displacement ellipsoids.

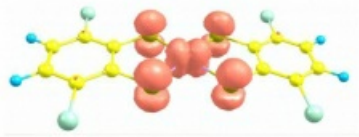


Fig. 1d Theoretical spin density from unrestricted DFT calculations. Isodensity value 0.002 e/Å^3.

Keywords: spin and charge density, nickel(III) complex, polarized neutrons