Poster Presentations

[MS13-P03] Charge Density Study of (CH3P(Ph)3)[Ni(bdtCl2)2].

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A wide range of technical applications of the dithiolate complexes, as well as their biological activity makes them interesting subjects for the research [1]. The complex (MeP(Ph)3) [Ni(bdtCl2)2] was prepared and his structure was determined by the means of single crystal X-ray diffraction. All X-ray data collections were performed on an Oxford Diffraction Gemini R four circle diffractometer, using Mo-Kα radiation at 100(1) K. ESR spectra of the (MeP(Ph)3) [Ni(bdtCl2)2] shows paramagnetic properties, which could be interpreted as unusual NiIII (d7 configuration) state of central atom. Magnetic measurements down to 2K shows that in Ni(III) complex there is one unpaired electron. A neutron diffraction experiment on the Ni complex was done very recent on the monochromatic D19 neutron diffractometer (ILL) with neutron radiation wavelength 0.948 at 15(2) K. Position of H atoms from the neutron experiment will be used for multipole refinement. Data collection strategy for charge density studies of (MeP(Ph)3) [Ni(bdtCl2)2] complex was as follows: 93 runs, 994601 diffractions, resolution till 0.46 . Data reduction was done by CrysAlis 171.35.19 and an average redundancy of 17.4 gives Rint 0.057 and R(σ) 0.024. The final refinement of crystal structure by SHELXL gives a R1-factor of 0.0192, for 6256 Fo > 4sig(Fo). After the multipole refinement R-values were: R(F)=0.0378 and Rall(F)= 0.0463 for all 194147 diffractions up to resolution 0.46 . The topological analysis was performed using XD package. This allows us to compare theoretical and experimental charge density as well as in the future (after having polarized neutron data) the experimental and theoretical spin densities in cooperation with our theoretical group, who has already published paper on theoretical spin densities [2].

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[1] Mrkvov‡ K., Kamen'ček J., Šindel‡ř Z., Kv'tek L., (2004). *Trans. Met. Chem.* **29**, 238 - 244.

[2] Hud‡k M., Jayatilaka D., Peraš'nov‡ L., Biskupič S., Kož'šek K. and Bučinsk. L., (2010). *Acta Cryst.* **A66**, 78-92.

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