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.


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