

CHEMICAL BONDING AND INTERMOLECULAR INTERACTIONS OF A NICKEL(II) COMPLEX

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A Nickel(II) complex, bis-(di-isopropyl-diseleno-phosphato)-Nickel(II), is a square planar complex, where Ni ion is bonded to four Se ligand. The electron density distribution is investigated by single crystal x-ray diffraction at 100K using Mo K α on a Kappa CCD diffractometer. It crystallized in space group is P-1, the inter-set agreement index, R_{int} , is 0.033, (total # reflections/unique reflection = 75997/11924) with the max resolution $(\sin\theta/\lambda)_{max}$ of 1.08 \AA^{-1} . The nickel atom is located at the inversion center. There are two different Ni-Se distances: one at 2.3615(6) \AA and the other at 2.3294(6) \AA . Interestingly, there is a short Se-Sc contact of 3.294 \AA between the neighboring molecules; which is roughly the same as intra molecular Se---Se contact distance. Thus there is a Se square network throughout the crystal. The aim of this study is not only looking into the chemical bonding interactions of this Ni complex but also search for the interesting intermolecular interactions through short contact of Se---Se interaction. The experimental electron density will be produced with multipole model. The electron density distribution of metal ligand and Se---Se interactions will be presented in terms of deformation density and respective Laplacian of density. The topological properties associated with bond critical points will also be discussed.