14-Diffraction Physics and Optics

Fig. 1. Charge densities of the three water molecules in NiSO$_4$·6H$_2$O. Water (1) is coordinated in the plane to Ni, water (2) is coordinated tetrahedrally to one Ni, water (3) is coordinated tetrahedrally to one Ni and one H-bond donor.

Fig. 2. Comparison of charge and spin densities around Ni$^{2+}$ in NiSO$_4$·6H$_2$O.

(a) RT
(b) 25 K
(c) 1.5 K


High-order low temperature X-ray diffraction data (Siemens P3/PC diffractometer, $\lambda_{Mo} = 0.71073 \AA$, T=100-150K) were collected for a long series of molecular crystals with different types of chemical bonds in order to elucidate some essential features of the electron density distribution (EDD) for these bonds. Among the organic compounds studied, highly strained spirocyclopropene derivatives (trihalogeno[1,3]diazirines] with an essential bond bending and new nitrogen-containing heterocycles (benzofuroxane, tetrazapentalene and tetrazine derivatives). An essential delocalization of the electron density in the π-regions was found in these aromatic heterocycles and the multipole analysis of EDD was performed. In the highly reactive phosphalkynes (Me$_2$N)$_2$C=PH$_2$, Cl$_2$C=P(N$_2$SiMe$_3$)$_2$, phosphalkyne Me$_2$C=C-P the position and orientation of the lone pairs at the P atoms was established. These compounds are low-melting liquids at ordinary conditions and suitable monocrystals were grown in situ from the melts directly or the diffractometer. Charge density analysis was also performed for carbanions (9-azido-9-carbarane,