06. CHARGE, SPIN AND MOMENTUM DENSITIES

06.7-8 ELECTRON DENSITY DISTRIBUTIONS IN Yb(CF₃SO₃)₃·9H₂O and Lu(CF₃SO₃)₃·9H₂O.

By A. Chatterjee, Department of Physics, University of Rajshahi, Rajshahi, Bangladesh.

It has long been held that the relative heaviness of the rare earth elements would limit the significance of X-ray diffraction analyses of their electron density in crystalline compounds. Their valence electron scattering is small in comparison to the total scattering. Present investigation showed that those rare earth compounds containing highly symmetrical crystal structures are not unfavourable for charge density work.

According to conventional wisdom, the 4f shell is highly symmetrical when it is half or completely filled. A completely filled 4f shell tends to be rather stable chemically, and it is suggested that 4f electrons play only a limited role in bonding.

The electron density distributions in crystalline Yb(CF₃SO₃)₃·9H₂O and Lu(CF₃SO₃)₃·9H₂O have been investigated on the basis of X-ray intensity data collected at room temperature (295 K). The perturbing effect on the metal environment due to bond formation was represented in a set of "deformation density" maps. The symmetry of the peaks in the immediate vicinity of the metal atom resembles that of a component of the tricontadipole (fifth order pole) resulting from a 4f-5d orbital product. Its close fit with the major features of the observed density suggests d-f hybridized bonding and is also consistent with the overall coordination geometry of the ligands. There is a lack of correspondence of the angular dependence of that fifth order pole further from the metal site.