06.X-01 CHARGE DENSITY STUDIES OF TRANSITION METAL ATOM CONTAINING SOLIDS.* By Philip Coppens, Department of Chemistry, State University of New York at Buffalo, Buffalo, New York 14214, USA.

Analysis of the errors in observed deformation densities leads to the conclusion that even though estimated standard deviations (e.s.d's) are larger near heavier atoms than near light atoms in the same crystal, e.s.d's in the vicinity of the atoms may vary little with atomic number when the heaviest atoms in different crystals are compared. In accordance with this result an increasing number of studies of transition metal atom containing solids have been performed in a number of laboratories. The experimental data have been used to derive d orbital occupancy within the crystal field approximation, to assess the effect of covalency in metal-ligand bonding and to study the nature of metal-metal bonding. They may be combined with other physical information as derived for example by Mossbauer or NQR spectroscopy.

Solids which will be discussed include a limited number of alloys and metal oxides, and a number of metalloorganic and coordination complexes exhibiting various degrees of metal-metal bonding.

Derived net atomic charges indicate the values to be quite dependent on the definition of atomic volume or the choice of atomic scattering factor. However, they are meaningful within a series of compounds once a specific definition has been selected.

For analysis of metal-ligand bonding a reference state described as the procomplex, in which bonding within the ligands has been allowed for, offers advantages over the commonly used promolecule reference state.

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06.X-02 MAGNETIC NEUTRON SCATTERING IN TRANSITION METALS AND THEIR COMPOUNDS. By P.J. Brown, I.L.L., 38042 Grenoble Cedex, France.

From magnetic neutron scattering one may obtain information about magnetic structure and magnetization distribution in solids having unpaired electrons. The polarized neutron technique thus compliments X-ray experiments and allows one to analyze magnetic interactions in transition metals, covalency in complex ions and therefore electronic structure of magnetic solids. The methods used in analyzing data are quite similar to those used in charge density studies. Several examples will be described which cover the case of metals, alloys and complex ions. The relationship between these types of experiments and other observations will be discussed.

06.X-03 ELECTRON DENSITIES IN MOMENTUM SPACE OF TRANSITION METALS AND THEIR COMPOUNDS.* By Stephan Berko, Brandeis University, Physics Department, Waltham MA 02254, USA.

The electron density in momentum space, $\rho(\vec{p})$, can be obtained from a measurement of the energy profiles of Compton scattered X-rays or γ-rays and from the angular correlation of 2γ-annihilation radiation in positron experiments. $\rho(\vec{p})$ is related to the square of the Fourier transform of the electron wavefunction in real space and thus provides information independent from the charge distribution obtained by diffraction experiments. The relationship between $\rho(\vec{p})$ and the electronic band structure will be discussed with examples drawn from recent experiments on transition metals and transition metal compounds. In metals the Fermi surface manifests itself as discussed in $\rho(\vec{p})$. In discussing insulators use can be made of the "$B(\vec{r})$" function, i.e. the Fourier transform of $\rho(\vec{p})$, which gives the autocorrelation of the wavefunction in real space.

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06.X-04 RECENT TABULATIONS (X-RAY MASS ATTENUATION DATA). By J.H. Hubbell, National Bureau of Standards, Washington, D.C. 20234, U.S.A.

The x-ray attenuation coefficient tables (Sec. 2.1, Hubbell et al) in the International Tables for X-Ray Crystallography (Vol. 4, 1974) are discussed and compared with other compilations, with theoretical estimates, and with recent measurements within and outside the crystallographic literature. Included in these measurements are some preliminary results from the X-Ray Attenuation Project (D.C. Creagh, Chmn.), inaugurated at the 1978 Warsaw IUCr Congress under sponsorship of the Commission on Crystallographic Apparatus, discussed in more detail elsewhere in this Microsymposium. Present theoretical knowledge of the individual photon-atom interactions (atomic photoeffect and pair and triplet production, in addition to scattering theory discussed in more detail elsewhere in this Microsymposium) is reviewed over a wide range of photon energies (100 eV to 100 GeV). Uncertainties in present tabulations are estimated as a function of photon energy and atomic number (Z = 1 to 100), and regions in most urgent need of further theoretical and/or experimental work are pointed out.