06.X-1 RECENT CHARGE DENSITY STUDIES[†]. By E. D. Stevens, Department of Chemistry, University of New Orleans, New Orleans, LA 70148, U.S.A.

Accurate x-ray intensity measurements have the potential to provide unique experimental information on the electronic structures of molecules and solids. As the accuracy of such studies gradually improves, experimental electron density measurements are being applied to an increasingly broad range of problems in physics, chemistry, and biology. Studies of inorganic and organometallic complexes including elements up through the second row transition metals are now routinely reported. Studies of moderately large molecules (up to 200 atoms) of biological interest also appear possible without excessive difficulty. The problem associated with the uncertainty in phases of reflections from acentric structures can be adequately overcome using multipole refinement techniques. A survey of recent experimental results will be presented.

The most interesting and challenging task for the future will be to use experimental electron density distributions to predict other molecular properties and especially chemical reactivity. The molecular electrostatic potential, a property which may also be obtained from x-ray diffraction data, is currently being studied as a means of estimating intermolecular interactions and the initial steps in chemical reactions. Several examples of experimental electrostatic potentials will also be presented.

[†]Research supported by grants from the National Institutes of Health and the National Science Foundation.

06.X-2 ACCURATE STRUCTURE FACTORS FROM PERFECT CRYSTALS. BY N. Kato, Department of Physics, Meijo University, Nagoya, Japan.

Pendellösung methods can determine crystal structure factors with an extremely high accuracy on the absolute scale. Since the early work of HKKK (J. Phys. Soc. Jpn., 1965, 20, 988), various methodologies have been proposed. Neither, however, seems absolutely superior than others and each has its own merits and demerits. More important are how and what experimental cares have been paid.
The accuracy has been improved about one decimal in the past two decades. It is estimated to be better than 0.05% in the best case of Si (Tanemura and Kato, Acta Cryst. A, 1972, 28, 69; Aldred and Hart, Proc. R. Soc. London A, 1973, 332, 223 and 239; Teworte and Bonse, Phys.Rev.B, 1984, 4, 2102; Saka and Kato Acta Cryst. A, 1986, 42, 469). Incidentally, in the neutron case (Shull, 1975), the nuclear scattering amplitude was determined with accuracy of 10^{-5}.
The measurable order of reflections is high as (8.8.8) (Hart, 1987, private communication). The measurement is explored to diamond, Ge, Al, Cu, Zn, InP, GaAs and quartz (Takama and Sato's group, Acta Cryst. A, 1980~1986). If one satisfies with the accuracy level of 0.5%, no longer the applicability is confined to the lower reflections of Si, as it was in 1965.
The most serious obstacle in the measurement is a long range strain. For obtaining the charge distribution from Fg values, the accurate knowledges of anomalous dispersion (f'+if") is required. As a case study, the experiment of Saka and Kato (1986) on Si together with the experimental work (Saka and Kato, Acta Cryst. A, 1987, in printing) and theoretical work (Omote and Kato, Acta Cryst. A, 1987, in printing) on f' will be reviewed. Fig.1 is the difference Fourier synthesis, in which Fg values of 30 reflections plus the 222 value of Fehlman and Fujimoto, (J. Phys. Soc. Jpn., 1975, 38, 208) are employed. All data are obtained by Pendellösung methods without additional modifications except of f' values calculated by Cromer and Liebermann (Acta Cryst. A, 1981, 37, 267).

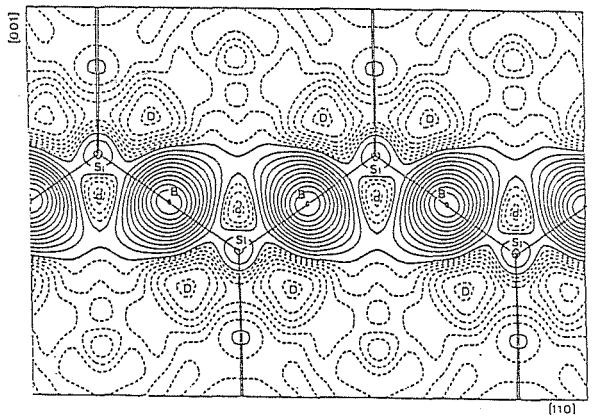

Fig.1. DFS map of Si. The step is 0.02 and 0.01 e/Å^3 for positive and negative contours of the deformation charge, respectively.

06.X-3 DETERMINATION OF MAGNETISATION DENSITIES IN VERY WEAKLY MAGNETIC SYSTEMS. by P.J. Brown, Institut Laue Langevin, Grenoble France.

One important advantage of using polarised neutrons to measure magnetisation densities is that it enables very weakly magnetic materials to be studied. This property of the polarised neutron technique has been exploited to probe the origins of the magnetisation process in some weakly paramagnetic and some diamagnetic systems. When the magnetic scattering is very weak it is not feasible to measure in a reasonable time a complete, or even a nearly complete set of magnetic structure factors. It is therefore necessary to analyse the few data available using fairly simple models which incorporate physically or chemically important parameters.

The possibility of obtaining useful information from rather sparse data will be illustrated using as examples the weakly paramagnetic cluster compound Nb_6I_{11} and the diamagnetism of carbon rings in graphite and napthalene.

As a further example of the use to which the sensitivity of the polarised neutron technique can be put, results obtained using the neutron spin-orbit interaction to probe acentric charge distributions will be reported.