06.1—2   DESIGN OF AN X-RAY SPECTROMETER FOR IN-ELASTIC SCATTERING EXPERIMENTS. By P.Pattison and W:Weyrich, Faculty of Chemistry, University of Konstanz, W.Germany.

We describe the performance parameters for an X-ray spectrometer which has been designed for inelastic, Compton scattering experiments in the energy range around 20 keV. For these relatively low energy X-rays, photoabsorption limits the choice of suitable samples to those containing predominantly elements up to the first transition metal series. Test results will be presented for single crystals of LiF, Be, Al and Si.

The spectrometer operates in a scanning mode, where focussing X-ray optics can be employed most efficiently. The radiation source is a 1.8 kW fine-focus Mo X-ray tube, followed by a fixed geometry logarithmic spiral Si (111) monochromator which selects the $MoK\alpha_1$ radiation. The monochromator delivers a photon flux on the sample of about 4×10^9 photons/sec in the $K\alpha_1$ line. The sample is positioned on the focal circle of a Johann curved crystal analyzer with a bending radius of 823mm. Using the Si (444) reflection, the achieved resolution of 60 eV at 17.5 keV provides a momentum resolution of 0.25 Å, in the measured Compton profile. The peak count-rate for a LiF sample, for example, is around 200 photons/sec, yielding a mean Compton count-rate of 50 counts/sec. This implies a measuring time of about 2 days for a data-set with 10^7 counts per profile. The reconstruction of the three-dimensional momentum density requires as input a minimum of about 10 directional Compton profiles (depending on the system under investigation, and the experimental resolution), resulting in a three-week measuring period for a full data-set. In comparison with earlier X-ray Compton spectrometers, the present system has several advantages which stem from the focussing optics. The primary radiation on the sample is monochromatic (within the natural line-width) and it is focussed, which reduces the required sample size dramatically. Even allowing for the intensity loss associated with the use of a monochromator, the Compton intensity on the detector is about a factor of 10 higher than the intensity achieved using a planar crystal analyzer without monochromator.

The combination of good resolution and statistics reached with this type of X-ray spectrometer provides us with a useful alternative to gamma-ray Compton spectroscopy, where the resolution is detector limited. The use of standard X-ray equipment implies that the spectrometer is an economical, in-house instrument which can easily be constructed in any X-ray laboratory.

06.1—3   DETERMINATION OF MOMENTUM DISTRIBUTIONS IN LIQUIDS AND SOLIDS USING A SPALLATION NEUTRON SOURCE. By P. E. Sokol, R. O. Simmons, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA, D. L. Price and R. O. Hilleke, Argonne National Laboratory, Argonne, Illinois, USA.

High flux spallation neutron sources have made inelastic scattering experiments possible at energy and momentum transfers higher than those readily accessible to reactor based sources. These high energy and momentum transfers allow us to approach the impulse limit and determine the momentum distribution of the scatterers directly. However, the asymmetry in the time distribution of neutrons emitted by a pulsed source causes problems in the determination of the dynamic structure factor from the experimental data. We will present a method for removing the effects of the incident neutron spectrum, as well as the geometrical effects, from the raw data. This allows us to accurately obtain the dynamic structure factor and the momentum distribution of the scatterer. Liquid and solid helium provide an ideal test case. The light mass and low binding energy of the helium atoms allow us to reach the impulse limit with modest momentum transfers of 15 A^{-1}. We will discuss the application of our procedures to these cases, and compare our results to the best present calculations for the momentum distributions.

06.2—1   COMPUTATIONAL CHEMICAL STUDIES OF THE PHOSPHORIC ACID MOLECULE IN CRYSTALLINE PHOSPHORIC ACID. By G. Moss and R. H. Blessing, Medical Foundation of Buffalo, Inc., 73 High Street, Buffalo, NY 14203, USA.

While numerous electron density studies of molecules containing first row atoms can be found in the literature, relatively fewer studies have been made of molecules containing second row atoms. As a preliminary to experimental electron density studies of metabolic phosphates we have performed a theoretical study of the phosphoric acid molecule in crystalline phosphoric acid in order to address the questions: (1) what new effects, if any, does a second row atom present to electron density studies, and (2) how extensively parameterized a pseudoatom model is required for a multipole analysis of the electron density.

Static structure factors have been calculated for the experimentally determined unit cell (Cole, F. E. (1966) Ph.D. Dissertation, Washington State University). The *ab initio* calculation of the phosphoric acid molecule with the crystal-structure geometry employed an extended basis set augmented with polarization functions. A multipole analysis of these structure factors has been made using the formalism of Hirshfeld (Hirshfeld, F. L., Israel J. of Chemistry (1977) 16, 168). The dependence of the pseudoatom fit on limited resolution, artificial parameter constraints and level of multipole expansion has been studied. The results show that, in this case, only the phosphorous pseudoatom requires multipole functions to fourth order.