12.X–5 POWDER PATTERN RECOGNITION AND STRUCTURE-SENSITIVE SEARCH-MATCH PROCEDURES. By Ludo K. Frevel, Department of Chemistry, The Johns Hopkins University, Baltimore, Maryland 21212, U.S.A.

A review will be presented covering the various methods for obtaining crystallographic information from the powder diffraction data of a single crystalline phase: appropriate nomograms for indexing uniaxial phases, application of the theory of homology to the splitting of hkl reflections, use of semilogarithmic charts (log d_ν versus I_ν) for establishing isomorphism with prototype crystal structures, computer programs for indexing powder patterns, and the applicability of calculated powder patterns. For multiphase powder patterns several SEARCH-MATCH strategies will be addressed. The crystallographic approach rather than the empirical "fingerprint" scheme will be emphasized. Two novel structure-sensitive SEARCH-MATCH programs will be outlined.

12.X–6 COMPARISON OF DIFFERENT EXPERIMENTAL TECHNIQUES USING THE RIETVELD METHOD. By B.T.M. Willis, Atomic Energy Research Establishment, Harwell, Oxfordshire, England.

In the Rietveld method of analysing powder diffraction data, the crystal structure is refined by fitting the entire profile of the diffraction pattern to a calculated profile. The method has been employed in all four categories of experimental technique, in which neutrons or X-rays are used as the primary source of radiation and in which the radiation is scattered at a fixed wavelength or over a wide range of wavelengths (Albinati and Willis, J. Appl. Cryst. (1982) 15, 361-374).

We shall discuss the relative merits of these different techniques and indicate where further improvements are desirable. We shall also refer to a problem which continues to provoke controversy, viz. whether the estimated standard deviations given by the conventional Rietveld analysis are valid or not.

12.X–7 COMPARISON OF PEAK ANGLE MEASUREMENTS OBTAINED WITH GUINIER CAMERA AND COUNTER DIFFRACTOMETER. By A. Brown, Studsvik Energiteknik AB, S-611 82 Nyköping, Sweden, and C. M. Foris, E. I. du Pont de Nemours & Co., Central Research and Development Dept., Wilmington, Delaware 19898, U.S.A.

Powder diffraction patterns are, in general, recorded by two primary methods. The camera utilizes x-ray sensitive film while the diffractometer employs a detector/slit system which is moved through the required angular range. Each approach has advantages and can also fulfill complementary functions in powder analysis and characterization. Both film and detector methods are subject, however, to systematic errors in intensity and 2Θ measurements. For the results to be compatible these errors must be identified and corrections applied. Errors in 2Θ can cause serious problems in the study of compositional variations in solid solutions and in phase identification and characterization. This is particularly so at a global level since published data for a compound may be referred to as a means of checking purity. A comparison has been made of 2Θ data obtained with different Guinier cameras and automated diffractometers. The Guinier cameras had subtractive geometry in common but were of different manufacture and/or cassette radius. Different methods were also used to measure the films. The diffractometers were set up with different configurations of the diffracted beam monochromator and the automatic divergence slit. The aim was to find procedures to reconcile 2Θ measurements obtained with these two techniques. The criterion is the precision of the cell parameters for several common materials and the agreement of results produced by the two approaches. The precision with which 2Θ can be estimated for an individual x-ray reflection and the systematic errors in this estimate have also been studied. Such errors can be produced by a possible non-linearity of the angular scale as well as specimen-dependent and/or instrumental factors. The silicon standard, SRM 640, was used as an internal calibrant for the Guinier films. Cell parameters for the same materials have been obtained from diffractometer measurements which were corrected for specimen transparency and displacement, flat specimen error, and beam divergence by purely numerical methods. Under suitable conditions, parameters obtained by these two techniques have deviations of 0.002% or less and agreement is within these limits. The procedures for achieving this level of agreement are discussed.