PS18.06.09 NEUTRON ATTENUATION CORRECTIONS FOR THE PARIS-EDINBURGH HIGH PRESSURE CELL. W.G.Marshall*, R.J.Nelmes*, J.S.Loveday*, J.M.Besson#. S.Klotz# and G.Hamel@. *Department of Physics and Astronomy, The University of Edinburgh, Edinburgh, EH9 3JZ, U.K.; #Physique des Milieux Condenses (CNRS URA 782), Universite P. et M. Curie, 4 Place Jussieu, Paris, France; @Departement des Hautes Pressions, Universite P. et M. Curie, 4 Place, Jussieu, Paris, France.

For data collected using the Paris-Edinburgh cell and time-of-flight neutron diffraction, it is important that accurate attenuation corrections are applied if reliable structural and thermal parameters are to be obtained. Because a direct measurement of the cell attenuation is time-consuming and can be made for only a limited number of sample/cell configurations, the approach followed has been one of performing a direct, first principles, calculation.

Direct calculation of the cell attenuation is a non-trivial problem: in general the attenuation is a function of not only the anvil and sample material, but also the neutron wavelength and the scattering angle. The results of a number of detailed experimental tests of the calculations, including direct measurements of the attenuation using a sample of vanadium, will be presented.

As a result of this effort, it is now possible to carry out, with confidence, full structural refinements of the high-quality diffraction data collected using the Paris-Edinburgh cell at pressures up to 25 GPa. This will be illustrated with results from a number of recent studies which rely heavily upon the accuracy of the attenuation calculations.

PS18.06.10 HIGH-PRESSURE STUDIES WITH KUMA. Damian Kucharczyk and Andrzej Katrusiak+, KUMA Diffraction, Akacjowa 15b, 53-122 Wroclaw, Poland; +Department of Crystal Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznan

A new programme for measuring reflection intensities of the crystals enclosed in high-pressure diamond-anvil cells of the Merrill-Bassett type has been prepared for the KUMA diffractometers. The main objective was to minimize the effects of high-pressure cell absorption [L.W.Finger and H.King, *Am. Mineralog.* 63 (1978) 337], and of the extinction of the diamond anvils [J.S.Loveday, M.I.McMahon and R.J.Nelmes, *J. Appl. Cryst.* 23 (1990) 392], without significantly prolonging the data collections. The programme contains several options allowing one to tackle the experimental difficulties. It is also aimed at facilitating the high pressure studies. It was demonstrated, that good quality structural data of the accuracy comparable to those from ambient-pressure measurements on bare crystals could be obtained in the preliminary high-pressure study on pentaerithritol, i.e. 2,2-bis(hydroxymethyl)-1,3-propanediol, crystals [A.Katrusiak, *Acta Crystallogr.* B51 (1995) 873].

PS18.06.11 IPA, A PROGRAM FOR PROCESSING POWDER DIFFRACTION IMAGES Ken Lagarec and Serge Desgreniers, Département de physique, Université d'Ottawa, Ottawa, CANADA, K1N 6N5

We describe a program and the underlying algorithms for processing powder diffraction images recorded on phosphor imaging plates (currently digitized by the FUJI BAS2000 laser scanner). The code, written in object-oriented C++, takes advantage of the recent availability of inexpensive and fast PCs and runs under the widespread Windows graphical interface. In order to produce, as the final goal, a 2Q-profile usable for refinement (e.g. a Rietveld analysis), the program accomplishes four main tasks on a digitized image showing partially complete Debye traces: i. a simplified image manipulation (e.g. loading, zooming, contrast enhancement, artefact removal); ii. image center finding, sample-to- detector calibration and calibration of the orientation of the image plane with respect to the incident X-ray beam direction; iii. intensity integration along the Debye traces; iv. azimuthal intensity profile generation. Algorithms used for planar orientation calibration and integration are partially based on a method described by Piltz *et al.* [1]. As an example, we show a powder diffraction image of a mixed sample of HfO_2 (monoclinic)/Mo (bcc) loaded in a Merrill-Bassett diamond anvil cell recorded at CHESS D1: the 2Q-profile generated by IPA is excellent as ascertained by a full Rietveld analysis.

[1] Piltz, R. O., McMahon, M. I., Crain, J., Hatton, P. D., Nelmes, R. J., Cernik, R. J. and Busnell-Wye, G., Rev. Sci. Instrum. **63**, 700 (1992).