K13 **Robotics and E-Science; Their Impact on Crystallography.** Colin Nave, *CCLRC Daresbury Laboratory, UK. E-mail: c.nave@dl.ac.uk*

**Keywords: Automation; Robotics; e-Science**

There is a long history of automation in crystallography with the development of computer controlled diffractometers being a good example of how automation can make data collection easier to carry out, faster and more reliable. These advantages apply to more recent developments in crystallography with robotic systems being applied to both sample preparation and crystallographic data collection. Automatic structure solution software has been in place some time for small molecule crystallography and is now being developed and applied for protein crystallography. These developments will enable significant changes to occur in the way structure determination by crystallography is carried out. Automation of the various stages makes it possible to link facilities for sample preparation, crystallisation, x-ray data collection, structure solution and structure deposition. These facilities could be in distant locations and the requirement is to allow collaborators to monitor and control the process, in a secure manner, from their home laboratory (or home). This is an example of the e-science concept which aims to provide necessary facilities for science over the internet. A description of such an approach, for the case of protein crystallography, will be given and examples from other crystallographic fields will also be covered. The difficulties with such an approach, as well as the advantages, will be described.

K14 **Neutron Scattering at High Pressure.** Stefan Klotz, *Physique des Milieux Condensés, Université P&M Curie, B77, 4 Place Jussieu, 75252 Paris, France. E-mail: Stk@pmc.jussieu.fr*

**Keywords: Neutron Scattering; High Pressure; Crystallography**

In this talk I will review the state of the art of neutron scattering under high pressure. Major progress in high pressure techniques and neutron instrumentation during the past decade now allows detailed crystallographic studies on a wide variety of fairly complex systems. The achievable pressures in such studies are several 10 GPa, and measurements under simultaneous high pressure and high temperatures up to 2000 K have been carried out. I will illustrate these possibilities by a number of recent powder neutron diffraction studies on simple molecular solids, minerals, magnetic systems, and even amorphous solids and liquids. Although most of this work concerns techniques exploiting the capability of the “Paris-Edinburgh” high pressure cell, complementary techniques using sapphire and diamond anvil methods will be presented. Prospects of single crystal techniques under high pressure will be discussed.