PS03.02.08 A TECHNIQUE TO RECOVER MISSING SCATTER INTENSITY INFORMATION AND REDUCE NOISE, REQUIRING NO *A PRIORI* KNOWLEDGE by Gary K Doherty[1] and George A. Poland[2] [1]Saacke Combustion Systems Ltd. Marshland Spur Farlington Portsmouth PO6 1RX England [2]University of Portsmouth PO1 2RY England.

A new technique is presented which recovers missing scatter intensity data, reduces the noise levels of the measured points and estimates the incoherent level when applied to experimental small angle scattering data.

The method differs from those of other authors in that only the measured data is used; no parameters need to be supplied, such as the number of splines or sinusoids to use, and no initial estimates of particle dimensions are required. The technique takes a new view of the work presented in Doherty & Poland (1996), both simplifying and extending the application of the same underlying principle.

Doherty, G. & Poland, G. A. (1996). *J. Appl. Cryst* **29**, 53-60

PS03.02.09 XTAL3.4: NEW RELEASE OF THE XTAL SYSTEM. S.R. Hall and D. du Boulay, Crystallography Centre, U. of Western Australia, Nedlands, 6009 Australia; G.S.D. King, Fisica-Chemische Geologie, KU Leuven, B-3001 Heverlee, Belgium; J.M. Stewart, Chemistry, U Maryland, Washington DC, USA; J.R. Hester, NIRIM, Namiki 1-1, Tsukuba, Ibaraki 305, Japan; and D. Grossie, Chemistry, Wright State University, Dayton OH, USA

The Xtal System is an integrated package of crystallographic programs for single crystal structure analysis. It facilitates calculations from processing raw diffraction intensities to the preparation of the publication diagrams, tables and submission files. For some calculation steps, several programs employing different algorithms are provided, enabling a choice of approaches and the ability to cross-check results. All calculations are integrated and share a common archive file.

Xtal3.4 is distributed at cost on an ISO-9660 CD-ROM and may be implemented on any computer supporting a Fortran and C compilers, and X11 graphics libraries. Executables are provided for the most unix, linux, VMS or DOS operating systems. The sources files are also supplied with implementation scripts so that Xtal3.4 may be installed on other machines, or adapted to locally available software.

User support is mainly via internet facilities. A web server provides users with the latest Xtal information. The WWW address is http://www.crystal.uwa.edu.au/xtal/. Newsletters will be airmailed as hardcopy to users but new and updated sources will be available via anonymous FTP from ftp.crystal.uwa.edu.au directory /xtal. General queries should be directed to xtal@crystal.uwa.edu.au.

PS03.02.10 DIRECT-SEARCHER SYSTEM (Ver. 3) FOR SOME ORGANIC COMPOUND ON PERSONAL COMPUTERS. K. Okada[1*)] and S. Okada[2)]. 1)Research & Development Center, Ricoh Co. Ltd., Tsuzuki-ku, Yokohama 224, Japan, 2)Faculty of Engineering, Science University of Tokyo, Shinjuku-ku, Tokyo 161, Japan.

The Direct-Searcher system version 3 (DS*System3) has been developed for automatic structure analysis of some organic compounds running on personal computers (PC). The DS*System3 running on Windows NT is the latest version developed for Cray-1 / CDC6600 (Ver.1, J.Chem.Soc.B,1969,940; Acta Cryst.1990, A46, C70) and mainframe / workstation / PC (Ver.2, Comput.Chem.1995, in press). An organic chemist as well as a crystallographer can get results very easily with his own well-known PC. This system consists of more than twenty crystallographic programs, and each program is improved and re-written in the Fortran language. The logical structure of DS*System3is simplified as three layers by using common and independent libraries for easy maintenance. The major improvements are: Loose limitation of no. of atoms, reflection and equiv.position; Color display; Plotter output; Change peak find algorithm; Adopt data base for space group and atomic scattering factor; add CIF facility; bag fixing. We found that the molecular skeleton takes usually less than 2 min with heavy-atom analysis (PSL3+Searcher3) and 15 min with direct methods (Dircter3) by a Pentium 100PC. Comparing the computational speed, the PC has a capability of 1.55 times a Cray-1, 3.93 times a HP9000/755,7.43 times a IBM3090-200E and 33.2 times a CDC6600. The crystal structure analysis of organic compounds has been carried out more than fifty with the heavy-atom analysis and more than thirty with the direct methods.

PS03.02.11 RESOLUTION ENHANCEMENT IN POWDER DIFFRACTION USING STABLE DECONVOLUTION. Derk Reefman, Philips Research, Prof. Holstlaan 4, 5656 AA Eindhoven, The Netherlands

A recently developed method will be presented for enhancing the resolution in powder diffraction to approximately 0.025 degrees 2theta, without loss of intensity. Enhancing the resolution in powder diffraction has always been a driving force for the development of sophisicated optics in the beam path of the X-Rays, like monochromators, mirrors, etc. This equipment has contributed significantly to the improvement of the resolution of todays diffractometers. Nevertheless, the everincreasing demands set by the increasingly complex materials which have to be characterized, ask for even higher resolution. For that reason, synchrotrons are extensively used nowadays.

However, the time allocation for a particular experiment on a synchrotron is limited and one would like to perform experiments with laboratory-equipment without significant loss of resolution. An approach to achieve this is to obtain the instrument function of the equipment of interest, and to correct the measured pattern for the instrumental aberrations. A classical method used to this end is the fourier approach of Stokes. This method has the drawback of becoming unstable for resolution enhancements by more then a factor of 1.5. Recently, it has been shown that application of Maximum Entropy (ME) deconvolution techniques can be used for resolution enhancements up to a factor of 3. A problem however are the computational resources needed. Nevertheless, continuing effort in this direction has now led to a method which, based on ME as well, provides robust access to a way to enhance the resolution of a complete wide range pattern within minutes.

PS03.02.12 EXPERIENCES PORTING CRYSTALLOGRAPHIC SOFTWARE TO MODERN USER INTERFACES: A WINDOWS VERSION OF THE *NRCVAX* PACKAGE. Peter S. White, Department of Chemistry, University of North Carolina, Chapel Hill, NC 27514, U.S.A. and Eric J. Gabe, Steacie Institute for Molecular Structure, National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada

NRCVAX is a complete suite of programs for the solution and refinement of crystal structures, designed to compile and run on a wide variety of computers. This has been achieved by writing the code in standard Fortran 77 and isolating any potential machine dependencies. The package relies on the operating system to provide a mechanism for starting routines which are interconnected by files containing the crystal and reflection data. The user interacts with the individual routines by means of a series of questions and answers. The system, whenever possible, suggests reasonable default answers which can be selected by pressing return.

This user interface is extremely powerful and easy to use, however, it is fast becoming an unnatural environment for new users,