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was inversely proportional to \bar{s} (the mean reciprocal radius for the observed reflections) and to \sqrt{p} (where p is the difference between the number of observed reflections, N_r , and the number of refined parameters, N_p). Further, $\bar{\sigma}(A)$ is shown to be proportional to the R-factor and to \sqrt{ZA} , where ZA is the number of atoms of A needed to give a scattering power at s which is equal to the scattering power of all atoms in the asymmetric unit.

The possibility of estimating $\bar{\sigma}(A)$ using some equation similar in form to that of Cruickshank is of interest in screening entries in the Cambridge Structural Database (CSD) prior to their inclusion in data analysis projects. The esd's of individual coordinates have only been included in the CSD for structures published since 1985. The only precision indicators available for ALL entries are the R-factor and a flag (AS) which categorizes the mean esd of a C-C bond length into four numerical bands: 0.001-0.005 (AS = 1), 0.006- 0.010 (AS=2), 0.011-0.030 (AS=3), and 0.031 and above (AS=4). Not only are the upper bands too broad, but AS is also unavailable for some 16% of CSD entries. Preliminary attempts to estimate $\bar{\sigma}(C-C)$, and hence $\bar{\sigma}(C)$, were described briefly by Allen & Doyle [Acta Cryst.(1987), A43, C291] but the number of entries having coordinate esd's was then too small (ca. 4000). We now extend the study to encompass the ca. 25,000 entries having esd's and with $R < 0.080$ that are currently available.

We have used the methods of correlation, simple linear regression and multiple linear regression to study the relationship between $\bar{\sigma}(C-C)$ (the dependent variable) and a variety of 'independent' variables which are available in each CSD entry or which can be calculated from the stored information. These include such items as: R-factor, Z_{max} (the maximum atomic number in the structure), ZA (as defined by Cruickshank), T (the temperature of data collection), N_a (the number of atoms in the asymmetric unit), etc. We find that only the R-factor and some function of the atomic numbers (Z) are sufficiently independent for use in regression procedures.

For a dataset of 25959 entries with $R < 0.08$ and $\bar{\sigma}(C-C)$ in the range 0.001 to 0.040, we find that an expression of the form:

$$\bar{\sigma}(C-C) = k R ZA$$

will estimate 75.5% of $\bar{\sigma}(C-C)$ values within 50% of their reported values (79% within + or - 0.005A of their reported values in absolute terms). Results obtained with regression expressions of the form

$$\bar{\sigma}(C-C) = a + k R ZA \text{ or } \bar{\sigma}(C-C) = a + bR + cZA$$

are marginally less effective estimators.

For 687 of these entries, we have added values of N_r/N_p (no. of observed reflections/no. of refined parameters) directly from the literature (these values are not available in the CSD). Here again the simplest regression, now $\bar{\sigma}(C-C) = k R ZA / (N_r/N_p)$ to follow Cruickshank's general philosophy, provides the best estimation, with 84.4% of the $\bar{\sigma}(C-C)$ being estimated within + or - 50% of their reported values (86% within 0.005A of the reported values in absolute terms).

A variety of graphical and numerical statistics concerning structural precision will be presented as general background to the correlation and regression experiments.

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SOFTWARE FOR X-RAY AND NEUTRON DIFFRACTION EXPERIMENT. By V.E. Anisimov, N.B. Bolotina, L.F. Malakhova*. Institute of Crystallography of Russian Academy of Sciences, Moscow, Russia.

New software was developed for certain 4-circle X-ray and neutron diffractometers controlled by a PC computer. The software is based on measurement techniques developed in our and other structural labs, experience of the diffraction measurements and capabilities of the PC computer. Some procedures of diffraction intensity measurements for perfect high symmetrical crystals, for

incommensurate modulated phases, for twins, for samples with restricted angle settings (eg. in diamond cell), for intensity distribution measurements in given part of reciprocal space are involved.

The software contains an effective procedure of automated unit cell determination, measurements in the general geometry of angle setting (azimuthal rotation) (Bolotina N.B. Kristallografiya, 1989, 34, 4, 993, Bolotina N.B., Chernaya T.S., Golubev A.M. Kristallografiya, 1990, 35, 2, 303) and correct calculation of optimum measurements time. Comprehensive calculation and results of the measurements are collected in the expanding table which is suitable for subsequent analysis and treatment of experimental information. The software is written in FORTRAN and MS-DOS system.

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RUNNING XRS-82 RIETVELD SYSTEM IN PC LEVEL MICRO COMPUTER UNDER MS-DOS OPERATING SYSTEM By Yihua XU.

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The XRS-82 Rietveld system is a useful package of programs for structural parameters refinement of powder diffraction data with whole pattern. The system had been written by Prof. Ch. Baerlocher and about fifty authors had great contributions (Ch. Baerlocher. The XRS-82 X-ray Rietvelds System. Institut fuer Kristallographie, ETH. Zurich, Switzerland). Many structures, especially for zeolites, had been refined by the system and good results obtained. Unfortunately it seems there are some limits to use the system; 1. The system needs a large memory of the computer. So only a few research workers, who have a big or super-computer, can use the system. 2. The system needs a set of step scan diffractometer data collected on a diffractometer. So the computer should be connected with a diffractometer or else the scanning data should be transmitted into the computer. It is not easy to do it for a big or super computer. 3. It is too expensive for running the system in large or a super computer. 4. Some programs for display and drawing must be modified in different computers, that is time-consuming. As it is well known, the micro personal computers, such as IBM PC/XT, AT 286, 386 or 486 and their compatible computers used in many research groups for many years, particularly in China. Some X-ray diffractometer have been supplied micro computer to control and collect data. So it is very convenient to use the XRS-82 system by more researchers if the system can be used in a micro computer. In order to run the system on a micro personal computer, we try to rewrite the system. Although it is difficult to load big programs into a small computer. In this paper we report the rewriting of the system on the Micro-Computer with MS-DOS V3.3 operating system. The XRS-82 system has 12 main programs: STEPCO, PEAK, SPRING, DATRDON, LOAD, CRYLSP, FOUR, BONDLA, PROPT, RELIST, PEKP and WRITU. All of these programs had been written in FORTRAN IV, and in super computer they would be loaded together and

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packed into a large executable programs, except STEP, PEAK, SPRIN and PROPT which are independent executable programs. The packed programs should be separated to be used in a micro computer. The least-squares refinement CRYLSP program can not be executed directly in a micro computer. We noticed that the CRYLSP program has a great array-A. If the array-A is moved out the program and modified as temporary data file, the program can be used on a micro computer with only 640K memory. In addition, the difference between FORTRAN-66 and IBM-FORTRAN-77, especially I/O formats, will be considered. Recently, the Micro computers have more and more functions, specially displaying and drawing graphics. We have written several programs for XRS-82. (1) To display and draw patterns in screen or plotter. The patterns are either observed or calculated as the results of STEP or CRYLSP programs. (2) To display and draw the atlas topologies framework structure or the ball-atoms in the unit cells. (3) To display and draw the electronic density of Fourier map and different Fourier map. These programs are necessary to run the XRS-82, written in both FORTRAN-77 and BASICA languages. In addition the MS-DOS can be used for running the system successively by both jobs. So that all input and output files have perpetual names themselves. The results of output file can be remained by copy. In order to check up the rewritten XRS-82 system, we compared the results of refinements for ZSM-39 and ZSM-5 structures on AT-386 computer with one result of the Honeywell DPS-8 computer in Aberdeen University of U. K. and in Jilin University. The results of refinements are reasonable and only have a little difference. In AT-386 computer, the calculating time of one step of refinement twice cycles is about 1-1.5 hr. for ZSM-39, having 9 atoms, 64 parameters and 76 reflections, and about 3-5 hr. for ZSM-5, having 38 atoms, 67 parameters and 1666 contributing reflections. I thank Prof. Ch. Baerlocher of Institut fuer Kristallographie, Prof. Ch. Baerlocher of Institut fuer Kristallographie, Prof. Ch. Baerlocher of Institut fuer Kristallographie, Prof. F.P. Glasser, Dr. Dent Glasser and Dr. R. A. Howie of Aberdeen University for many help.

PS-02.08.25 AB-INITIO SOLUTION OF MISFIT LAYER STRUCTURES BY AUTOMATIC PATTERSON AND DIRECT METHODS by Paul T.Beurskens*, Gezina Beurskens, and Erwin J.W.Lam, Crystallogr. Lab., Res. Inst. f. Materials, Univ. of Nijmegen, The Netherlands, Sander van Smaalen, Lab. of Chem. Physics, Materials Science Center, Univ. of Groningen, The Netherlands, and Hai-fu Fan, Inst. of Physics, Chinese Academy of Sciences, Beijing, China

A misfit layer compound is an intergrowth structure consisting of two or more types of layers. Each layers can approximately be described as a three-dimensional periodic structure with, however, mutually induced incommensurate modulations. The composite structure is best described as a periodic structure in higher dimensional space (S.van Smaalen (1992), Materials Sc. Forum 100 & 101, 173). We now consider the case of two layers, and reflection data indexed with 4-dim. indices hklm. Layer 1 is defined by the 'main' reflections hkl0 (3-dim. indices hkl), layer 2 is defined by the 'main' reflections 0klm (3-dim. indices klm), while all other reflections hklm (h,m=0) are the (usually weaker) 'satellite' reflections.

The last step (step4) in the present procedure is the determination of the phases of the satellites from the known phases of the main reflections of both layers by application of the Sayre equation in 4-dimensional superspace (Hao Quan, Lia Yi-wei & Fan Hai-fu (1987), Acta Cryst. A43, 820. Fan Hai-fu, S.van Smaalen, E. Lam & P.T.Beurskens (1993), Acta Cryst. A in press). The phases of the main reflections are determined as follows:

Step 1. Solve the 3-dim structure of layer 1 by routine application of a heavy atom structure solution program,

Step 2. Similarly, solve the 3-dim structure of layer2,

Step 3. Use the common origin, which is easily done by a shift function based on R2-minimalization. The four steps are imbedded in an automatic procedure which is incorporated in the DIRDIF system.

PS-02.08.26 TOWARD RAPID INORGANIC PHASE IDENTIFICATION FROM ELECTRON DIFFRACTION AND EDS DATA by Y.Le Page*, A.Chenite and J.R.Rodgers, National Research Council of Canada, Ottawa, K1A 0R6, Canada

The potential of electron diffraction for the phase identification of inorganic fine particles, e.g. environmental ones in our case, is considerable. Intense diffraction patterns of 1,000Å-size particles can be exposed in about 1 second, and semi-quantitative elemental analysis down to nitrogen obtained by energy-dispersive X-ray spectroscopy (EDS) in a minuter or so, off the same single particle. However, this potential is not fully developed. Measurement and analysis of diffraction patterns is time-consuming and leads to a typical accuracy of about 2% in reciprocal lengths. This accuracy, which can be explained by the accuracy in the length measurements used in the calculation of the reciprocal data, is often critical for successful phase identification by combination of semiquantitative EDS analysis and diffraction data. In addition, there are pitfalls in the search of cell databases with low-accuracy data.

Due to recent developments in the performance and cost of optical scanners, CCD cameras and computers, digitized electron diffraction patterns can be obtained and processed within minutes for a reasonable cost. The accuracy of measurements obtained by image processing of digitized data is comparable with that obtained manually, but many more positions of diffraction spots can be measured, allowing increased accuracy through least squares.

We have been developing experimental and computational methods for rapid phase identification. We will report on:

- image analysis of zero-level convergent-beam patterns;
- calibration of the camera constant;
- least-squares processing of zero-level data;
- least-squares extraction of 3-d cell from single CBED
- novel database search methods.