

02-Methods for Structure Determination and Analysis,  
Computing and Graphics

was inversely proportional to  $\bar{r}$  (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.

## PS-02.08.23

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.

## PS-02.08.24

RUNNING XRS-82 RIETVELD SYSTEM IN PC LEVEL MICRO COMPUTER UNDER MS-DOS OPERATING SYSTEM

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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