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A CRYSTALLOGRAPHIC COMPUTER PROGRAM LIBRARY FOR AN IBM - 360/40 COMPUTER

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ABSTRACT

An integrated set of computer programs for crystallographic works is discussed and some of the details are given.

ÖZET

Kristallografik çalışmalar için oluşturulan bilgisayar program takımı tartışılmakta ve bazı ayrıntıları verilmektedir.

INTRODUCTION

This work is a description of how authors solved the task of contructing an integrated set of programs for crystallographic work. Throughout the text, summary and the description of the various programs and their capabilities are given shortly to help the users working in this field. Several of the programs are not originally written by the authors but modified, in some cases to a large extent, and tested their correctness employing the data and outputs of the recent reliable reports in the international literature. Because of their great length the input instructions for the programs are not included here. However, these instructions and program write - ups are available in the program library called AR - NI in the Physics Department at the Faculty of Science in the University of Ankara.

PROGRAM SUMMARY

This work treats a set of crystallographic programs, some of which are well known to the users all over the world. Main frame of the programs are those of the ones actively used in the University of Uppsala, Sweden for CDC - 3600 machine. About one third of the programs are written at this department. The authors have tried to integrate all programs with different origins to make a flexible system and called this AR - NI program library for IBM 360/40 computer.

All the programs are written in FORTRAN IV and compiled with FORTRAN F compiler. Some of the programs require user-written subroutines in FORTRAN. However our aim has been to construct the programs in such a way that they should be useful to persons with very little programming experience. In most cases, user only has to punch the necessary control cards and include the crystallographic information required by the program.

The programs are stored on an active disk drive hence the compilation is unnecessary before execution and the access time to the programs is very short.

The largest quantity of data used in crystallographic work are the reflections. The information included for each reflection is given in Table — 1, and unformatted recording on the magnetic tape is used to store the reflection data of the various users.

TABLE — 1. Quantities stored for each reflection

1.	h	
2.	k	Milller indices
3.	l	
4.	FOBS	Observed structure factor (in some cases observed intensity)
5.	FCALC	Calculated structure factor (often blank)
6.	COSA	Cosine of the phase angle (often blank)
7.	SINA	Sine of the phase angle (often blank)
8.	SIGF	σ_F standard deviation of observed structure factor
9.	SF	Scale factor
10.	$\sin^2\Theta$	Θ = Bragg angel
11.	$\sin\Theta/\lambda$	
12.	NR	Number of reflection

It is assumed that the user has some knowledge of data organization, especially of the FORMAT concept.

DECRIPTION OF THE PROGRAMS

A simplified flow chart on the different steps in the use of programs is given in Fig. 1. Table — 2 lists some important features of the programs.

Fig. 1. Flow chart for AR - NI crystallographic program library for IBM 360/40 computer.

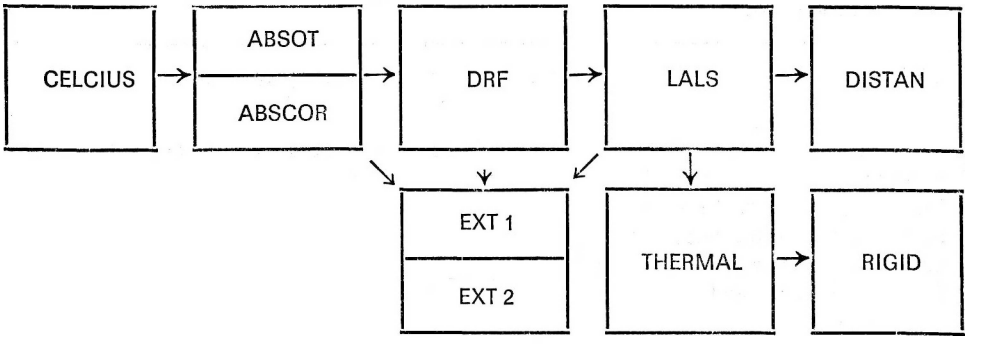

TABLE — 2. Some important features of the AR - NI Program library for the IBM 360/40 machine

Program and Programmer	The function of the program
CELCIUS J. Tegenfeldt, Uppsala, Sweden Modified by A. Aydın Uraz and N. Armağan	A least - squares program for the refinement of cell dimensions. All symmetries (not tested for triclinic). Input : h, k, l, Θ or $\sin^2\Theta$ Program length (6 4 Kbytes).
ABSOT P. Coppens, L. Leiserowitz and D. Rabinowich Modified and tested with the data given in ref. [1] by A. Aydın Uraz and N. Armağan	A numerical absorption correction program for equi - inclination Weissenberg geometry only [2, 3]. A modified TBAR (TMOD) is also calculated for each reflection processed for subsequent use in corrections for possible extinction effects. The expression used in applying an extinction correction is then F (CORR) = F (OBS) * (1 + G * F (CALC ** 2 * TMOD) ** 0.25 where G is the extinction parameter and F (CALC) is on an absolute scale. Program length (227 K bytes).
ABSCOR N. W. Alcock, England. Slightly modified adapted and completely tested with the sample data given in [1] by N. Armağan and A. Aydın Uraz	An analitical absorption correction program for all diffraction geometries. Provision for extinction correction has also been made by the program. Details of the method are given in ref. [1 - 11]. Program length (138 K bytes).

Program and Programmer	The function of the program
DRF A. Zalkin, Berkeley Calif., USA. The CDC - 3600 version of the program (R. Liminga and J.-O. Lundgren, Uppsala, Sweden) modified and tested with the structure reported in ref. [12] by A. Aydın Uraz and N. Armağan	Data reduction and Fourier program. This program 1. Calculates film factors and converts intensity values to the scale of the first film, when multiple - film technique is used (not tested). 2. Calculates Lorentz and polarization factor corrections for diffractometer (not tested) and Weissenberg data. 3. Stores the quantities given in TABLE — 1 of the reflection data on a magnetic tape for use in later calculations in DRF and LALS. 4. Calculates structure factors for upto 150 atoms. 5. Performs Fourier summations for all symmetries (three - dimensional and projections). The number of memory locations available for the Fourier summation is 10 000. Program length (138 K bytes).
EXT 1, EXT 2 A. Aydın Uraz and N. Armağan	This program applies in two steps the isotropic extinction correction [13, 14] to the data using the information obtainable from DRF, LALS, ABSCOR. Program lengths (19 K bytes and 17 K bytes respectively).
LALS A. Zalkin, Berkeley, Calif., USA The CDC - 3600 version of the program (R. Liminga, J. - O. Lundgren and C. - I. Brädén, Uppsala, Sweden) modified and tested with the structure, reported in [12] by N. Armağan and A. Aydın Uraz	Crystallographic least - squares program. This program minimizes the function $\Sigma w (\|F_o\| - \|F_c\|)^2$ according to the method of least squares [15, 16]. Full matrix (132 parameters) or diagonal approximation (350 parameters). Diagonal approximation alternative has not been checked due to the lack of an available data. The parameters that can be refined include scale factors (individual or over - all), atomic coordinates and isotropic or anisotropic individual atom temperature coefficients. The program uses — unit weights — weights (1/SIGMA * *2) supplied with the data — weights according to Hughes [17] — weights according to Cruickshank [18] A weight analysis is made in each cycle of the refinement [19]. Variance - covariance matrix can be stored on a magnetic tape when desired. Program length (137 K bytes).

Program and Programmer	The function of the program
DISTAN A. Zalkin, Berkeley, Calif., USA Modified and tested by N. Armağan and A. Aydın Uraz	Program DISTAN calculates bond distances and angles with standard deviations. The bond lengths can be corrected for thermal motion. The standard deviations are based on the standard deviations of the cell dimensions and positional parameters. No correlation between the parameters is considered. The output is a table with angles and two tables with distances, the last one arranged in a way suitable for publication with the distances listed in accending order. Program length (183 K bytes).
THERMAL A. Aydın Uraz and N. Armağan	The program calculates the eigen values and the eigen vectors of the atomic vibrational ellipsoids[20] using the thermal parameters directly obtainable form LALS. Program length (57 K bytes).
RIGID N. Armağan and A. Aydın Uraz	This program calculates translational and rotational vibration tensors and their eigen values and eigen vectors on the basis of rigid body assumption [20, 21]. Rigid body tensor calculations can be performed with respect to either — any desired orthogonal reference frame with a chosen origin or — inertial frame of a group of atoms which is considered as a rigid body. This program is used after the program THERMAL. Program length (79 K bytes).

CONCLUSION

Although the capabilities of the program library enable the user to perform most of the standard calculations in the crystallographic research, a program system of this kind may not be regarded complete. New programs should be introduced and alterations in the existing programs should frequently be made. Such changes include introduction of new options in the programs giving rise to new usage facilities. Work should also be performed to increase the calculating speed of the programs. The task of development of a program system is certainly nothing one can do in one's spare time. The need for the specially trained full time programmers at the research groups should be considered.

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