# A DIRECT-SEARCHER Automatic System (Version 3) for Some Organic Compounds Running on Personal Computers

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The DIRECT-SEARCHER system version 3 (DS*SYSTEM3) running on Windows NT and Windows 95 has been developed for automatic structure analysis of some organic compounds running on personal computers (PCs). An organic chemist as well as a crystallographer can get results very easily with their own familiar PC. The DS*SYSTEM3 reduces the limitation of the number of atoms and reflection data for the 32 bit operating system. The major improvements are as follows: loose limitation; adopt data bases for space groups and atomic scattering factors; add CIF and help facilities; and bag fixing. DS*SYSTEM3 prepares an output file to other molecular modeling and computational chemistry programs. This system consists of more than 20 crystallographic programs. We found that the molecular skeleton takes usually less than 2 min with the heavy-atom method (PSL3+SEARCHER3) and 15 min with direct methods (DIRCTER3) by a Pentium (100 MHz) PC. The crystal structure analysis of organic compounds has been carried out with more than 50 structures with the heavy-atom method and with more than 30 structures using the direct methods.

## INTRODUCTION

In the last few years, there have been significant changes in computer platforms, especially with the capability of personal computers (PCs) being able to exceed previous supercomputers in calculation speeds, available mass storages, 32 bit operating systems, and cost efficiency. On the other hand, many kinds of computers are still used for crystallographic computing such as supercomputers, mainframe computers (large computer), super-minicomputers, engineering workstations (EWS), and PCs. The reasons why traditional crystallographic computing systems are used is because they have become so prevalent over the years and use sophisticated software which is hardware dependent.

Computer systems and software used for the structure determination of organic compounds mentioned in *Acta Crystallogr., Sect. B* and *C* in the last three years (1993−1995) are summarized in Table 1. The following four program packages are now available to run on PCs: the SHELX-90 program system (1990)[31] from Cray to PCs, an interactive program system NRCVAX (1989)[9d] for large computers, EWS and PCs, the XTAL system (1987)[12d] for Cray-2, APOLLO, and PCs, and DS*SYSTEM (1990)[15] for large computers and PCs. Three individual programs are available on PCs: a PC version (1990)[32] of ORTEP, the ORTEX (1993)[33] for an interactive version of ORTEP, and the PARST (1983)[45] for calculating molecular structure parameters. At the International Union of Crystallography XVII congress and general assembly of 1996 (IUCr96, CGA17), several packages and individual programs running on Windows were reported.[47]

Using DS*SYSTEM3 an organic chemist as well as a crystallographer can get results very easily with their own well-known computer system that match the demands of the times. The crystal structure analysis of organic compounds has been carried out with more than 50 structures using the heavy-atom method and with more than 30 structures using the direct methods.

## DESCRIPTION

**DS*SYSTEM3.** The major improvements from the DS*SYSTEM2 (1995)[48] are as follows: (a) adopt layered approach; (b) loose limitation; (c) adopt data base; (d) display molecules on color CRT and prepare a HP-GL file; (e) add Crystallographic Information File (CIF)[49] facility and help file; (f) prepare an export file to other molecular modeling and computational chemistry programs, and (g) bag fixing.

The DS*SYSTEM3 consists of more than 20 main programs and subroutine libraries and is created using the layered approach. The bottom layer is the operating system. The utility layer consists of the subroutine libraries, and all subprograms are grouped into common and individual libraries. The application layer consists of main programs which have entries for calculation or drawing.

The DS*SYSTEM3 reduces the limitation of several data loosely for the 32 bit operating system, and the limitations are unified by using common libraries as shown in Table 2. These values are less troublesome in organic compounds.

As data bases, all space groups from triclinic to orthorhombic (263), including *b* and *c* unique axes and 50 atomic scattering factors (atom H to Bi) with the form $f(\sin\theta/\lambda) = \sum_{i=1}^{4} a_i \exp(-b_i \cdot \sin^2\theta/\lambda^2) + c$ based on the International Table[50] used usually in organic compounds, are registered in advance.

A chemist must prepare the CIF format to submit papers for *Acta Crystallogr., Sect. C (Cryst. Struct. Commun.*). Three programs (DISTAGL3, PARSTC3, and TABLES3) save the

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**Table 1.** Crystallographic Softwares Used for the Structure Determination of Organic Compounds

(a) Program Packages (Computing Systems)

| nucleus | | package name | ref. |
|---|---|---|---|
| manufacture | Japan (MAC) | CRYSTAN/CRYSTAN-GM(1977,92) | 1 |
| | The Netherlands (Enraf-Nonius) | SDP/SDP-PLUS/MolEN(1978,80,82,83,84,85,88,89,90) | 2 |
| | Germany/U.S.A. (Siemens) | SHELX/SHELXS/SHELXTL/SHELXTL-Plus[a] (1976,83,84,85,86,87,88,89,90,91,92)[a] | 3 |
| | Japan (Rigaku)/U.S.A. (MSC) | RCRYSTAN/TEXSAN(1985,87,89,90,92) | 4 |
| | U.S.A. (Syntex) | XTL(1973,76) | 5 |
| university | Italy (U. of Parma) | CRYSRULER(1986,87) | 6 |
| | England (U. of Oxford) | CRYSTALS(1985,93) | 7 |
| | Japan (Kyoto U.) | KPPXRAY(1991) | 8 |
| | Canada (NRC) | NCR System/NCRVAX(1973,81,87,89,90,92)[a] | 9 |
| | Germany (U. of Gottingen) | SHELX/SHELXS/SHELXTL/SHELXTL-Plus(1992,93,94,95)[a] | 10 |
| | Germany (Technische U.) | STRUX-III System(1987) | 11 |
| | Australia/Switzerland/U.S.A. (U. of Maryland, U. of W. Australia) | XRAY/Xtal(1970,76,80,89,92)[a] | 12 |
| society | USA (Ducham) | CRYM(1964) | 13 |
| | Japan (Sakurai) | UNICS(1967,79) | 14 |
| indivisual | Japan (Okada, Okada, Koyama) | DS*SYSTEM(1990,91)[a] | 15 |
| | Scotland (Mallinson and Muir) | GX Crystallographic Program System(1985) | 16 |

(b) Individual Programs

| category | program name | |
|---|---|---|
| structure analysis | DIRDIF (Beurskens et al. 1984,92)[17] | MTHRIL (Gilmore, 1984)[18] |
| | FASE (Yamaguchi, 1993)[19] | SIR (Cascarano et al., 1985,89,94)[20] |
| | MULTAN/RANTAN/SAYTAN (Main et al, 1980,81,82,88)[21] | UNIQUE (Cascarano et al., 1991)[22] |
| | XPACK (Yamaguchi, 1987)[23] | |
| patterson | XRAYRC (Vickery, 1971)[24] | |
| least-squares | ALLS (Lapp and Jacobson, 1979)[25] | CRYM (Ducham, 1984)[26] |
| fourier | FOUR (Powell and Jacobson, 1979)[27] | |
| molecular geometry | XANADU (Roberts and Sheldrick, 1975)[28] | |
| graphic | EUCLID/PLATON (Spek, 1982,90,91,92,93)[29] | GENPLOT (CGS, 1989)[30] |
| | ORTEP/ORTEP-II (Johnson, 1965,76)[31] | ORTEP (Breuggemann and Schmid, 1990)[32] [b] |
| | ORTEX (McArdle, 1993)[33] [b] | PEANUT (Hummel et al., 1990)[34] |
| | PLUTO (Motherwell et al., 1976,78)[35] | R3m (Riche, 1983)[36] |
| | SCHAKAL (Keller, 1988,92)[37] | Siemens (1989)[38] |
| | SNOOPI (Karailov, 1992)[39] | |
| literature survey | CSSR (SERC, 1984)[40] | |
| publication | ACTCIF (Riche, 1992)[41] | CIF2TEX/FCF2FOC (Kopf, 1992)[42] |
| | FUER (Larson, 1982,93)[43] | ORFFE (Busing et al., 1964)[44] |
| | PARST (Nardelli, 1983)[45] [b] | SWATAB (Swaminathan, 1989)[46] |

[a] Underlined system has the mainframe, EWS, and PC versions. [b] Underlined program is running on PCs.

CIF data as a file. The Help file is useful for the preparation of input data without consulting user manuals and documents.

The DS*SYSTEM3 consists of the following three groups as shown in Figure 1: (a) heavy-atom methods, (b) direct methods, and (c) other programs.

**Heavy-Atom Methods.** The theoretical and detailed descriptions of heavy-atom methods are described in previous papers.[51] The PSL3 and SEARCHER3 programs are improved in input/output and in the array usage of reflection data and the atomic parameters.

**PSL3 Program.** PSL3 calculates the Patterson function of Harker sections and/or lines and the possible atomic coordinates and height are stored by solving the Patterson matrix. Next PSL3 calculates the structure factor of possible atoms, stores the *R*-factor in increasing order, and compares the *R*-factor to identify the same atom. The heavy atom is positioned at a lower *R*-factor. Then PSL3 refines the heavy atom coordinates by full-matrix least-squares calculation and sorts the *R*-factor once more into increasing order. Finally the heavy atom is selected from the top of the list of *R*-factors.

**SEARCHER3 Program.** This program as shown in Figure 2 solves structures in all triclinic, monoclinic, and othorhombic space groups. The first part (A-part) calculates the structure factors and compares with NSF (number of input atoms) and NLS (maximum NSF). If NSF ≥ NLS, the B-part is started. The coordinates and peak height of the center of a Fourier peak is calculated, by use of a suitable second-order polynomial, from 27 values in two neighboring sections. Distances between input atoms and peaks are calculated, and new atoms (NLH) to be added in the next Fourier calculation are selected based on the "reasonable" interatomic distances (1.1−1.7 Å). If NSF ≥ NLS, the program goes into the B-part and is used for calculating the block-diagonal or full-matrix least-squares calculation, and determining which atomic positions are to be eliminated (Biso ≥ BCUT) for the next least-squares calculation. The selection of the atomic sites is based only on the temperature factor. The outputs of SEARCHER3 are projection diagrams of the molecules in a unit cell. The atomic coordinates are saved in a file which can be used as input to the next cycle of SEARCHER3.

**Direct Methods.** The theoretical and detailed descriptions of direct-methods are described in a previous paper.[52] In order to reduce the maximum limitations, several array usages are improved in optimization.

**DIRECTER3 Program.** The DIRECTER3 program is based on the symbolic addition method to solve the crystal

**Table 2.** Restrictions of DS*System3

(a) Reflection Data

| | | | |
|---|---|---|---|
| $\|h,k,l\|$ | ≤ | 98 | |
| no. of reflcns | ≤ | 200 000 | (AFCR3) |
| | | 1 000 | (DIRECTER3) |
| | | 10 000 | (LSBF3, SEARCHER3) |
| expand equiv reflcns | ≤ | 5 000 | |
| $\Sigma_2$ relationships | ≤ | 20 000 | (DIRECTER3) |

(b) Atomic Parameters

| | | | |
|---|---|---|---|
| no. of atoms | ≤ | 500 | |
| | | 1 500 | (ORTEP3, PLUTO3) |
| atomic kinds | ≤ | 10 | |
| equivalent positions | ≤ | 64 | |

(c) As NSF = no. of atoms, NAN = no. of anisotropic atoms, NV = no. of variables, NPAR = 2 + 5*(NSF + NAN),

MMAX =

$$\begin{cases} \text{NV} * (\text{NV}+1)/2 & \text{for full-matrix} \\ 3 + 55 * (\text{NAN} + 15 * (\text{NSF} - \text{NAN}) & \text{for block-matrix} \end{cases}$$

| | | | |
|---|---|---|---|
| 5 * NPAR + MMAX + NV | ≤ | 200 000 | (LSBF3) |
| NRD * 9 + NPAR * 6 + NSF * 10 | ≤ | 200 000 | (PSL3) |
| NRD * 9 + NPAR * 3 + MMAX + NV * 3 | ≤ | 200 000 | (SEARCHER3) |
| NV | ≤ | 5 002 | (LSBF3) |

(d) Fourier Summation and Peak Generation

| | | |
|---|---|---|
| grids in one section | ≤ | 200 × 200 |
| no. of max. peaks | ≤ | 5 000 |

structure without any human intervention and has been successful over a considerable range of space groups ($P\bar{1}$, $P2_1/c$, *Pbca*, $P2_1$, $P2_12_12_1$, etc.). The outputs of DIRECTER3 are the projection diagrams which are the same as for

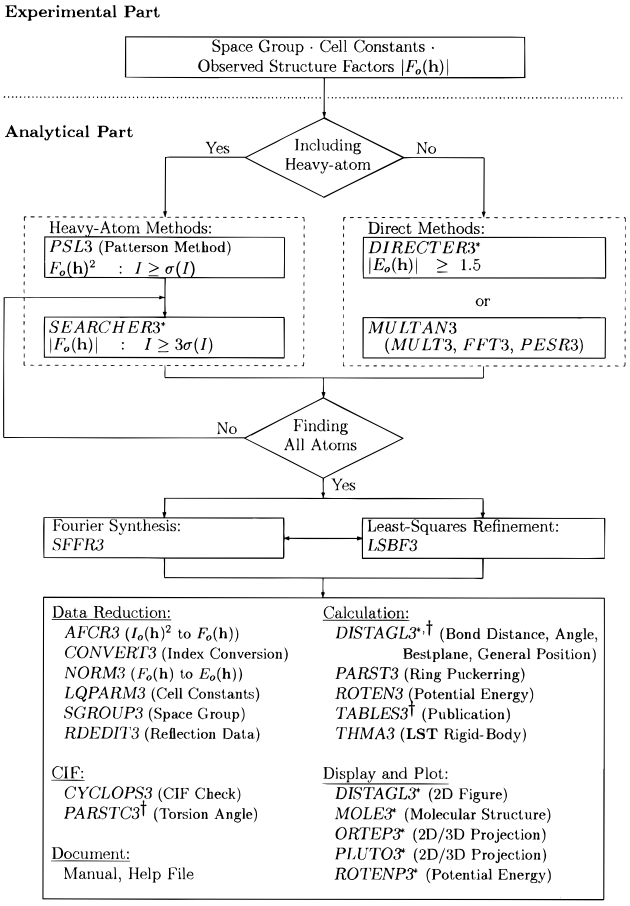


**Figure 1.** Layout of DS*SYSTEM3. Produce plot file (*) and CIF data (†).

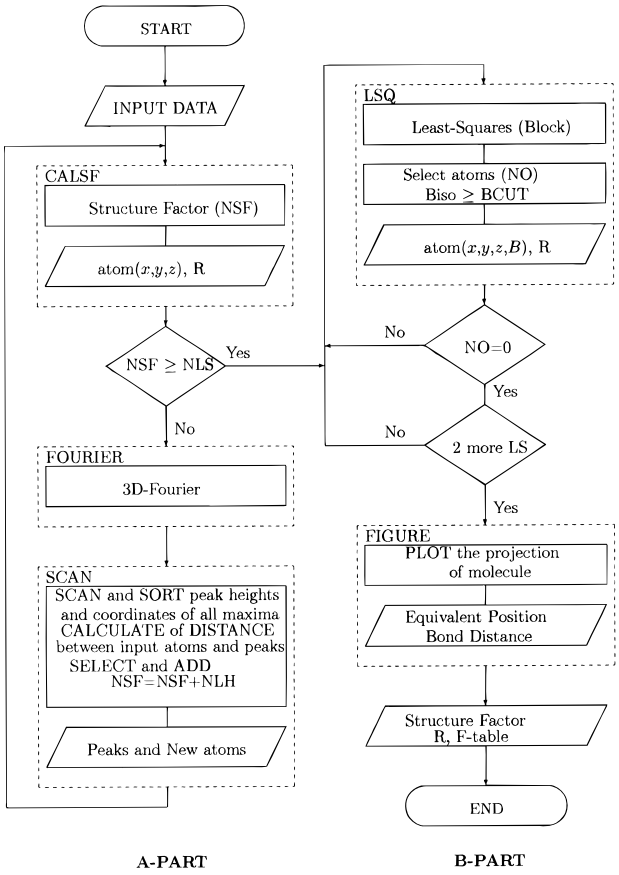


**Figure 2.** A simplified SEARCHER3 program layout.

SEARCHER3 and the atomic coordinates which are used as input for SEARCHER3.

**MULTAN3 Program.** The MULTAN3 program is conjugated into one program with MULT3, FFT3, and PESR3. The major alteration is the ability to use knowledge of molecular structure as described by Main.[53]

**Other Programs.** Several crystallographic programs are developed as "other programs". The theoretical and detailed descriptions of these programs are described in a previous paper.[54] The following programs are added or improved by DS*SYSTEM3.

**AFCR3 Program.** The output data of AFC (Automatic Four circle Controlled) manufactured by Rigaku Co. or Mac Science Co. include many experimental values (the standard reflections, flags, and IB1, BI2, T1, T2, ...) which are not used in the structure analysis. AFCR3 program edits the raw data and $F_o(\mathbf{h})$ data to prepare the necessary data considering the equivalent reflections and extinction rules which are treated depending upon the space group. The observed structure factor $F_o(\mathbf{h})$ is adjusted by the ratio of standard reflection of each block with decay corrections. If the reflection is counted twice or more, these reflections are deleted by option of the user (averaged, previous, or last).

**CONVERT3 Program.** The CONVERT3 program finds the reduced cell from cell constants and/or converts the cell constants, atomic coordinates, anisotropic temperature factors, and reflection indices. The calculation of the reduced cell is based on the Niggli reduction[55] and is performed by the unified algorithm of Křivý and Gruber.[56] The six scalar products of a rectangular matrix and the equivalent designation can be taken as the form of the Niggli reduced matrix

**Table 3.** Computer Speed using PSL3+SEARCHER3

| | | PSL[a] | | | SEARCHER[a] | | | |
|---|---|---|---|---|---|---|---|---|
| compd | formula space group | Cray-1 | 80386 (20 MHz) | Pentium (100 MHz) | CDC6600 | Cray-1 | 80386 (20 MHz) | Pentium (100 MHz) |
| X-83 | $C_{19}H_{20}O_2N_5SBr$ | $5.11_s$ | $4_m10_s$ | $9_s$ | $9_m33_s$ | $45.8_s$ | $57_m23_s$ | $10_s$ |
| | $P2_1/c$ | 0.568 | 27.8 | 1.000 | 57.3 | 4.58 | 344 | 1.00 |
| X-111 | $C_{19}H_{30}O_2S$ | $8.95_s$ | $6_m12_s$ | $27_s$ | $22_m03_s$ | $59.3_s$ | $1_h29_m39_s$ | $36_s$ |
| | $P2_12_12_1$ | 0.332 | 13.8 | 1.000 | 36.8 | 1.66 | 149 | 1.000 |
| X-114 | $C_{28}H_{37}O_7Br$ | $8.49_s$ | $16_m40_s$ | $16_s$ | $21_m01_s$ | $91.5_s$ | $1_h40_m00_s$ | $48_s$ |
| | $P2_12_12_1$ | 0.531 | 62.5 | 1.000 | 26.3 | 1.91 | 125 | 1.000 |
| X-144 | $C_{19}H_{22}O_3S$ | $11.96_s$ | $20_m09_s$ | $16_s$ | $14_m36_s$ | $56.4_s$ | $38_m14_s$ | $21_s$ |
| | $P1$ | 0.748 | 75.6 | 1.000 | 41.7 | 1.73 | 109 | 1.000 |
| X-149 | $C_{23}H_{20}O_5S$ | $7.52_s$ | $7_m14_s$ | $10_s$ | $20_m42_s$ | $107.4_s$ | $2_h09_m59_s$ | $41_s$ |
| | $Pna2_1$ | 0.752 | 43.4 | 1.000 | 30.3 | 2.62 | 190 | 1.000 |
| X-153 | $C_{14}H_{17}N_3O_3S$ | $23.30_s$ | $25_m58_s$ | $39_s$ | $22_m18_s$ | $53.3_s$ | $1_h33_m17_s$ | $38_s$ |
| | $C2/c$ | 0.597 | 39.9 | 1.000 | 35.2 | 1.41 | 147 | 1.000 |
| X-158 | $C_{27}H_{43}NOHI$ | $3.60_s$ | $3_m22_s$ | $10_s$ | $19_m44_s$ | $94.4_s$ | $47_m23_s$ | $24_s$ |
| | $P2_1$ | 0.360 | 20.2 | 1.000 | 49.3 | 3.93 | 118 | 1.000 |
| | ratio | 0.555 | 40.5 | 1.000 | 39.6 | 2.55 | 169 | 1.000 |

[a] Upper, actual CPU time; lower, ratio.

$$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{c}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} \end{pmatrix} = \begin{pmatrix} s_{11} & s_{22} & s_{33} \\ s_{23} & s_{31} & s_{12} \end{pmatrix} \quad (1)$$

where **a**, **b**, and **c** are old cell constants and $s_{ij}$ represents the scalar product between the axes $i$ and $j$. According to the Niggli matrix and the determination of the reduced cell type, the axes **a′**, **b′**, and **c′** of the new reduced cell are found from the axes of the reduced cell $t_1$, $t_2$, and $t_3$ with the aid of a transformation matrix by the band reduction method.

$$\begin{pmatrix} \mathbf{a}' \\ \mathbf{b}' \\ \mathbf{c}' \end{pmatrix} = \begin{pmatrix} u_1 & v_1 & w_1 \\ u_2 & v_2 & w_2 \\ u_3 & v_3 & w_3 \end{pmatrix} \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} \quad (2)$$

$t_n = u_n\mathbf{a} + v_n\mathbf{b} + w_n\mathbf{c}$ and the coefficients $u_n$, $v_n$, and $w_n$ depend on the Niggli matrix. Matrix conversions for cell parameters ($a'|$, $a|$), atomic coordinates ($x'|$, $x|$), anisotropic temperature factors (**B′**, **B**), and Miller indices ($h'|$, $h|$) are handled by reading a conversion matrix **Q**

$$\begin{aligned} a'| &= \mathbf{Q}\, a| \\ x'| &= \mathbf{R}\, x| \\ \mathbf{B}' &= \mathbf{R}\,\mathbf{B}\,\mathbf{R}^t \\ h'| &= \mathbf{Q}\, h| \end{aligned} \quad (3)$$

where **R** is an inverse matrix of $\mathbf{Q}^t$, $\mathbf{Q}^t$ is a transposed matrix of **Q**, and $\mathbf{R}^t$ is a transposed matrix of **R**.

**DISTAGL3 Program.** The DISTAGL3 program handles several calculations through keywords. We add a keyword *CSSR* for the molecular modeling and/or theoretical MO/MD/semiempirical calculations. This option causes the CSSR file to contain cell parameters, space group, Cartesian coordinates of atoms with their atomic types, and bonding connectivity. The user transfers this file to the CERIUS2 program[57] by file transfer protocol (FTP). The CERIUS2 computational chemistry program supports the SERC Daresbury Laboratory's Cambridge Structure Search and Retrieval (CSSR) file.[57]

**ORTEP3 Program.** The ORTEP3 program is the same version of ORTEP-III released in April 1996[58] where new capabilities of ORTEP3 include all ORTEP-III features and (a) allows the input of cell parameters, atomic parameters, and symmetries of DS*SYSTEM3; (b) adds HP-GL file (HP7580 file) + Screen output items: and (c) expands the number of atoms (1500) and bonds (2000).

**RDEDIT3 Program.** The RDEDIT3 program edits the reflection data to sort *hkl* or $|E_o(\mathbf{h})|$ in decreasing/increasing order, prints the maximum or minimum values of $F_o(\mathbf{h})$, and/or writes any format of reflection data.

**System Requirements in PCs.** The color CRT is used for communication with the PC, the monitoring of program execution, and for the display of molecular projections. Recommended PCs are IBMPC/AT or compatible, Pentium (100 MHz or faster), 16-64 MB memory, more than 1 GB hard disk space, and enhanced graphic color monitor (VGA, SVGA, XGA and ZGA). We use the RICOH SP10/PS laser printer which has HP-GL (plotter) emulator to draw molecular projections and handles A4/A3 paper size with 600 dots per inch.

**Software.** We use a screen editor and full set Fortran compiler[59] under MS-Windows NT 3.5x and/or MS-Windows 95 operating systems. We have developed the graphic library VGLIB3 which produces the HP-GL output requested for the submission to *Acta Crystallogr., Sect. C* and handles the basic color elements (point, line, fill area, and text) for a color CRT. 2D-projections, stereoscopic drawings, and molecular structures are drawn and displayed with arbitrary scale (1 Å = 0.1−10.0 cm).

## APPLICATIONS AND RESULTS

The DS*SYSTEM has been successful over a considerable range of normal space groups ($P\bar{1}$, $P2_1/c$, $Pbca$, $P2_1$, $P2_12_12_1$, and etc.). Table 3 and Table 4 indicate the actual ratios calculated by DS*SYSTEM3 in comparison with mainframe, EWS, and PCs based on several organic compounds solved by the DS*SYSTEM. The computational time has reduced dramatically over the last five years. Using a 32 bit PC (Pentium, 100 MHz), structure analysis for a small molecule with the heavy-atom method (PSL3+SEARCHER3) and direct methods (DIRECTER3) takes within 2 and 15 min, respectively. We found that the PC has a calculation speed of 1.55 of Cray-1, 3.93 of HP9000/755, 7.43 of IBM3090-200E, and 33.2 times of CDC6600.

## CONCLUSION

It is very important that chemical researchers are able to solve and determine molecular structures with a crystal-

**Table 4.** Computer Speed using DIRECTER3

| compd | formula space group | CDC6600[a] | 80386 (20 MHz)[a] | Pentium (100 MHz)[a] |
|---|---|---|---|---|
| X-1 | $C_{15}H_{16}O_4$ | $1_h33_m18_s$ | $1_h20_m34_s$ | $1_m10_s$ |
| | $P2_12_12_1$ | 80.0 | 69.1 | 1.000 |
| X-12 | $C_9H_{11}O_6N$ | $1_h19_m27_s$ | $10_h15_m08_s$ | $6_m24_s$ |
| | $C2$ | 12.4 | 96.1 | 1.000 |
| X-80 | $C_{11}H_{14}O$ | $14_m49_s$ | $53_m47_s$ | $36_s$ |
| | $P2_12_12_1$ | 24.7 | 92.4 | 1.000 |
| X-144 | $C_{19}H_{22}O_3S$ | $29_m12_s$ | $41_m04_s$ | $33_s$ |
| | $P1$ | 51.3 | 774.7 | 1.000 |
| X-164 | $C_{23}H_{32}O_7$ | $33_m56_s$ | $2_h13_m10_s$ | $1_m37_s$ |
| | $P2_1$ | 21.0 | 82.4 | 1.000 |
| K-85 | $C_{15}H_{24}O_2$ | | $25_h04_m24_s$ | $12_m35_s$ |
| | $P3_2$ | | 120 | 1.000 |
| K-88 | $C_{20}H_{30}O_2$ | | $5_h06_m01_s$ | $3_m51_s$ |
| | $P2_1$ | | 79.5 | 1.000 |
| | ratio | 37.9 | 87.7 | 1.000 |

[a] Upper, actual CPU time; lower, ratio.

lographic computing system on their own PCs. We should not neglect PCs that have high performances and laser printers that have the capabilities of printers, plotters, and a hardcopy. The noncrystallographers as well as crystallographers can determine the crystal structures of their own organic compounds by themselves using the DS*SYSTEM3 on PCs.

We will aim at the improvement of the user interface for input data and program execution, the import/export features of other crystallographic systems and/or computational chemistry packages, the preparation of the postscript output for the lastest laser printers, and the adjustment of new analytical programs such as *Shake-and-Bake (SnB)* computer program package (1995)[60] developed by Hauptman. This *(SnB)* program has solved *ca.* 24 structures with no failure in the 25−1000 or more independent non-H atom range.

**Program Availability.** The DS*SYSTEM3 has been fully tested under MS-Windows NT 3.51 and MS-Windows 95. These programs need 20 M byte of working disk space. A laser printer with HP-GL emulation is needed for drawing. Documentations, the Help, and latest executable files are available from K.O. upon request.

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