

# Display of Cross-Sections Showing Packing in Inclusion Compounds

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**Abstract.** A system of BASIC programs for a personal computer allowing the display of plane sections through crystal structures has been developed in order to analyse intermolecular contacts as well as the shape and size of intra- or intermolecular voids in the structure of inclusion compounds. The data consisting of lattice parameters, type of Bravais lattice, symmetry operations, and positional parameters of atoms in an asymmetric unit are stored in a data file, reusable and correctable. The structure is considered as an assembly of spherical atoms of given van der Waals radii. The section plane may be defined by either coordinates of three points or the crystallographic index. A series of sections parallel to the original one at a specified interval of distance may be calculated and displayed automatically, and memorized for further reviewing, modifying graphic features, etc. Hard copies may be prepared using a dot-matrix printer or plotting devices. The program may be applicable to any crystal structure with an arbitrary choice of atomic radii.

**Key words.** Crystal packing, personal computer display.

## 1. Introduction

A crystal structure can be understood in itself through the given set of crystal data and atomic coordinates described in the literature. However, it is often difficult, even for crystallographers, to make an image of the inclusion circumstances in a crystal of complicated structure. In such a case a simple program system for a personal computer is desirable to display the crystal packing. The program can also be used to design or estimate novel inclusion structures of selected host and guest species. The program system we have developed allows the display of plane sections through crystal structures, and is particularly useful in analysing intermolecular contacts between the host and the guest as well as the shape and size of intra- or intermolecular voids in the structures. The program written in BASIC was originally loaded on one of the most economic personal computers with an 8-bit CPU, the NEC-PC8001-MkII [1]; a revised version applicable to a 16-bit CPU computer the NEC-PC9801 is now commercially available [2].

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## 2. Program

### 2.1. OUTLINE

The principle of this program system WANDA is illustrated in the flow chart in Figure 1. The system is comprised of three main programs RAZ, DWA, and SAN. A data file is created by RAZ to memorize the file name, the file title, the lattice parameters, the type of Bravais lattice, the symmetry operations if necessary, the atomic coordinates, the atomic radii, and the colours in the display. By defining a section plane in DWA a work file is created to memorize the atoms to be displayed along with the plane equation, and the successive display of the section on a colour screen is executed by SAN. If one wants to have more sections parallel to the originally-defined plane at a given distance, the cycle between DWA and SAN is run until the required displays have been completed; each work file defined for each section is memorized in the disk. A complimentary program SHI is added to the system for review or printout of the contents of a data or work file, or for reviewing the contents of a work file.

For the execution of the whole program system a dual floppy disk unit is necessary:  $5\frac{1}{4}$ " in the original 8-bit CPU version and 8" in the revised 16-bit CPU version.

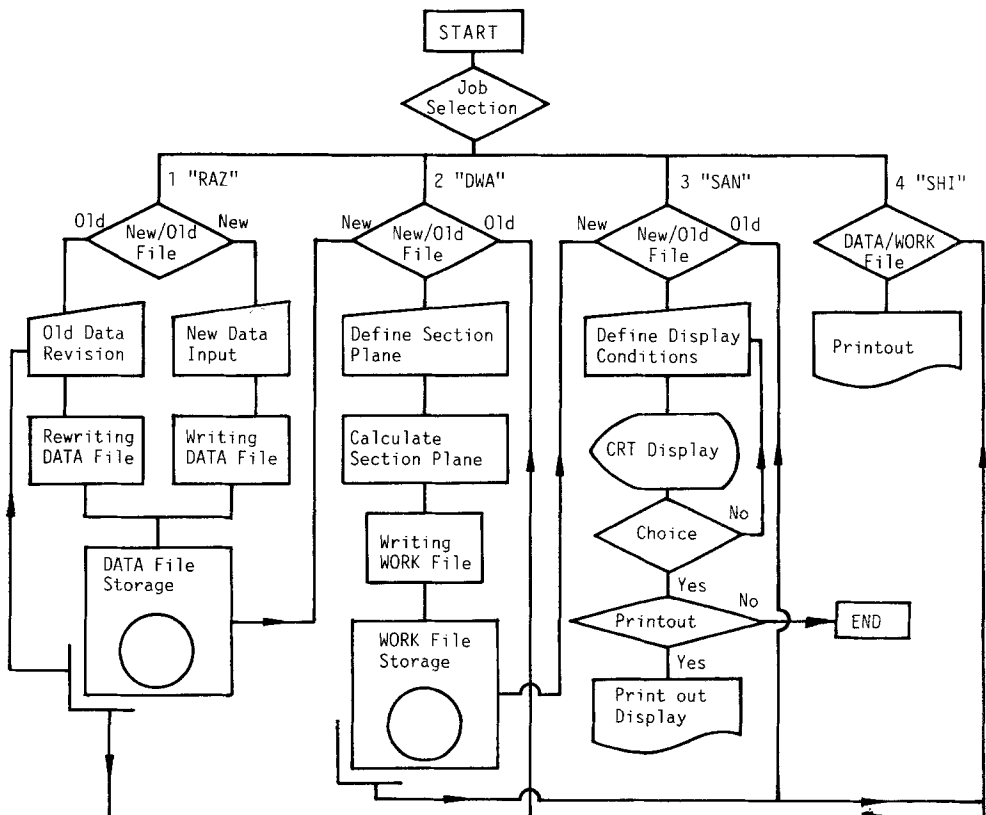


Fig. 1. Construction of the program system WANDA.

## 2.2. ALGORITHM AND FUNCTIONS

### 2.2.1. *RAZ*

Its function is to prepare a data file for a given crystal structure with a file name, a file title noting down information of the crystal within 256 letters, lattice parameters, type of Bravais lattice, symmetry operations, and atomic coordinates, van der Waals radius, and colour code for each atom. The space group emerges in the data file from the data inputted for lattice parameters, Bravais lattice type, presence or absence of inversion centre, and symmetry operations. If all the atoms to be displayed are on the special positions in the given space group, input of the operations related to the special ones is enough for the following calculations.

At each stage of input a question "data correct?" and y/n answer system is prepared. By calling the data file again the contents can be modified and/or corrected according to the enquiry system. After the correction or modification a new file name can be given independently of the previous file name but giving the same file name to the previous one cancels the previous file.

### 2.2.2. *DWA*

It first recalls the data file already prepared by *RAZ* from the disk. Then it defines the section plane by its crystallographic index or three points in the unit cell. The program calculates the orthogonalization matrix and the plane equation in orthogonal coordinates. Taking each atom from the input list, the program checks successively whether its sphere and the spheres of those generated by the symmetry operations are intersected by the defined plane. The approximate computing time estimated roughly from the volume of the unit cell is displayed along with the order number of the atom currently being considered by the program on the screen. Up to 278 atoms within the range of the unit cell  $\pm 2 \text{ \AA}$  intersected by the plane are memorized into a work file with the name of the data file followed by two digits. The program automatically runs the third part *SAN*.

### 2.2.3. *SAN*

As for *DWA*, a job selection is first done either by recalling the work file written previously or a review of already existing work files by referring to the data file name.

The scale and the mode of drawing are preset in the program: three scale factors,  $15.5 \times 9.5$ ,  $31 \times 19$ , and  $62 \times 38 \text{ \AA}^2$ , and four modes, to paint circles and print out, to paint circles but not to print out, open circles and print out, and open circles but not to print out. The most appropriate selection of the scale factor and the mode of display is ascertained by successive trials. Successive displays of the sections parallel to the original one with input of the number of planes and the interval in  $\text{\AA}$ , or display of non-parallel sections with input of the plane definition are available. In these processes, *DWA-SAN* cycles run automatically and the work file for each section is memorized into the disk.

In order to review already defined work files, the data file name and the number (last two digits) of the work file is called. After the selection of the scale factor and display mode, one can define the origin of the drawing on the screen.

### 3. Results

Examples of displays executed by this program system are shown for four types of clathrates, (i) quinol-host hydrogen chloride, **I**, [3], (ii) (deutero)hydrate of ethylene oxide, **II**, [4], (iii) 'Werner-type' bis(isothiocyanato)tetrakis(4-methylpyridine)-nickel(II)-*p*-xylene(1/1), **III**, [5], and (iv) 'Hofmann-dahxn-type' 1,6-diaminohexane-cadmium(II) tetracyanonickelate(II)-*o*-toluidine(1/1), **IV**, [6] in Figure 2; the data files were written according to the crystallographic data in the relevant references. Although Figure 2 shows the monochrome output from the printer, the original

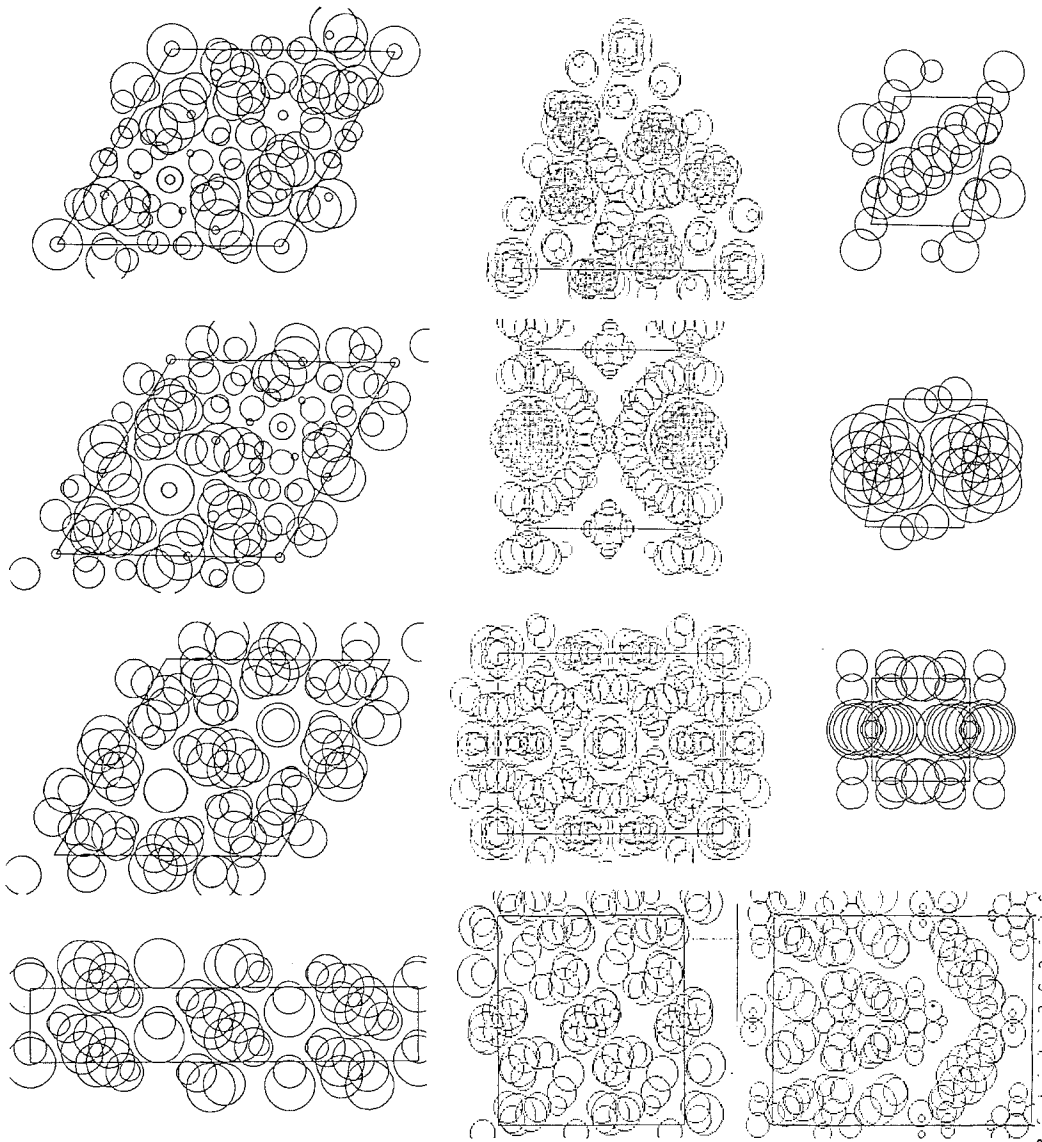


Fig. 2. Examples of display. Left upper to lower; a: (001), b: (003), c: (002), and d: (110) section of **I**; middle upper to lower; e: (111), f: (400), and g: (110) section of **II**, and h: (001) section of **III**; right upper to lower; i: (010), j: (020), and k: (200) section of **IV**, and l: (040) section of **III**.

colour display on the VDU is far better than the monochrome one for understanding the chemical structure. However, as the knowledge of the crystal structure should be presupposed to the users, enclathration of each guest molecule is recognizable on the monochrome output when the section is appropriately selected. For example, the (00 $l$ ) sections of I, a–c, on the printer-output show the positions of guest hydrogen chloride at each corner of the rhombus and at  $\frac{2}{3}, \frac{1}{3}, z$  and  $\frac{1}{3}, \frac{2}{3}, z$ , respectively. The (400) section of II, f, gives the image of guest ethylene oxide molecule in disorder centered at 0.25, 0, 0.5 clearly but it is difficult to judge the image at 0.25, 0, 0 either as that of the guest or of the host moiety, unless one knows the crystal structure in detail.

#### 4. Concluding Remark

As the four programs comprising WANDA can run independently with the respectively independent data and work files, it is possible to display an inclusion structure for both the cases in the presence and absence of the guest molecule. The section once calculated is reviewable as occasion demands with variable size and mode of display.

The program system WANDA is applicable to display arrangement of atoms and/or molecules on a cross section of any crystal including ionic and metallic ones, if the atomic radii are chosen for the relevant types of chemical bonding. Since the ionic and metallic radii are related to the distance of contact between two atomic species, a packing structure should be given by the same procedure as that applied to the inclusion compounds. However for a covalent crystal the display of the packing structure should give rise to too much vacancy if the covalent radii are applied.

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