Crystal data for diphenyl tin sulphide trimer and n-dibutyl(ethylene-1,2-dithiol)stannane. By N. R. KUNCHUR and SHAHIN BORHANI, Faculty of Science, University of Azarabadejan, Tabriz, Iran

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The compounds diphenyl tin sulphide trimer and n-dibutyl(ethylene-1,2-dithiol)stannane crystallize into space groups $P2_1$ and $C2$ respectively. The unit-cell parameters are reported.

Origin of specimen

Crystals of diphenyl tin sulphide trimer $[(C_6H_5)_2SnS]_3$ and n-dibutyl(ethylene-1,2-dithiol)stannane (S. CH$_2$. CH$_2$. S)Sn. n-Bu$_2$ were supplied by Dr R. C. Poller. The former compound crystallizes into needles along the $b$ axis, the latter into needles along the $a$ axis.

Crystal geometry

Unit-cell dimensions were determined on a General Electric XRD-6 diffractometer with a single-crystal orienter. For the compound $[(C_6H_5)_2SnS]_3$ the diffraction pattern showed monoclinic symmetry and only reflexions $0k0$ with $k$ odd were systematically absent indicating space group $P2_1$.

For $[\text{SCH}_2\text{CH}_2\text{S}]\text{Sn. n-Bu}_2$ the diffraction pattern showed monoclinic symmetry and only reflexions $hkl$ with $h + k$ odd were systematically absent. Hence the space group is $C2$, $Cm$ or $C2/m$. The presence of a mirror can be ruled out by consideration of the Patterson synthesis, molecular symmetry, and packing of molecules in the unit cell. The space group $C2$ is therefore indicated.

Crystal data

$[(C_6H_5)_2SnS]_3$

$a = 9.499 (3)$, $b = 21.739 (5)$, $c = 8.732 (3)$ Å, $\beta = 96.2^\circ$, $U = 1786.3 \text{ Å}^3$, $Z = 2$, $D_m = 1.69$ g cm$^{-3}$, $D_r = 1.70$ g cm$^{-3}$, space group $P2_1$.

$(\text{S. CH}_2\text{CH}_2. \text{S})\text{Sn. n-Bu}_2$

$a = 17.827 (5)$, $b = 7.867 (3)$, $c = 9.934 (3)$ Å, $\beta = 97.2^\circ$, $U = 1382.05 \text{ Å}^3$, $Z = 4$, $D_m = 1.55$ g cm$^{-3}$, $D_r = 1.56$ g cm$^{-3}$, space group $C2$.

Computer Program

A molecular packing plotter program.* By K. K. CHACKO and K. I. VARUGHESE,+ Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Madras-600025, India

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A general crystallographic molecular packing plotter program (Fortran) has been written for the IBM 1130 computer system with the IBM 1627 plotter. The program can plot the packing diagrams for all the three crystallographic projections and also indicates the hydrogen-bonded contacts.

The data preparation for the program is simple and essentially consists of the input coordinates of atoms in the asymmetric unit, the equivalent positions and the bonding matrix. The program can plot the packing diagram with respect to all the three crystallographic projections [i.e. the (100), (010) and (001) projections] or any desired projections as needed by the user. The program can also represent the hydrogen-bonded contacts and can plot the packing diagram of molecules (atoms) within the unit cell as well as that outside (if needed) to any suitable scale.

The molecular packing diagrams of two crystal structures are given below as examples to indicate the salient features of the program. Fig. 1 gives all the three crystallographic projections of the structure of L-thioproline (Chacko, 1974) indicating also the hydrogen-bonded contacts. The origin as well as the two axes of the projection are indicated in the figure and all the three projections are drawn in a 'right-handed' way with the third axis imagined to point upwards from the plane of the paper through the origin $O$. The atoms in the asymmetric unit (input coordinates) are shown in the projections and distinguished with their labelled names. Sometimes, particularly for oblique cells when one of the axes is much longer than the other, it is more convenient to represent the axes of a desired projection in a 'left-handed' way rather than in the usual 'right-handed' way of representation. This facility is also incorporated in the program as is indicated in Fig. 2 which gives the (010) projection of the structure of 1-aminocyclobutane carboxylic acid hydrochloride monohydrate (Chacko & Zand, 1975). Fig. 2(a) is plotted in a 'right-handed' way while Fig. 2(b) gives the packing diagram of the same (010) projection in a 'left-handed' way. The times taken to plot each projection shown in Figs. 1 and 2 are 3.6 and 4.2 min respectively.

The program is best suited to plot molecular packing
diagrams for small molecular structures, particularly for projections with minimum overlap between atoms. It could also be useful for general molecular model building. The IBM 1627 plotter subroutines \texttt{FPLOT}, \texttt{SCALF}, \texttt{POINT} and \texttt{FCHAR} are used in the program. Although this program has been written for the IBM 1130 computer system, it could be adapted to other computer systems with the IBM 1627 plotter. The maximum number of atoms per asymmetric unit is at present limited to 30 owing to the small core storage (8K) of the IBM 1130 system available in this department, but this number could easily be increased for computer systems with larger core. It is worth while mentioning that \textit{ORTEP} (Johnson, 1965) cannot be run on a small machine like the IBM 1130 as it requires a large core (50K). The Fortran listing and details of the data preparation of the program can be made available on request to one of us (K.K.C.).

References