Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.

Generation and best fitting of molecular models. By E. Gavuzzo, S. Pagliuca, V. Pavel and C. Quagliata, *Laboratorio di Chimica-fisica, Istituto Chimico, Università di Roma, Roma, Italy*

Two programs useful in crystallographic computation are described. The first permits the calculation of cartesian atomic coordinates from molecular interatomic distances and bond angles. The second obtains the best fit between two molecular models as a function of three rotation angles, by searching the smallest weighted sum of the distances between corresponding atoms.

Model-building program

The computation of cartesian atomic coordinates of molecular models is useful in dealing with many structural problems. A variety of programs for performing this calculation are available (Thompson, 1967; Hilderbrandt, 1969 and references cited therein). They take advantage of the knowledge of bond lengths and angles, dihedral or rotation angles and symmetry operations necessary to build up a molecule.

We have been interested in a program of this type in the course of attempts to solve the phase problem by potential energy calculations (Coiro, Giacomello & Giglio, 1971, and references quoted therein). However, we believe that it is easier, especially for asymmetric molecules, to describe the proper geometry as a function of distances between atoms, and bond angles only, without having to resort to the evaluation of torsion angles. Moreover the need to accomplish crystallographic computations with fractional atomic coordinates, defined in a triclinic system, has prompted us to write a suitable program in Fortran V for the Univac 1108 computer.

The cartesian coordinates of a minimum of three atoms, numbered 1, 2 and 3, must be given in an arbitrary rectangular framework $OXYZ$ together with the unit-cell parameters a, b, c, α, β, γ if fractional coordinates are desired. In addition, three translations along OX, OY, OZ and three rotation angles around OX, OY and OZ may be specified to obtain the appropriate orientation of the molecule, positioned in the orthogonal system $OXYZ$, with respect to the triclinic crystallographic axes Oa, Ob and Oc.

The fourth and the following atoms can be located by cards each containing these data:

$$i,j_1,d_{ij1},\ i,j_2,k_1,d_{iJ2} \text{ (or } a_{iJ2k_1}),$$
$$i,j_3,k_2,d_{iJ3} \text{ (or } a_{iJ3k_2}),\ h_x,h_y,h_z,n$$

allowing us to determine the coordinates of atom i, generally bonded to atom j_1. j_1, j_2, j_3, k_1 and k_2 are numbers which refer to atoms already known and d and a represent distances or angles respectively. k_1 and k_2 are zero when distances instead of angles are reported. The symbol n indicates the chemical species of i and may be used in a subsequent analysis of the packing energy and minimum residual (Damiani, Giglio, Liquori & Ripamonti, 1967).

Because it is possible to evaluate d_{ik_1} from a_{iJ2k_1} (by

means of Carnot's theorem for example), by putting the atom j_1 at the origin, the cartesian coordinates x_i, y_i, z_i of atom i become the unknown quantities of the three equations:

$$(x_i - x_{k_1})^2 + (y_i - y_{k_1})^2 + (z_i - z_{k_1})^2 = d_{ik_1}^2$$
$$(x_i - x_{k_2})^2 + (y_i - y_{k_2})^2 + (z_i - z_{k_2})^2 = d_{ik_2}^2$$
$$x_i^2 + y_i^2 + z_i^2 = d_{iJ1}^2$$

The choice between the two possible sets of roots is decided by one of the three numbers h_x, h_y, h_z, establishing if the right solution has x, y, or z greater $(+1)$ or less (-1).

The practical procedure for handling the program is illustrated in Table 1 for a 1-chlorine-1-butyne-3-one molecule containing nine atoms, as shown in Fig. 1. The following geometric parameters are presumed:

C(3)–C(4) = 1·20; C–C = 1·54; C–H = 1·08;
$$C–O = 1·24; C–Cl = 1·80 \text{ Å}$$

C(3)–C(4)–Cl(5) = C(2)–C(3)–C(4) = 180°;
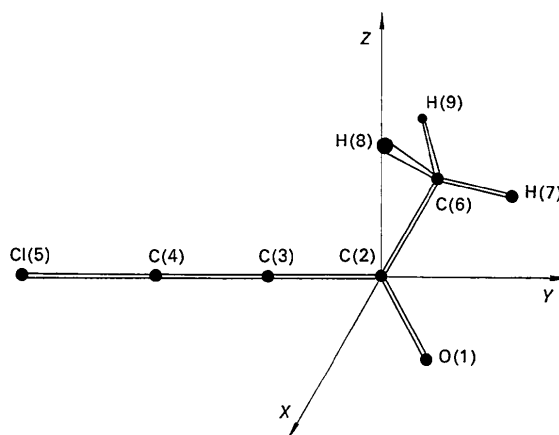C(3)–C(2)–C(6) = C(3)–C(2)–O(1) = C(6)–C(2)–O(1) = 120°.

Fig. 1. Structure of the molecule used in the explanatory example. Atoms 2 to 5 lie on the Y axis and atoms 1 to 7 in the YZ plane. Atoms 8 and 9 have x positive and negative respectively.

Table 1. *Scheme for the determination of atomic coordinates*

Atom i generated	i	j_1	d_{ij_1}	i	j_2	k_1	$d_{ij_2}(a_{ij_2k_1})$	i	j_3	k_2	$d_{ij_3}(a_{ij_3k_2})$	h_x	h_y	h_z	n
4	4	3	1·20	4	3	2	180·00	4	2	1	120·00	0	0	0	2
5	5	4	1·80	5	4	3	180·00	5	4	2	180·00	0	0	0	4
6	6	2	1·54	6	2	3	120·00	6	2	1	120·00	0	0	0	2
7	7	6	1·08	7	6	2	109·47	7	1	0	520·59	0	0	0	1
8	8	6	1·08	8	6	7	109·47	8	6	2	109·47	1	0	0	1
9	9	6	1·08	9	6	7	109·47	9	6	2	109·47	-1	0	0	1

The bond angles involving hydrogen atoms are all 109°28'. The number n, which refers to the chemical species, goes from 1 (hydrogen) to 4 (chlorine) increasing with the atomic number.

The output furnishes the cartesian atomic coordinates in Å (*OXYZ* framework) and the triclinic fractional ones (*Oabc* crystallographic system). In addition the program provides the listing of a squared matrix giving the distances between all the atoms.

Molecules best fitting program

It is often useful to compare an experimental molecule with a theoretical one. In crystallography, atomic positions obtained in Fourier syntheses or by least-squares refinement may be compared with standard models to find the right molecular orientation or some significant atomic displacement from the expected position.

Our program, written in Fortran V for the Univac 1108 computer, performs the calculations giving the atomic co-ordinates of the two molecules either as fractions of a triclinic crystallographic system or in ångströms in a rectangular framework.

The first molecule is rotated around three axes and the second one may be translated along three directions. The distances, d_i, between corresponding atoms i are calculated as a function of the Eulerian angles whenever the translations occur. It is possible to assign a weight w_i for every atom. The program stores the smallest $\sum_i w_i d_i$ and gives the values of the rotational parameters together with the d_i's and the fractional atomic coordinates of the rotated molecule in the triclinic unit cell.

We wish to thank Professor E. Giglio for helpful discussions. The authors acknowledge the Consiglio Nazionale delle Ricerche for the sponsorship of this work. A listing of the programs is available from the authors upon request.

References

Coiro, V. M., Giacomello, P. & Giglio, E. (1971). *Acta Cryst.* B27, 2112.

Damiani, A., Giglio, E., Liquori, A. M. & Ripamonti, A. (1967). *Acta Cryst.* 23, 681.

Hilderbrandt, R. L. (1969). *J. Chem. Phys.* 51, 1654.

Thompson, H. B. (1967). *J. Chem. Phys.* 47, 3407.

Die Kristallstruktur des Tetraargentotellurperchlorates, [Ag₄Te] [ClO₄]₂.

Von E. Schultze-Rhonhof, *Chemisches Institut der Universität Bonn, Deutschland (BRD)**

Tetrasilver tellurium perchlorate is cubic, space group $P2_13$ (T^4), with $a = 8.643 \pm 0.003$ Å. By using the coordinates of the silver tellurium cation in β-tetrasilver tellurium nitrate, β-[Ag₄Te] [NO₃]₂, and fitting the perchlorate group in accordance with its configuration in potassium perchlorate, an R value of 9,5 % was obtained for the 52 indepedent reflexions collected from zero-layer Weissenberg photographs.

Über Nitrate verschiedener Argentotellurkomplexe wurde bereits früher mehrfach berichtet (Lieser, 1960; Schultze-Rhonhof & Bergerhoff, 1966; Schultze-Rhonhof, 1969). Inzwischen ist es gelungen, einen dieser Komplexe auch als Perchlorat aufzufinden.

Nach der von Schultze-Rhonhof & Bergerhoff (1966) beschriebenen Darstellungsmethode, sinngemäss auf Perchlorat übertragen, entstehen schwarze, tetraederförmige Einkristalle von Tetraargentotellurperchlorat, [Ag₄Te] [ClO₄]₂, die in der kubischen Raumgruppe $P2_13$–T^4 mit einer Gitterkonstanten von $a = 8,643 \pm 0,003$ Å kristallisieren.

Weissenbergaufnahmen des Äquators zeigen grosse Ähnlichkeit mit solchen von β-Tetraargentotellurnitrat, β-[Ag₄Te] [NO₃]₂. Daher wurde als Strukturvorschlag versuchsweise ein Teil der Struktur dieser Verbindung (Schultze-Rhonhof, 1969), nämlich die des kationischen Tetraargentotellur-Komplexes, auf das [Ag₄Te] [ClO₄]₂ übertragen. In dieses Gerüst wurden die Perchloratgruppen als Festgruppen (Scheringer, 1963) derart eingefügt, dass sich optimale Abstände ergaben. Die Abmessungen der Perchloratgruppe wurden der Struktur des KClO₄ (Lee & Carpenter, 1959) entnommen. Mit diesen Parametern wurde für die 52 unabhängigen Reflexe des Äquators ein R-Wert ($R = \sum ||F_o| - |F_c||/\sum |F_o|$) von 9,5 % erhalten. Die beobachteten und berechneten Strukturfaktoren sind in Tabelle 1 wiedergegeben.

* Gegenwärtige Adresse: Vereinigte Aluminium-Werke AG., 53 Bonn 1, Gerichtsweg 48, Deutschland.