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 coordinates 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.

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

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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.

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Tabelle 1. *Beobachtete und berechnete Strukturfaktoren*

hkl	F_o	F_c	hkl	F_o	F_c	hkl	F_o	F_c	hkl	F_o	F_c	hkl	F_o	F_c
020	133	−176	210	26	−25	340	70	−80	460	19	−23	630	55	−66
040	260	+287	220	240	+274	350	220	−219	470	129	−133	640	98	−99
060	114	+112	230	42	+33	360	32	+33	510	31	−33	650	28	−41
080	77	−66	240	58	−77	370	14	−14	520	18	−16	710	29	+27
120	12	−27	250	84	−80	380	72	−66	530	33	+59	720	109	+110
130	74	+83	260	160	−162	410	269	−269	540	43	+46	730	144	−154
140	196	+185	270	94	+70	420	231	+225	550	89	−109	740	29	−23
150	120	+118	280	11	+3	430	31	+30	560	56	−57	810	45	+43
160	192	−196	310	168	−142	440	58	+65	610	51	+51	820	106	+102
170	85	+90	320	179	+206	450	38	−40	620	98	+120	830	108	−112
180	65	−73	330	58	−60									

Die vorliegende Untersuchung zeigt, dass die Struktur des Tetraargentotellurperchlorates das gleiche komplexe Gerüstkation enthält wie das β-Tetraargentotellurnitrat (Schultze-Rhonhof, 1969). Offenbar ist die Struktur dieses Gerüstkations von der Art des eingebauten Gegenanions weitgehend unabhängig. Aufgrund dieses Befundes wurde auf dreidimensionales Arbeiten und weitere Verfeinerung verzichtet.

Die notwendigen Rechnungen wurden mit Hilfe der Programmkette *BN-X-64* (Schultze-Rhonhof, 1966) auf der IBM 7090 der GMD in Bonn ausgeführt.

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On certain structural relations between racemic and optically active crystal structures.

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The occurrence of certain structural relations between racemic and optically active pairs is pointed out for some structures. When these relations occur, the determination of the structure of an optically active form can be derived from that of the racemic one or *vice versa*. Usually it is possible to recognize for such a pair of structures a conservative plane of close-packed isomorphous molecules whose repetitions by the appropriate symmetry elements generate the two structures.

Many cases of polymorphism consist of a different packing of identical molecular layers. This occurs whenever different crystalline modifications with nearly the same lattice energy can be generated by repetition of one plane of molecules through the operation of different symmetry elements; the conservative plane of molecules is one in which the molecules are close-packed with respect to each other. It is obvious that, when this phenomenon is recognized, the determination of the structure of a second form can be directly derived from that of the first one. It is interesting to note that this phenomenon may occur in the crystal structures of racemic and optically active pairs. Therefore, as mentioned above, the crystal structure of an optically active form can be derived from that of the racemic one or *vice versa*, as we shall see in the following. Simpson & Marsh (1966) have determined the crystal structure of L-alanine. Surprisingly they found that the L-form and DL-form (Donohue, 1950) show nearly the same structure as far as the molecular packing is concerned. On the basis of the solved structures, those authors showed that it was possible to derive the structure of the L-form by reversing sense and direction of a column of D molecules. The similarity of the two structures was clearly indicated by the fact that

the unit-cell parameters (see Table 1) were nearly identical. Furthermore the zero-level Weissenberg photographs taken along the *c* axes were only slightly different for the two compounds. From the packing of the racemic form we recognized one plane (*bc*) of close-packed *isomorphous* molecules related by a screw symmetry axis contained in the plane. Then we were able to generate the L-alanine crystal structure assuming as conservative the *bc* plane of the racemic structure. A good trial model for the optically active structure is obtained simply using the fractional coordinates of the crystallographically independent molecule of the racemic form, taking into account the proper shift of the origin due to the change in space group. Incidentally, the assumption of the existence of a conservative plane of molecules in the two structures allows the *a priori* prediction of the possible space groups and the unit-cell parameters for the optically active form once those of the racemic form are known and *vice versa*. In the case of the L-alanine structures for example, without taking into account packing considerations, we should expect as probable the $P2_1$, $P2_12_12_1$ or $P2_12_12$ space group and simple relations with the unit-cell parameters of the DL-alanine structure.

The same phenomenon occurs also for the ($\pm$) and (+)