meters derived from each of the corrected reflection angles θ_B against 2θ. If the line of regression is horizontal, a correct account has been made for the aberrations and the scatter of points is indicative of the random error. The method has been applied successfully to silicon, but much more experimental work is required to establish its full potential. It is hoped that it may be used to establish a basis for the empirical use of peak measurements which would then be applied to low symmetry substances where overlapping reflections may render the c.g. method impractical.

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The crystal data for the chloro and bromo derivatives of picrotoxinin.

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The chemistry of picrotoxinin ($C_{15}H_{16}O_6$) has been thoroughly investigated for many years. These efforts have culminated in the structure proposed by Conroy (1957).

Crystals of α- and β-chloro and bromopicrotoxinin ($C_{15}H_{15}O_6Cl$ and $C_{15}H_{15}O_6Br$) have been examined. It was not possible to prepare iodopicrotoxinin, see Slater *et al.* (1956). The α isomers were all prismatic in crystal habit, while the β isomers were acicular. It was found that α-bromopicrotoxinin crystallized in two forms, here called α_1 and α_2. The nature of the difference between these forms has not been determined. More than one form for α-chloropicrotoxinin has not been discovered.

The cell parameters for these compounds (see Table 1) were determined from oscillation and Weissenberg photographs and the crystal densities were determined by the method of flotation in a mixture of chloroform and bromoform.

The [a] Patterson projection for β-bromo and β-chloropicrotoxinin were almost identical and there was no difficulty in finding the heavy atom positions (see Table 2). Although the β isomers are thus isomorphous, the presence of the halogen atoms in a special position ($z = 0$) makes a structure determination by the heavy atom or isomorphous replacement method very difficult.

There was no similarity between the corresponding Patterson projections of any of the α isomers, from which it is inferred that their structures are all different.

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Table 2. *Halogen atom positions*

	$x_{hal.}$	$y_{hal.}$	$z_{hal.}$
β-Bromopicrotoxinin	0·312	0·796	0
β-Chloropicrotoxinin	0·31	0·80	0
α_1-Bromopicrotoxinin	0·295	0·027	0·335
α_2-Bromopicrotoxinin	0·316	0·062	0·435

The positions of the bromine atoms in α_1- and α_2-bromopicrotoxinin were uniquely determined from the Pattersons, but there was no unique interpretation of the α-chloropicrotoxinin Pattersons. The chlorine atom is probably at (0·340, 0·063, 0·410).

It has not been found possible to solve the structure of either α_1 or α_2-bromopicrotoxinin in projection because of the difficulty in recognizing any structural features in the approximate electron density maps. Three-dimensional structure determinations of both α_1- and α_2-bromopicrotoxinin are now in progress.

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Table 1. *Crystal data*

Compound	System	a (Å)	b (Å)	c (Å)	Å^3	D_m g.cm.$^{-3}$	D_x g.cm.$^{-3}$	Z	Space group
β-Bromopicrotoxinin	Tetragonal	7·08	—	28·30	1420	1·72	1·74	4	$P4_1$ or $P4_3$
β-Chloropicrotoxinin	Tetragonal	7·07	—	28·48	1425	—	—	4	$P4_1$ or $P4_3$
α_1-Bromopicrotoxinin	Orthorhombic	13·40	11·60	8·86	1378	1·78	1·80	4	$P2_12_12_1$
α_2-Bromopicrotoxinin	Orthorhombic	13·65	11·86	8·76	1420	1·76	1·75	4	$P2_12_12_1$
α-Chloropicrotoxinin	Orthorhombic	14·68	11·48	8·46	1425	—	—	4	$P2_12_12_1$