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Crystallographic study of an unknown compound from western red cedar.

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In a study of the substances occurring in the aqueous extracts of western red cedar, a compound of unknown structure with interesting chemical properties was isolated. In an effort to determine the structure, hydrobromide and hydroiodide derivatives were examined by X-ray methods. The crystal data are given in Table 1.

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Table 1. *Crystal data*

	Hydrobromide	Hydroiodide
Formula	$C_{24}H_{24}O_{12}$. HBr	$C_{24}H24O_{12}$. HI
Mol. wt.	585·4	632·4
Crystal system	Monoclinic	Monoclinic
a(Å)	6·13	6·20
b(Å)	19·16	19·37
c(Å)	10·80	10·86
β	107·1°	97·1°
U(Å^3)	1213	1294
D_m	1·59	1·62
Z	2	2
D_x	1·60	1·62
Space group	$P2_1$	$P2_1$
x (Br^- or I^-)	0·025	0·012
z (Br^- or I^-)	0·192	0·138

Using scintillation counter data for the hydrobromide and visual data for the hydroiodide, the heavy-atom coordinates were determined from the Harker sections (Table 1). Three-dimensional electron-density distributions were then computed; these had of course false mirror planes, and efforts were made to interpret them by introducing small numbers of light atoms, at first based on only the electron-density maps, and later with the added information that the compound is probably related to plicatic acid (Gardner, MacDonald & McLean, 1960). All the efforts were unsuccessful, and no further work is planned.

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Crystallographic data for ochotensimine methiodide.

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The alkaloids ochotensine and ochotensimine were isolated from *Corydalis ochotensis* by Manske (1940), who showed that ochotensimine is simply the *O*-methyl ether of the phenolic base ochotensine. A structure for ochotensimine has been proposed on the basis of nuclear magnetic resonance data (McLean & Lin, 1964), and an X-ray analysis of ochotensimine methiodide was undertaken to establish the structure directly. The data suggest that the crystals contain methanol of crystallization.

Crystal data

Ochotensimine methiodide, $C_{23}H_{26}O_4NI$ (probably $+CH_3OH$), M.W. 507·4 (539·4 with CH_3OH).

Orthorhombic, $a=7{\cdot}67\pm0{\cdot}02$, $b=11{\cdot}92\pm0{\cdot}02$, $c=52{\cdot}15\pm0{\cdot}10$ Å.

$U=4768$ Å^3.

$D_m=1{\cdot}50$, $Z=8$, $D_x=1{\cdot}41$ (1·50 with CH_3OH).

$F(000)=2192$.

Absent spectra: $h00$ when h is odd, $0k0$ when k is odd, $00l$ when l is odd. Space group $P2_12_12_1$.

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The intensities were estimated visually, and the coordinates of the two I^- ions in the asymmetric unit were determined from the three-dimensional Patterson function as:

	x	y	z
I(1)	0·04	0·063	0·250
I(2)	0	−0·170	−0·052

An electron-density distribution was computed; this had almost a false mirror plane at $x=0$, and many efforts to interpret it were unsuccessful. No further work is planned on this compound, but an analysis of ochotensine methiodide is being undertaken.

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