tainty as to which interatomic distance to use in computing a radius, in the case of complex structures having several different interatomic distances. Values of the atomic volume of pure elements were taken from the paper by Rudman (1965). Table 1 includes a list of relative atomic sizes in terms of the atomic volume of the Sc group element divided by the atomic volume of the Cu group element.

Nevitt (1963) has discussed the $MoSi_2$-type compounds and has observed that the ideal radius ratio is 1 (hence, the ideal volume ratio is also 1), many compounds having ratios which lie above the ideal value. When $MnAu_2$ (Hall & Royan, 1959) is also considered, the apparent range in volume ratios is from 0·718 for $MnAu_2$ to 2·424 for $YbAu_2$. However, so high a volume ratio for $YbAu_2$ is of questionable validity, because the atomic volume for pure Yb applies to divalent Yb, but there is reason to believe that Yb in $YbAu_2$ is nearly trivalent. As shown in Fig. 1, the c_0 and a_0 values for $YbAu_2$ lie on a smooth curve between Tm and Lu. The c/a and volume per formula weight values show only a small deviation. If Yb were divalent, the unit cell constants would be much larger. This effect was recently discussed by Kripyakevich, Gladyshevskii, Zarechnyuk, Evdokimenko, Zalutskii & Frankevich (1964). Therefore, the volume ratio for $YbAu_2$ should be computed from a lower unknown volume for trivalent Yb.

A better way to obtain a maximum limiting volume ratio for $MoSi_2$-type structures is by use of data for Y, Sm, and Gd compounds. The elements Y, Sm and Gd all have nearly the same atomic volume, but when alloyed with Ag and Au, only Y and Gd form the $MoSi_2$-type structure. Therefore, the maximum limiting volume for the Sc group–Au_2 series must lie close to the value for $GdAu_2$, *i.e.* 1·941.

A different limiting volume ratio is obtained from the Sc group-Cu_2 series. Only the smallest member of the Sc group, Sc itself, when alloyed with Cu, forms the $MoSi_2$-type structure (Table 1). The next smallest, Lu, forms the $CeCu_2$-type (Storm & Benson, 1963). Volume ratios are 2·119 for $ScCu_2$ and 2·50 for $LuCu_2$. The limiting volume ratio for the $MoSi_2$-type structure lies above 2·119 when the B element is Cu, and close to 1·941 when the B element is Au. Therefore, it is concluded that no single value can be assigned as the upper limit, but that the maximum limiting volume ratio is very approximately 2.

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The space group and lattice constants of the 2-, 3- and 4-iodosalicylideneanilines.

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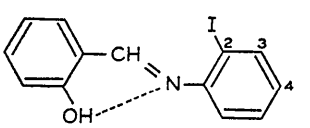
The space group and lattice constants of photochromic and thermochromic 2-, 3- and 4-iodo-salicylideneanilines have been determined.

The crystalline *N*-salicylideneanilines exhibit interesting color changes induced by ultraviolet irradiation (photochromic) or by temperature changes (thermochromic). These properties of the salicylideneanilines are a function of the crystal and molecular structure. Thermochromicity requires planar, close packed molecules, whereas photochromicity appears to require nonplanar molecules with a relatively open crystal structure (Cohen, 1964).

An X-ray study of the salicylideneanilines having chlorine or bromine in the 2-, 3- and 4-positions has previously been made (Cohen, Schmidt & Flavin, 1964). The 2-chloro and 2-bromo derivatives are isomorphous and are both photochromic. The 3-chloro- and 3-bromo derivatives are both thermochromic but are not isomorphous.

A recent infrared spectroscopic study (Cohen, 1966) of the phase system of the 4-chloro and 4-bromo derivatives shows that these materials exhibit 'structure mimicry'. (Sacconi, Clampolini & Speroni, 1965). This is the existence of two series of solid solutions in which the guest molecules (solute) adopt the molecular structures of the host molecules. These systems have been subject to an infrared examination (Dodd & Cohen, 1966) with particular emphasis on the vibrational modes of the halogen atoms. This work was extended to include the 2-, 3- and 4-iodo derivatives. For this purpose it was necessary to obtain structural information on the iodosalicylideneanilines (I). The iodine may be in the 2-, 3- or 4-position as indicated.

In this study, the space groups and lattice constants of the three iodo-substituted compounds have been determined. Precession, Weissenberg and rotation photographs were



$C_6H_4CH_2ON\,C_6H_4I$
(I)

taken of small single crystals of each substance with Mo $K\alpha$ radiation ($\lambda = 0{\cdot}7107$ Å) and Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å). The absorption coefficient is 2·77 mm^{-1} for Mo $K\alpha$ and 21·91 mm^{-1} for Cu $K\alpha$ radiation. Lattice constants were measured from the films, with due correction for film shrinkage. The densities were measured by flotation in an aqueous solution of zinc chloride at 24°C. The three iodo derivatives are yellow. The crystals were grown from aqueous ethanol. 2-Iodo-, 2-chloro- and 2-bromo-salicylideneaniline are isotypic: 3-iodo- and 3-bromo-salicylideneaniline are isotypic, but not with the 2-compounds.

The results of the X-ray study are summarized in Table 1. No further X-ray work on these compounds is contemplated.

I wish to thank Dr M. D. Cohen for supplying the crystals and for helpful discussions.

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Table 1. *Crystal data for the* 2,- 3- *and* 4-*iodo-salicylideneanilines*

Compound	Crystal system and space group	Lattice constants (24°C)	D_x	D_m	Z	m.p.	Morphology	Transformation*
2-Iodo-salicylidene-aniline	Orthorhombic $P2_12_12_1$ (D_2^4)	$a = 12{\cdot}953 \pm 0{\cdot}009$ Å $b = 7{\cdot}468 \pm 0{\cdot}009$ $c = 12{\cdot}525 \pm 0{\cdot}009$	1·77 g.cm^{-3}	1·773 ± 0·011 g.cm^{-3}	4	52·75 ± 0·25°C	Anhedral	Photochromic
3-Iodo-salicylidene-aniline	Monoclinic $P2_1$ (C_2^2)	$a = 13{\cdot}472 \pm 0{\cdot}008$ Å $b = 10{\cdot}353 \pm 0{\cdot}008$ $c = 4{\cdot}202 \pm 0{\cdot}008$ $\beta = 97°20' \pm 10'$	1·85 g.cm^{-3}	1·85 ± 0·02 g.cm^{-3}	2	95·5 ± 0·5°C	Lath shaped, elongated along b; a nearly perpendicular to lath; c in the plane of the lath	Thermochromic
4-Iodo-salicylidene-aniline	Orthorhombic *Pbma* (D_{2h}^{11}) or $Pb2_1a$ (C_{2v}^5)	$a = 6{\cdot}094 \pm 0{\cdot}008$ Å $b = 53{\cdot}70 \pm 0{\cdot}09$ $c = 7{\cdot}116 \pm 0{\cdot}008$	1·84 g.cm^{-3}	1·81 ± 0·03 g.cm^{-3}	8	126·9 ± 0·1°C	Lath shaped, elongated along a; b perpendicular to lath and c in the plane of the lath	Thermochromic

* Photochromic indicates a reversible color change when irradiated with ultraviolet light: Thermochromic refers to a reversible color change upon heating.