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**Crystallographic data for salicylaldehyde,  $C_7H_7O_2N$ .**\* By LYNNE L. MERRITT, JR. and EDITH SCHROEDER,  
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Salicylaldehyde is an organic reagent which forms complexes with a variety of metal ions, and which can, in some cases, be made specific by control of pH conditions of precipitation. This laboratory has been investigating the structures of chelating agents and of chelate complexes of analytical importance for the past few years. Recently the structure of nickel salicylaldehyde was reported by workers in this group (Merritt, Guare & Lessor, 1956). A study of the structure of salicylaldehyde has now been undertaken, and this paper constitutes a report on the preliminary work.

Using hexagonal crystals of salicylaldehyde, obtained from an alcohol solution of the compound, a preliminary X-ray survey has determined the unit cell and space group. From rotation, Weissenberg and precession photographs taken about the  $a$  and the  $c$  axes, using nickel-filtered  $Cu K\alpha$  radiation, the orthorhombic unit-cell dimensions were found to be

$$a = 12.69, b = 13.51, c = 7.98 \text{ \AA}.$$

The only systematic absences of reflections occurred for ( $h00$ ) when  $h$  is odd, ( $0k0$ ) when  $k$  is odd, and ( $00l$ ) when  $l$  is odd. Accordingly, the space group is determined as  $P2_12_12_1-D_2^7$ .

There are 8 molecules per unit cell. Density: calculated  $1.33 \text{ g.cm.}^{-3}$ ; observed (floatation)  $1.34 \text{ g.cm.}^{-3}$ .

The refractive indices were measured by means of standard refraction liquids:

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$$n_\alpha = 1.480, n_\beta = 1.76, 1.79 < n_\gamma < 1.80.$$

The powder pattern of salicylaldehyde was recorded with nickel-filtered  $Cu K\alpha$  radiation in a Debye-Scherrer camera of 57.3 mm. radius. The intensities were estimated visually by comparison with standard intensity strips prepared by timed exposures of one reflection from a single crystal. The data are summarized in Table 1.

Table 1. Powder diffraction data

$d$ (Å)	$I/I_0$	$d$ (Å)	$I/I_0$
6.76	0.42	3.08	0.21
6.32	0.15	2.96	0.07
5.99	0.13	2.89	0.15
5.68	0.28	2.78	0.10
5.10	0.23	2.64	0.09
4.58	0.36	2.36	0.12
3.97	0.21	2.20	0.09
3.65	1.00	1.98	0.08
3.38	0.51	1.79	0.08
3.26	0.67	1.67	0.06

Further work is in progress with the hope of completing a structure determination of this compound.

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#### Reference

MERRITT, L. L., JR., GUARE, C. & LESSOR, A. E., JR. (1956). *Acta Cryst.* In the Press.

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**Partial structure of bis-benzonitrile palladium chloride.** By J. R. HOLDEN and N. C. BAENZIGER,  
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In connexion with an investigation of some complexes of palladium chloride with ethylenic-type compounds (Holden & Baenziger, 1955) a partial structure of bis-benzonitrile palladium chloride (an intermediate in the preparation of the ethylenic complexes) was determined.

Long blade-shaped crystals of bis-benzonitrile palladium chloride showing no external symmetry were formed on a 'cold-finger' placed in a warm solution of palladium chloride in benzonitrile. Weissenberg and precession diagrams were taken with the X-ray beam normal to the needle axis of the crystal. The unit cell was found to be triclinic with the reduced primitive cell dimensions of

$$a = 5.79, b = 8.45, c = 8.71 \text{ \AA}, \\ \alpha = 117.4, \beta = 92.9, \gamma = 95.0^\circ.$$

The needle axis of the crystal is the short body diagonal

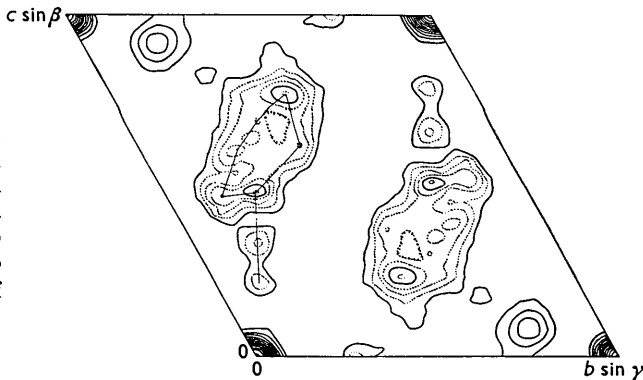


Fig. 1. Electron density projected along [100].