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Crystallographic data for triclinic 5-formylvanillic acid.*

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The unit cell and space group of monoclinic 5-formylvanillic acid, $C_9H_8O_5$, were reported from this laboratory (Morita & Kodama, 1964). A triclinic isomer melting at 227–228 °C has been isolated by slow crystallization of the compound from a solution in a mixture of dioxane and petroleum ether (b.p. 60–80 °C).

Crystal data

The crystal data were determined from rotation, Weissenberg, and precession photographs with Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å).

$a_0 = 6{\cdot}91$, $b_0 = 7{\cdot}93$, $c_0 = 9{\cdot}36$ Å.

$\alpha = 125°22'$, $\beta = 124°58'$, $\gamma = 58°40'$.

$V = 331{\cdot}2$ Å^3.

$D_m = 2{\cdot}0$, $D_x = 1{\cdot}9647$ g.cm^{-3}, $Z = 2$

Of the two possible space groups $P\bar{1}$ and $P1$, $P\bar{1}$ is preferred because the compound is optically inactive.

The Debye–Scherrer powder reflexions were indexed with the use of the unit-cell dimensions obtained from the single-crystal study and their intensities estimated visually. The powder data have been submitted for inclusion in the ASTM X-ray Powder Data File.

No further detailed analysis is contemplated.

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References

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The crystal structure of $YbZn_2$.*

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The determination of the crystal structure of $YbZn_2$ by single-crystal techniques is the subject of this communication.

Stoichiometric amounts of 99·5 % ytterbium and 99·999 % zinc were sealed under helium in a tantalum crucible, melted, and allowed to furnace-cool. Oscillation and Weissenberg photographs of a single crystal chosen from this alloy indicated the resulting compound to be orthorhombic, with $a = 4{\cdot}60$, $b = 7{\cdot}319$, $c = 7{\cdot}561$ Å. The values for b and c were obtained from an $0kl$ backreflection Weissenberg photograph. A Debye–Scherrer photograph, taken with Fe $K\alpha$ ($\lambda = 1{\cdot}93728$ Å) radiation, was subsequently indexed, and the final lattice parameters were found from a least-squares fit to the data to be:

$a = 4{\cdot}573 \pm 0{\cdot}002$, $b = 7{\cdot}325 \pm 0{\cdot}005$, $c = 7{\cdot}569 \pm 0{\cdot}004$ Å.

All hkl reflections with $h+k+l = 2n+1$ and $hk0$ reflections with $h = 2n+1$ are absent on the Weissenberg photographs, indicating that the space group is $Im2a$ (or $I2ma$) or $Imma$.

The intensities of 277 hkl reflections were measured on an equi-inclination Weissenberg counter diffractometer using an ω scan. Mo $K\alpha$ radiation was used, and data were recorded out to $\sin\theta = 0{\cdot}5$. Although the crystal was quite irregular in shape, it was approximated by a cylinder and absorption corrections were calculated according to Bond (1959).

The lattice parameters and possible space group for $YbZn_2$ indicated that it is isostructural with $CeCu_2$ (Larson & Cromer, 1961), and also YZn_2 (Sree Harsha & Ryba, 1964). Thus, there are four ytterbium atoms and eight zinc atoms in the equipoints 4(*e*) and 8(*h*), respectively, of the space group *Imma*. Using the positional parameters for YZn_2, a trial structure was refined with the full-matrix least-squares program of Busing, Martin & Levy (1962). The atomic scattering factors for ytterbium and zinc were taken from *International Tables for X-ray Crystallography* (1962), and were corrected for anomalous dispersion according to Dauben & Templeton (1955). Unit weights were assigned to all reflections. The results of this refinement are given in Table 1. The final residual for all observed reflections is 15 %. Observed and calculated $0kl$ structure factors are given in Table 2. An $0kl$ electron density projection confirmed the correctness of the structure. The high residual and the lack of better agreement between observed and calculated structure factors can probably be attributed to the irregular shape of the crystal and the high absorption of the ytterbium atom. Interatomic distances are given in Table 3; the standard deviations given were calculated by taking into account the standard deviations in both the positional parameters and the lattice parameters.

Metallographic examination of the alloy revealed the presence of extensive twinning. A thermal arrest, indicating a possible phase transition in $YbZn_2$, was observed at 683 ± 3 °C. This transition may be the cause of the twinning.

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Table 1. *Final parameters for* $YbZn_2$ *from the least-squares refinement*

Atom	Position	x	y	z	B(Å^2)
Yb	4e	0	$\frac{1}{4}$	$0{\cdot}5503 \pm 0{\cdot}0005$	$0{\cdot}91 \pm 0{\cdot}04$
Zn	8h	0	$0{\cdot}0587 \pm 0{\cdot}0009$	$0{\cdot}1641 \pm 0{\cdot}0009$	$1{\cdot}23 \pm 0{\cdot}08$