Zeitschrift für Kristallographie 165, 313–314 (1983)


# Synthesis and crystal structure of 2H—$CuAlO_2$

B. U. Köhler and M. Jansen

Institut für Anorganische Chemie der Universität, Callinstraße 9, D-3000 Hannover, Federal Republic of Germany

Received: August 30, 1983

*Synthesis / Crystal structure / 2H – $CuAlO_2$*

**Abstract.** 2H–$CuAlO_2$ was obtained by reaction of $Cu_2O$ and $Al_2O_3$ in a PbO flux. The crystal structure, which represents a 2H-stacking variant of the delafossite type of structure, was refined using single crystal X-ray diffractometer data ($P6_3/mmc$; $a = 285{,}8(2)$, $c = 1129{,}3(2)$ pm; $Z = 2$; $R = 0{,}057$; 122 independent observed reflexions).

## Experimental

*a) Preparation*

Crystals of 2H – $CuAlO_2$ were obtained in the form of hexagonal prisms or platelets by heating mixtures of $Cu_2O$, $Al_2O_3$ and PbO in the molar ratios 1.1:1:1 at 900 °C in an $Al_2O_3$-crucible for 48–96 h. In the course of this treatment PbO had evaporated and black (deep red in very thin sections) crystals of 2H – $CuAlO_2$ had formed. The excess of $Cu_2O$ was removed by washing with dilute nitric acid, the remaining traces of PbO by treating with 2n – NaOH.

*b) Crystal data, structure refinement*

The crystal system and possible space groups were determined from rotation, Weissenberg and precession photographs, the unit cell parameters were refined from Guinier powder data ($CuK_{\alpha_1}$, internal standard: low-quartz): hexagonal, $a = 285.8(2)$, $c = 1129.3(2)$ pm, $P6_3/mmc$, $D_{calc.} = 5.09$ Mg/m$^3$, $Z = 2$. The intensities of 2790 reflexions were measured using an automated diffractometer (CAD 4) and graphite-monochromated $MoK\alpha$ radiation (scan-width $= (1.3 + 0.35 \tan\theta)°$, horizontal detector aperture $= (1.3 + 1.0 \tan\theta)°$, scan mode $= \omega/\theta$). After averaging and applying LP-correction 122 unique structure factors remained for refinement. The final $R$-values are $R = 0.057$ and $R_w = 0.079$ with weights derived from counting statistics. The atomic parameters are given in Table 1.[1]

[1] Additional material to this paper can be ordered referring to the no. CSD 50577, names of the authors and citation of the paper at the Fachinformationszentrum Energie-Physik-Mathematik, D-7514 Eggenstein-Leopoldshafen 2, FRG

**Table 1.** Positional coordinates and anisotropic temperature factors of 2H – $CuAlO_2$, the thermal parameters are of the form $T = \exp. - (B_{11}h^2 \pm \ldots + B_{23}kl)$

| Atom | $x$ | $y$ | $z$ | $B_{11}$ | $B_{33}$ |
|---|---|---|---|---|---|
| Cu | 1/3 | 2/3 | 1/4 | 0.020(2) | 0.0004(1) |
| Al | 0 | 0 | 0 | 0.004(5) | 0.0004(1) |
| O | 1/3 | 2/3 | 0.0859(6) | 0.006(7) | 0.0006(3) |

Symmetry contraints: $B_{22} = B_{11}$, $B_{23} = B_{13} = O$, $B_{12} = B_{11}$

**Table 2.** Bond distances (pm) and angles (°) with e.s.d.'s

| | | | | |
|---|---|---|---|---|
| Cu – O | 185.3(5) | (2 ×) | O – Al – $O^{I}$ | 180 |
| Al – O | 191.4(3) | (6 ×) | O – Al – $O^{II}$ | 83.4(2) |
| O – Cu – O | 180° | | O – Al – $O^{III}$ | 96.6(2) |

Symmetry-code: (I) $-x, -y, -z$; (II) $-x, x, -z$; (III) $-y, -x, z$

Powder data of 2H – $CuAlO_2$

| $hkl$ | $d_{obs.}$ | $I_{obs.}$ | $hkl$ | $d_{obs.}$ | $I_{obs.}$ |
|---|---|---|---|---|---|
| 002 | 5.651 | 1 | 006 | 1.8819 | 1 |
| 004 | 2.8241 | 3 | 105 | 1.6687 | 3 |
| 101 | 2.4186 | 10 | 106 | 1.4987 | 3 |
| 102 | 2.2659 | 5 | 008 | 1.4118 | 1 |
| 103 | 2.0678 | 1 | 107 | 1.3512 | 2 |

## Discussion

2H – $CuAlO_2$ is isostructural with 2H – $CuFeO_2$, 2H – $AgFeO_2$ (Okomoto et al., 1972) and 2H – $AgAlO_2$ (Brachtel and Jansen, 1981) and is a stacking variant of R – $CuAlO_2$, delafossite type of structure, (Ishigawa et al., 1981). The oxygen atoms are stacked in the layer sequence ABBA... with Al in octahedral sites (AB) and Cu in linear coordination (BB). Bond distances and angles within the first coordination sphere of Al and Cu are given in Table 2.

*Acknowledgements.* This work was supported by Deutsche Forschungsgemeinschaft. The authors are indebted to Dr. Schmitz, Aachen, for collecting the intensity data.

## References

Brachtel, G., Jansen, M.: 2H – $AgAlO_2$. Cryst. Struct. Commun. **10,** 173 – 174 (1981)

Ishigawa, T., Kitazawa, A., Mizutani, N., Kato, M.: Single crystal growth and crystal structure refinement of copper aluminate ($CuAlO_2$). J. Solid State Chem. **40(2),** 170 – 174 (1981)

Okamoto, S., Okamoto, S. I., Ito, T.: Crystal structure of a new hexagonal phase of silver ferrite. Acta Crystallogr. **B 28,** 1774 – 1777 (1972)