# Crystal structure of ytterbium gold plumbide (2/2/1), $Yb_2Au_2Pb$

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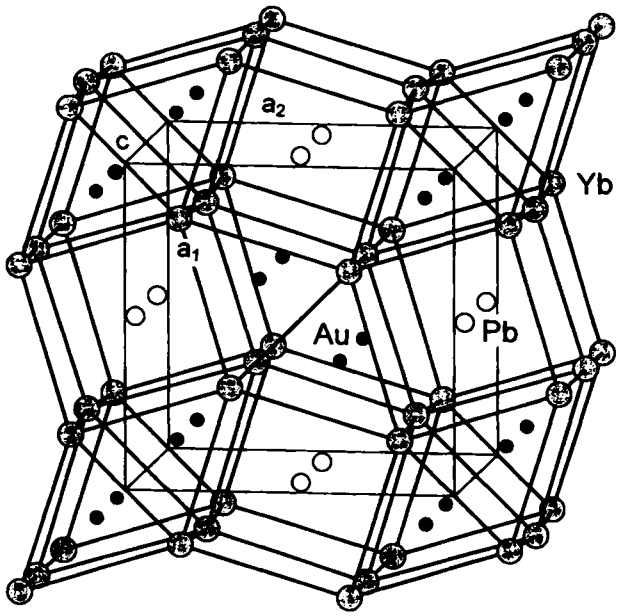


## Abstract

$Au_2PbYb_2$, tetragonal, $P4_2/mnm$ (No. 136), $a = 8.037(2)$ Å, $c = 7.465(2)$ Å, $V = 482.2$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.036$, $wR_{obs}(F^2) = 0.069$, $T = 293$ K.

## Source of material

The title compound was obtained from the elements (Yb 99.9%, Au and Pb 99.999%) by induction melting in a tantalum container sealed by arc welding under argon.

## Discussion

The phase $Yb_2Au_2Pb$ crystallizes in an ordered ternary variant of the $Zr_3Al_2$ type (Pearson code $tP20$), as the recently reported $Yb_2Pt_2Pb$ [1]. It is characterized by slabs of double trigonal prisms and cubes all formed by the Yb atoms. The trigonal prisms share a lateral face and are centered by gold, while the cubes are centered by lead atoms. Differently from the $U_3Si_2$ type, where the slab width corresponds to the $c$ lattice parameter, in the $Zr_3Al_2$-derived structures a certain atom displacement causes two slabs be stacked along $c$, doubling the lattice parameter. The shortest distances in $Yb_2Au_2Pb$ are Au—Au 2.790(2) Å, Yb2—Au 2.972(3) Å, Au—Pb 3.191(1) Å, Yb1—Pb 3.488(1) Å and Yb1—Yb2 3.736(1) Å.

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | metallic grey needle, size 0.03 × 0.04 × 0.14 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71069 Å) |
| μ: | 1336.40 cm$^{-1}$ |
| Diffractometer, scan mode: | Enraf-Nonius CAD4, ω/2θ |
| $2\theta_{max}$: | 59.92° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 1600, 413 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 229 |
| $N(param)_{refined}$: | 18 |
| Program: | SHELXL 97 [2] |

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## References

1. Pöttgen, R.; Arpe, P. E.; Felser, C.; Kussmann, D.; Müllmann, R.; Mosel, B. D.; Künnen, B.; Kotzyba, G.: Structure and properties of YbZnSn, YbAgSn, and $Yb_2Pt_2Pb$. J. Solid State Chem. **145** (1999) 668-677.
2. Sheldrick, G. M.: SHELXL-97, a program for refinement of crystal structures. University of Göttingen, Germany, 1997.

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Yb(1) | 4*g* | 0.3187(2) | $-x$ | 0 | 0.0225(9) | $U_{11}$ | 0.025(1) | 0.008(1) | 0 | 0 |
| Yb(2) | 4*f* | 0.1662(2) | $x$ | 0 | 0.0210(9) | $U_{11}$ | 0.024(1) | −0.0069(9) | 0 | 0 |
| Au | 8*j* | 0.37728(9) | $x$ | 0.2350(2) | 0.0174(3) | $U_{11}$ | 0.0317(7) | −0.0042(4) | −0.0006(5) | $U_{13}$ |
| Pb | 4*d* | 0 | 1/2 | 1/4 | 0.0173(4) | $U_{11}$ | 0.044(1) | 0 | 0 | 0 |

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