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Crystal structure of ytterbium gold aluminium, YbAuAl

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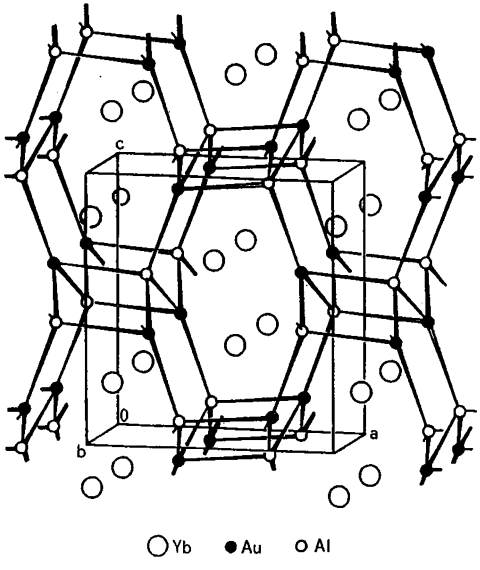

Source of material: The compound was prepared by melting the elements in stoichiometric amounts in corundum crucibles for 2 h at 1400 K and cooling to room temperature at a ratio of 100 K/h.
The title compound crystallizes in the NiSiTi (Co_2Si) structure type. Au- and Al-atoms form a framework of tetrahedra. The ytterbium atoms (CN = 16) occupy voids of this Au/Al-framework. Interatomic distances are: d(Yb-Yb) = 3.662(1)-3.735(1) Å, d(Yb-Au) = 3.022(2)-3.640(2) Å, d(Yb-Al) = 3.190(9)-3.3360(9) Å, d(Au-Al) = 2.645(9)-2.713(9) Å, d(Al-Al) = 3.425(14) Å.

Orthorhombic, Pnma (no 62), $a = 7.210(2)$, $b = 4.488(1)$, $c = 7.732(2)$ Å, V = 250.2 Å^3, Z = 4, $\varrho_m = 10.52$ g · cm^{-3}, R = 0.053.