

|                  |              |                                        |
|------------------|--------------|----------------------------------------|
| AuF <sub>3</sub> | <i>hP</i> 24 | (178) <i>P</i> 6 <sub>1</sub> 22 – cba |
|------------------|--------------|----------------------------------------|

# **AuF<sub>3</sub>** [2]

Structural features: Infinite twisted chains of vertex-linked AuF<sub>4</sub> squares are loosely interconnected to form a 3D-framework.

Zemva B. et al. (1991) [1]

AuF<sub>3</sub>

$a = 0.51508$ ,  $c = 1.62637$  nm,  $c/a = 3.158$ ,  $V = 0.3737$  nm<sup>3</sup>,  $Z = 6$

| site | Wyck.       | sym. | <i>x</i> | <i>y</i> | <i>z</i>                    | occ. | atomic environment             |
|------|-------------|------|----------|----------|-----------------------------|------|--------------------------------|
| F1   | 12 <i>c</i> | 1    | 0.5338   | 0.3099   | 0.4947                      |      | single atom Au                 |
| Au2  | 6 <i>b</i>  | ..2  | 0.2399   | 0.4798   | <sup>1</sup> / <sub>4</sub> |      | coplanar square F <sub>4</sub> |
| F3   | 6 <i>a</i>  | .2.  | 0.1639   | 0        | 0                           |      | non-colinear Au <sub>2</sub>   |

Experimental: powder, diffractometer, neutrons, time-of-flight, R<sub>p</sub> = 0.076

References: [1] Zemva B., Lutar K., Jesih A., Casteel W.J., Wilkinson A.P., Cox D.E., Von Dreele R.B., Borrmann H., Bartlett N. (1991), J. Am. Chem. Soc. 113, 4192-4198. [2] Einstein F.W.B., Rao P.R., Trotter J., Bartlett N. (1967), J. Chem. Soc. A 1967, 478-482.