

|   |              |   |
|---|--------------|---|
| Ba <sub>6</sub> EuCl <sub>2</sub> F <sub>12</sub> | <i>hP</i> 21 | (174) <i>P</i> -6 – k <sup>3</sup> j <sup>3</sup> fca |
|---|--------------|---|

**Ba<sub>6</sub>EuCl<sub>2</sub>F<sub>12</sub> ordered** [1]

Structural features: Infinite columns of base-linked Ba(Cl<sub>2</sub>F<sub>4</sub>)F<sub>3</sub> and EuF<sub>6</sub>F<sub>3</sub> tricapped trigonal prisms share atoms to form a 3D-framework with propeller-like columns. Ordering variant of Zr<sub>2</sub>Fe<sub>12</sub>P<sub>7</sub> antitype.

Kubel F. et al. (2000) [1]

Ba<sub>6</sub>Cl<sub>2</sub>EuF<sub>12</sub>

*a* = 1.05927, *c* = 0.41636 nm, *c/a* = 0.393, *V* = 0.4046 nm<sup>3</sup>, *Z* = 1

| site | Wyck.      | sym.        | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment  |
|------|------------|-------------|----------|----------|----------|------|---|
| F1   | 3 <i>k</i> | <i>m</i> .. | 0.0494   | 0.4371   | 1/2      |      | tetrahedron Ba <sub>4</sub>                               |
| F2   | 3 <i>k</i> | <i>m</i> .. | 0.2151   | 0.1166   | 1/2      |      | single atom Ba  |
| Ba3  | 3 <i>k</i> | <i>m</i> .. | 0.28778  | 0.40106  | 1/2      |      | monocapped trigonal prism F <sub>7</sub>                  |
| F4   | 3 <i>j</i> | <i>m</i> .. | 0.1223   | 0.2765   | 0        |      | tetrahedron EuBa <sub>3</sub>                             |
| Ba5  | 3 <i>j</i> | <i>m</i> .. | 0.41015  | 0.10935  | 0        |      | tricapped trigonal prism F <sub>7</sub> Cl <sub>2</sub>   |
| F6   | 3 <i>j</i> | <i>m</i> .. | 0.4299   | 0.3676   | 0        |      | tetrahedron Ba <sub>4</sub>                               |
| Cl7  | 1 <i>f</i> | -6..        | 2/3      | 1/3      | 1/2      |      | hexagonal prism Ba <sub>6</sub> F <sub>6</sub>            |
| Cl8  | 1 <i>c</i> | -6..        | 1/3      | 2/3      | 0        |      | sixcapped hexagonal prism Ba <sub>6</sub> F <sub>12</sub> |
| Eu9  | 1 <i>a</i> | -6..        | 0        | 0        | 0        |      | tricapped trigonal prism F <sub>9</sub>                   |

Experimental: single crystal, diffractometer, X-rays, *R* = 0.024, *T* = 293 K

References: [1] Kubel F., Bill H., Hagemann H. (2000), *Z. Anorg. Allg. Chem.* 626, 1721-1722.