

Ba₅Cu₄ClF₁₇*hP*81(189) *P*-62*m* – 1²kji⁴hg³feca**Ba₅Cu₄ClF₁₇** [1]

Structural features: CuF₆ octahedra, CuF₅ trigonal bipyramids and CuF₄ squares share vertices to form infinite chains (- octahedron - bipyramid - octahedron - square -) parallel to [001].

Fompeyrine J. et al. (1995) [1]

Ba₅ClCu₄F₁₇*a* = 1.0731, *c* = 1.2803 nm, *c/a* = 1.193, *V* = 1.2768 nm³, *Z* = 3

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------------|---------------------|-----------------------------|-----------------------------|-----------------------------|------|---|
| F1 | 12 <i>l</i> | 1 | 0.1449 | 0.5723 | 0.1642 | | single atom Cu |
| F2 | 12 <i>l</i> | 1 | 0.146 | 0.3871 | 0.3116 | | single atom Cu |
| F3 | 6 <i>k</i> | <i>m</i> .. | 0.1623 | 0.5309 | ¹ / ₂ | | single atom Cu |
| F4 | 6 <i>j</i> | <i>m</i> .. | 0.2041 | 0.3678 | 0 | | single atom Cu |
| F5 | 6 <i>i</i> | .. <i>m</i> | 0.2292 | 0 | 0.1443 | | non-colinear Cu ₂ |
| Cu6 | 6 <i>i</i> | .. <i>m</i> | 0.4031 | 0 | 0.2352 | | octahedron F ₆ |
| F7 | 6 <i>i</i> | .. <i>m</i> | 0.5678 | 0 | 0.351 | | non-colinear Cu ₂ |
| Ba8 | 6 <i>i</i> | .. <i>m</i> | 0.731 | 0 | 0.1928 | | monocapped square prism F ₉ |
| Ba9 | 4 <i>h</i> | 3.. | ¹ / ₃ | ² / ₃ | 0.3377 | | tricapped trigonal prism F ₉ |
| Ba10 | 3 <i>g</i> | <i>m</i> 2 <i>m</i> | 0.2429 | 0 | ¹ / ₂ | | square prism (cube) F ₈ |
| Cu11 | 3 <i>g</i> | <i>m</i> 2 <i>m</i> | 0.5762 | 0 | ¹ / ₂ | | trigonal bipyramid F ₅ |
| F12 | 3 <i>g</i> | <i>m</i> 2 <i>m</i> | 0.7541 | 0 | ¹ / ₂ | | single atom Cu |
| Cu13 | 3 <i>f</i> | <i>m</i> 2 <i>m</i> | 0.2418 | 0 | 0 | | square pyramid F ₄ Cl |
| Cl14 | 2 <i>e</i> | 3.. <i>m</i> | 0 | 0 | 0.3345 | | sixcapped hexagonal prism Ba ₆ F ₁₂ |
| Ba15 | 2 <i>c</i> | -6.. | ¹ / ₃ | ² / ₃ | 0 | | tricapped trigonal prism F ₉ |
| Cl16 | 1 <i>a</i> | -62 <i>m</i> | 0 | 0 | 0 | | coplanar triangle Cu ₃ |

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 ¹/₂Experimental: single crystal, diffractometer, X-rays, *R* = 0.034, *T* = 293 K

References: [1] Fompeyrine J., Nazabal V., Darriet J., Courbion G. (1995), Eur. J. Solid State Inorg. Chem. 32, 977-995.