| $Ba_{23}Cu_{12}Al_3O_{42}$ | *hP*164 | (186) $P6_3mc$ – $d^4c^{16}b^7a^3$ |
|---|---|---|

**$Ba_{46}Cu_{24}Al_6O_{84}$** [2]
Structural features: $Cu_6O_{15}$ units (rings formed by six $CuO_4$ squares sharing edges and vertices) and $AlO_4$ tetrahedra (partial substitution by $AlO_3$ ψ-tetrahedra).

VerNooy P.D. et al. (1990) [1]
$Al_{2.67}Ba_{23}Cu_{12}O_{42.31}$
$a$ = 1.31524, $c$ = 1.73122 nm, $c/a$ = 1.316, $V$ = 2.5935 nm$^3$, $Z$ = 2

| site | Wyck. | sym. | $x$ | $y$ | $z$ | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| O1 | 12*d* | 1 | 0.0063 | 0.3163 | 0.4202 | | single atom Cu |
| Cu2 | 12*d* | 1 | 0.03429 | 0.26764 | 0.19102 | | coplanar square $O_4$ |
| O3 | 12*d* | 1 | 0.3633 | 0.0217 | 0.1245 | | single atom Cu |
| Cu4 | 12*d* | 1 | 0.43527 | 0.06911 | 0.35205 | | coplanar square $O_4$ |
| O5 | 6*c* | .*m*. | 0.0733 | 0.9267 | 0.0357 | | single atom Al |
| O6 | 6*c* | .*m*. | 0.1016 | 0.8984 | 0.2587 | | non-colinear $Cu_2$ |
| Ba7 | 6*c* | .*m*. | 0.18879 | 0.81121 | 0.02267 | | tricapped trigonal prism $O_9$ |
| O8 | 6*c* | .*m*. | 0.1974 | 0.8026 | 0.1876 | | non-colinear $Cu_2$ |
| Ba9 | 6*c* | .*m*. | 0.22026 | 0.77974 | 0.35374 | | tricapped trigonal prism $O_9$ |
| O10 | 6*c* | .*m*. | 0.25925 | 0.74075 | 0.4975 | | single atom Al |
| O11 | 6*c* | .*m*. | 0.4078 | 0.5922 | 0.0287 | | single atom Al |
| Ba12 | 6*c* | .*m*. | 0.4472 | 0.5528 | 0.1897 | | 8-vertex polyhedron $O_8$ |
| O13 | 6*c* | .*m*. | 0.4707 | 0.5293 | 0.3524 | | non-colinear $Cu_2$ |
| Ba14 | 6*c* | .*m*. | 0.52753 | 0.47247 | 0.00885 | | square antiprism $O_8$ |
| O15 | 6*c* | .*m*. | 0.5704 | 0.4296 | 0.2872 | | non-colinear $Cu_2$ |
| Ba16 | 6*c* | .*m*. | 0.76457 | 0.23543 | 0.19549 | | monocapped trigonal prism $O_7$ |
| O17 | 6*c* | .*m*. | 0.78435 | 0.21565 | 0.357 | | non-colinear $Cu_2$ |
| Ba18 | 6*c* | .*m*. | 0.85921 | 0.14079 | 0.03279 | | square antiprism $O_8$ |
| O19 | 6*c* | .*m*. | 0.8799 | 0.1201 | 0.1948 | | non-colinear $Cu_2$ |
| Ba20 | 6*c* | .*m*. | 0.89903 | 0.10097 | 0.34836 | | 7-vertex polyhedron $O_7$ |
| Al21 | 2*b* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.0546 | 0.67 | tetrahedron $O_4$ |
| O22 | 2*b* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.1605 | 0.35 | colinear AlO |
| O23 | 2*b* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.2665 | 0.64 | |
| O24 | 2*b* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.3035 | 0.47 | |
| Al25 | 2*b* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.5292 | | tetrahedron $O_4$ |
| O26 | 2*b* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.6285 | 0.85 | single atom Al |
| Ba27 | 2*b* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.8835 | | 10-vertex polyhedron $O_9Al$ |
| Al28 | 2*a* | 3*m*. | 0 | 0 | 0.0 | | tetrahedron $O_4$ |
| Ba29 | 2*a* | 3*m*. | 0 | 0 | 0.17282 | | 10-vertex polyhedron $O_9Al$ |
| O30 | 2*a* | 3*m*. | 0 | 0 | 0.4001 | | single atom Al |

Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0 0.1165
Experimental: single crystal, diffractometer, X-rays, R = 0.018, T = 298 K

Remarks: When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Refinement of the site occupancies showed no significant deviation from unity except for those indicated here. Short interatomic distances for partly occupied site(s).

References: [1] VerNooy P.D., Dixon M.A., Hollander F.J., Stacy A.M. (1990), Inorg. Chem. 29, 2837-2841. [2] VerNooy P.D., Dixon M.A., Stacy A.M. (1988), Mater. Res. Soc. Symp. Proc. 99, 651-654.