| $Ba_{1.87}Al_{21}Pb_{0.47}O_{33.84}$ | *hP*89 | (187) *P*-6*m*2 – $n^9k^2j^3i^2h^3g^5$ |
|---|---|---|

**$(Ba,Pb)_{2.34}Al_{21}O_{33.84}$ form II** [1]
Structural features: Spinel-type slabs (close-packed O layers in c stacking, Al in octahedral and tetrahedral voids) and BaO layers (split O site, Ba near BR position) alternate along [001]; additional Ba and Pb are accommodated inside the slabs, accompanied by complex defects.

Iyi N. et al. (1985) [1]
$Al_{21.33}Ba_{1.90}O_{35.45}Pb_{0.38}$
$a$ = 0.56003, $c$ = 2.2922 nm, $c/a$ = 4.093, $V$ = 0.6226 nm$^3$, $Z$ = 1

| site | Wyck. | sym. | $x$ | $y$ | $z$ | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| Al1 | 6*n* | .*m*. | 0.16843 | 0.83157 | 0.1515 | 0.66 | 7-vertex polyhedron $O_6Al$ |
| O2 | 6*n* | .*m*. | 0.17933 | 0.82067 | 0.3048 | | tetrahedron $Al_4$ |
| Al3 | 6*n* | .*m*. | 0.18983 | 0.81017 | 0.0694 | 0.317 | |
| O4 | 6*n* | .*m*. | 0.49403 | 0.50597 | 0.2062 | | tetrahedron $Al_4$ |
| Al5 | 6*n* | .*m*. | 0.49933 | 0.50067 | 0.3573 | | octahedron $O_6$ |
| Al6 | 6*n* | .*m*. | 0.64173 | 0.35827 | 0.0741 | 0.332 | |
| O7 | 6*n* | .*m*. | 0.82733 | 0.17267 | 0.0827 | 0.278 | |
| O8 | 6*n* | .*m*. | 0.82753 | 0.17247 | 0.3996 | | non-coplanar triangle $Al_3$ |
| O9 | 6*n* | .*m*. | 0.83863 | 0.16137 | 0.108 | 0.793 | |
| O10 | 3*k* | *mm*2 | 0.01933 | 0.98067 | $^1/_2$ | 0.333 | |
| Ba11 | 3*k* | *mm*2 | 0.65353 | 0.34647 | $^1/_2$ | 0.334 | |
| Ba12 | 3*j* | *mm*2 | 0.01033 | 0.98967 | 0 | 0.228 | |
| O13 | 3*j* | *mm*2 | 0.24933 | 0.75067 | 0 | 0.33 | tetrahedron $O_2Al_2$ |
| O14 | 3*j* | *mm*2 | 0.59433 | 0.40567 | 0 | 0.393 | non-colinear $O_2$ |
| Al15 | 2*i* | 3*m*. | $^2/_3$ | $^1/_3$ | 0.2302 | | tetrahedron $O_4$ |
| O16 | 2*i* | 3*m*. | $^2/_3$ | $^1/_3$ | 0.3102 | | tetrahedron $Al_4$ |
| O17 | 2*h* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.1131 | | trigonal prism $Al_6$ |
| Al18 | 2*h* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.2532 | | octahedron $O_6$ |
| O19 | 2*h* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.3962 | | non-coplanar triangle $Al_3$ |
| O20 | 2*g* | 3*m*. | 0 | 0 | 0.2004 | 0.93 | |
| Ba21 | 2*g* | 3*m*. | 0 | 0 | 0.2202 | 0.106 | |
| Pb22 | 2*g* | 3*m*. | 0 | 0 | 0.2422 | 0.188 | |
| Al23 | 2*g* | 3*m*. | 0 | 0 | 0.2767 | 0.74 | |
| Al24 | 2*g* | 3*m*. | 0 | 0 | 0.4249 | | |

Transformation from published data: origin shift $^2/_3$ $^1/_3$ 0
Experimental: single crystal, diffractometer, X-rays, R = 0.030

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Iyi N., Inoue Z., Takekawa S., Kimura S. (1985), J. Solid State Chem. 60, 41-50.