

$\text{Ba}_5\text{Re}_3[\text{NO}_3]\text{O}_{15}$  $hP54$  $(185) P6_3cm - d^2c^4ba$ **Ba<sub>5</sub>(ReO<sub>5</sub>)<sub>3</sub>NO<sub>3</sub> [1]**Structural features: Single ReO<sub>5</sub> square pyramids and NO<sub>3</sub> trigonal units.

Aneas M. et al. (1983) [1]

 $\text{Ba}_5\text{NO}_{18}\text{Re}_3$  $a = 1.1054, c = 0.7718 \text{ nm}, c/a = 0.698, V = 0.8167 \text{ nm}^3, Z = 2$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	12 <i>d</i>	1	0.127	0.5794	0.2987		single atom Re
O2	12 <i>d</i>	1	0.1349	0.3925	0.4764		single atom Re
O3	6 <i>c</i>	.. <i>m</i>	0.1151	0	0.4752		single atom N
O4	6 <i>c</i>	.. <i>m</i>	0.2992	0	0.153		single atom Re
Re5	6 <i>c</i>	.. <i>m</i>	0.3933	0	0.3252		square pyramid O <sub>5</sub>
Ba6	6 <i>c</i>	.. <i>m</i>	0.7274	0	0.2784		bicapped square prism O <sub>10</sub>
Ba7	4 <i>b</i>	3.. <i></i>	$\frac{1}{3}$	$\frac{2}{3}$	0.0334		tricapped trigonal prism O <sub>9</sub>
N8	2 <i>a</i>	3.. <i>m</i>	0	0	0.0		non-coplanar triangle O <sub>3</sub>

Transformation from published data: origin shift 0 0 0.9666

Experimental: single crystal, diffractometer, X-rays, R = 0.064

References: [1] Aneas M., Picard J.P., Baud G., Besse J.P., Chevalier R. (1983), Mater. Chem. Phys. 8, 119-123.