

$\text{Ni}_9\text{Pb}_6\text{Te}_5\text{O}_{30}$

$hP100$

(182) $P6_322 - i^5h^3g^2f^2b$

$\text{Pb}_3\text{Ni}_{4.5}\text{Te}_{2.5}\text{O}_{15}$ [1]

Structural features: Infinite slabs of edge-linked NiO_6 and TeO_6 octahedra share vertices with units of two face-linked octahedra (a NiO_6 and a TeO_6 octahedron) to form a 3D-framework.

Wedel B. et al. (1998) [1]

$\text{Ni}_9\text{O}_{30}\text{Pb}_6\text{Te}_5$

$a = 1.02589$, $c = 1.3554$ nm, $c/a = 1.321$, $V = 1.2354$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.0084	0.3362	0.1717		non-coplanar triangle TeNi_2
O2	12i	1	0.1569	0.4847	0.3301		non-coplanar triangle TeNi_2
O3	12i	1	0.1649	0.1774	0.1716		non-coplanar triangle TeNi_2
O4	12i	1	0.4996	0.3291	0.1644		non-coplanar triangle TeNi_2
O5	12i	1	0.5246	0.1785	0.0024		non-coplanar TeNi_2
Te6	6h	..2	0.1674	0.3348	$\frac{1}{4}$		octahedron O_6
Ni7	6h	..2	0.5031	0.0062	$\frac{1}{4}$		octahedron O_6
Ni8	6h	..2	0.831	0.662	$\frac{1}{4}$		octahedron O_6
Pb9	6g	..2	0.2644	0	0		4-vertex polyhedron O_4
Pb10	6g	..2	0.6129	0	0		non-coplanar O_2
Ni11	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1116		octahedron O_6
Te12	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5981		octahedron O_6
Ni13	2b	3.2	0	0	$\frac{1}{4}$		octahedron O_6

Transformation from published data: $-x, -y, -z$; origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.046$

Remarks: In table 1 of [1] the Wyckoff position of former Ni(3) is misprinted as 6g instead of 6h.

References: [1] Wedel B., Sugiyama K., Müller Buschbaum H. (1998), Z. Naturforsch. B 53, 527-531.