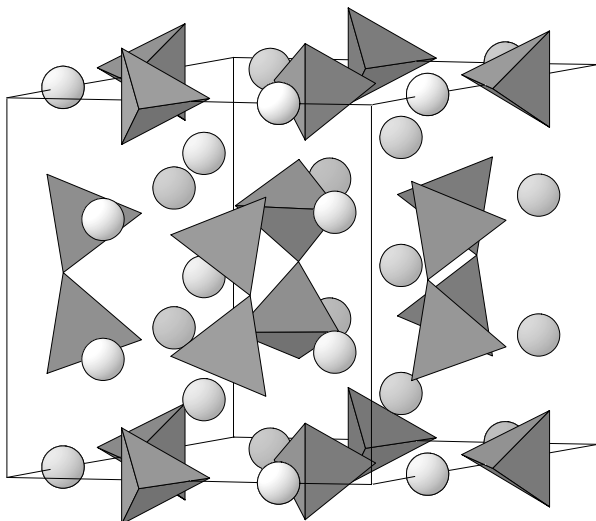


**Pb<sub>5</sub>Ge<sub>3</sub>O<sub>11</sub> paraelectric [2]**

Structural features: Slabs containing units of two vertex-linked GeO<sub>4</sub> tetrahedra (parallel to [001]) alternate with slabs containing single GeO<sub>4</sub> tetrahedra. See Fig. IV.90.

Fig. IV.90. **Pb<sub>5</sub>Ge<sub>3</sub>O<sub>11</sub> paraelectric**

Arrangement of GeO<sub>4</sub> tetrahedra and Pb atoms.

Iwata Y. (1977) [1]

Ge<sub>3</sub>O<sub>11</sub>Pb<sub>5</sub>

*a* = 1.026, *c* = 1.0696 nm, *c/a* = 1.042, *V* = 0.9751 nm<sup>3</sup>, *Z* = 3

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>l</i>	1	0.01237	0.41503	0.127		non-colinear GePb
O2	6 <i>l</i>	1	0.07637	0.22723	0.3401		single atom Ge
Ge3	6 <i>l</i>	1	0.27317	0.31853	0.3486		tetrahedron O <sub>4</sub>
O4	6 <i>l</i>	1	0.34247	0.24203	0.2377		single atom Ge
O5	6 <i>l</i>	1	0.35967	0.51163	0.3333		single atom Ge
Pb6	6 <i>l</i>	1	0.40367	0.06933	0.3158		non-coplanar triangle O <sub>3</sub>
O7	3 <i>k</i>	<i>m</i> ..	0.30807	0.26503	<sup>1</sup> / <sub>2</sub>		non-colinear Ge <sub>2</sub>
Ge8	3 <i>j</i>	<i>m</i> ..	0.05787	0.33713	0		tetrahedron O <sub>4</sub>
O9	3 <i>j</i>	<i>m</i> ..	0.18387	0.04443	0		single atom Ge
O10	3 <i>j</i>	<i>m</i> ..	0.25077	0.40703	0		non-colinear GePb
Pb11	3 <i>j</i>	<i>m</i> ..	0.40977	0.32763	0		6-vertex polyhedron O <sub>6</sub>
Pb12	2 <i>h</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1757		tricapped trigonal prism O <sub>9</sub>
Pb13	2 <i>g</i>	3..	0	0	0.1628		octahedron O <sub>6</sub>
Pb14	1 <i>d</i>	-6..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>2</sub>		trigonal prism O <sub>6</sub>
Pb15	1 <i>b</i>	-6..	0	0	<sup>1</sup> / <sub>2</sub>		tricapped trigonal prism O <sub>9</sub>

Transformation from published data: -*x*, -*y*, -*z*; origin shift <sup>1</sup>/<sub>3</sub> <sup>2</sup>/<sub>3</sub> <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, neutrons, *R* = 0.079, *T* = 473 K

Remarks: Phase stable at *T* > 450 K.

References: [1] Iwata Y. (1977), J. Phys. Soc. Jpn. 43, 961-967. [2] Newnham R.E., Wolfe R.W., Darlington C.N.W. (1973), J. Solid State Chem. 6, 378-383.