

$\text{Pb}_{4.925}[\text{VO}_4]_3\text{I}_{0.85}$	$hP70$	(176) $P6_3/m - i^4h^3f$
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**Pb<sub>9.85</sub>(VO<sub>4</sub>)<sub>6</sub>I<sub>1.7</sub>** [1], apatite family

Structural features: Infinite columns of base-linked PbO<sub>6</sub>O<sub>3</sub> tricapped trigonal prisms (partial vacancies ignored) share atoms with VO<sub>4</sub> tetrahedra (one split O site) to form a 3D-framework; I (displaced from the axis) in infinite columns of face-linked Pb<sub>6</sub> octahedra (split site) parallel to [001] (partial disorder).

Audubert F. et al. (1999) [1]

$\text{I}_{0.85}\text{O}_{12}\text{Pb}_{4.92}\text{V}_3$

$a = 1.0422$ ,  $c = 0.7467$  nm,  $c/a = 0.716$ ,  $V = 0.7024$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
I1	12i	1	0.027	0.028	0.021	0.142	
Pb2	12i	1	0.26525	0.26389	0.2224	0.493	
O3	12i	1	0.333	0.09	0.101	0.5	
O4	12i	1	0.383	0.089	0.041	0.5	
O5	6h	$m..$	0.1651	0.5014	$\frac{1}{4}$		single atom V
V6	6h	$m..$	0.4103	0.0284	$\frac{1}{4}$		
O7	6h	$m..$	0.6016	0.1226	$\frac{1}{4}$		single atom V
Pb8	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0097	0.982	tricapped trigonal prism O <sub>9</sub>

Transformation from published data: origin shift 0 0  $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.036, T = 293 K

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

References: [1] Audubert F., Savariault J.M., Lacout J.L. (1999), Acta Crystallogr. C 55, 271-273.