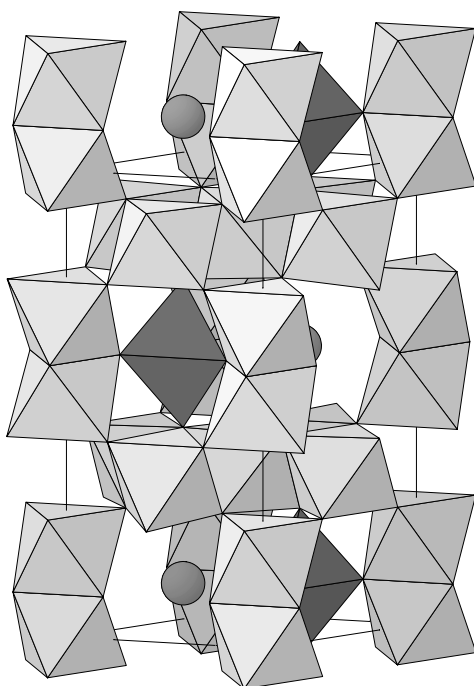


NaV₆O₁₁ It1 [1]

Structural features: Close-packed O₄ and NaO₃ layers in h stacking; V in octahedral and trigonal bipyramidal voids. Infinite slabs of edge-linked VO₆ octahedra share vertices with VO₅ trigonal bipyramids and pairs of face-linked VO₆ octahedra to form a 3D-framework. See Fig. IV.29.

Fig. IV.29. **NaV₆O₁₁ It1**

Arrangement of VO₅ trigonal bipyramids (dark), VO₆ octahedra (light) and Na atoms.

Kanke Y. et al. (1994) [1]

NaO₁₁V₆

$a = 0.57049$, $c = 1.30796$ nm, $c/a = 2.293$, $V = 0.3687$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>c</i>	. <i>m</i> .	0.16969	0.83031	0.27214		non-coplanar triangle V ₃
V2	6 <i>c</i>	. <i>m</i> .	0.50622	0.49378	0.35129		octahedron O ₆
O3	6 <i>c</i>	. <i>m</i> .	0.82898	0.17102	0.43448		non-coplanar triangle V ₃
O4	6 <i>c</i>	. <i>m</i> .	0.84718	0.15282	0.10099		coplanar triangle V ₃
Na5	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.10619		anticuboctahedron O ₁₂
O6	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.44036		tetrahedron V ₄
V7	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.59614		trigonal bipyramid O ₅
O8	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.75795		tetrahedron V ₄
V9	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		octahedron O ₆
V10	2 <i>a</i>	3 <i>m</i> .	0	0	0.2047		octahedron O ₆

Transformation from published data: origin shift 0 0 0.14871

Experimental: single crystal, diffractometer, X-rays, $R = 0.022$, $T = 200$ K

Remarks: Phase stable at $35 < T < 245$ K.

References: [1] Kanke Y., Izumi F., Morii Y., Akiba E., Funahashi S., Kato K., Isobe M., Takayama Muromachi E., Uchida Y. (1994), J. Solid State Chem. 112, 429-437.

