Crystal structure of sodium ytterbium diphosphate, NaYbP₂O₇

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Abstract

NaO₇P₂Yb, monoclinic, *P*12₁/*n*1 (no. 14), *a* = 9.0211(3) Å, *b* = 5.3571(4) Å, *c* = 12.7802(6) Å, β = 103.176(5)°, *V* = 601.4 Å³, *Z* = 4, *R*_{gt}(*F*) = 0.040, *wR*_{ref}(*F*²) = 0.110, *T* = 293 K.

Source of material

The NaYbP₂O₇ single crystals were grown. 3 g of Na₃P₃O₉ and 0.5 g of ytterbium oxide Yb₂O₃ as starting materials were mixed. They were progressively heated in platinum crucible to 1273 K for twenty days, then cooled and maintained at 873 K for ten hours. The excess of Na₃P₃O₉ was washed off with hot water and the crystals obtained were then isolated.

Discussion

The structure of NaYbP₂O₇ consists of YbO₆ polyhedra and P₂O₇^{4−} diphosphate groups which lie in planes parallel to (010), to form three-dimensional framework in which channels are noticed and where the sodium ions are located (*CN* 7). In PO₄ tetrahedra, the P—O distances vary from 1.481(6) Å to 1.605(5) Å. The shortest distances correspond to the external P—O connections, whereas largest of the distances P—O are those of the bridge. The values of O—P—O angles vary in the interval 105.0(3)° – 113.8(3)° and the angle of the P—O—P bridge has a value of 126.0°. These values are in conformity with the results found for the diphosphates [1]. Recently we have reported about the crystal structure of sodium and rare earth diphosphates such as NaEuP₂O₇ (monoclinic, space group *P*2₁/*n*) [2] and NaLaP₂O₇ (orthorhombic, space group *Pnma*) [3]. The coordination polyhedron of the rare earth atoms in these diphosphates is not the same. In the case of the NaLaP₂O₇ and NaEuP₂O₇, lanthanum and europium cations are coordinated by nine and eight oxygen atoms, respectively, whereas in NaYbP₂O₇ the coordination number is six. The difference of the rare earth coordination can be simply explained by the size effect of the cations, but electronic configuration of the rare earth may also play an important role. CsYbP₂O₇ crystallizes in the same space group as NaYbP₂O₇ [4]. But both are not isotopic and have, e.g., completely different lattice parameters.

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.10 × 0.13 × 0.30 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71073 Å)
μ :	161.39 cm ^{−1}
Diffractometer, scan mode:	Enraf-Nonius MACH 3, ω
2 θ _{max} :	59.98°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	1819, 1755
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 1532
<i>N</i> (<i>param</i>) _{refined} :	101
Programs:	SHELXS-97 [5], SHELXL-97 [6], WinGX [7], DIAMOND [8]

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Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Yb	4e	0.76943(2)	0.76384(4)	0.02359(2)	0.0062(2)	0.0140(2)	0.0038(2)	0.00031(7)	0.0000(1)	0.00018(7)
P(1)	4e	0.9716(2)	1.2512(2)	0.1536(2)	0.0059(7)	0.0135(7)	0.0039(7)	0.0000(4)	0.0001(6)	−0.0001(4)
P(2)	4e	0.5682(2)	0.2824(3)	−0.1180(1)	0.0065(7)	0.0143(6)	0.0032(7)	−0.0002(5)	−0.0011(5)	0.0005(5)
Na	4e	0.6384(4)	1.2280(5)	0.1931(3)	0.018(2)	0.021(1)	0.018(2)	0.0018(9)	0.002(1)	−0.0005(9)
O(1)	4e	1.0596(8)	1.2587(8)	0.0690(5)	0.017(3)	0.033(3)	0.006(2)	0.003(2)	0.005(2)	0.001(2)
O(2)	4e	0.8908(5)	1.0059(8)	0.1594(3)	0.015(2)	0.014(2)	0.005(2)	−0.002(2)	0.000(1)	0.001(1)
O(3)	4e	0.8605(5)	1.4693(8)	0.1458(3)	0.013(2)	0.016(2)	0.006(2)	0.005(2)	0.000(1)	0.002(2)
O(4)	4e	1.0948(5)	1.2793(8)	0.2647(4)	0.005(2)	0.021(2)	0.008(2)	−0.001(1)	0.001(2)	0.002(1)
O(5)	4e	0.6817(5)	0.1251(9)	−0.0422(3)	0.022(2)	0.022(2)	0.009(2)	0.002(2)	−0.004(2)	0.002(2)
O(6)	4e	0.4051(6)	0.2091(9)	−0.1231(4)	0.010(2)	0.029(2)	0.010(2)	−0.003(2)	0.007(2)	−0.005(2)
O(7)	4e	0.5931(5)	0.5593(8)	−0.0968(3)	0.016(2)	0.014(2)	0.010(2)	−0.001(2)	−0.003(2)	0.002(2)

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