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Potassium ytterbium diphosphate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(P–O) = 0.005 Å
R factor = 0.035
wR factor = 0.096
Data-to-parameter ratio = 19.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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$KYbP_2O_7$ consists of P_2O_7 double-tetrahedral groups connected to YbO_6 octahedra, forming a framework whose channels are occupied by K^+ cations.

Comment

Rare-earth containing compounds are widely used for optical applications such as colour displays, solid-state lasers, and sensors (Weber, 1999; Blasse & Grabmaier, 1994; Hashimoto *et al.*, 1991; Horchani-Naifer *et al.*, 2006). Yb^{3+}-doped crystals exhibit luminescence of Yb^{3+} from the charge-transfer state with emission in the near-UV–visible region and short radiative lifetimes (van Pieterson *et al.*, 2000; Guerassimova *et al.*, 2001; Chipaux *et al.*, 2002). Most matrices studied are glasses and single-crystal materials; here we report a new ytterbium single-crystal matrix prepared using a KH_2PO_4 flux. This material belongs to a family of alkali rare-earth diphosphates with the general formula $M^{I}LnP_2O_7$ (M^{I} = Na, K, Rb, Cs, NH_4; Ln = rare-earth element). $NaLnP_2O_7$ (Ln = La, Ce, Eu, Yb) crystallizes in the orthorhombic or monoclinic systems (Horchani-Naifer & Férid, 2005; Férid & Horchani-Naifer, 2004; Férid, Horchani *et al.*, 2004; Férid, Horchani-Naifer *et al.*, 2004). $KYbP_2O_7$ is monoclinic ($P2_1/c$) and is isotypic with $CsYbP_2O_7$ (Jansen *et al.*, 1991). The structure consists of YbO_6 octahedra and P_2O_7 diphosphate groups connected to form a three-dimensional framework containing channels in which the K^+ ions are located (Fig. 1). The P_2O_7 group is formed from two slightly distorted PO_4 tetrahedra (Fig. 2).

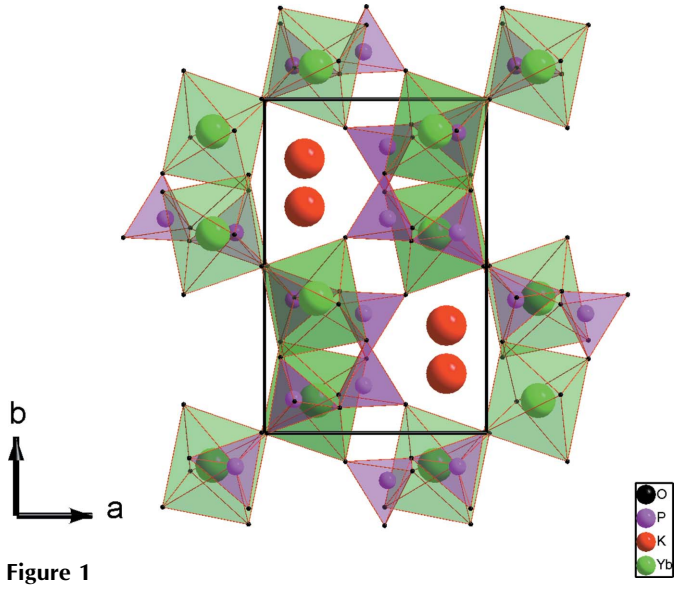

Figure 1
Projection of $KYbP_2O_7$ along the c-axis direction, showing the arrangement of YbO_6 octahedra and P_2O_7 groups, with K ions within channels.

In conformity with other diphosphates (Durif, 1995; Férid, 2006), the P—O distances range from 1.495 (5) to 1.612 (4) Å, the shortest corresponding to the terminal and the longest to the bridging O atoms.

Experimental

A mixture of KH_2PO_4 (10 g) and Yb_2O_3 (0.5 g) was gradually heated in a platinum crucible to 1273 K over 72 h, and then cooled and maintained at 873 K for 10 h. The crystals obtained were washed with hot water and hydrochloric acid.

Crystal data

$KYb(P_2O_7)$
M_r = 386.08
Monoclinic, $P2_1/c$
a = 7.538 (3) Å
b = 10.832 (2) Å
c = 8.537 (4) Å
β = 106.768 (7)°
V = 667.4 (4) Å^3
Z = 4
D_x = 3.842 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 15.10 mm^{-1}
T = 298 (2) K
Prism, colourless
0.18 × 0.17 × 0.17 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.223, T_{max} = 0.243
(expected range = 0.070–0.077)
10491 measured reflections
1957 independent reflections
1763 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 30.0°
2 standard reflections
every 150 reflections
intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.096
S = 1.17
1957 reflections
101 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 0.1042P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 4.91 e Å^{-3}
$\Delta\rho_{min}$ = −3.27 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0011 (1)

The highest peak and the deepest hole in the residual electron density are located 0.05 and 0.63 Å, respectively, from Yb.

Data collection: *CAD-4 EXPRESS* (Duisenberg, 1992; Macíček & Yordanov, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

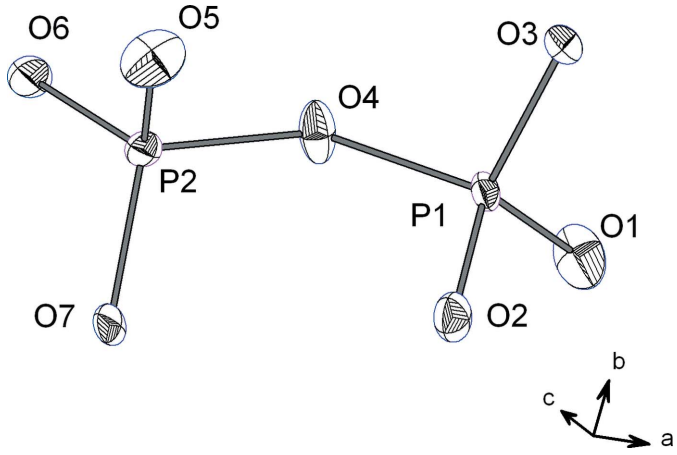

Figure 2
The P_2O_7 group, with displacement ellipsoids drawn at the 50% probability level.

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