

## A monoclinic polymorph of $\text{KY}(\text{PO}_3)_4$

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Received 30 April 2008; accepted 9 May 2008

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{P}-\text{O}) = 0.006$  Å;  $R$  factor = 0.048;  $wR$  factor = 0.138; data-to-parameter ratio = 12.2.

The title compound, potassium yttrium polyphosphate,  $\text{KY}(\text{PO}_3)_4$ , was synthesized using the flux method. The atomic arrangement consists of an infinite long-chain polyphosphate organization. Chains, with a period of four  $\text{PO}_4$  tetrahedra, run along the  $a$ -axis direction. Two other polymorphs of this phosphate are known, in space groups  $P21/n$  and  $C2/c$ .

### Related literature

For related structures, see: Durif (1995); Hamady *et al.* (1995); Hong *et al.* (1975); Malinowski (1990); Malinowski *et al.* (1988); Palkina *et al.* (1977). For earlier work on  $\text{KY}(\text{PO}_3)_4$ , see: Jouini *et al.* (2003). For related literature, see: Sun *et al.* (2004).

### Experimental

#### Crystal data

$\text{KY}(\text{PO}_3)_4$	$V = 469.7$ (2) Å <sup>3</sup>
$M_r = 443.89$	$Z = 2$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 7.2244$ (3) Å	$\mu = 7.40$ mm <sup>-1</sup>
$b = 8.2825$ (3) Å	$T = 298$ (2) K
$c = 7.854$ (4) Å	$0.16 \times 0.14 \times 0.13$ mm
$\beta = 91.735$ (3)°	

#### Data collection

Enraf–Nonius CAD-4 diffractometer	2011 independent reflections
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1996)	1904 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.321$ , $T_{\max} = 0.376$	$R_{\text{int}} = 0.081$
3651 measured reflections	2 standard reflections
	every 150 reflections
	intensity decay: 2%

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$	$\Delta\rho_{\text{max}} = 1.19$ e Å <sup>-3</sup>
$wR(F^2) = 0.138$	$\Delta\rho_{\text{min}} = -2.67$ e Å <sup>-3</sup>
$S = 1.13$	Absolute structure: Flack (1983),
2011 reflections	with 867 Friedel pairs
165 parameters	Flack parameter: 0.002 (9)
1 restraint	

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, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Ministry of Higher Education, Scientific Research and Technology of Tunisia.

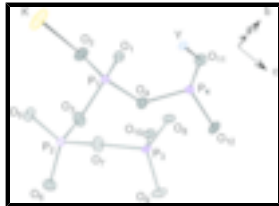
Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2073).

### References

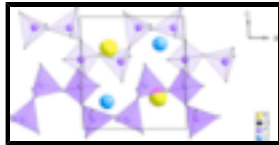
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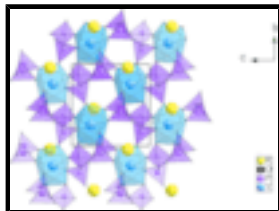




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