

A new polymorph of Lu(PO₃)₃

Anis Bejaoui, Karima Horchani-Naifer and Mokhtar Férid*

Unité de Recherches de Matériaux de Terres Rares, Centre National de Recherches en Sciences des Matériaux, BP 95 Hammam-Lif 2050, Tunisia
Correspondence e-mail: mokhtar.ferid@inrst.nrst.tn

Received 23 June 2008; accepted 14 July 2008

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{Lu}-\text{O}) = 0.005$ Å; R factor = 0.033; wR factor = 0.061; data-to-parameter ratio = 26.2.

A new polymorph of lutetium polyphosphate, Lu(PO₃)₃, was found to be isotopic with the trigonal form of Yb(PO₃)₃. Two of the three Lu atoms occupy special positions (Wyckoff positions *3a* and *3b*, site symmetry $\bar{3}$). The atomic arrangement consists of infinite helical polyphosphate chains running along the *c* axis, with a repeat period of 12 PO₄ tetrahedra, joined with LuO₆ octahedra.

Related literature

For syntheses and optical properties, see: Briche *et al.* (2006); Jouini, Férid, Gacon, Grosvalet *et al.* (2003); Jouini, Férid, Gacon & Trabelsi-Ayadi (2003); Ternane *et al.* (2005); Graia *et al.* (2003); Anisimova *et al.* (1992). For the monoclinic polymorph of Lu(PO₃)₃, see: Höppe & Sedlmaier (2007); Yuan *et al.* (2008).

Experimental

Crystal data

Lu(PO ₃) ₃	$Z = 24$
$M_r = 411.88$	Mo $K\alpha$ radiation
Trigonal, $R\bar{3}$	$\mu = 13.59$ mm ⁻¹
$a = 20.9106$ (6) Å	$T = 100$ (2) K
$c = 12.0859$ (7) Å	$0.18 \times 0.18 \times 0.17$ mm
$V = 4576.6$ (3) Å ³	

Data collection

Bruker APEXII CCD area-detector diffractometer	25139 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	4170 independent reflections
$T_{\min} = 0.102$, $T_{\max} = 0.104$	3609 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.054$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	159 parameters
$wR(F^2) = 0.060$	$\Delta\rho_{\text{max}} = 2.34$ e Å ⁻³
$S = 1.05$	$\Delta\rho_{\text{min}} = -2.07$ e Å ⁻³
4170 reflections	

Data collection: APEX2 (Bruker, 2005); cell refinement: APEX2; data reduction: APEX2; 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: FI2065).

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