

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## Lutetium ultraphosphate

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@inst.nrt.tn

Received 1 April 2008; accepted 2 May 2008

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{P}-\text{O}) = 0.002$  Å;  $R$  factor = 0.019;  $wR$  factor = 0.051; data-to-parameter ratio = 15.9.

The structure of the title compound,  $\text{LuP}_5\text{O}_{14}$ , comprises puckered eight-membered  $\text{PO}_4$  rings linked by the lutetium cations in a complex way, forming a three-dimensional framework. Each eight-membered phosphate ring shares a bridging tetrahedron with each of four adjacent tetrahedra, to form layers of  $\text{PO}_4$  tetrahedra. These layers are  $c/2$  in thickness and parallel to the  $ab$  plane. Each Lu ion is contained in one such layer, forming bonds to six O atoms in that layer and also to one O atom belonging to a tetrahedron in each of the layers lying above and below it. The  $\text{LuO}_8$  polyhedra are isolated from one another, since they share no common atoms. The Lu ions lie on twofold axes (special position  $4e$ ) and the shortest Lu...Lu distance is 5.703 (1) Å.

## Related literature

For related literature, see: Durif (1971); Hong (1974); Hong & Pierce (1974). For the classification of ultraphosphates, see: Bagieu-Beucher & Tranqui (1970).

## Experimental

## Crystal data

$\text{LuP}_5\text{O}_{14}$   
 $M_r = 553.82$

Monoclinic,  $C2/c$   
 $a = 12.8128$  (14) Å

$b = 12.6821$  (13) Å  
 $c = 12.3330$  (13) Å  
 $\beta = 91.295$  (3)°  
 $V = 2003.5$  (4) Å<sup>3</sup>  
 $Z = 8$

Mo  $K\alpha$  radiation  
 $\mu = 10.74$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 $0.20 \times 0.19 \times 0.18$  mm

## Data collection

Enraf-Nonius CAD-4 diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.121$ ,  $T_{\text{max}} = 0.145$   
10422 measured reflections

2912 independent reflections  
2734 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$   
2 standard reflections every 150 reflections  
intensity decay: 2%

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.019$   
 $wR(F^2) = 0.050$   
 $S = 1.08$   
2912 reflections

183 parameters  
 $\Delta\rho_{\text{max}} = 1.34$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.98$  e Å<sup>-3</sup>

Data collection: *CAD-4 EXPRESS* (Duisenberg, 1992; Enraf-Nonius, 1994; 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: BR2072).

## References

- Bagieu-Beucher, M. & Tranqui, D. (1970). *Bull. Soc. Fr. Mineral. Cristallogr.* **93**, 505–508.  
Brandenburg, K. (2001). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.  
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.  
Durif, A. (1971). *Bull. Soc. Fr. Mineral. Cristallogr.* **94**, 314–318.  
Enraf-Nonius (1994). *CAD-4 EXPRESS*. Enraf-Nonius, Delft, The Netherlands.  
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.  
Hong, H. Y.-P. (1974). *Acta Cryst.* **B30**, 468–474.  
Hong, H. Y.-P. & Pierce, J. W. (1974). *Mater. Res. Bull.* **9**, 179–190.  
Macíček, J. & Yordanov, A. (1992). *J. Appl. Cryst.* **25**, 73–80.  
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.



















