Crystal Structure of New Lanthanide Diphosphates

Francesco Capitelli[a], Brahim El Bali[b], Juan F. Piniella[c], *[a]IC-CNR, Bari, Italy. [b]Dépt. de Chimie, Faculté des Sciences Dhar Mehraz, BP 1796 Atlas, 30000 Fès, Morocco. [c]Dept. of Geology, Universitat Autònoma de Barcelona, Bellaterra, Spain.* E-mail: francesco.capitelli@ic.cnr.it

In the context of a general study on synthetic phosphates [1-2], the crystal structures of three new lanthanide diphosphates are presented: $KLnP_2O_7 \cdot 2H_2O$, where *Ln* is Gd, Tb and Yb. Suitable monocrystals were grown after the synthesis carried out using equimolar proportions of $K_4P_2O_7$ (dissolved in HCl) and $LnCl_3 \cdot 6H_2O$ as reagents. The structures, solved by X-ray diffraction methods (SIR97) and refined by full-matrix least squares (SHELXL-97), resulted to be isostructural within space group $P2_1/c$. In table 1 are presented the unit-cell parameters, the volumes and the final R_1 ($I \geq 2\sigma(I)$) values. The three-dimensional frameworks are made by zig-zag chains of KO_9 polyhedra down *c*, sharing edges with discrete LnO_7 polyhedra and P_2O_7 units; intricate hydrogen bonding networks complete the arrays.

Table 1

Ln	*a(Å)*	*b(Å)*	*c(Å)*	*β(°)*	*V(Å^3)*	R_1(%)
Gd	7.7522(2)	10.6732(8)	10.1375(7)	93.308(5)	837.39(9)	4.31
Tb	7.7380(6)	10.6360(8)	10.1060(7)	93.283(6)	830.37(11)	3.85
Yb	7.6791(3)	10.4992(7)	9.9554(9)	93.214(6)	801.39(10)	5.42

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