Crystal structure of tetradecaeuropium tetraphosphide tetraphosphidoaluminate polytriphosphide, $\text{Eu}_{14}(\text{P})_4(\text{AlP}_4)(\text{P}_3)$

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Table 1. Parameters used for the X-ray data collection

Crystal:	black plate, size 0.15 x 0.15 x 0.05 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	326.90 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	3
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	1554
Criterion for F_o :	$F_o > 4 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	61
Program:	SHELXTL-plus

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	Occ.	x	y	z	U_{iso}
P(4*)	16f	0.5	0.022(1)	0.272(1)	1/8	0.017(4)

Source of material: $\text{Eu}_{14}\text{AlP}_{11}$ was obtained as a by-product from the reaction of EuP with Al (ratio = 3:1) in a sealed niobium ampoule at 1375 K.

$\text{Eu}_{14}\text{AlP}_{11}$ is isostructural to $\text{Ca}_{14}\text{AlSb}_{11}$, $\text{Ca}_{14}\text{GaP}_{11}$, $\text{Ba}_{14}\text{InP}_{11}$ (see refs. 1-3). The structure contains isolated P^{3-} anions, asymmetrical $[\text{P}-\text{P}-\text{P}]^{7-}$ linear triads and tetrahedral $[\text{AlP}_4]^{9-}$ anions. The asymmetry of $[\text{P}-\text{P}-\text{P}]^{7-}$ is comparable to the corresponding unit in $\text{Ca}_{14}\text{GaP}_{11}$ (see ref. 2.). Bond lengths are: $[\text{P}-\text{P}-\text{P}]^{7-}$: $d(\text{P}-\text{P}) = 2.475 \text{ Å}$, 3.445 Å and $d(\text{Al}-\text{P}) = 2.467 \text{ Å}$. For a complete description of the structure family and further details on the asymmetric unit $[\text{X}_3]^{7-}$ ($\text{X} = \text{P}, \text{As}, \text{Sb}, \text{Bi}$) see ref. 3. The values of the U_{ij} parameter of Al might be influenced by the absorption correction.

$\text{AlEu}_{14}\text{P}_{11}$, tetragonal, $I4_1/acd$ (No. 142), $a = 15.913(1) \text{ Å}$, $c = 21.343(2) \text{ Å}$, $V = 5404.6 \text{ Å}^3$, $Z = 8$, $R(F) = 0.089$, $R_w(F) = 0.089$.

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu(1)	32g	0.0439(1)	0.0722(1)	0.17170(7)	0.021(1)	0.027(1)	0.0243(8)	-0.0055(7)	0.0038(6)	-0.0045(6)
Eu(2)	32g	0.0227(1)	0.3780(1)	0.00428(7)	0.0182(9)	0.020(1)	0.0272(8)	0.0022(6)	0.0012(6)	-0.0028(6)
Eu(3)	16e	0.3518(2)	0	1/4	0.020(1)	0.018(1)	0.025(1)	0	0	0.0020(9)
Eu(4)	32g	0.3450(1)	0.0715(1)	0.09433(7)	0.029(1)	0.0177(9)	0.0227(8)	-0.0001(7)	0.0053(7)	0.0009(6)
Al	8a	0	1/4	3/8	0.007(5)	U_{11}	0.026(8)	0	0	0
P(1)	16f	0.1315(7)	$x+1/4$	1/8	0.029(5)	U_{11}	0.024(5)	0.001(5)	0.260(3)	$-U_{13}$
P(2)	32g	0.3700(5)	0.2533(6)	0.0622(4)	0.017(4)	0.020(4)	0.025(3)	-0.004(3)	-0.004(3)	0.003(3)
P(3)	32g	0.1311(6)	0.0253(6)	0.0468(4)	0.023(5)	0.016(4)	0.021(3)	-0.006(3)	0.002(3)	0.003(3)

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