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Crystal structure of tetrasodium octaeuropium(II) [octaphosphido(3–)]-bis[diphosphido(4–)]tetraaluminate(III), $Na_4Eu_8[Al_4P_8(P_2)_2]$

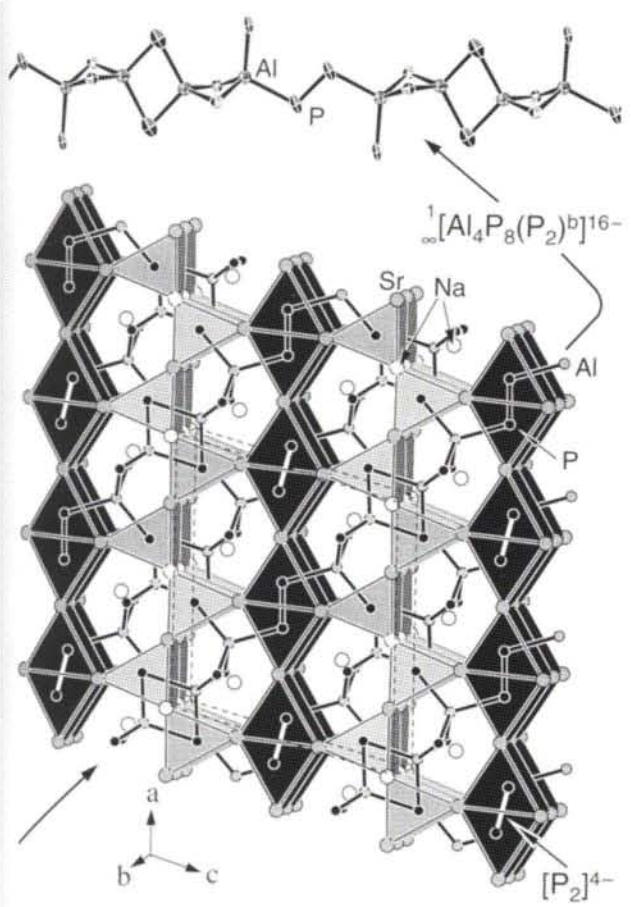
M. Somer

Koç University, Department of Chemistry, Cayir Cad. 5, TR-80860 Istinye-Istanbul, Turkey

W. Carrillo-Cabrera, K. Peters and H. G. von Schnering

Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

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Source of material: $Na_4Eu_8Al_4P_{12}$ is formed with phosphorous as byproduct from a mixture of NaP, EuP and AlP (ratio 1 : 2 : 1) in alumina crucible enclosed in a stainless steel ampoule at 1323 K.
The structure of $Na_4Eu_8Al_4P_{12}$ contains centrosymmetric chains of dimeric $[(Al_2P_4(P_2)^{)10-}]_2$ anions with terminal (t) exo$(P_2)^t$ ligands. Bond lengths: d(Al–P) = 2.36 Å to 2.44 Å (in the Al_2P_2 rings); $d(Al–P)^t$ = 2.34 Å, $d(Al–P_2)^t$ = 2.46 °A, $d(P–P)^t$ = 2.259 Å. The atoms of the anions are embedded in a matrix of condensed trigonal prisms formed by Eu and Na cations, and characterized by pentagonal channels. The structure is very similar to those reported in refs. 1, 2 and closely related to that of $Ca_5Al_2Sb_6$ (see ref. 3). The large anisotropy of Na2 indicates some displacement parallel (0 1 0) in the large pentagonal cavities.

$Al_4Eu_8Na_4P_{12}$, monoclinic, $C2/m$ (No. 12), a =13.404(1) Å, b =8.937(1) Å, c =11.474(1) Å, β =108.15(1)°, V =1306.1 Å^3, Z =2, $R(F)$ =0.056, $R_w(F)$ =0.055.

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

Crystal:	black plate, size 0.20 x 0.25 x 0.06
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	198.7 cm^{-1}
Diffractometer:	Siemens R3m/V
Scan mode:	ω
$T_{measurement}$:	293 K
$2\theta_{max}$:	55°
N(hkl)$_{unique}$:	1601
Criterion for F_o:	$F_o > 3\,\sigma(F_o)$
N($param$)$_{refined}$:	85
Program:	SHELXTL-plus

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

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na(1)	4*h*	0	0.3054(7)	1/2	0.018(3)	0.011(3)	0.022(4)	0	0.002(3)	0
Na(2)	4*i*	0.524(1)	0	0.262(1)	0.082(8)	0.017(4)	0.059(8)	0	0.013(6)	0
Eu(1)	8*j*	0.31376(4)	0.27026(7)	0.18273(5)	0.0181(4)	0.0123(4)	0.0092(4)	–0.0036(2)	0.0022(2)	0.0009(2)
Eu(2)	4*g*	0	0.24438(9)	0	0.0150(4)	0.0192(5)	0.0120(5)	0	0.0040(3)	0
Eu(3)	4*f*	1/4	1/4	1/2	0.0104(4)	0.0121(4)	0.0086(4)	–0.0017(2)	0.0027(3)	–0.0012(2)
Al(1)	4*i*	0.0311(3)	0	0.3833(4)	0.010(2)	0.011(2)	0.007(2)	0	0.002(2)	0
Al(2)	4*i*	0.1674(3)	0	0.2365(4)	0.008(2)	0.008(2)	0.009(2)	0	0.004(2)	0
P(1)	8*j*	0.0658(2)	0.2048(3)	0.2710(2)	0.013(1)	0.007(1)	0.009(1)	0.0011(9)	0.0032(9)	0.0011(9)
P(2)	4*i*	0.1397(3)	0	0.5983(4)	0.010(1)	0.010(2)	0.007(2)	0	0.002(1)	0
P(3)	4*i*	0.1765(3)	0	0.0256(4)	0.011(2)	0.011(2)	0.011(2)	0	0.004(1)	0
P(4)	4*i*	0.3392(3)	0	0.3708(4)	0.006(1)	0.011(2)	0.011(2)	0	0.000(1)	0
P(5)	4*i*	0.3389(3)	0	0.0055(4)	0.013(2)	0.012(2)	0.014(2)	0	0.006(1)	0

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