Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: PA1123). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A New Rare Earth Fluorocarbonate, $Na_2Eu(CO_3)F_3$

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Abstract

The structure of sodium europium fluorocarbonate, $Na_2Eu(CO_3)F_3$, obtained by hydrothermal growth, has been determined by single-crystal X-ray diffraction. The orthorhombic structure comprises EuO_3F_6 polyhedra linked by triangular faces and edges. Infinite EuO_2F_3 sheets in the *ab* plane are connected by the carbonate groups and Na atoms.

Comment

At high temperature (T = 1000 K), the study of the Na_2CO_3–LnF_3 system by hydrothermal growth leads only to $Na_3Ln_2(CO_3)_4F$ phases (Ln = La, Pr) (Mercier & Leblanc, 1993). At lower temperature, a new structure type, $Na_2Eu(CO_3)F_3$, is found. In the title compound, the cations adopt classical coordination numbers. Atoms Na1 and Na2 occupy the centres of NaO_4F_2 and NaO_2F_4 polyhedra, respectively. Each Eu atom is surrounded by three O atoms and six F atoms which form a tricapped triangular prism. It must be noted that the valence-bond analysis, as proposed by Brown (1982), is satisfied for all atoms. The EuO_3F_6 polyhedra are connected through the triangular faces formed by the F atoms and form infinite chains along *a*. These chains are linked together by O···O edges in order to build infinite $EuF_{6/2}O_{2/2}O$ sheets in the *ab* plane (Fig. 1). These sheets are shifted one from another along **c** and linked by Na atoms. One O atom of a carbonate group bonds solely to Na atoms. Only Na2 atoms are shown in Fig. 1, at the centre of pseudo-hexagonal cavities.

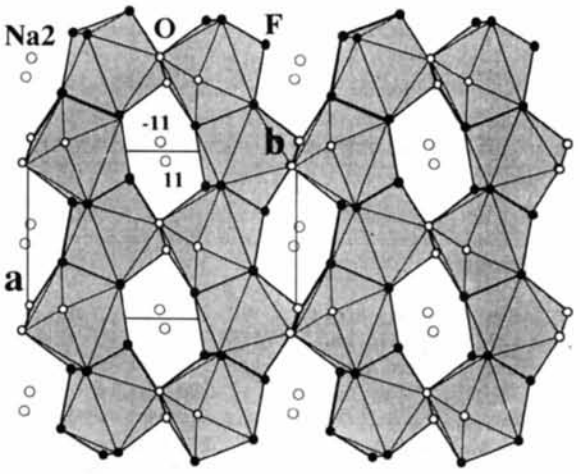

Fig. 1. Part of the structure of $Na_2Eu(CO_3)F_3$ showing a layer of EuO_3F_6 polyhedra in the *ab* plane.

Experimental

A mixture of Na_2CO_3 and EuF_3 in a 3/1 ratio under hydrothermal conditions (T = 650 K, P = 130 MPa) for 48 h leads to a new phase, $Na_2Eu(CO_3)F_3$. A parallelepipedic crystal was chosen for X-ray analysis by optical examination and its quality was tested with Laue photography.

Crystal data

$Na_2Eu(CO_3)F_3$
M_r = 314.94
Orthorhombic
Pbca
a = 6.596 (4) Å
b = 10.774 (4) Å
c = 14.090 (10) Å
V = 1001.3 (10) Å^3
Z = 8
D_x = 4.178 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 38 reflections
θ = 15.20–15.75°
μ = 12.713 mm^{-1}
T = 293 (2) K
Block
0.2 × 0.15 × 0.15 mm
Colourless

Data collection

Stoe Siemens AED four-circle diffractometer
$\omega/2\theta$ scans
1666 observed reflections [$I > 3\sigma(I)$]
R_{int} = 0.028

Absorption correction:
Gaussian integration
T_{min} = 0.173, T_{max} = 0.276
5195 measured reflections
2158 independent reflections

θ_{max} = 35.03°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 17$
$l = 0 \rightarrow 22$
3 standard reflections
frequency: 60 min
intensity variation: 4.7%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.0177
$wR(F^2)$ = 0.0451
S = 1.244
1666 reflections
92 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0179P)^2 + 3.1730P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.023
$\Delta\rho_{max}$ = 1.179 e Å^{-3}
$\Delta\rho_{min}$ = −1.197 e Å^{-3}

Extinction correction:
*SHELXL*93 (Sheldrick, 1994)
Extinction coefficient:
0.0083 (2)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
Eu	−0.00608 (2)	0.183349 (12)	0.014476 (9)	0.00726 (5)
Na1	0.2439 (2)	0.27913 (13)	0.25571 (10)	0.0169 (2)
Na2	−0.0541 (3)	0.00972 (14)	0.39257 (11)	0.0190 (3)
C	0.0008 (4)	0.5157 (3)	0.3229 (2)	0.0104 (4)
OX1	0.0059 (4)	0.4363 (2)	0.2575 (2)	0.0152 (4)
OX2	0.4449 (4)	0.1291 (2)	0.3127 (2)	0.0187 (5)
OX3	−0.0693 (4)	0.4864 (2)	0.4076 (2)	0.0115 (4)
F1	0.3011 (3)	0.2184 (2)	0.10300 (14)	0.0129 (3)
F2	0.2904 (3)	0.3381 (2)	0.41870 (14)	0.0141 (4)
F3	0.1491 (3)	0.1236 (2)	0.48054 (15)	0.0136 (3)

Table 2. *Selected geometric parameters* (Å, °)

Eu—F2^{i}	2.339 (2)	Na1—F2	2.403 (3)
Eu—F1^{ii}	2.341 (2)	Na1—OX1^{v}	2.426 (3)
Eu—F3^{i}	2.365 (2)	Na1—OX2^{i}	2.726 (3)
Eu—F3^{iii}	2.367 (2)	Na2—F3	2.200 (3)
Eu—F2^{iii}	2.387 (2)	Na2—OX1^{iv}	2.280 (3)
Eu—OX3^{iii}	2.405 (2)	Na2—F3^{vi}	2.377 (3)
Eu—F1	2.409 (2)	Na2—F1^{i}	2.443 (3)
Eu—OX3^{iv}	2.440 (2)	Na2—OX3^{vii}	2.506 (3)
Eu—OX2^{i}	2.525 (3)	Na2—F2^{viii}	2.565 (3)
Na1—OX2	2.239 (3)	C1—OX1	1.258 (3)
Na1—F1	2.281 (3)	C1—OX2^{ix}	1.281 (4)
Na1—OX1	2.309 (3)	C1—OX3	1.318 (4)
OX1—C1—OX2^{ix}	124.0 (3)	OX2^{ix}—C1—OX3	115.3 (3)
OX1—C1—OX3	120.6 (3)		

Symmetry codes: (i) $x - \frac{1}{2}, y, \frac{1}{2} - z$; (ii) $x - \frac{1}{2}, \frac{1}{2} - y, -z$; (iii) $x, \frac{1}{2} - y, z - \frac{1}{2}$; (iv) $-x, y - \frac{1}{2}, \frac{1}{2} - z$; (v) $\frac{1}{2} + x, y, \frac{1}{2} - z$; (vi) $-x, -y, 1 - z$; (vii) $-\frac{1}{2} - x, y - \frac{1}{2}, z$; (viii) $\frac{1}{2} - x, y - \frac{1}{2}, z$; (ix) $\frac{1}{2} - x, \frac{1}{2} + y, z$.

Data collection: *DIF*4 (Stoe & Cie, 1988*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1988*b*). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990), option *PATT*. Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1994). Molecular graphics: *STRUPLO*90 (Fischer, Le Lirzin, Kassner & Rüdinger, 1991).

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Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: PA1124). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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