Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å²)

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

	x	y	z	$U_{\rm eq}$
Hg	0.5236 (1)	−0.3888 (1)	0.6359 (1)	0.050 (1)
Cl(1)	0.5748 (2)	−0.3931 (9)	0.8514 (4)	0.046 (2)
Cl(2)	0.5417 (3)	−0.1002 (9)	0.6315 (5)	0.050 (3)
Cl(3)	0.5441 (3)	−0.6636 (8)	0.6038 (5)	0.049 (3)
C(11)	0.179 (1)	0.134 (3)	0.686 (2)	0.059 (1)
C(12)	0.229 (1)	0.209 (4)	0.731 (2)	0.083 (2)
C(13)	0.273 (1)	0.199 (3)	0.699 (2)	0.061 (1)
C(14)	0.2680 (9)	0.109 (3)	0.612 (2)	0.050 (1)
C(15)	0.2171 (9)	0.028 (3)	0.560 (2)	0.043 (10)
C(16)	0.1747 (10)	0.040 (3)	0.598 (2)	0.053 (1)
N(21)	0.3121 (7)	0.094 (2)	0.575 (1)	0.040 (8)
C(22)	0.364 (1)	0.122 (4)	0.649 (2)	0.078 (1)
C(23)	0.411 (2)	0.133 (4)	0.604 (2)	0.081 (1)
N(24)	0.4084 (10)	−0.016 (3)	0.545 (2)	0.069 (1)
C(25)	0.355 (1)	−0.045 (4)	0.467 (2)	0.074 (1)
C(26)	0.311 (1)	−0.054 (4)	0.513 (3)	0.088 (2)

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

Hg—Cl(1)	2.852 (5)	Hg—Cl(2)	2.365 (7)
Hg—Cl(3)	2.346 (7)	Hg—Cl(1^{i})	2.624 (7)
Cl(1)—Hg^{i}	2.624 (7)	C(11)—C(12)	1.37 (4)
C(11)—C(16)	1.42 (4)	C(12)—C(13)	1.35 (5)
C(13)—C(14)	1.38 (4)	C(14)—C(15)	1.42 (3)
C(14)—N(21)	1.42 (3)	C(15)—C(16)	1.38 (4)
N(21)—C(22)	1.41 (3)	N(21)—C(26)	1.47 (4)
C(22)—C(23)	1.55 (5)	C(23)—N(24)	1.44 (4)
N(24)—C(25)	1.45 (3)	C(25)—C(26)	1.48 (5)
Cl(1)—Hg—Cl(2)	90.9 (2)	Cl(1)—Hg—Cl(3)	98.0 (2)
Cl(2)—Hg—Cl(3)	148.5 (3)	Cl(1)—Hg—Cl(1^{i})	91.9 (2)
Cl(2)—Hg—Cl(1^{i})	102.8 (2)	Cl(3)—Hg—Cl(1^{i})	107.0 (2)
Hg—Cl(1)—Hg^{i}	88.1 (2)	C(12)—C(11)—C(16)	113.8 (3)
C(11)—C(12)—C(13)	126.7 (3)	C(12)—C(13)—C(14)	118.6 (2)
C(13)—C(14)—C(15)	118.7 (2)	C(13)—C(14)—N(21)	121.4 (2)
C(15)—C(14)—N(21)	119.9 (2)	C(14)—C(15)—C(16)	119.6 (2)
C(11)—C(16)—C(15)	122.5 (2)	C(14)—N(21)—C(22)	114.6 (2)
C(14)—N(21)—C(26)	116.3 (2)	C(22)—N(21)—C(26)	111.7 (2)
N(21)—C(22)—C(23)	113.9 (2)	C(22)—C(23)—N(24)	106.7 (2)
C(23)—N(24)—C(25)	114.3 (2)	N(24)—C(25)—C(26)	111.1 (2)
N(21)—C(26)—C(25)	111.3 (2)		

Symmetry code: (i) $1 - x, y, \frac{3}{2} - z$.

Preliminary oscillation and Weissenberg photographs showed a monoclinic crystal with systematic absences for the chosen cell consistent with the space group *C*2/*c*. Data reduction, structure solution and refinement were carried out using *SHELXTL/PC* (Sheldrick, 1993). The structure was solved by direct methods and refined successfully in the space group *C*2/*c*. Full-matrix least-squares refinement was carried out by minimizing $\Sigma w(F_o-F_c)^2$. The non-H atoms were refined anisotropically whereas H atoms were fixed isotropically to convergence. One H atom was not included.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1108). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Tetrakis(μ-DL-alanine-*O*:*O*′)octaaquadierbium(III) Hexaperchlorate

NING-HAI HU, ZENG-LIN WANG, CHUN-JI NIU AND JIA-ZUAN NI

Changchun Institute of Applied Chemistry,
Chinese Academy of Sciences, Changchun 130022,
People's Republic of China

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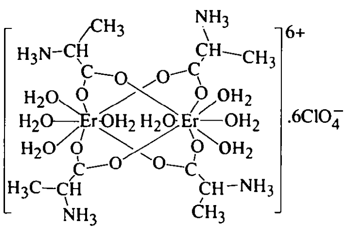
Abstract

The structure of the title compound, $[Er_2(C_3H_7NO_2)_4(H_2O)_8](ClO_4)_6$, consists of dimeric $[Er_2(\text{DL-alanine})_4(H_2O)_8]^{6+}$ cations and perchlorate anions. The four alanine molecules act as bridging ligands linking two Er^{3+} ions through their carboxyl O atoms. Each Er^{3+} ion is also coordinated by four water molecules to complete eightfold coordination in a square antiprism fashion. The perchlorate anions and the methyl groups of the alanine ligands are disordered.

Comment

Structural investigations of rare earth ion–amino acid complexes are of interest with respect to both the understanding of the biological effects of rare earth elements and the enrichment of lanthanide coordination chemistry. Previous studies have revealed that in these complexes the amino acid ligands are bonded to the rare earth ions (Ln^{3+}) through their carboxyl groups, while the amino groups are protonated and are not involved in the metal-ion coordination. The complexes usually adopt one of three types of structure, namely, dinuclear dimer, chain or network polymer. We report here the structure of an erbium complex with DL-alanine, (I), as part of crystallographic studies of rare earth ion–amino acid complexes.

The title compound crystallizes in the triclinic form having a dimeric unit similar to that in its monoclinic form reported by Zeng & Pan (1992). The disorder of the ligands and the perchlorate anions in the present structure could be responsible for the change in crystalline form.



(I)

The structure consists of dimeric $[Er_2$(DL-alanine)$_4(H_2O)_8]^{6+}$ cations and perchlorate anions. As expected, the alanine molecules occur in zwitterionic form with the amino groups protonated and the carboxyl groups deprotonated. The methyl groups are disordered over two positions corresponding to the D and L configurations.

Each alanine molecule acts as a bidentate bridging ligand. The two Er^{3+} ions are coordinated by four such ligands through their carboxyl O atoms, forming a dimeric unit around the $(\frac{1}{2},\frac{1}{2},0)$ crystallographic inversion centre. The planes of the two eight-membered rings in the dimeric unit are almost perpendicular to each other. The Er···Er distance is 4.364 (1) Å, which is considerably shorter than corresponding distances found in the chain structure of the Er^{3+}–proline complex [4.951 (1) and 4.980 (1) Å; Hu, Wang, Niu & Ni, 1993]. The average Er—O$_{\text{carboxyl}}$ bond length of 2.29 (1) Å and the average Er—O$_{\text{water}}$ distance of 2.40 (3) Å are in excellent agreement with the corresponding distances found in the monoclinic form of the complex [2.28 (1) and 2.39 (3) Å, respectively; Zeng & Pan, 1992], and are also consistent, within normal deviations, with those found in the Er^{3+}–proline complex [2.32 (2) and 2.41 (2) Å; Hu, Wang, Niu & Ni, 1993]. The coordination polyhedron around the Er^{3+} ion can be described as a distorted square antiprism in which one square is composed of four carboxyl O atoms with a maximum deviation of 0.066 (9) Å from the least-squares plane and the other comprises four water O atoms with a maximum deviation of 0.11 (1) Å. The perchlorate anions surround the dimeric cation and form hydrogen bonds with the coordinated water molecules and the amino groups.

Legendziewicz, Głowiak, Huskowska & Dao (1988) suggested that the structural type adopted by these complexes is related to the stoichiometric ratio of rare earth ion to amino acid. We have noticed that when perchlorate anions are present the structure is either network (Li & Pan, 1985; Csöregh, Kierkegaard, Legendziewicz & Huskowska, 1987; Wang, Niu, Hu & Ni, 1994), dimeric (Zheng & Pan, 1987; Dao, Głowiak, Huskowska & Legendziewicz, 1988; Zeng & Pan, 1992) or chain (Legendziewicz, Huskowska, Waskowska & Argay, 1984; Liu, Hu, Niu & Meng, 1992; Hu, Wang, Niu & Ni, 1993) when the rare earth ion to amino acid ratio is 1:1, 1:2 or 1:3, respectively. However, when Cl^- anions are present, a chain structure is also seen when the ratio is 1:1 (Głowiak, Dao, Legendziewicz & Huskowska, 1991) or 1:2 (Ma, Li, Lin & Xi, 1993).

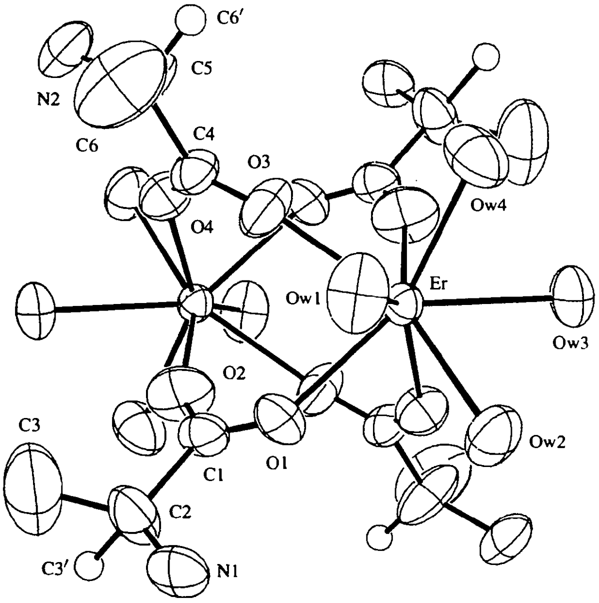


Fig. 1. The dimeric structure of the $[Er_2$(DL-alanine)$_4(H_2O)_8]^{6+}$ cation showing 50% probability displacement ellipsoids. The minor sites of the disordered atoms are shown as circles of arbitrary radii.

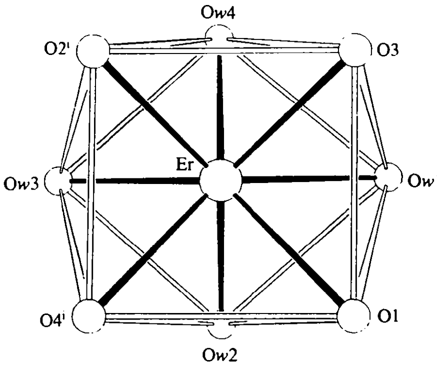


Fig. 2. The coordination polyhedron of the Er^{3+} ion.

Experimental

The title complex was prepared by mixing aqueous solutions of $[Er(ClO_4)_3]$ and DL-alanine in a 1:1 molar ratio at pH 4.0. Light-pink crystals formed after a few days by allowing the solution to stand at 280 K.

Crystal data

$[Er_2(C_3H_7NO_2)_4(H_2O)_8]$-$(ClO_4)_6$
$M_r = 1431.72$
Triclinic
$P\overline{1}$

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 20 reflections
$\theta = 2.8$–$13.2°$

$a = 11.028\,(2)$ Å
$b = 11.308\,(3)$ Å
$c = 10.988\,(3)$ Å
$\alpha = 117.10\,(2)°$
$\beta = 114.48\,(2)°$
$\gamma = 77.16\,(2)°$
$V = 1109.3\,(5)$ Å^3
$Z = 1$
$D_x = 2.14$ Mg m^{-3}

$\mu = 4.37$ mm^{-1}
$T = 294$ K
Columnar
0.42 × 0.36 × 0.28 mm
Light pink

Data collection

Nicolet *R3m/E* diffractometer
ω scans
Absorption correction:
  ψ scans (*XEMP*; Sheldrick, 1983)
  $T_{\rm min} = 0.71$, $T_{\rm max} = 0.94$
5100 measured reflections
4843 independent reflections
4146 observed reflections
  $[I > 3\sigma(I)]$

$R_{\rm int} = 0.014$
$\theta_{\rm max} = 27.0°$
$h = -14 \rightarrow 12$
$k = -14 \rightarrow 12$
$l = 0 \rightarrow 14$
2 standard reflections
  monitored every 98 reflections
  intensity decay: <1.4%

Refinement

Refinement on F
$R = 0.030$
$wR = 0.033$
$S = 1.39$
4146 reflections
345 parameters
H atoms not located
Unit weights applied

$(\Delta/\sigma)_{\rm max} = 0.01$
$\Delta\rho_{\rm max} = 0.54$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.67$ e Å^{-3}
Atomic scattering factors
  from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

$U_{\rm iso}$ for minor sites; $U_{\rm eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$ for others.

	Occupancy	x	y	z	$U_{\rm eq}/U_{\rm iso}$
Er	1.0	0.49962 (2)	0.60100 (2)	0.22290 (2)	0.0341 (1)
O(1)	1.0	0.6552 (4)	0.4272 (4)	0.1940 (5)	0.057 (2)
O(2)	1.0	0.6293 (5)	0.3347 (5)	−0.0402 (5)	0.075 (3)
N(1)	1.0	0.8458 (5)	0.2649 (5)	0.2706 (6)	0.060 (3)
C(1)	1.0	0.6810 (5)	0.3416 (5)	0.0860 (6)	0.047 (3)
C(2)	1.0	0.7857 (6)	0.2349 (6)	0.1106 (7)	0.066 (3)
C(3)	0.76	0.749 (2)	0.103 (1)	0.016 (1)	0.128 (9)
C(3′)	0.24	0.865 (4)	0.189 (5)	0.025 (5)	0.13 (2)
O(3)	1.0	0.3703 (4)	0.4229 (4)	0.0547 (5)	0.066 (2)
O(4)	1.0	0.3475 (4)	0.3263 (4)	−0.1802 (4)	0.054 (2)
N(2)	1.0	0.1524 (5)	0.1797 (5)	−0.2659 (6)	0.065 (3)
C(4)	1.0	0.3188 (5)	0.3448 (5)	−0.0749 (6)	0.045 (3)
C(5)	1.0	0.2097 (8)	0.2632 (8)	−0.1057 (7)	0.079 (4)
C(6)	0.65	0.222 (2)	0.211 (2)	−0.009 (2)	0.12 (1)
C(6′)	0.35	0.134 (2)	0.309 (3)	−0.016 (3)	0.102 (8)
O(*W*1)	1.0	0.4865 (5)	0.4748 (4)	0.3503 (5)	0.070 (3)
O(*W*2)	1.0	0.6703 (4)	0.6715 (4)	0.4575 (4)	0.068 (2)
O(*W*3)	1.0	0.4875 (4)	0.8406 (4)	0.3425 (4)	0.059 (2)
O(*W*4)	1.0	0.3054 (5)	0.6711 (5)	0.2809 (6)	0.076 (3)
Cl(1)	1.0	0.1248 (2)	0.0178 (2)	0.3320 (2)	0.075 (1)
O(5)	0.78	0.1139 (9)	−0.1192 (7)	0.238 (1)	0.139 (6)
O(6)	0.78	0.2510 (8)	0.037 (1)	0.441 (1)	0.152 (7)
O(7)	0.78	0.103 (1)	0.092 (1)	0.249 (1)	0.147 (9)
O(8)	0.78	0.0202 (8)	0.0567 (8)	0.385 (1)	0.110 (6)
O(5′)	0.22	0.104 (3)	0.151 (2)	0.445 (3)	0.108 (9)
O(6′)	0.22	0.014 (2)	−0.006 (4)	0.214 (3)	0.14 (1)
O(7′)	0.22	0.121 (4)	−0.063 (4)	0.406 (4)	0.18 (2)
O(8′)	0.22	0.249 (3)	0.021 (3)	0.336 (3)	0.100 (8)
Cl(2)	1.0	0.5724 (2)	0.1141 (2)	0.2840 (2)	0.081 (1)
O(9)	0.60	0.545 (1)	0.189 (1)	0.209 (2)	0.14 (1)
O(10)	0.60	0.541 (2)	0.158 (2)	0.406 (1)	0.19 (1)
O(11)	0.60	0.720 (1)	0.096 (1)	0.327 (2)	0.16 (1)
O(12)	0.60	0.533 (2)	−0.017 (1)	0.202 (2)	0.16 (1)
O(9′)	0.40	0.469 (2)	0.174 (2)	0.184 (2)	0.128 (6)
O(10′)	0.40	0.480 (2)	0.118 (2)	0.348 (3)	0.172 (9)
O(11′)	0.40	0.652 (2)	0.224 (2)	0.385 (3)	0.160 (8)
O(12′)	0.40	0.606 (3)	−0.003 (2)	0.195 (3)	0.20 (1)
Cl(3)	1.0	0.9252 (2)	0.4767 (2)	0.6670 (2)	0.080 (1)
O(13)	0.55	0.796 (1)	0.449 (1)	0.560 (1)	0.121 (8)
O(14)	0.55	0.919 (1)	0.461 (2)	0.788 (2)	0.16 (1)
O(15)	0.55	1.022 (1)	0.393 (2)	0.608 (2)	0.18 (1)
O(16)	0.55	0.952 (2)	0.607 (1)	0.718 (2)	0.20 (1)
O(13′)	0.45	0.800 (2)	0.522 (2)	0.668 (3)	0.195 (9)
O(14′)	0.45	1.025 (2)	0.523 (2)	0.794 (2)	0.158 (7)
O(15′)	0.45	0.932 (2)	0.342 (2)	0.606 (2)	0.128 (5)
O(16′)	0.45	0.931 (2)	0.535 (2)	0.575 (2)	0.154 (7)

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

Er—O(1)	2.301 (4)	Er—O(*W*1)	2.469 (7)
Er—O(2$^{\rm i}$)	2.255 (5)	Er—O(*W*2)	2.366 (4)
Er—O(3)	2.282 (4)	Er—O(*W*3)	2.414 (4)
Er—O(4$^{\rm i}$)	2.316 (6)	Er—O(*W*4)	2.353 (6)
O(1)—C(1)	1.239 (7)	O(3)—C(4)	1.240 (6)
O(2)—C(1)	1.233 (8)	O(4)—C(4)	1.240 (9)
N(1)—C(2)	1.495 (9)	N(2)—C(5)	1.489 (8)
C(1)—C(2)	1.510 (8)	C(4)—C(5)	1.51 (1)
C(2)—C(3)	1.41 (1)	C(5)—C(6)	1.39 (3)
C(2)—C(3′)	1.39 (5)	C(5)—C(6′)	1.40 (3)
O(1)—Er—O(2$^{\rm i}$)	122.5 (2)	O(3)—Er—O(*W*1)	71.3 (2)
O(1)—Er—O(3)	77.5 (1)	O(3)—Er—O(*W*2)	140.2 (2)
O(1)—Er—O(4$^{\rm i}$)	76.3 (2)	O(3)—Er—O(*W*3)	141.9 (1)
O(1)—Er—O(*W*1)	73.0 (2)	O(3)—Er—O(*W*4)	79.5 (2)
O(1)—Er—O(*W*2)	77.7 (1)	O(4$^{\rm i}$)—Er—O(*W*1)	141.4 (2)
O(1)—Er—O(*W*3)	140.2 (1)	O(4$^{\rm i}$)—Er—O(*W*2)	79.1 (2)
O(1)—Er—O(*W*4)	141.7 (2)	O(4$^{\rm i}$)—Er—O(*W*3)	74.2 (2)
O(2$^{\rm i}$)—Er—O(3)	76.8 (2)	O(4$^{\rm i}$)—Er—O(*W*4)	141.8 (2)
O(2$^{\rm i}$)—Er—O(4$^{\rm i}$)	76.9 (2)	O(*W*1)—Er—O(*W*2)	72.0 (2)
O(2$^{\rm i}$)—Er—O(*W*1)	140.2 (2)	O(*W*1)—Er—O(*W*3)	117.7 (2)
O(2$^{\rm i}$)—Er—O(*W*2)	143.0 (2)	O(*W*1)—Er—O(*W*4)	70.8 (2)
O(2$^{\rm i}$)—Er—O(*W*3)	75.6 (2)	O(*W*2)—Er—O(*W*3)	70.9 (1)
O(2$^{\rm i}$)—Er—O(*W*4)	80.8 (2)	O(*W*2)—Er—O(*W*4)	102.2 (2)
O(3)—Er—O(4$^{\rm i}$)	123.7 (2)	O(*W*3)—Er—O(*W*4)	70.5 (2)
O(1)—C(1)—O(2)	126.3 (5)	O(3)—C(4)—O(4)	127.2 (6)
O(1)—C(1)—C(2)	117.2 (6)	O(3)—C(4)—C(5)	115.6 (7)
O(2)—C(1)—C(2)	116.5 (5)	O(4)—C(4)—C(5)	117.2 (5)
N(1)—C(2)—C(1)	109.4 (5)	N(2)—C(5)—C(4)	109.7 (7)
N(1)—C(2)—C(3)	115.8 (9)	N(2)—C(5)—C(6)	118.6 (9)
C(1)—C(2)—C(3)	116.2 (7)	C(4)—C(5)—C(6)	120.2 (8)
N(1)—C(2)—C(3′)	121 (2)	N(2)—C(5)—C(6′)	122 (1)
C(1)—C(2)—C(3′)	116 (2)	C(4)—C(5)—C(6′)	121 (1)

Symmetry code: (i) $1 - x, 1 - y, -z$.

The structure was solved by heavy-atom methods and refined by block-diagonal least squares. The perchlorate groups and the methyl groups of the DL-alanine ligands were found to be disordered. The occupancy factors for the disordered atoms, each in two positions, were estimated on the basis of their electron densities. All non-H atoms were refined anisotropically, except for those with occupancy factors less than 0.5 which were refined isotropically. All calculations were performed using the *SHELXTL* program system (Sheldrick, 1983).

This work is supported by the Laboratory of Rare Earth Chemistry and Physics, Chinese Academy of Sciences, and by the Chinese National Program 'Basic Research of Rare Earth Science'.

Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the IUCr (Reference: KH1001). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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catena-Diaquatris(α-methylacrylato)-lanthanum(III)

Wei-min Lu,* Jing-bo Wu, Nan Dong and Wei-guo Chun

Department of Chemistry, University of Hangzhou, Hangzhou 310028, People's Republic of China

Jian-Ming Gu

Central Laboratory, University of Hangzhou, Hangzhou 310028, People's Republic of China

Ke-Li Liang

Department of Chemistry, University of Xing Jiang, Xing Jiang, People's Republic of China

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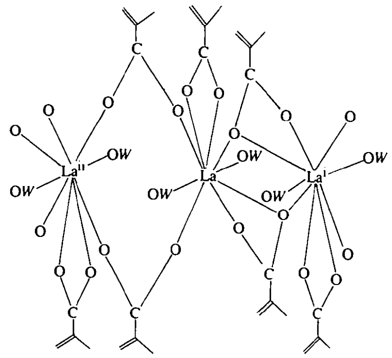
Abstract

The structure of *catena*-poly[{diaqua(methacrylato-*O*,*O*′)lanthanum-bis-μ-methacrylato-*O*,*O*′:*O*;*O*:*O*,*O*′-diaqua(methacrylato-*O*,*O*′)lanthanum}-bis-μ-methacrylato-*O*:*O*′;*O*:*O*′], $[La_2(C_4H_5O_2)_6(H_2O)_4]$, has been determined by single-crystal X-ray diffraction. Each La^{3+} ion is coordinated by seven O atoms from the methacrylato groups and by two water molecules which define a distorted tricapped trigonal prism. Each of the three independent methacrylato ligands bonds to the La^{III} ions in a different way. The crystal contains infinite chains running parallel to the **ab** direction.

Comment

The stereochemistry of complexes of rare earth ions with unsaturated carboxylic acids is of interest because of their potential use as extracting agents; in this context the effect of an α-C=C double bond on the coordination of the carboxylate group to rare earth ions may be significant. However, only a few molecular structures are known (Xue, Zhu & Yang, 1992; Hansson, 1975). The structure determination of the title complex, (I), was undertaken as part of a program of studies on rare earth metal complexes containing unsaturated carboxylic acids. Each complex contains a single independent La^{3+} ion which is coordinated by seven O atoms from five methacrylato groups and by two water molecules. The coordination polyhedron is a distorted tricapped trigonal prism.



(I)

Rare earth metal–carboxylate complexes are very often polymeric in the solid state, with the COO^- group bridging two or three metal ions. However, other bonding modes of the carboxyl groups also occur. Bidentate carboxyl groups are the least common because of the strained nature of the four-membered chelate ring. For this reason, cases where bridging and chelating carboxylate ligands occur in the same complex are very rare indeed. Unlike other polymeric Ln^{3+}–carboxylate complexes which contain either bidentate bridging ligands only (Ma, Li, Lin & Xi, 1993) or chelating and bidentate bridging ligands (Ma, Jin & Ni, 1993), the present compound contains pairs of La^{3+} ions linked by two distinctly different types of carboxylate bridge. One methacrylato group acts as a conventional bidentate bridging ligand, bonding to La