

C(5)	0.5419 (6)	0.9725 (4)	0.3670 (3)	0.038 (1)
C(4)	0.3979 (5)	0.8776 (3)	0.3725 (3)	0.035 (1)
N(4)	0.4349 (5)	0.7532 (3)	0.3713 (3)	0.048 (1)
N(3)	0.2142 (4)	0.9172 (3)	0.3819 (2)	0.0359 (9)
C(2)	0.1536 (6)	1.0447 (4)	0.3793 (3)	0.042 (1)
O(2)	-0.0135 (4)	1.0739 (3)	0.3816 (3)	0.064 (1)
N(1)	0.3001 (5)	1.1321 (3)	0.3729 (3)	0.046 (1)
C(6)	0.4882 (6)	1.0958 (4)	0.3662 (3)	0.041 (1)
C(7)	0.1891 (5)	0.6170 (4)	0.5943 (3)	0.039 (1)

Table 2. Selected geometric parameters (Å, °)

Sn(1)—Cl(1)	2.649 (1)	Sn(1)—Cl(2)	2.620 (1)
Sn(1)—C(7)	2.109 (4)	N(1)—C(2)	1.371 (5)
N(1)—C(6)	1.372 (5)	N(3)—C(2)	1.384 (5)
C(2)—O(2)	1.205 (5)	N(3)—C(4)	1.358 (5)
C(4)—C(5)	1.409 (5)	N(4)—C(4)	1.313 (6)
C(5)—C(6)	1.329 (6)		
Cl(1)—Sn(1)—Cl(2)	90.64 (4)	C(2)—N(3)—C(4)	125.0 (3)
C(7)—Sn(1)—Cl(1)	88.8 (1)	N(3)—C(4)—C(5)	118.3 (3)
C(7)—Sn(1)—Cl(2)	90.2 (1)	N(3)—C(4)—N(4)	119.0 (3)
C(2)—N(1)—C(6)	122.8 (3)	N(4)—C(4)—C(5)	122.8 (4)
N(1)—C(2)—N(3)	113.8 (3)	C(4)—C(5)—C(6)	117.9 (4)
N(1)—C(2)—O(2)	124.1 (4)	C(5)—C(6)—N(1)	122.1 (4)
N(3)—C(2)—O(2)	122.3 (4)		

Table 3. Hydrogen-bonding geometry (Å, °)

D—H...A	D—H	H...A	D...A	D—H...A
N(3)—H(3)...Cl(1 <sup>i</sup> )	0.97 (5)	2.18 (5)	3.139 (3)	169 (5)
N(4)—H(42)...Cl(1 <sup>ii</sup> )	0.75 (6)	2.55 (6)	3.289 (4)	168 (5)
N(1)—H(1)...Cl(2 <sup>iii</sup> )	0.94 (6)	2.34 (6)	3.256 (4)	165 (4)
N(4)—H(41)...Cl(2)	0.82 (6)	2.65 (6)	3.363 (4)	145 (5)

Symmetry codes: (i)  $-x, 1-y, 1-z$ ; (ii)  $1-x, 1-y, 1-z$ ; (iii)  $x, 1+y, z$ .

The structure was solved by the heavy-atom method and final scale factors, atomic coordinates and anisotropic displacement parameters were obtained by full-matrix least-squares refinement. H-atom positions were obtained from the electron density map and refined with a fixed displacement parameter ( $U_{\text{iso}} = 0.08 \text{ \AA}^2$ ). All calculations were performed on a MicroVAX computer using *SHELX76* (Sheldrick, 1976).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry, including intermolecular distances, have been deposited with the IUCr (Reference: NA1172). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

## References

- Bagieu-Beucher, M. (1990). *Acta Cryst.* **C46**, 238–240.
- Kabanos, T. A., Keramidias, A. D., Mentzafos, D., Russo, U., Terzis, A. & Tsangaris, J. M. (1992). *J. Chem. Soc. Dalton Trans.* pp. 2729–2733, and references therein.
- Matsubayashi, G., Ueyama, K. & Tanaka, T. (1985). *J. Chem. Soc. Dalton Trans.* pp. 465–469.
- McClure, R. J. & Craven, B. M. (1973). *Acta Cryst.* **B29**, 1234–1238.
- Nasser, F. A. K., Hossein, M. B., van der Helm, D. & Zuckerman, J. J. (1984). *Inorg. Chem.* **23**, 606–609.
- North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
- Sheldrick, G. M. (1976). *SHELX76. Program for Crystal Structure Determination*. Univ. of Cambridge, England.
- Smart, L. E. & Webster, M. W. (1976). *J. Chem. Soc. Dalton Trans.* pp. 1924–1926.
- Valle, G., Sánchez-González, A., Eitorre, R. & Plazzogna, G. (1988). *J. Organomet. Chem.* **348**, 49–53.

*Acta Cryst.* (1995), **C51**, 2295–2299

## Diaquabis(dichloroacetato)bis(1,10-phenanthroline)europium(III) Dichloroacetate and the Corresponding Erbium(III) Complex

WEIMIN LU, YIQIANG CHENG AND NAN DONG

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

JIANMING GU AND CHENG XU

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

(Received 10 October 1994; accepted 18 May 1995)

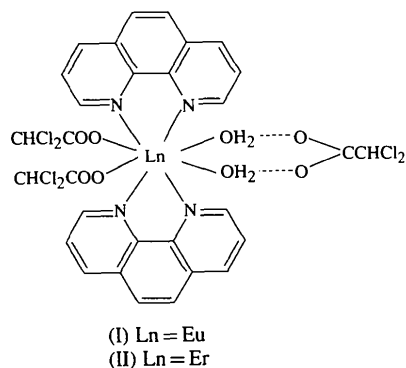
## Abstract

The title complexes, diaquabis(dichloroacetato)bis(1,10-phenanthroline)europium(III) dichloroacetate,  $[\text{Eu}(\text{CHCl}_2\text{CO}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]\text{CHCl}_2\text{CO}_2$ , and diaquabis(dichloroacetato)bis(1,10-phenanthroline)erbium(III) dichloroacetate,  $[\text{Er}(\text{CHCl}_2\text{CO}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]\text{CHCl}_2\text{CO}_2$ , are isostructural. The central atom in each is eight-coordinate and the coordination polyhedra are slightly distorted square antiprisms. The phenanthroline and dichloroacetato ligands compete to coordinate to the lanthanide ions. The structures of the series of lanthanide complexes  $\text{Ln} = \text{La}$  to  $\text{Yb}$  fall into two types, changing structure between  $\text{Sm}$  and  $\text{Eu}$ .

## Comment

Since the discovery of the lanthanide elements, the coordination chemistry of the trivalent lanthanide(III) ions has received considerable attention (Moeller, 1963; Choppin, 1989). Trivalent *f*-block ions are oxophilic and prefer to form coordination complexes with anionic or neutral ligands that have strong O and N-atom donor centres. The design of ligands capable of forming stable lanthanide(III) complexes would allow further study of the coordination properties of these ions. However, there are relatively few reports of lanthanide(III) complexes with heterocyclic amine bidentate ligands. Having completed our research on the complexes of lanthanide trichloroacetate with one bidentate heterocyclic amine ligand (Huang, Lu & Dong, 1990; Dong, Hong, Barton & Robertson, 1990; Mao, Lu & Dong, 1989), we studied the synthesis of the series of complexes of lanthanide(III) trichloroacetate or dichloroacetate (dea) with two bidentate heterocyclic amine

ligands, and have reported the preparation and molecular structures of Ln(CCl<sub>3</sub>CO<sub>2</sub>)<sub>3</sub>L<sub>2</sub>(H<sub>2</sub>O)<sub>*n*</sub> (Ln = La to Yb except Pm, *n* = 0–2, *L* = 1,10-phenanthroline or  $\alpha,\alpha$ -bipyridine) (Wang, Dong, Wu & Zheng, 1991; Cheng, Lu & Dong, 1993). In the preceding paper (Lu, Cheng, Dong, Xu & Chen, 1995), we reported the synthesis and single-crystal X-ray structures of the complexes [Ln(CHCl<sub>2</sub>CO<sub>2</sub>)<sub>3</sub>(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>(C<sub>2</sub>H<sub>5</sub>OH)(H<sub>2</sub>O)] (Ln = La to Sm), prepared by mixing the relevant lanthanide dichloroacetate hydrate with 1,10-phenanthroline (phen) in a mixed solvent of ethanol and water (1:1 v/v). These crystals all belong to the triclinic system with space group *P* $\bar{1}$  and have similar cell parameters. We continue this study in the present paper and describe the crystal structures of [Ln(CHCl<sub>2</sub>CO<sub>2</sub>)<sub>2</sub>(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]CHCl<sub>2</sub>CO<sub>2</sub> [Ln = Eu, (I), or Er, (II)].



The complexes are isostructural; the structure of the Eu complex is shown in Fig. 1. The central atom is eight-coordinate with four N atoms from two bidentate phen ligands and four O atoms from two monodentate dichloroacetato groups and two H<sub>2</sub>O ligands. The coordination polyhedron around the Eu<sup>3+</sup> or Er<sup>3+</sup> ion can be described as a slightly distorted square antiprism (Fig. 2). The groups of atoms O(1), O(8), N(1) and N(2), and O(3), O(7), N(3) and N(4), which are almost coplanar with deviations from the least-squares planes of less than 0.003 (7) and 0.144 (7) Å, respectively, for (I), and 0.016 (9) and 0.14 (1) Å, respectively, for (II), form two bent square planes, the dihedral angles between the mean planes being approximately 3 (1)°. The average bond distances in the two structures are: Eu—O(dca) 2.326 (3), Eu—O(H<sub>2</sub>O) 2.372 (4), Eu—N 2.594 (5), Er—O(dca) 2.273 (7), Er—O(H<sub>2</sub>O) 2.304 (8) and Er—N 2.527 (9) Å. Comparing both complexes, every metal–ligand bond length in (II) is shorter than the corresponding length in (I); this trend is expected for the whole series La to Er as a consequence of the lanthanide contraction.

The phenanthroline ligands possess local C<sub>2v</sub> symmetry. The structures of the phen ligands are iden-

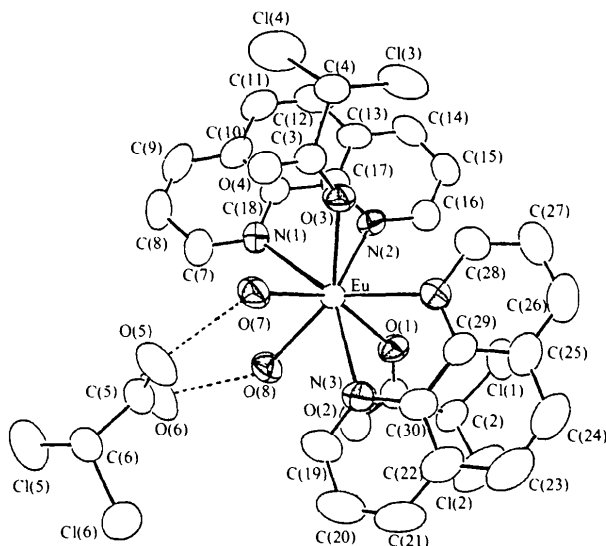


Fig. 1. The molecular structure and the numbering scheme for the europium complex. Displacement ellipsoids are shown at the 50% probability level.

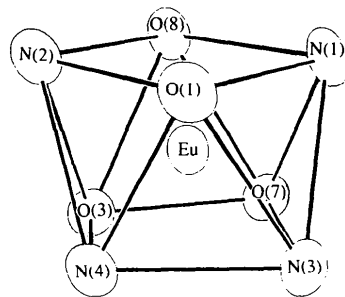


Fig. 2. The coordination polyhedron around the central atom.

tical and similar to those of the phen ligands in [Ln(CHCl<sub>2</sub>CO<sub>2</sub>)<sub>3</sub>(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>(C<sub>2</sub>H<sub>5</sub>OH)(H<sub>2</sub>O)] (Ln = La or Sm) (Lu, Cheng, Dong, Xu & Chen, 1995). The dihedral angle between the mean planes of the two phen groups is 24.4 (3)° for (I) and 24.9 (3)° for (II). As shown in Fig. 1 and Table 2, the uncoordinated dichloroacetate ion is connected to the water ligands through hydrogen bonds.

It should be noted that there is coordination competition between the phen and dichloroacetato ligands in the complexes of lanthanide dichloroacetate which have two phen ligands. In the complexes of the larger lanthanide ions, the central atom is nine-coordinate and three dca ions coordinate as monodentate ligands. In the complexes of the smaller lanthanide ions the coordination number is eight; two dca ions coordinate as monodentate ligands, one dca ion is uncoordinated, and the number of phen ligands is not

changed. This may be attributed to the chelating effect of the neutral phen ligand. This phenomenon did not manifest itself in the complexes of lanthanide trichloroacetate with one phenanthroline ligand (Dong, Hottg, Barton & Robertson, 1990). Moreover, not only does the coordination number of the central atom decrease as the radius of the central lanthanide ion decreases, but the ligand coordination changes; the ethanol ligand in  $[\text{La}(\text{CHCl}_2\text{CO}_2)_3(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{C}_2\text{H}_5\text{OH})(\text{H}_2\text{O})]$  (Lu, Cheng, Dong, Xu & Chen, 1995) is substituted by  $\text{H}_2\text{O}$  in  $[\text{Eu}(\text{CHCl}_2\text{CO}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]\text{CHCl}_2\text{CO}_2$ , even though both complexes are prepared by the same method.

The IR spectra of the series of complexes  $[\text{Ln}(\text{CHCl}_2\text{CO}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]\text{CHCl}_2\text{CO}_2$  (Ln = Eu, Tb, Dy, Ho, Er, Tm, Yb) are all similar and the compositions of the complexes are in fair agreement with their elemental analyses. The structures of the lanthanide complexes (Ln = La to Yb), therefore, fall into two types, changing structure between Sm and Eu.

## Experimental

The title complexes were prepared in the same manner as the complexes  $[\text{Ln}(\text{CHCl}_2\text{CO}_2)_3(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{C}_2\text{H}_5\text{OH})(\text{H}_2\text{O})]$  (Ln = La, Sm) (Lu, Cheng, Dong, Xu & Chen, 1995). The relevant lanthanide oxide was completely dissolved in dichloroacetic acid (Ln:CHCl<sub>2</sub>COOH = 1:1.4 mol ratio) to form a solution of the lanthanide dichloroacetate. After the solution had been slowly evaporated, the dry residue was recrystallized in water and the crystals were dried. 0.15 mmol of the relevant lanthanide dichloroacetate hydrate was then completely dissolved in 12 ml of a mixed solvent of ethanol and water (ethanol:water = 1:1 v/v) and mixed with a solution of 0.3 mmol of phen in the same solvent. Slow evaporation of the solution led, after a few days, to single crystals suitable for X-ray work. Analysis: calculated for (I) C 38.65, H 2.49, N 6.01, Eu 16.30%; found C 38.80, H 2.66, N 5.85, Eu 16.35%. Calculated for (II) C 38.03, H 2.45, N 5.91, Er 17.65%; found C 37.99, H 2.21, N 5.89, Er 17.71%. IR spectra:  $\nu_{\text{as}}(\text{COO}) \sim 1650$ ,  $\nu_{\text{s}}(\text{COO}) \sim 1380$ ,  $\nu_{\text{s}}(\text{C}=\text{C}) \sim 1528$ ,  $\nu_{\text{s}}(\text{C}=\text{N}) \sim 1600$ ,  $\nu_{\text{as}}(\text{C}-\text{H}) \sim 3000$ ,  $\nu_{\text{as}}(\text{O}-\text{H}) \sim 3450$ ,  $\nu(\text{C}-\text{H})$ , out of phen ring bend)  $\sim 727$  and  $845 \text{ cm}^{-1}$ .

### Compound (I)

#### Crystal data

$[\text{Eu}(\text{CHCl}_2\text{CO}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]\text{CHCl}_2\text{CO}_2$   
 $M_r = 932.2$   
 Monoclinic  
 $P2_1/c$   
 $a = 14.664 (2) \text{ \AA}$   
 $b = 13.913 (1) \text{ \AA}$   
 $c = 17.592 (8) \text{ \AA}$   
 $\beta = 102.65 (2)^\circ$   
 $V = 3502 (1) \text{ \AA}^3$   
 $Z = 4$   
 $D_x = 1.768 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation  
 $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 25 reflections  
 $\theta = 11.56\text{--}12.80^\circ$   
 $\mu = 2.31 \text{ mm}^{-1}$   
 $T = 293 \text{ K}$   
 Prism  
 $0.50 \times 0.30 \times 0.28 \text{ mm}$   
 Light pink

#### Data collection

Enraf–Nonius CAD-4 diffractometer  
 $\omega/2\theta$  scans  
 Absorption correction:  $\psi$  scan (North, Phillips & Mathews, 1968)  
 $T_{\text{min}} = 0.929$ ,  $T_{\text{max}} = 0.999$   
 6708 measured reflections  
 6170 independent reflections

#### Refinement

Refinement on  $F$   
 $R = 0.043$   
 $\omega R = 0.052$   
 $S = 3.556$   
 4511 reflections  
 442 parameters  
 H atoms refined isotropically  
 Unit weights applied

4511 observed reflections  
 $[I > 3\sigma(I)]$   
 $R_{\text{int}} = 0.028$   
 $\theta_{\text{max}} = 25^\circ$   
 $h = 0 \rightarrow 17$   
 $k = 0 \rightarrow 16$   
 $l = -20 \rightarrow 20$   
 3 standard reflections monitored every 200 reflections  
 intensity decay: 0.054%

$(\Delta/\sigma)_{\text{max}} = 0.02$   
 $\Delta\rho_{\text{max}} = 0.979 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.781 \text{ e \AA}^{-3}$   
 Extinction correction: none  
 Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

### Compound (II)

#### Crystal data

$[\text{Er}(\text{CHCl}_2\text{CO}_2)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]\text{CHCl}_2\text{CO}_2$   
 $M_r = 947.5$   
 Monoclinic  
 $P2_1/c$   
 $a = 14.564 (2) \text{ \AA}$   
 $b = 13.879 (2) \text{ \AA}$   
 $c = 17.505 (8) \text{ \AA}$   
 $\beta = 102.36 (2)^\circ$   
 $V = 3456 (1) \text{ \AA}^3$   
 $Z = 4$   
 $D_x = 1.823 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation  
 $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 25 reflections  
 $\theta = 10.36\text{--}14.58^\circ$   
 $\mu = 2.98 \text{ mm}^{-1}$   
 $T = 293 \text{ K}$   
 Needle  
 $0.50 \times 0.10 \times 0.10 \text{ mm}$   
 Light pink

#### Data collection

Enraf–Nonius CAD-4 diffractometer  
 $\omega/2\theta$  scans  
 Absorption correction:  $\psi$  scan (North, Phillips & Mathews, 1968)  
 $T_{\text{min}} = 0.938$ ,  $T_{\text{max}} = 0.999$   
 6614 measured reflections  
 6080 independent reflections

4090 observed reflections  
 $[I > 3\sigma(I)]$   
 $R_{\text{int}} = 0.064$   
 $\theta_{\text{max}} = 25^\circ$   
 $h = 0 \rightarrow 17$   
 $k = 0 \rightarrow 16$   
 $l = -20 \rightarrow 20$   
 3 standard reflections monitored every 200 reflections  
 intensity decay: 0.080%

#### Refinement

Refinement on  $F$   
 $R = 0.054$   
 $\omega R = 0.059$   
 $S = 4.478$   
 4090 reflections  
 442 parameters  
 H atoms refined isotropically  
 Unit weights applied

$(\Delta/\sigma)_{\text{max}} = 0.02$   
 $\Delta\rho_{\text{max}} = 0.849 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.786 \text{ e \AA}^{-3}$   
 Extinction correction: none  
 Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>) for (I) and (II)

$B_{eq} = (8\pi^2/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$				
	x	y	z	$B_{eq}$
<b>(I)</b>				
Eu	0.25558 (3)	0.33301 (3)	0.40467 (2)	3.011 (7)
Cl(1)	0.5389 (2)	0.1229 (2)	0.4718 (2)	8.03 (9)
Cl(2)	0.6046 (2)	0.2631 (3)	0.3754 (2)	10.5 (1)
Cl(3)	0.0199 (2)	0.0746 (2)	0.3888 (3)	10.0 (1)
Cl(4)	-0.0922 (3)	0.2161 (3)	0.4406 (2)	11.2 (1)
Cl(5)	0.2052 (3)	0.8626 (2)	0.4017 (2)	7.67 (9)
Cl(6)	0.3066 (2)	0.7919 (3)	0.2903 (2)	10.30 (9)
O(1)	0.4075 (4)	0.2816 (4)	0.4458 (4)	4.0 (1)
O(2)	0.5105 (5)	0.3945 (5)	0.4904 (6)	7.7 (2)
O(3)	0.1111 (4)	0.2527 (4)	0.3735 (4)	4.0 (1)
O(4)	-0.0131 (4)	0.3380 (5)	0.3184 (4)	4.5 (1)
O(5)	0.1462 (5)	0.6249 (5)	0.3087 (4)	6.0 (2)
O(6)	0.2547 (6)	0.6513 (5)	0.4164 (5)	7.0 (2)
O(7)	0.1464 (4)	0.4445 (4)	0.3367 (4)	4.1 (1)
O(8)	0.3305 (4)	0.4787 (4)	0.4556 (4)	4.6 (1)
N(1)	0.1772 (5)	0.3829 (5)	0.5168 (4)	3.8 (2)
N(2)	0.2491 (4)	0.2019 (5)	0.5082 (4)	3.3 (1)
N(3)	0.3381 (5)	0.3866 (5)	0.2941 (4)	4.0 (2)
N(4)	0.2727 (5)	0.2038 (5)	0.3035 (4)	3.9 (2)
C(1)	0.4874 (6)	0.3144 (7)	0.4661 (5)	4.3 (2)
C(2)	0.5713 (6)	0.2459 (7)	0.4639 (6)	4.7 (2)
C(3)	0.0267 (6)	0.2667 (6)	0.3509 (5)	3.5 (1)
C(4)	-0.0385 (6)	0.1831 (7)	0.3643 (6)	4.5 (2)
C(5)	0.2013 (6)	0.6740 (7)	0.3543 (5)	4.4 (2)
C(6)	0.2043 (6)	0.7797 (6)	0.3265 (6)	4.3 (2)
C(7)	0.1487 (7)	0.4711 (7)	0.5252 (6)	4.8 (2)
C(8)	0.0906 (7)	0.4937 (8)	0.5766 (6)	5.5 (2)
C(9)	0.0619 (7)	0.4243 (8)	0.6181 (6)	5.4 (2)
C(10)	0.0917 (6)	0.3299 (8)	0.6120 (5)	4.4 (2)
C(11)	0.0650 (7)	0.5207 (8)	0.6556 (6)	5.2 (2)
C(12)	0.0999 (6)	0.1606 (8)	0.6506 (6)	5.1 (2)
C(13)	0.1634 (6)	0.1403 (7)	0.6012 (5)	4.1 (2)
C(14)	0.2018 (7)	0.0500 (7)	0.5959 (5)	4.6 (2)
C(15)	0.2621 (6)	0.0373 (7)	0.5485 (6)	4.4 (2)
C(16)	0.2860 (6)	0.1145 (6)	0.5063 (6)	4.0 (2)
C(17)	0.1889 (6)	0.2160 (6)	0.5556 (5)	3.6 (2)
C(18)	0.1518 (5)	0.3117 (6)	0.5610 (5)	3.4 (2)
C(19)	0.3681 (7)	0.4759 (7)	0.2868 (6)	5.1 (2)
C(20)	0.4255 (7)	0.4997 (8)	0.2358 (6)	5.9 (3)
C(21)	0.4546 (7)	0.4328 (9)	0.1935 (6)	5.9 (3)
C(22)	0.4243 (6)	0.3375 (8)	0.1979 (5)	4.8 (2)
C(23)	0.4492 (7)	0.2588 (9)	0.1521 (6)	6.1 (3)
C(24)	0.4160 (7)	0.1686 (9)	0.1549 (5)	5.7 (2)
C(25)	0.3545 (7)	0.1463 (7)	0.2064 (5)	4.7 (2)
C(26)	0.3154 (8)	0.0553 (7)	0.2098 (6)	5.6 (3)
C(27)	0.2553 (8)	0.0407 (7)	0.2567 (6)	5.7 (3)
C(28)	0.2364 (7)	0.1151 (7)	0.3045 (5)	4.6 (2)
C(29)	0.3302 (6)	0.2201 (6)	0.2538 (5)	3.7 (2)
C(30)	0.3658 (6)	0.3175 (7)	0.2492 (5)	4.0 (2)
<b>(II)</b>				
Er	0.25473 (3)	0.33221 (3)	0.40576 (3)	2.755 (8)
Cl(1)	0.5372 (3)	0.1225 (3)	0.4727 (3)	8.1 (1)
Cl(2)	0.6033 (3)	0.2620 (5)	0.3759 (3)	9.8 (1)
Cl(3)	0.0185 (3)	0.0758 (3)	0.3916 (4)	9.5 (1)
Cl(4)	-0.0967 (3)	0.2188 (4)	0.4383 (3)	11.1 (1)
Cl(5)	0.2048 (4)	0.8596 (3)	0.4036 (3)	7.3 (1)
Cl(6)	0.3084 (3)	0.7923 (3)	0.2909 (3)	9.6 (1)
O(1)	0.4040 (5)	0.2825 (6)	0.4464 (5)	3.7 (2)
O(2)	0.5073 (6)	0.3926 (6)	0.4906 (7)	6.7 (3)
O(3)	0.1121 (5)	0.2542 (6)	0.3752 (5)	3.8 (2)
O(4)	-0.0118 (5)	0.3379 (6)	0.3184 (5)	4.1 (3)
O(5)	0.1492 (7)	0.6228 (6)	0.3090 (6)	5.8 (2)
O(6)	0.2567 (8)	0.6497 (6)	0.4169 (7)	6.7 (3)
O(7)	0.1499 (5)	0.4410 (5)	0.3379 (4)	3.6 (2)
O(8)	0.3296 (5)	0.4724 (6)	0.4581 (5)	3.9 (2)
N(1)	0.1767 (6)	0.3817 (7)	0.5146 (5)	3.4 (2)
N(2)	0.2497 (6)	0.2020 (7)	0.5068 (5)	3.1 (2)
N(3)	0.3367 (6)	0.3866 (7)	0.2980 (6)	3.5 (2)
N(4)	0.2709 (6)	0.2048 (7)	0.3083 (6)	3.7 (2)
<b>(I)</b>				
C(1)	0.4850 (8)	0.3135 (8)	0.4674 (7)	3.6 (3)
C(2)	0.5686 (8)	0.245 (1)	0.4650 (8)	4.3 (3)
C(3)	0.0263 (8)	0.2675 (8)	0.3505 (6)	3.1 (2)
C(4)	-0.0394 (8)	0.1835 (9)	0.3646 (8)	4.4 (3)
C(5)	0.2044 (8)	0.6720 (9)	0.3543 (7)	3.9 (2)
C(6)	0.2060 (9)	0.7783 (8)	0.3283 (7)	4.2 (3)
C(7)	0.1474 (9)	0.4709 (9)	0.5237 (8)	4.4 (3)
C(8)	0.0912 (9)	0.494 (1)	0.5766 (8)	5.0 (3)
C(9)	0.0614 (9)	0.423 (1)	0.6169 (8)	5.0 (3)
C(10)	0.0918 (7)	0.329 (1)	0.6111 (6)	4.0 (2)
C(11)	0.0651 (8)	0.250 (1)	0.6554 (7)	4.8 (3)
C(12)	0.0998 (8)	0.163 (1)	0.6499 (7)	4.7 (3)
C(13)	0.1645 (8)	0.1414 (9)	0.6012 (7)	3.7 (3)
C(14)	0.2030 (8)	0.0508 (9)	0.5957 (8)	4.2 (3)
C(15)	0.2633 (8)	0.0378 (9)	0.5474 (8)	4.3 (3)
C(16)	0.2860 (8)	0.1160 (9)	0.5052 (8)	4.1 (3)
C(17)	0.1893 (7)	0.2164 (8)	0.5551 (6)	3.2 (2)
C(18)	0.1518 (7)	0.3107 (8)	0.5595 (6)	3.1 (2)
C(19)	0.3660 (9)	0.475 (1)	0.2901 (8)	4.8 (3)
C(20)	0.4236 (9)	0.500 (1)	0.2389 (8)	5.9 (3)
C(21)	0.4523 (9)	0.431 (1)	0.1947 (7)	5.4 (3)
C(22)	0.4225 (8)	0.337 (1)	0.1999 (6)	4.3 (3)
C(23)	0.4469 (9)	0.261 (1)	0.1533 (8)	5.3 (3)
C(24)	0.4123 (9)	0.171 (1)	0.1570 (7)	5.2 (3)
C(25)	0.3519 (9)	0.1471 (9)	0.2094 (7)	4.3 (3)
C(26)	0.313 (1)	0.056 (1)	0.2131 (7)	5.1 (3)
C(27)	0.252 (1)	0.0419 (9)	0.2619 (8)	5.1 (3)
C(28)	0.2338 (9)	0.1168 (9)	0.3085 (7)	4.0 (3)
C(29)	0.3285 (7)	0.2213 (9)	0.2576 (7)	3.4 (2)
C(30)	0.3636 (7)	0.3168 (9)	0.2531 (6)	3.5 (2)
<b>(II)</b>				
Er—O(1)	2.301 (3)	Er—O(1)	2.245 (6)	
Eu—O(3)	2.351 (3)	Er—O(3)	2.301 (6)	
Eu—O(7)	2.359 (4)	Er—O(7)	2.289 (7)	
Eu—O(8)	2.385 (3)	Er—O(8)	2.318 (7)	
Eu—N(1)	2.586 (4)	Er—N(1)	2.514 (7)	
Eu—N(2)	2.593 (4)	Er—N(2)	2.540 (8)	
Eu—N(3)	2.615 (5)	Er—N(3)	2.553 (7)	
Eu—N(4)	2.580 (4)	Er—N(4)	2.501 (9)	
O(1)—Eu—O(3)	133.4 (1)	O(1)—Er—O(3)	133.9 (2)	
O(1)—Eu—O(7)	150.1 (1)	O(1)—Er—O(7)	149.2 (1)	
O(1)—Eu—O(8)	79.1 (1)	O(1)—Er—O(8)	77.9 (2)	
O(1)—Eu—N(1)	113.9 (2)	O(1)—Er—N(1)	114.0 (1)	
O(1)—Eu—N(2)	75.1 (2)	O(1)—Er—N(2)	74.4 (1)	
O(1)—Eu—N(3)	75.4 (1)	O(1)—Er—N(3)	75.6 (2)	
O(1)—Eu—N(4)	76.5 (1)	O(1)—Er—N(4)	76.9 (2)	
O(3)—Eu—O(7)	73.6 (1)	O(3)—Er—O(7)	73.8 (2)	
O(3)—Eu—O(8)	144.0 (1)	O(3)—Er—O(8)	144.2 (2)	
O(3)—Eu—N(1)	77.2 (2)	O(3)—Er—N(1)	76.8 (1)	
O(3)—Eu—N(2)	70.1 (1)	O(3)—Er—N(2)	70.6 (1)	
O(3)—Eu—N(3)	120.1 (1)	O(3)—Er—N(3)	120.6 (2)	
O(3)—Eu—N(4)	74.1 (1)	O(3)—Er—N(4)	73.8 (1)	
O(7)—Eu—O(8)	80.6 (1)	O(7)—Er—O(8)	81.8 (1)	
O(7)—Eu—N(1)	81.0 (1)	O(7)—Er—N(1)	81.6 (1)	
O(7)—Eu—N(2)	133.9 (1)	O(7)—Er—N(2)	135.6 (2)	
O(7)—Eu—N(3)	79.0 (1)	O(7)—Er—N(3)	77.7 (2)	
O(7)—Eu—N(4)	105.5 (2)	O(7)—Er—N(4)	105.1 (1)	
O(8)—Eu—N(1)	74.3 (1)	O(8)—Er—N(1)	73.9 (2)	
O(8)—Eu—N(2)	114.7 (1)	O(8)—Er—N(2)	113.7 (2)	
O(8)—Eu—N(3)	77.7 (1)	O(8)—Er—N(3)	77.8 (1)	
O(8)—Eu—N(4)	138.2 (2)	O(8)—Er—N(4)	139.1 (1)	
N(1)—Eu—N(2)	64.1 (2)	N(1)—Er—N(2)	65.2 (1)	
N(1)—Eu—N(3)	147.8 (1)	N(1)—Er—N(3)	146.9 (1)	
N(1)—Eu—N(4)	147.1 (1)	N(1)—Er—N(4)	146.4 (1)	
N(2)—Eu—N(3)	144.8 (2)	N(2)—Er—N(3)	144.4 (2)	
N(2)—Eu—N(4)	91.0 (1)	N(2)—Er—N(4)	89.7 (2)	
N(3)—Eu—N(4)	63.6 (2)	N(3)—Er—N(4)	65.0 (2)	
<b>D—H...A</b>				
O(7)—H(71)...O(5)	2.558 (5)	D—H...A	163.2 (3)	
O(7)—H(72)...O(4)	2.727 (4)		157.5 (2)	
O(8)—H(81)...O(6)	2.672 (5)		164.6 (2)	
O(8)—H(82)...O(2)	2.831 (5)		143.4 (3)	

## (II)

O(7)—H(71)···O(5)	2.571 (5)	160.1 (3)
O(7)—H(72)···O(4)	2.713 (5)	138.0 (3)
O(8)—H(81)···O(6)	2.713 (5)	146.6 (3)
O(8)—H(82)···O(2)	2.759 (5)	138.3 (3)

The data were corrected for Lorentz and polarization effects. All non-H atoms were located through Patterson and Fourier techniques and were refined by full-matrix least-squares methods including anisotropic displacement parameters. All H atoms were located by the same method and refined with isotropic displacement parameters in the last two cycles of refinement. Program used throughout the analysis: *SDP* (Frenz, 1985).

This work was partly supported by a National Natural Science Foundation Grant of China.

---

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KH1017). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

---

## References

- Cheng, Y. Q., Lu, W. M. & Dong, N. (1993). *Gaodexuexiao Huaxue Xuebao (Chem. J. Chin. Univ.)*, **14**, 1487–1491.
- Choppin, D. R. (1989). *Lanthanide Probes in Life, Chemical and Earth Sciences, Theory and Practice*, edited by J. C. G. Bunzli & G. R. Choppin, ch. 1. Amsterdam: Elsevier.
- Dong, N., Hong, W., Barton, R. J. & Robertson, B. E. (1990). *J. Coord. Chem.* **22**, 191–204.
- Frenz, B. A. (1985). *Enraf-Nonius SDP Structure Determination Package*. Version 1.1. Enraf-Nonius, Delft, The Netherlands.
- Huang, H. H., Lu, W. M. & Dong, N. (1990). *Wuji Huaxue (J. Inorg. Chem. China)*, **6**, 70–75.
- Lu, W. M., Cheng, Y. Q., Dong, N., Xu, C. & Chen, C. G. (1995). *Acta Cryst.* **C51**, 1756–1759.
- Mao, L., Lu, W. M. & Dong, N. (1989). *Jiegou Huaxue (J. Struct. Chem. China)*, **8**, 75–77.
- Moeller, T. (1963). *The Chemistry of the Lanthanides*, ch. 1. New York: Reinhold.
- North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
- Wang, J. R., Dong, N., Wu, G. & Zheng, P. J. (1991). *Gaodexuexiao Huaxue Xuebao (Chem. J. Chin. Univ.)*, **12**, 1284–1288.