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NOTE

Study on Novel Structure of Europium Complex

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A novel europium complex with the m.f. $C_{10}H_{21}Eu_2NO_{19}$ has been synthesized from a hydrothermal reaction and the crystal structure has been determined by means of single-crystal X-ray diffraction. Europium atom is coordinated by nine O atoms. The molecular structure stabilized by the O-H···O and O-H···N hydrogen-bonding interactions.

Key Words: Europium complex, Structure analysis.

Lanthanide complexes have attracted attention of researchers for interesting structures and potential applications in luminescent materials, catalysts and magnetic molecular materials, *etc*.[1-5]. Among lanthanide ions, europium(III) ion has received the most attention because of good luminescence with narrow bandwidth, large stokes shift and long luminescence lifetime. The Eu complexes are successfully applied in materials science as luminescent probes and sensory materials[6]. carboxylates are often used to construct the coordination polymers because of their rich coordination modes[7,8]. A large number of lanthanide carboxylate complexes have been reported with dimeric or 1-, 2- and 3-D polymeric structures due to variable coordination number of Ln(III) as well as coordination versatility of carboxylate[9-13]. In this paper, the novel Eu complex is reported.

All commercially obtained reagent-grade chemicals were used without further purification. A mixture of Eu_2O_3 (0.01 mmol, 0.004 g), dilute HNO_3, 2,2'-bipyridine (0.1 mmol, 0.016 g), K_2CrO_4 (0.1 mmol, 0.02 g), boric acid (0.1 mmol, 0.006 g) and tartaric acid (0.2 mmol, 0.03 g) were added into 20 mL water with 10 % (v/v) ethanol and heated for 6 h at 413 K. The solution was obtained by filtration after cooling the reaction to room temperature. Yellow block single crystals suitable for X-ray measurements were obtained after a few weeks.

The crystal structure of title europium complex with the m.f. $C_{10}H_{21}Eu_2NO_{19}$ is shown in Fig. 1. The crystal data and structure refinement is shown in Table-1. The Eu atom is

TABLE-1
CRYSTAL DATA AND STRUCTURE REFINEMENT FOR THE TITLE COMPLEX

Empirical formula	$C_{10}H_{21}Eu_2NO_{19}$
Formula weight	763.20
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 11.0821(12) Å, α = 90°, b = 9.6205(9) Å, β = 114.204(2)°, c = 10.1103(10) Å, γ = 90°
Volume	983.15(17) Å^3
Z, Calculated density	2, 2.578 Mg/m^3
Absorption coefficient	6.421 mm^{-1}
$F_{(000)}$	732
Crystal size	0.43 mm × 0.40 mm × 0.39 mm
Theta range for data collection	3.06-25.02°.
Limiting indices	-13 ⇐ h ⇐ 13, -11 ⇐ k ⇐ 11, -12 ⇐ l ⇐ 12
Reflections collected/unique	7439/1728 [$R_{(int)}$ = 0.0481]
Completeness to theta = 25.02	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.1885 and 0.1688
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	1728/0/175
Goodness-of-fit on F^2	1.064
Final R indices [I > 2σ(I)]	R_1 = 0.0317, wR_2 = 0.0700
R indices (all data)	R_1 = 0.0424, wR_2 = 0.0783
Largest diff. peak and hole	2.731 and -1.239 e Å^{-3}

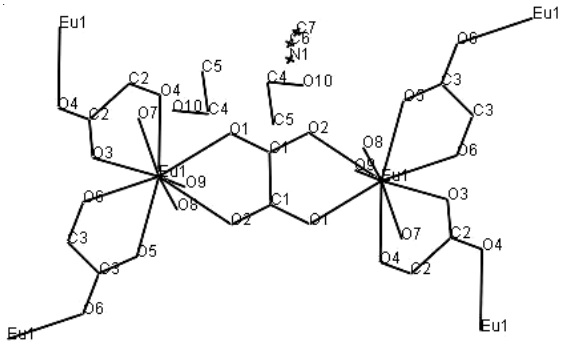

Fig. 1. Molecular structure of the Eu complex

coordinated by nine O atoms. One oxalic acid molecular bridges two Eu atoms. The Eu-O distances are in the range of 2.414-2.544 Å. The angles of O-Eu-O are in the range of 63.98-143.8º. The torsion angles of O(1)-Eu(1)-O(3)-C(2), O(3)-Eu(1)-O(1)-C(1), O(9)-Eu(1)-O(1)-C(1) are 5.6, 129.1 and 64.0º, respectively. Selected bond lengths and bond angles are shown in Table-2.

TABLE-2
SELECT BOND LENGTHS [Å] AND ANGLES [º] FOR THE TITLE COMPLEX

Eu(1)-O(5)	2.414(5)	O(7)-Eu(1)-O(3)	95.1(2)
Eu(1)-O(1)	2.423(5)	O(9)-Eu(1)-O(3)	71.84(19)
Eu(1)-O(7)	2.423(6)	O(5)-Eu(1)-O(8)	83.6(2)
Eu(1)-O(9)	2.429(5)	O(1)-Eu(1)-O(8)	81.0(2)
Eu(1)-O(3)	2.464(5)	O(7)-Eu(1)-O(8)	72.3(2)
Eu(1)-O(8)	2.477(6)	O(9)-Eu(1)-O(8)	137.3(2)
N(1)-C(6)	1.11(4)	C(2)-O(3)-Eu(1)	123.1(5)
O(1)-C(1)	1.242(9)	C(3)-O(5)-Eu(1)	121.4(5)
O(2)-C(1)	1.263(9)	O(8)-Eu(1)-O(4)#3	135.9(2)
O(5)-C(3)	1.244(9)	C(1)-O(1)-Eu(1)	121.2(5)
O(6)-C(3)	1.257(9)	C(1)-O(2)-Eu(1)#1	119.2(5)
O(9)-H(9D)	0.8501	C(2)-O(3)-Eu(1)	123.1(5)
O(10)-C(4)	1.42(4)	C(2)-O(4)-Eu(1)#3	120.1(5)
C(4)-H(4A)	0.9700	C(3)-O(5)-Eu(1)	121.4(5)
C(5)-H(5B)	0.9600	C(3)-O(6)-Eu(1)#2	119.2(5)
C(6)-C(7)	1.43(5)	Eu(1)-O(7)-H(7F)	134.6
C(7)-H(7C)	0.9600	Eu(1)-O(7)-H(7G)	116.2
O(5)-Eu(1)-O(1)	137.48(19)	H(7F)-O(7)-H(7G)	108.7
O(5)-Eu(1)-O(7)	137.06(19)	Eu(1)-O(8)-H(8C)	121.1
O(1)-Eu(1)-O(7)	73.71(19)	Eu(1)-O(8)-H(8D)	128.6
O(5)-Eu(1)-O(9)	76.1(2)	H(8C)-O(8)-H(8D)	108.6
O(1)-Eu(1)-O(9)	89.2(2)	Eu(1)-O(9)-H(9C)	118.2
O(7)-Eu(1)-O(9)	143.8(2)	O(5)-C(3)-O(6)	126.7(7)
O(5)-Eu(1)-O(3)	82.76(19)	N(1)-C(6)-C(7)	167(4)
O(1)-Eu(1)-O(3)	130.50(19)	–	–

The molecular structure stabilized by the O-H···O and O-H···N hydrogen-bonding interactions.

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