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Research Article

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Study on novel structure of Er complex, $C_{14}H_{19}ErN_2O_{14}$

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ABSTRACT

A novel Er complex $C_{14}H_{11}ErN_2O_{10}$●$4(H_2O)$ has been synthesized from a hydrothermal reaction and the crystal structure has been determined by means of single-crystal X-ray diffraction. Monoclinic, P21/c. a=14.0400(10) Å, b =11.2536(9) Å, c =12.9373(9) Å, $\alpha = 90^\circ$, $\beta = 102.010(6)^\circ$, $\gamma = 90^\circ$. V=1999.4 Å^3. Z=8. R_1 =0.0586, wR_2 = 0.1684, T=293(2) K. The Er atom is nine-coordinated by two N atoms from two 2,6-pyridine dicarboxylic acid moleculars and seven O atoms. The molecular structure stabilized by the O-H…O hydrogen-bonding interactions.

Keywords: Er complex; structure analysis; hydrogen bonding

INTRODUCTION

Lanthanide complexation chemistry has been investigated widely many years and much progress has been made for the applications as bioactive probes for magnetic resonance and luminescence [1-3]. The design of new molecular-based magnetic materials, combining lanthanide ions with organic radicals as magnetic ligand center, has attracted great amount interest for creation of single-molecule magnets and single-chain magnets [4-9]. Nitronyl nitroxide radicals are particularly attractive because of their exceptional stability and easy chemical modification and Er complex is reported [10]. 2,6-pyridine dicarboxylic acid show as multifunctional ligands for bridging ligands in metal complexes with five coordination sites involving the oxygen atoms of the carboxylate groups and the nitrogen atom of the pyridine ring [11-16]. In this paper, the novel Er complex is reported.

EXPERIMENTAL SECTION

All commercially obtained reagent-grade chemicals were used without further purication. A mixture of Er_2O_3 (0.01 mmol, 0.004g), dilute HNO_3, 2,6-bipyridine dicarboxylic acid (0.1mmol, 0.02g), boric acid (0.2mmol, 0.012g) and serine (0.1mmol, 0.01g) were added into 10 mL water with 10%(v/v) ethanol and heated for 10h at 403K. The solution was obtained by filtration after cooling the reaction to room temperature. Colorless single crystals suitable for X-ray measurements were obtained after a few weeks.

The crystal data was collected on a Bruker smart CCD Area Detector.

A colorless block single crystal with dimensions of 0.17 x 0.09 x 0.05 mm was selected for measurement. Diffraction data of the single crystal were collected by ψ-ω scan mode using a graphite-monochromatic Mo *K*α rediation (λ=0.71073 Å) at 293(2) K on a Bruker Smart Apex CCD diffractometer.

RESULTS AND DISCUSSION

The title complex crystal structure is shown in Fig.1. It is built up Er atom, two 2,6-pyridine dicarboxylic acid and four water molecular. The crystal data and structure refinement is shown in Table 1. The Er atom is nine-coordinated by two N atoms from two 2,6-pyridine dicarboxylic acid moleculars and seven O atoms. The distances d(Er-O) are in the range of 2.454-2.561 Å. The bond lengths d(Er-N) are 2.623 and 2.630 Å. The angles of O3-Er1-O1, N1-Er1-N2, O1-Er1-N2 are 122.2, 111.8, 72.3°, respectively. Selected bond lengths and bond angles are shown in Table 2.

The molecular structure stabilized by the O-H…O hydrogen bonding interactions.

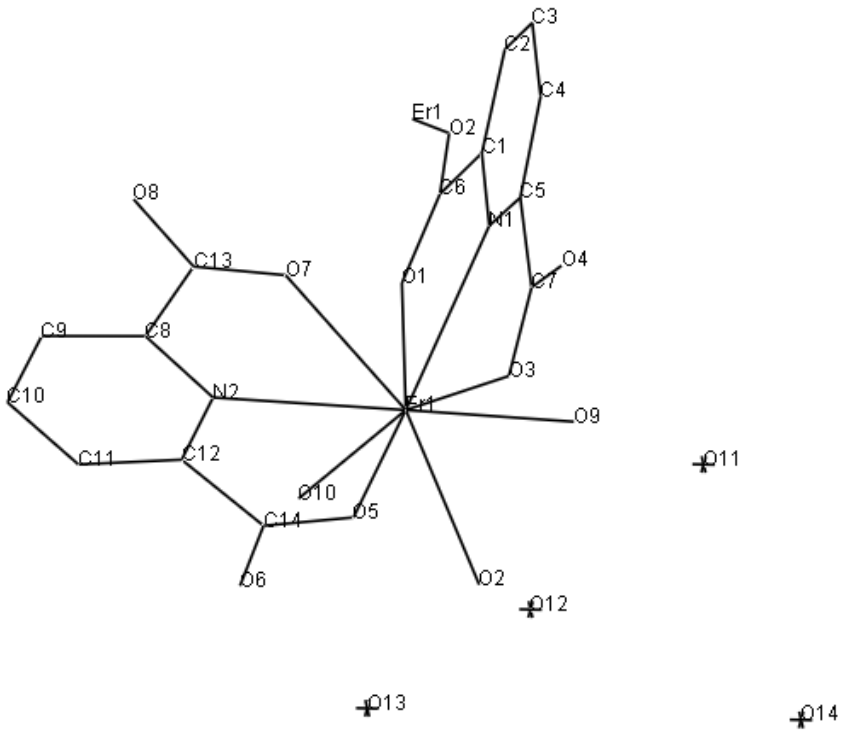

Fig.1 The molecular structure of $C_{14}H_{19}ErN_2O_{14}$

Table 1. Crystal data and structure refinement for the title complex

Empirical formula	$C_7H_{9.5}Er_{0.50}NO_7$
Formula weight	302.78
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 14.0400(10) Å alpha = 90°. b = 11.2536(9) Å beta = 102.010(6)°. c = 12.9373(9) Å gamma = 90°.
Volume	1999.4(3) $Å^3$
Z, Calculated density	8, 2.012 Mg/m^3
Absorption coefficient	4.275 mm^{-1}
F(000)	1184
Crystal size	0.17 x 0.09 x 0.05 mm
Theta range for data collection	2.42 to 25.02°.
Limiting indices	-16<=h<=16, -13<=k<=12, -15<=l<=14
Reflections collected / unique	7666 / 3532 [R(int) = 0.0588]
Completeness to theta = 25.02	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8147 and 0.5302
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3532 / 816 / 280
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0586, wR2 = 0.1484
R indices (all data)	R1 = 0.0826, wR2 = 0.1684
Largest diff. peak and hole	1.405 and -1.867 e.$Å^{-3}$

Table 2. Select bond lengths [Å] and angles [°] for the title complex

Er(1)-O(9)	2.454(7)
Er(1)-O(10)	2.477(6)
Er(1)-O(5)	2.486(7)
Er(1)-O(3)	2.509(6)
Er(1)-O(1)	2.540(7)
Er(1)-O(7)	2.561(7)
Er(1)-N(1)	2.623(8)
Er(1)-N(2)	2.630(8)
N(1)-C(1)	1.328(12)
N(2)-C(12)	1.311(13)
O(1)-C(6)	1.248(12)
O(9)-Er(1)-O(10)	141.8(2)
O(9)-Er(1)-O(5)	80.8(2)
O(10)-Er(1)-O(5)	97.8(2)
O(9)-Er(1)-O(3)	85.9(2)
O(10)-Er(1)-O(3)	78.6(2)
O(5)-Er(1)-O(3)	153.2(2)
O(9)-Er(1)-O(1)	72.6(2)
O(10)-Er(1)-O(1)	144.4(2)
O(5)-Er(1)-O(1)	75.6(2)
O(3)-Er(1)-O(1)	122.2(2)
O(9)-Er(1)-O(7)	140.4(2)
O(10)-Er(1)-O(7)	71.6(2)
O(5)-Er(1)-O(7)	122.8(2)
O(3)-Er(1)-O(7)	81.7(2)
O(1)-Er(1)-O(7)	82.7(2)
O(9)-Er(1)-N(1)	75.5(2)
O(10)-Er(1)-N(1)	124.1(3)
O(5)-Er(1)-N(1)	135.2(2)
O(3)-Er(1)-N(1)	61.6(2)
O(1)-Er(1)-N(1)	61.3(2)
O(7)-Er(1)-N(1)	65.5(2)
O(9)-Er(1)-N(2)	133.6(3)
O(10)-Er(1)-N(2)	73.9(2)
O(2)#1-Er(1)-N(2)	118.4(2)
O(5)-Er(1)-N(2)	61.7(2)
O(3)-Er(1)-N(2)	139.2(2)
O(1)-Er(1)-N(2)	72.3(2)
O(7)-Er(1)-N(2)	61.4(2)
N(1)-Er(1)-N(2)	111.8(2)
C(1)-N(1)-C(5)	118.5(9)
C(1)-N(1)-Er(1)	121.3(6)
C(5)-N(1)-Er(1)	118.7(6)
C(12)-N(2)-C(8)	119.8(8)
C(12)-N(2)-Er(1)	119.2(6)
C(8)-N(2)-Er(1)	120.7(6)
C(6)-O(1)-Er(1)	126.2(6)
C(6)-O(2)-Er(1)#2	142.3(6)
C(7)-O(3)-Er(1)	125.4(6)
C(14)-O(5)-Er(1)	126.7(7)
C(13)-O(7)-Er(1)	123.9(7)
N(1)-C(1)-C(2)	123.1(9)
N(1)-C(1)-C(6)	113.6(8)
N(2)-C(8)-C(13)	113.7(8)
N(2)-C(12)-C(14)	116.0(8)

CONCLUSION

A novel Er complex $C_{14}H_{11}ErN_2O_{10}\bullet 4(H_2O)$ has been synthesized from a hydrothermal reaction and the crystal structure has been determined by means of single-crystal X-ray diffraction.

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