Hai-Ping Wang*, Lu Chen, Jia-Jun Liang and Guo-Peng Huang

The crystal structure of (1-(pyridin-2-yl)-N-(pyridin-2-ylmethyl)-N-((1-(4-vinylbenzyl)-1H-benzo[d]imidazol-2-yl)methyl) methanamine-κ⁴N,N’,N″,N‴) tris(nitrato-κO,O’)-erbium(III), C₂₉H₂₇ErN₈O₉

Abstract
C₂₉H₂₇ErN₈O₉, triclinic, P₁ (no. 2), a = 8.6681(2) Å, b = 13.0695(3) Å, c = 14.1408(4) Å, α = 80.130(2)°, β = 86.409(2)°, γ = 75.761(2)°, V = 1529.43(4) Å³, Z = 2, Rgt(F) = 0.0382, wRref(F²) = 0.1110, T = 295 K.

Crystal: Colourless block
Size: 0.10 × 0.02 × 0.02 mm
Wavelength: Cu Kα radiation (1.54184 Å)
µ: 5.68 mm⁻¹
Diffractometer, scan mode: XtaLAB Synergy, ω
θmax, completeness: 77.5°, >99 %
N(hkl)measured, N(hkl)unique, Rint: 18,450, 6022, 0.046
Criterion for Iobs, N(hkl)gt: Iobs > 2σ(Iobs), 5507
N(param)refined: 434
Programs: CrysAlisPro [1], SHELX [2, 3], Olex2 [4]

Table 1: Data collection and handling.

<table>
<thead>
<tr>
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</tr>
</thead>
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</table>

2-(pyridin-2-yl)-N-((1-(4-vinylbenzyl)-1H-benzo[d]imidazol-2-yl)methyl) methanamine was prepared according to previous reports [5, 6]. A solution of above (0.01 mmol) in acetonitrile (5 mL) was added to a stirred solution of Er(NO₃)₃·6H₂O (0.01 mmol) in acetonitrile (5 mL) at room temperature for 1 h. After filtration, slow diffusion of diethyl ether into the filtrate over 72 h afforded block crystals.

2 Experimental details
All hydrogen atoms were refined isotropic on calculated positions using a riding model with their Uiso values constrained to 1.5 times the Ueq of their pivot atoms.

3 Comment
A lot of tripodal ligands-sensitized lanthanide complexes, which combine the outstanding optical properties of the lanthanide cations and the characteristics of strong light absorption yield and multidentate chelate ligands, have been studied in light-conversion molecular devices and organic light-emitting devices [7–9]. The application of these excellent molecular-based materials has been relatively limited, however, because of the poor machining performance of luminescent lanthanide complexes. Constructed a styrene unit on the skeleton of tripodal ligands, a lanthanide complexes was designed and synthesized and could...
be copolymerized with other monomers to prepare a metallopolymers.

Er(III) is surrounded in a 10-coordinating environment. One apical N, two pyridine N, one benzimidazole N, and six nitrate O atoms participate in coordination with the Er$^{3+}$ center. The two pyridine and one benzimidazole rings are linked by the apical N show a fan-like configuration. The Er–O bond lengths range are 2.386(4)–2.516(4) Å, while the Er–N bond lengths are 2.539(4)–2.905(4) Å. The N–Er–O bond angles range are 66.09(4)°–174.19(13)°, the N–Er–N bond angles range are 62.66(13)°–110.42(14)° and O–Er–O bond angles range are 50.60(13)°–124.23(15)°. These values were close to those reported for related compounds [10, 11]. All C–C and C–N bond lengths and angles are in the expected range.

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**References**


