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Tris(nitrato-κ^2O,O')bis(1,10-phenanthroline-κ^2N,N')ytterbium(III)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.014 Å
R factor = 0.033
wR factor = 0.079
Data-to-parameter ratio = 11.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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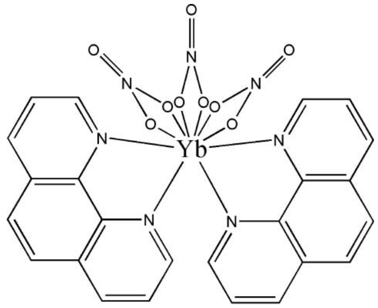
In the title compound, $[Yb(NO_3)_3(C_{12}H_8N_2)_2]$, two bidentate 1,10-phenanthroline ligands and three bidentate nitrate anions are coordinated to the Yb cation. A crystallographic twofold rotation axis passes through the Yb atom and one nitrate group. The molecules are linked into a three-dimensional network by five C—H···O hydrogen bonds.

Comment

1,10-Phenanthroline (phen) is a bidentate chelating reagent which can not only act as a terminal ligand but also, potentially, give rise to supramolecular interactions such as aromatic stacking to form interesting structures (Marinescu *et al.*, 2005; Chen & Liu, 2002). 1-Hydroxypyridine-2(1*H*)-thionato-*S*,*O* (pyrithione) and its metal derivatives have found numerous biochemical applications (Lobana *et al.*, 1999) and are widely used as fungicidal materials. As part of our investigation of the reactions between pyrithione and phen with metals, we attempted to design and synthesize a mixed-ligand rare earth metal complex. However, the crystalline product we isolated was the title compound, (I) (Fig. 1), a complex of ytterbium(III) containing no pyrithione ligand.



(I)

In complex (I), the Yb^{III} centre is ten-coordinated by four N atoms of two chelating phen ligands and six O donors of three nitrate anions. A crystallographic twofold rotation axis passes through Yb, N2 and O5.

In the crystal structure of (I), the molecules are linked into sheets parallel to the (010) plane by C—H···O hydrogen bonds, generating $R_2^2(12)$ and $R_1^2(4)$ rings (Bernstein *et al.*, 1995) (Fig. 2). Neighbouring sheets are connected by two C—H···O hydrogen bonds (Fig. 3), resulting in a three-dimensional network structure.

Experimental

A solution of equimolar quantities (2 mmol) of sodium pyrithione and 1,10-phenanthroline in ethanol (20 ml) was stirred for 20 min,

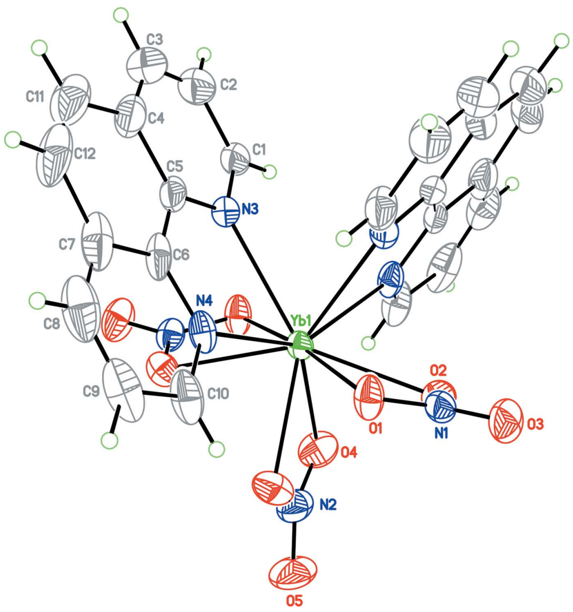


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator $-x+1, y, -z+\frac{3}{2}$

and then a solution of ytterbium(III) nitrate (1 mmol) in ethanol (10 ml) was added. The reaction mixture was stirred continuously for 2 h at room temperature and then filtered. X-ray quality crystals of (I) were obtained by evaporation of an aqueous solution over a period of about one month.

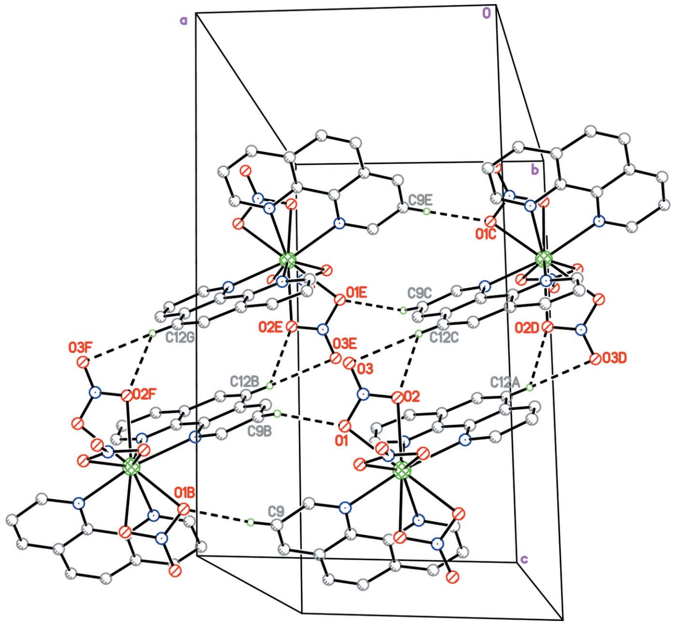


Figure 2
A portion of the crystal struture of (I), showing the formation of a hydrogen-bonded sheet built up from C—H⋯O hydrogen bonds (dashed lines). For clarity, H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (A) $1-x, y, \frac{3}{2}-z$; (B) $2-x, y, \frac{3}{2}-z$; (C) $-\frac{1}{2}+x, \frac{3}{2}-y, -\frac{1}{2}+z$; (D) $\frac{1}{2}-x, \frac{3}{2}-y, 1-z$; (E) $\frac{3}{2}-x, \frac{3}{2}-y, 1-z$; (F) $1-x, y, z$; (G) $\frac{1}{2}+x, \frac{3}{2}-y, -\frac{1}{2}+z$.]

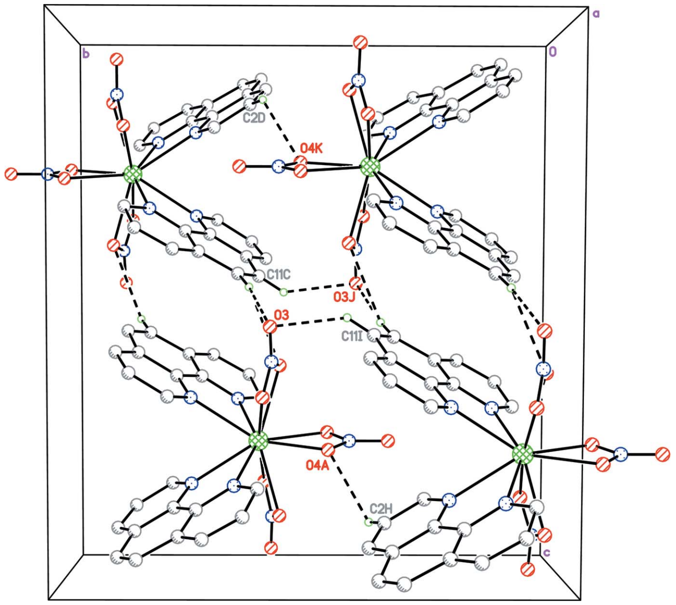


Figure 3
A different view of the crystal structure of (I), showing the formation of a three-dimensional network structure built up from C—H⋯O hydrogen bonds (dashed lines). For clarity, H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (A) $1-x, y, \frac{3}{2}-z$; (C) $-\frac{1}{2}+x, \frac{3}{2}-y, -\frac{1}{2}+z$; (D) $\frac{1}{2}-x, \frac{3}{2}-y, 1-z$; (H) $\frac{1}{2}+x, -\frac{1}{2}+y, z$; (I) $\frac{3}{2}-x, -\frac{1}{2}+y, \frac{3}{2}-z$; (J) $1-x, 1-y, 1-z$; (K) $x, 1-y, -\frac{1}{2}+z$.]

Crystal data

$[\mathrm{Yb(NO_3)_3(C_{12}H_8N_2)_2}]$
$M_r = 719.48$
Monoclinic, $C2/c$
$a = 9.456$ (2) Å
$b = 15.451$ (3) Å
$c = 17.104$ (3) Å
$\beta = 93.687$ (2)°
$V = 2493.8$ (8) Å^3
$Z = 4$
$D_x = 1.916$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.82$ mm^{-1}
$T = 298$ (2) K
Block, yellow
0.46 × 0.16 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.273$, $T_{\max} = 0.701$
6189 measured reflections
2162 independent reflections
1885 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}} = 0.040$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.079$
$S = 1.04$
2162 reflections
187 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.0077P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.00$ e Å^{-3}
$\Delta\rho_{\min} = -0.68$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Yb1—O4	2.400 (5)	Yb1—O1	2.481 (5)
Yb1—O2	2.451 (4)	Yb1—N3	2.533 (5)
Yb1—N4	2.452 (5)		

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Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O3^{i}	0.93	2.67	3.595 (12)	173
C12—H12···O2^{i}	0.93	2.70	3.412 (10)	134
C9—H9···O1^{ii}	0.93	2.43	3.234 (9)	145
C11—H11···O3^{iii}	0.93	2.53	3.253 (10)	135
C2—H2···O4^{iv}	0.93	2.71	3.309 (11)	123

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+2, y, -z+\frac{3}{2}$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

All H atoms were located in difference Fourier maps and were subsequently treated as riding atoms, with C—H distances of 0.93 Å and with $U_{\rm iso}(\rm H) = 1.2U_{\rm eq}(\rm C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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