Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2,4-Dioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylato-κ^2O^4,O^5)(4-oxido-2-oxo-1,2-dihydropyrimidine-5-carboxylato-κ^2O^4,O^5)bis(1,10-phenanthroline-κ^2N,N')yttrium(III) dihydrate

Wei Xiong, Huihui Xing, Yan Su and Zilu Chen*

College of Chemistry and Chemical Engineering, Guangxi Normal University, Yucai Road 15, Guilin 541004, People's Republic of China
Correspondence e-mail: chenziluczl@yahoo.co.uk

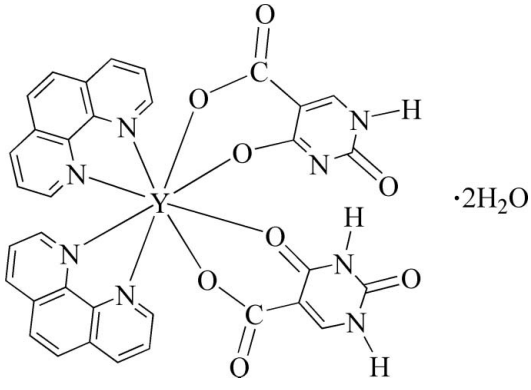
Received 22 July 2008; accepted 9 August 2008

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.097; data-to-parameter ratio = 13.1.

In the title compound, $[Y(C_5H_2N_2O_4)(C_5H_3N_2O_4)(C_{12}H_8N_2)_2]\cdot 2H_2O$, the Y^{III} ion lies on a twofold rotation axis and exhibits a distorted square-antiprismatic coordination geometry. It is chelated by two 1,10-phenanthroline ligands, a 2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate monoanion and a 4-oxido-2-oxo-1,2-dihydropyrimidine-5-carboxylate dianion. The H atom involved in an N—H···N hydrogen bond between the 1,2-dihydropyrimidine units has half occupancy and is disordered around a twofold rotation axis.

Related literature

For the crystal structures of the isostructural Er, Eu, Tb and Yb complexes, see: Sun & Jin (2004); Xing *et al.* (2008). For other related literature, see: Tobiki *et al.* (1980); Castan *et al.* (1990).



Experimental

Crystal data

$[Y(C_5H_2N_2O_4)(C_5H_3N_2O_4)(C_{12}H_8N_2)_2]\cdot 2H_2O$
M_r = 794.53
Monoclinic, $C2/c$
a = 17.1740 (13) Å
b = 14.4385 (11) Å
c = 13.2365 (10) Å
β = 100.881 (1)°
V = 3223.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 295 (2) K
0.24 × 0.08 × 0.06 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.660, T_{max} = 0.895
12035 measured reflections
3152 independent reflections
2986 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.096
S = 1.21
3152 reflections
240 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Y1—O2	2.247 (2)	Y1—N1	2.547 (3)
Y1—O1	2.302 (2)	Y1—N2	2.573 (3)
O2^i—Y1—O2	89.15 (13)	N1—Y1—N1^i	77.82 (13)
O2—Y1—O1^i	81.79 (9)	O2—Y1—N2^i	148.38 (8)
O2—Y1—O1	74.69 (8)	O1—Y1—N2^i	74.55 (8)
O1^i—Y1—O1	146.81 (11)	N1—Y1—N2^i	73.15 (9)
O2^i—Y1—N1	147.62 (8)	O2—Y1—N2	79.43 (9)
O2—Y1—N1	105.31 (9)	O1—Y1—N2	122.30 (9)
O1^i—Y1—N1	135.17 (8)	N1—Y1—N2	63.90 (9)
O1—Y1—N1	74.65 (9)	N2^i—Y1—N2	124.07 (12)

Symmetry code: (i) $-x+2, y, -z+\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{ii}	0.86	2.04	2.898 (3)	178
N1—H1···O1^{ii}	0.86	2.60	3.160 (4)	124
N2—H2···N2^{iii}	0.86	1.81	2.669 (5)	174
O5—H5A···O4^{iv}	0.85	2.14	2.970 (4)	164
O5—H5B···O2^{v}	0.85	2.14	2.985 (4)	173

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank the Science Foundation of Guangxi Province, China (Guikeqing 0542021) and the Scientific Research Foundation for Returned Overseas Chinese Scholars, State Education Ministry, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2161).

References

Bruker (1998). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Castan, P., Colacio-Rodriguez, E., Beauchamp, A. L., Cros, S. & Wimmer, J. (1990). *J. Inorg. Biochem.* **38**, 225–239.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sun, C.-Y. & Jin, L.-P. (2004). *Polyhedron*, **23**, 2227–2233.

Tobiki, H., Yamada, H., Nakatsaka, I., Shimago, K., Eda, Y., Noguchi, H., Komatsu, T. & Nakagome, T. (1980). *Yakugaku Zasshi*, **100**, 38–48.

Xing, H.-H., Chen, Z.-L. & Ng, S. W. (2008). *Acta Cryst.* E**64**, m418.

supplementary materials

Acta Cryst. (2008). E**64**, m1166-m1167 [**doi:10.1107/S1600536808025701**]

(2,4-Dioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylato-κ^2O^4,O^5)(4-oxido-2-oxo-1,2-dihydropyrimidine-5-carboxylato-κ^2O^4,O^5)bis(1,10-phenanthroline-κ^2N,N')yttrium(III) dihydrate

W. Xiong, H. Xing, Y. Su and Z. Chen

Comment

2,4-Dioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylic acid has attracted much attention because of its potential biological activity and pharmaceutical properties, such as anticancer, antibacterial and antihypertensive properties (Tobiki *et al.*, 1980; Castan *et al.*, 1990). Here we report the crystal structure of Y^{III} complex with 2,4-dioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylic acid and 1,10-phenenthroline as ligands. The title complex turned out to be isostructural with the analogues Eu, Tb, Yb (Sun & Jin, 2004) and Er (Xing *et al.*, 2008) complexes; see Sun & Jin (2004) for their detailed description.

Experimental

A mixture of 2,4-dihydroxypyrimidine-5-carboxylic acid (0.0312 g, 0.2 mmol), $YCl_3.6H_2O$ (0.0607 g, 0.2 mmol), phenanthroline dihydrate (0.0396 g, 0.2 mmol), NaOH (0.0160 g, 0.4 mmol) and water (15 ml) was sealed in a 25 ml, Teflon-lined stainless-steel reactor and heated to 383 K for 120 h. It was then cooled over 48 h to give colourless crystals in 70% yield. Elemental analysis calculated for $C_{34}H_{25}N_8O_{10}Y$: C 51.40, H 3.17, N 14.10%; found: C 51.77, H 3.29, N 14.49%.

Refinement

H atoms of the water molecule were located in a difference Fourier map and allowed to ride on their parent atom [U_{iso}(H) = 1.5U_{eq}(O)]. Other H atoms were placed at calculated positions (C—H = 0.93 Å and N—H = 0.86 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C, N). The pyrimidine hydrogen atom H4 is shared by two N—H groups and thus has an occupancy factor of 0.5.

Figures

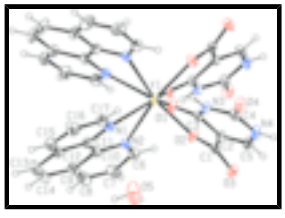


Fig. 1. The molecular structure of the title compound with the atom-numbering scheme and 30% displacement ellipsoids.

(2,4-Dioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylato- κ^2O^4,O^5)(4-oxido-2-oxo-1,2-dihydropyrimidine-5-carboxylato-κ^2O^4,O^5)bis(1,10-phenanthroline- κ^2N,N')yttrium(III) dihydrate

Crystal data

$[Y(C_5H_2N_2O_4)(C_5H_3N_2O_4)(C_{12}H_8N_2)_2]\cdot 2H_2O$	$F_{000} = 1616$
$M_r = 794.53$	$D_x = 1.637$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 7855 reflections
$a = 17.1740$ (13) Å	$\theta = 2.3$–27.9º
$b = 14.4385$ (11) Å	$\mu = 1.89$ mm^{-1}
$c = 13.2365$ (10) Å	$T = 295$ (2) K
$\beta = 100.8810$ (10)º	Prism, colourless
$V = 3223.2$ (4) Å^3	0.24 × 0.08 × 0.06 mm
$Z = 4$	

Data collection

Bruker APEXII diffractometer	3152 independent reflections
Radiation source: fine-focus sealed tube	2986 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.035$
$T = 295$(2) K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -21\rightarrow21$
$T_{min} = 0.660$, $T_{max} = 0.895$	$k = -17\rightarrow17$
12035 measured reflections	$l = -16\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.096$	$w = 1/[\sigma^2(F_o^2) + (0.0141P)^2 + 9.88P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.21$	$(\Delta/\sigma)_{max} < 0.001$
3152 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
240 parameters	$\Delta\rho_{min} = -0.51$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Y1	1.0000	0.88802 (3)	0.2500	0.02339 (12)	
N1	0.90591 (16)	0.75076 (19)	0.2117 (2)	0.0324 (6)	
N2	0.96510 (16)	0.80446 (19)	0.4073 (2)	0.0304 (6)	
N3	0.83326 (16)	1.02589 (19)	−0.0065 (2)	0.0297 (6)	
H3	0.8379	0.9842	−0.0514	0.036*	
N4	0.78240 (19)	1.1684 (2)	0.0310 (2)	0.0387 (7)	
H4	0.7585	1.2199	0.0131	0.046*	0.50
O1	0.90470 (14)	0.93356 (15)	0.11247 (17)	0.0329 (6)	
O2	0.93006 (14)	0.99886 (16)	0.31195 (17)	0.0337 (6)	
O3	0.84729 (15)	1.10907 (17)	0.34049 (17)	0.0371 (6)	
O4	0.76917 (16)	1.11986 (18)	−0.13684 (19)	0.0451 (7)	
C1	0.8770 (2)	1.0594 (2)	0.2805 (2)	0.0272 (7)	
C2	0.84980 (19)	1.0723 (2)	0.1678 (2)	0.0269 (7)	
C3	0.86584 (18)	1.0066 (2)	0.0941 (2)	0.0248 (7)	
C4	0.7937 (2)	1.1063 (2)	−0.0423 (3)	0.0324 (7)	
C5	0.8085 (2)	1.1498 (2)	0.1311 (3)	0.0358 (8)	
H5	0.7976	1.1928	0.1788	0.043*	
C6	0.9900 (2)	0.8317 (3)	0.5036 (3)	0.0386 (8)	
H6	1.0089	0.8920	0.5148	0.046*	
C7	0.9896 (3)	0.7758 (3)	0.5890 (3)	0.0512 (11)	
H7	1.0074	0.7982	0.6552	0.061*	
C8	0.9624 (3)	0.6872 (3)	0.5735 (3)	0.0599 (12)	
H8	0.9626	0.6483	0.6296	0.072*	
C9	0.9342 (2)	0.6545 (3)	0.4735 (3)	0.0463 (10)	
C10	0.9355 (2)	0.7169 (2)	0.3922 (3)	0.0327 (8)	
C11	0.9042 (2)	0.6886 (2)	0.2883 (3)	0.0325 (8)	
C12	0.8716 (2)	0.5993 (2)	0.2699 (3)	0.0419 (9)	
C13	0.8735 (3)	0.5372 (3)	0.3546 (4)	0.0607 (13)	
H13	0.8534	0.4776	0.3423	0.073*	
C14	0.9036 (3)	0.5634 (3)	0.4513 (4)	0.0618 (13)	
H14	0.9045	0.5215	0.5048	0.074*	
C15	0.8370 (2)	0.5768 (3)	0.1686 (4)	0.0510 (11)	
H15	0.8148	0.5185	0.1533	0.061*	

C16	0.8357 (2)	0.6401 (3)	0.0926 (3)	0.0490 (10)
H16	0.8119	0.6262	0.0252	0.059*
C17	0.8707 (2)	0.7264 (3)	0.1173 (3)	0.0397 (9)
H17	0.8693	0.7693	0.0647	0.048*
O5	0.6925 (3)	0.1887 (2)	0.6600 (3)	0.0956 (14)
H51	0.6793	0.2454	0.6644	0.143*
H52	0.7082	0.1681	0.7208	0.143*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Y1	0.0287 (2)	0.0187 (2)	0.0207 (2)	0.000	−0.00062 (16)	0.000
N1	0.0322 (16)	0.0288 (15)	0.0352 (16)	−0.0037 (12)	0.0040 (12)	−0.0035 (12)
N2	0.0318 (15)	0.0294 (15)	0.0297 (15)	−0.0002 (12)	0.0051 (12)	0.0008 (12)
N3	0.0389 (16)	0.0276 (15)	0.0204 (13)	0.0051 (12)	0.0001 (12)	−0.0021 (11)
N4	0.057 (2)	0.0273 (15)	0.0278 (15)	0.0107 (14)	−0.0016 (14)	0.0018 (12)
O1	0.0421 (14)	0.0265 (12)	0.0255 (12)	0.0100 (10)	−0.0052 (10)	−0.0034 (9)
O2	0.0441 (14)	0.0324 (13)	0.0226 (12)	0.0133 (11)	0.0011 (10)	0.0006 (10)
O3	0.0510 (15)	0.0374 (14)	0.0227 (12)	0.0125 (12)	0.0064 (11)	−0.0021 (10)
O4	0.0562 (17)	0.0369 (15)	0.0358 (14)	0.0044 (13)	−0.0074 (12)	0.0002 (12)
C1	0.0345 (18)	0.0240 (16)	0.0224 (16)	−0.0025 (14)	0.0032 (13)	0.0017 (13)
C2	0.0328 (17)	0.0263 (16)	0.0207 (16)	0.0053 (14)	0.0031 (13)	0.0002 (13)
C3	0.0284 (16)	0.0237 (16)	0.0209 (15)	−0.0008 (13)	0.0014 (13)	0.0007 (12)
C4	0.0373 (19)	0.0291 (18)	0.0280 (17)	−0.0006 (15)	−0.0012 (14)	0.0021 (14)
C5	0.050 (2)	0.0292 (18)	0.0263 (18)	0.0094 (16)	0.0031 (16)	−0.0026 (14)
C6	0.039 (2)	0.042 (2)	0.0339 (19)	−0.0026 (17)	0.0042 (16)	−0.0029 (16)
C7	0.056 (3)	0.070 (3)	0.028 (2)	−0.010 (2)	0.0082 (18)	0.0061 (19)
C8	0.066 (3)	0.069 (3)	0.044 (2)	−0.008 (2)	0.009 (2)	0.024 (2)
C9	0.048 (2)	0.043 (2)	0.048 (2)	−0.0034 (19)	0.0101 (19)	0.0158 (19)
C10	0.0306 (18)	0.0296 (18)	0.0384 (19)	−0.0007 (14)	0.0078 (15)	0.0034 (15)
C11	0.0311 (18)	0.0269 (17)	0.0399 (19)	−0.0005 (14)	0.0072 (15)	−0.0017 (15)
C12	0.042 (2)	0.0279 (19)	0.058 (2)	−0.0074 (16)	0.0137 (19)	−0.0027 (17)
C13	0.074 (3)	0.030 (2)	0.080 (3)	−0.018 (2)	0.017 (3)	0.004 (2)
C14	0.076 (3)	0.042 (3)	0.068 (3)	−0.017 (2)	0.016 (3)	0.021 (2)
C15	0.051 (2)	0.035 (2)	0.069 (3)	−0.0161 (19)	0.016 (2)	−0.018 (2)
C16	0.047 (2)	0.050 (2)	0.049 (2)	−0.0137 (19)	0.0063 (19)	−0.022 (2)
C17	0.039 (2)	0.039 (2)	0.040 (2)	−0.0064 (17)	0.0052 (16)	−0.0062 (16)
O5	0.145 (4)	0.059 (2)	0.067 (2)	0.004 (2)	−0.017 (2)	−0.0089 (19)

Geometric parameters (Å, °)

Y1—O2^{i}	2.247 (2)	C2—C3	1.423 (4)
Y1—O2	2.247 (2)	C5—H5	0.9300
Y1—O1^{i}	2.302 (2)	C6—C7	1.391 (5)
Y1—O1	2.302 (2)	C6—H6	0.9300
Y1—N1	2.547 (3)	C7—C8	1.362 (6)
Y1—N1^{i}	2.547 (3)	C7—H7	0.9300
Y1—N2^{i}	2.573 (3)	C8—C9	1.403 (6)

Y1—N2	2.573 (3)	C8—H8	0.9300
N1—C17	1.329 (4)	C9—C10	1.407 (5)
N1—C11	1.358 (4)	C9—C14	1.426 (6)
N2—C6	1.326 (4)	C10—C11	1.439 (5)
N2—C10	1.363 (4)	C11—C12	1.408 (5)
N3—C3	1.373 (4)	C12—C15	1.399 (6)
N3—C4	1.383 (4)	C12—C13	1.431 (6)
N3—H3	0.8600	C13—C14	1.342 (6)
N4—C5	1.343 (4)	C13—H13	0.9300
N4—C4	1.362 (4)	C14—H14	0.9300
N4—H4	0.8600	C15—C16	1.355 (6)
O1—C3	1.247 (4)	C15—H15	0.9300
O2—C1	1.275 (4)	C16—C17	1.395 (5)
O3—C1	1.248 (4)	C16—H16	0.9300
O4—C4	1.258 (4)	C17—H17	0.9300
C1—C2	1.489 (4)	O5—H51	0.8533
C2—C5	1.364 (4)	O5—H52	0.8518
$O2^{i}$—Y1—O2	89.15 (13)	C3—C2—C1	122.6 (3)
$O2^{i}$—Y1—$O1^{i}$	74.69 (8)	O1—C3—N3	117.7 (3)
O2—Y1—$O1^{i}$	81.79 (9)	O1—C3—C2	126.6 (3)
$O2^{i}$—Y1—O1	81.79 (8)	N3—C3—C2	115.7 (3)
O2—Y1—O1	74.69 (8)	O4—C4—N4	122.7 (3)
$O1^{i}$—Y1—O1	146.81 (11)	O4—C4—N3	121.5 (3)
$O2^{i}$—Y1—N1	147.62 (8)	N4—C4—N3	115.8 (3)
O2—Y1—N1	105.31 (9)	N4—C5—C2	124.8 (3)
$O1^{i}$—Y1—N1	135.17 (8)	N4—C5—H5	117.6
O1—Y1—N1	74.65 (9)	C2—C5—H5	117.6
$O2^{i}$—Y1—$N1^{i}$	105.31 (9)	N2—C6—C7	124.0 (4)
O2—Y1—$N1^{i}$	147.62 (8)	N2—C6—H6	118.0
$O1^{i}$—Y1—$N1^{i}$	74.65 (9)	C7—C6—H6	118.0
O1—Y1—$N1^{i}$	135.17 (8)	C8—C7—C6	118.5 (4)
N1—Y1—$N1^{i}$	77.82 (13)	C8—C7—H7	120.7
$O2^{i}$—Y1—$N2^{i}$	79.43 (8)	C6—C7—H7	120.7
O2—Y1—$N2^{i}$	148.38 (8)	C7—C8—C9	120.4 (4)
$O1^{i}$—Y1—$N2^{i}$	122.30 (9)	C7—C8—H8	119.8
O1—Y1—$N2^{i}$	74.55 (8)	C9—C8—H8	119.8
N1—Y1—$N2^{i}$	73.15 (9)	C8—C9—C10	117.0 (4)
$N1^{i}$—Y1—$N2^{i}$	63.90 (9)	C8—C9—C14	123.6 (4)
$O2^{i}$—Y1—N2	148.38 (8)	C10—C9—C14	119.4 (4)
O2—Y1—N2	79.43 (9)	N2—C10—C9	122.8 (3)
$O1^{i}$—Y1—N2	74.55 (8)	N2—C10—C11	117.7 (3)
O1—Y1—N2	122.30 (9)	C9—C10—C11	119.5 (3)
N1—Y1—N2	63.90 (9)	N1—C11—C12	122.7 (3)
$N1^{i}$—Y1—N2	73.15 (9)	N1—C11—C10	118.0 (3)

N2^{i}—Y1—N2	124.07 (12)	C12—C11—C10	119.3 (3)
C17—N1—C11	117.1 (3)	C15—C12—C11	117.5 (4)
C17—N1—Y1	123.5 (2)	C15—C12—C13	123.2 (4)
C11—N1—Y1	117.9 (2)	C11—C12—C13	119.3 (4)
C6—N2—C10	117.4 (3)	C14—C13—C12	121.2 (4)
C6—N2—Y1	123.8 (2)	C14—C13—H13	119.4
C10—N2—Y1	117.0 (2)	C12—C13—H13	119.4
C3—N3—C4	125.9 (3)	C13—C14—C9	121.2 (4)
C3—N3—H3	117.0	C13—C14—H14	119.4
C4—N3—H3	117.0	C9—C14—H14	119.4
C5—N4—C4	120.3 (3)	C16—C15—C12	119.9 (4)
C5—N4—H4	119.9	C16—C15—H15	120.0
C4—N4—H4	119.9	C12—C15—H15	120.0
C3—O1—Y1	132.1 (2)	C15—C16—C17	118.8 (4)
C1—O2—Y1	140.2 (2)	C15—C16—H16	120.6
O3—C1—O2	122.6 (3)	C17—C16—H16	120.6
O3—C1—C2	118.5 (3)	N1—C17—C16	123.9 (4)
O2—C1—C2	118.8 (3)	N1—C17—H17	118.1
C5—C2—C3	117.2 (3)	C16—C17—H17	118.1
C5—C2—C1	120.2 (3)	H51—O5—H52	108.2
O2^{i}—Y1—N1—C17	−8.9 (4)	C4—N3—C3—O1	−174.8 (3)
O2—Y1—N1—C17	104.9 (3)	C4—N3—C3—C2	6.6 (5)
O1^{i}—Y1—N1—C17	−161.4 (3)	C5—C2—C3—O1	177.5 (3)
O1—Y1—N1—C17	35.9 (3)	C1—C2—C3—O1	−1.8 (5)
N1^{i}—Y1—N1—C17	−108.3 (3)	C5—C2—C3—N3	−4.0 (5)
N2^{i}—Y1—N1—C17	−42.2 (3)	C1—C2—C3—N3	176.7 (3)
N2—Y1—N1—C17	174.6 (3)	C5—N4—C4—O4	178.8 (4)
O2^{i}—Y1—N1—C11	157.1 (2)	C5—N4—C4—N3	−0.5 (5)
O2—Y1—N1—C11	−89.1 (2)	C3—N3—C4—O4	176.4 (3)
O1^{i}—Y1—N1—C11	4.6 (3)	C3—N3—C4—N4	−4.3 (5)
O1—Y1—N1—C11	−158.1 (3)	C4—N4—C5—C2	2.7 (6)
N1^{i}—Y1—N1—C11	57.7 (2)	C3—C2—C5—N4	−0.3 (6)
N2^{i}—Y1—N1—C11	123.8 (3)	C1—C2—C5—N4	179.0 (3)
N2—Y1—N1—C11	−19.3 (2)	C10—N2—C6—C7	1.8 (5)
O2^{i}—Y1—N2—C6	7.0 (4)	Y1—N2—C6—C7	−162.4 (3)
O2—Y1—N2—C6	−63.6 (3)	N2—C6—C7—C8	0.4 (6)
O1^{i}—Y1—N2—C6	20.7 (3)	C6—C7—C8—C9	−1.3 (7)
O1—Y1—N2—C6	−127.8 (3)	C7—C8—C9—C10	0.0 (7)
N1—Y1—N2—C6	−176.6 (3)	C7—C8—C9—C14	−178.8 (5)
N1^{i}—Y1—N2—C6	99.0 (3)	C6—N2—C10—C9	−3.2 (5)
N2^{i}—Y1—N2—C6	139.5 (3)	Y1—N2—C10—C9	162.2 (3)
O2^{i}—Y1—N2—C10	−157.3 (2)	C6—N2—C10—C11	176.5 (3)
O2—Y1—N2—C10	132.1 (2)	Y1—N2—C10—C11	−18.1 (4)
O1^{i}—Y1—N2—C10	−143.6 (2)	C8—C9—C10—N2	2.3 (6)
O1—Y1—N2—C10	67.9 (2)	C14—C9—C10—N2	−178.8 (4)
N1—Y1—N2—C10	19.1 (2)	C8—C9—C10—C11	−177.4 (4)

N1^{i}—Y1—N2—C10	−65.3 (2)	C14—C9—C10—C11	1.5 (6)
N2^{i}—Y1—N2—C10	−24.8 (2)	C17—N1—C11—C12	4.1 (5)
O2^{i}—Y1—O1—C3	−68.1 (3)	Y1—N1—C11—C12	−162.8 (3)
O2—Y1—O1—C3	23.3 (3)	C17—N1—C11—C10	−174.4 (3)
O1^{i}—Y1—O1—C3	−23.2 (3)	Y1—N1—C11—C10	18.7 (4)
N1—Y1—O1—C3	134.3 (3)	N2—C10—C11—N1	−0.2 (5)
N1^{i}—Y1—O1—C3	−171.6 (3)	C9—C10—C11—N1	179.6 (3)
N2^{i}—Y1—O1—C3	−149.3 (3)	N2—C10—C11—C12	−178.7 (3)
N2—Y1—O1—C3	89.8 (3)	C9—C10—C11—C12	1.1 (5)
O2^{i}—Y1—O2—C1	72.0 (3)	N1—C11—C12—C15	−2.7 (6)
O1^{i}—Y1—O2—C1	146.7 (4)	C10—C11—C12—C15	175.7 (3)
O1—Y1—O2—C1	−9.7 (3)	N1—C11—C12—C13	178.8 (4)
N1—Y1—O2—C1	−78.6 (3)	C10—C11—C12—C13	−2.8 (6)
N1^{i}—Y1—O2—C1	−170.0 (3)	C15—C12—C13—C14	−176.4 (5)
N2^{i}—Y1—O2—C1	4.0 (4)	C11—C12—C13—C14	2.0 (7)
N2—Y1—O2—C1	−137.6 (4)	C12—C13—C14—C9	0.6 (8)
Y1—O2—C1—O3	176.0 (2)	C8—C9—C14—C13	176.5 (5)
Y1—O2—C1—C2	−4.6 (5)	C10—C9—C14—C13	−2.3 (7)
O3—C1—C2—C5	15.4 (5)	C11—C12—C15—C16	−0.1 (6)
O2—C1—C2—C5	−164.0 (3)	C13—C12—C15—C16	178.4 (4)
O3—C1—C2—C3	−165.3 (3)	C12—C15—C16—C17	1.3 (6)
O2—C1—C2—C3	15.2 (5)	C11—N1—C17—C16	−2.8 (5)
Y1—O1—C3—N3	158.7 (2)	Y1—N1—C17—C16	163.3 (3)
Y1—O1—C3—C2	−22.8 (5)	C15—C16—C17—N1	0.2 (6)

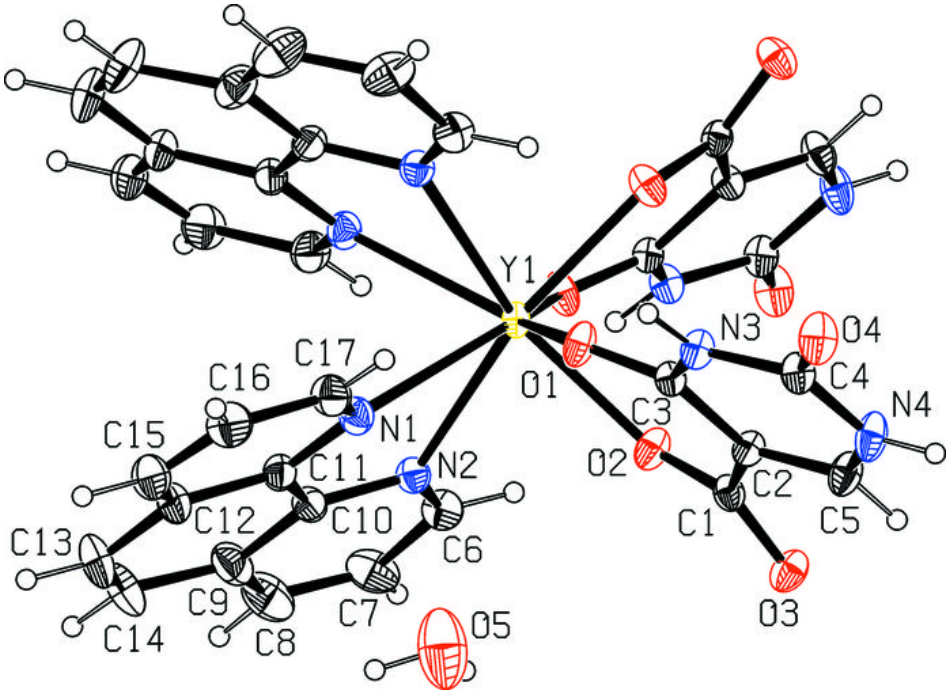
Symmetry codes: (i) −*x*+2, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O3^{ii}	0.86	1.99	2.853 (4)	178
N3—H3···O2^{ii}	0.86	2.63	3.189 (4)	124
N4—H4···N4^{iii}	0.86	1.81	2.667 (6)	174
O5—H51···O3^{iv}	0.85	2.15	2.998 (4)	173
O5—H52···O4^{v}	0.85	2.10	2.935 (4)	169

Symmetry codes: (ii) *x*, −*y*+2, *z*−1/2; (iii) −*x*+3/2, −*y*+5/2, −*z*; (iv) −*x*+3/2, −*y*+3/2, −*z*+1; (v) *x*, *y*−1, *z*+1.

Fig. 1


Y1
O1
N3
O4
C4
N4
C3
O2
C2
C1
C5
O3
C17
C16
N1
C15
C11
N2
C12
C10
C6
C13
C9
C7
C14
C8
O5