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Dichloridobis(methanol-κO)[*cis*-(±)-2,4,5-tris(pyridin-2-yl)-2-imidazoline-κ^3N^2,N^3,N^4]ytterbium(III) chloride

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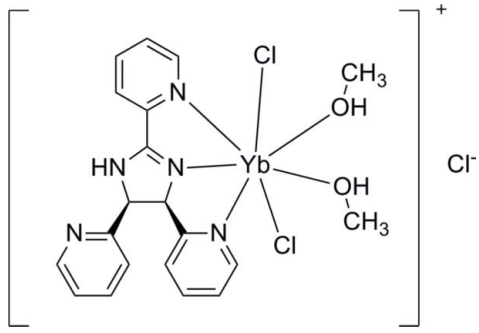
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.011 Å; R factor = 0.035; wR factor = 0.091; data-to-parameter ratio = 14.3.

In the crystal structure of the title complex, $[YbCl_2(C_{18}H_{15}N_5)(CH_3OH)_2]Cl$, the pseudo-pentagonal–bipyramidal coordination geometry of the Yb^{III} cation is composed of three N atoms from one *cis*-(±)-2,4,5-tris(pyridin-2-yl)-imidazoline (H*L*) ligand, two O atoms from two methanol molecules and two Cl^- anions. Chains are formed along [010] through N—H···Cl, O—H···Cl and O—H···N hydrogen bonds.

Related literature

For background to the synthesis of H*L*, see: Later *et al.* (1998); Fernandes *et al.* (2007). For metal complexes with H*L*, see: Parra-Hake *et al.* (2000); Campos-Gaxiola *et al.* (2007, 2008, 2010). For related Yb (III) complexes, see: Li *et al.* (2007); Xu *et al.* (2009); Stojanovic *et al.* (2010); Okawara *et al.* (2012). For potential applications of polypyridyl chelating ligands in magnetic, electronic and luminescent devices, see: Freidzon *et al.* (2011); Maynard *et al.* (2009); Thomas *et al.* (2012).



Experimental

Crystal data

$[YbCl_2(C_{18}H_{15}N_5)(CH_4O)_2]Cl$
M_r = 644.82
Triclinic, $P\overline{1}$
a = 9.2401 (13) Å
b = 9.8390 (14) Å
c = 13.3765 (19) Å
α = 99.978 (2)°
β = 94.616 (2)°
γ = 92.145 (2)°
V = 1192.2 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.29 mm^{-1}
T = 293 K
0.34 × 0.29 × 0.24 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.32, T_{max} = 0.43
11582 measured reflections
4178 independent reflections
3995 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 1.08
4178 reflections
292 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.10 e Å^{-3}
$\Delta\rho_{min}$ = −1.35 e Å^{-3}

Table 1
Selected bond lengths (Å).

Yb1—Cl1	2.5220 (19)	Yb1—N4	2.556 (6)
Yb1—Cl2	2.5834 (18)	Yb1—O1	2.289 (5)
Yb1—N1	2.268 (5)	Yb1—O2	2.287 (5)
Yb1—N3	2.579 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H10′···N5^{i}	0.84	1.86	2.681 (3)	164
O2—H20′···Cl3^{i}	0.84	2.19	2.956 (3)	152
N2—H2′···Cl3	0.86	2.25	3.096 (3)	167

Symmetry code: (i) $x, y-1, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus-NT* (Bruker 2001); data reduction: *SAINT-Plus-NT*; program(s) used to solve structure: *SHELXTL-NT* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2554).

References

Bruker (2000). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SAINT-Plus-NT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Campos-Gaxiola, J. J., Höpfl, H. & Parra-Hake, M. (2007). *J. Mex. Chem. Soc.* **51**, 27–32.
Campos-Gaxiola, J. J., Höpfl, H. & Parra-Hake, M. (2008). *Inorg. Chim. Acta*, **361**, 248–254.
Campos-Gaxiola, J. J., Höpfl, H. & Parra-Hake, M. (2010). *Inorg. Chim. Acta*, **363**, 1179–1185.
Fernandes, C., Horn, A. Jr, Howie, A. R., Schripsema, J., Skakle, J. M. & Wardell, J. L. (2007). *J. Mol. Struct.* **837**, 274–283.
Freidzon, A. Y., Scherbinin, A. V., Bagaturyants, A. A. & Alfimov, M. V. (2011). *J. Phys. Chem. A*, **115**, 4565–4573.
Later, M. L., Phillips, M., Ortega, F., Aguirre, G., Somanathan, R. & Walsh, P. J. (1998). *Tetrahedron Lett.* **39**, 4785–4788.
Li, X. L., Dai, F. R., Zhang, L. Y., Zhu, Y. M., Peng, Q. & Chen, Z. N. (2007). *Organometallics*, **26**, 4483–4490.
Maynard, B. A., Smith, P. A., Ladner, L., Jaleel, A., Beedoe, N., Crawford, C., Assefa, Z. & Sykora, R. E. (2009). *Inorg. Chem.* **48**, 6425–6453.
Okawara, T., Feng, J., Abe, M. & Hisaeda, Y. (2012). *Acta Cryst.* E**68**, m29–m30.
Parra-Hake, M., Larter, M. L., Gantzel, P., Aguirre, G., Ortega, F., Somanathan, R. & Walsh, P. J. (2000). *Inorg. Chem.* **39**, 5400–5403.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stojanovic, M., Robinson, N. J., Chen, X., Smith, P. A. & Sykora, R. E. (2010). *J. Solid State Chem.* **183**, 933–939.
Thomas, R. B., Smith, P. A., Jaleel, A., Vogel, P., Crawford, C., Assefa, Z. & Sykora, R. E. (2012). *Inorg. Chem.* **51**, 3399–3408.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Xu, H. B., Zhang, L. Y., Chen, X. M., Li, X. L. & Chen, Z. N. (2009). *Cryst. Growth Des.* **9**, 569–576.

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Acta Cryst. (2012). E**68**, m815–m816 [doi:10.1107/S1600536812022052]

Dichloridobis(methanol-κO)[*cis*-(±)-2,4,5-tris(pyridin-2-yl)-2-imidazoline-κ^3N^2,N^3,N^4]ytterbium(III) chloride

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S1. Comment

The synthesis and characterization of lanthanide complexes supported by polypiridyl chelating ligands has attracted continuous interest, due to the potential application of these compounds in magnetic, electronic and luminescent devices (Maynard *et al.*, 2009; Freidzon *et al.*, 2011; Thomas *et al.*, 2012). A handful of transition metal complexes based on the HL ligand have been prepared (Parra-Hake *et al.* Campos-Gaxiola *et al.*, 2007, 2008 and 2010), but to date there are no reports on complexes containing rare earth elements. Herein, we report on the structure of a mononuclear Yb^{III} complex (Scheme 1), which was synthesized by reaction of $YbCl_3{\cdot}6H_2O$ with *cis*-(±)-2,4,5-tri(2-pyridyl)imidazoline at room temperature in methanol.

In the title complex, the central Yb^{III} ion is seven-coordinated by three nitrogen atoms from one tridentate chelate ligand, two oxygen atoms from two methanol molecules and two Cl^- anions [Yb—N, 2.268 (5)–2.579 (5) Å; Yb—O 2.287 (4)–2.289 (4) Å; Yb—Cl 2.5219 (18)–2.5834 (17) Å (Table 1)] and displays a pseudo-pentagonal-bipyramidal geometry (Fig. 1). In the crystal structure the complex molecules are linked through N—H···Cl, O—H···Cl and O—H···N hydrogen bonds to form linear supramolecular chains along [010] (Table 2, Fig 2).

S2. Experimental

A mixture of *cis*-(±)-2,4,5-tri(2-pyridyl)imidazoline (HL) (0.05 g, 0.166 mmol) and $YbCl_3{\cdot}6H_2O$ (0.063 g, 0.166 mmol) dissolved in methanol (3 ml) was stirred for 2 h at room temperature to give a colorless solution. The product was crystallized at room temperature by gas phase diffusion of diethyl ether into the reaction mixture, providing colorless crystals which were dried under vacuo. Yield: 71%. IR (KBr): 3320, 3060, 3155, 2894, 1631, 1592, 1471, 1437, 1338, 1280, 1260, 1162, 1007 and 691 cm^{-1}. TGA Calcd for $2CH_3OH$: 9.94. Found: 8.76% (30–200 °C).

S3. Refinement

C—H atoms were positioned geometrically and constrained using the riding-model approximation [C—H_{aryl} = 0.93 Å, $U_{iso}(H_{aryl}) = 1.2\ U_{eq}(C)$]. The coordinates of the O—H and N—H hydrogen atoms were refined with distances restraints: O—H = 0.840±0.001 Å, N—H = 0.860±0.001 Å and [$U_{iso}(H) = 1.5\ U_{eq}(O,N)$].

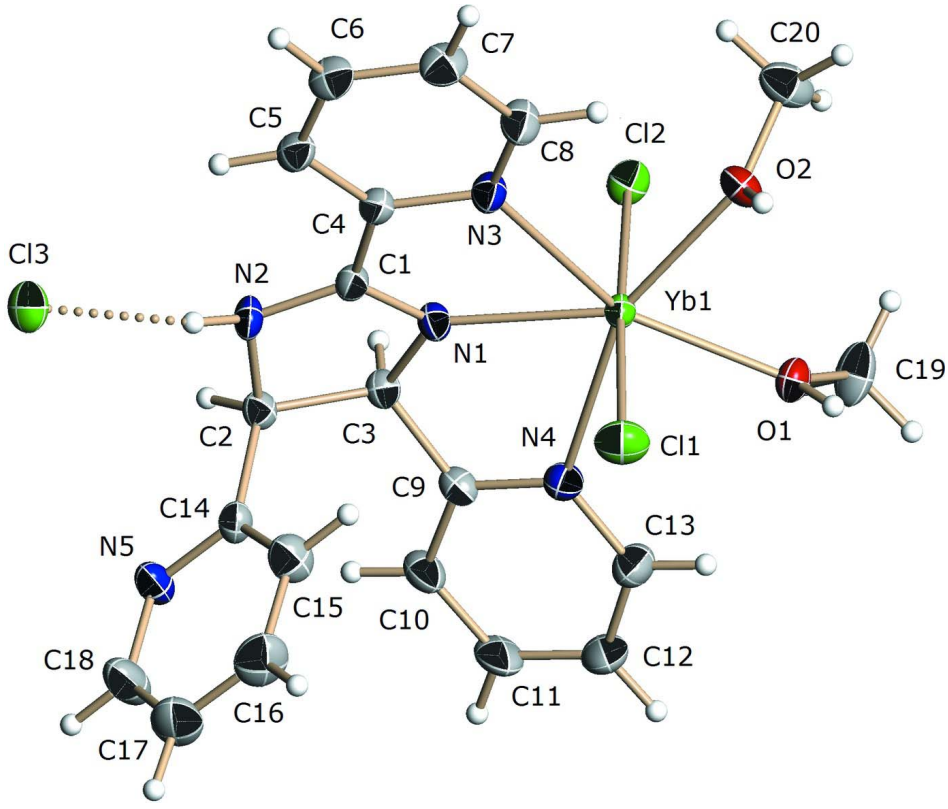

Figure 1

Perspective view of the molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids.

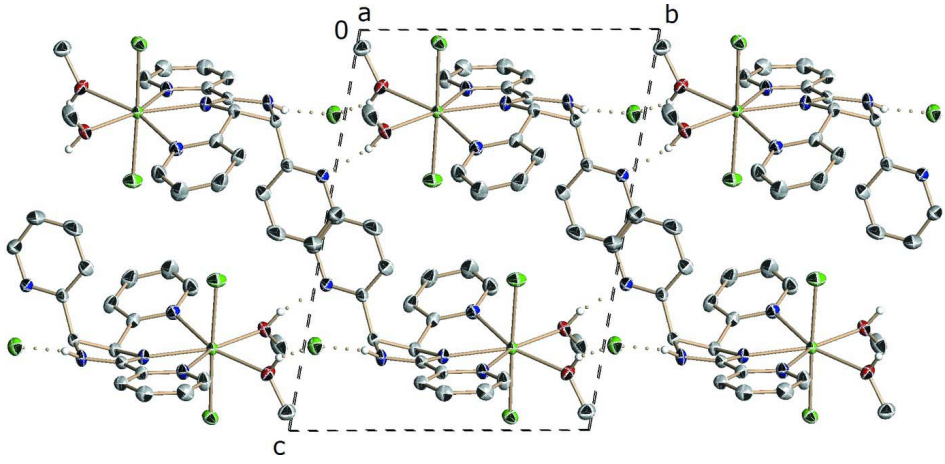

Figure 2

Perspective view of a fragment of the linear supramolecular chain along [010] with the N—H···Cl, O—H···Cl and O—H···N hydrogen bonds shown as dashed lines.

Dichloridobis(methanol-κO)[*cis*-(±)-2,4,5-tris(pyridin-2-yl)-2- imidazoline-κ^3N^2,N^3,N^4]ytterbium(III) chloride

Crystal data

$[YbCl_2(C_{18}H_{15}N_5)(CH_4O)_2]Cl$
$M_r = 644.82$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.2401$ (13) Å
$b = 9.8390$ (14) Å
$c = 13.3765$ (19) Å
$\alpha = 99.978$ (2)°
$\beta = 94.616$ (2)°
$\gamma = 92.145$ (2)°
$V = 1192.2$ (3) Å^3
$Z = 2$
$F(000) = 630$
$D_x = 1.796$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7905 reflections
$\theta = 2.2$–$28.3°$
$\mu = 4.29$ mm^{-1}
$T = 293$ K
Rectangular prism, colorless
0.34 × 0.29 × 0.24 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.32$, $T_{max} = 0.43$
11582 measured reflections
4178 independent reflections
3995 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.091$
$S = 1.08$
4178 reflections
292 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 3.5218P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.10$ e Å^{-3}
$\Delta\rho_{min} = -1.35$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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}
Yb1	0.21176 (3)	0.30381 (2)	0.204195 (19)	0.02770 (10)
Cl1	0.3560 (2)	0.3299 (2)	0.37530 (14)	0.0560 (5)

Cl2	0.05316 (18)	0.26855 (19)	0.03273 (13)	0.0444 (4)
Cl3	0.57461 (18)	0.96378 (19)	0.21144 (15)	0.0486 (4)
N1	0.2212 (5)	0.5280 (5)	0.1839 (4)	0.0333 (12)
N2	0.3278 (6)	0.7350 (5)	0.1816 (5)	0.0383 (13)
H2′	0.400 (5)	0.794 (6)	0.199 (6)	0.057*
N3	0.4539 (6)	0.3892 (5)	0.1471 (4)	0.0381 (13)
N4	0.0248 (6)	0.4541 (6)	0.2944 (4)	0.0406 (13)
N5	0.1688 (7)	0.9593 (6)	0.3636 (4)	0.0458 (14)
O1	0.0623 (5)	0.1401 (5)	0.2518 (4)	0.0382 (10)
H10′	0.099 (8)	0.097 (7)	0.296 (4)	0.057*
O2	0.3170 (5)	0.1033 (5)	0.1423 (4)	0.0411 (11)
H20′	0.380 (6)	0.076 (8)	0.182 (5)	0.062*
C1	0.3387 (7)	0.5981 (6)	0.1703 (5)	0.0343 (14)
C2	0.1917 (7)	0.7706 (6)	0.2265 (5)	0.0339 (14)
H2	0.1415	0.8351	0.1894	0.041*
C3	0.1082 (6)	0.6265 (6)	0.2014 (5)	0.0331 (14)
H3	0.0496	0.6223	0.1364	0.040*
C4	0.4686 (7)	0.5258 (6)	0.1447 (5)	0.0343 (14)
C5	0.5934 (7)	0.5880 (7)	0.1193 (5)	0.0394 (15)
H5	0.6006	0.6827	0.1198	0.047*
C6	0.7078 (7)	0.5061 (8)	0.0931 (5)	0.0443 (17)
H6	0.7925	0.5443	0.0739	0.053*
C7	0.6944 (8)	0.3692 (8)	0.0961 (6)	0.0490 (18)
H7	0.7709	0.3131	0.0795	0.059*
C8	0.5684 (7)	0.3130 (8)	0.1235 (6)	0.0476 (18)
H8	0.5619	0.2190	0.1258	0.057*
C9	0.0099 (7)	0.5825 (7)	0.2750 (5)	0.0362 (14)
C10	−0.0956 (8)	0.6658 (7)	0.3153 (6)	0.0475 (18)
H10	−0.1044	0.7539	0.2998	0.057*
C11	−0.1872 (9)	0.6178 (8)	0.3785 (7)	0.061 (2)
H11	−0.2592	0.6727	0.4058	0.073*
C12	−0.1719 (10)	0.4893 (9)	0.4010 (7)	0.066 (2)
H12	−0.2320	0.4550	0.4444	0.079*
C13	−0.0643 (9)	0.4108 (8)	0.3574 (6)	0.057 (2)
H13	−0.0535	0.3230	0.3730	0.068*
C14	0.2201 (7)	0.8352 (7)	0.3373 (5)	0.0366 (14)
C15	0.2982 (9)	0.7722 (8)	0.4064 (6)	0.0537 (19)
H15	0.3318	0.6847	0.3863	0.064*
C16	0.3266 (10)	0.8398 (10)	0.5062 (6)	0.068 (2)
H16	0.3800	0.7994	0.5541	0.082*
C17	0.2734 (11)	0.9683 (10)	0.5321 (6)	0.072 (3)
H17	0.2910	1.0173	0.5982	0.087*
C18	0.1945 (12)	1.0233 (9)	0.4596 (6)	0.072 (3)
H18	0.1571	1.1096	0.4783	0.087*
C19	−0.0775 (8)	0.0814 (9)	0.2119 (7)	0.064 (2)
H19A	−0.1374	0.1524	0.1938	0.096*
H19B	−0.1211	0.0390	0.2625	0.096*
H19C	−0.0684	0.0128	0.1526	0.096*

C20	0.2876 (9)	0.0171 (8)	0.0451 (6)	0.060 (2)
H20A	0.1852	−0.0063	0.0328	0.090*
H20B	0.3396	−0.0658	0.0437	0.090*
H20C	0.3183	0.0654	−0.0067	0.090*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Yb1	0.02727 (15)	0.02462 (15)	0.03167 (16)	0.00041 (10)	0.00363 (10)	0.00598 (10)
Cl1	0.0528 (11)	0.0726 (13)	0.0401 (10)	0.0067 (9)	−0.0046 (8)	0.0065 (9)
Cl2	0.0398 (9)	0.0511 (10)	0.0430 (9)	−0.0013 (7)	−0.0055 (7)	0.0154 (8)
Cl3	0.0381 (9)	0.0455 (10)	0.0607 (11)	−0.0070 (7)	−0.0054 (8)	0.0111 (8)
N1	0.030 (3)	0.027 (3)	0.044 (3)	0.002 (2)	0.006 (2)	0.006 (2)
N2	0.038 (3)	0.026 (3)	0.053 (3)	−0.003 (2)	0.007 (3)	0.013 (3)
N3	0.036 (3)	0.034 (3)	0.046 (3)	−0.001 (2)	0.007 (2)	0.010 (2)
N4	0.042 (3)	0.039 (3)	0.042 (3)	0.006 (3)	0.010 (3)	0.007 (3)
N5	0.065 (4)	0.033 (3)	0.037 (3)	0.006 (3)	−0.006 (3)	0.003 (2)
O1	0.035 (2)	0.036 (3)	0.045 (3)	0.0003 (19)	0.000 (2)	0.016 (2)
O2	0.041 (3)	0.035 (3)	0.043 (3)	0.005 (2)	−0.002 (2)	−0.004 (2)
C1	0.040 (4)	0.032 (3)	0.033 (3)	−0.002 (3)	0.004 (3)	0.009 (3)
C2	0.039 (3)	0.029 (3)	0.035 (3)	0.006 (3)	0.000 (3)	0.009 (3)
C3	0.030 (3)	0.031 (3)	0.038 (3)	0.001 (3)	0.000 (3)	0.006 (3)
C4	0.035 (3)	0.033 (3)	0.035 (3)	−0.001 (3)	0.004 (3)	0.006 (3)
C5	0.036 (4)	0.042 (4)	0.039 (4)	−0.007 (3)	0.003 (3)	0.007 (3)
C6	0.027 (3)	0.057 (5)	0.048 (4)	−0.007 (3)	0.002 (3)	0.009 (3)
C7	0.037 (4)	0.058 (5)	0.055 (5)	0.011 (3)	0.010 (3)	0.014 (4)
C8	0.041 (4)	0.039 (4)	0.067 (5)	0.010 (3)	0.016 (3)	0.014 (4)
C9	0.030 (3)	0.035 (4)	0.041 (4)	0.002 (3)	0.001 (3)	−0.001 (3)
C10	0.043 (4)	0.038 (4)	0.059 (5)	0.005 (3)	0.012 (3)	−0.003 (3)
C11	0.058 (5)	0.051 (5)	0.071 (6)	0.009 (4)	0.033 (4)	−0.007 (4)
C12	0.073 (6)	0.058 (5)	0.071 (6)	−0.001 (4)	0.045 (5)	0.007 (4)
C13	0.065 (5)	0.049 (5)	0.062 (5)	0.008 (4)	0.025 (4)	0.018 (4)
C14	0.040 (4)	0.032 (3)	0.038 (4)	−0.004 (3)	−0.003 (3)	0.010 (3)
C15	0.064 (5)	0.047 (4)	0.050 (4)	0.012 (4)	−0.007 (4)	0.013 (4)
C16	0.079 (6)	0.079 (6)	0.048 (5)	0.003 (5)	−0.013 (4)	0.024 (4)
C17	0.107 (8)	0.065 (6)	0.040 (5)	−0.004 (5)	−0.008 (5)	0.004 (4)
C18	0.128 (9)	0.043 (5)	0.043 (5)	0.013 (5)	−0.002 (5)	0.000 (4)
C19	0.044 (4)	0.063 (5)	0.088 (6)	−0.017 (4)	−0.010 (4)	0.036 (5)
C20	0.071 (5)	0.057 (5)	0.049 (5)	0.024 (4)	−0.003 (4)	0.001 (4)

Geometric parameters (Å, º)

Yb1—Cl1	2.5220 (19)	C5—C6	1.384 (10)
Yb1—Cl2	2.5834 (18)	C5—H5	0.93
Yb1—N1	2.268 (5)	C6—C7	1.355 (11)
Yb1—N3	2.579 (5)	C6—H6	0.93
Yb1—N4	2.556 (6)	C7—C8	1.373 (10)
Yb1—O1	2.289 (5)	C7—H7	0.9301

Yb1—O2	2.287 (5)	C8—H8	0.9303
N1—C1	1.306 (8)	C9—C10	1.380 (10)
N1—C3	1.457 (8)	C10—C11	1.370 (12)
N2—C1	1.338 (8)	C10—H10	0.9302
N2—C2	1.465 (9)	C11—C12	1.359 (12)
N2—H2′	0.86 (6)	C11—H11	0.9302
N3—C4	1.352 (9)	C12—C13	1.386 (12)
N3—C8	1.346 (9)	C12—H12	0.9294
N4—C13	1.333 (10)	C13—H13	0.9303
N4—C9	1.343 (9)	C14—C15	1.373 (10)
N5—C14	1.326 (9)	C15—C16	1.384 (11)
N5—C18	1.327 (10)	C15—H15	0.9294
O1—C19	1.419 (9)	C16—C17	1.372 (14)
O1—H10′	0.84 (6)	C16—H16	0.9303
O2—C20	1.424 (10)	C17—C18	1.365 (13)
O2—H20′	0.84 (6)	C17—H17	0.9295
C1—C4	1.453 (9)	C18—H18	0.9304
C2—C14	1.506 (9)	C19—H19A	0.9601
C2—C3	1.559 (9)	C19—H19B	0.9598
C2—H2	0.9797	C19—H19C	0.9595
C3—C9	1.496 (9)	C20—H20A	0.96
C3—H3	0.9797	C20—H20B	0.9599
C4—C5	1.379 (9)	C20—H20C	0.96

N1—Yb1—O2	138.18 (18)	N1—C3—H3	107.27
N1—Yb1—O1	141.84 (17)	C2—C3—H3	107.27
O2—Yb1—O1	77.76 (17)	C9—C3—H3	107.29
N1—Yb1—Cl1	99.05 (14)	N3—C4—C5	123.1 (6)
O2—Yb1—Cl1	92.85 (12)	N3—C4—C1	112.6 (5)
O1—Yb1—Cl1	89.06 (12)	C5—C4—C1	124.3 (6)
N1—Yb1—N4	64.63 (18)	C4—C5—C6	118.3 (6)
O2—Yb1—N4	156.52 (18)	C4—C5—H5	120.84
O1—Yb1—N4	78.77 (17)	C6—C5—H5	120.83
Cl1—Yb1—N4	87.06 (14)	C7—C6—C5	118.9 (6)
N1—Yb1—N3	65.20 (17)	C5—C6—H6	120.5
O2—Yb1—N3	76.74 (17)	C7—C6—H6	120.57
O1—Yb1—N3	152.94 (17)	C6—C7—C8	120.3 (7)
Cl1—Yb1—N3	83.32 (13)	C6—C7—H7	119.81
N4—Yb1—N3	126.44 (17)	C8—C7—H7	119.9
N1—Yb1—Cl2	83.18 (14)	N3—C8—C7	122.3 (7)
O2—Yb1—Cl2	86.99 (12)	N3—C8—H8	118.86
O1—Yb1—Cl2	87.74 (12)	C7—C8—H8	118.87
Cl1—Yb1—Cl2	176.75 (6)	N4—C9—C10	122.1 (6)
N4—Yb1—Cl2	91.79 (13)	N4—C9—C3	115.9 (5)
N3—Yb1—Cl2	99.79 (13)	C10—C9—C3	121.9 (6)
N1—Yb1—C1	19.51 (17)	C11—C10—C9	119.5 (7)
O2—Yb1—C1	121.66 (17)	C9—C10—H10	120.28
O1—Yb1—C1	160.52 (16)	C11—C10—H10	120.24

Cl1—Yb1—C1	91.30 (12)	C12—C11—C10	119.4 (7)
N4—Yb1—C1	81.80 (17)	C10—C11—H11	120.3
N3—Yb1—C1	46.10 (16)	C12—C11—H11	120.28
Cl2—Yb1—C1	91.55 (12)	C11—C12—C13	118.2 (7)
C1—N1—C3	106.9 (5)	C11—C12—H12	120.93
C1—N1—Yb1	125.0 (4)	C13—C12—H12	120.96
C3—N1—Yb1	127.2 (4)	N4—C13—C12	123.6 (7)
C1—N2—H2′	124 (4)	N4—C13—H13	118.21
C2—N2—H2′	116 (4)	C12—C13—H13	118.1
C1—N2—C2	108.6 (5)	N5—C14—C15	121.8 (6)
C8—N3—C4	117.0 (6)	N5—C14—C2	115.8 (5)
C8—N3—Yb1	126.7 (4)	C15—C14—C2	122.4 (6)
C4—N3—Yb1	116.2 (4)	C14—C15—C16	119.7 (7)
C13—N4—C9	117.2 (6)	C14—C15—H15	120.18
C13—N4—Yb1	123.8 (5)	C16—C15—H15	120.2
C9—N4—Yb1	119.0 (4)	C17—C16—C15	117.8 (8)
C14—N5—C18	118.5 (6)	C15—C16—H16	121.05
C19—O1—Yb1	132.4 (4)	C17—C16—H16	121.09
Yb1—O1—H10′	116 (5)	C18—C17—C16	119.2 (8)
C19—O1—H10′	111 (5)	C16—C17—H17	120.4
C20—O2—Yb1	128.2 (4)	C18—C17—H17	120.42
Yb1—O2—H20′	116 (5)	N5—C18—C17	122.9 (8)
C20—O2—H20′	116 (5)	O1—C19—H19C	109.45
N1—C1—N2	115.4 (6)	H19A—C19—H19C	109.51
N1—C1—C4	119.7 (6)	H19B—C19—H19C	109.53
N2—C1—C4	124.9 (6)	O1—C19—H19B	109.44
N2—C2—C14	111.0 (5)	H19A—C19—H19B	109.48
N2—C2—C3	99.8 (5)	O1—C19—H19A	109.42
C14—C2—C3	117.1 (5)	O2—C20—H20C	109.44
N2—C2—H2	109.54	H20A—C20—H20C	109.47
C3—C2—H2	109.5	H20B—C20—H20C	109.47
C14—C2—H2	109.48	O2—C20—H20B	109.48
N1—C3—C9	109.5 (5)	H20A—C20—H20B	109.48
N1—C3—C2	104.6 (5)	O2—C20—H20A	109.48
C9—C3—C2	120.3 (5)		

O2—Yb1—N1—C1	−37.1 (6)	N4—Yb1—C1—N1	−27.2 (5)
O1—Yb1—N1—C1	167.7 (4)	N3—Yb1—C1—N1	166.5 (6)
Cl1—Yb1—N1—C1	67.6 (5)	C1—N2—C2—C14	104.9 (6)
N4—Yb1—N1—C1	150.0 (6)	C1—N2—C2—C3	−19.3 (6)
N3—Yb1—N1—C1	−10.7 (5)	C1—N1—C3—C9	−146.0 (5)
Cl2—Yb1—N1—C1	−114.8 (5)	Yb1—N1—C3—C9	23.8 (7)
O2—Yb1—N1—C3	154.9 (4)	C1—N1—C3—C2	−15.8 (6)
O1—Yb1—N1—C3	−0.3 (6)	Yb1—N1—C3—C2	154.0 (4)
Cl1—Yb1—N1—C3	−100.4 (5)	N2—C2—C3—N1	20.8 (6)
N4—Yb1—N1—C3	−18.1 (5)	C14—C2—C3—N1	−99.1 (6)
N3—Yb1—N1—C3	−178.7 (5)	N2—C2—C3—C9	144.2 (6)
Cl2—Yb1—N1—C3	77.2 (5)	C14—C2—C3—C9	24.4 (8)

N1—Yb1—N3—C8	−176.1 (6)	C8—N3—C4—C5	0.1 (10)
O2—Yb1—N3—C8	−13.8 (6)	Yb1—N3—C4—C5	177.6 (5)
O1—Yb1—N3—C8	6.1 (8)	C8—N3—C4—C1	179.4 (6)
Cl1—Yb1—N3—C8	80.7 (6)	Yb1—N3—C4—C1	−3.0 (7)
N4—Yb1—N3—C8	162.1 (5)	N1—C1—C4—N3	−5.8 (9)
Cl2—Yb1—N3—C8	−98.3 (6)	N2—C1—C4—N3	174.4 (6)
N1—Yb1—N3—C4	6.7 (4)	N1—C1—C4—C5	173.5 (6)
O2—Yb1—N3—C4	168.9 (5)	N2—C1—C4—C5	−6.3 (10)
O1—Yb1—N3—C4	−171.1 (4)	N3—C4—C5—C6	1.4 (10)
Cl1—Yb1—N3—C4	−96.5 (4)	C1—C4—C5—C6	−177.9 (6)
N4—Yb1—N3—C4	−15.2 (5)	C4—C5—C6—C7	−1.8 (10)
Cl2—Yb1—N3—C4	84.4 (4)	C5—C6—C7—C8	0.7 (11)
N1—Yb1—N4—C13	−173.7 (7)	C4—N3—C8—C7	−1.2 (11)
O2—Yb1—N4—C13	18.1 (9)	Yb1—N3—C8—C7	−178.4 (5)
O1—Yb1—N4—C13	17.3 (6)	C6—C7—C8—N3	0.8 (12)
Cl1—Yb1—N4—C13	−72.3 (6)	C13—N4—C9—C10	−2.0 (10)
N3—Yb1—N4—C13	−151.8 (6)	Yb1—N4—C9—C10	175.4 (5)
Cl2—Yb1—N4—C13	104.7 (6)	C13—N4—C9—C3	−178.1 (6)
N1—Yb1—N4—C9	9.0 (4)	Yb1—N4—C9—C3	−0.7 (7)
O2—Yb1—N4—C9	−159.1 (4)	N1—C3—C9—N4	−12.3 (8)
O1—Yb1—N4—C9	−159.9 (5)	C2—C3—C9—N4	−133.4 (6)
Cl1—Yb1—N4—C9	110.5 (5)	N1—C3—C9—C10	171.6 (6)
N3—Yb1—N4—C9	31.0 (6)	C2—C3—C9—C10	50.5 (9)
Cl2—Yb1—N4—C9	−72.5 (5)	N4—C9—C10—C11	1.0 (11)
N1—Yb1—O1—C19	60.5 (8)	C3—C9—C10—C11	176.9 (7)
O2—Yb1—O1—C19	−102.9 (7)	C9—C10—C11—C12	0.5 (13)
Cl1—Yb1—O1—C19	164.0 (7)	C10—C11—C12—C13	−0.9 (14)
N4—Yb1—O1—C19	76.8 (7)	C9—N4—C13—C12	1.7 (12)
N3—Yb1—O1—C19	−122.7 (7)	Yb1—N4—C13—C12	−175.6 (7)
Cl2—Yb1—O1—C19	−15.4 (7)	C11—C12—C13—N4	−0.2 (14)
N1—Yb1—O2—C20	−75.2 (7)	C18—N5—C14—C15	0.0 (11)
O1—Yb1—O2—C20	89.4 (6)	C18—N5—C14—C2	−177.9 (7)
Cl1—Yb1—O2—C20	177.9 (6)	N2—C2—C14—N5	123.6 (6)
N4—Yb1—O2—C20	88.7 (7)	C3—C2—C14—N5	−122.8 (6)
N3—Yb1—O2—C20	−99.7 (6)	N2—C2—C14—C15	−54.3 (8)
Cl2—Yb1—O2—C20	1.1 (6)	C3—C2—C14—C15	59.4 (9)
C3—N1—C1—N2	3.7 (8)	N5—C14—C15—C16	−0.9 (12)
Yb1—N1—C1—N2	−166.4 (4)	C2—C14—C15—C16	176.9 (7)
C3—N1—C1—C4	−176.1 (5)	C14—C15—C16—C17	0.5 (13)
Yb1—N1—C1—C4	13.8 (8)	C15—C16—C17—C18	0.6 (15)
C2—N2—C1—N1	11.2 (8)	C14—N5—C18—C17	1.2 (14)
C2—N2—C1—C4	−169.0 (6)	C16—C17—C18—N5	−1.5 (16)
Cl1—Yb1—C1—N1	−114.0 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H10′···N5^{i}	0.84	1.86	2.681 (3)	164

O2—H20′···Cl3^{i}	0.84	2.19	2.956 (3)	152
N2—H2′···Cl3	0.86	2.25	3.096 (3)	167

Symmetry code: (i) x, $y-1$, z.