

Poly[bis[*diaqua(isonicotinato-κ²O,O')*dysprosium(III)][bis(*isonicotinato-κO*)copper(II)]tetra-(*μ₃-isonicotinato-κ³O:O':N*)

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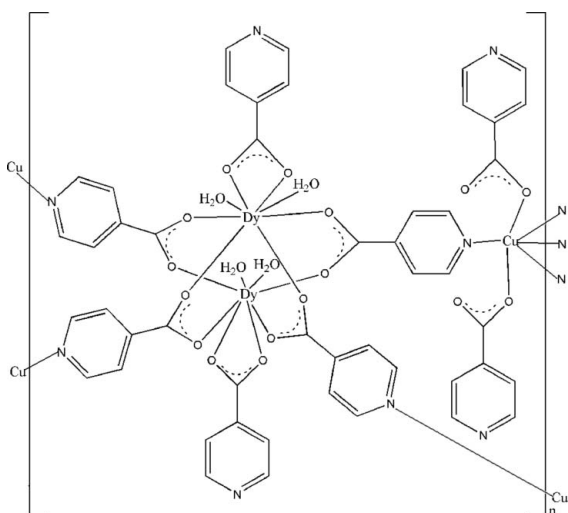
Received 21 August 2007; accepted 7 September 2007

Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.025; wR factor = 0.058; data-to-parameter ratio = 12.4.

The title compound, $\{[\text{Dy}(\text{C}_6\text{H}_4\text{NO}_2)(\text{H}_2\text{O})_2]_2[\text{Cu}(\text{C}_6\text{H}_4\text{NO}_2)_2](\text{C}_6\text{H}_4\text{NO}_2)_4\}_n$, is a three-dimensional coordination polymer. The six-coordinate Cu^{II} atom, lying on an inversion center, is bonded to two O atoms from two monodentate isonicotinate ligands and four N atoms from four bridging isonicotinate ligands. Two Dy^{III} atoms form a centrosymmetric dinuclear unit and each Dy^{III} atom is eight-coordinated by six O atoms from five different isonicotinate ligands and two O atoms from two water molecules. These metal coordination units are connected by the bridging isonicotinate ligands, generating a three-dimensional network. The crystal structure is further stabilized by hydrogen bonds.

Related literature

For related literature, see: Coats *et al.* (1998); Kahn *et al.* (1999); Sanz *et al.* (1996).



Experimental

Crystal data

$[\text{Dy}_2\text{Cu}(\text{C}_6\text{H}_4\text{NO}_2)_8(\text{H}_2\text{O})_4]$	$V = 2565.4 (8) \text{ \AA}^3$
$M_r = 1437.43$	$Z = 2$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 9.456 (1) \text{ \AA}$	$\mu = 3.38 \text{ mm}^{-1}$
$b = 14.966 (3) \text{ \AA}$	$T = 294 (2) \text{ K}$
$c = 18.166 (4) \text{ \AA}$	$0.54 \times 0.42 \times 0.28 \text{ mm}$
$\beta = 93.74 (1)^\circ$	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	5313 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	4638 independent reflections
$T_{\text{min}} = 0.199$, $T_{\text{max}} = 0.391$	3853 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.058$	$\Delta\rho_{\text{max}} = 0.61 \text{ e \AA}^{-3}$
$S = 1.03$	$\Delta\rho_{\text{min}} = -0.89 \text{ e \AA}^{-3}$
4638 reflections	
375 parameters	
4 restraints	

Table 1

Selected bond lengths (Å).

Dy—O7	2.298 (3)	Dy—O6	2.433 (3)
Dy—O2 ⁱ	2.300 (3)	Dy—O5	2.513 (3)
Dy—O8 ⁱ	2.313 (3)	Cu—O3	1.976 (3)
Dy—O1	2.324 (3)	Cu—N1	2.004 (3)
Dy—O10	2.366 (3)	Cu—N4 ⁱⁱ	2.639 (4)
Dy—O9	2.409 (3)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O9—H9A \cdots O4 ⁱⁱⁱ	0.81 (3)	1.98 (3)	2.778 (4)	169 (5)
O9—H9B \cdots N3 ^{iv}	0.82 (3)	2.07 (3)	2.883 (5)	176 (5)
O10—H10A \cdots O5 ^v	0.82 (3)	1.98 (2)	2.784 (4)	166 (5)
O10—H10B \cdots N2 ^{vi}	0.81 (4)	1.99 (2)	2.796 (5)	169 (6)

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

This work was supported by the Construct Program of the Key Discipline in Hunan Province and Hunan Provincial Natural Science Foundation of China (grant No. 06 J J2015).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2080).

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supplementary materials

Acta Cryst. (2007). E63, m2526-m2527 [doi:10.1107/S1600536807043899]

Poly[bis[*diaqua(isonicotinato- κ^2O,O')dysprosium(III)]*][bis(isonicotinato- κO)copper(II)]tetra(μ_3 -isonicotinato- $\kappa^3O:O':N$)

D.-Z. Kuang, Y.-L. Feng, Y.-L. Peng and Y.-F. Deng

Comment

In the past few years, more extensive attention had been paid to the research on the chemistry of heterometallic complexes containing simultaneously lanthanide and transition metal ions (Costs *et al.*, 1998; Kahn *et al.*, 1999; Sanz *et al.*, 1996). As an extension of this research, we report here the structure of the title compound, a new heterometallic coordination polymer,

In the title compound (Fig. 1), the Cu^{II} atom lies on an inversion center and is six-coordinated by two O atoms from two monodentate isonicotinate ligands and four N atoms from the other four isonicotinate ligands. Thus the Cu^{II} atom has a slight distorted octahedral coordination geometry. The Dy^{III} atom is eight-coordinated by six O atoms from five different isonicotinate ligands and two O atoms from two water molecules in a square antiprism geometry (Table 1). The adjacent Cu and Dy coordination units are bridged by the tridentate isonicotinate ligands, forming a three-dimensional network structure (Fig. 2).

Experimental

A mixture of CuO (0.082 g, 1.0 mmol), Dy₂O₃ (0.181 g, 0.5 mmol), isonicotinic acid (0.248 g, 2.0 mmol), H₂O (10 ml, 0.55 mmol) and two drops of acetic acid, with a pH value about 2.0, was sealed in a 25 ml Teflon-lined reaction vessel at 443 K for 5 d. The reaction mixture was cooled to room temperature over a period of 48 h. The product was collected by filtration, washed with water and air-dried. Blue block crystals suitable for X-ray analysis were obtained. Analysis, calculated for C₄₈H₄₀CuDy₂N₈O₂₀: C 40.11, H 2.80, N 7.80%; found: C 40.05; H 2.59, N 7.97%.

Refinement

H atoms bonded to C atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of water molecules were found from difference Fourier maps and refined isotropically with a restraint of O—H = 0.82 (1) Å.

Figures

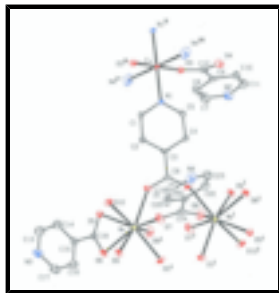


Fig. 1. The asymmetric unit of the title compound, together with symmetry-related atoms to complete the coordination units. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $-x + 1, -y, -z + 1$; (iii) $-x + 1/2, y - 1/2, -z + 3/2$; (iv) $1/2 + x, 1/2 - y, -1/2 + z$.]

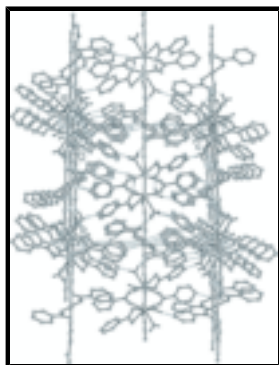


Fig. 2. A view of the three-dimensional structure of the title compound. Dotted lines denote hydrogen bonds.

Poly[bis[*diaqua*(isonicotinato- κ 2O,*O'*)dysprosium(III)] [bis(isonicotinato- κ O)copper(II)]tetra(μ 3-isonicotinato- κ 3O:*O'*:*N*)

Crystal data

[Dy₂Cu(C₆H₄NO₂)₈(H₂O)₄]

$M_r = 1437.43$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2yn$

$a = 9.456(1)\ \text{\AA}$

$b = 14.966(3)\ \text{\AA}$

$c = 18.166(4)\ \text{\AA}$

$\beta = 93.74(1)^\circ$

$V = 2565.4(8)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 1410$

$D_x = 1.861\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 4174 reflections

$\theta = 2.6\text{--}14.6^\circ$

$\mu = 3.38\ \text{mm}^{-1}$

$T = 294(2)\ \text{K}$

Block, blue

$0.54 \times 0.42 \times 0.28\ \text{mm}$

Data collection

Bruker SMART 1000 CCD area-detector diffractometer

Radiation source: normal-focus sealed tube

Monochromator: graphite

$T = 294(2)\ \text{K}$

ϕ and ω scans

4638 independent reflections

3853 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\text{max}} = 25.3^\circ$

$\theta_{\text{min}} = 1.8^\circ$

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
 $T_{\min} = 0.199$, $T_{\max} = 0.391$
5313 measured reflections

$h = 0 \rightarrow 11$
 $k = 0 \rightarrow 17$
 $l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.058$
 $S = 1.03$
4638 reflections
375 parameters
4 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
 $w = 1/[\sigma^2(F_o^2) + (0.0289P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.61 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.89 \text{ e } \text{\AA}^{-3}$
Extinction correction: SHELXL97
Extinction coefficient: 0.00120 (9)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Dy	0.195701 (18)	0.583911 (12)	0.500576 (9)	0.01381 (7)
Cu	0.5000	0.0000	0.5000	0.01940 (16)
O1	0.2280 (3)	0.43001 (18)	0.50421 (17)	0.0337 (8)
O2	0.0274 (3)	0.3543 (2)	0.50973 (19)	0.0402 (8)
O3	0.3581 (3)	-0.05366 (19)	0.42852 (15)	0.0255 (7)
O4	0.1845 (3)	-0.1225 (2)	0.48600 (15)	0.0345 (8)
O5	0.3964 (3)	0.56810 (18)	0.41742 (14)	0.0243 (6)
O6	0.2726 (3)	0.69240 (19)	0.41176 (15)	0.0298 (7)
O7	0.1052 (4)	0.5477 (2)	0.61110 (16)	0.0390 (8)
O8	-0.0907 (3)	0.4660 (2)	0.61044 (16)	0.0398 (8)
O9	0.2216 (3)	0.7219 (2)	0.56835 (17)	0.0281 (7)
O10	0.4068 (3)	0.5705 (2)	0.57715 (16)	0.0272 (7)
N1	0.3863 (3)	0.1131 (2)	0.49738 (16)	0.0168 (7)
N2	0.0145 (4)	-0.1238 (3)	0.2173 (2)	0.0425 (11)
N3	0.5756 (5)	0.7292 (3)	0.1969 (2)	0.0467 (11)
N4	0.0917 (4)	0.4501 (4)	0.8722 (2)	0.0475 (12)
C1	0.4533 (4)	0.1926 (3)	0.4982 (2)	0.0230 (9)
H1	0.5517	0.1933	0.4988	0.028*
C2	0.3828 (4)	0.2722 (3)	0.4983 (2)	0.0215 (9)
H2	0.4329	0.3257	0.4987	0.026*
C3	0.2366 (4)	0.2729 (3)	0.4979 (2)	0.0194 (9)
C4	0.1649 (4)	0.1919 (3)	0.4943 (2)	0.0221 (9)
H4	0.0664	0.1900	0.4919	0.027*
C5	0.2442 (4)	0.1140 (3)	0.4944 (2)	0.0220 (9)

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H5	0.1964	0.0597	0.4924	0.026*
C6	0.1574 (4)	0.3599 (3)	0.5038 (2)	0.0220 (9)
C7	0.1288 (6)	-0.0714 (4)	0.2280 (3)	0.0491 (15)
H7	0.1616	-0.0417	0.1875	0.059*
C8	0.2008 (5)	-0.0592 (3)	0.2961 (2)	0.0385 (12)
H8	0.2775	-0.0202	0.3008	0.046*
C9	0.1591 (4)	-0.1045 (3)	0.3564 (2)	0.0227 (9)
C10	0.0435 (4)	-0.1607 (3)	0.3463 (2)	0.0300 (10)
H10	0.0117	-0.1931	0.3857	0.036*
C11	-0.0242 (5)	-0.1681 (3)	0.2768 (3)	0.0374 (12)
H11	-0.1016	-0.2064	0.2709	0.045*
C12	0.2395 (4)	-0.0932 (3)	0.4307 (2)	0.0230 (9)
C13	0.6322 (6)	0.6681 (4)	0.2435 (3)	0.0545 (16)
H13	0.7200	0.6444	0.2337	0.065*
C14	0.5697 (5)	0.6376 (4)	0.3052 (3)	0.0424 (13)
H14	0.6148	0.5950	0.3357	0.051*
C15	0.4397 (4)	0.6712 (3)	0.3210 (2)	0.0255 (9)
C16	0.3780 (5)	0.7340 (3)	0.2730 (2)	0.0397 (12)
H16	0.2901	0.7584	0.2814	0.048*
C17	0.4488 (6)	0.7599 (4)	0.2122 (3)	0.0497 (14)
H17	0.4051	0.8014	0.1801	0.060*
C18	0.3660 (4)	0.6428 (3)	0.3878 (2)	0.0192 (9)
C19	0.1568 (5)	0.5134 (4)	0.8384 (3)	0.0528 (16)
H19	0.2187	0.5495	0.8671	0.063*
C20	0.1418 (5)	0.5311 (4)	0.7644 (2)	0.0373 (12)
H20	0.1930	0.5767	0.7438	0.045*
C21	0.0486 (4)	0.4793 (3)	0.7215 (2)	0.0214 (9)
C22	-0.0190 (4)	0.4097 (3)	0.7547 (2)	0.0292 (10)
H22	-0.0812	0.3723	0.7275	0.035*
C23	0.0088 (5)	0.3974 (4)	0.8296 (3)	0.0418 (13)
H23	-0.0334	0.3490	0.8516	0.050*
C24	0.0185 (4)	0.4987 (3)	0.6407 (2)	0.0210 (9)
H9A	0.223 (5)	0.7683 (18)	0.545 (2)	0.043 (16)*
H9B	0.178 (4)	0.734 (3)	0.6043 (15)	0.033 (13)*
H10A	0.468 (4)	0.533 (2)	0.572 (3)	0.043 (16)*
H10B	0.433 (6)	0.592 (4)	0.6169 (17)	0.08 (2)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Dy	0.01477 (10)	0.01319 (10)	0.01358 (10)	0.00195 (9)	0.00165 (6)	0.00091 (8)
Cu	0.0195 (3)	0.0130 (3)	0.0247 (4)	0.0058 (3)	-0.0065 (3)	-0.0050 (3)
O1	0.0367 (19)	0.0121 (16)	0.052 (2)	0.0043 (14)	0.0036 (15)	0.0001 (14)
O2	0.0233 (17)	0.0296 (19)	0.068 (2)	0.0145 (15)	0.0071 (16)	0.0005 (17)
O3	0.0259 (16)	0.0243 (16)	0.0250 (15)	0.0031 (13)	-0.0088 (12)	-0.0052 (12)
O4	0.045 (2)	0.0325 (18)	0.0256 (17)	0.0004 (16)	0.0011 (15)	0.0013 (14)
O5	0.0253 (15)	0.0255 (17)	0.0229 (14)	0.0021 (13)	0.0075 (12)	0.0046 (12)
O6	0.0399 (18)	0.0192 (16)	0.0324 (16)	0.0038 (14)	0.0184 (14)	0.0026 (13)

O7	0.054 (2)	0.042 (2)	0.0232 (16)	-0.0082 (18)	0.0164 (15)	0.0048 (15)
O8	0.0355 (18)	0.060 (2)	0.0224 (16)	-0.0039 (18)	-0.0074 (14)	-0.0027 (16)
O9	0.0396 (18)	0.0194 (17)	0.0267 (17)	-0.0007 (15)	0.0140 (14)	-0.0017 (14)
O10	0.0242 (16)	0.0313 (19)	0.0248 (16)	0.0093 (15)	-0.0086 (13)	-0.0053 (14)
N1	0.0174 (16)	0.0169 (17)	0.0158 (15)	0.0039 (14)	-0.0022 (13)	-0.0021 (13)
N2	0.048 (3)	0.041 (2)	0.035 (2)	-0.007 (2)	-0.0195 (19)	0.005 (2)
N3	0.063 (3)	0.040 (3)	0.041 (2)	0.004 (2)	0.029 (2)	0.011 (2)
N4	0.041 (2)	0.082 (4)	0.019 (2)	0.003 (3)	-0.0027 (18)	0.009 (2)
C1	0.016 (2)	0.022 (2)	0.031 (2)	-0.0044 (18)	0.0064 (17)	-0.0001 (18)
C2	0.016 (2)	0.018 (2)	0.030 (2)	-0.0011 (17)	-0.0006 (16)	-0.0022 (18)
C3	0.023 (2)	0.014 (2)	0.022 (2)	0.0114 (17)	0.0023 (17)	0.0010 (16)
C4	0.015 (2)	0.021 (2)	0.030 (2)	0.0027 (17)	0.0022 (17)	-0.0006 (18)
C5	0.028 (2)	0.014 (2)	0.024 (2)	-0.0027 (18)	0.0012 (17)	-0.0031 (16)
C6	0.024 (2)	0.021 (2)	0.021 (2)	0.0081 (18)	-0.0023 (17)	-0.0011 (17)
C7	0.060 (3)	0.052 (4)	0.033 (3)	-0.018 (3)	-0.016 (2)	0.017 (3)
C8	0.042 (3)	0.036 (3)	0.036 (3)	-0.016 (2)	-0.015 (2)	0.013 (2)
C9	0.023 (2)	0.019 (2)	0.025 (2)	0.0030 (18)	-0.0035 (17)	-0.0009 (17)
C10	0.027 (2)	0.030 (3)	0.032 (2)	-0.004 (2)	0.0017 (19)	-0.002 (2)
C11	0.032 (3)	0.036 (3)	0.042 (3)	-0.008 (2)	-0.011 (2)	-0.004 (2)
C12	0.029 (2)	0.014 (2)	0.025 (2)	0.0058 (19)	-0.0040 (17)	-0.0054 (18)
C13	0.051 (3)	0.055 (4)	0.063 (4)	0.017 (3)	0.039 (3)	0.019 (3)
C14	0.036 (3)	0.047 (3)	0.046 (3)	0.011 (2)	0.017 (2)	0.018 (2)
C15	0.027 (2)	0.027 (2)	0.023 (2)	-0.001 (2)	0.0096 (18)	-0.0005 (18)
C16	0.045 (3)	0.038 (3)	0.039 (3)	0.012 (2)	0.018 (2)	0.012 (2)
C17	0.063 (4)	0.044 (3)	0.044 (3)	0.010 (3)	0.020 (3)	0.019 (3)
C18	0.0154 (19)	0.023 (2)	0.019 (2)	-0.0054 (18)	-0.0009 (16)	0.0014 (17)
C19	0.043 (3)	0.093 (5)	0.023 (3)	-0.017 (3)	-0.001 (2)	-0.017 (3)
C20	0.036 (3)	0.053 (3)	0.023 (2)	-0.014 (2)	0.0017 (19)	-0.004 (2)
C21	0.021 (2)	0.029 (2)	0.0154 (19)	0.0051 (19)	0.0068 (16)	-0.0001 (17)
C22	0.030 (2)	0.033 (3)	0.024 (2)	-0.002 (2)	0.0009 (18)	0.000 (2)
C23	0.052 (3)	0.043 (3)	0.031 (3)	0.005 (3)	0.014 (2)	0.014 (2)
C24	0.024 (2)	0.025 (2)	0.0138 (19)	0.0036 (19)	-0.0014 (17)	-0.0001 (17)

Geometric parameters (Å, °)

Dy—O7	2.298 (3)	C1—C2	1.365 (5)
Dy—O2 ⁱ	2.300 (3)	C1—H1	0.9300
Dy—O8 ⁱ	2.313 (3)	C2—C3	1.382 (5)
Dy—O1	2.324 (3)	C2—H2	0.9300
Dy—O10	2.366 (3)	C3—C4	1.388 (6)
Dy—O9	2.409 (3)	C3—C6	1.510 (5)
Dy—O6	2.433 (3)	C4—C5	1.386 (6)
Dy—O5	2.513 (3)	C4—H4	0.9300
Dy—C18	2.828 (4)	C5—H5	0.9300
Cu—O3	1.976 (3)	C7—C8	1.385 (6)
Cu—O3 ⁱⁱ	1.976 (3)	C7—H7	0.9300
Cu—N1	2.004 (3)	C8—C9	1.369 (6)
Cu—N1 ⁱⁱ	2.004 (3)	C8—H8	0.9300

supplementary materials

Cu—N4 ⁱⁱⁱ	2.639 (4)	C9—C10	1.382 (6)
O1—C6	1.243 (5)	C9—C12	1.515 (5)
O2—C6	1.244 (5)	C10—C11	1.384 (6)
O2—Dy ⁱ	2.300 (3)	C10—H10	0.9300
O3—C12	1.271 (5)	C11—H11	0.9300
O4—C12	1.240 (5)	C13—C14	1.378 (6)
O5—C18	1.266 (5)	C13—H13	0.9300
O6—C18	1.253 (5)	C14—C15	1.376 (6)
O7—C24	1.248 (5)	C14—H14	0.9300
O8—C24	1.239 (5)	C15—C16	1.385 (6)
O8—Dy ⁱ	2.313 (3)	C15—C18	1.499 (5)
O9—H9A	0.81 (3)	C16—C17	1.384 (6)
O9—H9B	0.82 (3)	C16—H16	0.9300
O10—H10A	0.82 (3)	C17—H17	0.9300
O10—H10B	0.81 (4)	C19—C20	1.368 (6)
N1—C5	1.341 (5)	C19—H19	0.9300
N1—C1	1.348 (5)	C20—C21	1.377 (6)
N2—C11	1.339 (6)	C20—H20	0.9300
N2—C7	1.340 (6)	C21—C22	1.382 (6)
N3—C17	1.331 (6)	C21—C24	1.504 (5)
N3—C13	1.334 (6)	C22—C23	1.381 (6)
N4—C19	1.304 (7)	C22—H22	0.9300
N4—C23	1.325 (7)	C23—H23	0.9300
O7—Dy—O2 ⁱ	76.94 (12)	C3—C2—H2	120.2
O7—Dy—O8 ⁱ	121.52 (12)	C2—C3—C4	118.6 (4)
O2 ⁱ —Dy—O8 ⁱ	73.71 (12)	C2—C3—C6	120.4 (4)
O7—Dy—O1	78.31 (12)	C4—C3—C6	120.9 (3)
O2 ⁱ —Dy—O1	121.25 (11)	C5—C4—C3	118.1 (3)
O8 ⁱ —Dy—O1	75.69 (12)	C5—C4—H4	120.9
O7—Dy—O10	79.29 (11)	C3—C4—H4	120.9
O2 ⁱ —Dy—O10	144.72 (12)	N1—C5—C4	123.3 (4)
O8 ⁱ —Dy—O10	141.53 (11)	N1—C5—H5	118.3
O1—Dy—O10	78.16 (11)	C4—C5—H5	118.3
O7—Dy—O9	77.68 (11)	O1—C6—O2	126.1 (4)
O2 ⁱ —Dy—O9	76.06 (11)	O1—C6—C3	117.4 (4)
O8 ⁱ —Dy—O9	138.25 (12)	O2—C6—C3	116.4 (4)
O1—Dy—O9	145.75 (11)	N2—C7—C8	123.5 (5)
O10—Dy—O9	73.66 (11)	N2—C7—H7	118.3
O7—Dy—O6	151.75 (11)	C8—C7—H7	118.3
O2 ⁱ —Dy—O6	89.43 (11)	C9—C8—C7	120.0 (4)
O8 ⁱ —Dy—O6	76.52 (11)	C9—C8—H8	120.0
O1—Dy—O6	129.48 (10)	C7—C8—H8	120.0
O10—Dy—O6	99.76 (11)	C8—C9—C10	117.5 (4)
O9—Dy—O6	75.05 (10)	C8—C9—C12	120.3 (4)
O7—Dy—O5	147.35 (11)	C10—C9—C12	122.2 (4)
O2 ⁱ —Dy—O5	135.54 (10)	C9—C10—C11	119.0 (4)

O8 ⁱ —Dy—O5	75.13 (10)	C9—C10—H10	120.5
O1—Dy—O5	79.68 (10)	C11—C10—H10	120.5
O10—Dy—O5	72.79 (10)	N2—C11—C10	124.2 (4)
O9—Dy—O5	109.42 (10)	N2—C11—H11	117.9
O6—Dy—O5	52.71 (9)	C10—C11—H11	117.9
O7—Dy—C18	165.56 (11)	O4—C12—O3	127.4 (4)
O2 ⁱ —Dy—C18	112.24 (11)	O4—C12—C9	118.0 (4)
O8 ⁱ —Dy—C18	72.62 (11)	O3—C12—C9	114.6 (4)
O1—Dy—C18	104.46 (11)	N3—C13—C14	124.5 (5)
O10—Dy—C18	87.36 (11)	N3—C13—H13	117.7
O9—Dy—C18	93.40 (11)	C14—C13—H13	117.7
O6—Dy—C18	26.21 (10)	C15—C14—C13	119.1 (5)
O5—Dy—C18	26.58 (10)	C15—C14—H14	120.4
O3—Cu—O3 ⁱⁱ	180.000 (1)	C13—C14—H14	120.4
O3—Cu—N1	89.27 (12)	C14—C15—C16	117.4 (4)
O3 ⁱⁱ —Cu—N1	90.73 (12)	C14—C15—C18	122.3 (4)
O3—Cu—N1 ⁱⁱ	90.73 (12)	C16—C15—C18	120.2 (4)
O3 ⁱⁱ —Cu—N1 ⁱⁱ	89.27 (12)	C17—C16—C15	119.2 (4)
N1—Cu—N1 ⁱⁱ	180.00 (17)	C17—C16—H16	120.4
O3—Cu—N4 ⁱⁱⁱ	102.43 (12)	C15—C16—H16	120.4
O3 ⁱⁱ —Cu—N4 ⁱⁱⁱ	77.57 (12)	N3—C17—C16	124.0 (5)
N1—Cu—N4 ⁱⁱⁱ	93.04 (14)	N3—C17—H17	118.0
N1 ⁱⁱ —Cu—N4 ⁱⁱⁱ	86.96 (14)	C16—C17—H17	118.0
C6—O1—Dy	140.1 (3)	O6—C18—O5	121.4 (3)
C6—O2—Dy ⁱ	150.7 (3)	O6—C18—C15	119.2 (4)
C12—O3—Cu	137.0 (3)	O5—C18—C15	119.3 (4)
C18—O5—Dy	90.7 (2)	O6—C18—Dy	59.05 (19)
C18—O6—Dy	94.7 (2)	O5—C18—Dy	62.69 (19)
C24—O7—Dy	143.9 (3)	C15—C18—Dy	172.3 (3)
C24—O8—Dy ⁱ	144.4 (3)	N4—C19—C20	125.5 (5)
Dy—O9—H9A	118 (3)	N4—C19—H19	117.3
Dy—O9—H9B	124 (3)	C20—C19—H19	117.3
H9A—O9—H9B	105 (5)	C19—C20—C21	118.0 (5)
Dy—O10—H10A	125 (3)	C19—C20—H20	121.0
Dy—O10—H10B	133 (4)	C21—C20—H20	121.0
H10A—O10—H10B	102 (5)	C20—C21—C22	118.3 (4)
C5—N1—C1	117.4 (3)	C20—C21—C24	121.2 (4)
C5—N1—Cu	123.0 (3)	C22—C21—C24	120.5 (4)
C1—N1—Cu	119.6 (3)	C23—C22—C21	117.8 (4)
C11—N2—C7	115.7 (4)	C23—C22—H22	121.1
C17—N3—C13	115.7 (4)	C21—C22—H22	121.1
C19—N4—C23	115.9 (4)	N4—C23—C22	124.3 (5)
N1—C1—C2	122.8 (3)	N4—C23—H23	117.8
N1—C1—H1	118.6	C22—C23—H23	117.8
C2—C1—H1	118.6	O8—C24—O7	126.3 (4)
C1—C2—C3	119.7 (4)	O8—C24—C21	117.1 (4)

supplementary materials

C1—C2—H2 120.2 O7—C24—C21 116.5 (4)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$; (iii) $-x+1/2, y-1/2, -z+3/2$.

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O9—H9A...O4 ^{iv}	0.81 (3)	1.98 (3)	2.778 (4)	169 (5)
O9—H9B...N3 ^v	0.82 (3)	2.07 (3)	2.883 (5)	176 (5)
O10—H10A...O5 ^{vi}	0.82 (3)	1.98 (2)	2.784 (4)	166 (5)
O10—H10B...N2 ^{vii}	0.81 (4)	1.99 (2)	2.796 (5)	169 (6)

Symmetry codes: (iv) $x, y+1, z$; (v) $x-1/2, -y+3/2, z+1/2$; (vi) $-x+1, -y+1, -z+1$; (vii) $x+1/2, -y+1/2, z+1/2$.

Fig. 1

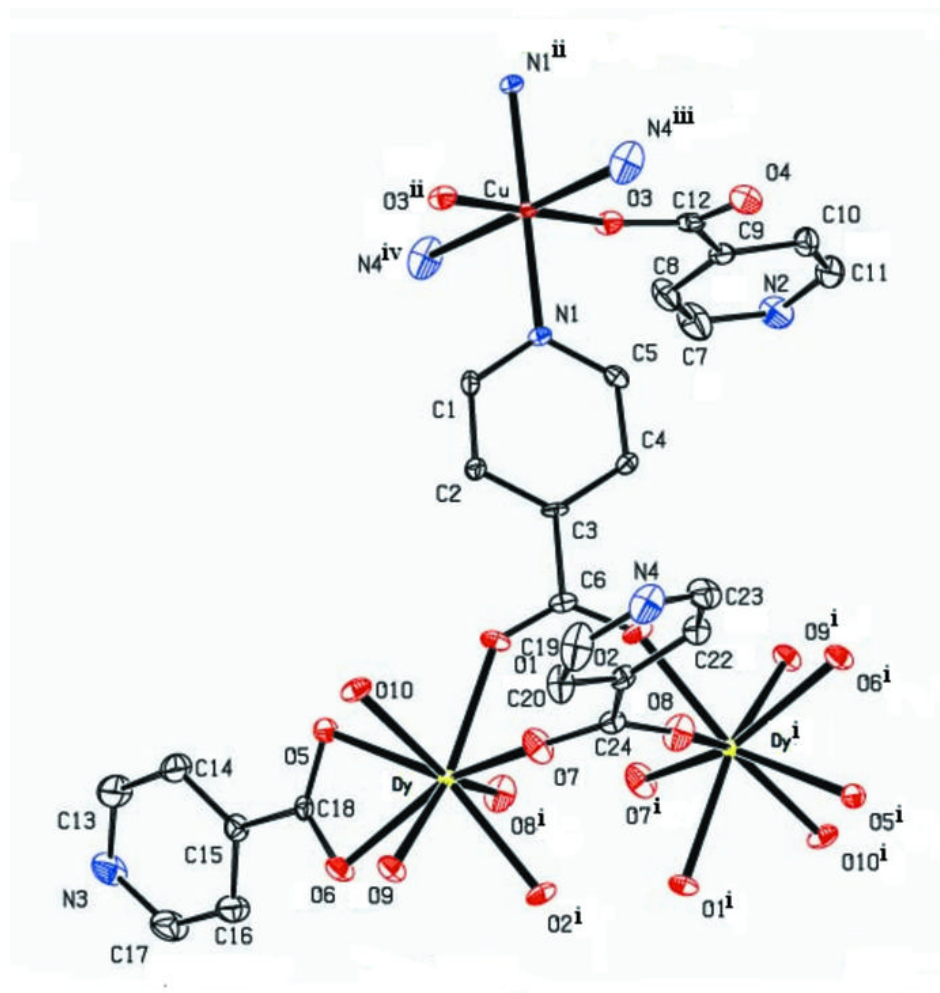


Fig. 2

