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Tris(1,10-phenanthrolinium) tris(pyridine-2,6-dicarboxylato)yttriate(III) dimethyl sulfoxide solvate pentahydrate

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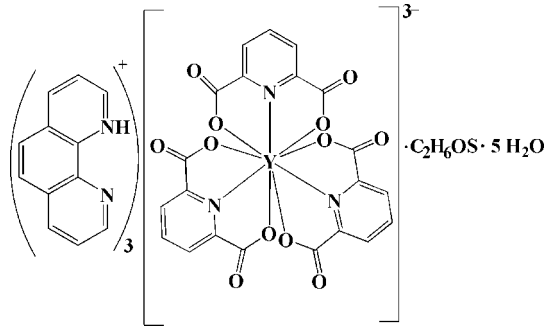
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.008 Å; R factor = 0.054; wR factor = 0.131; data-to-parameter ratio = 14.9.

The title compound, $(C_{12}H_9N_2)_3[Y(C_7H_3NO_4)_3]\cdot C_2H_6OS\cdot 5H_2O$ or $(phenH)_3[Y(pydc)_3]\cdot DMSO\cdot 5H_2O$ (phenH is 1,10-phenanthrolinium, pydc is pyridine-2,6-dicarboxylate and DMSO is dimethyl sulfoxide), was synthesized by the reaction of YCl_3 with the proton-transfer compound $(phenH)_2(pydc)$ in DMSO as solvent. The nine donor atoms of the three $pydc^{2-}$ fragments form a distorted tricapped trigonal–prismatic arrangement around the Y^{III} centre. Considerable π–π and C—H$\cdots\pi$ stacking interactions between the aromatic rings of $pydc^{2-}$ [centroid–centroid distances 3.659 (4) and 3.662 (4) Å], and between the CH groups of DMSO with the benzene rings of the $pydc^{2-}$ fragments, are observed. In the crystal structure, a wide range of non-covalent interactions consisting of hydrogen bonding [of the types O—H$\cdots$O, O—H$\cdots$S, N—H$\cdots$O and C—H$\cdots$O], ion pairing, π–π and C—H$\cdots\pi$ stacking connect the various components into a supramolecular structure.

Related literature

For related literature, see: Aghabozorg, Attar Gharamaleki, Ghadermazi *et al.* (2007); Aghabozorg, Attar Gharamaleki, Ghasemikhah *et al.* (2007); Aghabozorg, Daneshvar *et al.* (2007); Brayshaw *et al.* (2005); Tancrez *et al.* (2005).



Experimental

Crystal data

$(C_{12}H_9N_2)_3[Y(C_7H_3NO_4)_3]\cdot C_2H_6OS\cdot 5H_2O$
M_r = 1296.08
Triclinic, $P\overline{1}$
a = 10.4185 (14) Å
b = 10.9689 (14) Å
c = 14.3844 (19) Å
α = 70.599 (2)°
β = 81.174 (2)°
γ = 63.298 (2)°
V = 1385.1 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 150 (2) K
0.30 × 0.20 × 0.17 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.719, T_{max} = 0.825
15984 measured reflections
11832 independent reflections
8989 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.131
S = 1.00
11832 reflections
795 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}
Absolute structure: Flack (1983), 5621 Friedel pairs
Flack parameter: −0.004 (4)

Table 1
Selected geometric parameters (Å, °).

Y1—O5	2.362 (3)	Y1—O4	2.421 (3)
Y1—O9	2.374 (3)	Y1—N3	2.481 (4)
Y1—O8	2.386 (3)	Y1—N2	2.490 (4)
Y1—O12	2.398 (3)	Y1—N1	2.500 (4)
Y1—O1	2.415 (3)		
O5—Y1—O9	80.12 (11)	O9—Y1—O4	78.84 (11)
O8—Y1—O12	78.83 (11)	N3—Y1—N2	121.88 (12)
O8—Y1—O1	77.80 (11)	N3—Y1—N1	121.09 (13)
O12—Y1—O1	78.82 (11)	N2—Y1—N1	116.97 (12)
O5—Y1—O4	77.91 (11)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O14—H14A···O10^{i}	0.95	1.84	2.734 (5)	156
O14—H14B···O3^{ii}	0.95	1.82	2.757 (5)	169
O15—H15A···O11^{i}	0.95	2.02	2.854 (5)	146
O15—H15B···O2	0.95	1.89	2.824 (5)	166
O16—H16A···O17^{iii}	0.95	1.73	2.678 (5)	175
O16—H16B···O15^{iv}	0.95	1.84	2.769 (5)	165
O17—H17A···O14^{v}	0.95	1.91	2.859 (5)	180
O17—H17B···O18^{vi}	0.95	2.03	2.804 (5)	138
O17—H17B···O6^{i}	0.95	2.60	3.192 (5)	121
O18—H18A···O13	0.95	1.85	2.789 (5)	169
O18—H18A···S1	0.95	2.77	3.650 (4)	155
O18—H18B···O4^{ii}	0.95	1.90	2.849 (5)	177
N4—H4A···O7	0.95	1.88	2.680 (5)	140
N6—H6A···O13	0.95	1.84	2.673 (5)	146
N9—H9···O16	0.95	1.69	2.612 (6)	161
C3—H3···O11^{i}	0.95	2.49	3.319 (7)	146
C5—H5···O6^{i}	0.95	2.59	3.277 (8)	129
C22—H22···O8	0.95	2.33	3.056 (6)	132
C29—H29···O6^{vii}	0.95	2.51	3.380 (7)	152
C31—H31···O11^{vi}	0.95	2.41	3.357 (7)	174
C34—H34···O18	0.95	2.53	3.446 (7)	162
C36—H36···O12^{viii}	0.95	2.46	3.384 (6)	164
C39—H39···O2^{ix}	0.95	2.54	3.438 (7)	159
C42—H42···O14^{v}	0.95	2.36	3.247 (7)	155
C54—H54···O9	0.95	2.44	3.275 (6)	146
C55—H55···O10	0.95	2.40	3.244 (7)	147
C59—H59A···O10	0.98	2.55	3.381 (9)	143
C58—H58C···Cg1^{i}	0.98	2.84	3.424 (7)	119

Symmetry codes: (i) $x+1, y, z$; (ii) $x+1, y-1, z$; (iii) $x, y-1, z$; (iv) $x, y-1, z+1$; (v) $x-1, y+1, z$; (vi) $x, y+1, z$; (vii) $x, y+1, z-1$; (viii) $x+1, y-1, z+1$; (ix) $x, y, z+1$. $Cg1$ is the centroid of atoms N3,C16–C20.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 2005); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2178).

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supplementary materials

Acta Cryst. (2007). E**63**, m3170-m3171 [**doi:10.1107/S1600536807060047**]

Tris(1,10-phenanthrolinium) tris(pyridine-2,6-dicarboxylato)yttriate(III) dimethyl sulfoxide solvate pentahydrate

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Comment

Just as there is a field of *molecular chemistry* based on the covalent bond, there is a field of *supramolecular chemistry*, the chemistry of molecular assemblies and of the intermolecular bond. The non-covalent interactions such as ion pairing, hydrogen bonding and π–π stacking are observed in these ionic compounds. The importance of weak hydrogen bonds in the context of crystal engineering, molecular recognition and supramolecular chemistry has been well recognized in recent years. Recently, we have defined a plan to prepare water soluble proton transfer compounds as novel self-assembled systems that can function as suitable ligands in the synthesis of metal complexes. In this regard, we have reported cases in which proton transfer from pyridine-2,6-dicarboxylic acid, $pydcH_2$, and benzene-1,2,4,5-tetracarboxylicacid, $btcH_4$, to propane-1,3-diamine (pn) and 1,10-phenanthroline, (phen), results in the formation of self-assembled $(pnH_2)(pydc).(pydcH_2)\cdot 2.5H_2O$, $(pnH_2)_2(btc)\cdot 2H_2O$ and $(phenH)_4(btcH_3)_2(btcH_2)$ systems, respectively. Our attempts to obtain single crystals of the proton transfer compound $(phenH)_2(pydc)$ were not successful. The resulting compounds with some remaining sites as electron donors can coordinate to metal ions (Aghabozorg, Attar Gharamaleki Ghadermazi *et al.*, 2007; Aghabozorg, Attar Gharamaleki, Ghasemikhah *et al.*, 2007; Aghabozorg, Daneshvar *et al.*, 2007, and references therein).

The molecular structure of the anion of the title compound, $(phenH)_3[Y(pydc)_3]\cdot DMSO\cdot 5H_2O$ is presented in Fig. 1, while its disposition with respect to the remaining constituents is illustrated in Fig. 2. Bond lengths and angles are presented in Table 1. Fig. 3 presents the hydrogen bonding between its components. Also hydrogen bond lengths are given separately in Table 2.

In the structure, Y^{III} is coordinated by three $pydc^{2-}$ groups as tridentate ligands, and a nine coordinate complex results. For balancing the charge, three protonated 1,10-phenanthrolines, $(phenH)^+$, exist.

The sum of the bond angles, N1—Y1—N2, N1—Y1—N3 and N2—Y1—N3 equals to 359.94° and indicates that Y^{III} is located in the center of N1N2N3 plane. The three O atoms O1, O8 and O12 form a triangle and the other three, O4, O5 and O9 form another triangle around the Y^{III}. Considering the angles between the oxygen atoms, a prismatic geometry consisting of the six O atoms and three nitrogen caps on its faces is proposed (Fig. 4). This anion has been previously reported to have a tricapped prismatic geometry (Tancrez *et al.*, 2005; Brayshaw, *et al.*, 2005).

In the structure of the $(phenH)_3[Y(pydc)_3]\cdot DMSO\cdot 5H_2O$ complex, the spaces between two layers of $[Y(pydc)_3]^{3-}$ anions are filled with $(phenH)^+$ cations, DMSO and water molecules (Fig. 5). A noticeable feature of the title compound is the presence of a C–H···π stacking interactions between a C—H group of DMSO molecules with an aromatic ring of a $pydc^{2-}$ unit. The C—H···π distance (measured to the centre of phenyl ring) is 2.84 Å for C58—H58C···*Cg*(1) (1 + *x*, *y*, *z*) with the angles of 119°, [*Cg*(1) is the centroid of N3,C16—C20] (Fig. 6). Also a considerable π-π stacking interactions between aromatic rings of pyridine-2,6-dicarboxylate fragments with distances of 3.659 (4) Å for X1B···X1A (*x*, *y*, *z*) and 3.662 (4) Å

for X1A···X1C (1 + *x*, −1 + *y*, 1 + *z*) are observed (Fig. 7). A wide range of non-covalent interactions consisting of hydrogen bonding (of the type O—H···O, O—H···S, N—H···O and C—H···O with D···A ranging from 2.612 (6) Å to 3.650 (4) Å, ion pairing, π–π and C—H···π stacking connect the various components into a supramolecular structure (Table 2, Fig. 2 and Fig. 3).

Experimental

The proton transfer compound of $(phenH)_2(pydc)$ was prepared according to our reported procedure. A solution of YCl_3 (0.05 mmol, 11 mg) in dimethylsulfoxide (DMSO) (5 ml) was added to a stirring solution of $(phenH)_2(pydc)$ (0.095 mmol, 50 mg) in DMSO (5 ml). The volume of the resulting suspension was increased by adding 5 ml H_2O at room temperature. Due to the high viscosity of DMSO solvent, the crystallization time for the title complex was very long, so that it took about nine months for the colorless crystals to be obtained from the solution.

Refinement

Hydrogen atoms were positioned geometrically and refined with a riding model (including torsional freedom for methyl groups), with C—H = 0.95–0.98 Å, and with U(H) constrained to be 1.2 (1.5 for methyl groups) times U_{eq} of the carrier atom. Hydrogen atoms on phen were initially found in a difference Fourier map and placed with no ambiguity.

Figures

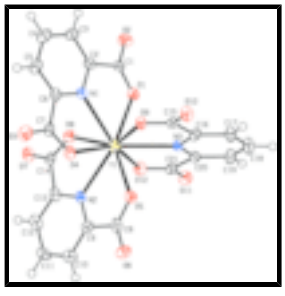


Fig. 1. The structure of the anion of the title compound showing the atom-numbering scheme and displacement ellipsoids at the 50% probability level.

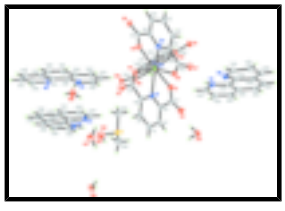


Fig. 2. The anion, cations, DMSO and water molecules with their atom numbering and thermal ellipsoids at the 50% probability level are shown.

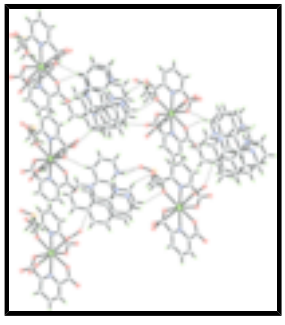


Fig. 3. The hydrogen bonding between different components of the title compound.

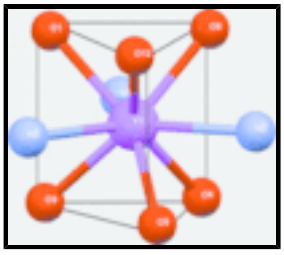


Fig. 4. Coordination environment of the central Y atom.

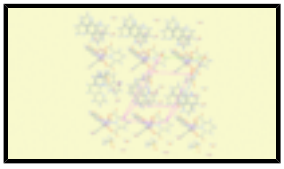


Fig. 5. A packing diagram as viewed down the *a* axis. The space between the two layers of $[Y(pydc)_3]^{3-}$ fragments is filled with a layer of $(phenH)^+$ cations, DMSO and water molecules.

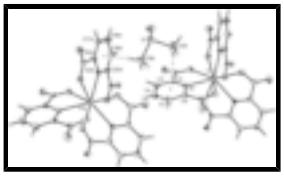


Fig. 6. C–H···π stacking interactions between C—H groups of DMSO with aromatic rings of $pydc^{2-}$ units. The C—H···π distances (measured to the centre of phenyl ring) are 2.840 Å for C58—H58C···*Cg*(1) (1 + *x*, *y*, *z*) with the angles of 119° [*Cg*(1) is the centroid of N3,C16—C20]

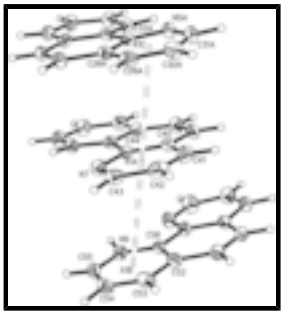


Fig. 7. π-π stacking interactions between aromatic rings of pyridine-2,6-dicarboxylate fragments with distances of 3.659 (4) Å for X1B···X1A (*x*, *y*, *z*) and 3.662 (4) Å for X1A···X1C (1 + *x*, −1 + *y*, 1 + *z*).

Tris(1,10-phenanthrolinium) tris(pyridine-2,6-dicarboxylato)yttriumate dimethyl sulfoxide pentahydrate

Crystal data

$(C_{12}H_9N_2)_3[Y(C_7H_3NO_4)_3]\cdot C_2H_6OS\cdot 5H_2O$	$Z = 1$
$M_r = 1296.08$	$F_{000} = 668$
Triclinic, *P*1	$D_x = 1.554$ Mg m^{-3}
a = 10.4185 (14) Å	Mo *K*α radiation λ = 0.71073 Å
b = 10.9689 (14) Å	Cell parameters from 5015 reflections
c = 14.3844 (19) Å	θ = 2.2–26.9º
α = 70.599 (2)º	μ = 1.18 mm^{-1}
β = 81.174 (2)º	*T* = 150 (2) K
γ = 63.298 (2)º	Block, colourless
V = 1385.1 (3) Å^3	0.30 × 0.20 × 0.17 mm

Data collection

Bruker SMART 1000 diffractometer	11832 independent reflections
Radiation source: fine-focus sealed tube	8989 reflections with $I > 2\sigma(I)$

Monochromator: graphite	R_{int} = 0.045
Detector resolution: 8.3 pixels mm^{-1}	θ_{max} = 27.6º
T = 150(2) K	θ_{min} = 1.5º
ω scans	h = −13→13
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	k = −14→14
T_{min} = 0.719, T_{max} = 0.825	l = −18→18
15984 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.054	$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.131	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.70 e Å^{-3}
11832 reflections	$\Delta\rho_{min}$ = −0.85 e Å^{-3}
795 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983), 5621 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.004 (4)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Y1	−0.11333 (4)	1.34289 (4)	0.10288 (3)	0.01762 (11)
S1	0.57322 (16)	0.90591 (15)	0.26814 (10)	0.0275 (3)
C1	0.1728 (5)	1.2743 (5)	−0.0431 (4)	0.0211 (11)
C2	0.2177 (5)	1.3214 (5)	0.0298 (3)	0.0201 (10)
C3	0.3466 (5)	1.3313 (5)	0.0244 (3)	0.0233 (11)
H3	0.4166	1.3018	−0.0239	0.028*
C4	0.3713 (6)	1.3855 (6)	0.0914 (4)	0.0285 (13)
H4	0.4582	1.3950	0.0883	0.034*

C5	0.2700 (6)	1.4250 (6)	0.1616 (4)	0.0267 (11)
H5	0.2849	1.4628	0.2075	0.032*
C6	0.1447 (5)	1.4084 (5)	0.1641 (3)	0.0191 (10)
C7	0.0253 (6)	1.4468 (5)	0.2388 (4)	0.0210 (12)
C8	−0.4004 (6)	1.3917 (6)	0.2435 (4)	0.0210 (12)
C9	−0.4383 (5)	1.5452 (5)	0.1780 (3)	0.0200 (10)
C10	−0.5669 (6)	1.6627 (6)	0.1831 (4)	0.0257 (11)
H10	−0.6392	1.6518	0.2296	0.031*
C11	−0.5869 (5)	1.7963 (6)	0.1186 (4)	0.0258 (12)
H11	−0.6740	1.8780	0.1198	0.031*
C12	−0.4786 (6)	1.8093 (5)	0.0525 (3)	0.0253 (11)
H12	−0.4895	1.9003	0.0092	0.030*
C13	−0.3546 (5)	1.6882 (5)	0.0505 (3)	0.0208 (10)
C14	−0.2305 (5)	1.6851 (5)	−0.0200 (3)	0.0171 (10)
C15	0.0479 (5)	1.0031 (5)	0.2240 (4)	0.0191 (11)
C16	−0.0399 (5)	0.9977 (5)	0.1514 (3)	0.0197 (10)
C17	−0.0407 (5)	0.8733 (5)	0.1476 (4)	0.0249 (11)
H17	0.0158	0.7833	0.1920	0.030*
C18	−0.1265 (6)	0.8829 (6)	0.0769 (4)	0.0315 (13)
H18	−0.1305	0.7997	0.0735	0.038*
C19	−0.2050 (6)	1.0148 (5)	0.0123 (4)	0.0239 (11)
H19	−0.2605	1.0233	−0.0381	0.029*
C20	−0.2014 (5)	1.1354 (5)	0.0223 (3)	0.0182 (10)
C21	−0.2849 (5)	1.2869 (5)	−0.0419 (4)	0.0195 (11)
C22	−0.0197 (6)	1.6003 (6)	−0.2235 (4)	0.0274 (12)
H22	0.0015	1.5435	−0.1568	0.033*
C23	0.0303 (6)	1.5373 (6)	−0.2976 (4)	0.0300 (12)
H23	0.0865	1.4369	−0.2820	0.036*
C24	0.0000 (6)	1.6179 (6)	−0.3936 (4)	0.0271 (11)
H24	0.0349	1.5734	−0.4445	0.033*
C25	−0.0831 (5)	1.7670 (6)	−0.4174 (4)	0.0240 (11)
C26	−0.1224 (5)	1.8588 (6)	−0.5159 (4)	0.0250 (11)
H26	−0.0943	1.8187	−0.5691	0.030*
C27	−0.1994 (6)	2.0022 (6)	−0.5345 (4)	0.0274 (12)
H27	−0.2254	2.0611	−0.6003	0.033*
C28	−0.2424 (5)	2.0666 (5)	−0.4547 (4)	0.0218 (10)
C29	−0.3192 (6)	2.2141 (6)	−0.4711 (4)	0.0277 (12)
H29	−0.3473	2.2770	−0.5358	0.033*
C30	−0.3530 (6)	2.2658 (6)	−0.3917 (4)	0.0290 (12)
H30	−0.4074	2.3652	−0.4003	0.035*
C31	−0.3064 (6)	2.1705 (6)	−0.2977 (4)	0.0260 (11)
H31	−0.3282	2.2087	−0.2439	0.031*
C32	−0.2051 (5)	1.9802 (6)	−0.3578 (3)	0.0215 (11)
C33	−0.1271 (5)	1.8279 (5)	−0.3387 (3)	0.0210 (10)
C34	0.6437 (6)	0.6252 (6)	0.5886 (4)	0.0276 (12)
H34	0.6778	0.5757	0.5404	0.033*
C35	0.6634 (6)	0.5496 (6)	0.6878 (4)	0.0294 (12)
H35	0.7084	0.4481	0.7080	0.035*
C36	0.6179 (6)	0.6217 (6)	0.7562 (4)	0.0268 (11)

H36	0.6337	0.5698	0.8242	0.032*
C37	0.5478 (5)	0.7724 (5)	0.7274 (4)	0.0238 (11)
C38	0.4972 (6)	0.8541 (6)	0.7952 (4)	0.0269 (11)
H38	0.5084	0.8062	0.8639	0.032*
C39	0.4333 (6)	0.9990 (6)	0.7635 (4)	0.0275 (12)
H39	0.4031	1.0514	0.8098	0.033*
C40	0.4112 (5)	1.0732 (6)	0.6606 (4)	0.0235 (11)
C41	0.3423 (6)	1.2238 (6)	0.6245 (4)	0.0298 (12)
H41	0.3114	1.2796	0.6688	0.036*
C42	0.3207 (6)	1.2879 (6)	0.5268 (4)	0.0322 (13)
H42	0.2775	1.3893	0.5014	0.039*
C43	0.3627 (5)	1.2033 (6)	0.4629 (4)	0.0280 (12)
H43	0.3421	1.2502	0.3947	0.034*
C44	0.4522 (5)	0.9982 (6)	0.5910 (4)	0.0198 (11)
C45	0.5276 (5)	0.8437 (6)	0.6255 (3)	0.0231 (11)
C46	0.2254 (6)	0.7322 (6)	0.8653 (4)	0.0370 (14)
H46	0.2690	0.6307	0.8882	0.044*
C47	0.1944 (7)	0.8066 (7)	0.9344 (4)	0.0343 (15)
H47	0.2178	0.7564	1.0019	0.041*
C48	0.1301 (6)	0.9523 (6)	0.9030 (4)	0.0316 (13)
H48	0.1078	1.0047	0.9488	0.038*
C49	0.0967 (5)	1.0254 (6)	0.8022 (4)	0.0255 (11)
C50	0.0286 (5)	1.1781 (6)	0.7624 (4)	0.0255 (11)
H50	0.0019	1.2362	0.8048	0.031*
C51	0.0026 (5)	1.2391 (6)	0.6651 (4)	0.0260 (11)
H51	−0.0429	1.3405	0.6402	0.031*
C52	0.0411 (5)	1.1570 (6)	0.5982 (4)	0.0253 (11)
C53	0.0167 (6)	1.2180 (6)	0.4955 (4)	0.0287 (12)
H53	−0.0267	1.3189	0.4675	0.034*
C54	0.0557 (6)	1.1312 (6)	0.4368 (4)	0.0270 (12)
H54	0.0347	1.1715	0.3684	0.032*
C55	0.1259 (6)	0.9844 (6)	0.4771 (4)	0.0262 (11)
H55	0.1571	0.9246	0.4356	0.031*
C56	0.1094 (5)	1.0079 (5)	0.6353 (3)	0.0205 (10)
C57	0.1364 (5)	0.9385 (5)	0.7395 (3)	0.0235 (11)
C58	0.6083 (6)	1.0556 (6)	0.2559 (4)	0.0354 (13)
H58A	0.5611	1.0964	0.3099	0.053*
H58B	0.5708	1.1281	0.1928	0.053*
H58C	0.7122	1.0245	0.2584	0.053*
C59	0.3837 (6)	0.9890 (8)	0.2812 (5)	0.0442 (16)
H59A	0.3456	0.9176	0.2952	0.066*
H59B	0.3416	1.0644	0.2200	0.066*
H59C	0.3591	1.0308	0.3357	0.066*
O1	0.0544 (4)	1.2653 (4)	−0.0241 (2)	0.0232 (7)
O2	0.2516 (4)	1.2526 (4)	−0.1156 (3)	0.0313 (9)
O3	0.0386 (4)	1.4951 (5)	0.3015 (3)	0.0365 (10)
O4	−0.0820 (4)	1.4254 (3)	0.2307 (2)	0.0224 (7)
O5	−0.2825 (4)	1.2997 (4)	0.2228 (2)	0.0237 (8)
O6	−0.4872 (4)	1.3728 (4)	0.3087 (2)	0.0279 (8)

O7	−0.2408 (4)	1.7992 (3)	−0.0822 (2)	0.0246 (8)
O8	−0.1265 (4)	1.5639 (4)	−0.0103 (2)	0.0236 (7)
O9	0.0411 (3)	1.1243 (3)	0.2129 (2)	0.0203 (7)
O10	0.1179 (4)	0.8896 (4)	0.2879 (2)	0.0265 (8)
O11	−0.3584 (4)	1.3055 (4)	−0.1099 (2)	0.0259 (8)
O12	−0.2730 (4)	1.3829 (3)	−0.0188 (2)	0.0237 (7)
O13	0.6314 (4)	0.8034 (4)	0.3684 (3)	0.0361 (9)
O14	1.1684 (4)	0.6103 (4)	0.3790 (3)	0.0316 (9)
H14A	1.1241	0.7112	0.3509	0.038*
H14B	1.1132	0.5811	0.3518	0.038*
O15	0.3899 (4)	1.4263 (4)	−0.2256 (3)	0.0348 (9)
H15A	0.4473	1.4139	−0.1748	0.042*
H15B	0.3575	1.3589	−0.1823	0.042*
O16	0.3079 (5)	0.6530 (4)	0.6028 (3)	0.0427 (11)
H16A	0.3558	0.6304	0.5450	0.051*
H16B	0.3491	0.5671	0.6552	0.051*
O17	0.4315 (4)	1.5831 (4)	0.4392 (3)	0.0385 (10)
H17A	0.3441	1.5920	0.4192	0.046*
H17B	0.5123	1.5408	0.4010	0.046*
O18	0.7177 (4)	0.5189 (4)	0.3788 (3)	0.0319 (9)
H18A	0.6773	0.6181	0.3723	0.038*
H18B	0.7830	0.4854	0.3294	0.038*
N1	0.1196 (4)	1.3584 (4)	0.0993 (3)	0.0173 (8)
N2	−0.3370 (4)	1.5585 (4)	0.1120 (3)	0.0195 (8)
N3	−0.1199 (4)	1.1258 (4)	0.0899 (3)	0.0173 (8)
N4	−0.0982 (4)	1.7415 (4)	−0.2452 (3)	0.0210 (9)
H4A	−0.1184	1.7820	−0.1927	0.025*
N5	−0.2338 (4)	2.0302 (4)	−0.2794 (3)	0.0230 (9)
N6	0.5770 (4)	0.7673 (4)	0.5610 (3)	0.0223 (9)
H6A	0.5711	0.8177	0.4927	0.027*
N7	0.4295 (4)	1.0614 (4)	0.4924 (3)	0.0240 (9)
N8	0.1977 (5)	0.7944 (5)	0.7706 (3)	0.0279 (10)
N9	0.1502 (4)	0.9265 (5)	0.5734 (3)	0.0235 (9)
H9	0.2104	0.8272	0.5973	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Y1	0.0206 (2)	0.0181 (2)	0.0154 (2)	−0.0093 (2)	−0.00083 (17)	−0.00465 (17)
S1	0.0338 (8)	0.0343 (8)	0.0200 (7)	−0.0186 (7)	0.0039 (6)	−0.0110 (6)
C1	0.015 (3)	0.017 (3)	0.028 (3)	−0.005 (2)	0.003 (2)	−0.007 (2)
C2	0.021 (3)	0.017 (2)	0.018 (2)	−0.007 (2)	−0.0003 (19)	−0.003 (2)
C3	0.020 (2)	0.031 (3)	0.018 (2)	−0.012 (2)	0.0012 (19)	−0.005 (2)
C4	0.028 (3)	0.039 (3)	0.023 (3)	−0.020 (3)	−0.005 (2)	−0.005 (3)
C5	0.034 (3)	0.034 (3)	0.020 (2)	−0.021 (3)	−0.005 (2)	−0.007 (2)
C6	0.023 (2)	0.018 (2)	0.018 (2)	−0.009 (2)	−0.0027 (19)	−0.005 (2)
C7	0.030 (3)	0.023 (3)	0.017 (2)	−0.016 (3)	0.000 (2)	−0.008 (2)
C8	0.036 (3)	0.021 (3)	0.009 (2)	−0.013 (3)	−0.005 (2)	−0.004 (2)

C9	0.023 (3)	0.028 (3)	0.013 (2)	−0.014 (2)	−0.0002 (19)	−0.008 (2)
C10	0.026 (3)	0.032 (3)	0.018 (2)	−0.010 (2)	−0.002 (2)	−0.009 (2)
C11	0.022 (3)	0.029 (3)	0.021 (3)	−0.004 (2)	0.001 (2)	−0.012 (2)
C12	0.032 (3)	0.021 (3)	0.019 (2)	−0.005 (2)	−0.008 (2)	−0.006 (2)
C13	0.031 (3)	0.022 (3)	0.012 (2)	−0.011 (2)	−0.0037 (19)	−0.0079 (19)
C14	0.024 (3)	0.019 (3)	0.014 (2)	−0.013 (2)	−0.0023 (19)	−0.005 (2)
C15	0.018 (3)	0.022 (3)	0.019 (2)	−0.010 (2)	0.000 (2)	−0.006 (2)
C16	0.023 (2)	0.023 (3)	0.016 (2)	−0.014 (2)	−0.0001 (19)	−0.003 (2)
C17	0.031 (3)	0.018 (3)	0.024 (3)	−0.010 (2)	−0.008 (2)	−0.003 (2)
C18	0.040 (3)	0.023 (3)	0.035 (3)	−0.012 (3)	−0.010 (3)	−0.010 (2)
C19	0.033 (3)	0.026 (3)	0.020 (2)	−0.016 (2)	−0.007 (2)	−0.008 (2)
C20	0.017 (2)	0.019 (2)	0.019 (2)	−0.007 (2)	−0.0017 (19)	−0.007 (2)
C21	0.017 (2)	0.027 (3)	0.019 (2)	−0.011 (2)	−0.0014 (19)	−0.007 (2)
C22	0.027 (3)	0.025 (3)	0.026 (3)	−0.011 (2)	0.001 (2)	−0.003 (2)
C23	0.033 (3)	0.026 (3)	0.032 (3)	−0.012 (3)	0.003 (2)	−0.012 (2)
C24	0.029 (3)	0.032 (3)	0.025 (3)	−0.015 (3)	0.006 (2)	−0.014 (2)
C25	0.022 (3)	0.029 (3)	0.026 (3)	−0.015 (2)	0.006 (2)	−0.011 (2)
C26	0.027 (3)	0.036 (3)	0.022 (3)	−0.018 (3)	0.006 (2)	−0.016 (2)
C27	0.029 (3)	0.037 (3)	0.015 (2)	−0.016 (3)	−0.001 (2)	−0.005 (2)
C28	0.023 (3)	0.025 (3)	0.019 (2)	−0.013 (2)	−0.003 (2)	−0.004 (2)
C29	0.026 (3)	0.032 (3)	0.023 (3)	−0.013 (3)	−0.004 (2)	−0.003 (2)
C30	0.031 (3)	0.018 (3)	0.036 (3)	−0.009 (2)	−0.005 (2)	−0.005 (2)
C31	0.030 (3)	0.026 (3)	0.024 (3)	−0.010 (2)	0.002 (2)	−0.013 (2)
C32	0.020 (3)	0.027 (3)	0.019 (2)	−0.011 (2)	−0.001 (2)	−0.007 (2)
C33	0.024 (3)	0.027 (3)	0.019 (2)	−0.016 (2)	−0.002 (2)	−0.007 (2)
C34	0.030 (3)	0.021 (3)	0.028 (3)	−0.006 (2)	0.000 (2)	−0.010 (2)
C35	0.033 (3)	0.022 (3)	0.024 (3)	−0.010 (2)	−0.001 (2)	0.000 (2)
C36	0.027 (3)	0.028 (3)	0.019 (3)	−0.010 (2)	−0.004 (2)	0.002 (2)
C37	0.021 (3)	0.025 (3)	0.024 (3)	−0.009 (2)	0.000 (2)	−0.007 (2)
C38	0.031 (3)	0.031 (3)	0.013 (2)	−0.011 (3)	−0.002 (2)	−0.003 (2)
C39	0.030 (3)	0.038 (3)	0.022 (3)	−0.017 (3)	0.001 (2)	−0.013 (2)
C40	0.020 (3)	0.030 (3)	0.025 (3)	−0.012 (2)	−0.001 (2)	−0.011 (2)
C41	0.028 (3)	0.026 (3)	0.038 (3)	−0.011 (2)	0.004 (2)	−0.014 (3)
C42	0.026 (3)	0.020 (3)	0.047 (3)	−0.008 (2)	−0.004 (3)	−0.006 (3)
C43	0.024 (3)	0.026 (3)	0.029 (3)	−0.011 (2)	−0.003 (2)	−0.001 (2)
C44	0.018 (2)	0.025 (3)	0.017 (2)	−0.010 (2)	0.0005 (19)	−0.005 (2)
C45	0.022 (3)	0.030 (3)	0.020 (2)	−0.014 (2)	0.000 (2)	−0.006 (2)
C46	0.046 (4)	0.028 (3)	0.025 (3)	−0.009 (3)	−0.006 (3)	0.000 (2)
C47	0.037 (4)	0.042 (4)	0.014 (3)	−0.012 (3)	−0.002 (2)	−0.002 (3)
C48	0.031 (3)	0.047 (4)	0.021 (3)	−0.017 (3)	0.002 (2)	−0.016 (3)
C49	0.024 (3)	0.037 (3)	0.024 (3)	−0.016 (3)	0.003 (2)	−0.016 (2)
C50	0.023 (3)	0.027 (3)	0.029 (3)	−0.007 (2)	0.000 (2)	−0.017 (2)
C51	0.026 (3)	0.021 (3)	0.030 (3)	−0.008 (2)	−0.002 (2)	−0.011 (2)
C52	0.025 (3)	0.030 (3)	0.025 (3)	−0.014 (2)	−0.002 (2)	−0.009 (2)
C53	0.032 (3)	0.026 (3)	0.026 (3)	−0.014 (3)	−0.008 (2)	0.000 (2)
C54	0.031 (3)	0.033 (3)	0.019 (2)	−0.018 (3)	−0.004 (2)	−0.003 (2)
C55	0.030 (3)	0.034 (3)	0.019 (3)	−0.017 (3)	0.004 (2)	−0.011 (2)
C56	0.019 (2)	0.027 (3)	0.019 (2)	−0.011 (2)	0.001 (2)	−0.009 (2)
C57	0.025 (3)	0.029 (3)	0.019 (2)	−0.013 (2)	0.003 (2)	−0.009 (2)

C58	0.044 (3)	0.032 (3)	0.035 (3)	−0.023 (3)	0.005 (3)	−0.009 (3)
C59	0.041 (4)	0.070 (5)	0.042 (4)	−0.034 (4)	0.006 (3)	−0.028 (3)
O1	0.0274 (19)	0.0265 (19)	0.0204 (17)	−0.0142 (16)	0.0033 (14)	−0.0104 (15)
O2	0.031 (2)	0.043 (2)	0.028 (2)	−0.018 (2)	0.0092 (17)	−0.0211 (19)
O3	0.041 (2)	0.058 (3)	0.034 (2)	−0.030 (2)	0.0090 (18)	−0.033 (2)
O4	0.0299 (19)	0.0225 (18)	0.0167 (16)	−0.0108 (16)	−0.0029 (14)	−0.0076 (14)
O5	0.028 (2)	0.0233 (19)	0.0205 (17)	−0.0120 (17)	0.0043 (15)	−0.0079 (15)
O6	0.029 (2)	0.036 (2)	0.0180 (18)	−0.0179 (19)	0.0040 (15)	−0.0045 (16)
O7	0.035 (2)	0.0182 (18)	0.0184 (17)	−0.0110 (17)	−0.0005 (15)	−0.0025 (14)
O8	0.0233 (19)	0.0223 (19)	0.0205 (17)	−0.0085 (17)	0.0006 (14)	−0.0028 (14)
O9	0.0236 (18)	0.0159 (17)	0.0204 (17)	−0.0075 (15)	−0.0049 (14)	−0.0032 (14)
O10	0.031 (2)	0.0187 (19)	0.0239 (19)	−0.0076 (17)	−0.0105 (16)	0.0004 (15)
O11	0.027 (2)	0.031 (2)	0.0206 (18)	−0.0103 (18)	−0.0087 (15)	−0.0080 (16)
O12	0.0256 (19)	0.0220 (18)	0.0216 (17)	−0.0085 (16)	−0.0068 (14)	−0.0036 (14)
O13	0.052 (3)	0.026 (2)	0.0247 (19)	−0.0127 (19)	0.0007 (18)	−0.0055 (16)
O14	0.040 (2)	0.0213 (19)	0.035 (2)	−0.0134 (18)	−0.0141 (17)	−0.0036 (16)
O15	0.035 (2)	0.038 (2)	0.0256 (19)	−0.0154 (19)	−0.0090 (17)	0.0014 (17)
O16	0.058 (3)	0.028 (2)	0.025 (2)	−0.003 (2)	0.0015 (19)	−0.0096 (18)
O17	0.035 (2)	0.054 (3)	0.031 (2)	−0.018 (2)	0.0026 (17)	−0.021 (2)
O18	0.034 (2)	0.025 (2)	0.030 (2)	−0.0073 (18)	0.0042 (17)	−0.0099 (17)
N1	0.0173 (19)	0.017 (2)	0.0138 (18)	−0.0063 (17)	0.0002 (15)	−0.0022 (15)
N2	0.024 (2)	0.020 (2)	0.0183 (19)	−0.0097 (18)	0.0009 (16)	−0.0095 (16)
N3	0.0168 (19)	0.018 (2)	0.0181 (19)	−0.0070 (17)	0.0006 (15)	−0.0076 (16)
N4	0.020 (2)	0.021 (2)	0.021 (2)	−0.0089 (19)	0.0018 (17)	−0.0063 (18)
N5	0.028 (2)	0.024 (2)	0.019 (2)	−0.011 (2)	−0.0001 (18)	−0.0082 (18)
N6	0.023 (2)	0.023 (2)	0.017 (2)	−0.0074 (19)	−0.0015 (17)	−0.0042 (18)
N7	0.024 (2)	0.024 (2)	0.019 (2)	−0.009 (2)	−0.0005 (17)	−0.0032 (18)
N8	0.036 (3)	0.026 (2)	0.021 (2)	−0.013 (2)	−0.0019 (19)	−0.0062 (19)
N9	0.025 (2)	0.027 (2)	0.019 (2)	−0.013 (2)	0.0031 (17)	−0.0066 (18)

Geometric parameters (Å, °)

Y1—O5	2.362 (3)	C30—C31	1.401 (7)
Y1—O9	2.374 (3)	C30—H30	0.9500
Y1—O8	2.386 (3)	C31—N5	1.325 (6)
Y1—O12	2.398 (3)	C31—H31	0.9500
Y1—O1	2.415 (3)	C32—N5	1.350 (6)
Y1—O4	2.421 (3)	C32—C33	1.438 (7)
Y1—N3	2.481 (4)	C33—N4	1.348 (6)
Y1—N2	2.490 (4)	C34—N6	1.331 (6)
Y1—N1	2.500 (4)	C34—C35	1.384 (7)
S1—O13	1.513 (4)	C34—H34	0.9500
S1—C59	1.774 (6)	C35—C36	1.362 (7)
S1—C58	1.786 (5)	C35—H35	0.9500
C1—O2	1.244 (6)	C36—C37	1.410 (7)
C1—O1	1.263 (6)	C36—H36	0.9500
C1—C2	1.520 (7)	C37—C45	1.411 (7)
C2—N1	1.339 (6)	C37—C38	1.425 (7)
C2—C3	1.384 (6)	C38—C39	1.355 (7)

C3—C4	1.394 (7)	C38—H38	0.9500
C3—H3	0.9500	C39—C40	1.428 (7)
C4—C5	1.369 (7)	C39—H39	0.9500
C4—H4	0.9500	C40—C44	1.401 (7)
C5—C6	1.392 (7)	C40—C41	1.411 (7)
C5—H5	0.9500	C41—C42	1.349 (8)
C6—N1	1.333 (6)	C41—H41	0.9500
C6—C7	1.516 (7)	C42—C43	1.407 (8)
C7—O3	1.240 (6)	C42—H42	0.9500
C7—O4	1.269 (6)	C43—N7	1.328 (6)
C8—O6	1.233 (6)	C43—H43	0.9500
C8—O5	1.261 (6)	C44—N7	1.360 (6)
C8—C9	1.530 (7)	C44—C45	1.449 (7)
C9—N2	1.332 (6)	C45—N6	1.345 (6)
C9—C10	1.394 (7)	C46—N8	1.316 (6)
C10—C11	1.390 (7)	C46—C47	1.400 (8)
C10—H10	0.9500	C46—H46	0.9500
C11—C12	1.387 (7)	C47—C48	1.363 (8)
C11—H11	0.9500	C47—H47	0.9500
C12—C13	1.381 (7)	C48—C49	1.414 (7)
C12—H12	0.9500	C48—H48	0.9500
C13—N2	1.348 (6)	C49—C57	1.411 (7)
C13—C14	1.511 (7)	C49—C50	1.434 (7)
C14—O7	1.243 (5)	C50—C51	1.346 (7)
C14—O8	1.260 (6)	C50—H50	0.9500
C15—O10	1.247 (6)	C51—C52	1.425 (7)
C15—O9	1.255 (6)	C51—H51	0.9500
C15—C16	1.522 (6)	C52—C56	1.399 (7)
C16—N3	1.341 (6)	C52—C53	1.414 (7)
C16—C17	1.387 (6)	C53—C54	1.366 (7)
C17—C18	1.403 (7)	C53—H53	0.9500
C17—H17	0.9500	C54—C55	1.383 (7)
C18—C19	1.379 (7)	C54—H54	0.9500
C18—H18	0.9500	C55—N9	1.328 (6)
C19—C20	1.395 (6)	C55—H55	0.9500
C19—H19	0.9500	C56—N9	1.356 (6)
C20—N3	1.336 (6)	C56—C57	1.445 (7)
C20—C21	1.516 (7)	C57—N8	1.348 (6)
C21—O11	1.242 (6)	C58—H58A	0.9800
C21—O12	1.264 (6)	C58—H58B	0.9800
C22—N4	1.335 (6)	C58—H58C	0.9800
C22—C23	1.371 (7)	C59—H59A	0.9800
C22—H22	0.9500	C59—H59B	0.9800
C23—C24	1.364 (7)	C59—H59C	0.9800
C23—H23	0.9500	O14—H14A	0.9499
C24—C25	1.410 (7)	O14—H14B	0.9500
C24—H24	0.9500	O15—H15A	0.9501
C25—C33	1.417 (7)	O15—H15B	0.9501
C25—C26	1.432 (7)	O16—H16A	0.9499

C26—C27	1.357 (8)	O16—H16B	0.9501
C26—H26	0.9500	O17—H17A	0.9500
C27—C28	1.453 (7)	O17—H17B	0.9499
C27—H27	0.9500	O18—H18A	0.9499
C28—C32	1.396 (7)	O18—H18B	0.9502
C28—C29	1.398 (7)	N4—H4A	0.9499
C29—C30	1.370 (7)	N6—H6A	0.9501
C29—H29	0.9500	N9—H9	0.9500
O5—Y1—O9	80.12 (11)	C29—C30—H30	120.3
O5—Y1—O8	129.11 (11)	C31—C30—H30	120.3
O9—Y1—O8	143.86 (11)	N5—C31—C30	123.9 (5)
O5—Y1—O12	87.24 (11)	N5—C31—H31	118.1
O9—Y1—O12	129.23 (11)	C30—C31—H31	118.1
O8—Y1—O12	78.83 (11)	N5—C32—C28	124.3 (5)
O5—Y1—O1	146.72 (11)	N5—C32—C33	116.6 (4)
O9—Y1—O1	85.57 (11)	C28—C32—C33	119.1 (5)
O8—Y1—O1	77.80 (11)	N4—C33—C25	119.3 (5)
O12—Y1—O1	78.82 (11)	N4—C33—C32	120.2 (4)
O5—Y1—O4	77.91 (11)	C25—C33—C32	120.5 (5)
O9—Y1—O4	78.84 (11)	N6—C34—C35	119.8 (5)
O8—Y1—O4	86.76 (11)	N6—C34—H34	120.1
O12—Y1—O4	145.62 (11)	C35—C34—H34	120.1
O1—Y1—O4	128.50 (11)	C36—C35—C34	119.7 (5)
O5—Y1—N3	74.91 (12)	C36—C35—H35	120.2
O9—Y1—N3	64.97 (11)	C34—C35—H35	120.2
O8—Y1—N3	135.60 (12)	C35—C36—C37	120.8 (5)
O12—Y1—N3	64.26 (12)	C35—C36—H36	119.6
O1—Y1—N3	71.81 (11)	C37—C36—H36	119.6
O4—Y1—N3	137.61 (12)	C36—C37—C45	117.1 (5)
O5—Y1—N2	64.65 (12)	C36—C37—C38	123.6 (5)
O9—Y1—N2	137.89 (12)	C45—C37—C38	119.3 (5)
O8—Y1—N2	64.46 (12)	C39—C38—C37	121.3 (4)
O12—Y1—N2	73.53 (12)	C39—C38—H38	119.4
O1—Y1—N2	136.49 (12)	C37—C38—H38	119.4
O4—Y1—N2	72.09 (12)	C38—C39—C40	120.3 (5)
N3—Y1—N2	121.88 (12)	C38—C39—H39	119.8
O5—Y1—N1	137.25 (12)	C40—C39—H39	119.8
O9—Y1—N1	74.06 (11)	C44—C40—C41	116.9 (5)
O8—Y1—N1	69.83 (12)	C44—C40—C39	120.9 (5)
O12—Y1—N1	135.39 (11)	C41—C40—C39	122.2 (5)
O1—Y1—N1	64.36 (11)	C42—C41—C40	119.6 (5)
O4—Y1—N1	64.18 (12)	C42—C41—H41	120.2
N3—Y1—N1	121.09 (13)	C40—C41—H41	120.2
N2—Y1—N1	116.97 (12)	C41—C42—C43	119.3 (5)
O13—S1—C59	106.4 (3)	C41—C42—H42	120.3
O13—S1—C58	105.0 (3)	C43—C42—H42	120.3
C59—S1—C58	98.2 (3)	N7—C43—C42	123.7 (5)
O2—C1—O1	126.5 (5)	N7—C43—H43	118.1
O2—C1—C2	118.4 (4)	C42—C43—H43	118.1

O1—C1—C2	115.1 (4)	N7—C44—C40	124.1 (5)
N1—C2—C3	121.5 (4)	N7—C44—C45	117.7 (4)
N1—C2—C1	114.7 (4)	C40—C44—C45	118.2 (4)
C3—C2—C1	123.8 (4)	N6—C45—C37	119.6 (5)
C2—C3—C4	118.5 (5)	N6—C45—C44	120.5 (4)
C2—C3—H3	120.7	C37—C45—C44	119.9 (4)
C4—C3—H3	120.7	N8—C46—C47	124.0 (5)
C5—C4—C3	119.8 (5)	N8—C46—H46	118.0
C5—C4—H4	120.1	C47—C46—H46	118.0
C3—C4—H4	120.1	C48—C47—C46	118.8 (5)
C4—C5—C6	118.3 (4)	C48—C47—H47	120.6
C4—C5—H5	120.9	C46—C47—H47	120.6
C6—C5—H5	120.9	C47—C48—C49	119.9 (5)
N1—C6—C5	122.1 (4)	C47—C48—H48	120.1
N1—C6—C7	114.6 (4)	C49—C48—H48	120.1
C5—C6—C7	123.3 (4)	C57—C49—C48	115.9 (5)
O3—C7—O4	125.5 (5)	C57—C49—C50	120.2 (5)
O3—C7—C6	119.1 (4)	C48—C49—C50	123.9 (5)
O4—C7—C6	115.4 (4)	C51—C50—C49	120.1 (5)
O6—C8—O5	128.2 (5)	C51—C50—H50	120.0
O6—C8—C9	117.1 (5)	C49—C50—H50	120.0
O5—C8—C9	114.7 (4)	C50—C51—C52	122.3 (5)
N2—C9—C10	121.4 (5)	C50—C51—H51	118.9
N2—C9—C8	113.8 (4)	C52—C51—H51	118.9
C10—C9—C8	124.7 (4)	C56—C52—C53	117.8 (5)
C11—C10—C9	118.4 (5)	C56—C52—C51	118.6 (4)
C11—C10—H10	120.8	C53—C52—C51	123.6 (5)
C9—C10—H10	120.8	C54—C53—C52	119.7 (5)
C12—C11—C10	119.5 (5)	C54—C53—H53	120.1
C12—C11—H11	120.2	C52—C53—H53	120.1
C10—C11—H11	120.2	C53—C54—C55	119.9 (5)
C13—C12—C11	119.0 (5)	C53—C54—H54	120.0
C13—C12—H12	120.5	C55—C54—H54	120.0
C11—C12—H12	120.5	N9—C55—C54	120.5 (5)
N2—C13—C12	121.2 (5)	N9—C55—H55	119.7
N2—C13—C14	113.9 (4)	C54—C55—H55	119.7
C12—C13—C14	124.9 (4)	N9—C56—C52	120.2 (4)
O7—C14—O8	126.4 (4)	N9—C56—C57	119.2 (5)
O7—C14—C13	118.1 (4)	C52—C56—C57	120.6 (4)
O8—C14—C13	115.5 (4)	N8—C57—C49	124.3 (5)
O10—C15—O9	126.7 (4)	N8—C57—C56	117.5 (4)
O10—C15—C16	118.0 (4)	C49—C57—C56	118.2 (5)
O9—C15—C16	115.3 (4)	S1—C58—H58A	109.5
N3—C16—C17	121.6 (4)	S1—C58—H58B	109.5
N3—C16—C15	114.1 (4)	H58A—C58—H58B	109.5
C17—C16—C15	124.3 (4)	S1—C58—H58C	109.5
C16—C17—C18	118.7 (4)	H58A—C58—H58C	109.5
C16—C17—H17	120.7	H58B—C58—H58C	109.5
C18—C17—H17	120.7	S1—C59—H59A	109.5

C19—C18—C17	119.2 (5)	S1—C59—H59B	109.5
C19—C18—H18	120.4	H59A—C59—H59B	109.5
C17—C18—H18	120.4	S1—C59—H59C	109.5
C18—C19—C20	118.8 (4)	H59A—C59—H59C	109.5
C18—C19—H19	120.6	H59B—C59—H59C	109.5
C20—C19—H19	120.6	C1—O1—Y1	125.6 (3)
N3—C20—C19	121.8 (4)	C7—O4—Y1	125.4 (3)
N3—C20—C21	113.9 (4)	C8—O5—Y1	126.9 (3)
C19—C20—C21	124.3 (4)	C14—O8—Y1	126.2 (3)
O11—C21—O12	126.5 (5)	C15—O9—Y1	125.9 (3)
O11—C21—C20	118.3 (4)	C21—O12—Y1	125.8 (3)
O12—C21—C20	115.1 (4)	H14A—O14—H14B	102.1
N4—C22—C23	119.9 (5)	H15A—O15—H15B	90.8
N4—C22—H22	120.0	H16A—O16—H16B	105.2
C23—C22—H22	120.0	H17A—O17—H17B	113.6
C24—C23—C22	120.4 (5)	H18A—O18—H18B	118.2
C24—C23—H23	119.8	C6—N1—C2	119.7 (4)
C22—C23—H23	119.8	C6—N1—Y1	120.4 (3)
C23—C24—C25	120.1 (5)	C2—N1—Y1	119.9 (3)
C23—C24—H24	119.9	C9—N2—C13	120.4 (4)
C25—C24—H24	119.9	C9—N2—Y1	119.8 (3)
C24—C25—C33	117.4 (5)	C13—N2—Y1	119.8 (3)
C24—C25—C26	123.7 (5)	C20—N3—C16	120.0 (4)
C33—C25—C26	118.9 (5)	C20—N3—Y1	120.7 (3)
C27—C26—C25	121.0 (5)	C16—N3—Y1	119.4 (3)
C27—C26—H26	119.5	C22—N4—C33	122.6 (5)
C25—C26—H26	119.5	C22—N4—H4A	116.8
C26—C27—C28	120.7 (5)	C33—N4—H4A	119.6
C26—C27—H27	119.7	C31—N5—C32	116.2 (4)
C28—C27—H27	119.7	C34—N6—C45	123.1 (4)
C32—C28—C29	117.8 (5)	C34—N6—H6A	118.6
C32—C28—C27	119.8 (5)	C45—N6—H6A	118.1
C29—C28—C27	122.4 (5)	C43—N7—C44	116.3 (4)
C30—C29—C28	118.4 (5)	C46—N8—C57	117.1 (5)
C30—C29—H29	120.8	C55—N9—C56	121.8 (5)
C28—C29—H29	120.8	C55—N9—H9	118.2
C29—C30—C31	119.3 (5)	C56—N9—H9	119.3
O2—C1—C2—N1	172.6 (4)	N3—Y1—O4—C7	112.1 (4)
O1—C1—C2—N1	−5.4 (6)	N2—Y1—O4—C7	−129.9 (4)
O2—C1—C2—C3	−5.0 (8)	N1—Y1—O4—C7	3.4 (4)
O1—C1—C2—C3	176.9 (5)	O6—C8—O5—Y1	−176.2 (4)
N1—C2—C3—C4	−2.0 (7)	C9—C8—O5—Y1	4.1 (6)
C1—C2—C3—C4	175.5 (5)	O9—Y1—O5—C8	153.6 (4)
C2—C3—C4—C5	1.2 (7)	O8—Y1—O5—C8	−2.6 (4)
C3—C4—C5—C6	0.5 (7)	O12—Y1—O5—C8	−75.8 (4)
C4—C5—C6—N1	−1.4 (7)	O1—Y1—O5—C8	−140.5 (4)
C4—C5—C6—C7	179.4 (5)	O4—Y1—O5—C8	73.0 (4)
N1—C6—C7—O3	−179.5 (5)	N3—Y1—O5—C8	−139.9 (4)
C5—C6—C7—O3	−0.2 (7)	N2—Y1—O5—C8	−2.7 (4)

N1—C6—C7—O4	0.6 (6)	N1—Y1—O5—C8	100.4 (4)
C5—C6—C7—O4	179.8 (5)	O7—C14—O8—Y1	−176.1 (3)
O6—C8—C9—N2	177.3 (4)	C13—C14—O8—Y1	2.6 (5)
O5—C8—C9—N2	−3.0 (6)	O5—Y1—O8—C14	−1.9 (4)
O6—C8—C9—C10	−4.1 (7)	O9—Y1—O8—C14	−139.5 (3)
O5—C8—C9—C10	175.6 (4)	O12—Y1—O8—C14	75.2 (4)
N2—C9—C10—C11	−1.2 (7)	O1—Y1—O8—C14	156.0 (4)
C8—C9—C10—C11	−179.8 (4)	O4—Y1—O8—C14	−73.4 (4)
C9—C10—C11—C12	−0.9 (7)	N3—Y1—O8—C14	108.7 (4)
C10—C11—C12—C13	1.8 (7)	N2—Y1—O8—C14	−1.7 (3)
C11—C12—C13—N2	−0.6 (7)	N1—Y1—O8—C14	−137.1 (4)
C11—C12—C13—C14	177.4 (4)	O10—C15—O9—Y1	−172.5 (4)
N2—C13—C14—O7	177.0 (4)	C16—C15—O9—Y1	7.1 (6)
C12—C13—C14—O7	−1.2 (7)	O5—Y1—O9—C15	72.6 (4)
N2—C13—C14—O8	−1.9 (6)	O8—Y1—O9—C15	−139.5 (3)
C12—C13—C14—O8	179.9 (4)	O12—Y1—O9—C15	−5.6 (4)
O10—C15—C16—N3	175.4 (4)	O1—Y1—O9—C15	−77.3 (4)
O9—C15—C16—N3	−4.2 (6)	O4—Y1—O9—C15	152.1 (4)
O10—C15—C16—C17	−4.1 (7)	N3—Y1—O9—C15	−5.3 (4)
O9—C15—C16—C17	176.3 (4)	N2—Y1—O9—C15	105.4 (4)
N3—C16—C17—C18	0.6 (7)	N1—Y1—O9—C15	−141.8 (4)
C15—C16—C17—C18	−179.9 (5)	O11—C21—O12—Y1	−173.9 (4)
C16—C17—C18—C19	1.2 (8)	C20—C21—O12—Y1	7.1 (6)
C17—C18—C19—C20	−2.8 (8)	O5—Y1—O12—C21	−79.9 (4)
C18—C19—C20—N3	2.6 (8)	O9—Y1—O12—C21	−5.0 (4)
C18—C19—C20—C21	−178.5 (5)	O8—Y1—O12—C21	149.4 (4)
N3—C20—C21—O11	176.7 (4)	O1—Y1—O12—C21	69.8 (4)
C19—C20—C21—O11	−2.2 (7)	O4—Y1—O12—C21	−143.6 (3)
N3—C20—C21—O12	−4.2 (6)	N3—Y1—O12—C21	−5.3 (4)
C19—C20—C21—O12	176.9 (5)	N2—Y1—O12—C21	−144.2 (4)
N4—C22—C23—C24	−0.2 (8)	N1—Y1—O12—C21	103.8 (4)
C22—C23—C24—C25	0.1 (8)	C5—C6—N1—C2	0.6 (7)
C23—C24—C25—C33	2.5 (7)	C7—C6—N1—C2	179.9 (4)
C23—C24—C25—C26	−178.6 (5)	C5—C6—N1—Y1	−176.9 (4)
C24—C25—C26—C27	−178.2 (5)	C7—C6—N1—Y1	2.3 (5)
C33—C25—C26—C27	0.7 (7)	C3—C2—N1—C6	1.2 (7)
C25—C26—C27—C28	0.7 (8)	C1—C2—N1—C6	−176.6 (4)
C26—C27—C28—C32	−0.4 (7)	C3—C2—N1—Y1	178.7 (3)
C26—C27—C28—C29	178.7 (5)	C1—C2—N1—Y1	1.0 (5)
C32—C28—C29—C30	0.3 (7)	O5—Y1—N1—C6	−32.8 (4)
C27—C28—C29—C30	−178.8 (5)	O9—Y1—N1—C6	−87.9 (3)
C28—C29—C30—C31	1.8 (7)	O8—Y1—N1—C6	93.5 (3)
C29—C30—C31—N5	−2.1 (8)	O12—Y1—N1—C6	141.7 (3)
C29—C28—C32—N5	−2.4 (7)	O1—Y1—N1—C6	179.3 (4)
C27—C28—C32—N5	176.7 (5)	O4—Y1—N1—C6	−2.8 (3)
C29—C28—C32—C33	179.5 (4)	N3—Y1—N1—C6	−134.6 (3)
C27—C28—C32—C33	−1.4 (7)	N2—Y1—N1—C6	48.1 (4)
C24—C25—C33—N4	−5.1 (7)	O5—Y1—N1—C2	149.7 (3)
C26—C25—C33—N4	175.9 (4)	O9—Y1—N1—C2	94.5 (3)

C24—C25—C33—C32	176.4 (4)	O8—Y1—N1—C2	−84.0 (3)
C26—C25—C33—C32	−2.5 (7)	O12—Y1—N1—C2	−35.8 (4)
N5—C32—C33—N4	6.2 (7)	O1—Y1—N1—C2	1.8 (3)
C28—C32—C33—N4	−175.6 (4)	O4—Y1—N1—C2	179.6 (4)
N5—C32—C33—C25	−175.4 (4)	N3—Y1—N1—C2	47.9 (4)
C28—C32—C33—C25	2.9 (7)	N2—Y1—N1—C2	−129.4 (3)
N6—C34—C35—C36	−1.9 (8)	C10—C9—N2—C13	2.5 (7)
C34—C35—C36—C37	1.6 (8)	C8—C9—N2—C13	−178.8 (4)
C35—C36—C37—C45	−0.1 (7)	C10—C9—N2—Y1	−177.8 (3)
C35—C36—C37—C38	179.8 (5)	C8—C9—N2—Y1	0.8 (5)
C36—C37—C38—C39	178.5 (5)	C12—C13—N2—C9	−1.6 (7)
C45—C37—C38—C39	−1.6 (8)	C14—C13—N2—C9	−179.8 (4)
C37—C38—C39—C40	2.0 (8)	C12—C13—N2—Y1	178.7 (3)
C38—C39—C40—C44	1.3 (7)	C14—C13—N2—Y1	0.5 (5)
C38—C39—C40—C41	178.6 (5)	O5—Y1—N2—C9	0.7 (3)
C44—C40—C41—C42	−0.7 (7)	O9—Y1—N2—C9	−35.5 (4)
C39—C40—C41—C42	−178.1 (5)	O8—Y1—N2—C9	−179.2 (4)
C40—C41—C42—C43	2.2 (8)	O12—Y1—N2—C9	95.5 (3)
C41—C42—C43—N7	−3.2 (8)	O1—Y1—N2—C9	148.3 (3)
C41—C40—C44—N7	−0.1 (7)	O4—Y1—N2—C9	−84.1 (3)
C39—C40—C44—N7	177.3 (5)	N3—Y1—N2—C9	51.3 (4)
C41—C40—C44—C45	177.8 (4)	N1—Y1—N2—C9	−131.5 (3)
C39—C40—C44—C45	−4.8 (7)	O5—Y1—N2—C13	−179.7 (4)
C36—C37—C45—N6	−1.0 (7)	O9—Y1—N2—C13	144.2 (3)
C38—C37—C45—N6	179.0 (4)	O8—Y1—N2—C13	0.4 (3)
C36—C37—C45—C44	178.0 (4)	O12—Y1—N2—C13	−84.8 (3)
C38—C37—C45—C44	−2.0 (7)	O1—Y1—N2—C13	−32.0 (4)
N7—C44—C45—N6	2.1 (7)	O4—Y1—N2—C13	95.5 (3)
C40—C44—C45—N6	−175.9 (4)	N3—Y1—N2—C13	−129.0 (3)
N7—C44—C45—C37	−176.9 (4)	N1—Y1—N2—C13	48.2 (4)
C40—C44—C45—C37	5.1 (7)	C19—C20—N3—C16	−0.8 (7)
N8—C46—C47—C48	0.9 (10)	C21—C20—N3—C16	−179.7 (4)
C46—C47—C48—C49	−0.3 (9)	C19—C20—N3—Y1	178.8 (3)
C47—C48—C49—C57	−1.2 (7)	C21—C20—N3—Y1	−0.1 (5)
C47—C48—C49—C50	179.7 (5)	C17—C16—N3—C20	−0.8 (7)
C57—C49—C50—C51	−0.1 (7)	C15—C16—N3—C20	179.6 (4)
C48—C49—C50—C51	179.0 (5)	C17—C16—N3—Y1	179.5 (3)
C49—C50—C51—C52	−0.3 (8)	C15—C16—N3—Y1	0.0 (5)
C50—C51—C52—C56	−0.6 (8)	O5—Y1—N3—C20	96.6 (3)
C50—C51—C52—C53	−179.3 (5)	O9—Y1—N3—C20	−177.4 (4)
C56—C52—C53—C54	2.0 (7)	O8—Y1—N3—C20	−34.6 (4)
C51—C52—C53—C54	−179.4 (5)	O12—Y1—N3—C20	2.3 (3)
C52—C53—C54—C55	−3.5 (8)	O1—Y1—N3—C20	−83.8 (3)
C53—C54—C55—N9	3.0 (8)	O4—Y1—N3—C20	148.5 (3)
C53—C52—C56—N9	0.1 (7)	N2—Y1—N3—C20	50.2 (4)
C51—C52—C56—N9	−178.6 (4)	N1—Y1—N3—C20	−126.9 (3)
C53—C52—C56—C57	−179.4 (4)	O5—Y1—N3—C16	−83.7 (3)
C51—C52—C56—C57	1.9 (7)	O9—Y1—N3—C16	2.2 (3)
C48—C49—C57—N8	2.4 (7)	O8—Y1—N3—C16	145.1 (3)

C50—C49—C57—N8	−178.4 (4)	O12—Y1—N3—C16	−178.0 (4)
C48—C49—C57—C56	−177.8 (4)	O1—Y1—N3—C16	95.9 (3)
C50—C49—C57—C56	1.3 (7)	O4—Y1—N3—C16	−31.8 (4)
N9—C56—C57—N8	−2.0 (7)	N2—Y1—N3—C16	−130.1 (3)
C52—C56—C57—N8	177.6 (4)	N1—Y1—N3—C16	52.8 (4)
N9—C56—C57—C49	178.2 (4)	C23—C22—N4—C33	−2.5 (7)
C52—C56—C57—C49	−2.2 (7)	C25—C33—N4—C22	5.3 (7)
O2—C1—O1—Y1	−169.9 (4)	C32—C33—N4—C22	−176.3 (4)
C2—C1—O1—Y1	7.9 (6)	C30—C31—N5—C32	0.0 (7)
O5—Y1—O1—C1	−144.4 (4)	C28—C32—N5—C31	2.2 (7)
O9—Y1—O1—C1	−79.9 (4)	C33—C32—N5—C31	−179.6 (4)
O8—Y1—O1—C1	67.8 (4)	C35—C34—N6—C45	0.7 (8)
O12—Y1—O1—C1	148.6 (4)	C37—C45—N6—C34	0.7 (7)
O4—Y1—O1—C1	−8.0 (4)	C44—C45—N6—C34	−178.2 (5)
N3—Y1—O1—C1	−145.0 (4)	C42—C43—N7—C44	2.3 (7)
N2—Y1—O1—C1	97.5 (4)	C40—C44—N7—C43	−0.7 (7)
N1—Y1—O1—C1	−5.5 (4)	C45—C44—N7—C43	−178.6 (4)
O3—C7—O4—Y1	176.5 (4)	C47—C46—N8—C57	0.3 (9)
C6—C7—O4—Y1	−3.5 (6)	C49—C57—N8—C46	−2.0 (8)
O5—Y1—O4—C7	163.1 (4)	C56—C57—N8—C46	178.3 (5)
O9—Y1—O4—C7	81.0 (4)	C54—C55—N9—C56	−0.9 (7)
O8—Y1—O4—C7	−65.7 (4)	C52—C56—N9—C55	−0.7 (7)
O12—Y1—O4—C7	−130.5 (4)	C57—C56—N9—C55	178.9 (4)
O1—Y1—O4—C7	5.9 (4)		

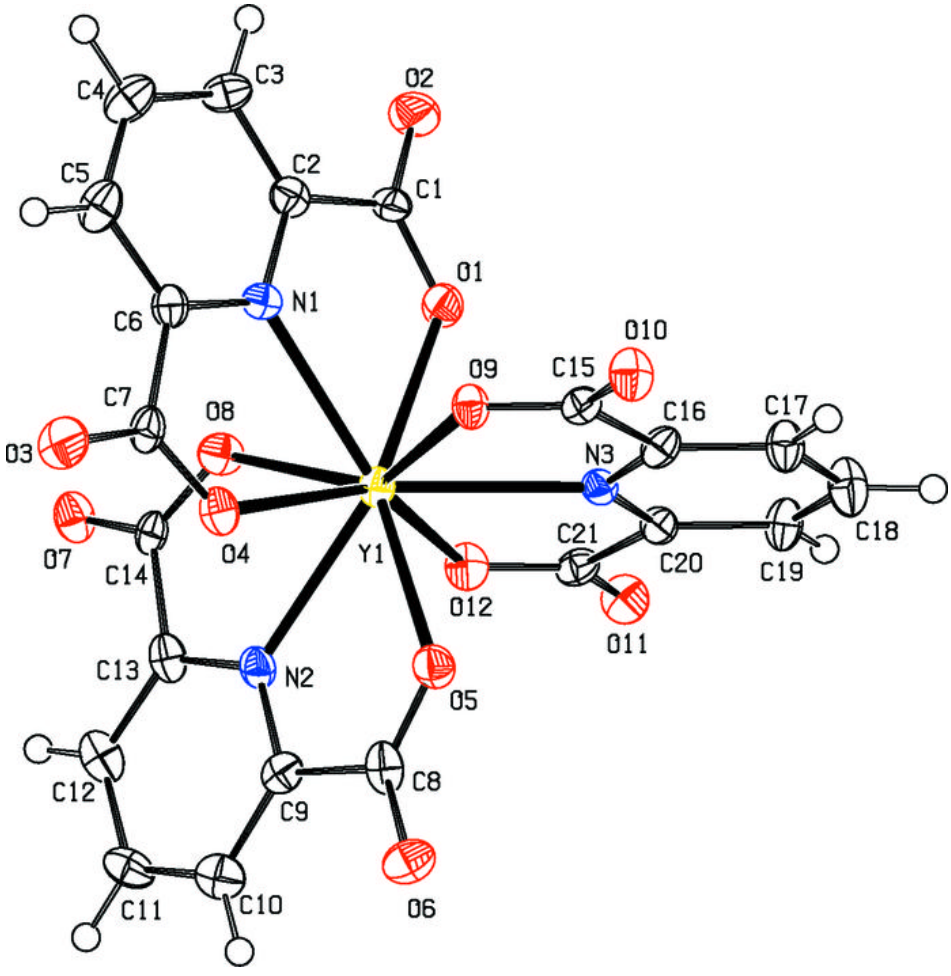
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O14—H14A···O10^{i}	0.95	1.84	2.734 (5)	156
O14—H14B···O3^{ii}	0.95	1.82	2.757 (5)	169
O15—H15A···O11^{i}	0.95	2.02	2.854 (5)	146
O15—H15B···O2	0.95	1.89	2.824 (5)	166
O16—H16A···O17^{iii}	0.95	1.73	2.678 (5)	175
O16—H16B···O15^{iv}	0.95	1.84	2.769 (5)	165
O17—H17A···O14^{v}	0.95	1.91	2.859 (5)	180
O17—H17B···O18^{vi}	0.95	2.03	2.804 (5)	138
O17—H17B···O6^{i}	0.95	2.60	3.192 (5)	121
O18—H18A···O13	0.95	1.85	2.789 (5)	169
O18—H18A···S1	0.95	2.77	3.650 (4)	155
O18—H18B···O4^{ii}	0.95	1.90	2.849 (5)	177
N4—H4A···O7	0.95	1.88	2.680 (5)	140
N6—H6A···O13	0.95	1.84	2.673 (5)	146
N9—H9···O16	0.95	1.69	2.612 (6)	161
C3—H3···O11^{i}	0.95	2.49	3.319 (7)	146
C5—H5···O6^{i}	0.95	2.59	3.277 (8)	129
C22—H22···O8	0.95	2.33	3.056 (6)	132
C29—H29···O6^{vii}	0.95	2.51	3.380 (7)	152

C31—H31···O11^{vi}	0.95	2.41	3.357 (7)	174
C34—H34···O18	0.95	2.53	3.446 (7)	162
C36—H36···O12^{viii}	0.95	2.46	3.384 (6)	164
C39—H39···O2^{ix}	0.95	2.54	3.438 (7)	159
C42—H42···O14^{v}	0.95	2.36	3.247 (7)	155
C54—H54···O9	0.95	2.44	3.275 (6)	146
C55—H55···O10	0.95	2.40	3.244 (7)	147
C59—H59A···O10	0.98	2.55	3.381 (9)	143
C58—H58C···Cg1 (N3,C16-C20)^{i}	0.98	2.84	3.424 (7)	119

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*+1, *y*−1, *z*; (iii) *x*, *y*−1, *z*; (iv) *x*, *y*−1, *z*+1; (v) *x*−1, *y*+1, *z*; (vi) *x*, *y*+1, *z*; (vii) *x*, *y*+1, *z*−1; (viii) *x*+1, *y*−1, *z*+1; (ix) *x*, *y*, *z*+1.

Fig. 1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C5
C2
C1
O1
N1
C6
O10
O9
C15
C7
C16
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O3
N3
O7
O4
Y1
C21
C18
C14
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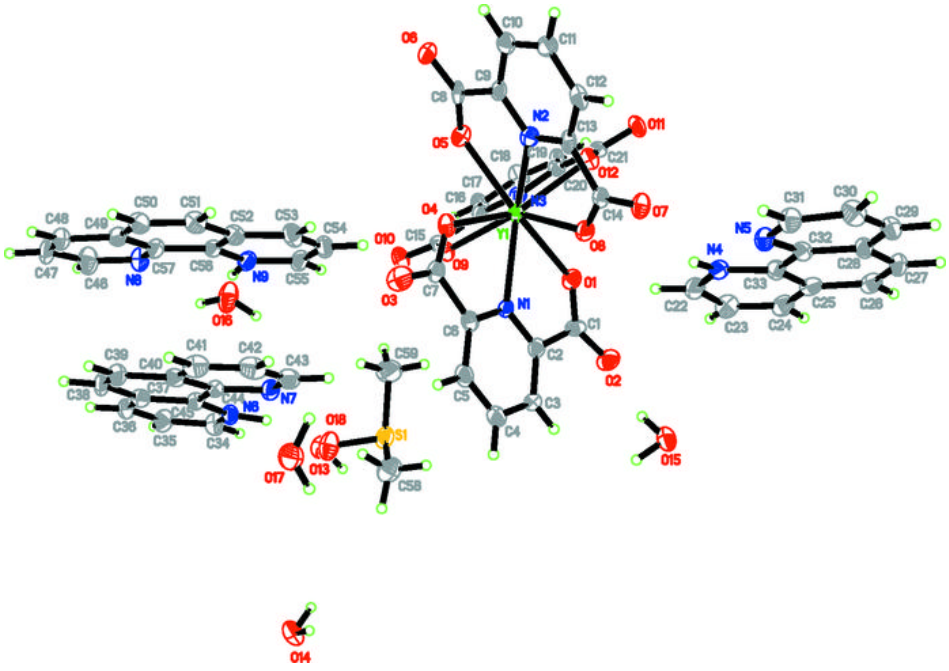
C19
O12
O11
C13
N2
O5
C12
C8
C9
O6
C11
C10

Fig. 2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C16
N3
C14
O7
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O8
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C7
O1
N1
C6
C1
C2
O2
C5
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C4
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C34
C31
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C28
C27
C33
C22
C25
C26
C23
C24

Fig. 3

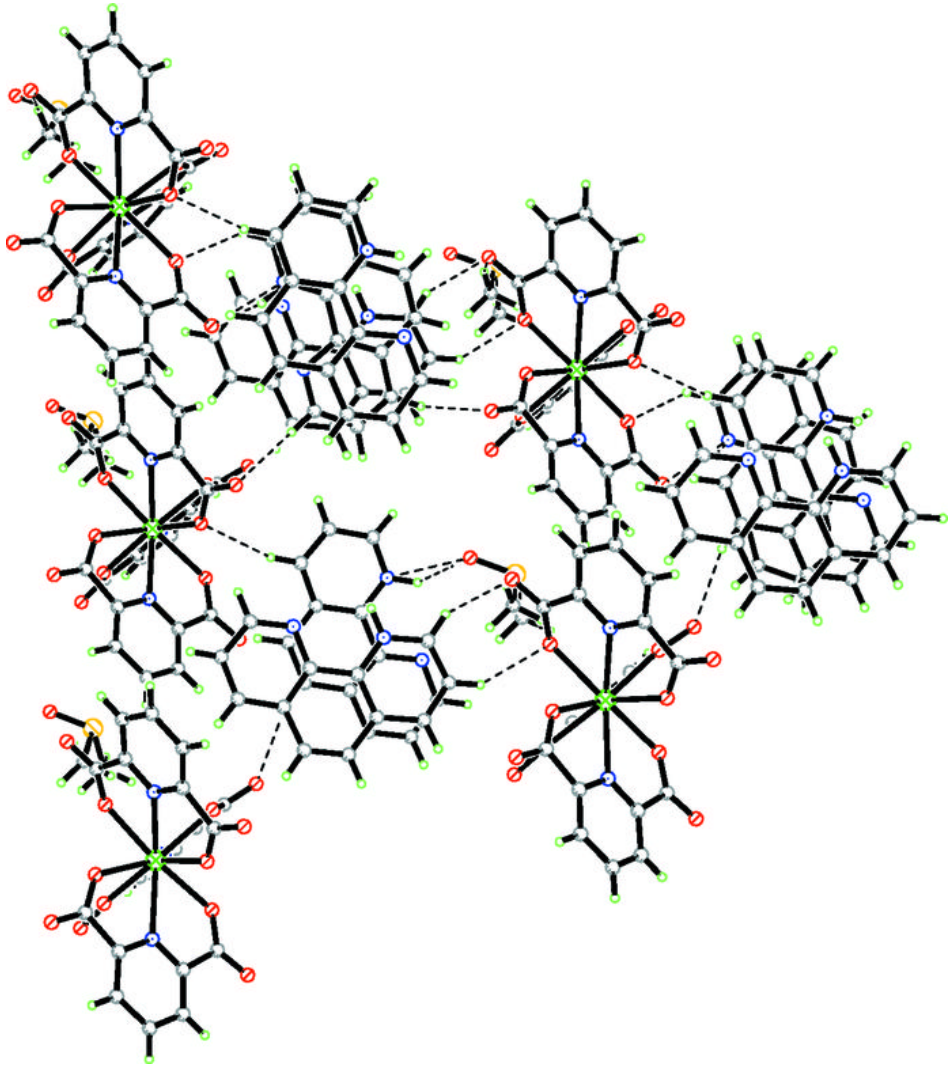


Fig. 4

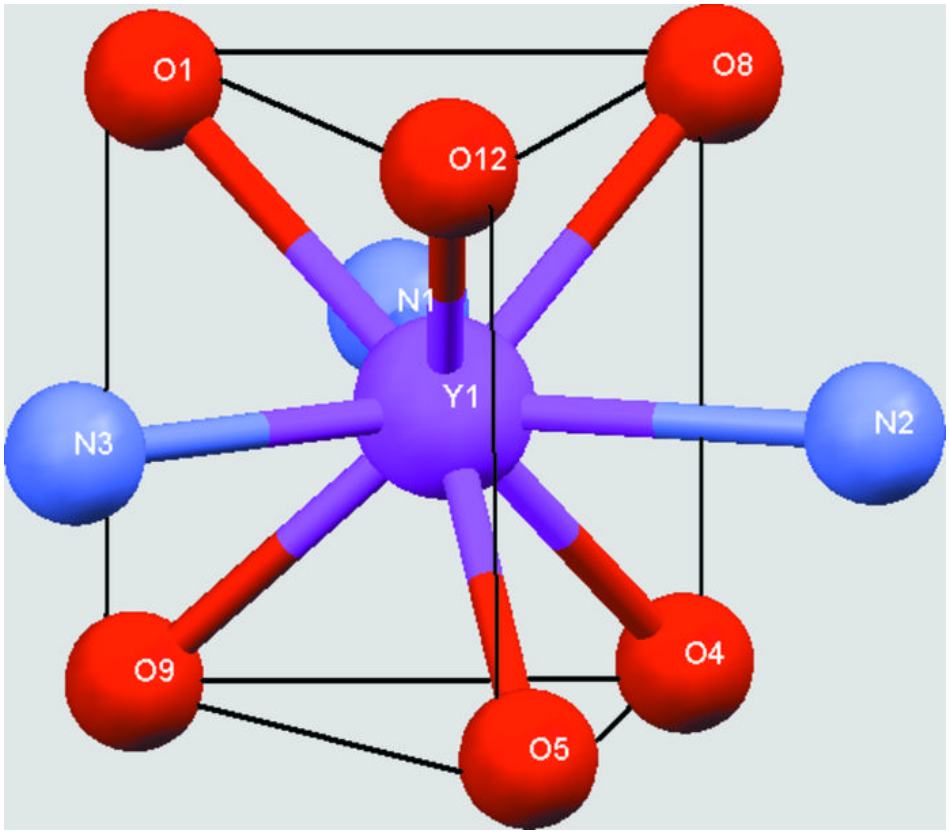


Fig. 5

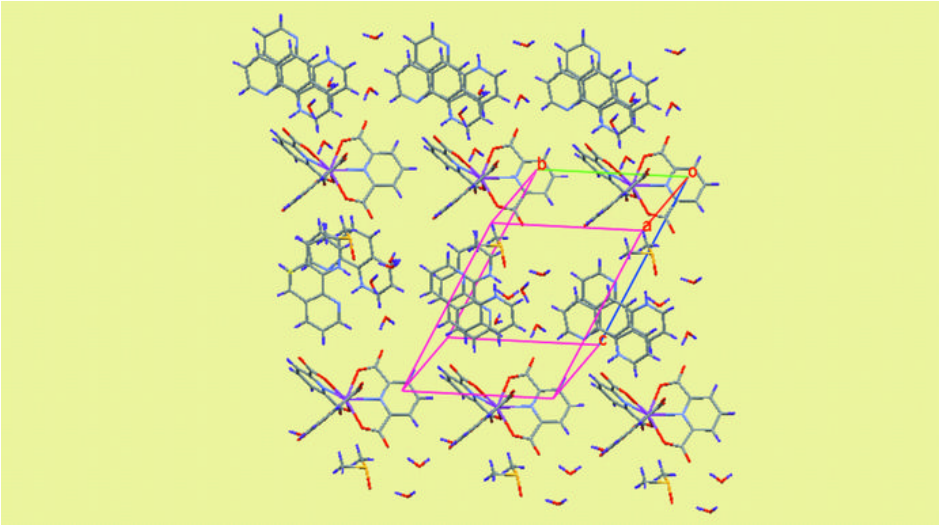


Fig. 6

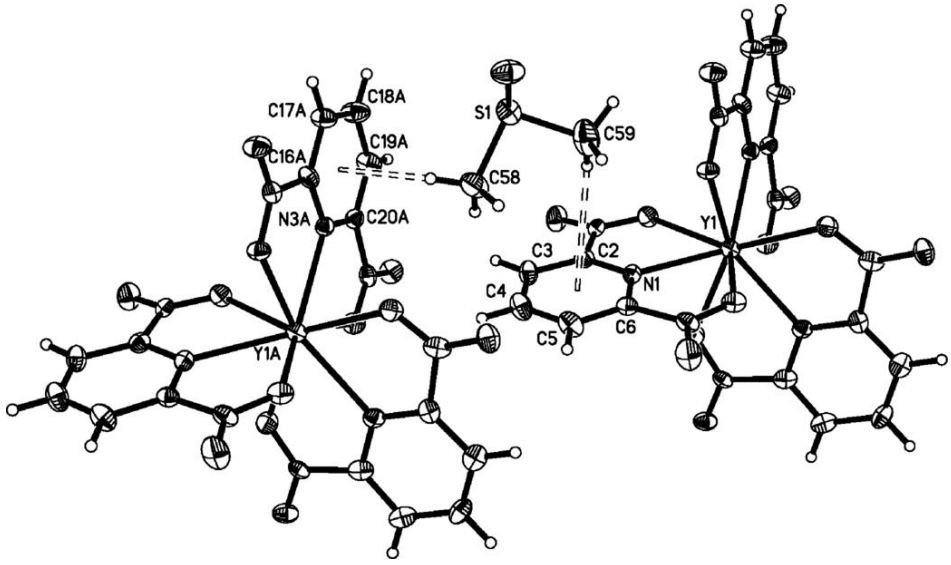
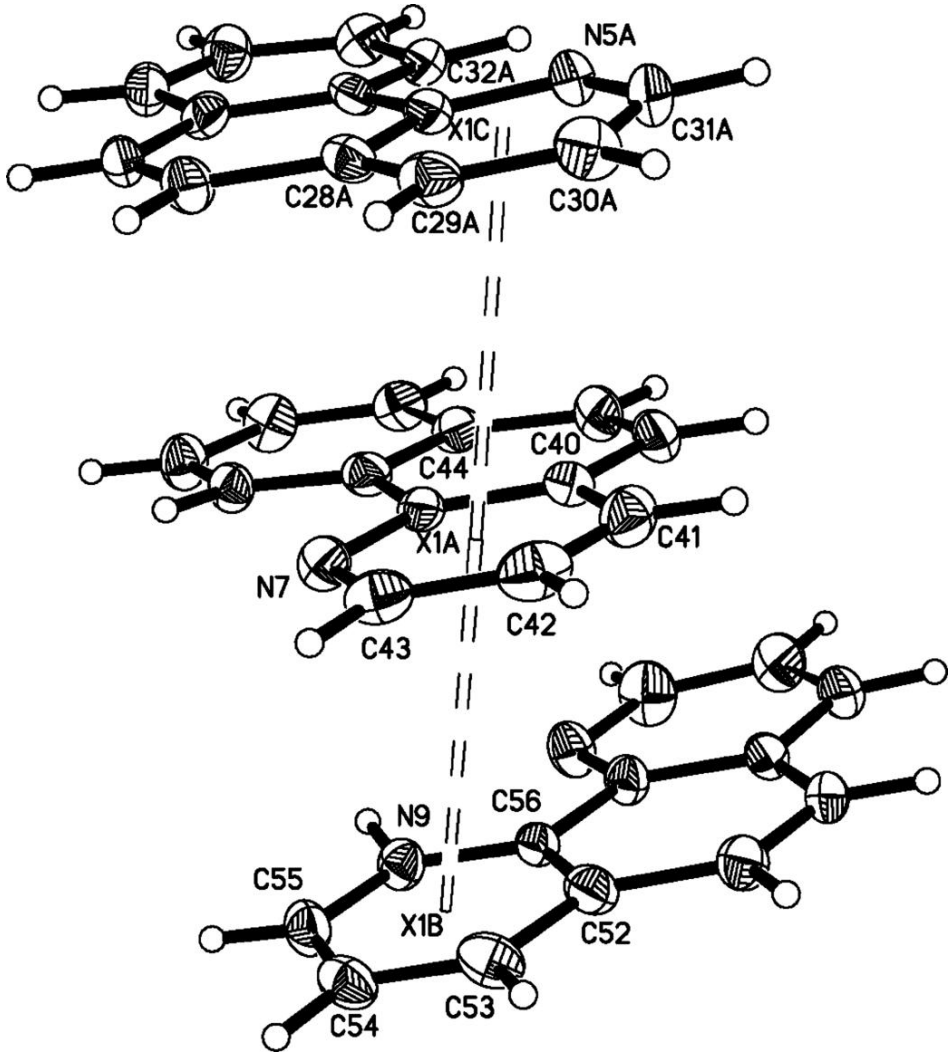


Fig. 7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C41
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C56
N9
C55
X1B
C52
C53
C54