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4,4′-Bipyridinediium triaquabis(pyridine-2,6-dicarboxylato)strontium(II) trihydrate

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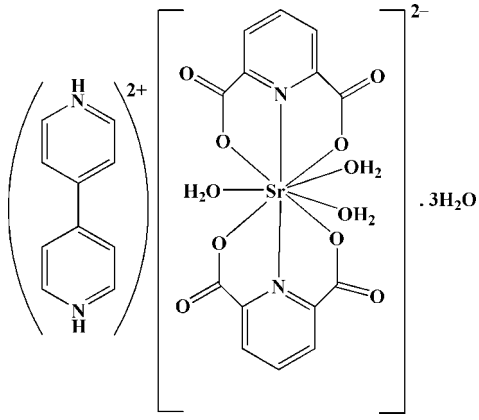
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.027; wR factor = 0.074; data-to-parameter ratio = 29.0.

The reaction of strontium(II) nitrate with pyridine-2,6-dicarboxylic acid, ($pydcH_2$) and 4,4′-bipyridine (bipy) in a 1:2:4 molar ratio leads to the formation of the title compound, $(C_{10}H_{10}N_2)[Sr(C_7H_3NO_4)_2(H_2O)_3]\cdot 3H_2O$, or $(bipyH_2)$-$[Sr(pydc)_2(H_2O)_3]\cdot 3H_2O$, in aqueous solution. This compound is composed of an anionic complex, $[Sr(pydc)_2(H_2O)_3]^{2-}$, a protonated 4,4′-bipyridine as a counter-ion, $(bipyH_2)^{2+}$ (site symmetry $\overline{1}$), and three uncoordinated water molecules. The anion is a nine-coordinate complex, with a distorted tricapped trigonal–prismatic geometry around the Sr^{II} atom. The coordination environment consists of two tridentate pyridine-2,6-dicarboxylate, $(pydc)^{2-}$, groups and three O atoms of the coordinated water molecules. In the crystal structure, intermolecular O—H···O, N—H···O and C—H···O hydrogen bonds, π–π stacking between two aromatic rings [with distances of 3.5723 (7)–3.7494 (7) Å] and C—O···π stacking [distance of 3.5228 (12) Å] connect the various components into a supramolecular structure.

Related literature

For related literature, see: Aghabozorg, Attar Gharamaleki, Ghadermaz *et al.* (2007); Aghabozorg, Attar Gharamaleki, Ghasemikhah *et al.* (2007); Aghabozorg, Daneshvar *et al.* (2007).



Experimental

Crystal data

$(C_{10}H_{10}N_2)[Sr(C_7H_3NO_4)_2(H_2O)_3]\cdot 3H_2O$
M_r = 684.12
Triclinic, $P\overline{1}$
a = 6.9994 (1) Å
b = 11.6876 (2) Å
c = 17.9748 (3) Å
α = 104.120 (1)°
β = 100.975 (1)°
γ = 95.901 (1)°
V = 1382.63 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.03 mm^{-1}
T = 296 (2) K
0.49 × 0.26 × 0.16 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.436, T_{max} = 0.737
32412 measured reflections
11270 independent reflections
10117 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.074
S = 1.07
11270 reflections
388 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sr1—O8	2.6199 (9)	Sr1—O1	2.6858 (9)
Sr1—O9	2.6223 (10)	Sr1—O4	2.6970 (9)
Sr1—O10	2.6239 (10)	Sr1—N2	2.7299 (10)
Sr1—O11	2.6580 (9)	Sr1—N1	2.7504 (10)
Sr1—O5	2.6633 (10)		
O8—Sr1—O10	77.70 (3)	O1—Sr1—N2	119.01 (3)
O8—Sr1—O11	87.84 (3)	O4—Sr1—N2	120.81 (3)
O10—Sr1—O11	70.77 (3)	O9—Sr1—N1	85.89 (3)
O9—Sr1—O5	69.08 (3)	O5—Sr1—N1	107.88 (3)
O1—Sr1—O4	118.22 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1S—H1A···O3S^{i}	0.95	1.90	2.8462 (17)	175
O1S—H1B···O6	0.94	1.81	2.7370 (16)	173
O2S—H2B···O6	0.95	1.79	2.7358 (16)	172
O2S—H2A···O3S^{ii}	0.95	1.83	2.7800 (15)	178
O3S—H3A···O3^{iii}	0.95	1.79	2.7216 (14)	166
O3S—H3B···O2	0.95	1.75	2.7016 (15)	175
O9—H9B···O2S^{iv}	0.95	1.85	2.8043 (15)	177
O10—H10B···O1S^{v}	0.95	1.85	2.8008 (15)	174
O10—H10A···O2^{vi}	0.95	1.84	2.7864 (14)	174
O11—H11B···O7^{vii}	0.95	1.74	2.6773 (13)	171
O11—H11A···O1^{vi}	0.95	1.91	2.8013 (13)	156
O11—H11A···O2^{vi}	0.95	2.63	3.4752 (14)	148
N3—H3C···O3^{iv}	0.95	1.60	2.5500 (13)	175
N4—H4C···O8^{i}	0.95	1.67	2.6081 (13)	171
N4—H4C···O7^{i}	0.95	2.57	3.1285 (15)	118
C16—H16···O5^{viii}	0.93	2.31	3.2097 (16)	162
C19—H19···O9	0.93	2.49	3.2130 (17)	135
C20—H20···O5	0.93	2.51	3.4087 (16)	162
C21—H21···O1^{i}	0.93	2.58	3.2867 (18)	133
C22—H22···O2S^{iv}	0.93	2.57	3.4867 (19)	167
C24—H24···O2S^{ix}	0.93	2.39	3.2888 (18)	164
C25—H25···O7^{i}	0.93	2.37	3.0280 (17)	127

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

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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2021).

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supplementary materials

Acta Cryst. (2007). E**63**, m3089-m3090 [**doi:10.1107/S1600536807058722**]

4,4'-Bipyridinediium triaquabis(pyridine-2,6-dicarboxylato)strontium(II) trihydrate

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Comment

Intermolecular intractions, such as hydrogen bonding, π-π stacking, ion pairing and donor-acceptor intractions, are famous for making aggregates of molecules. One or more of these interactions may result in the formation of specific and spontaneous self-associations or self-associated compounds. Research has shown that hydrogen bonding plays a key role in the preparation of self-assembled compounds. There is a very close relationship between hydrogen bonding and the formation of proton transfer compounds (Aghabozorg, Attar, Ghadermazi *et al.*, 2007; Aghabozorg, Attar, Ghasemikhah *et al.*, 2007; Aghabozorg, Daneshvar *et al.*, 2007).

Here, we report on the synthesis and crystal structure of the title compound, (I). Selected bond lengths and angles are given in Table 1. Compound (I) is composed of an anionic complex, $[Sr(pydc)_2(H_2O)_3]^{2-}$, a protonated 4,4'-bipyridine as a counter ion, $(bipyH_2)^{2+}$, and three uncoordinated water molecules (Fig. 1).

The Sr^{II} atom is nine-coordinated by two pyridine-2,6-dicarboxylate, $(pydc)^{2-}$, groups, which act as a tridentate ligand through two O atom and one N atom, and three O atoms of coordinated waters molecules. The dihedral angle between the two $(pydc)^{2-}$ planes is 37.30 (6)°.

The sum of bond angles, N2—Sr1—O4, O4—Sr1—O1 and O1—Sr1—N2 is equal to 358.04° and indicates that Sr^{II} is located in the center of the O1O4N2 plane. The three O atoms, O8, O10 and O11, form a triangle and atoms, O5, O9 and N1, form another triangle around the Sr^{II} atom. Considering the angles between the atoms (Table 1), it is found that they are almost eclipsed. So a prism consisting of the five O atoms and one N atom and three caps on its faces is proposed. The coordination polyhedron can be descibed as a highly distorted tricapped trigonal prism.

An important feature of compound (I) is the presence of π-π and C—O···π stacking interactions. The π-π stacking between aromatic rings *Cg*1 [*Cg*1: N1/C2—C6] and *Cg*3 [*Cg*3: N3/C17—C19] with distances of 3.5723 (7) Å (*x*, *y*, *z*), *Cg*2 [*Cg*2: N2/C9—C13] and *Cg*4 [*Cg*4: N4/C21—C25] with distances of 3.5941 (8)Å (1 − *x*, 1 − *y*, −*z*), *Cg*1 and *Cg*1 with distances of 3.6836 (7)Å (1 − *x*, −*y*, 1 − *z*) and *Cg*3 and *Cg*3 with distances of 3.7494 (7) Å (2 − *x*, 1 − *y*, 1 − *z*) are observed (Fig. 2). The C—O···π distances are 3.5228 (12) Å (−*x*, −*y*, −*z*) (Fig. 3). Intermolecular O—H···O, N—H···O and C—H···O hydrogen bonds with D···A distances ranging from 2.5500 (15) Å to 3.4867 (19) Å (Table 2) seem to be effective in the stabilization of the crystal structure. This results in the formation of an interesting supramolecular structure (Fig. 4).

Experimental

A solution of $Sr(NO_3)_2$ (106 mg, 0.5 mmol) in water (5 ml) was added to an aqueous solution of pyridine-2,6-dicarboxylic acid (167 mg, 1 mmol) and 4,4'-bipyridine (312 mg, 2 mmol) in water (10 ml) in a 1:2:4 molar ratio and refluxed for an hour. Colorless crystals of (I) were obtained after allowing the mixture to stand for two weeks at room temperature.

Refinement

(type here to add refinement details)

Figures

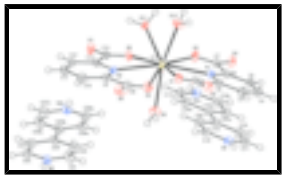

Fig. 1. The molecular structure of the title compound (I), with displacement ellipsoids drawn at the 50% probability level.

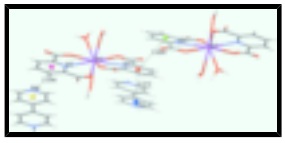

Fig. 2. π-π Stacking interactions between *Cg*1 [N1/C2—C6] and *Cg*3 [N3/C17—C19], *Cg*2 [N2/C9—C13] and *Cg*4 [N4/C21—C25] and two *Cg*1 [N1/C2—C6] of (I). The average distances between the planes are 3.5723 (7) Å (*x*, *y*, *z*), 3.5941 (8) Å (1 − *x*, 1 − *y*, −*z*) and 3.6836 (7) Å (1 − *x*, −*y*, 1 − *z*), respectively.

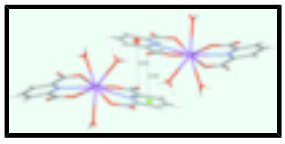

Fig. 3. The C—O···π stacking interactions of the carbonyl groups of the $(pydc)^{2-}$ fragments. The C—O···π distances [measured to the centre of the ring (N2/C9—C13)] are 3.5228 (12) Å (−*x*, −*y*, −*z*).

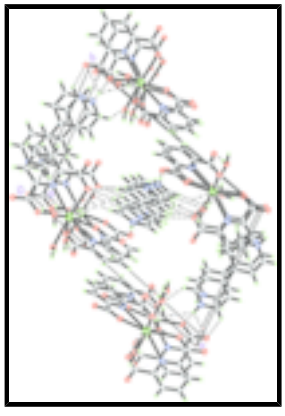

Fig. 4. The crystal packing of compound (I). Hydrogen bonds are shown as dashed lines.

4,4'-Bipyridindiium triaquabis(pyridine-2,6-dicarboxylato)strontium(II) trihydrate

Crystal data

$(C_{10}H_{10}N_2)[Sr(C_7H_3NO_4)_2(H_2O)_3]\cdot 3H_2O$	$Z = 2$
$M_r = 684.12$	$F_{000} = 700$
Triclinic, $P\overline{1}$	$D_x = 1.643$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.9994$ (1) Å	Cell parameters from 19317 reflections
$b = 11.6876$ (2) Å	$\theta = 2.4$–$30.6°$
$c = 17.9748$ (3) Å	$\mu = 2.03$ mm^{-1}
$\alpha = 104.120$ (1)°	$T = 296$ (2) K
$\beta = 100.975$ (1)°	Block, colourless

γ = 95.901 (1)°	0.49 × 0.26 × 0.16 mm
V = 1382.63 (4) Å^3	

Data collection

Bruker SMART 1000 diffractometer	11270 independent reflections
Radiation source: fine-focus sealed tube	10117 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.018
Detector resolution: 100 pixels mm^{-1}	θ_{max} = 36.0°
T = 296(2) K	θ_{min} = 1.2°
ω scans	h = −10→11
Absorption correction: multi-scan (SADABS; Bruker, 1998)	k = −19→16
T_{min} = 0.436, T_{max} = 0.737	l = −27→27
32412 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.027	H-atom parameters constrained
$wR(F^2)$ = 0.074	$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.5264P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
11270 reflections	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
388 parameters	$\Delta\rho_{min}$ = −0.45 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Sr1	0.307652 (15)	0.128882 (9)	0.237424 (6)	0.01445 (3)
O1	0.60785 (14)	0.00307 (8)	0.24267 (5)	0.02076 (16)

O1S	0.32246 (19)	0.72765 (10)	0.27767 (8)	0.0391 (3)
H1A	0.4569	0.7223	0.2961	0.047*
H1B	0.2497	0.6507	0.2622	0.047*
O2	0.82991 (15)	−0.08672 (9)	0.30428 (6)	0.02578 (19)
O2S	−0.26586 (17)	0.49429 (9)	0.23393 (7)	0.0313 (2)
H2B	−0.1292	0.5007	0.2344	0.038*
H2A	−0.2676	0.5677	0.2707	0.038*
O3	0.22149 (14)	0.25616 (9)	0.50121 (5)	0.02306 (18)
O3S	0.71963 (18)	−0.29136 (9)	0.34024 (6)	0.0293 (2)
H3A	0.7463	−0.2663	0.3961	0.035*
H3B	0.7656	−0.2212	0.3270	0.035*
O4	0.18013 (14)	0.20685 (10)	0.37060 (5)	0.02483 (19)
O5	0.26973 (16)	0.35859 (9)	0.26076 (6)	0.0273 (2)
O6	0.11805 (17)	0.50023 (9)	0.22108 (8)	0.0351 (3)
O7	0.24198 (16)	−0.03028 (9)	−0.03564 (5)	0.02638 (19)
O8	0.31399 (14)	0.00750 (8)	0.09486 (5)	0.01968 (16)
O9	0.63918 (15)	0.25817 (9)	0.23992 (7)	0.0274 (2)
H9A	0.7511	0.2240	0.2284	0.033*
H9B	0.6671	0.3385	0.2378	0.033*
O10	0.14922 (15)	−0.08710 (9)	0.23239 (7)	0.0273 (2)
H10B	0.2128	−0.1501	0.2450	0.033*
H10A	0.0341	−0.0885	0.2531	0.033*
O11	−0.08144 (13)	0.10537 (9)	0.19017 (5)	0.02129 (17)
H11B	−0.1249	0.0785	0.1345	0.026*
H11A	−0.1589	0.0581	0.2131	0.026*
N1	0.50015 (14)	0.09789 (9)	0.37780 (6)	0.01496 (16)
N2	0.20743 (15)	0.22243 (8)	0.11289 (6)	0.01635 (17)
N3	0.91685 (15)	0.35890 (9)	0.49464 (6)	0.01948 (18)
H3C	1.0254	0.3163	0.4964	0.023*
N4	0.41975 (17)	0.79713 (9)	0.05747 (7)	0.0220 (2)
H4C	0.3948	0.8769	0.0730	0.026*
C1	0.70090 (17)	−0.01926 (10)	0.30273 (7)	0.01692 (19)
C2	0.65680 (16)	0.04143 (10)	0.38089 (7)	0.01547 (18)
C3	0.77792 (18)	0.03998 (12)	0.45150 (7)	0.0205 (2)
H3	0.8856	−0.0005	0.4516	0.025*
C4	0.73572 (18)	0.09976 (12)	0.52175 (7)	0.0212 (2)
H4	0.8165	0.1020	0.5698	0.025*
C5	0.57031 (18)	0.15618 (11)	0.51890 (7)	0.0178 (2)
H5	0.5369	0.1960	0.5650	0.021*
C6	0.45556 (16)	0.15184 (10)	0.44566 (7)	0.01495 (18)
C7	0.27066 (17)	0.20877 (10)	0.43679 (7)	0.01640 (19)
C8	0.18459 (19)	0.40237 (11)	0.20962 (8)	0.0221 (2)
C9	0.15631 (17)	0.33162 (10)	0.12402 (8)	0.0192 (2)
C10	0.0827 (2)	0.37711 (12)	0.06158 (9)	0.0253 (2)
H10	0.0496	0.4536	0.0709	0.030*
C11	0.0593 (2)	0.30680 (13)	−0.01467 (9)	0.0258 (3)
H11	0.0097	0.3354	−0.0572	0.031*
C12	0.11055 (19)	0.19322 (12)	−0.02696 (8)	0.0215 (2)
H12	0.0952	0.1439	−0.0775	0.026*

C13	0.18595 (17)	0.15537 (10)	0.03903 (7)	0.01627 (19)
C14	0.25074 (17)	0.03444 (10)	0.03112 (7)	0.01667 (19)
C15	0.58895 (16)	0.47071 (10)	0.49884 (7)	0.01624 (19)
C16	0.71839 (18)	0.47043 (11)	0.56843 (7)	0.0204 (2)
H16	0.6959	0.5088	0.6170	0.024*
C17	0.87996 (18)	0.41260 (12)	0.56417 (8)	0.0211 (2)
H17	0.9647	0.4109	0.6104	0.025*
C19	0.79738 (18)	0.35895 (11)	0.42720 (7)	0.0195 (2)
H19	0.8260	0.3213	0.3796	0.023*
C20	0.63196 (17)	0.41406 (11)	0.42711 (7)	0.0186 (2)
H20	0.5498	0.4136	0.3798	0.022*
C21	0.4775 (3)	0.74127 (12)	0.11225 (9)	0.0314 (3)
H21	0.4966	0.7818	0.1651	0.038*
C22	0.5096 (3)	0.62398 (12)	0.09167 (8)	0.0312 (3)
H22	0.5489	0.5858	0.1305	0.037*
C23	0.48263 (19)	0.56312 (10)	0.01228 (8)	0.0202 (2)
C24	0.42385 (19)	0.62453 (11)	−0.04326 (8)	0.0210 (2)
H24	0.4050	0.5869	−0.0966	0.025*
C25	0.39352 (19)	0.74164 (11)	−0.01906 (8)	0.0219 (2)
H25	0.3544	0.7823	−0.0564	0.026*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01633 (5)	0.01467 (5)	0.01249 (5)	0.00548 (3)	0.00343 (3)	0.00248 (3)
O1	0.0245 (4)	0.0243 (4)	0.0169 (4)	0.0106 (3)	0.0082 (3)	0.0063 (3)
O1S	0.0376 (6)	0.0235 (5)	0.0527 (7)	0.0066 (4)	−0.0001 (5)	0.0107 (5)
O2	0.0284 (5)	0.0283 (5)	0.0301 (5)	0.0189 (4)	0.0160 (4)	0.0121 (4)
O2S	0.0322 (5)	0.0231 (4)	0.0361 (6)	0.0056 (4)	0.0094 (4)	0.0017 (4)
O3	0.0228 (4)	0.0325 (5)	0.0173 (4)	0.0163 (4)	0.0084 (3)	0.0051 (3)
O3S	0.0422 (6)	0.0250 (4)	0.0216 (4)	0.0089 (4)	0.0092 (4)	0.0047 (4)
O4	0.0241 (4)	0.0359 (5)	0.0166 (4)	0.0170 (4)	0.0044 (3)	0.0064 (4)
O5	0.0348 (5)	0.0209 (4)	0.0234 (4)	0.0091 (4)	0.0067 (4)	−0.0013 (3)
O6	0.0335 (5)	0.0170 (4)	0.0525 (7)	0.0115 (4)	0.0117 (5)	0.0005 (4)
O7	0.0374 (5)	0.0247 (4)	0.0145 (4)	0.0094 (4)	0.0032 (4)	0.0007 (3)
O8	0.0299 (4)	0.0158 (3)	0.0140 (4)	0.0086 (3)	0.0045 (3)	0.0034 (3)
O9	0.0231 (4)	0.0208 (4)	0.0391 (6)	0.0056 (3)	0.0104 (4)	0.0061 (4)
O10	0.0259 (5)	0.0239 (4)	0.0394 (6)	0.0081 (4)	0.0151 (4)	0.0142 (4)
O11	0.0192 (4)	0.0287 (4)	0.0166 (4)	0.0045 (3)	0.0044 (3)	0.0068 (3)
N1	0.0154 (4)	0.0165 (4)	0.0146 (4)	0.0063 (3)	0.0052 (3)	0.0041 (3)
N2	0.0165 (4)	0.0139 (4)	0.0190 (4)	0.0037 (3)	0.0046 (3)	0.0042 (3)
N3	0.0164 (4)	0.0190 (4)	0.0237 (5)	0.0078 (3)	0.0060 (4)	0.0037 (4)
N4	0.0271 (5)	0.0142 (4)	0.0248 (5)	0.0060 (4)	0.0094 (4)	0.0015 (4)
C1	0.0178 (5)	0.0163 (4)	0.0199 (5)	0.0060 (4)	0.0092 (4)	0.0057 (4)
C2	0.0150 (4)	0.0165 (4)	0.0169 (5)	0.0057 (4)	0.0056 (4)	0.0052 (4)
C3	0.0174 (5)	0.0254 (5)	0.0199 (5)	0.0109 (4)	0.0033 (4)	0.0060 (4)
C4	0.0193 (5)	0.0277 (6)	0.0164 (5)	0.0087 (4)	0.0015 (4)	0.0054 (4)
C5	0.0200 (5)	0.0211 (5)	0.0132 (4)	0.0068 (4)	0.0047 (4)	0.0039 (4)

C6	0.0150 (4)	0.0157 (4)	0.0153 (4)	0.0057 (3)	0.0049 (4)	0.0036 (3)
C7	0.0166 (4)	0.0180 (4)	0.0164 (5)	0.0076 (4)	0.0063 (4)	0.0041 (4)
C8	0.0211 (5)	0.0146 (5)	0.0298 (6)	0.0039 (4)	0.0087 (5)	0.0014 (4)
C9	0.0168 (5)	0.0152 (4)	0.0268 (6)	0.0042 (4)	0.0058 (4)	0.0065 (4)
C10	0.0225 (6)	0.0202 (5)	0.0371 (7)	0.0072 (4)	0.0058 (5)	0.0139 (5)
C11	0.0229 (6)	0.0283 (6)	0.0305 (6)	0.0059 (5)	0.0023 (5)	0.0181 (5)
C12	0.0200 (5)	0.0251 (5)	0.0199 (5)	0.0026 (4)	0.0012 (4)	0.0101 (4)
C13	0.0156 (4)	0.0164 (4)	0.0171 (5)	0.0023 (4)	0.0030 (4)	0.0059 (4)
C14	0.0185 (5)	0.0159 (4)	0.0155 (5)	0.0025 (4)	0.0042 (4)	0.0039 (4)
C15	0.0148 (4)	0.0139 (4)	0.0187 (5)	0.0046 (3)	0.0039 (4)	0.0009 (4)
C16	0.0189 (5)	0.0228 (5)	0.0186 (5)	0.0092 (4)	0.0040 (4)	0.0015 (4)
C17	0.0190 (5)	0.0244 (5)	0.0197 (5)	0.0093 (4)	0.0033 (4)	0.0036 (4)
C19	0.0182 (5)	0.0196 (5)	0.0208 (5)	0.0069 (4)	0.0072 (4)	0.0018 (4)
C20	0.0163 (5)	0.0194 (5)	0.0181 (5)	0.0061 (4)	0.0035 (4)	0.0003 (4)
C21	0.0548 (9)	0.0175 (5)	0.0239 (6)	0.0117 (6)	0.0153 (6)	0.0021 (5)
C22	0.0587 (10)	0.0180 (5)	0.0205 (6)	0.0130 (6)	0.0145 (6)	0.0045 (4)
C23	0.0253 (5)	0.0131 (4)	0.0227 (5)	0.0045 (4)	0.0098 (4)	0.0018 (4)
C24	0.0220 (5)	0.0163 (5)	0.0227 (5)	0.0053 (4)	0.0048 (4)	0.0008 (4)
C25	0.0228 (5)	0.0166 (5)	0.0256 (6)	0.0064 (4)	0.0055 (4)	0.0030 (4)

Geometric parameters (Å, °)

Sr1—O8	2.6199 (9)	N4—H4C	0.9500
Sr1—O9	2.6223 (10)	C1—C2	1.5153 (16)
Sr1—O10	2.6239 (10)	C2—C3	1.3907 (16)
Sr1—O11	2.6580 (9)	C3—C4	1.3870 (17)
Sr1—O5	2.6633 (10)	C3—H3	0.9300
Sr1—O1	2.6858 (9)	C4—C5	1.3888 (17)
Sr1—O4	2.6970 (9)	C4—H4	0.9300
Sr1—N2	2.7299 (10)	C5—C6	1.3920 (16)
Sr1—N1	2.7504 (10)	C5—H5	0.9300
O1—C1	1.2499 (15)	C6—C7	1.5143 (15)
O1S—H1A	0.9500	C8—C9	1.5230 (18)
O1S—H1B	0.9352	C9—C10	1.3911 (18)
O2—C1	1.2591 (14)	C10—C11	1.385 (2)
O2S—H2B	0.9500	C10—H10	0.9300
O2S—H2A	0.9499	C11—C12	1.3874 (19)
O3—C7	1.2821 (14)	C11—H11	0.9300
O3S—H3A	0.9501	C12—C13	1.3952 (16)
O3S—H3B	0.9500	C12—H12	0.9300
O4—C7	1.2307 (15)	C13—C14	1.5105 (16)
O5—C8	1.2433 (17)	C15—C16	1.3988 (17)
O6—C8	1.2643 (15)	C15—C20	1.4012 (16)
O7—C14	1.2391 (14)	C15—C15^{i}	1.484 (2)
O8—C14	1.2725 (14)	C16—C17	1.3807 (16)
O9—H9A	0.9500	C16—H16	0.9300
O9—H9B	0.9501	C17—H17	0.9300
O10—H10B	0.9500	C19—C20	1.3816 (16)
O10—H10A	0.9501	C19—H19	0.9300

O11—H11B	0.9501	C20—H20	0.9300
O11—H11A	0.9500	C21—C22	1.3835 (19)
N1—C2	1.3358 (14)	C21—H21	0.9300
N1—C6	1.3390 (14)	C22—C23	1.3973 (18)
N2—C13	1.3386 (15)	C22—H22	0.9300
N2—C9	1.3391 (15)	C23—C24	1.3910 (18)
N3—C19	1.3353 (16)	C23—C23^{ii}	1.493 (2)
N3—C17	1.3401 (16)	C24—C25	1.3827 (17)
N3—H3C	0.9500	C24—H24	0.9300
N4—C21	1.3327 (19)	C25—H25	0.9300
N4—C25	1.3382 (17)		
O8—Sr1—O9	87.77 (3)	N1—C2—C1	116.49 (10)
O8—Sr1—O10	77.70 (3)	C3—C2—C1	120.87 (10)
O9—Sr1—O10	143.16 (3)	C4—C3—C2	119.01 (10)
O8—Sr1—O11	87.84 (3)	C4—C3—H3	120.5
O9—Sr1—O11	143.04 (3)	C2—C3—H3	120.5
O10—Sr1—O11	70.77 (3)	C3—C4—C5	118.61 (11)
O8—Sr1—O5	117.81 (3)	C3—C4—H4	120.7
O9—Sr1—O5	69.08 (3)	C5—C4—H4	120.7
O10—Sr1—O5	147.32 (3)	C4—C5—C6	118.60 (10)
O11—Sr1—O5	80.80 (3)	C4—C5—H5	120.7
O8—Sr1—O1	70.16 (3)	C6—C5—H5	120.7
O9—Sr1—O1	68.30 (3)	N1—C6—C5	122.84 (10)
O10—Sr1—O1	74.93 (3)	N1—C6—C7	114.85 (10)
O11—Sr1—O1	142.46 (3)	C5—C6—C7	122.31 (10)
O5—Sr1—O1	136.17 (3)	O4—C7—O3	125.13 (11)
O8—Sr1—O4	160.45 (3)	O4—C7—C6	119.40 (10)
O9—Sr1—O4	111.64 (3)	O3—C7—C6	115.48 (10)
O10—Sr1—O4	87.33 (3)	O5—C8—O6	126.75 (13)
O11—Sr1—O4	75.27 (3)	O5—C8—C9	117.22 (10)
O5—Sr1—O4	69.72 (3)	O6—C8—C9	116.02 (12)
O1—Sr1—O4	118.22 (3)	N2—C9—C10	122.18 (12)
O8—Sr1—N2	59.48 (3)	N2—C9—C8	115.40 (11)
O9—Sr1—N2	77.25 (3)	C10—C9—C8	122.43 (11)
O10—Sr1—N2	120.88 (3)	C11—C10—C9	119.02 (12)
O11—Sr1—N2	69.00 (3)	C11—C10—H10	120.5
O5—Sr1—N2	59.38 (3)	C9—C10—H10	120.5
O1—Sr1—N2	119.01 (3)	C10—C11—C12	119.34 (12)
O4—Sr1—N2	120.81 (3)	C10—C11—H11	120.3
O8—Sr1—N1	127.75 (3)	C12—C11—H11	120.3
O9—Sr1—N1	85.89 (3)	C11—C12—C13	117.86 (12)
O10—Sr1—N1	77.18 (3)	C11—C12—H12	121.1
O11—Sr1—N1	124.65 (3)	C13—C12—H12	121.1
O5—Sr1—N1	107.88 (3)	N2—C13—C12	123.13 (11)
O1—Sr1—N1	59.37 (3)	N2—C13—C14	115.44 (10)
O4—Sr1—N1	59.06 (3)	C12—C13—C14	121.43 (11)
N2—Sr1—N1	161.65 (3)	O7—C14—O8	124.69 (11)
C1—O1—Sr1	125.70 (7)	O7—C14—C13	118.75 (10)

H1A—O1S—H1B	108.4	O8—C14—C13	116.55 (10)
H2B—O2S—H2A	100.3	C16—C15—C20	118.14 (10)
H3A—O3S—H3B	102.8	C16—C15—C15^{i}	120.77 (13)
C7—O4—Sr1	124.53 (8)	C20—C15—C15^{i}	121.09 (13)
C8—O5—Sr1	124.51 (8)	C17—C16—C15	119.27 (11)
C14—O8—Sr1	126.81 (7)	C17—C16—H16	120.4
Sr1—O9—H9A	122.7	C15—C16—H16	120.4
Sr1—O9—H9B	131.0	N3—C17—C16	121.18 (11)
H9A—O9—H9B	104.4	N3—C17—H17	119.4
Sr1—O10—H10B	128.6	C16—C17—H17	119.4
Sr1—O10—H10A	113.2	N3—C19—C20	120.96 (11)
H10B—O10—H10A	106.2	N3—C19—H19	119.5
Sr1—O11—H11B	112.5	C20—C19—H19	119.5
Sr1—O11—H11A	117.0	C19—C20—C15	119.50 (11)
H11B—O11—H11A	108.8	C19—C20—H20	120.2
C2—N1—C6	118.24 (10)	C15—C20—H20	120.2
C2—N1—Sr1	120.39 (7)	N4—C21—C22	121.02 (13)
C6—N1—Sr1	120.81 (7)	N4—C21—H21	119.5
C13—N2—C9	118.47 (10)	C22—C21—H21	119.5
C13—N2—Sr1	120.70 (7)	C21—C22—C23	119.67 (13)
C9—N2—Sr1	120.37 (8)	C21—C22—H22	120.2
C19—N3—C17	120.93 (10)	C23—C22—H22	120.2
C19—N3—H3C	122.7	C24—C23—C22	117.74 (11)
C17—N3—H3C	116.2	C24—C23—C23^{ii}	121.00 (14)
C21—N4—C25	120.82 (11)	C22—C23—C23^{ii}	121.26 (15)
C21—N4—H4C	119.5	C25—C24—C23	119.94 (12)
C25—N4—H4C	119.6	C25—C24—H24	120.0
O1—C1—O2	125.84 (11)	C23—C24—H24	120.0
O1—C1—C2	117.22 (10)	N4—C25—C24	120.81 (12)
O2—C1—C2	116.93 (11)	N4—C25—H25	119.6
N1—C2—C3	122.62 (10)	C24—C25—H25	119.6
O8—Sr1—O1—C1	−163.64 (10)	C6—N1—C2—C3	−2.12 (17)
O9—Sr1—O1—C1	100.68 (10)	Sr1—N1—C2—C3	169.43 (9)
O10—Sr1—O1—C1	−81.53 (10)	C6—N1—C2—C1	179.50 (10)
O11—Sr1—O1—C1	−106.00 (10)	Sr1—N1—C2—C1	−8.94 (13)
O5—Sr1—O1—C1	86.46 (10)	O1—C1—C2—N1	10.68 (16)
O4—Sr1—O1—C1	−3.02 (11)	O2—C1—C2—N1	−170.11 (11)
N2—Sr1—O1—C1	161.19 (9)	O1—C1—C2—C3	−167.72 (11)
N1—Sr1—O1—C1	2.29 (9)	O2—C1—C2—C3	11.49 (17)
O8—Sr1—O4—C7	125.26 (11)	N1—C2—C3—C4	−0.27 (19)
O9—Sr1—O4—C7	−62.04 (11)	C1—C2—C3—C4	178.03 (11)
O10—Sr1—O4—C7	85.47 (11)	C2—C3—C4—C5	1.79 (19)
O11—Sr1—O4—C7	156.28 (11)	C3—C4—C5—C6	−0.94 (19)
O5—Sr1—O4—C7	−118.26 (11)	C2—N1—C6—C5	3.04 (17)
O1—Sr1—O4—C7	14.16 (12)	Sr1—N1—C6—C5	−168.47 (9)
N2—Sr1—O4—C7	−149.76 (10)	C2—N1—C6—C7	−177.30 (10)
N1—Sr1—O4—C7	8.83 (10)	Sr1—N1—C6—C7	11.18 (13)
O8—Sr1—O5—C8	28.13 (12)	C4—C5—C6—N1	−1.53 (18)

O9—Sr1—O5—C8	103.72 (11)	C4—C5—C6—C7	178.85 (11)
O10—Sr1—O5—C8	−83.98 (12)	Sr1—O4—C7—O3	172.81 (9)
O11—Sr1—O5—C8	−54.48 (11)	Sr1—O4—C7—C6	−7.15 (16)
O1—Sr1—O5—C8	117.86 (10)	N1—C6—C7—O4	−2.99 (16)
O4—Sr1—O5—C8	−132.08 (11)	C5—C6—C7—O4	176.66 (12)
N2—Sr1—O5—C8	16.49 (10)	N1—C6—C7—O3	177.05 (10)
N1—Sr1—O5—C8	−178.05 (10)	C5—C6—C7—O3	−3.29 (17)
O9—Sr1—O8—C14	−84.81 (10)	Sr1—O5—C8—O6	160.40 (11)
O10—Sr1—O8—C14	129.27 (10)	Sr1—O5—C8—C9	−19.52 (16)
O11—Sr1—O8—C14	58.49 (10)	C13—N2—C9—C10	−0.18 (18)
O5—Sr1—O8—C14	−19.93 (11)	Sr1—N2—C9—C10	−172.45 (9)
O1—Sr1—O8—C14	−152.51 (10)	C13—N2—C9—C8	179.89 (10)
O4—Sr1—O8—C14	88.40 (13)	Sr1—N2—C9—C8	7.62 (13)
N2—Sr1—O8—C14	−8.31 (9)	O5—C8—C9—N2	7.03 (17)
N1—Sr1—O8—C14	−167.86 (9)	O6—C8—C9—N2	−172.89 (11)
O8—Sr1—N1—C2	20.85 (10)	O5—C8—C9—C10	−172.90 (12)
O9—Sr1—N1—C2	−63.12 (9)	O6—C8—C9—C10	7.17 (18)
O10—Sr1—N1—C2	83.95 (9)	N2—C9—C10—C11	0.7 (2)
O11—Sr1—N1—C2	139.34 (8)	C8—C9—C10—C11	−179.34 (12)
O5—Sr1—N1—C2	−129.58 (8)	C9—C10—C11—C12	−0.3 (2)
O1—Sr1—N1—C2	4.04 (8)	C10—C11—C12—C13	−0.60 (19)
O4—Sr1—N1—C2	178.58 (10)	C9—N2—C13—C12	−0.81 (17)
N2—Sr1—N1—C2	−86.25 (12)	Sr1—N2—C13—C12	171.43 (9)
O8—Sr1—N1—C6	−167.81 (8)	C9—N2—C13—C14	178.74 (10)
O9—Sr1—N1—C6	108.22 (9)	Sr1—N2—C13—C14	−9.02 (13)
O10—Sr1—N1—C6	−104.72 (9)	C11—C12—C13—N2	1.20 (18)
O11—Sr1—N1—C6	−49.32 (9)	C11—C12—C13—C14	−178.32 (11)
O5—Sr1—N1—C6	41.75 (9)	Sr1—O8—C14—O7	−173.87 (9)
O1—Sr1—N1—C6	175.37 (10)	Sr1—O8—C14—C13	7.26 (15)
O4—Sr1—N1—C6	−10.08 (8)	N2—C13—C14—O7	−177.24 (11)
N2—Sr1—N1—C6	85.09 (12)	C12—C13—C14—O7	2.32 (18)
O8—Sr1—N2—C13	8.61 (8)	N2—C13—C14—O8	1.70 (16)
O9—Sr1—N2—C13	103.60 (9)	C12—C13—C14—O8	−178.75 (11)
O10—Sr1—N2—C13	−41.56 (9)	C20—C15—C16—C17	−1.47 (18)
O11—Sr1—N2—C13	−91.73 (9)	C15^{i}—C15—C16—C17	178.44 (14)
O5—Sr1—N2—C13	176.66 (10)	C19—N3—C17—C16	−0.5 (2)
O1—Sr1—N2—C13	47.58 (9)	C15—C16—C17—N3	1.3 (2)
O4—Sr1—N2—C13	−148.63 (8)	C17—N3—C19—C20	−0.18 (19)
N1—Sr1—N2—C13	127.28 (10)	N3—C19—C20—C15	−0.01 (19)
O8—Sr1—N2—C9	−179.30 (10)	C16—C15—C20—C19	0.83 (18)
O9—Sr1—N2—C9	−84.30 (9)	C15^{i}—C15—C20—C19	−179.07 (13)
O10—Sr1—N2—C9	130.54 (8)	C25—N4—C21—C22	−0.8 (2)
O11—Sr1—N2—C9	80.37 (9)	N4—C21—C22—C23	0.5 (3)
O5—Sr1—N2—C9	−11.25 (8)	C21—C22—C23—C24	0.0 (2)
O1—Sr1—N2—C9	−140.32 (8)	C21—C22—C23—C23^{ii}	179.49 (17)
O4—Sr1—N2—C9	23.47 (10)	C22—C23—C24—C25	−0.2 (2)
N1—Sr1—N2—C9	−60.62 (14)	C23^{ii}—C23—C24—C25	−179.68 (14)
Sr1—O1—C1—O2	173.40 (9)	C21—N4—C25—C24	0.6 (2)

Sr1—O1—C1—C2	−7.47 (15)	C23—C24—C25—N4	−0.1 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1S—H1A···O3S^{iii}	0.95	1.90	2.8462 (17)	175
O1S—H1B···O6	0.94	1.81	2.7370 (16)	173
O2S—H2B···O6	0.95	1.79	2.7358 (16)	172
O2S—H2A···O3S^{iv}	0.95	1.83	2.7800 (15)	178
O3S—H3A···O3^{v}	0.95	1.79	2.7216 (14)	166
O3S—H3B···O2	0.95	1.75	2.7016 (15)	175
O9—H9B···O2S^{vi}	0.95	1.85	2.8043 (15)	177
O10—H10B···O1S^{vii}	0.95	1.85	2.8008 (15)	174
O10—H10A···O2^{viii}	0.95	1.84	2.7864 (14)	174
O11—H11B···O7^{ix}	0.95	1.74	2.6773 (13)	171
O11—H11A···O1^{viii}	0.95	1.91	2.8013 (13)	156
O11—H11A···O2^{viii}	0.95	2.63	3.4752 (14)	148
N3—H3C···O3^{vi}	0.95	1.60	2.5500 (13)	175
N4—H4C···O8^{iii}	0.95	1.67	2.6081 (13)	171
N4—H4C···O7^{iii}	0.95	2.57	3.1285 (15)	118
C16—H16···O5^{i}	0.93	2.31	3.2097 (16)	162
C19—H19···O9	0.93	2.49	3.2130 (17)	135
C20—H20···O5	0.93	2.51	3.4087 (16)	162
C21—H21···O1^{iii}	0.93	2.58	3.2867 (18)	133
C22—H22···O2S^{vi}	0.93	2.57	3.4867 (19)	167
C24—H24···O2S^{x}	0.93	2.39	3.2888 (18)	164
C25—H25···O7^{iii}	0.93	2.37	3.0280 (17)	127

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

Fig. 1

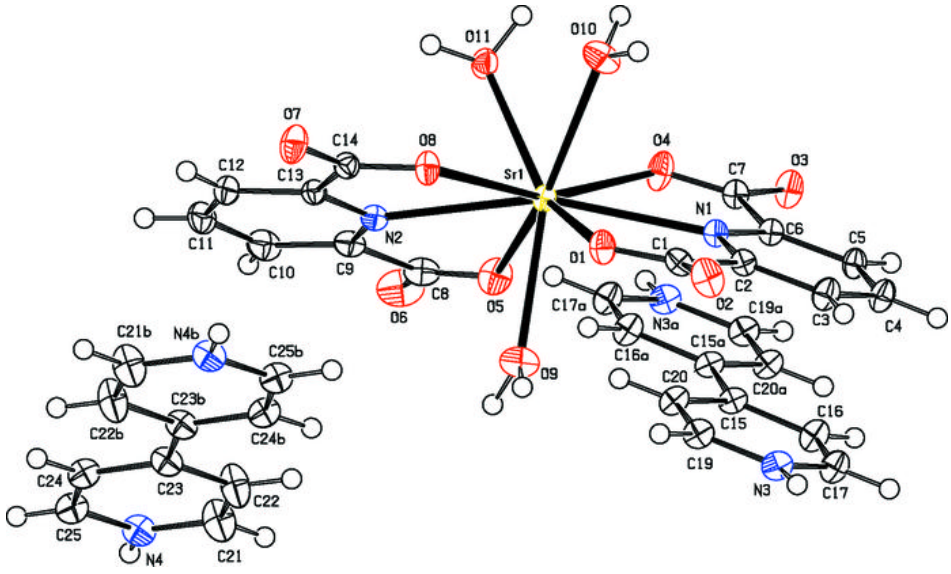
O11
O10
O7
C14
O8
C12
C13
Sr1
O4
C7
O3
N1
C6
C5
C11
N2
C1
O1
C2
C10
C9
C8
O5
O2
C19a
C3
C4
C17a
N3a
O6
C16a
C15a
C21b
N4b
C25b
O9
C20
C20a
C23b
C16
C22b
C24b
C15
C24
C23
C22
C19
N3
C17
C25
C21
N4

Fig. 2

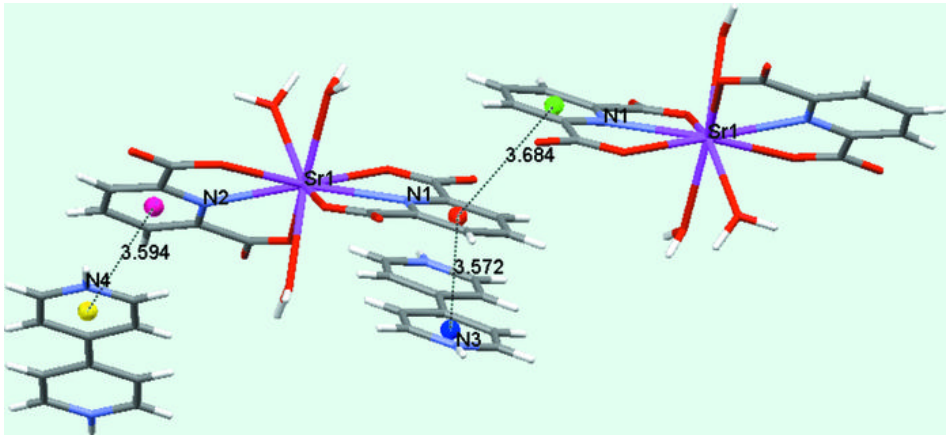

Fig. 3

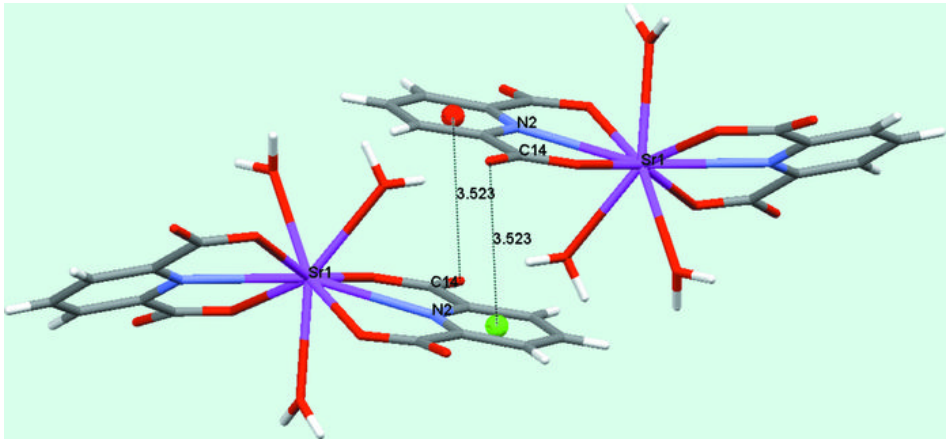

Fig. 4