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Poly[aqua(dimethyl sulfoxide)(μ_4-pyridine-2,5-dicarboxylato)calcium(II)]

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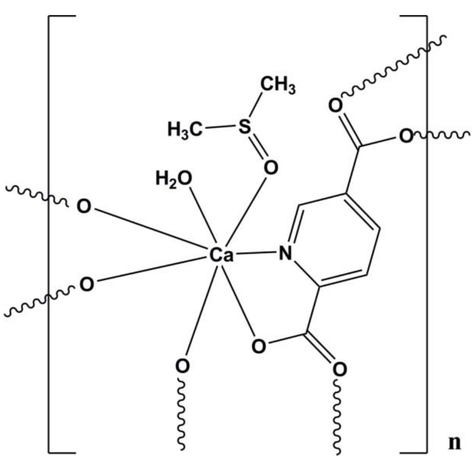
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.097; data-to-parameter ratio = 19.1.

In the polymeric title compound, $[Ca(C_7H_3NO_4)(H_2O)(C_2H_6OS)]_n$, the Ca^{II} ion is coordinated in a distorted pentagonal–bipyramidal $CdNO_6$ geometry. The crystal packing is stabilized by O—H⋯O hydrogen bonds and π–π stacking interactions between the aromatic rings of pyridine-2,5-dicarboxylate with centroid–centroid distances of 3.6166 (13) Å.

Related literature

For related coordination polymers involving pyridine-2,5-dicarboxylic acid, see: Aghabozorg, Derikvand *et al.* (2008); Aghabozorg, Manteghi & Sheshmani (2008); Xu *et al.* (2008); Sun *et al.* (2006); Çolak *et al.* (2010); Wang *et al.* (2009); Xie *et al.* (2009).



Experimental

Crystal data

$[Ca(C_7H_3NO_4)(H_2O)(C_2H_6OS)]$	V = 1228.7 (4) Å^3
M_r = 301.34	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 10.449 (2) Å	μ = 0.70 mm^{-1}
b = 11.450 (2) Å	T = 298 K
c = 10.325 (2) Å	0.27 × 0.15 × 0.15 mm
β = 95.93 (3)°	

Data collection

Stoe IPDS II diffractometer	2718 reflections with $I > 2\sigma(I)$
8616 measured reflections	R_{int} = 0.041
3302 independent reflections	

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.097	$\Delta\rho_{max}$ = 0.44 e Å^{-3}
S = 1.11	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
3302 reflections	
173 parameters	

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O6—H6B⋯O3^i	0.84 (3)	2.00 (3)	2.782 (2)	155 (3)
O6—H6A⋯O1^{ii}	0.82 (4)	1.96 (4)	2.739 (2)	158 (3)

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $x, -y+\frac{5}{2}, z-\frac{1}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5441).

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Poly[aqua(dimethyl sulfoxide)(μ_4-pyridine-2,5-dicarboxylato)calcium(II)]

Hoda Pasdar, Zahra Safari, Hossein Aghabozorg, Behrouz Notash and Masoud Mirzaei

S1. Comment

Extended frameworks of coordination polymers based on transition metal ions and multifunctional bridging ligands are currently of great interest because of their intriguing topologies and their potential applications (Sun *et al.*, 2006; Wang *et al.*, 2009; Xie, *et al.*, 2009). Pyridine-2,5-dicarboxylic acid (py-2,5- dcH_2) has unique features because of the presence of two carboxylate groups (O donor atoms) and the pyridine ring (N donor atom), which aids to increase the dimensionality of the assembled covalent network. Therefore, it is most likely that py-2,5-dcH_2 will form low symmetric structures with metals (Aghabozorg, Derikvand, *et al.*, 2008; Xu *et al.*, 2008; Çolak *et al.*, 2010). Our research group has recently focused on one-pot synthesis of water soluble self-assembly systems that can function as suitable ligands in the synthesis of metal complexes (Aghabozorg, Manteghi & Sheshmani, 2008).

The title compound consists of one deprotonated 2,5-pydc unit, one water molecule, and one dimethylsulfoxide molecule. The asymmetric unit of the title compound is shown in Fig. 1. In the the title compound, Ca^{II} ion is 7-coordinated in a NO_6 environment. Its geometry is distorted pentagonal bipyramidal. Pentagonal plane is constructed by one oxygen from water, one nitrogen and three oxygen atoms from the (py-2,5-dc)$^{2-}$ and axial positions occupied by two oxygen atoms from (py-2,5-dc)$^{2-}$ and dimethylsulfoxide moieties. A perspective view of the coordination environment around the Ca^{II} ion is shown in Fig. 2. The crystal structure of title compound shows that the compound is a two-dimensional polymer $[Ca(C_7H_3NO_4)(H_2O)(C_2H_6SO)]_n$. The polymeric structure of title compound is shown in Fig. 3. There are O—H···O hydrogen bonds between hydrogen atoms of water molecules and oxygen atoms of py-2,5-dc (Table 2). There is also π–π stacking interactions (Fig. 4) between two aromatic rings of (py-2,5-dc)$^{2-}$ with centroid–centroid distances of 3.6166 (13) Å.

S2. Experimental

A mixture of $CaCl_2$ (0.627 g), pyridine-2,5-dicarboxylic acid (0.1519 g), 1,4-butanediammine (1 ml) in 6 ml DMSO was stirred at room temprature for 2 hrs.The solution was filtered, and the filtrate was stand at room temprature. After two days, colorless block shape crystals of the title compound were obtained (m.p 249°C).

S3. Refinement

The hydrogen atoms of the water molecule were found in a difference Fourier map and refined isotropically. The C—H protons were positioned geometrically and refined as riding atoms with C—H = 0.93 Å and Uiso(H) = 1.2 Ueq(C) for aromatic C—H and C—H = 0.96 Å and Uiso(H) = 1.5 Ueq(C) for methyl groups.

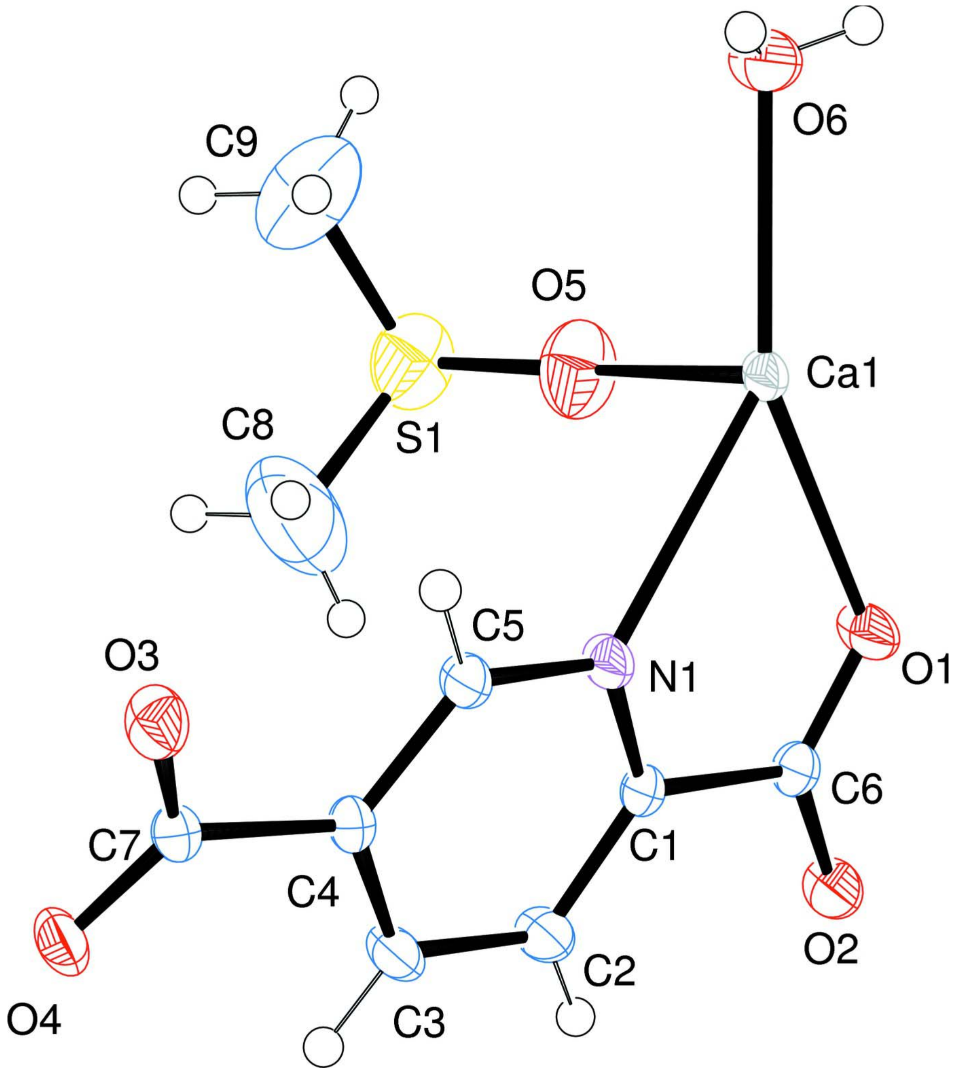

Figure 1

The asymetric unit of title compound with displacement ellipsoids drawn at 50% probability level.

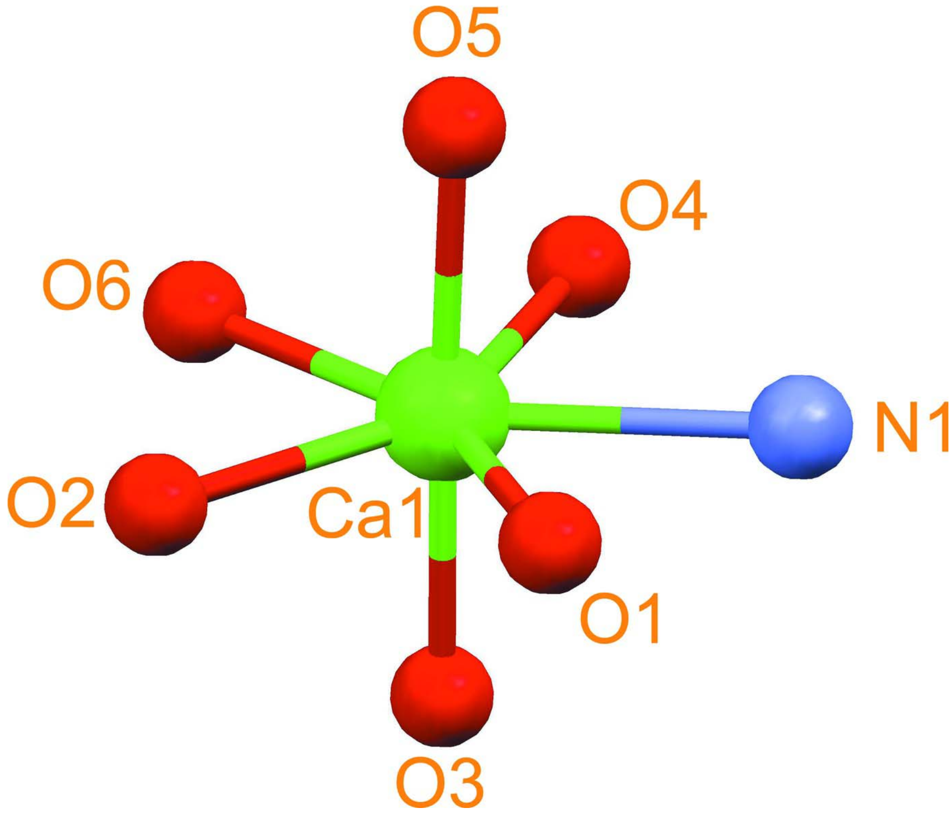

Figure 2

The coordination environment around the Ca(II) ion in the title compound.

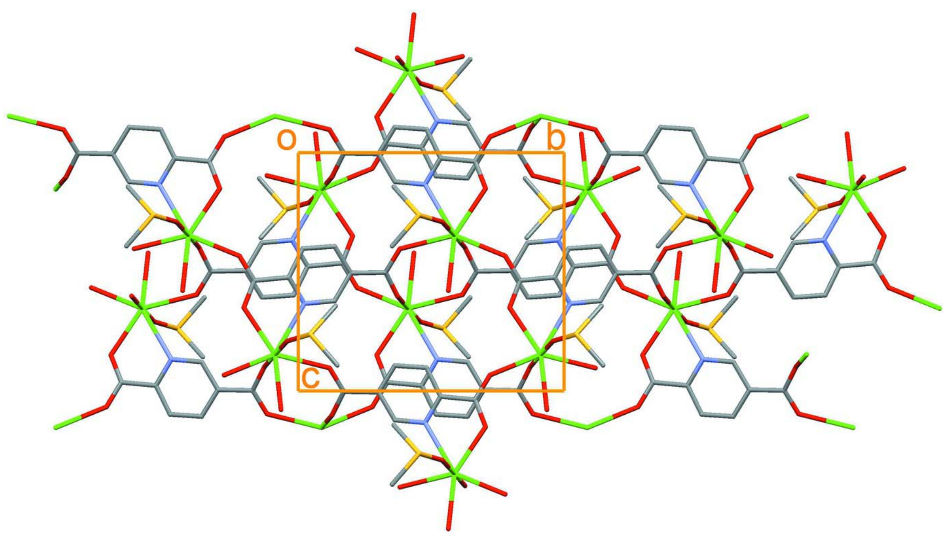

Figure 3

A view of the two-dimensional structure of the title compound down the *a*-axis. Hydrogen atoms have been ommited for clarity.

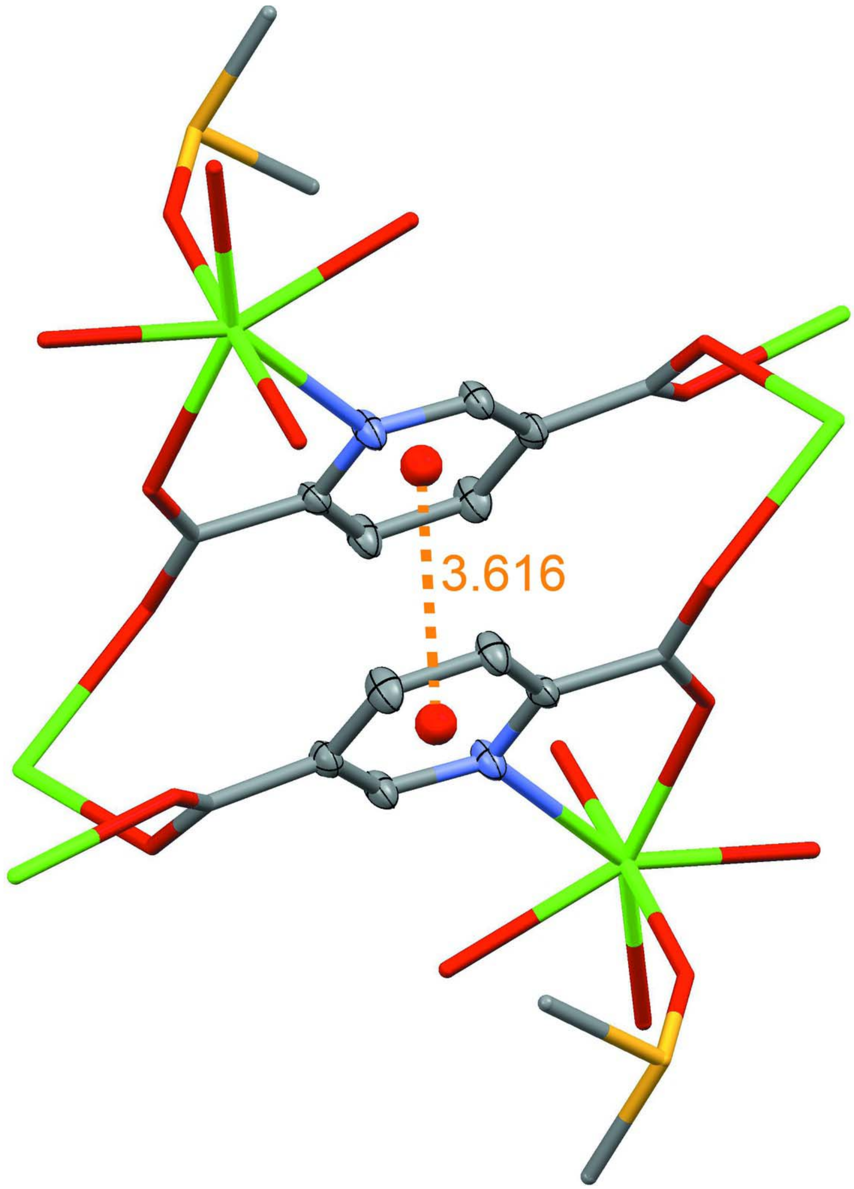

Figure 4

The packing diagram of title compound showing intermolecular π-π interaction (dashed lines) between pyridine rings of py-2,5-dc.

Poly[aqua(dimethyl sulfoxide)(μ_4-pyridine-2,5-dicarboxylato)calcium(II)]

Crystal data

$[Ca(C_7H_3NO_4)(C_2H_6OS)(H_2O)]$
M_r = 301.34
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.449 (2) Å
b = 11.450 (2) Å
c = 10.325 (2) Å
β = 95.93 (3)°
V = 1228.7 (4) Å^3
Z = 4
F(000) = 624.0
D_x = 1.629 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3302 reflections
θ = 2.7–29.1°
μ = 0.70 mm^{-1}

T = 298 K	0.27 × 0.15 × 0.15 mm
Block, colorless	

Data collection

Stoe IPDS II diffractometer	3302 independent reflections
Radiation source: fine-focus sealed tube	2718 reflections with $I > 2\sigma(I)$
Graphite monochromator	R_{int} = 0.041
Detector resolution: 0.15 mm pixels mm^{-1}	θ_{max} = 29.1°, θ_{min} = 2.7°
rotation method scans	$h = -14 \rightarrow 13$
8616 measured reflections	$k = -13 \rightarrow 15$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.097	$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 0.5537P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.11	$(\Delta/\sigma)_{max}$ = 0.001
3302 reflections	$\Delta\rho_{max}$ = 0.44 e Å^{-3}
173 parameters	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
0 restraints	
Primary atom site location: structure-invariant direct methods	

Special details

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

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

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

	x	y	z	U_{iso}*/U_{eq}
Ca1	0.67926 (4)	1.08747 (3)	0.15351 (3)	0.01937 (10)
S1	1.00299 (7)	0.95463 (8)	0.23803 (8)	0.0533 (2)
O5	0.89654 (19)	1.04175 (19)	0.2093 (2)	0.0525 (5)
C9	0.9931 (4)	0.8533 (4)	0.1082 (4)	0.0836 (13)
H9A	0.9068	0.8237	0.0933	0.125*
H9B	1.0515	0.7899	0.1298	0.125*
H9C	1.0155	0.8914	0.0308	0.125*
C8	0.9511 (5)	0.8595 (5)	0.3569 (5)	0.114 (2)
H8A	0.9386	0.9031	0.4340	0.171*
H8B	1.0151	0.8003	0.3777	0.171*
H8C	0.8715	0.8234	0.3237	0.171*
N1	0.63254 (17)	0.97721 (13)	0.36682 (15)	0.0212 (3)
C5	0.6057 (2)	0.86315 (16)	0.37822 (17)	0.0207 (4)
H5	0.5735	0.8228	0.3037	0.025*

C1	0.67172 (18)	1.03533 (15)	0.47695 (17)	0.0176 (3)
C3	0.6660 (2)	0.86337 (17)	0.60687 (18)	0.0245 (4)
H3	0.6803	0.8252	0.6866	0.029*
C2	0.6872 (2)	0.98248 (17)	0.59788 (18)	0.0237 (4)
H2	0.7114	1.0262	0.6723	0.028*
C4	0.62317 (19)	0.80212 (15)	0.49489 (17)	0.0191 (3)
C7	0.59970 (19)	0.67151 (16)	0.49754 (18)	0.0203 (4)
O3	0.53823 (15)	0.62711 (12)	0.39822 (14)	0.0265 (3)
O4	0.64566 (17)	0.61761 (13)	0.59638 (14)	0.0311 (4)
O2	0.72123 (17)	1.22148 (12)	0.56666 (14)	0.0307 (3)
O1	0.69341 (17)	1.20480 (12)	0.34958 (13)	0.0307 (3)
C6	0.6974 (2)	1.16520 (15)	0.46351 (18)	0.0209 (4)
O6	0.7022 (2)	1.06481 (15)	−0.07874 (15)	0.0350 (4)
H6A	0.685 (3)	1.127 (3)	−0.116 (3)	0.055 (9)*
H6B	0.643 (3)	1.019 (3)	−0.106 (3)	0.043 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0298 (2)	0.01175 (16)	0.01607 (16)	0.00106 (14)	−0.00007 (13)	0.00002 (13)
S1	0.0306 (3)	0.0622 (5)	0.0649 (5)	0.0089 (3)	−0.0054 (3)	−0.0029 (4)
O5	0.0371 (10)	0.0517 (12)	0.0662 (13)	0.0085 (9)	−0.0062 (9)	−0.0013 (10)
C9	0.077 (3)	0.074 (3)	0.103 (3)	0.005 (2)	0.025 (2)	−0.026 (2)
C8	0.109 (4)	0.128 (4)	0.109 (4)	0.062 (3)	0.038 (3)	0.066 (3)
N1	0.0341 (9)	0.0119 (7)	0.0173 (7)	−0.0012 (6)	0.0011 (6)	0.0000 (5)
C5	0.0321 (10)	0.0128 (8)	0.0169 (8)	−0.0009 (7)	0.0012 (7)	−0.0013 (6)
C1	0.0235 (9)	0.0118 (8)	0.0177 (8)	0.0012 (6)	0.0026 (7)	−0.0012 (6)
C3	0.0383 (11)	0.0187 (9)	0.0159 (8)	−0.0018 (8)	0.0000 (8)	0.0034 (7)
C2	0.0371 (11)	0.0170 (8)	0.0165 (8)	−0.0043 (8)	0.0000 (7)	−0.0022 (7)
C4	0.0252 (9)	0.0122 (8)	0.0200 (8)	0.0005 (7)	0.0034 (7)	0.0013 (6)
C7	0.0280 (10)	0.0133 (8)	0.0200 (8)	0.0001 (7)	0.0049 (7)	0.0014 (6)
O3	0.0342 (8)	0.0172 (6)	0.0272 (7)	−0.0041 (6)	−0.0019 (6)	−0.0016 (5)
O4	0.0573 (10)	0.0150 (6)	0.0203 (7)	0.0015 (6)	−0.0002 (7)	0.0039 (5)
O2	0.0549 (10)	0.0151 (6)	0.0212 (7)	−0.0016 (6)	0.0003 (6)	−0.0042 (5)
O1	0.0598 (10)	0.0131 (6)	0.0191 (6)	−0.0043 (6)	0.0029 (7)	0.0003 (5)
C6	0.0307 (10)	0.0116 (8)	0.0206 (8)	0.0003 (7)	0.0031 (7)	−0.0021 (6)
O6	0.0622 (12)	0.0181 (7)	0.0253 (7)	−0.0083 (8)	0.0076 (7)	−0.0010 (6)

Geometric parameters (Å, º)

Ca1—O3^{i}	2.3249 (16)	C5—C4	1.388 (2)
Ca1—O5	2.343 (2)	C5—H5	0.9300
Ca1—O1	2.4214 (15)	C1—C2	1.382 (3)
Ca1—O2^{ii}	2.4215 (15)	C1—C6	1.520 (2)
Ca1—O4^{iii}	2.4377 (15)	C3—C2	1.386 (3)
Ca1—O6	2.4484 (17)	C3—C4	1.386 (3)
Ca1—N1	2.6278 (16)	C3—H3	0.9300
Ca1—H6B	2.78 (3)	C2—H2	0.9300

S1—O5	1.501 (2)	C4—C7	1.516 (2)
S1—C8	1.768 (5)	C7—O4	1.246 (2)
S1—C9	1.768 (4)	C7—O3	1.260 (2)
C9—H9A	0.9600	O3—Ca1^{iv}	2.3249 (16)
C9—H9B	0.9600	O4—Ca1^{v}	2.4377 (15)
C9—H9C	0.9600	O2—C6	1.248 (2)
C8—H8A	0.9600	O2—Ca1^{vi}	2.4215 (15)
C8—H8B	0.9600	O1—C6	1.257 (2)
C8—H8C	0.9600	O6—H6A	0.82 (4)
N1—C5	1.344 (2)	O6—H6B	0.84 (3)
N1—C1	1.344 (2)		

O3^{i}—Ca1—O5	178.05 (7)	S1—C8—H8A	109.5
O3^{i}—Ca1—O1	93.30 (6)	S1—C8—H8B	109.5
O5—Ca1—O1	86.82 (7)	H8A—C8—H8B	109.5
O3^{i}—Ca1—O2^{ii}	87.06 (6)	S1—C8—H8C	109.5
O5—Ca1—O2^{ii}	94.87 (7)	H8A—C8—H8C	109.5
O1—Ca1—O2^{ii}	79.09 (5)	H8B—C8—H8C	109.5
O3^{i}—Ca1—O4^{iii}	91.12 (6)	C5—N1—C1	117.08 (16)
O5—Ca1—O4^{iii}	87.47 (7)	C5—N1—Ca1	126.80 (12)
O1—Ca1—O4^{iii}	137.02 (5)	C1—N1—Ca1	113.85 (11)
O2^{ii}—Ca1—O4^{iii}	143.87 (5)	N1—C5—C4	123.73 (17)
O3^{i}—Ca1—O6	89.31 (7)	N1—C5—H5	118.1
O5—Ca1—O6	91.53 (8)	C4—C5—H5	118.1
O1—Ca1—O6	150.93 (5)	N1—C1—C2	122.99 (16)
O2^{ii}—Ca1—O6	72.13 (5)	N1—C1—C6	116.64 (16)
O4^{iii}—Ca1—O6	71.77 (5)	C2—C1—C6	120.37 (16)
O3^{i}—Ca1—N1	91.41 (6)	C2—C3—C4	118.80 (17)
O5—Ca1—N1	86.89 (7)	C2—C3—H3	120.6
O1—Ca1—N1	64.30 (5)	C4—C3—H3	120.6
O2^{ii}—Ca1—N1	143.22 (5)	C1—C2—C3	119.12 (18)
O4^{iii}—Ca1—N1	72.87 (5)	C1—C2—H2	120.4
O6—Ca1—N1	144.64 (5)	C3—C2—H2	120.4
O3^{i}—Ca1—H6B	78.5 (6)	C3—C4—C5	118.12 (17)
O5—Ca1—H6B	102.0 (6)	C3—C4—C7	121.52 (16)
O1—Ca1—H6B	162.4 (7)	C5—C4—C7	120.34 (17)
O2^{ii}—Ca1—H6B	84.9 (7)	O4—C7—O3	126.02 (18)
O4^{iii}—Ca1—H6B	59.5 (7)	O4—C7—C4	117.00 (18)
O6—Ca1—H6B	17.1 (7)	O3—C7—C4	116.95 (17)
N1—Ca1—H6B	130.7 (7)	C7—O3—Ca1^{iv}	132.07 (13)
O5—S1—C8	105.83 (18)	C7—O4—Ca1^{v}	135.17 (13)
O5—S1—C9	107.57 (19)	C6—O2—Ca1^{vi}	139.02 (14)
C8—S1—C9	97.1 (3)	C6—O1—Ca1	125.13 (12)
S1—O5—Ca1	151.24 (14)	O2—C6—O1	126.64 (17)
S1—C9—H9A	109.5	O2—C6—C1	116.68 (16)
S1—C9—H9B	109.5	O1—C6—C1	116.68 (16)
H9A—C9—H9B	109.5	Ca1—O6—H6A	110 (2)
S1—C9—H9C	109.5	Ca1—O6—H6B	105 (2)

H9A—C9—H9C	109.5	H6A—O6—H6B	106 (3)
H9B—C9—H9C	109.5		
C8—S1—O5—Ca1	−51.3 (4)	C4—C3—C2—C1	−3.5 (3)
C9—S1—O5—Ca1	51.7 (3)	C2—C3—C4—C5	1.1 (3)
O1—Ca1—O5—S1	124.5 (3)	C2—C3—C4—C7	179.23 (19)
O2^{ii}—Ca1—O5—S1	−156.7 (3)	N1—C5—C4—C3	2.6 (3)
O4^{iii}—Ca1—O5—S1	−12.9 (3)	N1—C5—C4—C7	−175.50 (18)
O6—Ca1—O5—S1	−84.5 (3)	C3—C4—C7—O4	−14.9 (3)
N1—Ca1—O5—S1	60.1 (3)	C5—C4—C7—O4	163.15 (18)
O3^{i}—Ca1—N1—C5	89.08 (17)	C3—C4—C7—O3	166.78 (19)
O5—Ca1—N1—C5	−89.97 (18)	C5—C4—C7—O3	−15.2 (3)
O1—Ca1—N1—C5	−177.93 (18)	O4—C7—O3—Ca1^{iv}	88.3 (2)
O2^{ii}—Ca1—N1—C5	176.05 (15)	C4—C7—O3—Ca1^{iv}	−93.54 (19)
O4^{iii}—Ca1—N1—C5	−1.66 (16)	O3—C7—O4—Ca1^{v}	10.8 (3)
O6—Ca1—N1—C5	−1.7 (2)	C4—C7—O4—Ca1^{v}	−167.38 (13)
O3^{i}—Ca1—N1—C1	−108.68 (14)	O3^{i}—Ca1—O1—C6	103.41 (18)
O5—Ca1—N1—C1	72.27 (14)	O5—Ca1—O1—C6	−74.64 (18)
O1—Ca1—N1—C1	−15.69 (13)	O2^{ii}—Ca1—O1—C6	−170.23 (18)
O2^{ii}—Ca1—N1—C1	−21.71 (19)	O4^{iii}—Ca1—O1—C6	8.2 (2)
O4^{iii}—Ca1—N1—C1	160.58 (14)	O6—Ca1—O1—C6	−162.06 (16)
O6—Ca1—N1—C1	160.53 (13)	N1—Ca1—O1—C6	13.44 (16)
C1—N1—C5—C4	−3.8 (3)	Ca1^{vi}—O2—C6—O1	37.1 (4)
Ca1—N1—C5—C4	157.96 (15)	Ca1^{vi}—O2—C6—C1	−143.44 (16)
C5—N1—C1—C2	1.2 (3)	Ca1—O1—C6—O2	170.04 (17)
Ca1—N1—C1—C2	−162.86 (15)	Ca1—O1—C6—C1	−9.4 (3)
C5—N1—C1—C6	−177.95 (17)	N1—C1—C6—O2	173.06 (18)
Ca1—N1—C1—C6	18.0 (2)	C2—C1—C6—O2	−6.1 (3)
N1—C1—C2—C3	2.4 (3)	N1—C1—C6—O1	−7.5 (3)
C6—C1—C2—C3	−178.49 (18)	C2—C1—C6—O1	173.34 (19)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6*B*···O3^{iii}	0.84 (3)	2.00 (3)	2.782 (2)	155 (3)
O6—H6*A*···O1^{ii}	0.82 (4)	1.96 (4)	2.739 (2)	158 (3)

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