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Bis(1*H*-benzotriazole-4-sulfonato-κ^2N^3,O)(2,2′-bipyridyl-κ^2N,N')cadmium

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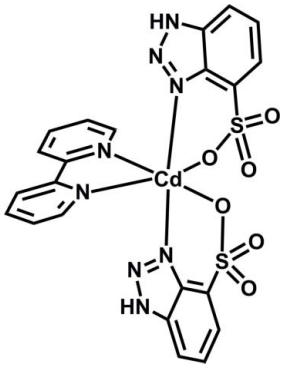
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.028; wR factor = 0.075; data-to-parameter ratio = 17.0.

In the title complex, $[Cd(C_6H_4N_3O_3S)_2(C_{10}H_8N_2)]$, the Cd^{2+} cation is located on a twofold rotation axis and is coordinated by two N and two O atoms from two symmetry-related benzotriazole-4-sulfonate anions and two N atoms from a 2,2-bipyridyl ligand, displaying a distorted CdN_4O_2 octahedral geometry. The crystal structure is stabilized by N—H···O and C—H···O hydrogen-bonding interactions.

Related literature

For a related structure, see: Xia *et al.* (2010).



Experimental

Crystal data

$[Cd(C_6H_4N_3O_3S)_2(C_{10}H_8N_2)]$ M_r = 664.95
Monoclinic, $C2/c$
a = 8.148 (4) Å
b = 17.207 (7) Å
c = 17.720 (8) Å
β = 103.29 (1)°
V = 2417.8 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.805, T_{max} = 0.805
8519 measured reflections
3009 independent reflections
2866 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.075
S = 1.05
3009 reflections
177 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3*N*···O2^{i}	0.93	1.86	2.776 (3)	167
C3—H3···O3^{ii}	0.93	2.55	3.255 (3)	133
C7—H7···O2^{iii}	0.93	2.56	3.204 (3)	127

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2474).

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supporting information

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Bis(1*H*-benzotriazole-4-sulfonato-κ^2N^3,O)(2,2′-bipyridyl-κ^2N,N')cadmium

Xiao-Hong Zhu and Xiao-Chun Cheng

S1. Comment

Benzotriazole-4-sulfonic acid is often used as a ligand to synthesize complexes for its variable coordination modes. Herein, we report the crystal structure of title complex. The asymmetric unit consists of half of a cadmium ion, half of a 2,2-bipyridyl molecule, and a benzotriazole-4-sulfonate anion. The Cd ion is located on a two fold axis and coordinated by two N atoms from two different benzotriazole-4-sulfonate anions, two N atoms from 2,2-bipyridyl molecule, and two sulfonate O atoms from two different benzotriazole-4-sulfonate anions, displaying a distorted CdN_4O_2 octahedral geometry (Fig. 1). Both benzotriazole-4-sulfonate and 2,2-bipyridyl display bidentate chelating coordinating mode. In the crystal structure, there exist O—H···N and C—H···O hydrogen bonds (Table 1). Sulfonate O atoms as hydrogen bonding acceptor play a very important role in the formation of these hydrogen bonding interactions.

S2. Experimental

A mixture of cadmium perchlorate hexahydrate (83.9 mg, 0.2 mmol), benzotriazole-4-sulfonic acid (39.8 mg, 0.2 mmol), 2,2-bipyridyl (31.2 mg, 0.2 mmol) and potassium hydroxide (11.2 mg, 0.2 mmol) in 12 ml H_2O was sealed in a 16 ml Teflon-lined stainless steel container and heated to 393 K for 3 days. After cooling to room temperature, colorless block crystals of the title complex were obtained.

S3. Refinement

The hydrogen atoms bonded to C atoms were located in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The hydrogen atom bonded to N3 was found from a difference Fourier map and fixed at that positio with U_{iso}(H) = 1.2U_{eq}(N).

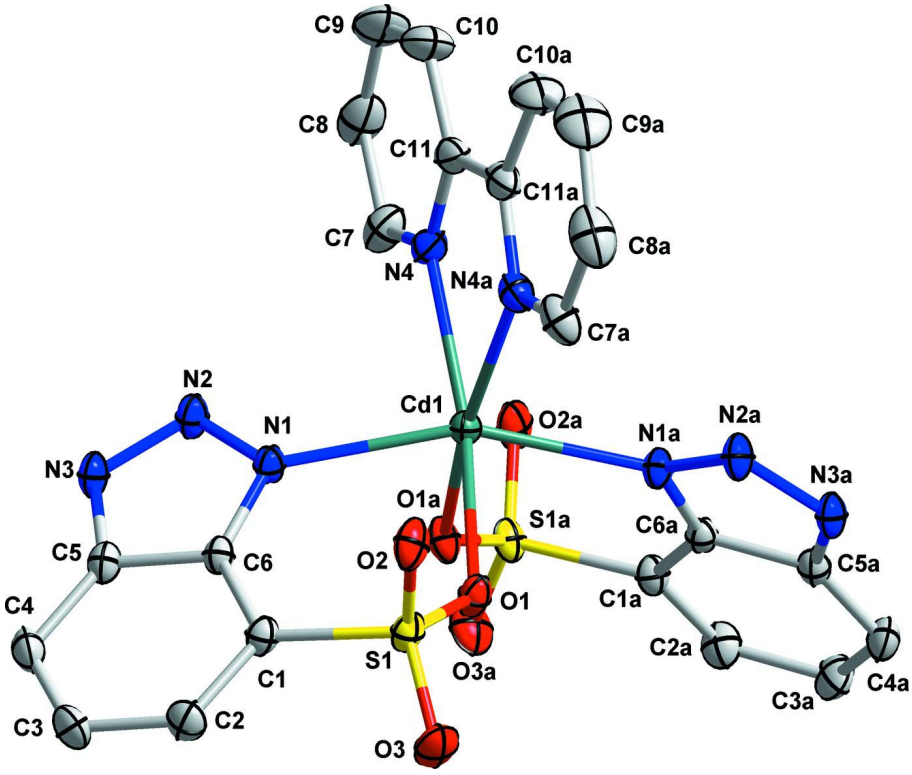

Figure 1

The coordination environment of Cd ion in the title complex with the ellipsoids drawn at the 30% probability level. The hydrogen atoms have been omitted for clarity. symmetry code: a: -x, y, -z+1/2.

Bis(1*H*-benzotriazole-4-sulfonato-κ^2N^3,O)(2,2′- bipyridyl-κ^2N,N')cadmium

Crystal data

$[Cd(C_6H_4N_3O_3S)_2(C_{10}H_8N_2)]$
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Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 8.148$ (4) Å
$b = 17.207$ (7) Å
$c = 17.720$ (8) Å
$\beta = 103.29$ (1)°
$V = 2417.8$ (19) Å^3
$Z = 4$
$F(000) = 1328$
$D_x = 1.827$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6866 reflections
$\theta = 2.4$–28.4°
$\mu = 1.14$ mm^{-1}
$T = 293$ K
Block, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.805$, $T_{max} = 0.805$
8519 measured reflections
3009 independent reflections
2866 reflections with $I > 2\sigma(I)$
$R_{int} = 0.073$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.4°$
$h = -9\rightarrow10$
$k = -22\rightarrow22$
$l = -23\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.075$
$S = 1.05$
3009 reflections
177 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 1.8012P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.82$ e Å^{-3}
$\Delta\rho_{min} = -0.64$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.0973 (2)	−0.10519 (11)	0.06169 (11)	0.0286 (3)
C2	−0.1066 (3)	−0.15816 (14)	0.00234 (12)	0.0388 (4)
H2	−0.2059	−0.1860	−0.0150	0.047*
C3	0.0298 (3)	−0.17160 (14)	−0.03310 (13)	0.0449 (5)
H3	0.0179	−0.2085	−0.0724	0.054*
C4	0.1784 (3)	−0.13203 (14)	−0.01131 (12)	0.0400 (5)
H4	0.2683	−0.1409	−0.0344	0.048*
C5	0.1872 (2)	−0.07701 (12)	0.04815 (11)	0.0297 (4)
C6	0.0555 (2)	−0.06363 (10)	0.08486 (10)	0.0252 (3)
C7	0.3344 (3)	0.12261 (16)	0.31089 (13)	0.0445 (5)
H7	0.3858	0.0742	0.3206	0.053*
C8	0.4326 (4)	0.18893 (19)	0.32763 (15)	0.0573 (7)
H8	0.5472	0.1855	0.3504	0.069*
C9	0.3560 (4)	0.26011 (18)	0.30959 (19)	0.0681 (9)
H9	0.4197	0.3055	0.3180	0.082*
C10	0.1860 (4)	0.26376 (15)	0.27930 (18)	0.0601 (7)
H10	0.1331	0.3116	0.2676	0.072*
C11	0.0927 (3)	0.19536 (12)	0.26615 (11)	0.0376 (4)
Cd1	0.0000	0.017130 (9)	0.2500	0.02575 (8)
N1	0.1089 (2)	−0.00941 (9)	0.14217 (10)	0.0281 (3)
N2	0.2645 (2)	0.01101 (11)	0.14125 (11)	0.0340 (4)
N3	0.3117 (2)	−0.02916 (11)	0.08527 (10)	0.0329 (3)
H3N	0.4172	−0.0247	0.0738	0.039*
N4	0.1685 (2)	0.12587 (10)	0.28136 (10)	0.0338 (3)
O1	−0.18547 (17)	−0.07919 (9)	0.19035 (8)	0.0335 (3)

O2	−0.3547 (2)	−0.02209 (10)	0.07349 (10)	0.0410 (4)
O3	−0.3666 (2)	−0.16108 (11)	0.09518 (10)	0.0492 (4)
S1	−0.26613 (5)	−0.09167 (3)	0.10818 (3)	0.02965 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0243 (8)	0.0342 (9)	0.0272 (8)	−0.0016 (7)	0.0055 (6)	0.0006 (7)
C2	0.0396 (11)	0.0449 (11)	0.0311 (9)	−0.0085 (9)	0.0066 (8)	−0.0059 (8)
C3	0.0592 (14)	0.0445 (12)	0.0351 (10)	−0.0033 (10)	0.0190 (10)	−0.0119 (9)
C4	0.0450 (11)	0.0463 (11)	0.0340 (10)	0.0051 (9)	0.0200 (9)	−0.0028 (9)
C5	0.0265 (8)	0.0363 (9)	0.0277 (8)	0.0035 (7)	0.0090 (7)	0.0043 (7)
C6	0.0231 (8)	0.0290 (8)	0.0239 (7)	0.0021 (6)	0.0062 (6)	0.0020 (6)
C7	0.0413 (11)	0.0528 (13)	0.0381 (10)	−0.0126 (10)	0.0065 (9)	0.0050 (9)
C8	0.0529 (15)	0.0773 (19)	0.0404 (12)	−0.0292 (14)	0.0078 (11)	−0.0097 (12)
C9	0.082 (2)	0.0547 (17)	0.0692 (18)	−0.0351 (15)	0.0195 (16)	−0.0240 (14)
C10	0.082 (2)	0.0328 (11)	0.0678 (17)	−0.0149 (12)	0.0225 (15)	−0.0123 (11)
C11	0.0582 (13)	0.0297 (9)	0.0283 (9)	−0.0072 (9)	0.0169 (8)	−0.0039 (7)
Cd1	0.02654 (11)	0.02444 (11)	0.02832 (11)	0.000	0.01050 (7)	0.000
N1	0.0234 (7)	0.0339 (8)	0.0281 (7)	−0.0031 (6)	0.0082 (6)	−0.0019 (6)
N2	0.0260 (8)	0.0460 (10)	0.0319 (8)	−0.0047 (6)	0.0104 (6)	−0.0015 (7)
N3	0.0233 (7)	0.0456 (9)	0.0318 (8)	−0.0004 (6)	0.0108 (6)	0.0007 (7)
N4	0.0384 (8)	0.0337 (8)	0.0301 (7)	−0.0077 (7)	0.0094 (6)	0.0010 (6)
O1	0.0291 (7)	0.0433 (8)	0.0283 (6)	−0.0103 (6)	0.0074 (5)	−0.0003 (5)
O2	0.0244 (7)	0.0578 (11)	0.0427 (8)	0.0073 (6)	0.0117 (6)	0.0099 (7)
O3	0.0450 (9)	0.0546 (10)	0.0499 (9)	−0.0275 (8)	0.0149 (7)	−0.0115 (8)
S1	0.0219 (2)	0.0385 (2)	0.0286 (2)	−0.00741 (16)	0.00572 (16)	−0.00111 (17)

Geometric parameters (Å, º)

C1—C2	1.381 (3)	C9—H9	0.9300
C1—C6	1.412 (2)	C10—C11	1.391 (3)
C1—S1	1.774 (2)	C10—H10	0.9300
C2—C3	1.415 (3)	C11—N4	1.344 (3)
C2—H2	0.9300	C11—C11^{i}	1.487 (5)
C3—C4	1.365 (3)	Cd1—N4	2.3114 (18)
C3—H3	0.9300	Cd1—N4^{i}	2.3114 (18)
C4—C5	1.406 (3)	Cd1—O1	2.3267 (15)
C4—H4	0.9300	Cd1—O1^{i}	2.3267 (15)
C5—N3	1.354 (3)	Cd1—N1	2.3293 (19)
C5—C6	1.397 (3)	Cd1—N1^{i}	2.3293 (19)
C6—N1	1.374 (2)	N1—N2	1.319 (2)
C7—N4	1.334 (3)	N2—N3	1.336 (3)
C7—C8	1.386 (3)	N3—H3N	0.9310
C7—H7	0.9300	O1—S1	1.4690 (15)
C8—C9	1.378 (5)	O2—S1	1.4587 (17)
C8—H8	0.9300	O3—S1	1.4363 (16)
C9—C10	1.367 (5)		

C2—C1—C6	116.48 (18)	N4—Cd1—N4^{i}	71.91 (10)
C2—C1—S1	121.87 (15)	N4—Cd1—O1	166.80 (5)
C6—C1—S1	121.63 (14)	N4^{i}—Cd1—O1	100.35 (7)
C1—C2—C3	122.3 (2)	N4—Cd1—O1^{i}	100.35 (7)
C1—C2—H2	118.8	N4^{i}—Cd1—O1^{i}	166.80 (5)
C3—C2—H2	118.8	O1—Cd1—O1^{i}	89.15 (8)
C4—C3—C2	121.9 (2)	N4—Cd1—N1	92.23 (6)
C4—C3—H3	119.0	N4^{i}—Cd1—N1	106.18 (6)
C2—C3—H3	119.0	O1—Cd1—N1	79.50 (6)
C3—C4—C5	115.9 (2)	O1^{i}—Cd1—N1	84.43 (6)
C3—C4—H4	122.0	N4—Cd1—N1^{i}	106.18 (6)
C5—C4—H4	122.0	N4^{i}—Cd1—N1^{i}	92.23 (6)
N3—C5—C6	104.12 (17)	O1—Cd1—N1^{i}	84.43 (6)
N3—C5—C4	132.63 (19)	O1^{i}—Cd1—N1^{i}	79.50 (6)
C6—C5—C4	123.20 (18)	N1—Cd1—N1^{i}	157.38 (8)
N1—C6—C5	108.02 (16)	N2—N1—C6	108.28 (16)
N1—C6—C1	131.83 (17)	N2—N1—Cd1	120.41 (13)
C5—C6—C1	120.12 (17)	C6—N1—Cd1	128.60 (12)
N4—C7—C8	122.2 (3)	N1—N2—N3	108.25 (16)
N4—C7—H7	118.9	N2—N3—C5	111.32 (17)
C8—C7—H7	118.9	N2—N3—H3N	123.9
C9—C8—C7	118.3 (3)	C5—N3—H3N	124.8
C9—C8—H8	120.9	C7—N4—C11	119.6 (2)
C7—C8—H8	120.9	C7—N4—Cd1	123.54 (16)
C10—C9—C8	119.7 (2)	C11—N4—Cd1	116.87 (15)
C10—C9—H9	120.1	S1—O1—Cd1	130.56 (8)
C8—C9—H9	120.1	O3—S1—O2	113.99 (11)
C9—C10—C11	119.5 (3)	O3—S1—O1	112.90 (10)
C9—C10—H10	120.3	O2—S1—O1	111.29 (10)
C11—C10—H10	120.3	O3—S1—C1	106.89 (10)
N4—C11—C10	120.7 (2)	O2—S1—C1	105.86 (9)
N4—C11—C11^{i}	117.13 (12)	O1—S1—C1	105.16 (9)
C10—C11—C11^{i}	122.13 (17)		

C6—C1—C2—C3	1.0 (3)	Cd1—N1—N2—N3	162.45 (12)
S1—C1—C2—C3	−177.47 (18)	N1—N2—N3—C5	0.0 (2)
C1—C2—C3—C4	−0.9 (4)	C6—C5—N3—N2	0.4 (2)
C2—C3—C4—C5	−0.3 (3)	C4—C5—N3—N2	−177.0 (2)
C3—C4—C5—N3	178.3 (2)	C8—C7—N4—C11	0.8 (3)
C3—C4—C5—C6	1.4 (3)	C8—C7—N4—Cd1	178.65 (18)
N3—C5—C6—N1	−0.6 (2)	C10—C11—N4—C7	1.4 (3)
C4—C5—C6—N1	177.08 (18)	C11^{i}—C11—N4—C7	−179.5 (2)
N3—C5—C6—C1	−179.00 (16)	C10—C11—N4—Cd1	−176.55 (19)
C4—C5—C6—C1	−1.3 (3)	C11^{i}—C11—N4—Cd1	2.5 (3)
C2—C1—C6—N1	−177.84 (19)	N4^{i}—Cd1—N4—C7	−178.8 (2)
S1—C1—C6—N1	0.6 (3)	O1—Cd1—N4—C7	−123.2 (3)
C2—C1—C6—C5	0.1 (3)	O1^{i}—Cd1—N4—C7	12.25 (18)

S1—C1—C6—C5	178.54 (14)	N1—Cd1—N4—C7	−72.49 (17)
N4—C7—C8—C9	−3.0 (4)	N1^{i}—Cd1—N4—C7	94.20 (17)
C7—C8—C9—C10	2.9 (5)	N4^{i}—Cd1—N4—C11	−0.92 (11)
C8—C9—C10—C11	−0.8 (5)	O1—Cd1—N4—C11	54.7 (3)
C9—C10—C11—N4	−1.4 (4)	O1^{i}—Cd1—N4—C11	−169.89 (14)
C9—C10—C11—C11^{i}	179.6 (3)	N1—Cd1—N4—C11	105.37 (15)
C5—C6—N1—N2	0.7 (2)	N1^{i}—Cd1—N4—C11	−87.93 (15)
C1—C6—N1—N2	178.77 (19)	N4—Cd1—O1—S1	9.9 (3)
C5—C6—N1—Cd1	−160.36 (13)	N4^{i}—Cd1—O1—S1	62.73 (12)
C1—C6—N1—Cd1	17.7 (3)	O1^{i}—Cd1—O1—S1	−126.49 (14)
N4—Cd1—N1—N2	29.31 (15)	N1—Cd1—O1—S1	−41.99 (12)
N4^{i}—Cd1—N1—N2	101.12 (15)	N1^{i}—Cd1—O1—S1	153.99 (12)
O1—Cd1—N1—N2	−161.04 (16)	Cd1—O1—S1—O3	176.99 (11)
O1^{i}—Cd1—N1—N2	−70.88 (15)	Cd1—O1—S1—O2	−53.35 (14)
N1^{i}—Cd1—N1—N2	−115.61 (15)	Cd1—O1—S1—C1	60.81 (13)
N4—Cd1—N1—C6	−171.67 (16)	C2—C1—S1—O3	21.9 (2)
N4^{i}—Cd1—N1—C6	−99.86 (16)	C6—C1—S1—O3	−156.48 (16)
O1—Cd1—N1—C6	−2.02 (15)	C2—C1—S1—O2	−99.96 (19)
O1^{i}—Cd1—N1—C6	88.15 (16)	C6—C1—S1—O2	81.66 (17)
N1^{i}—Cd1—N1—C6	43.42 (15)	C2—C1—S1—O1	142.14 (17)
C6—N1—N2—N3	−0.4 (2)	C6—C1—S1—O1	−36.25 (18)

Symmetry code: (i) −*x*, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*N*···O2^{ii}	0.93	1.86	2.776 (3)	167
C3—H3···O3^{iii}	0.93	2.55	3.255 (3)	133
C7—H7···O2^{i}	0.93	2.56	3.204 (3)	127

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