Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure of oxamyl

Eunjin Kwon, Ki-Min Park,* Hyunjin Park and Tae Ho Kim*

Department of Chemistry (BK21 plus) and Research Institute of Natural Sciences, Gyeongsang National University, Jinju 52828, Republic of Korea. *Correspondence e-mail: kmpark@gnu.ac.kr, thkim@gnu.ac.kr

Received 8 November 2016
Accepted 12 November 2016

Edited by J. Simpson, University of Otago, New Zealand

Keywords: crystal structure; acaricide; insecticide; nematicide; oxamyl.

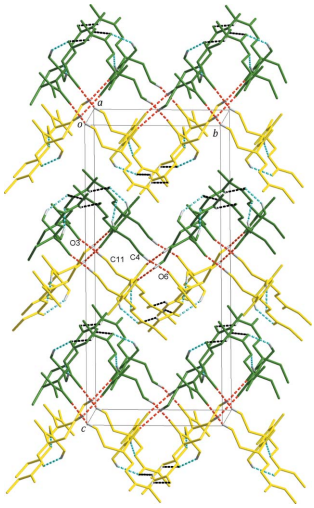
CCDC reference: 1516996

Supporting information: this article has supporting information at journals.iucr.org/e

The title compound, $C_7H_{13}N_3O_3S$ [systematic name: (*Z*)-methyl 2-dimethylamino-*N*-(methylcarbamoyloxy)-2-oxoethanimidothioate], is an oxime carbamate acaride, insecticide and nematicide. The asymmetric unit comprises two independent molecules, *A* and *B*. The dihedral angles between the mean planes [r.m.s. deviations = 0.0017 (*A*) and 0.0016 Å (*B*)] of the acetamide and oxyimino groups are 88.80 (8)° for *A* and 87.05 (8)° for *B*. In the crystal, N/C—H···O hydrogen bonds link adjacent molecules, forming chains along the *a* axis. The chains are further linked by C—H···O hydrogen bonds, resulting in a three-dimensional network with alternating rows of *A* and *B* molecules in the *bc* plane stacked along the *a*-axis direction. The structure was refined as an inversion twin with a final BASF parameter of 0.16 (9).

1. Chemical context

Oxamyl [(*N*,*N*-dimethyl-2-methylcarbamoyloximino-2-(dimethylsulfanyl)acetamide] is a carbamate compound used in a wide range of agricultural situations. It is systemic and active as an insecticide or a nematicide. It is used for the control of nematodes in vegetables, bananas, pineapple, peanuts, cotton, soya beans, tobacco, potatoes, sugar beet, and other crops. It is also used in India for controlling the growth of nematodes on vegetable crops (Mohammad *et al.*, 2015; Agarwal *et al.*, 2016). In addition, oxamyl was classified by the World Health Organization (WHO) as highly hazardous (class IB) (Al-Dabbas *et al.*, 2014). Oxamyl can be integrated with horse manure, sesame-oil-cake, or *Bacillus thuringiensis* to improve eggplant growth response and reduce development of the nematode *Meloidogyne incognita* (Osman *et al.*, 2009). Also, oxamyl has a very high water solubility (280 g/L at 298 K) and low sorption solubility affinity to soils. As a result of these properties, oxamyl easily migrates into the water compartment (Mazellier *et al.*, 2010). Herein, we report the molecular and crystal structure of oxamyl.



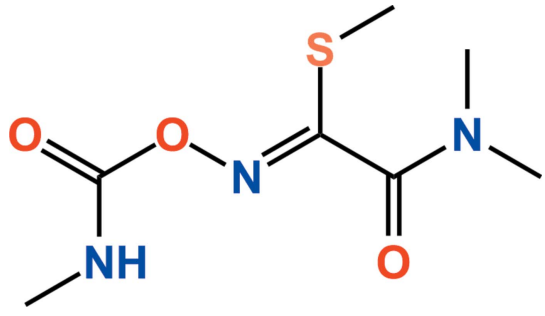


Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.88	2.13	2.871 (3)	142
N4—H4N···O4^{ii}	0.88	2.04	2.794 (3)	142
C4—H4B···O6^{iii}	0.98	2.54	3.075 (4)	114
C6—H6B···O2^{iv}	0.98	2.60	3.518 (4)	156
C7—H7B···O1^{iv}	0.98	2.52	3.431 (4)	155
C11—H11B···O3^{v}	0.98	2.53	3.042 (4)	113
C13—H13B···O4^{iv}	0.98	2.53	3.440 (4)	155
C14—H14B···O5^{iv}	0.98	2.59	3.554 (4)	168

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

2. Structural commentary

The asymmetric unit of oxamyl comprises two independent molecules, *A* and *B* (Fig. 1). The compound consists of carbamate, acetamide, methylthio and oxyimino functional groups. The dihedral angles between the mean planes [r.m.s. deviations = 0.0017 (*A*) and 0.0016 Å (*B*)] of the acetamide and oxyimino groups are 88.80 (8) for *A* and 87.05 (8)° for *B*. All bond lengths and bond angles are normal and comparable to those observed in methomyl [systematic name: (*E*)-methyl *N*-(methylcarbamoyl)oxyethanimidothioate] which adopts similar crystal structure (Takusagawa & Jacobson, 1977).

3. Supramolecular features

The crystal structure is stabilized by several N—H···O and C—H···O hydrogen bonds (Table 1). Adjacent *A* molecules form intermolecular N1—H1N···O1 hydrogen bonds. In addition, C6—H6B···O2 and C7—H7B···O1 hydrogen bonds between the carbamate and dimethylamine groups generate $R_2^2(8)$ inversion dimers. These contacts link the *A* molecules into double chains along the *a* axis. A closely similar situation obtains for the *B* molecules, with intermolecular N4—H4N···O4 hydrogen bonds together with C13—H13B···O4 and C14—H14B···O5 $R_2^2(8)$ inversion dimers also forming a double chain, this time solely of *B* molecules, parallel to the one described previously, again along the *a* axis, Fig. 2. The *A* and *B* double chains are further linked by C4—H4B···O6 and C11—H11B···O3 contacts, Table 1, to give a three-dimensional network with alternating rows of *A* and *B* molecules in the *bc* plane stacked along the *a*-axis direction, Fig. 3.

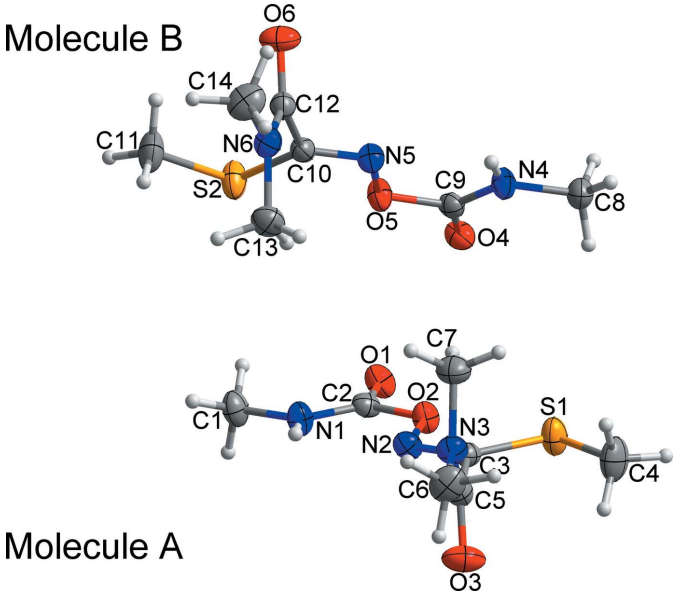


Figure 1
The asymmetric unit of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

4. Synthesis and crystallization

The title compound was purchased from Dr Ehrenstorfer GmbH. Slow evaporation of its solution in CH_3OH gave single crystals suitable for X-ray analysis.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All C-bound H atoms were positioned geometrically [with d(N—H) = 0.88 Å, $U_{iso} = 1.2U_{eq}$(C) for N—H group, $U_{iso} = 1.5U_{eq}$(C) for methyl group, d(C—H) = 0.98 Å]. The crystal studied was an inversion twin with a 0.84 (9):0.16 (9) domain ratio.

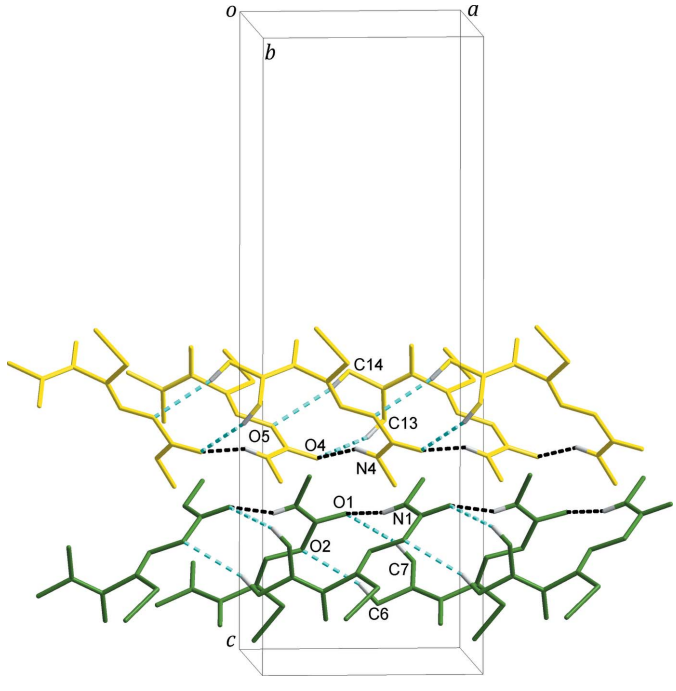


Figure 2
The double chains formed through intermolecular N—H···O (black dashed lines) and C—H···O (sky-blue dashed lines) hydrogen bonds. The *A* and *B* molecules are shown in green and yellow, respectively. H atoms not involved in intermolecular interactions have been omitted for clarity.

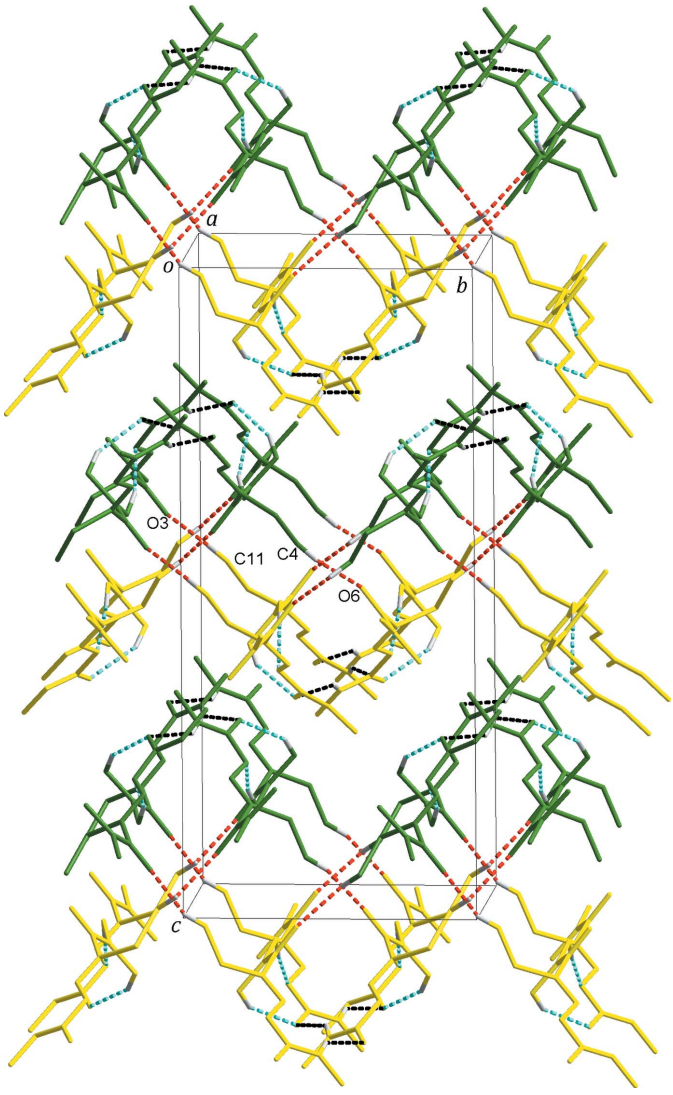


Figure 3
The three-dimensional network made up of molecules *A* (green) and *B* (yellow). Black dashed lines represent intermolecular N—H···O hydrogen bonds. The C—H···O hydrogen bonds are shown as sky-blue (between each molecule *A* or *B*) and red (between molecules *A* and *B*) dashed lines, respectively. H atoms not involved in intermolecular interactions have been omitted for clarity.

Acknowledgements

This research was supported by the Basic Science Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (No. 2015R1D1A4A01020317).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_7H_{13}N_3O_3S$
M_r	219.26
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	173
a, b, c (Å)	8.3367 (4), 10.7752 (5), 24.1016 (12)
V (Å^3)	2165.04 (18)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.29
Crystal size (mm)	0.50 × 0.14 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.665, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19300, 5238, 4655
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.090, 1.04
No. of reflections	5238
No. of parameters	262
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.23
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.16 (9)

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2010) and *publCIF* (Westrip, 2010).

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supporting information

Acta Cryst. (2016). E**72**, 1816-1818 [https://doi.org/10.1107/S2056989016018168]

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

(*Z*)-[(Dimethylcarbamoyl)(methylsulfanyl)methylidene]amino *N*-methylcarbamate

Crystal data

$C_7H_{13}N_3O_3S$
$M_r = 219.26$
Orthorhombic, $Pca2_1$
$a = 8.3367$ (4) Å
$b = 10.7752$ (5) Å
$c = 24.1016$ (12) Å
$V = 2165.04$ (18) Å^3
$Z = 8$
$F(000) = 928$
$D_x = 1.345$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6335 reflections
$\theta = 2.5$–$27.8°$
$\mu = 0.29$ mm^{-1}
$T = 173$ K
Plate, colourless
0.50 × 0.14 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min} = 0.665$, $T_{max} = 0.746$
19300 measured reflections
5238 independent reflections
4655 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.7°$
$h = -11 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -32 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.090$
$S = 1.04$
5238 reflections
262 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.3998P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.16 (9)

Special details

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

Refinement. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.55678 (10)	0.32807 (7)	0.87717 (3)	0.0373 (2)
S2	0.97239 (10)	0.16264 (7)	0.54545 (3)	0.0376 (2)
O1	0.8636 (3)	0.13823 (18)	0.74085 (9)	0.0308 (5)
O2	0.6589 (2)	0.17413 (17)	0.79576 (8)	0.0270 (4)
O3	0.2966 (3)	0.0966 (2)	0.91570 (10)	0.0431 (6)
O4	1.2851 (3)	0.36802 (18)	0.67471 (9)	0.0307 (5)
O5	1.0771 (3)	0.32628 (17)	0.62210 (9)	0.0282 (5)
O6	0.7167 (3)	0.3997 (2)	0.50123 (10)	0.0403 (6)
N1	0.6479 (3)	0.0112 (2)	0.73350 (10)	0.0290 (5)
H1N	0.5497	−0.0037	0.7451	0.035*
N2	0.5009 (3)	0.1328 (2)	0.81132 (10)	0.0272 (5)
N3	0.1571 (3)	0.2143 (2)	0.85463 (10)	0.0303 (6)
N4	1.0729 (3)	0.4993 (2)	0.67852 (10)	0.0287 (5)
H4N	0.9764	0.5151	0.6655	0.034*
N5	0.9217 (3)	0.3683 (2)	0.60490 (10)	0.0261 (5)
N6	0.5764 (3)	0.2808 (2)	0.56227 (10)	0.0291 (6)
C1	0.7188 (4)	−0.0672 (3)	0.69115 (14)	0.0348 (7)
H1A	0.7844	−0.0164	0.6662	0.052*
H1B	0.6335	−0.1079	0.6699	0.052*
H1C	0.7863	−0.1304	0.7088	0.052*
C2	0.7298 (4)	0.1050 (2)	0.75477 (12)	0.0244 (6)
C3	0.4493 (4)	0.2044 (3)	0.84969 (11)	0.0242 (6)
C4	0.4197 (5)	0.3917 (4)	0.92805 (16)	0.0481 (10)
H4A	0.3255	0.4260	0.9091	0.072*
H4B	0.4736	0.4576	0.9490	0.072*
H4C	0.3858	0.3259	0.9536	0.072*
C5	0.2909 (3)	0.1659 (3)	0.87589 (13)	0.0271 (6)
C6	0.0028 (4)	0.1835 (4)	0.88024 (16)	0.0398 (8)
H6A	0.0171	0.1138	0.9059	0.060*
H6B	−0.0742	0.1604	0.8513	0.060*
H6C	−0.0376	0.2557	0.9007	0.060*
C7	0.1526 (4)	0.3046 (3)	0.80973 (14)	0.0372 (7)
H7A	0.1188	0.3853	0.8243	0.056*
H7B	0.0764	0.2770	0.7813	0.056*
H7C	0.2597	0.3122	0.7933	0.056*
C8	1.1426 (4)	0.5816 (3)	0.71943 (13)	0.0348 (7)
H8A	1.1834	0.5326	0.7507	0.052*
H8B	1.0607	0.6396	0.7327	0.052*

H8C	1.2311	0.6281	0.7026	0.052*
C9	1.1516 (4)	0.4014 (2)	0.66055 (11)	0.0242 (6)
C10	0.8681 (4)	0.2936 (2)	0.56845 (11)	0.0240 (6)
C11	0.8379 (5)	0.0982 (3)	0.49430 (15)	0.0462 (9)
H11A	0.7431	0.0641	0.5129	0.069*
H11B	0.8928	0.0320	0.4739	0.069*
H11C	0.8049	0.1635	0.4684	0.069*
C12	0.7109 (4)	0.3295 (2)	0.54159 (13)	0.0267 (6)
C13	0.5720 (4)	0.1938 (3)	0.60790 (14)	0.0366 (7)
H13A	0.5364	0.1126	0.5944	0.055*
H13B	0.4972	0.2238	0.6363	0.055*
H13C	0.6795	0.1861	0.6240	0.055*
C14	0.4231 (4)	0.3106 (4)	0.53622 (15)	0.0420 (8)
H14A	0.4301	0.3922	0.5184	0.063*
H14B	0.3386	0.3120	0.5645	0.063*
H14C	0.3976	0.2476	0.5083	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0356 (4)	0.0368 (4)	0.0393 (4)	−0.0072 (3)	0.0091 (4)	−0.0137 (4)
S2	0.0352 (4)	0.0330 (4)	0.0447 (5)	0.0083 (3)	−0.0103 (4)	−0.0155 (4)
O1	0.0210 (10)	0.0284 (10)	0.0428 (12)	−0.0018 (9)	0.0060 (9)	−0.0027 (9)
O2	0.0212 (10)	0.0271 (10)	0.0325 (11)	−0.0017 (8)	0.0047 (9)	−0.0055 (8)
O3	0.0392 (14)	0.0478 (13)	0.0423 (13)	0.0036 (11)	0.0085 (11)	0.0196 (11)
O4	0.0246 (11)	0.0275 (10)	0.0401 (12)	−0.0007 (9)	−0.0058 (10)	0.0029 (9)
O5	0.0211 (10)	0.0257 (10)	0.0379 (12)	0.0023 (8)	−0.0061 (9)	−0.0072 (9)
O6	0.0342 (13)	0.0476 (12)	0.0393 (12)	0.0008 (11)	−0.0035 (10)	0.0185 (11)
N1	0.0227 (12)	0.0282 (11)	0.0360 (13)	−0.0003 (10)	0.0061 (10)	−0.0077 (10)
N2	0.0233 (13)	0.0265 (12)	0.0318 (13)	−0.0011 (11)	0.0054 (11)	0.0001 (10)
N3	0.0269 (13)	0.0338 (13)	0.0303 (13)	−0.0022 (11)	0.0031 (11)	0.0026 (10)
N4	0.0259 (12)	0.0261 (11)	0.0343 (12)	0.0015 (10)	−0.0078 (10)	−0.0065 (10)
N5	0.0204 (12)	0.0268 (11)	0.0310 (13)	0.0025 (10)	−0.0039 (10)	−0.0028 (10)
N6	0.0242 (13)	0.0338 (12)	0.0293 (13)	−0.0019 (10)	−0.0014 (10)	−0.0019 (10)
C1	0.0351 (17)	0.0295 (15)	0.0398 (17)	0.0018 (13)	0.0061 (14)	−0.0103 (12)
C2	0.0232 (15)	0.0219 (12)	0.0281 (14)	0.0057 (11)	0.0031 (12)	0.0023 (11)
C3	0.0265 (15)	0.0235 (13)	0.0225 (13)	0.0020 (12)	0.0005 (11)	0.0021 (11)
C4	0.047 (2)	0.052 (2)	0.045 (2)	0.0018 (18)	0.0094 (18)	−0.0225 (17)
C5	0.0276 (15)	0.0256 (13)	0.0282 (14)	−0.0014 (11)	0.0051 (13)	−0.0014 (12)
C6	0.0255 (15)	0.055 (2)	0.0388 (17)	−0.0041 (15)	0.0053 (16)	−0.0005 (16)
C7	0.0364 (18)	0.0385 (17)	0.0368 (17)	0.0014 (14)	−0.0027 (15)	0.0072 (14)
C8	0.0439 (19)	0.0293 (14)	0.0311 (15)	−0.0019 (14)	−0.0055 (14)	−0.0050 (12)
C9	0.0236 (14)	0.0225 (13)	0.0266 (13)	−0.0036 (11)	−0.0002 (12)	0.0020 (11)
C10	0.0262 (15)	0.0210 (12)	0.0249 (13)	0.0001 (12)	0.0008 (11)	0.0001 (11)
C11	0.048 (2)	0.0461 (19)	0.045 (2)	0.0003 (17)	−0.0105 (17)	−0.0213 (16)
C12	0.0277 (15)	0.0253 (12)	0.0271 (14)	0.0005 (11)	−0.0025 (13)	−0.0024 (12)
C13	0.0346 (18)	0.0368 (16)	0.0383 (18)	−0.0050 (14)	0.0050 (14)	0.0040 (14)
C14	0.0240 (15)	0.057 (2)	0.045 (2)	0.0030 (15)	−0.0041 (15)	0.0001 (16)

Geometric parameters (Å, º)

S1—C3	1.737 (3)	C1—H1A	0.9800
S1—C4	1.811 (3)	C1—H1B	0.9800
S2—C10	1.748 (3)	C1—H1C	0.9800
S2—C11	1.805 (3)	C3—C5	1.521 (4)
O1—C2	1.218 (4)	C4—H4A	0.9800
O2—C2	1.371 (3)	C4—H4B	0.9800
O2—N2	1.440 (3)	C4—H4C	0.9800
O3—C5	1.216 (4)	C6—H6A	0.9800
O4—C9	1.219 (4)	C6—H6B	0.9800
O5—C9	1.378 (3)	C6—H6C	0.9800
O5—N5	1.434 (3)	C7—H7A	0.9800
O6—C12	1.233 (4)	C7—H7B	0.9800
N1—C2	1.323 (4)	C7—H7C	0.9800
N1—C1	1.451 (4)	C8—H8A	0.9800
N1—H1N	0.8800	C8—H8B	0.9800
N2—C3	1.279 (4)	C8—H8C	0.9800
N3—C5	1.334 (4)	C10—C12	1.512 (4)
N3—C7	1.455 (4)	C11—H11A	0.9800
N3—C6	1.464 (4)	C11—H11B	0.9800
N4—C9	1.315 (4)	C11—H11C	0.9800
N4—C8	1.448 (4)	C13—H13A	0.9800
N4—H4N	0.8800	C13—H13B	0.9800
N5—C10	1.272 (4)	C13—H13C	0.9800
N6—C12	1.334 (4)	C14—H14A	0.9800
N6—C13	1.445 (4)	C14—H14B	0.9800
N6—C14	1.460 (4)	C14—H14C	0.9800
C3—S1—C4	102.89 (16)	N3—C6—H6C	109.5
C10—S2—C11	102.61 (16)	H6A—C6—H6C	109.5
C2—O2—N2	114.5 (2)	H6B—C6—H6C	109.5
C9—O5—N5	114.6 (2)	N3—C7—H7A	109.5
C2—N1—C1	120.5 (2)	N3—C7—H7B	109.5
C2—N1—H1N	119.8	H7A—C7—H7B	109.5
C1—N1—H1N	119.8	N3—C7—H7C	109.5
C3—N2—O2	108.1 (2)	H7A—C7—H7C	109.5
C5—N3—C7	124.6 (3)	H7B—C7—H7C	109.5
C5—N3—C6	118.9 (3)	N4—C8—H8A	109.5
C7—N3—C6	116.3 (3)	N4—C8—H8B	109.5
C9—N4—C8	121.0 (3)	H8A—C8—H8B	109.5
C9—N4—H4N	119.5	N4—C8—H8C	109.5
C8—N4—H4N	119.5	H8A—C8—H8C	109.5
C10—N5—O5	108.5 (2)	H8B—C8—H8C	109.5
C12—N6—C13	124.1 (3)	O4—C9—N4	126.9 (3)
C12—N6—C14	119.2 (3)	O4—C9—O5	115.2 (2)
C13—N6—C14	116.6 (3)	N4—C9—O5	117.9 (3)
N1—C1—H1A	109.5	N5—C10—C12	116.0 (2)

N1—C1—H1B	109.5	N5—C10—S2	123.7 (2)
H1A—C1—H1B	109.5	C12—C10—S2	120.1 (2)
N1—C1—H1C	109.5	S2—C11—H11A	109.5
H1A—C1—H1C	109.5	S2—C11—H11B	109.5
H1B—C1—H1C	109.5	H11A—C11—H11B	109.5
O1—C2—N1	126.2 (3)	S2—C11—H11C	109.5
O1—C2—O2	115.7 (2)	H11A—C11—H11C	109.5
N1—C2—O2	118.1 (3)	H11B—C11—H11C	109.5
N2—C3—C5	115.3 (2)	O6—C12—N6	124.7 (3)
N2—C3—S1	124.4 (2)	O6—C12—C10	117.4 (3)
C5—C3—S1	119.9 (2)	N6—C12—C10	117.9 (3)
S1—C4—H4A	109.5	N6—C13—H13A	109.5
S1—C4—H4B	109.5	N6—C13—H13B	109.5
H4A—C4—H4B	109.5	H13A—C13—H13B	109.5
S1—C4—H4C	109.5	N6—C13—H13C	109.5
H4A—C4—H4C	109.5	H13A—C13—H13C	109.5
H4B—C4—H4C	109.5	H13B—C13—H13C	109.5
O3—C5—N3	125.1 (3)	N6—C14—H14A	109.5
O3—C5—C3	117.4 (3)	N6—C14—H14B	109.5
N3—C5—C3	117.4 (3)	H14A—C14—H14B	109.5
N3—C6—H6A	109.5	N6—C14—H14C	109.5
N3—C6—H6B	109.5	H14A—C14—H14C	109.5
H6A—C6—H6B	109.5	H14B—C14—H14C	109.5

C2—O2—N2—C3	179.8 (2)	S1—C3—C5—N3	93.6 (3)
C9—O5—N5—C10	178.1 (2)	C8—N4—C9—O4	0.0 (5)
C1—N1—C2—O1	3.0 (5)	C8—N4—C9—O5	179.2 (2)
C1—N1—C2—O2	−178.2 (3)	N5—O5—C9—O4	−178.6 (2)
N2—O2—C2—O1	179.9 (2)	N5—O5—C9—N4	2.1 (3)
N2—O2—C2—N1	1.0 (3)	O5—N5—C10—C12	−174.7 (2)
O2—N2—C3—C5	−173.4 (2)	O5—N5—C10—S2	0.4 (3)
O2—N2—C3—S1	−0.5 (3)	C11—S2—C10—N5	−179.2 (3)
C4—S1—C3—N2	179.3 (3)	C11—S2—C10—C12	−4.2 (3)
C4—S1—C3—C5	−8.0 (3)	C13—N6—C12—O6	176.8 (3)
C7—N3—C5—O3	175.0 (3)	C14—N6—C12—O6	0.1 (4)
C6—N3—C5—O3	−0.1 (5)	C13—N6—C12—C10	−1.4 (4)
C7—N3—C5—C3	−2.4 (4)	C14—N6—C12—C10	−178.1 (3)
C6—N3—C5—C3	−177.5 (3)	N5—C10—C12—O6	85.8 (3)
N2—C3—C5—O3	89.3 (3)	S2—C10—C12—O6	−89.5 (3)
S1—C3—C5—O3	−84.0 (3)	N5—C10—C12—N6	−95.9 (3)
N2—C3—C5—N3	−93.1 (3)	S2—C10—C12—N6	88.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1^{i}	0.88	2.13	2.871 (3)	142
N4—H4*N*···O4^{ii}	0.88	2.04	2.794 (3)	142
C4—H4*B*···O6^{iii}	0.98	2.54	3.075 (4)	114

C6—H6*B*···O2^{iv}	0.98	2.60	3.518 (4)	156
C7—H7*B*···O1^{iv}	0.98	2.52	3.431 (4)	155
C11—H11*B*···O3^{v}	0.98	2.53	3.042 (4)	113
C13—H13*B*···O4^{iv}	0.98	2.53	3.440 (4)	155
C14—H14*B*···O5^{iv}	0.98	2.59	3.554 (4)	168

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