Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-[(*E*)-2-(4-Ethoxyphenyl)ethenyl]-1-methylpyridinium 4-chlorobenzenesulfonate monohydrate[1]

Suchada Chantrapromma,[a]*§ Kullapa Chanawanno[a] and Hoong-Kun Fun[b]¶

[a]Crystal Materials Research Unit, Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand, and [b]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: suchada.c@psu.ac.th

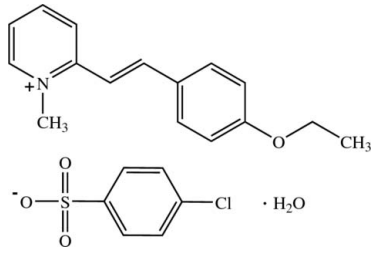
Received 5 December 2010; accepted 21 December 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.141; data-to-parameter ratio = 28.1.

In the title compound, $C_{16}H_{18}NO^{+}\cdot C_6H_4ClO_3S^{-}\cdot H_2O$, the cation exists in an E configuration with respect to the ethenyl bond and is slightly twisted with a dihedral angle of 9.85 (5)° between the pyridinium and the benzene rings. The anion is inclined to the cation with the dihedral angles between the benzene ring of the anion and the pyridinium and benzene rings of the cation of 78.33 (6) and 68.73 (6)°, respectively. In the crystal, the cations and anions are arranged alternately into head-to-head ribbons along the c axis, with the cationic ribbons stacked along the b axis. The crystal is consolidated by O—H···O hydrogen bonds, weak C—H···O and C—H···π interactions. π–π interactions with centroid–centroid distances of 3.6111 (7) and 3.6466 (7) Å are also observed.

Related literature

For background to and the biological activity of quaternary ammonium compounds, see: Armitage *et al.* (1929); Browning *et al.* (1922); Chanawanno *et al.* (2010); Chantrapromma *et al.* (2010); Wainwright & Kristiansen (2003). For related structures, see: Fun *et al.* (2010). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{16}H_{18}NO^{+}\cdot C_6H_4ClO_3S^{-}\cdot H_2O$
M_r = 449.94
Monoclinic, $P2_1/c$
a = 9.7568 (5) Å
b = 6.5284 (3) Å
c = 34.6568 (15) Å
β = 104.784 (1)°
V = 2134.43 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 100 K
0.45 × 0.32 × 0.13 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.873, T_{max} = 0.962
30082 measured reflections
7670 independent reflections
6483 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.141
S = 1.11
7670 reflections
273 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

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

*Cg*2 and *Cg*3 are the centroids of the C8–C13 and C17–C22 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*W*1···O4^{i}	0.91	1.95	2.8148 (16)	158
O1*W*—H2*W*1···O2	0.82	2.11	2.9265 (14)	173
C1—H1*A*···O1*W*^{ii}	0.93	2.23	3.1544 (17)	176
C2—H2*A*···O1*W*^{iii}	0.93	2.44	3.2200 (17)	142
C4—H4*A*···O2^{i}	0.93	2.50	3.3768 (17)	158
C6—H6*A*···O3^{iv}	0.93	2.56	3.4308 (17)	155
C13—H13*A*···O3^{iv}	0.93	2.51	3.3859 (17)	157
C16—H16*A*···O4^{v}	0.96	2.57	3.3766 (18)	142
C16—H16*B*···O3^{iv}	0.96	2.50	3.1307 (17)	124
C22—H22*A*···O4	0.93	2.56	2.9246 (17)	104
C9—H9*A*···*Cg*3^{i}	0.93	2.90	3.5924 (13)	132
C12—H12*A*···*Cg*3^{iv}	0.93	2.96	3.7431 (13)	143
C15—H15*C*···*Cg*2^{vi}	0.96	2.87	3.6918 (14)	145

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

The authors thank the Prince of Songkla University for a research grant. They also thank the Malaysian Government

[1] This paper is dedicated to His Majesty King Bhumibol Adulyadej of Thailand (King Rama IX) on the occasion of his 83th Birthday Anniversary which fell on December 5th, 2010.
§ Thomson Reuters ResearcherID: A-5085-2009.
¶ Additional correspondence author, e-mail: hkfun@usm.my. Thomson Reuters ResearcherID: A-3561-2009.

and Universiti Sains Malaysia for the Research University grant No. 1001/PFIZIK/811160.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2539).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Armitage, G., Gordon, J., Cohen, J. B. & Ellingworth, S. (1929). *Lancet*, **2**, 968–971.
Browning, C. H., Cohen, J. B. & Gulbransen, R. (1922). *Br. Med. J.* **1**, 514–515.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chanawanno, K., Chantrapromma, S., Anantapong, T., Kanjana-Opas, A. & Fun, H.-K. (2010). *Eur. J. Med. Chem.* **45**, 4199–4208.
Chantrapromma, S., Chanawanno, K. & Fun, H.-K. (2010). *Acta Cryst.* E**66**, o1975–o1976.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Fun, H.-K., Chanawanno, K. & Chantrapromma, S. (2010). *Acta Cryst.* E**66**, o305–o306.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wainwright, M. & Kristiansen, J. E. (2003). *Int. J. Antimicrob. Ag.* **22**, 479–486.

supporting information

Acta Cryst. (2011). E**67**, o515–o516 [doi:10.1107/S1600536810053572]

2-[(*E*)-2-(4-Ethoxyphenyl)ethenyl]-1-methylpyridinium 4-chlorobenzenesulfonate monohydrate

Suchada Chantrapromma, Kullapa Chanawanno and Hoong-Kun Fun

S1. Comment

Various quaternary ammonium compounds, such as styryl pyridinium derivatives, exhibit antiseptic properties (Armitage *et al.*, 1929; Browning *et al.*, 1922; Wainwright & Kristiansen, 2003). From our previous investigation on bioactive styryl pyridinium compounds, we found that dimethylaminostyryl pyridinium 4-substituted-benzenesulfonates possess high activity against both susceptible and methicillin-resistant *Staphylococcus aureus* (MRSA) (Chanawanno *et al.*, 2010). In continuing our on-going research on biologically-active quaternary ammonium compounds (Chanawanno *et al.*, 2010; Chantrapromma *et al.*, 2010), the title pyridinium derivative (I) was synthesized. Our results show that (I) is moderately active against the MRSA with the MIC value = 75 μg/ml, whereas it is inactive against susceptible *Staphylococcus aureus*. Herein we report the crystal structure of (I).

In the title compound (Fig. 1), the cation exists in an *E* configuration with respect to the ethenyl bond [torsion angle C5—C6—C7—C8 = 179.53 (11)°]. The cation is slightly twisted with a dihedral angle between the N1/C1–C5 pyridinium and C8–C13 benzene rings of 9.85 (5)°. The ethoxy group is slightly twisted from the mean plane of the attached benzene ring with the torsion angle C11–O1–C14–C15 = -174.84 (10)°. The 4-chlorobenzenesulfonate anion is inclined to the cation as indicated by the dihedral angles between the benzene ring of the anion and the pyridinium and benzene rings of the cation of 78.33 (6) and 68.73 (6)°, respectively. The water molecule forms an O—H···O hydrogen bond with the anion (Table 1). Bond distances in (I) have normal values (Allen *et al.*, 1987) and are comparable to those observed in a related structure (Fun *et al.*, 2010).

In the crystal (Fig. 2), cations and anions are arranged alternatively into head-to-head ribbons along the *c* axis, with the cationic ribbons stacked along the *b* axis. The water molecules are linked to the anions by O—H···O hydrogen bonds and to the cations by C—H···O weak interactions. The crystal is consolidated by O—H···O hydrogen bonds, weak C—H···O and C—H···π interactions (Table 1). π–π interactions with distances $Cg_1\cdots Cg_1$ = 3.6466 (7) Å (symmetry code; 2-x, 2-y, 1-z) and $Cg_1\cdots Cg_2$ = 3.6466 (7) Å (symmetry code; x, 1+y, z) are observed (Cg_1, Cg_2 and Cg_3 are the centroids of N1/C1–C5, C8–C13 and C17–C22 rings, respectively).

S2. Experimental

The title compound was prepared according to our reported procedure (Chanawanno *et al.*, 2010). Yellow block-shaped single crystal of the title compound suitable for *x*-ray structure determination were recrystallized from methanol by slow evaporation of the solvent at room temperature after a few weeks. M. p. 458-459 K.

S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with d(O-H) = 0.82 and 0.91 Å, d(C-H) = 0.93 Å for aromatic and CH and 0.96 Å for CH_3 atoms. The U_{iso} values were constrained to be $1.5U_{eq}$ of the

carrier atom for methyl H atoms and 1.2U_{eq} for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is located at 0.60 Å from atom C4 and the deepest hole is located at 0.53 Å from atom S1.

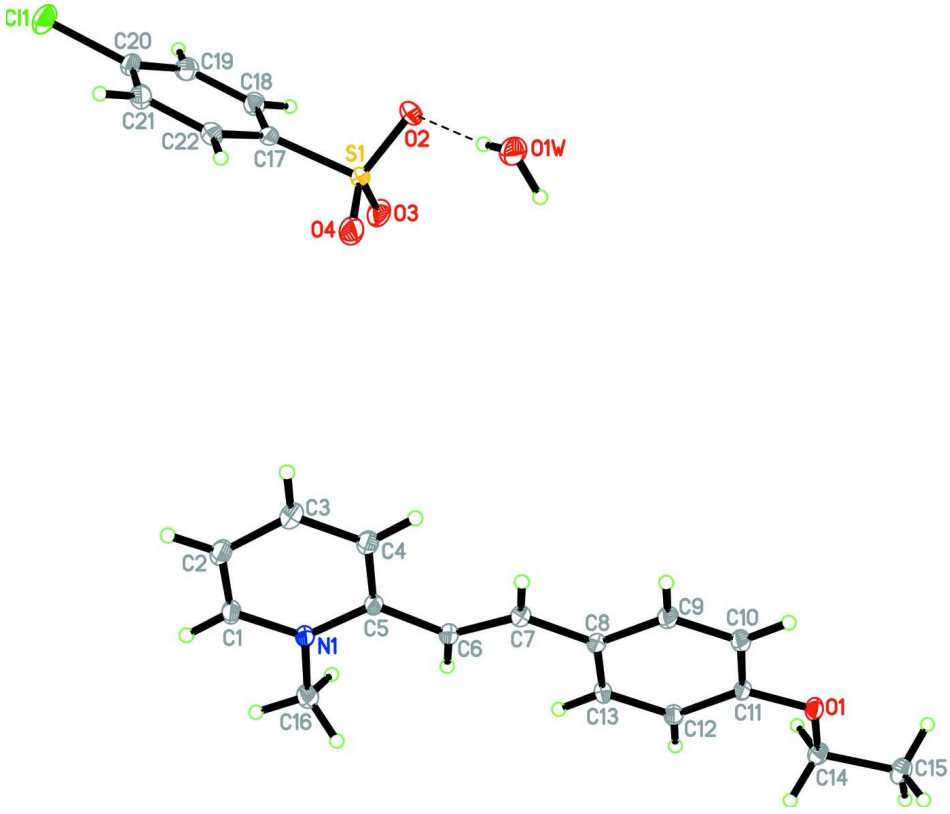


Figure 1

The molecular structure of the title compound, with 50% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen bond was shown as dashed line.

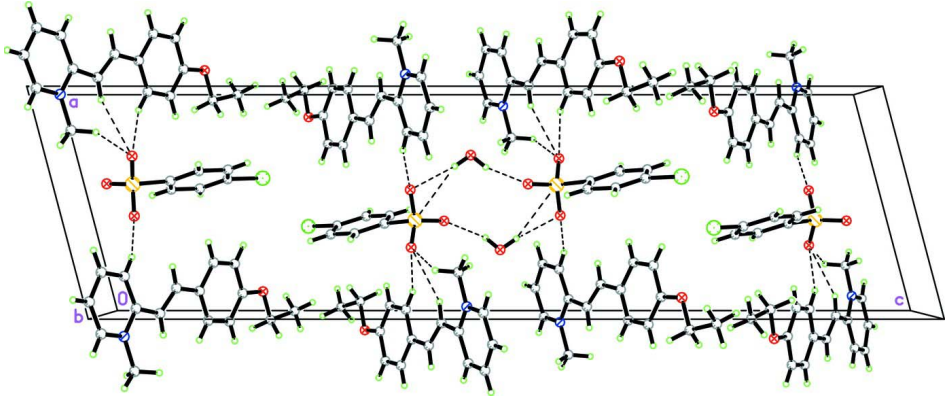


Figure 2

The crystal packing of the title compound viewed down the *b* axis. Hydrogen bonds were shown as dashed lines.

2-[(*E*)-2-(4-Ethoxyphenyl)ethenyl]-1-methylpyridinium 4-chlorobenzenesulfonate monohydrate

Crystal data

$C_{16}H_{18}NO^+ \cdot C_6H_4ClO_3S^- \cdot H_2O$
$M_r = 449.94$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.7568$ (5) Å
$b = 6.5284$ (3) Å
$c = 34.6568$ (15) Å
$\beta = 104.784$ (1)°
$V = 2134.43$ (17) Å^3
$Z = 4$
$F(000) = 944$
$D_x = 1.400$ Mg m^{-3}
Melting point = 458–459 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7670 reflections
$\theta = 2.7$–$32.5°$
$\mu = 0.31$ mm^{-1}
$T = 100$ K
Block, yellow
0.45 × 0.32 × 0.13 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.873$, $T_{max} = 0.962$
30082 measured reflections
7670 independent reflections
6483 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 32.5°$, $\theta_{min} = 2.7°$
$h = -14 \rightarrow 14$
$k = -9 \rightarrow 9$
$l = -52 \rightarrow 52$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.141$
$S = 1.11$
7670 reflections
273 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
$w = 1/[\sigma^2(F_o^2) + (0.0825P)^2 + 0.5425P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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. 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}
Cl1	0.61088 (4)	1.16478 (6)	0.733973 (10)	0.02817 (10)
S1	0.57932 (3)	0.55765 (5)	0.591654 (9)	0.01591 (8)

O1	0.90170 (9)	−0.18011 (14)	0.30285 (3)	0.01455 (17)
O2	0.44294 (10)	0.45645 (16)	0.58702 (3)	0.02007 (19)
O3	0.69824 (11)	0.41862 (18)	0.60401 (3)	0.0256 (2)
O4	0.58242 (13)	0.68270 (18)	0.55696 (3)	0.0281 (2)
N1	1.05293 (11)	0.97676 (16)	0.44598 (3)	0.01308 (18)
C1	1.03405 (14)	1.15606 (19)	0.46387 (3)	0.0154 (2)
H1A	1.1125	1.2364	0.4755	0.018*
C2	0.90154 (14)	1.2210 (2)	0.46519 (3)	0.0167 (2)
H2A	0.8895	1.3445	0.4773	0.020*
C3	0.78515 (14)	1.0976 (2)	0.44795 (4)	0.0172 (2)
H3A	0.6943	1.1377	0.4486	0.021*
C4	0.80564 (13)	0.9157 (2)	0.42988 (4)	0.0156 (2)
H4A	0.7280	0.8333	0.4186	0.019*
C5	0.94160 (12)	0.85327 (18)	0.42827 (3)	0.0125 (2)
C6	0.96936 (13)	0.66430 (18)	0.40911 (3)	0.0135 (2)
H6A	1.0627	0.6205	0.4132	0.016*
C7	0.86537 (13)	0.55033 (19)	0.38569 (3)	0.0141 (2)
H7A	0.7730	0.5972	0.3823	0.017*
C8	0.88342 (12)	0.36117 (18)	0.36522 (3)	0.01223 (19)
C9	0.76163 (12)	0.2621 (2)	0.34228 (3)	0.0150 (2)
H9A	0.6729	0.3189	0.3406	0.018*
C10	0.77130 (12)	0.0822 (2)	0.32213 (4)	0.0148 (2)
H10A	0.6894	0.0186	0.3073	0.018*
C11	0.90392 (12)	−0.00427 (18)	0.32398 (3)	0.01176 (19)
C12	1.02673 (12)	0.09169 (19)	0.34644 (3)	0.0131 (2)
H12A	1.1153	0.0351	0.3478	0.016*
C13	1.01532 (12)	0.27234 (19)	0.36666 (3)	0.0131 (2)
H13A	1.0973	0.3357	0.3815	0.016*
C14	1.03411 (12)	−0.28231 (19)	0.30496 (3)	0.0143 (2)
H14A	1.0752	−0.3321	0.3318	0.017*
H14B	1.1008	−0.1893	0.2977	0.017*
C15	1.00046 (14)	−0.4587 (2)	0.27591 (4)	0.0183 (2)
H15A	1.0860	−0.5317	0.2761	0.028*
H15B	0.9593	−0.4071	0.2496	0.028*
H15C	0.9347	−0.5495	0.2836	0.028*
C16	1.20000 (13)	0.9193 (2)	0.44648 (4)	0.0182 (2)
H16A	1.2635	1.0262	0.4590	0.027*
H16B	1.2073	0.9000	0.4196	0.027*
H16C	1.2247	0.7942	0.4612	0.027*
C17	0.59473 (12)	0.7331 (2)	0.63174 (3)	0.0141 (2)
C18	0.63847 (13)	0.6617 (2)	0.67086 (4)	0.0172 (2)
H18A	0.6637	0.5250	0.6757	0.021*
C19	0.64444 (13)	0.7944 (2)	0.70261 (4)	0.0186 (2)
H19A	0.6739	0.7480	0.7288	0.022*
C20	0.60549 (13)	0.9978 (2)	0.69447 (4)	0.0178 (2)
C21	0.56337 (14)	1.0721 (2)	0.65572 (4)	0.0183 (2)
H21A	0.5385	1.2090	0.6509	0.022*
C22	0.55904 (13)	0.9387 (2)	0.62424 (4)	0.0168 (2)

H22A	0.5323	0.9865	0.5981	0.020*
O1W	0.28876 (11)	0.44954 (18)	0.50268 (3)	0.0249 (2)
H1W1	0.3425	0.3848	0.4886	0.037*
H2W1	0.3382	0.4499	0.5257	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.03033 (18)	0.0307 (2)	0.02448 (16)	−0.00245 (14)	0.00880 (13)	−0.01471 (13)
S1	0.01448 (13)	0.01772 (15)	0.01687 (14)	−0.00511 (10)	0.00646 (10)	−0.00574 (10)
O1	0.0143 (4)	0.0133 (4)	0.0160 (4)	−0.0007 (3)	0.0037 (3)	−0.0052 (3)
O2	0.0146 (4)	0.0231 (5)	0.0224 (4)	−0.0076 (3)	0.0045 (3)	−0.0059 (4)
O3	0.0161 (4)	0.0260 (5)	0.0345 (5)	0.0022 (4)	0.0063 (4)	−0.0133 (4)
O4	0.0444 (6)	0.0246 (5)	0.0195 (4)	−0.0121 (5)	0.0161 (4)	−0.0056 (4)
N1	0.0164 (4)	0.0110 (4)	0.0123 (4)	−0.0023 (4)	0.0045 (3)	−0.0013 (3)
C1	0.0217 (5)	0.0119 (5)	0.0127 (4)	−0.0028 (4)	0.0049 (4)	−0.0019 (4)
C2	0.0238 (6)	0.0132 (5)	0.0136 (5)	0.0003 (4)	0.0057 (4)	−0.0017 (4)
C3	0.0198 (5)	0.0167 (5)	0.0152 (5)	0.0019 (4)	0.0049 (4)	−0.0024 (4)
C4	0.0158 (5)	0.0155 (5)	0.0157 (5)	−0.0008 (4)	0.0043 (4)	−0.0031 (4)
C5	0.0158 (5)	0.0114 (5)	0.0109 (4)	−0.0016 (4)	0.0044 (4)	−0.0008 (4)
C6	0.0158 (5)	0.0114 (5)	0.0138 (4)	−0.0014 (4)	0.0049 (4)	−0.0018 (4)
C7	0.0153 (5)	0.0135 (5)	0.0146 (5)	−0.0012 (4)	0.0056 (4)	−0.0022 (4)
C8	0.0143 (4)	0.0115 (5)	0.0116 (4)	−0.0016 (4)	0.0045 (3)	−0.0017 (4)
C9	0.0126 (4)	0.0167 (5)	0.0165 (5)	−0.0007 (4)	0.0050 (4)	−0.0044 (4)
C10	0.0122 (4)	0.0164 (5)	0.0156 (5)	−0.0026 (4)	0.0032 (4)	−0.0042 (4)
C11	0.0139 (4)	0.0111 (5)	0.0105 (4)	−0.0013 (4)	0.0036 (3)	−0.0016 (4)
C12	0.0126 (4)	0.0128 (5)	0.0138 (4)	−0.0005 (4)	0.0031 (4)	−0.0018 (4)
C13	0.0133 (4)	0.0124 (5)	0.0132 (4)	−0.0024 (4)	0.0025 (4)	−0.0020 (4)
C14	0.0162 (5)	0.0125 (5)	0.0143 (4)	0.0021 (4)	0.0042 (4)	−0.0008 (4)
C15	0.0225 (6)	0.0149 (5)	0.0172 (5)	0.0032 (4)	0.0043 (4)	−0.0032 (4)
C16	0.0156 (5)	0.0181 (6)	0.0216 (5)	−0.0030 (4)	0.0057 (4)	−0.0040 (4)
C17	0.0114 (4)	0.0163 (5)	0.0153 (5)	−0.0029 (4)	0.0046 (4)	−0.0035 (4)
C18	0.0157 (5)	0.0174 (6)	0.0180 (5)	−0.0009 (4)	0.0032 (4)	−0.0019 (4)
C19	0.0169 (5)	0.0232 (6)	0.0151 (5)	−0.0020 (5)	0.0030 (4)	−0.0022 (4)
C20	0.0149 (5)	0.0206 (6)	0.0184 (5)	−0.0027 (4)	0.0052 (4)	−0.0079 (5)
C21	0.0174 (5)	0.0155 (6)	0.0220 (5)	−0.0015 (4)	0.0051 (4)	−0.0038 (4)
C22	0.0158 (5)	0.0179 (6)	0.0169 (5)	−0.0028 (4)	0.0045 (4)	−0.0015 (4)
O1W	0.0202 (4)	0.0337 (6)	0.0203 (4)	−0.0034 (4)	0.0042 (4)	−0.0082 (4)

Geometric parameters (Å, º)

Cl1—C20	1.7405 (13)	C10—C11	1.3982 (16)
S1—O3	1.4491 (11)	C10—H10A	0.9300
S1—O2	1.4573 (10)	C11—C12	1.3994 (16)
S1—O4	1.4599 (11)	C12—C13	1.3906 (16)
S1—C17	1.7772 (12)	C12—H12A	0.9300
O1—C11	1.3587 (14)	C13—H13A	0.9300
O1—C14	1.4392 (14)	C14—C15	1.5096 (17)

N1—C1	1.3589 (16)	C14—H14A	0.9700
N1—C5	1.3662 (15)	C14—H14B	0.9700
N1—C16	1.4791 (16)	C15—H15A	0.9600
C1—C2	1.3724 (18)	C15—H15B	0.9600
C1—H1A	0.9300	C15—H15C	0.9600
C2—C3	1.3960 (18)	C16—H16A	0.9600
C2—H2A	0.9300	C16—H16B	0.9600
C3—C4	1.3808 (18)	C16—H16C	0.9600
C3—H3A	0.9300	C17—C18	1.3939 (17)
C4—C5	1.4025 (17)	C17—C22	1.3938 (18)
C4—H4A	0.9300	C18—C19	1.3899 (18)
C5—C6	1.4587 (16)	C18—H18A	0.9300
C6—C7	1.3496 (16)	C19—C20	1.390 (2)
C6—H6A	0.9300	C19—H19A	0.9300
C7—C8	1.4570 (16)	C20—C21	1.3878 (19)
C7—H7A	0.9300	C21—C22	1.3886 (18)
C8—C13	1.4008 (16)	C21—H21A	0.9300
C8—C9	1.4071 (16)	C22—H22A	0.9300
C9—C10	1.3820 (17)	O1W—H1W1	0.9078
C9—H9A	0.9300	O1W—H2W1	0.8195

O3—S1—O2	112.85 (7)	C13—C12—C11	119.52 (11)
O3—S1—O4	114.23 (7)	C13—C12—H12A	120.2
O2—S1—O4	111.89 (7)	C11—C12—H12A	120.2
O3—S1—C17	105.73 (6)	C12—C13—C8	121.61 (10)
O2—S1—C17	105.74 (5)	C12—C13—H13A	119.2
O4—S1—C17	105.53 (6)	C8—C13—H13A	119.2
C11—O1—C14	118.27 (9)	O1—C14—C15	106.27 (10)
C1—N1—C5	121.91 (10)	O1—C14—H14A	110.5
C1—N1—C16	117.21 (10)	C15—C14—H14A	110.5
C5—N1—C16	120.88 (10)	O1—C14—H14B	110.5
N1—C1—C2	121.32 (11)	C15—C14—H14B	110.5
N1—C1—H1A	119.3	H14A—C14—H14B	108.7
C2—C1—H1A	119.3	C14—C15—H15A	109.5
C1—C2—C3	118.55 (12)	C14—C15—H15B	109.5
C1—C2—H2A	120.7	H15A—C15—H15B	109.5
C3—C2—H2A	120.7	C14—C15—H15C	109.5
C4—C3—C2	119.62 (12)	H15A—C15—H15C	109.5
C4—C3—H3A	120.2	H15B—C15—H15C	109.5
C2—C3—H3A	120.2	N1—C16—H16A	109.5
C3—C4—C5	121.07 (11)	N1—C16—H16B	109.5
C3—C4—H4A	119.5	H16A—C16—H16B	109.5
C5—C4—H4A	119.5	N1—C16—H16C	109.5
N1—C5—C4	117.53 (11)	H16A—C16—H16C	109.5
N1—C5—C6	119.01 (10)	H16B—C16—H16C	109.5
C4—C5—C6	123.46 (11)	C18—C17—C22	120.23 (11)
C7—C6—C5	122.79 (11)	C18—C17—S1	119.24 (10)
C7—C6—H6A	118.6	C22—C17—S1	120.49 (9)

C5—C6—H6A	118.6	C19—C18—C17	120.14 (12)
C6—C7—C8	126.46 (11)	C19—C18—H18A	119.9
C6—C7—H7A	116.8	C17—C18—H18A	119.9
C8—C7—H7A	116.8	C20—C19—C18	118.72 (12)
C13—C8—C9	117.74 (11)	C20—C19—H19A	120.6
C13—C8—C7	123.90 (10)	C18—C19—H19A	120.6
C9—C8—C7	118.35 (10)	C21—C20—C19	121.92 (12)
C10—C9—C8	121.29 (11)	C21—C20—Cl1	118.95 (11)
C10—C9—H9A	119.4	C19—C20—Cl1	119.13 (10)
C8—C9—H9A	119.4	C20—C21—C22	118.88 (12)
C9—C10—C11	120.12 (11)	C20—C21—H21A	120.6
C9—C10—H10A	119.9	C22—C21—H21A	120.6
C11—C10—H10A	119.9	C21—C22—C17	120.08 (12)
O1—C11—C10	115.42 (10)	C21—C22—H22A	120.0
O1—C11—C12	124.87 (10)	C17—C22—H22A	120.0
C10—C11—C12	119.72 (11)	H1W1—O1W—H2W1	104.3

C5—N1—C1—C2	0.44 (17)	O1—C11—C12—C13	179.64 (11)
C16—N1—C1—C2	−179.42 (11)	C10—C11—C12—C13	−0.06 (17)
N1—C1—C2—C3	0.53 (18)	C11—C12—C13—C8	0.17 (18)
C1—C2—C3—C4	−0.49 (18)	C9—C8—C13—C12	−0.45 (17)
C2—C3—C4—C5	−0.49 (19)	C7—C8—C13—C12	−179.79 (11)
C1—N1—C5—C4	−1.39 (16)	C11—O1—C14—C15	−174.84 (10)
C16—N1—C5—C4	178.46 (11)	O3—S1—C17—C18	−38.98 (11)
C1—N1—C5—C6	179.12 (10)	O2—S1—C17—C18	80.92 (11)
C16—N1—C5—C6	−1.03 (16)	O4—S1—C17—C18	−160.37 (10)
C3—C4—C5—N1	1.41 (17)	O3—S1—C17—C22	143.13 (10)
C3—C4—C5—C6	−179.12 (11)	O2—S1—C17—C22	−96.96 (11)
N1—C5—C6—C7	−169.32 (11)	O4—S1—C17—C22	21.75 (11)
C4—C5—C6—C7	11.22 (18)	C22—C17—C18—C19	1.09 (18)
C5—C6—C7—C8	179.53 (11)	S1—C17—C18—C19	−176.80 (9)
C6—C7—C8—C13	−1.26 (19)	C17—C18—C19—C20	0.29 (18)
C6—C7—C8—C9	179.40 (12)	C18—C19—C20—C21	−1.11 (19)
C13—C8—C9—C10	0.64 (18)	C18—C19—C20—Cl1	179.38 (10)
C7—C8—C9—C10	−179.99 (11)	C19—C20—C21—C22	0.52 (19)
C8—C9—C10—C11	−0.54 (19)	Cl1—C20—C21—C22	−179.97 (10)
C14—O1—C11—C10	−177.17 (10)	C20—C21—C22—C17	0.88 (18)
C14—O1—C11—C12	3.12 (17)	C18—C17—C22—C21	−1.69 (18)
C9—C10—C11—O1	−179.49 (11)	S1—C17—C22—C21	176.17 (9)
C9—C10—C11—C12	0.24 (18)		

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of the C8–C13 and C17–C22 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O4^{i}	0.91	1.95	2.8148 (16)	158
O1*W*—H2*W*1···O2	0.82	2.11	2.9265 (14)	173
C1—H1*A*···O1*W*^{ii}	0.93	2.23	3.1544 (17)	176

C2—H2*A*···O1*W*^{iii}	0.93	2.44	3.2200 (17)	142
C4—H4*A*···O2^{i}	0.93	2.50	3.3768 (17)	158
C6—H6*A*···O3^{iv}	0.93	2.56	3.4308 (17)	155
C13—H13*A*···O3^{iv}	0.93	2.51	3.3859 (17)	157
C16—H16*A*···O4^{v}	0.96	2.57	3.3766 (18)	142
C16—H16*B*···O3^{iv}	0.96	2.50	3.1307 (17)	124
C22—H22*A*···O4	0.93	2.56	2.9246 (17)	104
C9—H9*A*···*Cg*3^{i}	0.93	2.90	3.5924 (13)	132
C12—H12*A*···*Cg*3^{iv}	0.93	2.96	3.7431 (13)	143
C15—H15*C*···*Cg*2^{vi}	0.96	2.87	3.6918 (14)	145

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