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# (*E*)-2-[4-(Dimethylamino)styryl]-1-methylpyridinium 4-methylbenzenesulfonate monohydrate[1]

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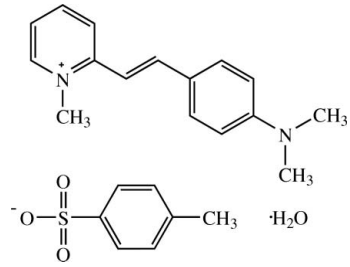
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.053; $wR$ factor = 0.156; data-to-parameter ratio = 14.6.

The cation of the title compound, $C_{16}H_{19}N_2^+\cdot C_7H_7O_3S^-\cdot H_2O$, exists in the $E$ configuration with respect to the C=C double bond and is essentially planar, the dihedral angle between the pyridinium and benzene rings being 3.55 (13)°. In the crystal, $\pi$-conjugated planes of cations and anions are inclined to each other at 84.30 (11)°. The crystal structure is stabilized by O—H···O hydrogen bonds and weak C—H···O interactions, which link the cations, anions and water molecules into chains along the $b$ axis. These chains are stacked along the $a$ axis by $\pi$–$\pi$ interactions with centroid–centroid distances of 3.6032 (16) and 3.6462 (16) Å.

## Related literature

For bond-length data, see Allen *et al.* (1987). For background to and applications of quarternary ammonium compounds and sulfonamides, see: Barlow *et al.* (1937); Ohkura *et al.* (2003); Pernak *et al.* (2001). For related structures, see: Chanawanno *et al.* (2010); Kobkeatthawin *et al.* (2009). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



## Experimental

### Crystal data

$C_{16}H_{19}N_2^+\cdot C_7H_7O_3S^-\cdot H_2O$
$M_r$ = 428.53
Triclinic, $P\overline{1}$
$a$ = 7.3469 (9) Å
$b$ = 9.8860 (12) Å
$c$ = 15.5541 (19) Å
$\alpha$ = 75.801 (3)°
$\beta$ = 79.438 (3)°
$\gamma$ = 76.865 (2)°
$V$ = 1056.8 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.19 mm$^{-1}$
$T$ = 100 K
0.47 × 0.13 × 0.06 mm

### Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.919, $T_{max}$ = 0.989
15705 measured reflections
4122 independent reflections
3307 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.156
$S$ = 1.11
4122 reflections
282 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$W$1···O2 | 0.83 (5) | 1.96 (5) | 2.774 (3) | 170 (4) |
| O1$W$—H2$W$1···O1$^{i}$ | 0.94 (4) | 1.99 (4) | 2.906 (3) | 167 (3) |
| C1—H1$A$···O1$^{ii}$ | 0.93 | 2.55 | 3.424 (3) | 157 |
| C2—H2$A$···O1$^{iii}$ | 0.93 | 2.54 | 3.382 (4) | 150 |
| C4—H4$A$···O1$W$ | 0.93 | 2.35 | 3.222 (4) | 157 |
| C6—H6$A$···O3$^{iv}$ | 0.93 | 2.53 | 3.456 (4) | 176 |
| C9—H9$A$···O2 | 0.93 | 2.49 | 3.376 (3) | 158 |
| C13—H13$A$···O3$^{iv}$ | 0.93 | 2.49 | 3.390 (4) | 164 |
| C14—H14$B$···O1$^{ii}$ | 0.96 | 2.56 | 3.479 (4) | 161 |

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

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).

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¶ Additional correspondence author, e-mail: hkfun@usm.my. Thomson Reuters ResearcherID: A-3561-2009.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5034).

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# supporting information

*Acta Cryst.* (2010). E**66**, o1975–o1976 [https://doi.org/10.1107/S1600536810026309]

## (*E*)-2-[4-(Dimethylamino)styryl]-1-methylpyridinium 4-methylbenzenesulfonate monohydrate

**Suchada Chantrapromma, Kullapa Chanawanno and Hoong-Kun Fun**

### S1. Comment

Quarternary ammonium compounds and sulfonamide drugs are the interesting antibacterial agents. They are widely used in industrial disinfection and hospital treatment (Barlow *et al.*, 1937; Ohkura *et al.*, 2003). Pyridinium derivatives represent a class of synthetic quarternary ammonium compounds that show significant antibacterial activity. (Pernak *et al.*, 2001). The title compound was synthesized based on the combination of pyridinium and sulfonamide chemophores in order to yield a potent disinfectant. Our biological actvity results showed that the title compound was moderately active against Gram-positive bacteria *ie* Methicillin-Resistant *Staphylococcus aureus* with the MIC = 37.5 $\mu$g/ml. However it was inactive against the Gram-negative bacteria we tested which are *Pseudomonas aeruginosa*, *Salmonella typhi* and *Shigella sonnei* (Chanawanno *et al.*, 2010). Herein its crystal structure is reported.

Fig. 1 shows the asymmetric unit of the title compound (I) which consists of the $C_{16}H_{19}N_2^+$ cation, $C_7H_7O_3S^-$ anion and one $H_2O$ molecule. The cation exists in the *E* configuration with respect to the C6═C7 double bond [1.343 (4) Å]. The cation is essentially planar with the dihedral angle between the pyridinium and the dimethylaminophenyl rings being 3.55 (13)° and with the torsion angle C5–C6–C7–C8 = 176.3 (3)°. Both methyl groups of dimethylamino moiety are slightly twisted from the mean plane of the attached C8–C13 ring as indicated by the torsion angles C15—N2–C11–C10 = 9.3 (4)° and C16–N2–C11–C12 = 3.5 (4)°. The relative arrangement of cation and anion is shown by the interplanar angle between the mean plane of the $\pi$-conjugate system (C1–C13/N1) of the cation and the C17–C22 benzene ring of the anion being 84.30 (11)°. The bond lengths (Allen *et al.*, 1987) and angles in (I) are in normal ranges and comparable with a related structure (Kobkeatthawin *et al.*, 2009).

In the crystal packing, all O atoms of the sulfonate group are involved in weak C—H···O interactions (Table 1). The cation is linked to both the anion and water molecule by weak C—H···O interactions, and the anion is linked to the water molecule by O—H···O hydrogen bond. These three molecules are linked into chains along the *b* axis (Table 1, Fig. 2). These chains are stacked along the *a* axis (Fig. 2) by $\pi$–$\pi$ interactions with the distances $Cg_1\cdots Cg_1$ = 3.6032 (16) Å (symmetry code: 2 - *x*, 2 - *y*, -*z*) and $Cg_1\cdots Cg_2$ = 3.6462 (16) Å (symmetry code: 1 - *x*, *y*, *z*); $Cg_1$ and $Cg_2$ are the centroids of the N1/C1–C5 and C8–C13 rings, respectively.

### S2. Experimental

The title compound was prepared by the reported procedure (Chanawanno *et al.*, 2010). Orange needle-shaped single crystals of the title compound suitable for *x*-ray structure determination were recrystalized from methanol by slow evaporation of the solvent at room temperature after a few weeks. Mp. 468–469 K.

### S3. Refinement

Water H atoms were located in difference maps and refined isotropically. The remaining H atoms were placed in calculated positions with d(C—H) = 0.93 Å, $U_{iso}$=1.2$U_{eq}$(C) for aromatic and CH and 0.96 Å, $U_{iso}$ = 1.5$U_{eq}$(C) for $CH_3$ atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is located at 1.08 Å from O1 and the deepest hole is located at 0.85 Å from S1.

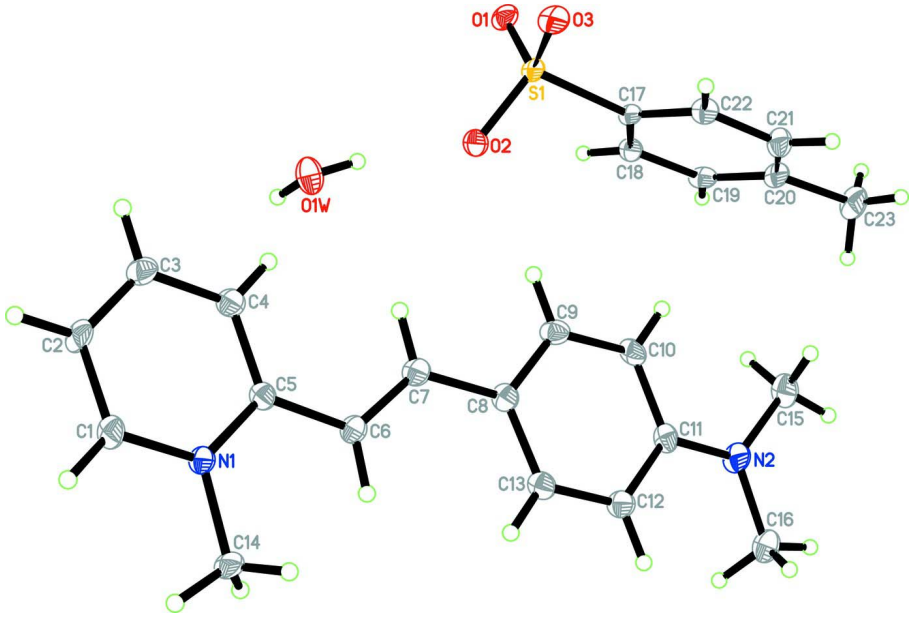


**Figure 1**

The asymmetric unit of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

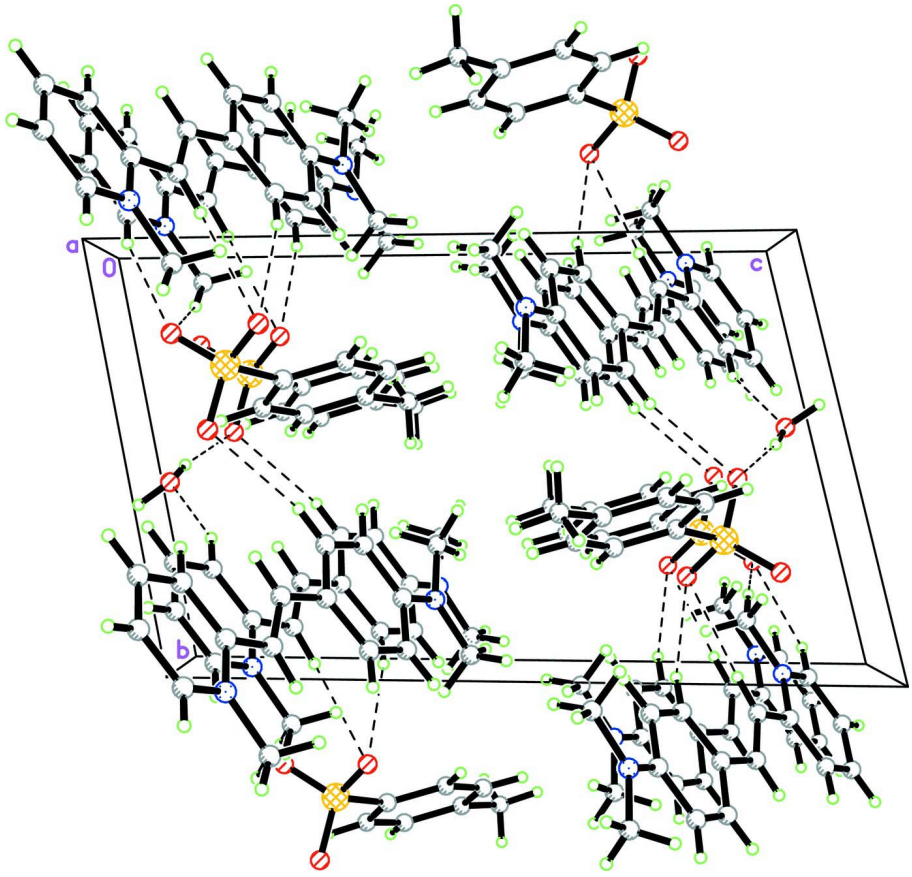


**Figure 2**

The crystal packing of (I) viewed along the *a* axis. The O—H···O hydrogen bonds and weak C—H···O interactions are drawn as dashed lines.

### (*E*)-2-[4-(Dimethylamino)styryl]-1-methylpyridinium 4-methylbenzenesulfonate monohydrate

*Crystal data*

$C_{16}H_{19}N_2^+ \cdot C_7H_7O_3S^- \cdot H_2O$
$M_r = 428.53$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.3469\ (9)$ Å
$b = 9.8860\ (12)$ Å
$c = 15.5541\ (19)$ Å
$\alpha = 75.801\ (3)°$
$\beta = 79.438\ (3)°$
$\gamma = 76.865\ (2)°$
$V = 1056.8\ (2)$ Å$^3$
$Z = 2$
$F(000) = 456$
$D_x = 1.347$ Mg m$^{-3}$
Melting point = 468–469 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4122 reflections
$\theta = 1.4–26.0°$
$\mu = 0.19$ mm$^{-1}$
$T = 100$ K
Needle, orange
0.47 × 0.13 × 0.06 mm

*Data collection*

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.919$, $T_{max} = 0.989$
15705 measured reflections
4122 independent reflections

3307 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.4°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -19 \rightarrow 19$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.156$
$S = 1.11$
4122 reflections
282 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 1.5338P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.51$ e Å$^{-3}$
$\Delta\rho_{min} = -0.56$ 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 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 1.0171 (3) | 0.9737 (2) | 0.12371 (15) | 0.0145 (5) |
| N2 | −0.1299 (3) | 0.8266 (3) | 0.39380 (16) | 0.0215 (5) |
| C1 | 1.1969 (4) | 0.9572 (3) | 0.08076 (18) | 0.0176 (6) |
| H1A | 1.2683 | 1.0256 | 0.0766 | 0.021* |
| C2 | 1.2745 (4) | 0.8414 (3) | 0.04353 (19) | 0.0198 (6) |
| H2A | 1.3976 | 0.8309 | 0.0143 | 0.024* |
| C3 | 1.1662 (4) | 0.7399 (3) | 0.05011 (18) | 0.0189 (6) |
| H3A | 1.2161 | 0.6606 | 0.0252 | 0.023* |
| C4 | 0.9842 (4) | 0.7579 (3) | 0.09382 (18) | 0.0170 (6) |
| H4A | 0.9115 | 0.6905 | 0.0975 | 0.020* |
| C5 | 0.9067 (4) | 0.8750 (3) | 0.13271 (18) | 0.0152 (5) |
| C6 | 0.7180 (4) | 0.8965 (3) | 0.18253 (18) | 0.0166 (6) |
| H6A | 0.6710 | 0.9821 | 0.2007 | 0.020* |
| C7 | 0.6089 (4) | 0.7978 (3) | 0.20334 (18) | 0.0177 (6) |
| H7A | 0.6566 | 0.7156 | 0.1812 | 0.021* |
| C8 | 0.4235 (4) | 0.8062 (3) | 0.25704 (18) | 0.0166 (5) |
| C9 | 0.3246 (4) | 0.6955 (3) | 0.26819 (19) | 0.0182 (6) |
| H9A | 0.3816 | 0.6174 | 0.2431 | 0.022* |
| C10 | 0.1460 (4) | 0.6991 (3) | 0.31509 (18) | 0.0168 (6) |

| | | | | |
|---|---|---|---|---|
| H10A | 0.0860 | 0.6230 | 0.3223 | 0.020* |
| C11 | 0.0532 (4) | 0.8173 (3) | 0.35233 (18) | 0.0163 (5) |
| C12 | 0.1546 (4) | 0.9257 (3) | 0.34420 (18) | 0.0176 (6) |
| H12A | 0.0992 | 1.0026 | 0.3707 | 0.021* |
| C13 | 0.3347 (4) | 0.9203 (3) | 0.29778 (18) | 0.0172 (6) |
| H13A | 0.3980 | 0.9937 | 0.2935 | 0.021* |
| C14 | 0.9449 (4) | 1.1036 (3) | 0.16027 (19) | 0.0186 (6) |
| H14A | 0.8340 | 1.1563 | 0.1345 | 0.028* |
| H14B | 1.0398 | 1.1612 | 0.1460 | 0.028* |
| H14C | 0.9142 | 1.0774 | 0.2241 | 0.028* |
| C15 | −0.2224 (4) | 0.7057 (3) | 0.4121 (2) | 0.0236 (6) |
| H15A | −0.2238 | 0.6787 | 0.3570 | 0.035* |
| H15B | −0.3496 | 0.7309 | 0.4400 | 0.035* |
| H15C | −0.1552 | 0.6275 | 0.4515 | 0.035* |
| C16 | −0.2284 (4) | 0.9532 (3) | 0.4263 (2) | 0.0248 (6) |
| H16A | −0.2241 | 1.0353 | 0.3784 | 0.037* |
| H16B | −0.1688 | 0.9626 | 0.4740 | 0.037* |
| H16C | −0.3574 | 0.9455 | 0.4481 | 0.037* |
| S1 | 0.39079 (9) | 0.30482 (7) | 0.18364 (5) | 0.01550 (19) |
| O1 | 0.3624 (3) | 0.2330 (2) | 0.11664 (13) | 0.0202 (4) |
| O2 | 0.4315 (3) | 0.4458 (2) | 0.14332 (13) | 0.0214 (5) |
| O3 | 0.5235 (3) | 0.2178 (2) | 0.24342 (14) | 0.0205 (4) |
| C17 | 0.1685 (3) | 0.3327 (3) | 0.25164 (18) | 0.0138 (5) |
| C18 | 0.0064 (4) | 0.3932 (3) | 0.21068 (18) | 0.0157 (5) |
| H18A | 0.0153 | 0.4239 | 0.1488 | 0.019* |
| C19 | −0.1682 (4) | 0.4069 (3) | 0.26349 (19) | 0.0170 (6) |
| H19A | −0.2767 | 0.4449 | 0.2364 | 0.020* |
| C20 | −0.1835 (4) | 0.3651 (3) | 0.35578 (19) | 0.0182 (6) |
| C21 | −0.0197 (4) | 0.3085 (3) | 0.39579 (19) | 0.0196 (6) |
| H21A | −0.0280 | 0.2819 | 0.4578 | 0.024* |
| C22 | 0.1561 (4) | 0.2916 (3) | 0.34368 (18) | 0.0166 (6) |
| H22A | 0.2647 | 0.2529 | 0.3707 | 0.020* |
| C23 | −0.3743 (4) | 0.3757 (3) | 0.4126 (2) | 0.0266 (7) |
| H23A | −0.3581 | 0.3418 | 0.4746 | 0.040* |
| H23B | −0.4472 | 0.3190 | 0.3963 | 0.040* |
| H23C | −0.4389 | 0.4730 | 0.4031 | 0.040* |
| O1W | 0.7344 (3) | 0.5643 (2) | 0.04598 (15) | 0.0251 (5) |
| H1W1 | 0.645 (7) | 0.524 (5) | 0.070 (3) | 0.056 (13)* |
| H2W1 | 0.699 (5) | 0.618 (4) | −0.009 (3) | 0.033 (10)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0088 (10) | 0.0153 (11) | 0.0197 (11) | −0.0024 (9) | −0.0005 (9) | −0.0051 (9) |
| N2 | 0.0114 (12) | 0.0250 (13) | 0.0286 (13) | −0.0059 (10) | 0.0045 (10) | −0.0096 (10) |
| C1 | 0.0078 (12) | 0.0207 (14) | 0.0230 (14) | −0.0019 (10) | −0.0013 (10) | −0.0038 (11) |
| C2 | 0.0083 (13) | 0.0234 (14) | 0.0237 (14) | 0.0021 (11) | 0.0016 (11) | −0.0049 (11) |
| C3 | 0.0164 (14) | 0.0163 (13) | 0.0209 (14) | 0.0024 (11) | −0.0021 (11) | −0.0034 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4 | 0.0140 (13) | 0.0148 (13) | 0.0213 (14) | −0.0014 (10) | −0.0025 (11) | −0.0032 (11) |
| C5 | 0.0115 (13) | 0.0154 (13) | 0.0180 (13) | −0.0019 (10) | −0.0030 (10) | −0.0019 (10) |
| C6 | 0.0109 (13) | 0.0168 (13) | 0.0203 (14) | −0.0003 (10) | −0.0005 (10) | −0.0040 (11) |
| C7 | 0.0113 (13) | 0.0174 (13) | 0.0231 (14) | −0.0003 (10) | −0.0018 (11) | −0.0046 (11) |
| C8 | 0.0105 (13) | 0.0167 (13) | 0.0211 (14) | −0.0016 (10) | −0.0023 (10) | −0.0022 (10) |
| C9 | 0.0136 (14) | 0.0154 (13) | 0.0251 (14) | −0.0002 (11) | −0.0034 (11) | −0.0050 (11) |
| C10 | 0.0129 (13) | 0.0149 (13) | 0.0239 (14) | −0.0069 (10) | −0.0024 (11) | −0.0026 (11) |
| C11 | 0.0102 (13) | 0.0192 (13) | 0.0179 (13) | −0.0028 (10) | −0.0011 (10) | −0.0018 (10) |
| C12 | 0.0149 (13) | 0.0166 (13) | 0.0213 (14) | −0.0028 (11) | −0.0015 (11) | −0.0052 (11) |
| C13 | 0.0117 (13) | 0.0175 (13) | 0.0221 (14) | −0.0035 (10) | −0.0024 (11) | −0.0028 (11) |
| C14 | 0.0114 (13) | 0.0176 (13) | 0.0275 (15) | −0.0020 (10) | 0.0016 (11) | −0.0100 (11) |
| C15 | 0.0147 (14) | 0.0294 (16) | 0.0268 (15) | −0.0090 (12) | 0.0022 (12) | −0.0054 (12) |
| C16 | 0.0145 (14) | 0.0289 (16) | 0.0283 (16) | −0.0032 (12) | 0.0053 (12) | −0.0082 (13) |
| S1 | 0.0063 (3) | 0.0145 (3) | 0.0248 (4) | −0.0030 (2) | 0.0034 (2) | −0.0058 (3) |
| O1 | 0.0130 (10) | 0.0195 (10) | 0.0287 (11) | −0.0047 (8) | 0.0046 (8) | −0.0104 (8) |
| O2 | 0.0116 (10) | 0.0181 (10) | 0.0320 (11) | −0.0049 (8) | 0.0060 (8) | −0.0052 (8) |
| O3 | 0.0055 (9) | 0.0211 (10) | 0.0332 (11) | 0.0004 (7) | −0.0020 (8) | −0.0057 (8) |
| C17 | 0.0055 (12) | 0.0123 (12) | 0.0236 (14) | −0.0031 (9) | 0.0029 (10) | −0.0064 (10) |
| C18 | 0.0112 (13) | 0.0150 (13) | 0.0210 (14) | −0.0029 (10) | −0.0015 (10) | −0.0040 (10) |
| C19 | 0.0086 (12) | 0.0130 (13) | 0.0296 (15) | 0.0001 (10) | −0.0039 (11) | −0.0059 (11) |
| C20 | 0.0087 (13) | 0.0195 (13) | 0.0269 (15) | −0.0050 (10) | 0.0044 (11) | −0.0086 (11) |
| C21 | 0.0153 (14) | 0.0233 (14) | 0.0196 (14) | −0.0052 (11) | 0.0006 (11) | −0.0043 (11) |
| C22 | 0.0091 (13) | 0.0171 (13) | 0.0244 (14) | −0.0032 (10) | −0.0028 (10) | −0.0049 (11) |
| C23 | 0.0117 (14) | 0.0357 (17) | 0.0310 (16) | −0.0056 (12) | 0.0055 (12) | −0.0098 (13) |
| O1W | 0.0169 (11) | 0.0311 (12) | 0.0287 (12) | −0.0126 (9) | 0.0002 (9) | −0.0038 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.360 (3) | C14—H14A | 0.9600 |
| N1—C5 | 1.372 (3) | C14—H14B | 0.9600 |
| N1—C14 | 1.480 (3) | C14—H14C | 0.9600 |
| N2—C11 | 1.374 (3) | C15—H15A | 0.9600 |
| N2—C15 | 1.450 (4) | C15—H15B | 0.9600 |
| N2—C16 | 1.454 (4) | C15—H15C | 0.9600 |
| C1—C2 | 1.371 (4) | C16—H16A | 0.9600 |
| C1—H1A | 0.9300 | C16—H16B | 0.9600 |
| C2—C3 | 1.390 (4) | C16—H16C | 0.9600 |
| C2—H2A | 0.9300 | S1—O3 | 1.454 (2) |
| C3—C4 | 1.378 (4) | S1—O2 | 1.4553 (19) |
| C3—H3A | 0.9300 | S1—O1 | 1.464 (2) |
| C4—C5 | 1.396 (4) | S1—C17 | 1.780 (3) |
| C4—H4A | 0.9300 | C17—C22 | 1.381 (4) |
| C5—C6 | 1.456 (4) | C17—C18 | 1.396 (4) |
| C6—C7 | 1.343 (4) | C18—C19 | 1.389 (4) |
| C6—H6A | 0.9300 | C18—H18A | 0.9300 |
| C7—C8 | 1.458 (4) | C19—C20 | 1.384 (4) |
| C7—H7A | 0.9300 | C19—H19A | 0.9300 |
| C8—C13 | 1.402 (4) | C20—C21 | 1.395 (4) |

| | | | |
|---|---|---|---|
| C8—C9 | 1.406 (4) | C20—C23 | 1.511 (4) |
| C9—C10 | 1.377 (4) | C21—C22 | 1.392 (4) |
| C9—H9A | 0.9300 | C21—H21A | 0.9300 |
| C10—C11 | 1.411 (4) | C22—H22A | 0.9300 |
| C10—H10A | 0.9300 | C23—H23A | 0.9600 |
| C11—C12 | 1.407 (4) | C23—H23B | 0.9600 |
| C12—C13 | 1.383 (4) | C23—H23C | 0.9600 |
| C12—H12A | 0.9300 | O1W—H1W1 | 0.83 (5) |
| C13—H13A | 0.9300 | O1W—H2W1 | 0.94 (4) |

| | | | |
|---|---|---|---|
| C1—N1—C5 | 121.8 (2) | H14A—C14—H14B | 109.5 |
| C1—N1—C14 | 117.0 (2) | N1—C14—H14C | 109.5 |
| C5—N1—C14 | 121.2 (2) | H14A—C14—H14C | 109.5 |
| C11—N2—C15 | 120.3 (2) | H14B—C14—H14C | 109.5 |
| C11—N2—C16 | 120.6 (2) | N2—C15—H15A | 109.5 |
| C15—N2—C16 | 118.9 (2) | N2—C15—H15B | 109.5 |
| N1—C1—C2 | 121.1 (2) | H15A—C15—H15B | 109.5 |
| N1—C1—H1A | 119.5 | N2—C15—H15C | 109.5 |
| C2—C1—H1A | 119.5 | H15A—C15—H15C | 109.5 |
| C1—C2—C3 | 118.9 (2) | H15B—C15—H15C | 109.5 |
| C1—C2—H2A | 120.5 | N2—C16—H16A | 109.5 |
| C3—C2—H2A | 120.5 | N2—C16—H16B | 109.5 |
| C4—C3—C2 | 119.4 (2) | H16A—C16—H16B | 109.5 |
| C4—C3—H3A | 120.3 | N2—C16—H16C | 109.5 |
| C2—C3—H3A | 120.3 | H16A—C16—H16C | 109.5 |
| C3—C4—C5 | 121.5 (2) | H16B—C16—H16C | 109.5 |
| C3—C4—H4A | 119.3 | O3—S1—O2 | 113.73 (11) |
| C5—C4—H4A | 119.3 | O3—S1—O1 | 113.30 (12) |
| N1—C5—C4 | 117.3 (2) | O2—S1—O1 | 111.86 (12) |
| N1—C5—C6 | 118.9 (2) | O3—S1—C17 | 106.05 (12) |
| C4—C5—C6 | 123.8 (2) | O2—S1—C17 | 105.69 (11) |
| C7—C6—C5 | 122.8 (2) | O1—S1—C17 | 105.35 (11) |
| C7—C6—H6A | 118.6 | C22—C17—C18 | 120.5 (2) |
| C5—C6—H6A | 118.6 | C22—C17—S1 | 120.3 (2) |
| C6—C7—C8 | 126.8 (3) | C18—C17—S1 | 119.2 (2) |
| C6—C7—H7A | 116.6 | C19—C18—C17 | 119.1 (2) |
| C8—C7—H7A | 116.6 | C19—C18—H18A | 120.4 |
| C13—C8—C9 | 117.2 (2) | C17—C18—H18A | 120.4 |
| C13—C8—C7 | 123.7 (2) | C20—C19—C18 | 121.2 (2) |
| C9—C8—C7 | 119.0 (2) | C20—C19—H19A | 119.4 |
| C10—C9—C8 | 122.1 (2) | C18—C19—H19A | 119.4 |
| C10—C9—H9A | 119.0 | C19—C20—C21 | 118.9 (2) |
| C8—C9—H9A | 119.0 | C19—C20—C23 | 120.9 (3) |
| C9—C10—C11 | 120.6 (2) | C21—C20—C23 | 120.2 (3) |
| C9—C10—H10A | 119.7 | C22—C21—C20 | 120.6 (3) |
| C11—C10—H10A | 119.7 | C22—C21—H21A | 119.7 |
| N2—C11—C12 | 121.5 (2) | C20—C21—H21A | 119.7 |
| N2—C11—C10 | 121.1 (2) | C17—C22—C21 | 119.6 (2) |

| | | | |
|---|---|---|---|
| C12—C11—C10 | 117.4 (2) | C17—C22—H22A | 120.2 |
| C13—C12—C11 | 121.5 (2) | C21—C22—H22A | 120.2 |
| C13—C12—H12A | 119.3 | C20—C23—H23A | 109.5 |
| C11—C12—H12A | 119.3 | C20—C23—H23B | 109.5 |
| C12—C13—C8 | 121.1 (2) | H23A—C23—H23B | 109.5 |
| C12—C13—H13A | 119.5 | C20—C23—H23C | 109.5 |
| C8—C13—H13A | 119.5 | H23A—C23—H23C | 109.5 |
| N1—C14—H14A | 109.5 | H23B—C23—H23C | 109.5 |
| N1—C14—H14B | 109.5 | H1W1—O1W—H2W1 | 105 (4) |

| | | | |
|---|---|---|---|
| C5—N1—C1—C2 | 0.8 (4) | C9—C10—C11—N2 | 175.4 (3) |
| C14—N1—C1—C2 | −178.9 (3) | C9—C10—C11—C12 | −3.8 (4) |
| N1—C1—C2—C3 | 0.1 (4) | N2—C11—C12—C13 | −176.0 (3) |
| C1—C2—C3—C4 | −0.1 (4) | C10—C11—C12—C13 | 3.1 (4) |
| C2—C3—C4—C5 | −0.8 (4) | C11—C12—C13—C8 | −0.1 (4) |
| C1—N1—C5—C4 | −1.7 (4) | C9—C8—C13—C12 | −2.3 (4) |
| C14—N1—C5—C4 | 178.1 (2) | C7—C8—C13—C12 | 176.7 (3) |
| C1—N1—C5—C6 | 177.6 (2) | O3—S1—C17—C22 | 8.8 (2) |
| C14—N1—C5—C6 | −2.6 (4) | O2—S1—C17—C22 | −112.3 (2) |
| C3—C4—C5—N1 | 1.7 (4) | O1—S1—C17—C22 | 129.2 (2) |
| C3—C4—C5—C6 | −177.6 (3) | O3—S1—C17—C18 | −169.54 (19) |
| N1—C5—C6—C7 | −172.2 (3) | O2—S1—C17—C18 | 69.4 (2) |
| C4—C5—C6—C7 | 7.1 (4) | O1—S1—C17—C18 | −49.1 (2) |
| C5—C6—C7—C8 | 176.3 (3) | C22—C17—C18—C19 | −2.3 (4) |
| C6—C7—C8—C13 | −2.3 (4) | S1—C17—C18—C19 | 176.08 (19) |
| C6—C7—C8—C9 | 176.7 (3) | C17—C18—C19—C20 | 1.6 (4) |
| C13—C8—C9—C10 | 1.6 (4) | C18—C19—C20—C21 | 0.1 (4) |
| C7—C8—C9—C10 | −177.4 (3) | C18—C19—C20—C23 | −177.9 (2) |
| C8—C9—C10—C11 | 1.5 (4) | C19—C20—C21—C22 | −1.3 (4) |
| C15—N2—C11—C12 | −171.6 (3) | C23—C20—C21—C22 | 176.7 (2) |
| C16—N2—C11—C12 | 3.5 (4) | C18—C17—C22—C21 | 1.1 (4) |
| C15—N2—C11—C10 | 9.3 (4) | S1—C17—C22—C21 | −177.2 (2) |
| C16—N2—C11—C10 | −175.6 (3) | C20—C21—C22—C17 | 0.7 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*W*1···O2 | 0.83 (5) | 1.96 (5) | 2.774 (3) | 170 (4) |
| O1*W*—H2*W*1···O1$^{i}$ | 0.94 (4) | 1.99 (4) | 2.906 (3) | 167 (3) |
| C1—H1*A*···O1$^{ii}$ | 0.93 | 2.55 | 3.424 (3) | 157 |
| C2—H2*A*···O1$^{iii}$ | 0.93 | 2.54 | 3.382 (4) | 150 |
| C4—H4*A*···O1*W* | 0.93 | 2.35 | 3.222 (4) | 157 |
| C6—H6*A*···O3$^{iv}$ | 0.93 | 2.53 | 3.456 (4) | 176 |
| C9—H9*A*···O2 | 0.93 | 2.49 | 3.376 (3) | 158 |
| C13—H13*A*···O3$^{iv}$ | 0.93 | 2.49 | 3.390 (4) | 164 |

| | | | | |
|---|---|---|---|---|
| C14—H14*B*···O1$^{ii}$ | 0.96 | 2.56 | 3.479 (4) | 161 |
| C22—H22*A*···O3 | 0.93 | 2.51 | 2.894 (3) | 105 |

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