

# Hexaaquanickel(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

 Xi-Shi Tai,<sup>a\*</sup> Jun Xu,<sup>b</sup> Yi-Min Feng<sup>a</sup> and Zu-Pei Liang<sup>a</sup>

<sup>a</sup>Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China, and <sup>b</sup>Weifang Institute of Supervision and Inspection, on Product Quality, Weifang 261031, People's Republic of China  
Correspondence e-mail: taixishi@lzu.edu.cn

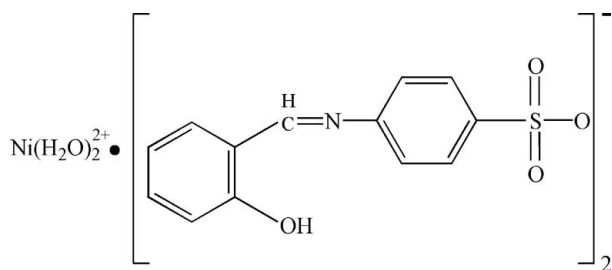
Received 16 May 2008; accepted 21 May 2008

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.011$  Å;  $R$  factor = 0.067;  $wR$  factor = 0.138; data-to-parameter ratio = 13.0.

In the title compound,  $[\text{Ni}(\text{H}_2\text{O})_6](\text{C}_{13}\text{H}_{10}\text{NO}_4\text{S})_2$ , the nickel(II) atom, lying on a center of symmetry, is six-coordinated by six aqua O-atom donors. The dihedral angle between the two benzene rings is  $33.1(3)^\circ$ . The crystal structure is stabilized by aqua-anion  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds. Intramolecular  $\text{O}-\text{H}\cdots\text{N}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen-bonding interactions occur in the anion.

## Related literature

For related literature, see: Tai & Feng (2008); Tai *et al.* (2003, 2008); Tai, Yin & Feng (2007); Tai, Yin & Hao (2007); Tai, Yin, Feng & Kong (2007); Wang *et al.* (2007).



## Experimental

### Crystal data

$[\text{Ni}(\text{H}_2\text{O})_6](\text{C}_{13}\text{H}_{10}\text{NO}_4\text{S})_2$   
 $M_r = 719.37$   
 Monoclinic,  $P2_1/c$   
 $a = 6.3047(6)$  Å  
 $b = 35.193(3)$  Å  
 $c = 9.3536(10)$  Å  
 $\beta = 131.822(2)^\circ$

$V = 1546.6(3)$  Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.83$  mm<sup>-1</sup>  
 $T = 298(2)$  K  
 $0.43 \times 0.38 \times 0.25$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (*SADABS*; Bruker, 2000)  
 $T_{\min} = 0.716$ ,  $T_{\max} = 0.819$   
 7465 measured reflections  
 2661 independent reflections  
 2428 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.032$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$   
 $wR(F^2) = 0.137$   
 $S = 1.28$   
 2661 reflections  
 205 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.32$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.00$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O4}-\text{H4}\cdots\text{N1}$	0.82	1.86	2.595 (9)	148
$\text{O5}-\text{H5A}\cdots\text{O1}^{\text{i}}$	0.85	1.96	2.737 (6)	151
$\text{O5}-\text{H5B}\cdots\text{O2}^{\text{ii}}$	0.85	1.98	2.751 (6)	150
$\text{O6}-\text{H6A}\cdots\text{O3}^{\text{i}}$	0.85	1.95	2.764 (7)	161
$\text{O6}-\text{H6B}\cdots\text{O1}^{\text{iii}}$	0.85	1.97	2.768 (8)	156
$\text{O7}-\text{H7A}\cdots\text{O2}$	0.85	2.00	2.757 (8)	148
$\text{O7}-\text{H7B}\cdots\text{O3}^{\text{ii}}$	0.85	2.00	2.769 (7)	150
$\text{C2}-\text{H2}\cdots\text{O3}$	0.93	2.56	2.917 (7)	104

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

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

The authors thank the National Natural Science Foundation of China (20671073), the Natural Science Foundation of Shandong (Y2007B60), the Science and Technology Foundation of Weifang and Weifang University for research grants.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2568).

## References

- Bruker (2000). *SMART, SAINT and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Tai, X.-S. & Feng, Y.-M. (2008). *Acta Cryst.* **E64**, o707.
- Tai, X.-S., Feng, Y.-M. & Zhang, H.-X. (2008). *Acta Cryst.* **E64**, m502.
- Tai, X. S., Yin, J. & Feng, Y. M. (2007). *Z. Kristallogr. New Cryst. Struct.* **222**, 398–400.
- Tai, X. S., Yin, J., Feng, Y. M. & Kong, F. Y. (2007). *Chin. J. Inorg. Chem.* **23**, 1812–1814.
- Tai, X.-S., Yin, J. & Hao, M.-Y. (2007). *Acta Cryst.* **E63**, m1061–m1062.
- Tai, X.-S., Yin, X.-H., Tan, M.-Y. & Li, Y.-Z. (2003). *Acta Cryst.* **E59**, o681–o682.
- Wang, L.-H., Yin, J. & Tai, X.-S. (2007). *Acta Cryst.* **E63**, m1664.

## supporting information

*Acta Cryst.* (2008). E64, m893 [doi:10.1107/S1600536808015262]

## Hexaaquanickel(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

Xi-Shi Tai, Jun Xu, Yi-Min Feng and Zu-Pei Liang

### S1. Comment

As part of our ongoing studies of the coordination chemistry of Schiffbase ligands (Tai *et al.*, 2003; (Tai, Yin & Feng, 2007; Tai, Yin, Feng & Kong, 2007; Tai, Yin & Hao, 2007; Wang *et al.*, 2007; Tai *et al.*, 2008; Tai *et al.*, 2008), we now report the synthesis and structure of the title compound, (I), (Fig. 1).

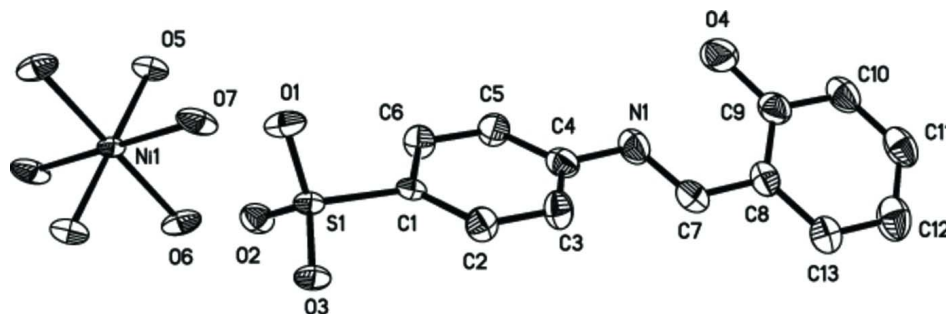
In the molecule of (I), the nickel (II) center is six-coordinate with six O donor of H<sub>2</sub>O. The C7—N1 [1.288 (8) Å] is close to double-bond. Otherwise, the geometrical parameters for (I) are normal. The dihedral angle between the two benzene rings is 33.1°. The packing is stabilized by O<sub>water</sub>—H···O<sub>anion</sub> hydrogen bonds. The intramolecular O—H···N and C—H···O hydrogen bonding interactions occur in the anion. (Table 1).

### S2. Experimental

1 mmol of Ni(CH<sub>3</sub>COO)<sub>2</sub>·4H<sub>2</sub>O was added to a solution of salicylaldehyde-4-aminobenzene sulfonic acid (1 mmol) in 10 ml of 95% ethanol. The mixture was stirred for 2 h at refluxing temperature. Evaporating some ethanol, clear blocks of (I) were obtained after one weeks.

### S3. Refinement

The H atoms were placed geometrically (C—H = 0.93 Å and O—H = 0.82-0.85 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5U_{\text{eq}}(\text{carrier})$ .



**Figure 1**

The molecular structure of (I) showing 30% displacement ellipsoids.

## Hexaaquanickel(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

### Crystal data

[Ni(H<sub>2</sub>O)<sub>6</sub>](C<sub>13</sub>H<sub>10</sub>NO<sub>4</sub>S)<sub>2</sub>

$M_r = 719.37$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 6.3047$  (6) Å

$b = 35.193$  (3) Å

$c = 9.3536$  (10) Å

$\beta = 131.822$  (2)°

$V = 1546.6 (3) \text{ \AA}^3$   
 $Z = 2$   
 $F(000) = 748$   
 $D_x = 1.545 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 4537 reflections

$\theta = 2.9\text{--}27.7^\circ$   
 $\mu = 0.83 \text{ mm}^{-1}$   
 $T = 298 \text{ K}$   
 Block, colourless  
 $0.43 \times 0.38 \times 0.25 \text{ mm}$

*Data collection*

Bruker SMART CCD area-detector  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2000)  
 $T_{\min} = 0.716$ ,  $T_{\max} = 0.819$

7465 measured reflections  
 2661 independent reflections  
 2428 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.032$   
 $\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 2.3^\circ$   
 $h = -7 \rightarrow 5$   
 $k = -41 \rightarrow 40$   
 $l = -9 \rightarrow 11$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.067$   
 $wR(F^2) = 0.137$   
 $S = 1.28$   
 2661 reflections  
 205 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0161P)^2 + 4.8144P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.32 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -1.00 \text{ e \AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.5000	1.0000	1.0000	0.0310 (2)
N1	0.4029 (11)	0.76969 (14)	0.4874 (8)	0.0565 (13)
O1	0.3354 (7)	0.95021 (11)	0.3248 (5)	0.0486 (10)
O2	0.6843 (8)	0.94957 (11)	0.6726 (5)	0.0462 (9)
O3	0.8302 (7)	0.93929 (10)	0.4933 (5)	0.0392 (8)
O4	0.0669 (10)	0.71618 (13)	0.4256 (8)	0.0767 (14)
H4	0.1257	0.7379	0.4400	0.115*
O5	0.2072 (7)	0.97532 (11)	0.9978 (5)	0.0474 (9)
H5A	0.2819	0.9621	1.0975	0.071*
H5B	0.0852	0.9623	0.8972	0.071*
O6	0.7945 (8)	0.96016 (12)	1.1929 (6)	0.0549 (11)

H6A	0.8124	0.9592	1.2913	0.082*
H6B	0.9559	0.9642	1.2273	0.082*
O7	0.3791 (8)	0.96590 (13)	0.7796 (6)	0.0600 (12)
H7A	0.4709	0.9703	0.7444	0.090*
H7B	0.2009	0.9665	0.6838	0.090*
S1	0.6046 (2)	0.93471 (4)	0.49681 (17)	0.0319 (3)
C1	0.5566 (9)	0.88532 (14)	0.4986 (7)	0.0313 (10)
C2	0.6556 (12)	0.86005 (16)	0.4406 (8)	0.0451 (13)
H2	0.7524	0.8689	0.4039	0.054*
C3	0.6082 (14)	0.82145 (16)	0.4382 (9)	0.0529 (15)
H3	0.6758	0.8042	0.4012	0.063*
C4	0.4623 (12)	0.80853 (16)	0.4899 (9)	0.0483 (14)
C5	0.3614 (13)	0.83417 (16)	0.5454 (9)	0.0509 (15)
H5	0.2614	0.8253	0.5795	0.061*
C6	0.4079 (12)	0.87246 (15)	0.5503 (8)	0.0438 (13)
H6	0.3404	0.8896	0.5878	0.053*
C7	0.5721 (13)	0.74368 (17)	0.5168 (9)	0.0525 (15)
H7	0.7384	0.7507	0.5446	0.063*
C8	0.5084 (15)	0.70327 (16)	0.5074 (9)	0.0527 (14)
C9	0.2544 (14)	0.69149 (18)	0.4569 (9)	0.0589 (17)
C10	0.1982 (16)	0.65268 (18)	0.4407 (9)	0.0643 (18)
H10	0.0295	0.6445	0.4068	0.077*
C11	0.3845 (17)	0.6265 (2)	0.4733 (9)	0.068 (2)
H11	0.3396	0.6008	0.4588	0.082*
C12	0.6424 (19)	0.6376 (2)	0.5281 (11)	0.077 (2)
H12	0.7726	0.6196	0.5549	0.092*
C13	0.7008 (15)	0.67614 (18)	0.5417 (9)	0.0610 (17)
H13	0.8689	0.6840	0.5739	0.073*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ni1	0.0214 (4)	0.0436 (5)	0.0287 (4)	−0.0007 (4)	0.0170 (4)	−0.0012 (4)
N1	0.060 (3)	0.044 (3)	0.061 (3)	−0.010 (2)	0.038 (3)	−0.004 (2)
O1	0.0284 (19)	0.064 (2)	0.048 (2)	0.0099 (18)	0.0234 (19)	0.0211 (19)
O2	0.042 (2)	0.056 (2)	0.051 (2)	−0.0096 (18)	0.035 (2)	−0.0105 (18)
O3	0.0269 (17)	0.055 (2)	0.041 (2)	−0.0029 (16)	0.0250 (16)	0.0003 (17)
O4	0.056 (3)	0.059 (3)	0.094 (4)	−0.008 (2)	0.042 (3)	0.002 (3)
O5	0.0309 (19)	0.074 (3)	0.035 (2)	−0.0104 (19)	0.0206 (17)	−0.0005 (19)
O6	0.038 (2)	0.082 (3)	0.055 (3)	0.018 (2)	0.035 (2)	0.025 (2)
O7	0.036 (2)	0.100 (3)	0.053 (3)	−0.023 (2)	0.033 (2)	−0.033 (2)
S1	0.0229 (6)	0.0420 (7)	0.0311 (6)	−0.0014 (5)	0.0181 (5)	0.0003 (5)
C1	0.021 (2)	0.041 (3)	0.027 (2)	−0.004 (2)	0.014 (2)	−0.002 (2)
C2	0.053 (3)	0.049 (3)	0.047 (3)	−0.003 (3)	0.039 (3)	−0.004 (3)
C3	0.066 (4)	0.046 (3)	0.054 (4)	−0.006 (3)	0.043 (3)	−0.012 (3)
C4	0.041 (3)	0.046 (3)	0.049 (3)	−0.007 (3)	0.026 (3)	0.001 (3)
C5	0.054 (4)	0.046 (3)	0.068 (4)	−0.004 (3)	0.047 (4)	0.001 (3)
C6	0.053 (3)	0.044 (3)	0.053 (3)	−0.004 (3)	0.043 (3)	0.001 (3)

C7	0.050 (4)	0.056 (4)	0.048 (4)	-0.014 (3)	0.031 (3)	-0.009 (3)
C8	0.059 (4)	0.045 (3)	0.047 (3)	-0.008 (3)	0.032 (3)	-0.008 (3)
C9	0.050 (4)	0.049 (4)	0.048 (4)	-0.003 (3)	0.021 (3)	0.002 (3)
C10	0.065 (4)	0.049 (4)	0.055 (4)	-0.014 (3)	0.030 (4)	-0.002 (3)
C11	0.082 (5)	0.050 (4)	0.051 (4)	-0.013 (4)	0.035 (4)	0.000 (3)
C12	0.098 (6)	0.049 (4)	0.079 (5)	0.000 (4)	0.057 (5)	0.002 (4)
C13	0.068 (4)	0.052 (4)	0.063 (4)	-0.007 (3)	0.044 (4)	-0.007 (3)

*Geometric parameters (Å, °)*

Ni1—O5 <sup>i</sup>	2.028 (3)	C1—C2	1.388 (7)
Ni1—O5	2.028 (3)	C2—C3	1.388 (8)
Ni1—O7 <sup>i</sup>	2.043 (4)	C2—H2	0.9300
Ni1—O7	2.043 (4)	C3—C4	1.371 (8)
Ni1—O6	2.049 (4)	C3—H3	0.9300
Ni1—O6 <sup>i</sup>	2.049 (4)	C4—C5	1.389 (8)
N1—C7	1.288 (8)	C5—C6	1.373 (8)
N1—C4	1.414 (7)	C5—H5	0.9300
O1—S1	1.458 (4)	C6—H6	0.9300
O2—S1	1.459 (4)	C7—C8	1.465 (8)
O3—S1	1.454 (3)	C7—H7	0.9300
O4—C9	1.333 (8)	C8—C9	1.397 (9)
O4—H4	0.8209	C8—C13	1.402 (9)
O5—H5A	0.8494	C9—C10	1.394 (8)
O5—H5B	0.8492	C10—C11	1.357 (10)
O6—H6A	0.8500	C10—H10	0.9300
O6—H6B	0.8498	C11—C12	1.396 (10)
O7—H7A	0.8497	C11—H11	0.9300
O7—H7B	0.8504	C12—C13	1.387 (9)
S1—C1	1.767 (5)	C12—H12	0.9300
C1—C6	1.387 (7)	C13—H13	0.9300
O5 <sup>i</sup> —Ni1—O5	180.0 (2)	C3—C2—H2	120.5
O5 <sup>i</sup> —Ni1—O7 <sup>i</sup>	90.78 (15)	C1—C2—H2	120.5
O5—Ni1—O7 <sup>i</sup>	89.22 (15)	C4—C3—C2	120.4 (5)
O5 <sup>i</sup> —Ni1—O7	89.22 (15)	C4—C3—H3	119.8
O5—Ni1—O7	90.78 (15)	C2—C3—H3	119.8
O7 <sup>i</sup> —Ni1—O7	180.000 (2)	C3—C4—C5	119.9 (5)
O5 <sup>i</sup> —Ni1—O6	89.99 (15)	C3—C4—N1	123.2 (6)
O5—Ni1—O6	90.01 (15)	C5—C4—N1	116.9 (5)
O7 <sup>i</sup> —Ni1—O6	90.23 (18)	C6—C5—C4	120.6 (5)
O7—Ni1—O6	89.77 (18)	C6—C5—H5	119.7
O5 <sup>i</sup> —Ni1—O6 <sup>i</sup>	90.01 (15)	C4—C5—H5	119.7
O5—Ni1—O6 <sup>i</sup>	89.99 (15)	C5—C6—C1	119.1 (5)
O7 <sup>i</sup> —Ni1—O6 <sup>i</sup>	89.77 (18)	C5—C6—H6	120.4
O7—Ni1—O6 <sup>i</sup>	90.23 (18)	C1—C6—H6	120.4
O6—Ni1—O6 <sup>i</sup>	180.000 (3)	N1—C7—C8	121.5 (6)
C7—N1—C4	120.7 (5)	N1—C7—H7	119.3

C9—O4—H4	109.5	C8—C7—H7	119.3
Ni1—O5—H5A	112.9	C9—C8—C13	119.8 (6)
Ni1—O5—H5B	112.8	C9—C8—C7	121.0 (6)
H5A—O5—H5B	110.6	C13—C8—C7	119.1 (6)
Ni1—O6—H6A	111.7	O4—C9—C8	122.0 (6)
Ni1—O6—H6B	111.9	O4—C9—C10	119.4 (6)
H6A—O6—H6B	109.6	C8—C9—C10	118.6 (7)
Ni1—O7—H7A	113.0	C11—C10—C9	121.4 (7)
Ni1—O7—H7B	112.9	C11—C10—H10	119.3
H7A—O7—H7B	110.5	C9—C10—H10	119.3
O3—S1—O1	111.7 (2)	C10—C11—C12	120.9 (7)
O3—S1—O2	112.3 (2)	C10—C11—H11	119.5
O1—S1—O2	112.5 (2)	C12—C11—H11	119.5
O3—S1—C1	106.6 (2)	C13—C12—C11	118.7 (8)
O1—S1—C1	107.3 (2)	C13—C12—H12	120.6
O2—S1—C1	105.9 (2)	C11—C12—H12	120.6
C6—C1—C2	120.8 (5)	C12—C13—C8	120.5 (7)
C6—C1—S1	119.0 (4)	C12—C13—H13	119.7
C2—C1—S1	120.2 (4)	C8—C13—H13	119.7
C3—C2—C1	119.0 (5)		
O3—S1—C1—C6	163.8 (4)	C2—C1—C6—C5	0.6 (8)
O1—S1—C1—C6	-76.3 (5)	S1—C1—C6—C5	177.7 (4)
O2—S1—C1—C6	44.1 (5)	C4—N1—C7—C8	-177.6 (5)
O3—S1—C1—C2	-19.0 (5)	N1—C7—C8—C9	3.2 (10)
O1—S1—C1—C2	100.8 (4)	N1—C7—C8—C13	-179.6 (6)
O2—S1—C1—C2	-138.8 (4)	C13—C8—C9—O4	179.1 (6)
C6—C1—C2—C3	-1.1 (8)	C7—C8—C9—O4	-3.8 (10)
S1—C1—C2—C3	-178.2 (4)	C13—C8—C9—C10	-0.4 (10)
C1—C2—C3—C4	0.8 (9)	C7—C8—C9—C10	176.8 (6)
C2—C3—C4—C5	-0.1 (10)	O4—C9—C10—C11	-179.3 (6)
C2—C3—C4—N1	178.9 (6)	C8—C9—C10—C11	0.2 (10)
C7—N1—C4—C3	29.9 (9)	C9—C10—C11—C12	1.3 (11)
C7—N1—C4—C5	-151.1 (6)	C10—C11—C12—C13	-2.4 (11)
C3—C4—C5—C6	-0.4 (10)	C11—C12—C13—C8	2.2 (10)
N1—C4—C5—C6	-179.5 (6)	C9—C8—C13—C12	-0.8 (10)
C4—C5—C6—C1	0.2 (9)	C7—C8—C13—C12	-178.0 (6)

Symmetry code: (i)  $-x+1, -y+2, -z+2$ .

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O4—H4 $\cdots$ N1	0.82	1.86	2.595 (9)	148
O5—H5A $\cdots$ O1 <sup>ii</sup>	0.85	1.96	2.737 (6)	151
O5—H5B $\cdots$ O2 <sup>iii</sup>	0.85	1.98	2.751 (6)	150
O6—H6A $\cdots$ O3 <sup>ii</sup>	0.85	1.95	2.764 (7)	161
O6—H6B $\cdots$ O1 <sup>iv</sup>	0.85	1.97	2.768 (8)	156

---

O7—H7A···O2	0.85	2.00	2.757 (8)	148
O7—H7B···O3 <sup>iii</sup>	0.85	2.00	2.769 (7)	150
C2—H2···O3	0.93	2.56	2.917 (7)	104

---

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