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Crystal structure and theoretical study of (2*E*)-1-[4-hydroxy-3-(morpholin-4-ylmethyl)-phenyl]-3-(thiophen-2-yl)prop-2-en-1-one

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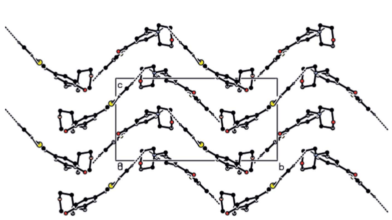
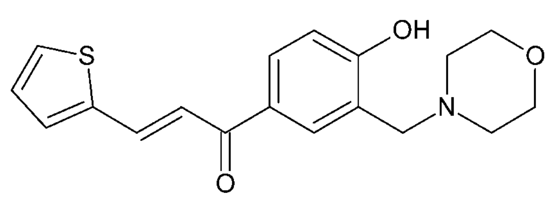
In the title compound, $C_{18}H_{19}NO_3S$, the morpholine ring adopts a chair conformation. The thiophene ring forms dihedral angles of 26.04 (9) and 74.07 (10)° with the benzene ring and the mean plane of the morpholine ring, respectively. The molecular conformation is stabilized by an O—H···N hydrogen bond. In the crystal, molecules are connected through C—H···O hydrogen bonds, forming wave-like layers parallel to the *ab* plane, which are further linked into a three-dimensional network by C—H···π interactions involving the benzene rings and the methylene H atoms of the morpholine rings.



1. Chemical context

Chalcones, *viz* 1,3-diaryl-2-propene-1-ones, are major component of many natural products as well as important precursors for many synthetic manipulations (Das *et al.*, 2006; Yerdelen *et al.*, 2015; Gul *et al.*, 2009). Chalcones and their synthetic analogues display a wide range of biological activities such as anticancer, antimalarial, antibacterial, anti-inflammatory, antifungal, antioxidant, anti-*HIV*, anti-protozoal, and carbonic anhydrase inhibiting activities (Das *et al.*, 2006; Yerdelen *et al.*, 2015; Gul *et al.*, 2007, 2009; Bilginer *et al.*, 2013, 2014; Yamali *et al.*, 2016; Singh *et al.*, 2014).



Mannich bases are an important class of compounds in medicinal chemistry. The Mannich reaction can be considered as a substitution reaction of a suitable compound in which one or more aminomethylation processes happen, depending on the nature of the reactants. The biological activities of Mannich bases may result from their chemical structures or from the production of α,β-unsaturated ketone moieties (Roman, 2015). The title compound was designed with the expectation of observing an increased bioactivity or cytotoxicity in a molecule including both chalcone and Mannich base pharmakophores.

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

*Cg*1 is the centroid of the C8–C13 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O*···N1	0.83 (2)	1.94 (2)	2.6834 (18)	149 (3)
C1—H1···O1^{i}	0.93	2.38	3.249 (2)	156
C2—H2···O2^{ii}	0.93	2.57	3.417 (2)	152
C16—H16*A*···*Cg*1^{iii}	0.97	2.88	3.789 (2)	157
C18—H18*B*···*Cg*1^{iv}	0.97	2.70	3.6010 (18)	154

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

2. Structural commentary

In the title compound (Fig. 1), the morpholine ring (N1/O3/C15–C18) adopts a chair conformation with puckering parameters Q_T = 0.5776 (18) Å, θ = 0.00 (19)°, φ = 308 (12)°. The benzene ring (C8–C13) forms dihedral angles of 26.04 (9) and 79.95 (8)° with the thiophene ring (S1/C1–C4) and the mean plane of the morpholine ring, respectively. The values of all bond lengths and angles in the title compound are unexceptional. The molecular conformation is enforced by an intramolecular O—H···N hydrogen bond (Table 1).

3. Supramolecular features

In the crystal, molecules are linked by intermolecular C—H···O hydrogen bonds, forming wave-like layers parallel to the *ab* plane (Table 1, Fig. 2). C—H···π interactions are observed between the benzene rings and the methylene hydrogen atoms of the morpholine rings in adjacent layers, forming a three-dimensional network.

4. Database survey

A search of the Cambridge Structural Database (Version 5.39, update May 2018; Groom *et al.*, 2016) for the 2-(morpholinomethyl)phenol substructure yielded two hits, namely BOPMEY (Fun *et al.*, 1999) and IHUBIW (Xie *et al.*, 2003). In both compounds, the amine N atoms of the morpholine rings and the hydroxy groups of the phenol fragments are engaged in intramolecular hydrogen bonds.

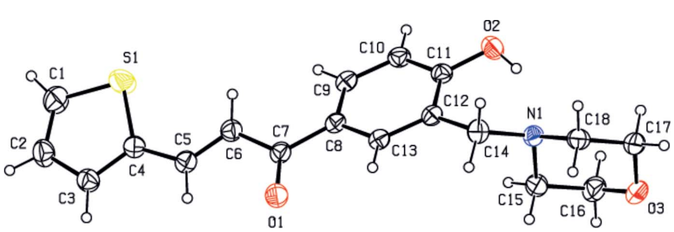


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level

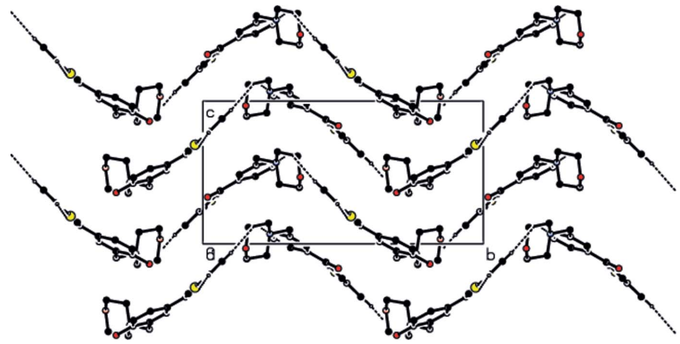


Figure 2
The molecular packing of the title compound viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

5. Theoretical calculations

A quantum-chemical calculation was performed using the *CNDO* (Complete Neglect of Differential Overlap; Pople & Beveridge, 1970) approximation. A view of the calculated molecule is shown in Fig. 3. The charges at atoms S1, O1, O2, O3 and N1 are −0.049, −0.336, −0.271, −0.224 and −0.145 e^{-}, respectively. The calculated dipole moment of the title molecule is *ca* 2.881 Debye. The *HOMO* and *LUMO* energy levels are −10.3681 and 1.4009 eV, respectively.

In addition, the geometrical optimization calculations of the title compound were performed using the *PM3* (Parameterized Model number 3) method (Stewart, 1989*a,b*) in *WinMopac7.2*. A view of the molecule calculated with *PM3* is shown in Fig. 4. The net charges at atoms S1, O1, O2, O3 and N1 are 0.321, −0.230, −0.260, −0.321 and −0.070 e^{-}, respectively. The calculated dipole moment of the title molecule is *ca* 1.176 Debye. The *HOMO* and *LUMO* energy levels are

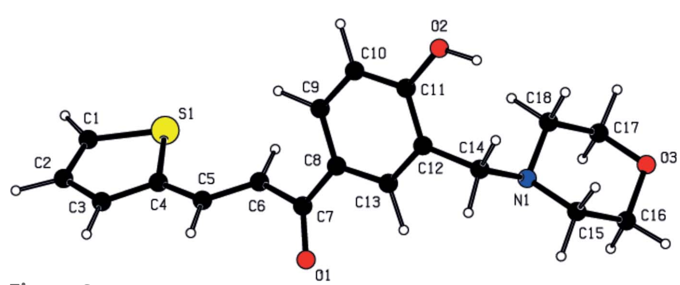


Figure 3
Spatial view of the title compound calculated using the *CNDO* method.

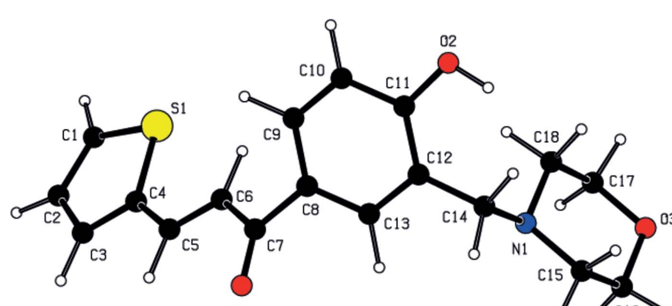


Figure 4
Spatial view of the title compound calculated using the *PM3* method

Table 2
Comparison of experimental (X-ray), theoretical (*CNDO* and *PM3*) parameters (Å, °) of the title compound.

Bond/Angle	X-ray	*CNDO*	PM3
S1—C1	1.705 (2)	1.7663	1.7194
S1—C4	1.720 (2)	1.7758	1.7449
O1—C7	1.224 (2)	1.2143	1.2196
O2—C11	1.354 (2)	1.3565	1.3663
O3—C16	1.419 (2)	1.4208	1.4149
O3—C17	1.422 (2)	1.4209	1.4153
N1—C14	1.472 (2)	1.4606	1.4916
N1—C15	1.469 (2)	1.4573	1.4914
N1—C18	1.469 (2)	1.4567	1.4906
C1—S1—C4	92.20 (9)	88.91	91.38
C16—O3—C17	109.29 (13)	110.44	112.79
C14—N1—C15	111.86 (13)	111.15	112.06
C14—N1—C18	110.61 (13)	111.92	112.86
C15—N1—C18	109.09 (13)	109.64	111.62
S1—C1—C2	111.75 (15)	111.11	112.58
S1—C4—C5	123.58 (12)	126.03	125.76
S1—C4—C3	109.79 (12)	109.88	111.11
O1—C7—C6	120.42 (14)	119.03	122.82
O1—C7—C8	119.90 (14)	123.49	121.52
O2—C11—C10	118.59 (14)	119.87	115.22
O2—C11—C12	121.18 (14)	122.06	123.98
N1—C14—C12	112.14 (12)	112.35	111.21
N1—C15—C16	109.98 (14)	110.79	109.89
O3—C16—C15	111.42 (17)	109.89	112.44
O3—C17—C18	111.22 (14)	110.05	112.30
N1—C18—C17	109.80 (15)	110.73	110.02

−0.1724 and 0.0829 eV, respectively. These calculations were performed assuming the molecule to be isolated and in an absolute vacuum. A comparison between experimental and calculated bond lengths (r.m.s. deviations of 0.029 and 0.016 Å for *CNDO* and *PM3*, respectively) and angles (r.m.s. deviations of 1.601 and 1.915° for *CNDO* and *PM3*, respectively) is given in Table 2. The *PM3* method gave the lowest values for *HOMO*, *LUMO* and dipole moments.

6. Synthesis and crystallization

A mixture of paraformaldehyde (0.13 g, 4.3 mmol) and morpholine (0.37 g, 4.3 mmol) in acetonitrile (5 ml) was refluxed at 353 K for 30 min. A solution of a suitable chalcone in acetonitrile (25 ml), [1-(4-hydroxyphenyl)-3-(thiophene-2-yl)-2-propene-1-one (1 g, 4.3 mmol)], was added into the reaction flask under continuous heating. The reaction progress was monitored by TLC. The reaction stopped after 8 h when the chalcone compound was consumed in the reaction medium, and the solvent was removed under vacuum. The residue was purified by column chromotography (SiO_2; $CHCl_3$: MeOH 9:1 *v*/*v*). Yield 32%, m.p. 424–426 K. Crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution.

7. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 3. C-bound H atoms were placed in calculated positions with C—H = 0.93–0.97 Å and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$. The hydroxy H atom was found in a difference-Fourier map and refined with $U_{iso}(H) = 1.5U_{eq}(O)$. 15 outliers (5 4 6, $\overline{8}$ 14 1, 5 3 2, 3 4 2, $\overline{1}$ 3 1, $\overline{6}$ 16 4, $\overline{4}$ 11 1, $\overline{7}$ 7 9, $\overline{2}$ 11 1, 2 2 10, 0 5 12, $\overline{8}$ 13 1, $\overline{6}$ 13 3, 0 15 4, $\overline{6}$ 17 4) were omitted in the final cycles of refinement.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{19}NO_3S$
M_r	329.40
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, *b*, *c* (Å)	9.4939 (5), 18.5548 (10), 9.5068 (5)
β (°)	96.788 (3)
V (Å^3)	1662.95 (15)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.21
Crystal size (mm)	0.81 × 0.50 × 0.48
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.882, 0.905
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33902, 4168, 3373
R_{int}	0.033
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.670
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.050, 0.138, 1.03
No. of reflections	4168
No. of parameters	211
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.25

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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supporting information

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Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

(2*E*)-1-[4-Hydroxy-3-(morpholin-4-ylmethyl)phenyl]-3-(thiophen-2-yl)prop-2-en-1-one

Crystal data

$C_{18}H_{19}NO_3S$
M_r = 329.40
Monoclinic, $P2_1/n$
a = 9.4939 (5) Å
b = 18.5548 (10) Å
c = 9.5068 (5) Å
β = 96.788 (3)°
V = 1662.95 (15) Å^3
Z = 4
$F(000)$ = 696
D_x = 1.316 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9868 reflections
θ = 2.2–28.4°
μ = 0.21 mm^{-1}
T = 293 K
Prism, colourless
0.81 × 0.50 × 0.48 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
T_{min} = 0.882, T_{max} = 0.905
33902 measured reflections
4168 independent reflections
3373 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 28.5°, θ_{min} = 2.2°
h = −12→12
k = −24→24
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.138
S = 1.03
4168 reflections
211 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2 + 0.4859P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.3316 (2)	−0.02309 (12)	0.2121 (3)	0.0720 (6)
H1	0.235465	−0.019863	0.221873	0.086*
C2	0.3860 (2)	−0.06817 (11)	0.1231 (2)	0.0623 (5)
H2	0.331381	−0.099790	0.063433	0.075*
C3	0.53423 (18)	−0.06285 (9)	0.12897 (19)	0.0522 (4)
H3	0.587701	−0.090438	0.073164	0.063*
C4	0.59198 (16)	−0.01301 (8)	0.22504 (17)	0.0441 (3)
C5	0.74016 (16)	0.00373 (8)	0.25820 (17)	0.0447 (3)
H5	0.802258	−0.022598	0.209531	0.054*
C6	0.79903 (17)	0.05204 (9)	0.34953 (18)	0.0465 (4)
H6	0.741687	0.080254	0.400249	0.056*
C7	0.95402 (16)	0.06168 (8)	0.37183 (17)	0.0433 (3)
C8	1.01520 (15)	0.12698 (8)	0.44638 (15)	0.0398 (3)
C9	0.93436 (16)	0.18710 (8)	0.47309 (16)	0.0435 (3)
H9	0.836671	0.186378	0.448048	0.052*
C10	0.99807 (17)	0.24766 (8)	0.53638 (17)	0.0456 (3)
H10	0.943157	0.287658	0.552522	0.055*
C11	1.14360 (16)	0.24932 (8)	0.57615 (15)	0.0410 (3)
C12	1.22777 (15)	0.18990 (8)	0.54966 (15)	0.0390 (3)
C13	1.16227 (15)	0.13017 (8)	0.48509 (15)	0.0397 (3)
H13	1.217489	0.090658	0.466589	0.048*
C14	1.38542 (17)	0.19118 (9)	0.59817 (18)	0.0473 (4)
H14A	1.401057	0.181264	0.698985	0.057*
H14B	1.431423	0.153440	0.549728	0.057*
C15	1.45567 (19)	0.27260 (10)	0.41787 (17)	0.0533 (4)
H15A	1.360309	0.272216	0.368303	0.064*
H15B	1.508851	0.233930	0.380183	0.064*
C16	1.5255 (2)	0.34382 (12)	0.3944 (2)	0.0645 (5)
H16A	1.529884	0.350654	0.293866	0.077*
H16B	1.468902	0.382512	0.427116	0.077*
C17	1.65806 (19)	0.33755 (12)	0.6150 (2)	0.0603 (5)
H17A	1.601485	0.375827	0.649325	0.072*
H17B	1.752902	0.340669	0.665265	0.072*
C18	1.59421 (16)	0.26603 (10)	0.64480 (18)	0.0507 (4)
H18A	1.652343	0.227514	0.613763	0.061*
H18B	1.591062	0.260745	0.745894	0.061*
N1	1.45003 (13)	0.26102 (7)	0.56999 (13)	0.0425 (3)
O1	1.03248 (13)	0.01683 (7)	0.32762 (15)	0.0605 (3)
O2	1.20139 (14)	0.30917 (7)	0.64087 (14)	0.0548 (3)

O3	1.66467 (14)	0.34704 (8)	0.46745 (15)	0.0686 (4)
S1	0.45988 (5)	0.02779 (3)	0.30547 (7)	0.0781 (2)
H1O	1.2875 (19)	0.3090 (18)	0.633 (3)	0.117*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0407 (9)	0.0815 (14)	0.0932 (15)	0.0020 (9)	0.0062 (9)	−0.0139 (12)
C2	0.0505 (10)	0.0600 (11)	0.0743 (13)	−0.0078 (8)	−0.0017 (9)	−0.0083 (9)
C3	0.0508 (9)	0.0475 (9)	0.0585 (10)	0.0007 (7)	0.0072 (7)	−0.0053 (7)
C4	0.0416 (8)	0.0406 (8)	0.0499 (8)	0.0049 (6)	0.0046 (6)	0.0006 (6)
C5	0.0417 (8)	0.0414 (7)	0.0515 (8)	0.0031 (6)	0.0073 (6)	0.0028 (6)
C6	0.0419 (8)	0.0443 (8)	0.0538 (9)	0.0012 (6)	0.0084 (7)	−0.0019 (7)
C7	0.0426 (8)	0.0413 (8)	0.0470 (8)	−0.0013 (6)	0.0094 (6)	0.0031 (6)
C8	0.0394 (7)	0.0408 (7)	0.0405 (7)	−0.0009 (6)	0.0098 (6)	0.0044 (6)
C9	0.0370 (7)	0.0476 (8)	0.0472 (8)	0.0017 (6)	0.0102 (6)	0.0029 (6)
C10	0.0451 (8)	0.0430 (8)	0.0505 (9)	0.0060 (6)	0.0132 (7)	−0.0018 (6)
C11	0.0468 (8)	0.0414 (7)	0.0359 (7)	−0.0002 (6)	0.0086 (6)	0.0015 (6)
C12	0.0388 (7)	0.0417 (7)	0.0367 (7)	0.0007 (6)	0.0052 (6)	0.0066 (6)
C13	0.0401 (7)	0.0372 (7)	0.0427 (7)	0.0034 (6)	0.0090 (6)	0.0049 (6)
C14	0.0427 (8)	0.0468 (8)	0.0509 (9)	0.0011 (6)	−0.0012 (6)	0.0040 (7)
C15	0.0532 (9)	0.0672 (11)	0.0389 (8)	−0.0119 (8)	0.0035 (7)	−0.0032 (7)
C16	0.0651 (11)	0.0769 (13)	0.0532 (10)	−0.0191 (10)	0.0138 (8)	0.0029 (9)
C17	0.0433 (9)	0.0802 (13)	0.0587 (10)	−0.0145 (8)	0.0114 (7)	−0.0211 (9)
C18	0.0379 (8)	0.0673 (11)	0.0461 (8)	0.0016 (7)	0.0016 (6)	−0.0121 (7)
N1	0.0376 (6)	0.0507 (7)	0.0388 (6)	−0.0043 (5)	0.0032 (5)	−0.0020 (5)
O1	0.0456 (6)	0.0539 (7)	0.0837 (9)	0.0002 (5)	0.0151 (6)	−0.0174 (6)
O2	0.0554 (7)	0.0482 (6)	0.0605 (7)	−0.0024 (5)	0.0059 (6)	−0.0127 (5)
O3	0.0540 (7)	0.0911 (10)	0.0646 (8)	−0.0251 (7)	0.0234 (6)	−0.0133 (7)
S1	0.0495 (3)	0.0889 (4)	0.0965 (4)	0.0074 (2)	0.0111 (3)	−0.0427 (3)

Geometric parameters (Å, º)

C1—C2	1.336 (3)	C11—C12	1.402 (2)
C1—S1	1.705 (2)	C12—C13	1.379 (2)
C1—H1	0.9300	C12—C14	1.513 (2)
C2—C3	1.406 (2)	C13—H13	0.9300
C2—H2	0.9300	C14—N1	1.472 (2)
C3—C4	1.368 (2)	C14—H14A	0.9700
C3—H3	0.9300	C14—H14B	0.9700
C4—C5	1.439 (2)	C15—N1	1.469 (2)
C4—S1	1.7197 (16)	C15—C16	1.507 (3)
C5—C6	1.325 (2)	C15—H15A	0.9700
C5—H5	0.9300	C15—H15B	0.9700
C6—C7	1.473 (2)	C16—O3	1.419 (2)
C6—H6	0.9300	C16—H16A	0.9700
C7—O1	1.2239 (19)	C16—H16B	0.9700
C7—C8	1.487 (2)	C17—O3	1.422 (2)

C8—C9	1.394 (2)	C17—C18	1.500 (3)
C8—C13	1.403 (2)	C17—H17A	0.9700
C9—C10	1.380 (2)	C17—H17B	0.9700
C9—H9	0.9300	C18—N1	1.4691 (19)
C10—C11	1.389 (2)	C18—H18A	0.9700
C10—H10	0.9300	C18—H18B	0.9700
C11—O2	1.3538 (19)	O2—H1O	0.830 (18)

C2—C1—S1	111.75 (15)	C8—C13—H13	118.9
C2—C1—H1	124.1	N1—C14—C12	112.14 (12)
S1—C1—H1	124.1	N1—C14—H14A	109.2
C1—C2—C3	113.02 (18)	C12—C14—H14A	109.2
C1—C2—H2	123.5	N1—C14—H14B	109.2
C3—C2—H2	123.5	C12—C14—H14B	109.2
C4—C3—C2	113.24 (16)	H14A—C14—H14B	107.9
C4—C3—H3	123.4	N1—C15—C16	109.98 (14)
C2—C3—H3	123.4	N1—C15—H15A	109.7
C3—C4—C5	126.63 (15)	C16—C15—H15A	109.7
C3—C4—S1	109.79 (12)	N1—C15—H15B	109.7
C5—C4—S1	123.58 (12)	C16—C15—H15B	109.7
C6—C5—C4	127.99 (15)	H15A—C15—H15B	108.2
C6—C5—H5	116.0	O3—C16—C15	111.42 (17)
C4—C5—H5	116.0	O3—C16—H16A	109.3
C5—C6—C7	120.90 (15)	C15—C16—H16A	109.3
C5—C6—H6	119.6	O3—C16—H16B	109.3
C7—C6—H6	119.6	C15—C16—H16B	109.3
O1—C7—C6	120.42 (14)	H16A—C16—H16B	108.0
O1—C7—C8	119.90 (14)	O3—C17—C18	111.22 (14)
C6—C7—C8	119.67 (13)	O3—C17—H17A	109.4
C9—C8—C13	118.09 (14)	C18—C17—H17A	109.4
C9—C8—C7	123.12 (14)	O3—C17—H17B	109.4
C13—C8—C7	118.69 (13)	C18—C17—H17B	109.4
C10—C9—C8	120.57 (14)	H17A—C17—H17B	108.0
C10—C9—H9	119.7	N1—C18—C17	109.80 (15)
C8—C9—H9	119.7	N1—C18—H18A	109.7
C9—C10—C11	120.48 (14)	C17—C18—H18A	109.7
C9—C10—H10	119.8	N1—C18—H18B	109.7
C11—C10—H10	119.8	C17—C18—H18B	109.7
O2—C11—C10	118.59 (14)	H18A—C18—H18B	108.2
O2—C11—C12	121.18 (14)	C18—N1—C15	109.09 (13)
C10—C11—C12	120.23 (14)	C18—N1—C14	110.61 (13)
C13—C12—C11	118.39 (13)	C15—N1—C14	111.86 (13)
C13—C12—C14	121.74 (13)	C11—O2—H1O	108 (2)
C11—C12—C14	119.80 (13)	C16—O3—C17	109.29 (13)
C12—C13—C8	122.22 (13)	C1—S1—C4	92.20 (9)
C12—C13—H13	118.9		

S1—C1—C2—C3	0.3 (3)	C10—C11—C12—C14	−177.78 (14)

C1—C2—C3—C4	0.4 (3)	C11—C12—C13—C8	−0.4 (2)
C2—C3—C4—C5	178.40 (16)	C14—C12—C13—C8	176.60 (13)
C2—C3—C4—S1	−0.9 (2)	C9—C8—C13—C12	0.9 (2)
C3—C4—C5—C6	179.33 (18)	C7—C8—C13—C12	177.50 (13)
S1—C4—C5—C6	−1.5 (3)	C13—C12—C14—N1	140.07 (14)
C4—C5—C6—C7	179.26 (15)	C11—C12—C14—N1	−42.94 (19)
C5—C6—C7—O1	−13.9 (3)	N1—C15—C16—O3	58.3 (2)
C5—C6—C7—C8	165.08 (15)	O3—C17—C18—N1	−59.52 (19)
O1—C7—C8—C9	166.04 (15)	C17—C18—N1—C15	56.66 (17)
C6—C7—C8—C9	−12.9 (2)	C17—C18—N1—C14	−179.90 (13)
O1—C7—C8—C13	−10.4 (2)	C16—C15—N1—C18	−55.98 (19)
C6—C7—C8—C13	170.68 (14)	C16—C15—N1—C14	−178.68 (15)
C13—C8—C9—C10	−0.3 (2)	C12—C14—N1—C18	167.76 (13)
C7—C8—C9—C10	−176.70 (14)	C12—C14—N1—C15	−70.41 (17)
C8—C9—C10—C11	−0.8 (2)	C15—C16—O3—C17	−59.5 (2)
C9—C10—C11—O2	−178.50 (14)	C18—C17—O3—C16	60.1 (2)
C9—C10—C11—C12	1.3 (2)	C2—C1—S1—C4	−0.7 (2)
O2—C11—C12—C13	179.13 (13)	C3—C4—S1—C1	0.90 (15)
C10—C11—C12—C13	−0.7 (2)	C5—C4—S1—C1	−178.40 (16)
O2—C11—C12—C14	2.0 (2)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C8–C13 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1*O*···N1	0.83 (2)	1.94 (2)	2.6834 (18)	149 (3)
C1—H1···O1^{i}	0.93	2.38	3.249 (2)	156
C2—H2···O2^{ii}	0.93	2.57	3.417 (2)	152
C5—H5···O1	0.93	2.45	2.786 (2)	101
C16—H16*A*···*Cg*1^{iii}	0.97	2.88	3.789 (2)	157
C18—H18*B*···*Cg*1^{iv}	0.97	2.70	3.6010 (18)	154

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iii) *x*+1/2, −*y*+1/2, *z*−1/2; (iv) *x*+1/2, −*y*+1/2, *z*+1/2.