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4-(Acetylamino)phenyl benzenesulfonate

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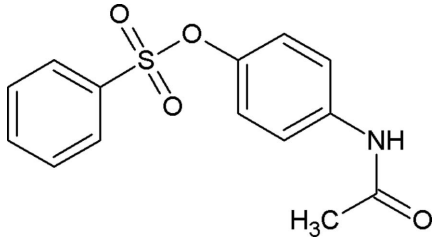
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.104; data-to-parameter ratio = 15.8.

The phenyl and acetylaminophenyl rings of the title compound, $C_{14}H_{13}NO_4S$, are at an angle of 71.57 (5)°, with the acetylamino group rotated by 16.3 (1)° from coplanarity with the ring to which it is attached. The structure is stabilized by the presence of N—H···O hydrogen bonds which create infinite one-dimensional chains along [010]; weak C—H···O interactions are also present.

Related literature

For a detailed account of the molecular and supramolecular architectures of aromatic sulfonates, see Manivannan *et al.* (2005) and references cited therein.

For related literature, see: Alford *et al.* (1991); Bernstein *et al.* (1995); Desiraju *et al.* (1999); Etter (1990); Jiang *et al.* (1990); Narayanan & Krakow (1983); Spungin *et al.* (1992); Tharakan *et al.* (1992); Yachi *et al.* (1989).



Experimental

Crystal data

$C_{14}H_{13}NO_4S$
M_r = 291.31
Monoclinic, $P2_1/n$
a = 11.9028 (14) Å
b = 8.7768 (9) Å
c = 13.7394 (15) Å
β = 110.144 (4)°
V = 1347.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 120 (2) K
0.32 × 0.28 × 0.20 mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.869, T_{max} = 1.000
(expected range 0.922–0.951)
9274 measured reflections
3637 independent reflections
2983 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.104
S = 1.04
3637 reflections
230 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N17—H17···O8^{i}	0.84 (2)	2.09 (2)	2.9272 (17)	173.3 (18)
C6—H6···O19^{ii}	0.92 (2)	2.55 (2)	3.269 (2)	135.5 (18)
C7—H7···O10^{iii}	0.97 (2)	2.59 (2)	3.5360 (19)	166.6 (16)
C16—H16···O9^{iii}	0.947 (19)	2.539 (19)	3.3783 (19)	147.9 (15)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2025).

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supplementary materials

Acta Cryst. (2007). E**63**, o3544 [**doi:10.1107/S1600536807034332**]

4-(Acetylamino)phenyl benzenesulfonate

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Comment

Aromatic sulfonates are used in monitoring the merging of lipids (Yachi *et al.*, 1989) and in many other fields (Spungin *et al.*, 1992, Tharakan *et al.*,1992, Alford *et al.*, 1991, Jiang *et al.*, 1990, Narayanan & Krakow, 1983). An X-ray study of the title compound (I) was undertaken in order to determine its crystal and molecular structure owing to the biological importance of its analogues. The molecular structure of (I) is shown in Fig. 1 with selected geometric parameters provided in Table 1. The S—C, S—O and S=O bond lengths are comparable with those found in related structures previously reported by our research group (Manivannan *et al.* 2005 & references cited therein).

A Newman projection along the O10—S1 bond is provided in Fig. 2. Using C11 as a reference point, the orientations of the two sulfonyl oxygen atoms (O8 and O9) and the phenyl carbon (C2) have been deduced from the corresponding torsion angles (C11–O10–S1–O8/O9/C2). Helical nomenclature is employed to assign + or -synclinal (*sc*) and +antiperiplanar (*ap*) conformations. The C2–S1–O10–C11 torsion angle of −61.6 (1)° corresponds to +synclinal conformation. The dihedral angle between the mean planes of the phenyl and acetylaminophenyl C_6 rings of 71.58 (8)° shows that the two rings are not coplanar. This is similar to that reported by us for other aromatic sulfonates (Manivannan *et al.* 2005 & references cited therein). The acetylamino group (N17 C18 O19 C20) is twisted by 16.3 (1)° from the mean plane of the phenyl ring (C11—C16) to which it is attached.

The crystal structure of (I) is stabilized by the presence of an intermolecular N—H···O hydrogen bond, along with several weak C—H···O interactions (Desiraju *et al.*, 1999) (Table 2, Fig. 3). The symmetry related N—H···O interactions generate a cooperative infinite one-dimensional chain along [010], while the C7—H7···O10 (−*x* + 1, −*y* + 1, −*z* + 1) interactions generate an $R^2_2(10)$ motif (Etter, *et al.*, 1990; Bernstein *et al.*, 1995).

Experimental

Benzenesulfonyl chloride (10 mmol), dissolved in acetone, was added dropwise to *N*-(4-hydroxyphenyl)acetamide (10 mmol) in aqueous NaOH (8 ml, 5%) with constant stirring. The precipitant (6.0 mmol, yield 60%) was filtered and recrystallized from aqueous ethanol.

Refinement

Hydrogen atoms were positioned geometrically (aromatic C—H = 0.95 Å, methyl C—H = 0.98 Å and N—H = 0.88 Å) and refined using a riding model. The H atom isotropic displacement parameters were fixed; U_{iso}(aromatic H) = 1.2 *x* U_{eq} of the parent atom; U_{iso}(methyl H) = 1.5 *x* U_{eq} of the parent atom; U_{iso}(N—H) = 1.2 *x* U_{eq} of the parent atom.

Figures

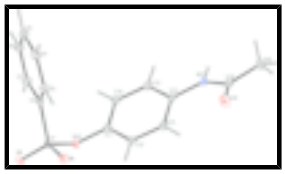

Fig. 1. The asymmetric unit of (I) with the atoms labelled and displacement ellipsoids depicted at the 50% probability level for the non-H atoms. H-atoms are drawn as spheres of arbitrary radius.

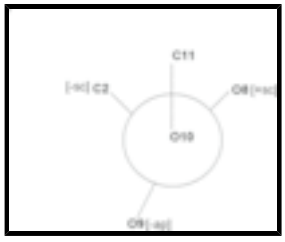

Fig. 2. A Newman projection along the O10—S1 bond with C11 as a reference point, +/-*sc* = +/-synclinal, -*ap* = -antiperiplanar.

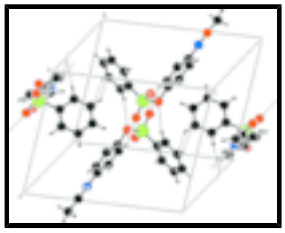

Fig. 3. The molecular packing viewed down the *a*-axis. Dashed lines represent the weak C—H···O interactions.

N-[4-(Acetylamino)phenyl]benzenesulfonate

Crystal data

$C_{14}H_{13}NO_4S$	F_{000} = 608
M_r = 291.31	D_x = 1.436 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 386-387 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.9028 (14) Å	Cell parameters from 5029 reflections
b = 8.7768 (9) Å	θ = 2.8–29.9º
c = 13.7394 (15) Å	μ = 0.25 mm^{-1}
β = 110.144 (4)º	T = 120 (2) K
V = 1347.5 (3) Å^3	Block, colourless
Z = 4	0.32 × 0.28 × 0.20 mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer	3637 independent reflections
Radiation source: fine-focus sealed tube	2983 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
Detector resolution: 8 pixels mm^{-1}	θ_{max} = 30.0º
T = 120(2) K	θ_{min} = 2.0º
ω scans	h = −16→9
Absorption correction: multi-scan	k = −11→11

(SADABS; Sheldrick, 1998a)
T_{min} = 0.869, T_{max} = 1.000
9274 measured reflections

l = −19→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.104
S = 1.04
3637 reflections
230 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 0.484P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Extinction correction: none

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.68262 (3)	0.63484 (4)	0.48846 (3)	0.02158 (11)
C2	0.75999 (13)	0.57481 (16)	0.61551 (11)	0.0203 (3)
C3	0.88245 (14)	0.60072 (18)	0.65761 (12)	0.0264 (3)
C4	0.94228 (15)	0.5596 (2)	0.75990 (13)	0.0304 (3)
C5	0.88100 (15)	0.4921 (2)	0.81739 (12)	0.0297 (3)
C6	0.75873 (16)	0.4664 (2)	0.77403 (13)	0.0308 (4)
C7	0.69649 (14)	0.50892 (19)	0.67272 (12)	0.0274 (3)
O8	0.76729 (10)	0.68778 (12)	0.44310 (9)	0.0277 (2)
O9	0.58457 (10)	0.73088 (13)	0.48467 (9)	0.0304 (3)
O10	0.61972 (9)	0.48512 (12)	0.43025 (8)	0.0229 (2)
C11	0.69032 (12)	0.35872 (16)	0.42162 (11)	0.0203 (3)
C12	0.76458 (13)	0.36714 (17)	0.36377 (11)	0.0225 (3)
C13	0.82522 (14)	0.23759 (17)	0.35126 (11)	0.0228 (3)
C14	0.81121 (13)	0.10049 (17)	0.39774 (11)	0.0204 (3)

C15	0.73370 (14)	0.09522 (17)	0.45465 (12)	0.0232 (3)
C16	0.67308 (13)	0.22412 (17)	0.46683 (12)	0.0236 (3)
N17	0.86890 (12)	−0.03536 (15)	0.38809 (10)	0.0231 (3)
C18	0.96450 (13)	−0.05347 (18)	0.35576 (12)	0.0249 (3)
O19	1.01465 (12)	0.05343 (14)	0.33170 (12)	0.0423 (3)
C20	1.00092 (16)	−0.2161 (2)	0.35039 (14)	0.0291 (3)
H3	0.9265 (18)	0.651 (2)	0.6176 (16)	0.035 (5)*
H4	1.0294 (19)	0.578 (2)	0.7907 (16)	0.037 (5)*
H5	0.9233 (19)	0.461 (2)	0.8887 (16)	0.041 (6)*
H6	0.720 (2)	0.421 (2)	0.8139 (17)	0.044 (6)*
H7	0.6112 (19)	0.493 (2)	0.6414 (15)	0.034 (5)*
H12	0.7745 (16)	0.462 (2)	0.3331 (14)	0.026 (5)*
H13	0.8753 (17)	0.244 (2)	0.3133 (14)	0.028 (5)*
H15	0.7254 (15)	0.002 (2)	0.4843 (13)	0.021 (4)*
H16	0.6220 (17)	0.221 (2)	0.5066 (15)	0.032 (5)*
H17	0.8453 (17)	−0.117 (2)	0.4077 (14)	0.027 (5)*
H20A	0.949 (2)	−0.270 (2)	0.3034 (17)	0.040*
H20B	1.0039 (19)	−0.273 (2)	0.4107 (17)	0.040*
H20C	1.076 (2)	−0.222 (2)	0.3411 (16)	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02313 (18)	0.01753 (17)	0.02454 (18)	0.00093 (13)	0.00880 (14)	0.00177 (13)
C2	0.0214 (7)	0.0166 (6)	0.0234 (7)	−0.0002 (5)	0.0083 (5)	−0.0008 (5)
C3	0.0236 (7)	0.0261 (7)	0.0302 (8)	−0.0047 (6)	0.0100 (6)	0.0006 (6)
C4	0.0228 (7)	0.0334 (9)	0.0318 (8)	−0.0030 (7)	0.0055 (6)	−0.0006 (7)
C5	0.0317 (8)	0.0338 (8)	0.0227 (7)	0.0035 (7)	0.0082 (6)	0.0007 (6)
C6	0.0308 (8)	0.0373 (9)	0.0289 (8)	−0.0001 (7)	0.0160 (7)	0.0052 (7)
C7	0.0224 (7)	0.0320 (8)	0.0296 (8)	−0.0013 (6)	0.0112 (6)	0.0019 (6)
O8	0.0348 (6)	0.0221 (5)	0.0297 (6)	−0.0057 (5)	0.0155 (5)	0.0014 (4)
O9	0.0313 (6)	0.0255 (6)	0.0337 (6)	0.0101 (5)	0.0102 (5)	0.0035 (5)
O10	0.0194 (5)	0.0217 (5)	0.0263 (5)	−0.0003 (4)	0.0061 (4)	−0.0012 (4)
C11	0.0177 (6)	0.0203 (7)	0.0208 (6)	−0.0009 (5)	0.0039 (5)	−0.0026 (5)
C12	0.0247 (7)	0.0221 (7)	0.0206 (6)	−0.0034 (6)	0.0075 (6)	0.0018 (5)
C13	0.0241 (7)	0.0245 (7)	0.0217 (7)	−0.0032 (6)	0.0104 (6)	−0.0006 (5)
C14	0.0199 (6)	0.0209 (7)	0.0205 (6)	−0.0040 (5)	0.0070 (5)	−0.0035 (5)
C15	0.0264 (7)	0.0195 (7)	0.0265 (7)	−0.0048 (6)	0.0126 (6)	−0.0002 (6)
C16	0.0230 (7)	0.0243 (7)	0.0261 (7)	−0.0045 (6)	0.0119 (6)	−0.0016 (6)
N17	0.0266 (6)	0.0186 (6)	0.0270 (6)	−0.0030 (5)	0.0129 (5)	−0.0018 (5)
C18	0.0229 (7)	0.0277 (7)	0.0244 (7)	−0.0002 (6)	0.0086 (6)	−0.0019 (6)
O19	0.0382 (7)	0.0309 (6)	0.0720 (10)	0.0004 (6)	0.0370 (7)	0.0054 (6)
C20	0.0255 (8)	0.0287 (8)	0.0325 (8)	0.0019 (6)	0.0090 (7)	−0.0044 (7)

Geometric parameters (Å, °)

S1—O8	1.4326 (11)	C11—C16	1.382 (2)
S1—O9	1.4260 (11)	C12—C13	1.389 (2)
S1—O10	1.5857 (11)	C12—H12	0.958 (19)

S1—C2	1.7509 (15)	C13—C14	1.399 (2)
C2—C3	1.389 (2)	C13—H13	0.920 (19)
C2—C7	1.390 (2)	C14—C15	1.401 (2)
C3—C4	1.387 (2)	C14—N17	1.4047 (19)
C3—H3	0.99 (2)	C15—C16	1.383 (2)
C4—C5	1.380 (2)	C15—H15	0.937 (18)
C4—H4	0.99 (2)	C16—H16	0.947 (19)
C5—C6	1.388 (2)	N17—C18	1.366 (2)
C5—H5	0.97 (2)	N17—H17	0.84 (2)
C6—C7	1.384 (2)	C18—O19	1.2173 (19)
C6—H6	0.92 (2)	C18—C20	1.501 (2)
C7—H7	0.97 (2)	C20—H20A	0.86 (2)
O10—C11	1.4211 (17)	C20—H20B	0.96 (2)
C11—C12	1.379 (2)	C20—H20C	0.94 (2)
O8—S1—O9	118.81 (7)	C11—C12—C13	119.40 (14)
O8—S1—O10	109.27 (6)	C11—C12—H12	120.1 (11)
O9—S1—O10	103.48 (6)	C13—C12—H12	120.5 (11)
O8—S1—C2	108.91 (7)	C12—C13—C14	119.93 (14)
O9—S1—C2	110.92 (7)	C12—C13—H13	119.0 (12)
O10—S1—C2	104.38 (6)	C14—C13—H13	121.1 (12)
C3—C2—C7	121.97 (14)	C13—C14—C15	119.22 (14)
C3—C2—S1	118.81 (12)	C13—C14—N17	123.24 (13)
C7—C2—S1	119.16 (11)	C15—C14—N17	117.52 (13)
C4—C3—C2	118.57 (15)	C16—C15—C14	120.81 (14)
C4—C3—H3	119.7 (12)	C16—C15—H15	121.8 (11)
C2—C3—H3	121.6 (12)	C14—C15—H15	117.4 (11)
C5—C4—C3	120.25 (15)	C11—C16—C15	118.71 (14)
C5—C4—H4	120.5 (12)	C11—C16—H16	120.6 (12)
C3—C4—H4	119.2 (12)	C15—C16—H16	120.7 (12)
C4—C5—C6	120.45 (15)	C18—N17—C14	128.20 (13)
C4—C5—H5	120.4 (12)	C18—N17—H17	114.3 (13)
C6—C5—H5	119.2 (12)	C14—N17—H17	117.4 (13)
C7—C6—C5	120.46 (15)	O19—C18—N17	122.68 (15)
C7—C6—H6	120.8 (14)	O19—C18—C20	122.87 (14)
C5—C6—H6	118.7 (14)	N17—C18—C20	114.44 (14)
C6—C7—C2	118.29 (15)	C18—C20—H20A	114.2 (14)
C6—C7—H7	121.6 (12)	C18—C20—H20B	112.1 (13)
C2—C7—H7	120.1 (12)	H20A—C20—H20B	99.6 (19)
C11—O10—S1	119.93 (9)	C18—C20—H20C	111.4 (13)
C12—C11—C16	121.90 (14)	H20A—C20—H20C	109.6 (19)
C12—C11—O10	121.39 (13)	H20B—C20—H20C	109.4 (18)
C16—C11—O10	116.49 (13)		
O9—S1—C2—C3	−125.43 (13)	S1—O10—C11—C12	−66.20 (16)
O8—S1—C2—C3	7.12 (14)	S1—O10—C11—C16	119.02 (12)
O10—S1—C2—C3	123.73 (12)	C16—C11—C12—C13	−0.8 (2)
O9—S1—C2—C7	51.76 (14)	O10—C11—C12—C13	−175.30 (13)
O8—S1—C2—C7	−175.69 (12)	C11—C12—C13—C14	−0.4 (2)
O10—S1—C2—C7	−59.08 (13)	C12—C13—C14—C15	1.4 (2)

C7—C2—C3—C4	−0.2 (2)	C12—C13—C14—N17	179.59 (13)
S1—C2—C3—C4	176.95 (12)	C13—C14—C15—C16	−1.2 (2)
C2—C3—C4—C5	1.1 (3)	N17—C14—C15—C16	−179.52 (14)
C3—C4—C5—C6	−0.8 (3)	C12—C11—C16—C15	1.0 (2)
C4—C5—C6—C7	−0.4 (3)	O10—C11—C16—C15	175.73 (13)
C5—C6—C7—C2	1.3 (3)	C14—C15—C16—C11	0.1 (2)
C3—C2—C7—C6	−1.0 (2)	C13—C14—N17—C18	16.3 (2)
S1—C2—C7—C6	−178.09 (13)	C15—C14—N17—C18	−165.51 (15)
O9—S1—O10—C11	−177.78 (10)	C14—N17—C18—O19	1.2 (3)
O8—S1—O10—C11	54.72 (12)	C14—N17—C18—C20	−177.61 (14)
C2—S1—O10—C11	−61.64 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O8	0.99 (2)	2.51 (2)	2.892 (2)	102.6 (14)
C12—H12···O8	0.958 (19)	2.513 (18)	3.0140 (19)	112.7 (13)
C13—H13···O19	0.920 (19)	2.308 (19)	2.861 (2)	118.3 (14)
N17—H17···O8^{i}	0.84 (2)	2.09 (2)	2.9272 (17)	173.3 (18)
C6—H6···O19^{ii}	0.92 (2)	2.55 (2)	3.269 (2)	135.5 (18)
C7—H7···O10^{iii}	0.97 (2)	2.59 (2)	3.5360 (19)	166.6 (16)
C16—H16···O9^{iii}	0.947 (19)	2.539 (19)	3.3783 (19)	147.9 (15)

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

Fig. 1

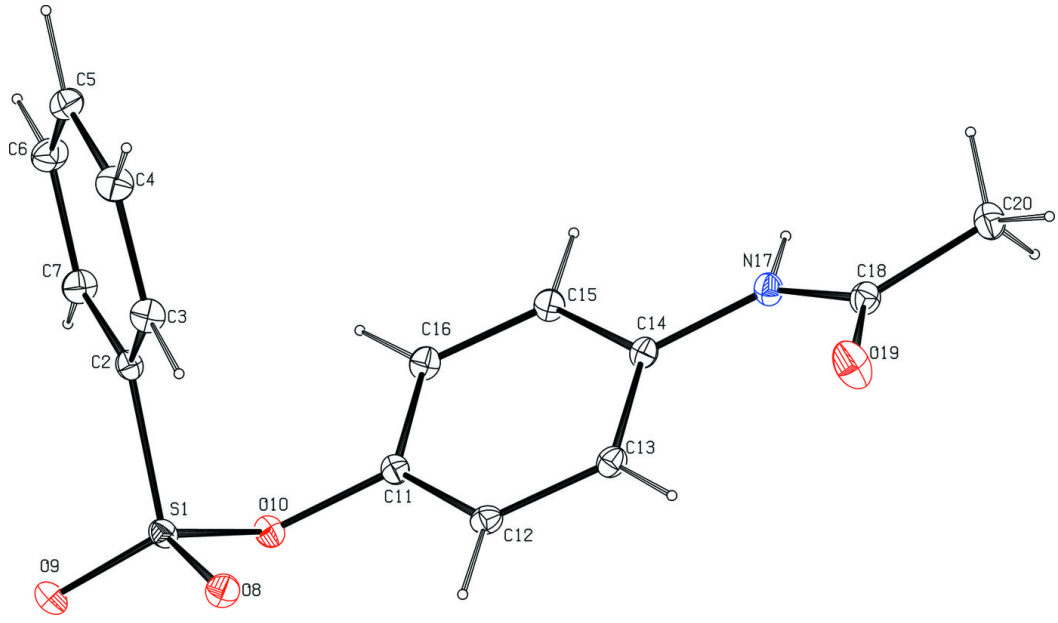
C5
C6
C4
C7
C3
C2
S1
O10
O9
O8
C11
C12
C13
C16
C15
C14
N17
C18
O19
C20

Fig. 2

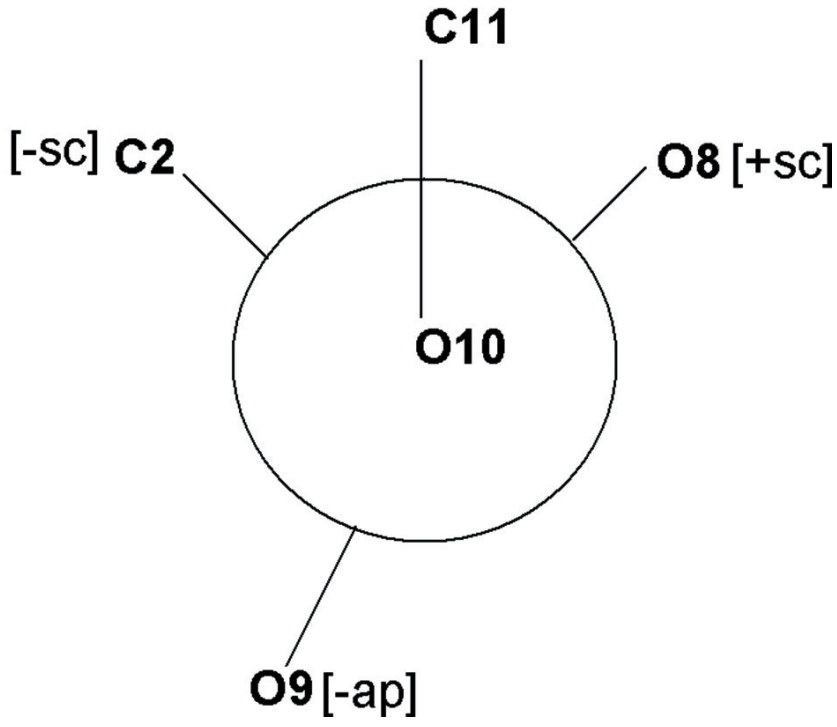

Fig. 3