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2-(3,4-Dichlorobenzoylmethyl)-1,2-benziso-thiazol-3(2*H*)-one 1,1-dioxide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.107
Data-to-parameter ratio = 15.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title molecule, $C_{15}H_9Cl_2NO_4S$, all bond lengths and angles are within normal ranges. In the crystal structure, the molecules are linked into a three-dimensional network *via* weak C—H···O hydrogen bonds.

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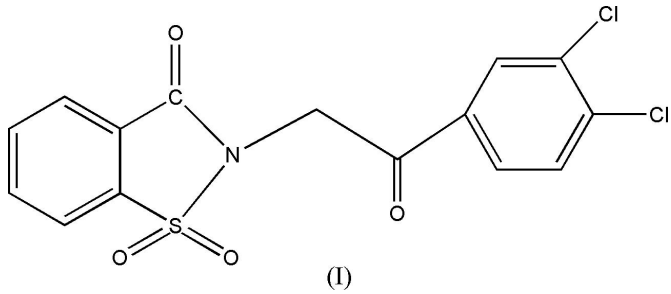
Comment

Saccharin was the earliest synthetic sweetener widely applied in the synthesis of drugs. Many pharmaceuticals originated from saccharin, such as the anti-inflammatory and antirheumatic drug Meloxicam (Xu *et al.*, 1999). We report here the crystal structure of the title compound, (I), containing the saccharin moiety.



(I)

In (I), all bond lengths and angles (Table 1) within the saccharin moiety are similar to those found in the series of *N*-saccharin acids (Feeder & Jones, 1996), *N*-saccharin peracids (Feeder & Jones, 1994) and *N*-(2-nitrophenylthio)saccharin (Glidewell *et al.*, 2000). The C1–C7/N1/S1 ring system and 1,2-dichloro-4-methylbenzene moiety are essentially planar [the maximum deviations are 0.040 (3) and 0.013 (2) Å for N1 and

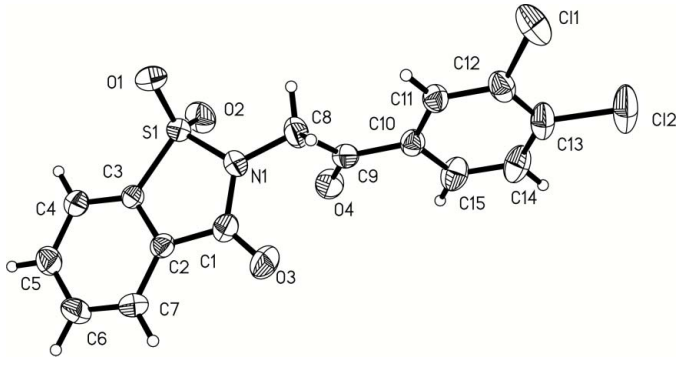


Figure 1
View of (I), with displacement ellipsoids drawn at the 40% probability level.

C15, respectively], making a dihedral angle of 66.71 (4)°. The crystal packing (Fig. 2) is stabilized by weak C—H···O intermolecular hydrogen bonds (Table 2).

Experimental

The title compound was prepared by the reaction of sodium saccharin (4.17 g, 0.02 mol), 2-bromo-1-(3,4-dichlorophenyl)ethanone (5.36 g, 0.02 mol) and potassium hydroxide (1.12 g, 0.02 mol) in acetone (20 ml) at room temperature (292 K) for 5 h. The solid product obtained (6.73 g, yield 91.0%) was recrystallized from ethyl acetate at room temperature to give colourless crystals suitable for X-ray measurements.

Crystal data

$C_{15}H_9Cl_2NO_4S$
M_r = 370.19
Monoclinic, $P2_1/c$
a = 7.7987 (13) Å
b = 11.324 (2) Å
c = 17.750 (3) Å
β = 100.625 (3)°
V = 1540.7 (5) Å^3
Z = 4
D_x = 1.596 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2407 reflections
θ = 3.0–24.8°
μ = 0.57 mm^{-1}
T = 294 (2) K
Block, colourless
0.28 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.840, T_{max} = 0.902
8484 measured reflections
3132 independent reflections
2036 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 26.3°
$h = -9 \rightarrow 8$
$k = -14 \rightarrow 14$
$l = -22 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
S = 1.01
3132 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 0.48P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.4204 (19)	N1—C1	1.391 (3)
S1—O2	1.424 (2)	N1—C8	1.452 (3)
S1—N1	1.663 (2)	O3—C1	1.207 (3)
S1—C3	1.751 (2)		
O1—S1—O2	116.91 (12)	C1—N1—S1	115.09 (17)
C3—S1—N1—C1	2.9 (2)	N1—C8—C9—C10	−164.2 (2)

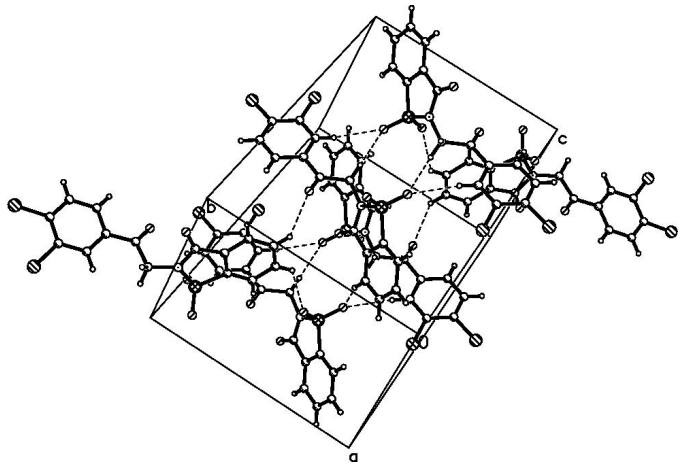


Figure 2
A packing diagram for (I). The intermolecular C—H···O hydrogen bonds are indicated by dashed lines.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O4^{i}	0.93	2.53	3.355 (3)	148
C5—H5···O2^{i}	0.93	2.53	3.167 (3)	126
C6—H6···O4^{ii}	0.93	2.41	3.161 (3)	138
C8—H8B···O1^{iii}	0.97	2.51	3.202 (3)	128
C11—H11···O1^{iii}	0.93	2.53	3.430 (3)	163

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

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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