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[(2-Nitrophenyl)sulfinyl]acetic acid

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In the title compound, $C_8H_7NO_5S$, all bond lengths and angles are normal. Intermolecular O—H···O hydrogen bonds link the molecules into helical chains running along the *b* axis. The crystal packing is further stabilized by weak intermolecular C—H···O interactions.

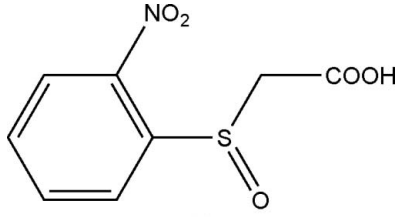
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.086
Data-to-parameter ratio = 15.6

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

Comment

Simple carboxylic acids containing the nitrophenyl group exhibit a variety of supramolecular aggregation patterns (Glidewell *et al.*, 2002). In recent years, the crystal structures of several 4-nitrophenyl carboxylic acids have been reported, namely, (4-nitrophenoxy)acetic acid (Gao *et al.*, 2006*a*); (4-nitrophenylsulfanyl)acetic acid (Glidewell *et al.*, 2002; Gao *et al.*, 2006*b*) and (4-nitrophenylsulfinyl)acetic acid (Glidewell *et al.*, 2003). In contrast, less attention has been paid to 2-nitrophenyl carboxylic acids. The title compound, (I), belongs to the latter family of compounds.



(I)

In (I) (Fig. 1), all bond lengths and angles are normal (Allen *et al.*, 1987). The nitro group is twisted out the benzene ring

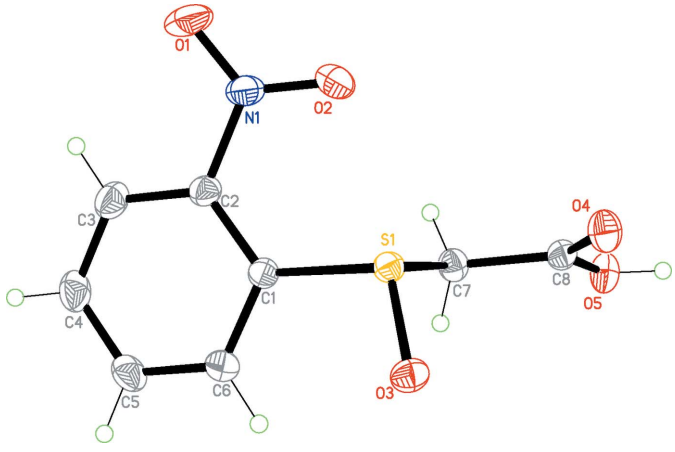


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level.

plane by 13.4 (2)°. Intermolecular O—H···O hydrogen bonds (Table 1) link the molecules into helical chains running along the *b* axis (Fig. 2). The crystal packing is further stabilized by weak intermolecular C—H···O interactions (Table 1).

Experimental

2-Nitrophenylthioacetic acid was prepared by the nucleophilic reaction of chloroacetic acid (9.4 g, 0.1 mol) and 2-nitrothiophenol (15.5 g, 0.1 mol) under basic conditions. 2-Nitrophenylthioacetic acid (21.3 g, 0.1 mol) was then oxidized using 30% aqueous hydrogen peroxide (30 ml) in acetic anhydride solution (50 ml), producing [(2-nitrophenyl)sulfinyl]acetic acid (Nobles *et al.*, 1965). Crystals of (I) suitable for single-crystal X-ray diffraction were grown by slow evaporation of an ethanol solution.

Crystal data

$C_8H_7NO_5S$
M_r = 229.21
Monoclinic, $P2_1/c$
a = 13.809 (3) Å
b = 7.7892 (16) Å
c = 8.7858 (18) Å
β = 97.47 (3)°
V = 937.0 (3) Å^3
Z = 4
D_x = 1.625 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 291 (2) K
Block, yellow
0.18 × 0.16 × 0.14 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.941, T_{max} = 0.953
8862 measured reflections
2133 independent reflections
1770 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.04
2133 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 0.1946P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H7···O3^{i}	0.82	1.83	2.6422 (17)	168
C3—H1···O1^{ii}	0.93	2.49	3.223 (2)	136
C7—H6···O4^{iii}	0.97	2.51	3.262 (2)	135

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{5}{2}, z-\frac{1}{2}$.

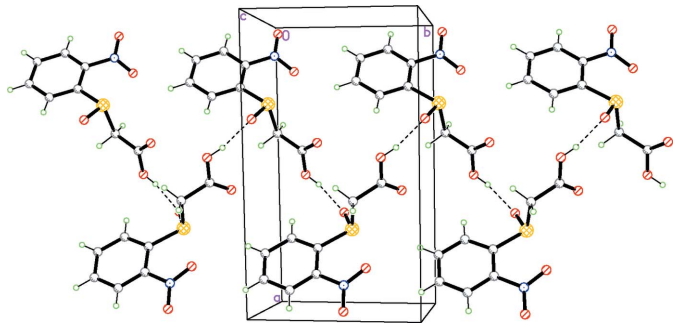


Figure 2
A portion of the crystal packing, showing the hydrogen bonded helical chain. Dashed lines indicate intermolecular O—H···O hydrogen bonds.

All H atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 ($C_{aromatic}$) or 0.97 Å ($C_{methylene}$) and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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