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N-(4-Methoxy-2-nitrophenyl)-*N*-(methylsulfonyl)acetamide

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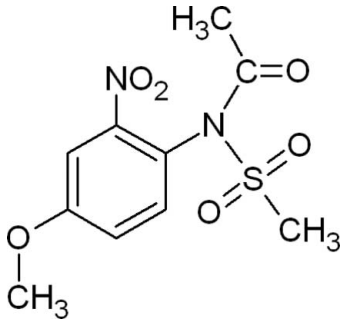
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.128; data-to-parameter ratio = 18.0.

In the title compound, $C_{10}H_{12}N_2O_6S$, the nitro group is twisted slightly out of the plane of the aromatic ring, forming a dihedral angle of 20.79 (1)°. In the crystal, the molecules arrange themselves as a chain along the *a* axis through intermolecular C—H···O interactions.

Related literature

For the synthesis of sulfur-containing heterocyclic compounds, see: Siddiqui *et al.* (2007); Wen *et al.* (2006); Zhang *et al.* (2006). For related structures, see: Zhang *et al.* (2006); Wen *et al.* (2005); Zia-ur-Rehman *et al.* (2008).



Experimental

Crystal data

$C_{10}H_{12}N_2O_6S$
M_r = 288.29
Monoclinic, $P2_1/n$
a = 7.1512 (2) Å
b = 15.4303 (5) Å
c = 11.3217 (3) Å
β = 91.769 (2)°
V = 1248.70 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 296 K
0.21 × 0.11 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.958, T_{max} = 0.974
14122 measured reflections
3102 independent reflections
2101 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.128
S = 1.05
3102 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10B···O3^{i}	0.96	2.50	3.453 (3)	169

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SMART* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2918).

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supporting information

Acta Cryst. (2009). E**65**, o941 [doi:10.1107/S1600536809011799]

N-(4-Methoxy-2-nitrophenyl)-*N*-(methylsulfonyl)acetamide

Muhammad Zia-ur-Rehman, Amir Sepehrianazar, Muhammad Ali, Waseeq Ahmad Siddiqui and Nagihan Çaylak

S1. Comment

N-(Substituted phenyl)acetamides are considered as important intermediates in organic synthesis. A large number of heterocyclic compounds such as 2,5-piperazinedione (Wen *et al.*, 2006), (quinolin-8-yloxy) acetamide (Zhang *et al.*, 2006) and 2,2-(1,3,4-thiadiazolyl-2,5-dithio)diacetamide (Wen *et al.*, 2005) are being efficiently synthesized starting from such acetamides. In the present paper, the structure of *N*-(4-Methoxy-2-nitrophenyl)-*N*-(methylsulfonyl)acetamide has been determined as part of a research program involving the synthesis and biological evaluation of sulfur containing heterocyclic compounds (Siddiqui *et al.*, 2007).

In the molecule (Fig. 1), the bond lengths and bond angles are similar to those in the related molecules (Wen *et al.*, 2006; Zhang *et al.*, 2006) and are within in normal ranges. The nitro group is slightly twisted out of the plane of the aromatic ring. Each molecule is linked to its neighbour by inter molecular C—H···O interactions forming a chain along the *a* axis (Table 1 and Fig. 2).

S2. Experimental

A mixture of *N*-(4-methoxy-2-nitrophenyl)methane sulfonamide (2.462507 g; 10.0 mmoles) and acetic anhydride (10.0 ml) was heated to reflux for half an hour and then poued over crushed ice. Resultant solids were then washed with cold water and dried under reduced pressure. Yellow crystals were obtained by slow evaporation of an ethanolic solution over a period of two days.

S3. Refinement

H atoms bound to C were placed in geometric positions (C—H distance = 0.93 to 0.96 Å) using a riding model with U_{iso}(H) = 1.2 U_{eq}(C) or U_{iso}(H) = 1.5 U_{eq}(C_{methyl}).

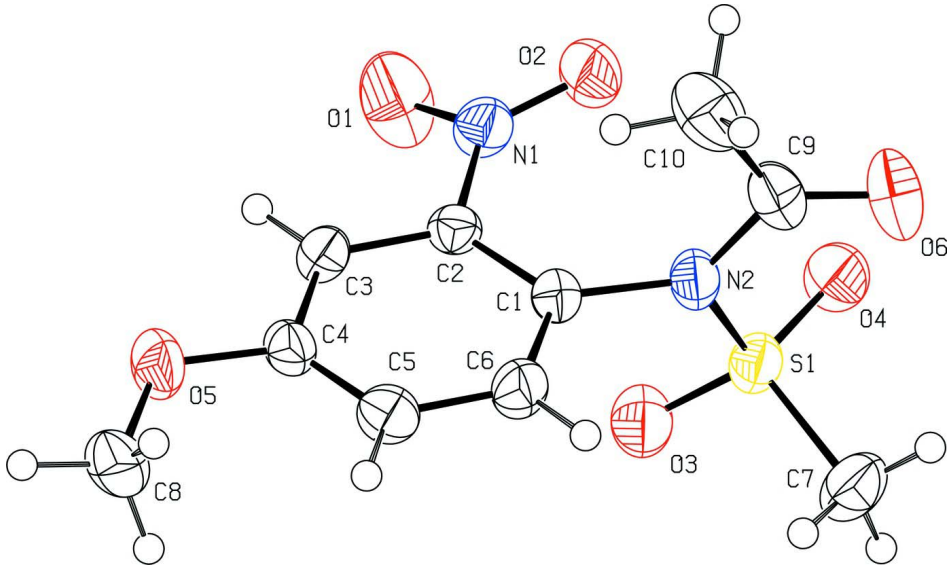

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

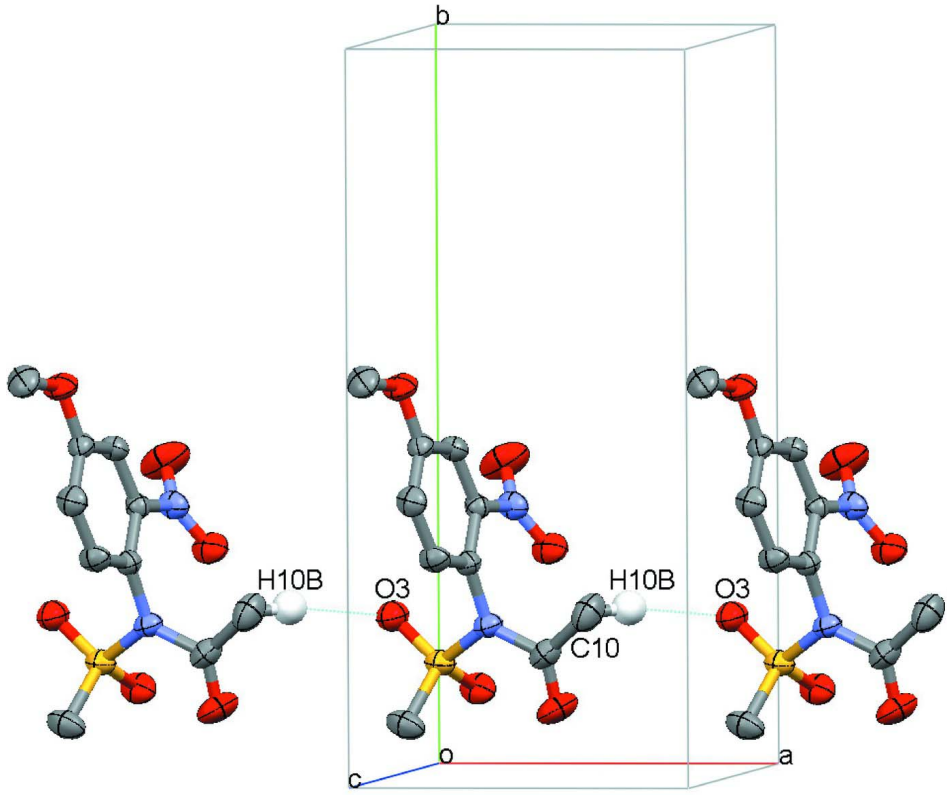

Figure 2

Perspective view of the crystal packing showing inter molecular C—H···O interactions (dashed lines) along *a*. H atoms not involved in hydrogen bonding have been omitted for clarity.

N-(4-Methoxy-2-nitrophenyl)-N-(methylsulfonyl)acetamide

Crystal data

$C_{10}H_{12}N_2O_6S$
$M_r = 288.29$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.1512$ (2) Å
$b = 15.4303$ (5) Å
$c = 11.3217$ (3) Å
$\beta = 91.769$ (2)°
$V = 1248.70$ (6) Å^3
$Z = 4$
$F(000) = 600$
$D_x = 1.533$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3173 reflections
$\theta = 2.6$–$26.8°$
$\mu = 0.29$ mm^{-1}
$T = 296$ K
Needles, yellow
0.21 × 0.11 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.958$, $T_{max} = 0.974$
14122 measured reflections
3102 independent reflections
2101 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$
$h = -8 \rightarrow 9$
$k = -20 \rightarrow 20$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.128$
$S = 1.05$
3102 reflections
172 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
$w = 1/[\sigma^2(F_o^2) + (0.0614P)^2 + 0.2596P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.23442 (8)	0.16533 (4)	0.86323 (4)	0.03679 (18)
O1	0.3919 (3)	0.43383 (14)	0.73036 (15)	0.0788 (7)
O2	0.5342 (3)	0.31646 (11)	0.76949 (14)	0.0535 (5)
O3	0.0897 (2)	0.22746 (11)	0.84351 (15)	0.0493 (4)

O4	0.3188 (2)	0.12704 (11)	0.76361 (13)	0.0489 (4)
O5	0.1853 (2)	0.54616 (10)	1.10272 (14)	0.0473 (4)
O6	0.6008 (3)	0.10620 (12)	0.94545 (17)	0.0634 (5)
N1	0.4337 (3)	0.37563 (12)	0.79726 (15)	0.0390 (4)
N2	0.3979 (2)	0.21872 (11)	0.94551 (14)	0.0353 (4)
C1	0.3511 (3)	0.30400 (13)	0.98604 (17)	0.0311 (4)
C2	0.3598 (3)	0.37840 (13)	0.91680 (16)	0.0296 (4)
C3	0.3029 (3)	0.45779 (13)	0.95680 (17)	0.0334 (5)
H3	0.3089	0.5064	0.9084	0.040*
C4	0.2359 (3)	0.46491 (14)	1.07076 (18)	0.0341 (5)
C5	0.2273 (3)	0.39268 (15)	1.14165 (18)	0.0413 (6)
H5	0.1845	0.3973	1.2181	0.050*
C6	0.2828 (3)	0.31336 (15)	1.09848 (18)	0.0393 (5)
H6	0.2740	0.2647	1.1464	0.047*
C7	0.1573 (4)	0.08423 (16)	0.9575 (2)	0.0538 (7)
H7A	0.2552	0.0425	0.9707	0.081*
H7B	0.0497	0.0561	0.9222	0.081*
H7C	0.1245	0.1095	1.0316	0.081*
C8	0.1068 (4)	0.55680 (17)	1.2166 (2)	0.0525 (7)
H8A	0.0775	0.6168	1.2288	0.079*
H8B	0.1955	0.5379	1.2766	0.079*
H8C	−0.0053	0.5228	1.2209	0.079*
C9	0.5736 (3)	0.18093 (16)	0.97108 (19)	0.0431 (6)
C10	0.7164 (4)	0.23869 (19)	1.0292 (2)	0.0590 (7)
H10A	0.6632	0.2951	1.0409	0.089*
H10B	0.8226	0.2436	0.9798	0.089*
H10C	0.7552	0.2146	1.1042	0.089*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0472 (4)	0.0292 (3)	0.0344 (3)	−0.0019 (2)	0.0066 (2)	−0.0012 (2)
O1	0.1238 (19)	0.0701 (14)	0.0443 (10)	0.0384 (13)	0.0293 (11)	0.0251 (10)
O2	0.0705 (12)	0.0439 (10)	0.0476 (9)	0.0051 (9)	0.0257 (8)	−0.0059 (8)
O3	0.0464 (10)	0.0414 (10)	0.0595 (10)	0.0024 (8)	−0.0069 (8)	−0.0045 (8)
O4	0.0640 (11)	0.0455 (10)	0.0378 (8)	−0.0032 (8)	0.0122 (7)	−0.0081 (7)
O5	0.0607 (11)	0.0338 (9)	0.0480 (9)	0.0058 (8)	0.0120 (8)	−0.0095 (7)
O6	0.0757 (14)	0.0435 (11)	0.0705 (12)	0.0253 (10)	−0.0037 (10)	−0.0059 (9)
N1	0.0486 (12)	0.0364 (11)	0.0324 (9)	−0.0029 (9)	0.0081 (8)	0.0001 (8)
N2	0.0418 (11)	0.0276 (10)	0.0367 (9)	0.0042 (8)	0.0042 (7)	−0.0011 (7)
C1	0.0328 (11)	0.0271 (11)	0.0335 (10)	0.0007 (9)	0.0034 (8)	−0.0016 (8)
C2	0.0292 (11)	0.0312 (11)	0.0285 (9)	−0.0022 (9)	0.0037 (7)	−0.0016 (8)
C3	0.0378 (12)	0.0283 (11)	0.0341 (10)	−0.0029 (9)	0.0017 (8)	0.0015 (8)
C4	0.0320 (12)	0.0313 (12)	0.0391 (11)	0.0008 (9)	0.0029 (8)	−0.0084 (9)
C5	0.0494 (14)	0.0428 (14)	0.0324 (10)	−0.0010 (11)	0.0126 (9)	−0.0037 (10)
C6	0.0499 (14)	0.0333 (12)	0.0353 (10)	0.0013 (10)	0.0103 (9)	0.0060 (9)
C7	0.0731 (18)	0.0406 (14)	0.0486 (13)	−0.0138 (13)	0.0156 (12)	0.0016 (11)
C8	0.0554 (16)	0.0489 (15)	0.0540 (14)	0.0012 (12)	0.0161 (12)	−0.0194 (12)

C9	0.0476 (14)	0.0426 (14)	0.0394 (11)	0.0143 (11)	0.0041 (10)	0.0010 (10)
C10	0.0478 (16)	0.0689 (19)	0.0597 (15)	0.0149 (14)	−0.0081 (12)	−0.0093 (14)

Geometric parameters (Å, º)

S1—O3	1.4234 (17)	C3—H3	0.9300
S1—O4	1.4239 (15)	C4—C5	1.376 (3)
S1—N2	1.6868 (19)	C5—C6	1.381 (3)
S1—C7	1.745 (2)	C5—H5	0.9300
O1—N1	1.207 (2)	C6—H6	0.9300
O2—N1	1.209 (2)	C7—H7A	0.9600
O5—C4	1.357 (2)	C7—H7B	0.9600
O5—C8	1.432 (3)	C7—H7C	0.9600
O6—C9	1.206 (3)	C8—H8A	0.9600
N1—C2	1.469 (2)	C8—H8B	0.9600
N2—C9	1.407 (3)	C8—H8C	0.9600
N2—C1	1.437 (3)	C9—C10	1.493 (3)
C1—C6	1.385 (3)	C10—H10A	0.9600
C1—C2	1.393 (3)	C10—H10B	0.9600
C2—C3	1.372 (3)	C10—H10C	0.9600
C3—C4	1.394 (3)		
O3—S1—O4	118.63 (10)	C4—C5—H5	120.2
O3—S1—N2	104.23 (9)	C6—C5—H5	120.2
O4—S1—N2	109.67 (10)	C5—C6—C1	122.1 (2)
O3—S1—C7	109.68 (13)	C5—C6—H6	119.0
O4—S1—C7	109.68 (11)	C1—C6—H6	119.0
N2—S1—C7	103.83 (11)	S1—C7—H7A	109.5
C4—O5—C8	117.47 (18)	S1—C7—H7B	109.5
O2—N1—O1	122.44 (18)	H7A—C7—H7B	109.5
O2—N1—C2	119.68 (18)	S1—C7—H7C	109.5
O1—N1—C2	117.88 (18)	H7A—C7—H7C	109.5
C9—N2—C1	121.94 (18)	H7B—C7—H7C	109.5
C9—N2—S1	120.69 (15)	O5—C8—H8A	109.5
C1—N2—S1	117.36 (14)	O5—C8—H8B	109.5
C6—C1—C2	117.03 (19)	H8A—C8—H8B	109.5
C6—C1—N2	118.78 (18)	O5—C8—H8C	109.5
C2—C1—N2	124.09 (17)	H8A—C8—H8C	109.5
C3—C2—C1	122.09 (17)	H8B—C8—H8C	109.5
C3—C2—N1	116.68 (18)	O6—C9—N2	119.8 (2)
C1—C2—N1	121.22 (18)	O6—C9—C10	124.3 (2)
C2—C3—C4	119.31 (19)	N2—C9—C10	116.0 (2)
C2—C3—H3	120.3	C9—C10—H10A	109.5
C4—C3—H3	120.3	C9—C10—H10B	109.5
O5—C4—C5	125.15 (19)	H10A—C10—H10B	109.5
O5—C4—C3	114.93 (19)	C9—C10—H10C	109.5
C5—C4—C3	119.91 (19)	H10A—C10—H10C	109.5
C4—C5—C6	119.54 (19)	H10B—C10—H10C	109.5

O3—S1—N2—C9	−172.42 (16)	O1—N1—C2—C1	160.0 (2)
O4—S1—N2—C9	−44.42 (19)	C1—C2—C3—C4	0.7 (3)
C7—S1—N2—C9	72.73 (18)	N1—C2—C3—C4	−178.38 (18)
O3—S1—N2—C1	6.58 (17)	C8—O5—C4—C5	−3.8 (3)
O4—S1—N2—C1	134.58 (15)	C8—O5—C4—C3	177.00 (19)
C7—S1—N2—C1	−108.27 (16)	C2—C3—C4—O5	179.21 (19)
C9—N2—C1—C6	−85.2 (3)	C2—C3—C4—C5	−0.1 (3)
S1—N2—C1—C6	95.8 (2)	O5—C4—C5—C6	179.9 (2)
C9—N2—C1—C2	98.7 (2)	C3—C4—C5—C6	−0.9 (3)
S1—N2—C1—C2	−80.3 (2)	C4—C5—C6—C1	1.4 (4)
C6—C1—C2—C3	−0.3 (3)	C2—C1—C6—C5	−0.7 (3)
N2—C1—C2—C3	175.92 (19)	N2—C1—C6—C5	−177.2 (2)
C6—C1—C2—N1	178.73 (19)	C1—N2—C9—O6	172.7 (2)
N2—C1—C2—N1	−5.0 (3)	S1—N2—C9—O6	−8.3 (3)
O2—N1—C2—C3	158.5 (2)	C1—N2—C9—C10	−7.6 (3)
O1—N1—C2—C3	−21.0 (3)	S1—N2—C9—C10	171.38 (17)
O2—N1—C2—C1	−20.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*B*···O3^{i}	0.96	2.50	3.453 (3)	169

Symmetry code: (i) *x*+1, *y*, *z*.