Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Methoxyphenoxy)acetohydrazide

Gang Liu* and Jie Gao

College of Food Engineering, Jilin Teachers' Institute of Engineering and Technology, 130052 Changchun, Jilin, People's Republic of China
Correspondence e-mail: lg2003915@163.com

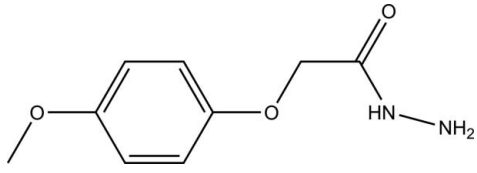
Received 5 April 2012; accepted 28 May 2012

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.089; data-to-parameter ratio = 11.6.

The title compound, $C_9H_{12}N_2O_3$, was synthesized by the reaction of ethyl 2-(4-methoxyphenoxy)acetate with hydrazine hydrate in ethanol. In the acetohydrazide group, the N—N bond is relatively short [1.413 (2) Å], suggesting some degree of electronic delocalization in the molecule. In the crystal, molecules are linked into sheets lying parallel to the *ab* plane by N—H···N and N—H···O hydrogen bonds.

Related literature

For general background to and the biological activity of hydrazides, see: Khattab (2005); Ozdemir *et al.* (2009); Ashiq *et al.* (2009); Zhang & Shi (2009). For related structures, see: Dutkiewicz *et al.* (2009); Fun *et al.* (2009, 2010*a*,*b*, 2011).



Experimental

Crystal data

$C_9H_{12}N_2O_3$
M_r = 196.21
Orthorhombic, $P2_12_12_1$
a = 4.0964 (17) Å
b = 6.382 (3) Å
c = 35.608 (14) Å
V = 930.9 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 K
0.30 × 0.25 × 0.18 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.969, T_{max} = 0.981
4782 measured reflections
1631 independent reflections
1503 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.089
S = 0.88
1631 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3^{i}	0.89 (2)	2.51 (2)	3.155 (2)	130.4 (16)
N1—H1···N2^{ii}	0.88 (2)	2.18 (2)	2.984 (2)	152.2 (18)
N2—H2B···O3^{iii}	0.91 (2)	2.13 (2)	3.027 (2)	167.5 (18)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2352).

References

Ashiq, U., Jamal, R. A., Tahir, M. N., Yousuf, S. & Khan, I. U. (2009). *Acta Cryst.* E**65**, o1551.
Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dutkiewicz, G., Chidan Kumar, C. S., Narayana, B., Yathirajan, H. S. & Kubicki, M. (2009). *Acta Cryst.* E**65**, o3189.
Fun, H.-K., Quah, C. K., Isloor, A. M., Sunil, D. & Shetty, P. (2010*a*). *Acta Cryst.* E**66**, o31–o32.
Fun, H.-K., Quah, C. K., Isloor, A. M., Sunil, D. & Shetty, P. (2010*b*). *Acta Cryst.* E**66**, o53–o54.
Fun, H.-K., Quah, C. K., Malladi, S. M. V. A. & Isloor, A. M. (2011). *Acta Cryst.* E**67**, o165.
Fun, H.-K., Quah, C. K., Sujith, K. V. & Kalluraya, B. (2009). *Acta Cryst.* E**65**, o1184–o1185.
Khattab, S. N. (2005). *Molecules*, **10**, 1218-1228.
Ozdemir, A., Turan-Zitouni, G., Kaplancikli, Z. A. & Tunali, Y. (2009). *J. Enzyme Inhib. Med. Chem.* **24**, 825-831.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, Y.-X. & Shi, Z.-Q. (2009). *Acta Cryst.* E**65**, o1538.

supplementary materials

Acta Cryst. (2012). E**68**, o1969 [doi:10.1107/S160053681202435X]

2-(4-Methoxyphenoxy)acetohydrazide

Gang Liu and Jie Gao

Comment

Hydrazides have been of great interest for many years because they have different biological activities and been used for the synthesis of various heterocyclic compounds (Khattab, 2005; Dutkiewicz *et al.*, 2009; Ozdemir *et al.*, 2009; Ashiq *et al.*, 2009; Zhang & Shi, 2009; Fun *et al.*, 2009, 2010*a*,*b*, 2011). In order to search for new hydrazide compounds with higher bioactivity, the title compound, was synthesized. Its molecular and crystal structures were determined. The molecular structure is shown in Fig. 1. In the crystal structure (Fig. 2), molecules are linked into infinite two-dimensional networks by the classical intermolecular N–H···N and N–H···O hydrogen bonds. For parameters of these interactions, see Table 1.

Experimental

The title compound was synthesized by the reaction of 2-(4-methoxyphenoxy)acetate (1 mmol) with hydrazine hydrate 85% (1.1 mmol) in ethanol (15 ml) under reflux conditions (338 K) for 5 h. The solvent was removed and the solid product recrystallized from ethanol. After six days colourless crystals suitable for X-ray diffraction study were obtained.

Refinement

The H atoms attached to N atoms were located in a difference Fourier map and allowed to refined freely. The remaining H atoms were placed in calculated positions (C–H = 0.93-0.97Å) and refined as riding atoms and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C), respectively. The 609 Friedel pairs were measured.

Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

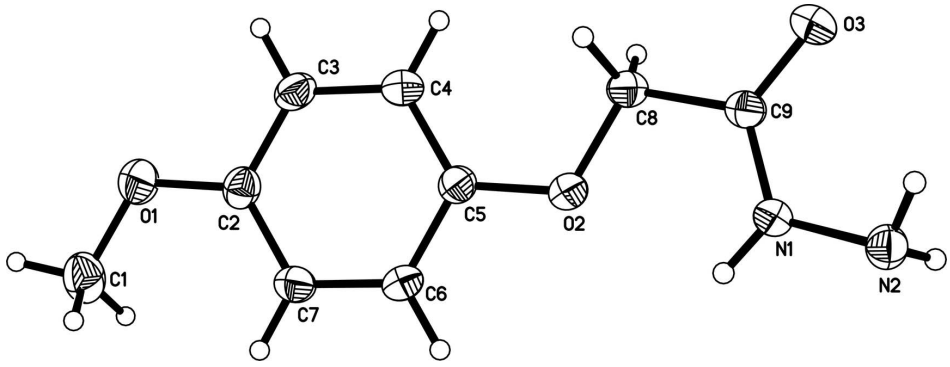


Figure 1

The molecular structure of title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

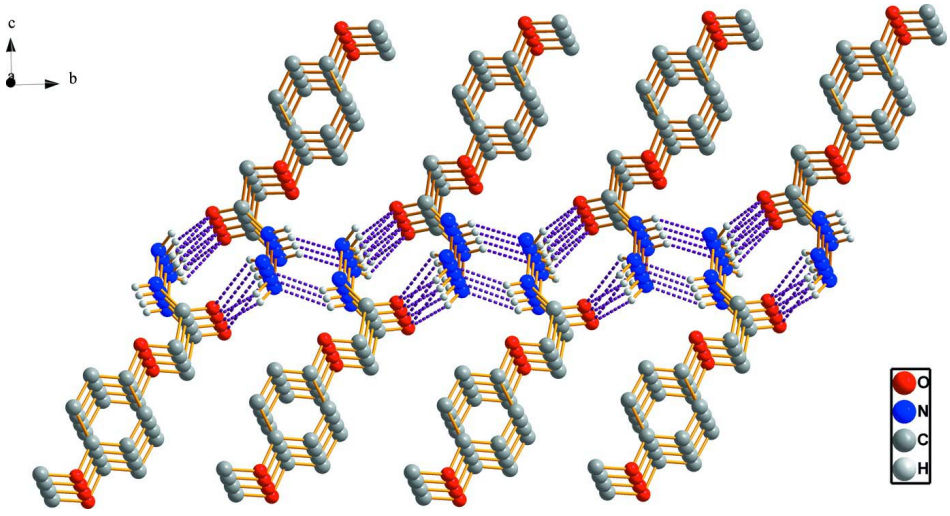


Figure 2

The structure of the infinite two-dimensional networks formed *via* hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonds have been omitted for clarity.

2-(4-Methoxyphenoxy)acetohydrazide

Crystal data

$C_9H_{12}N_2O_3$
$M_r = 196.21$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 4.0964\ (17)$ Å
$b = 6.382\ (3)$ Å
$c = 35.608\ (14)$ Å
$V = 930.9\ (7)$ Å^3
$Z = 4$

$F(000) = 416$
$D_x = 1.400$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2044 reflections
$\theta = 2.3$–$25.2°$
$\mu = 0.11$ mm^{-1}
$T = 298$ K
Block, colourless
0.30 × 0.25 × 0.18 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.969, T_{max} = 0.981

4782 measured reflections
1631 independent reflections
1503 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.1°, θ_{min} = 1.1°
h = −4→4
k = −7→7
l = −42→37

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.089
S = 0.88
1631 reflections
140 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.070P)^2 + 0.087P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.7470 (4)	0.5028 (2)	0.28285 (3)	0.0575 (4)
O3	−0.2287 (3)	1.24787 (16)	0.45169 (3)	0.0492 (3)
O2	0.2900 (3)	0.86238 (18)	0.41321 (3)	0.0475 (3)
N1	−0.0331 (4)	0.9456 (2)	0.47495 (3)	0.0375 (3)
N2	−0.2052 (4)	0.9626 (2)	0.50921 (4)	0.0409 (4)
C1	0.9213 (6)	0.3121 (3)	0.28446 (6)	0.0622 (6)
H1A	1.1128	0.3301	0.2997	0.093*
H1B	0.9844	0.2712	0.2596	0.093*
H1C	0.7852	0.2055	0.2953	0.093*
C3	0.4850 (5)	0.7769 (3)	0.31370 (4)	0.0445 (4)
H3	0.4583	0.8404	0.2904	0.053*
C7	0.6851 (5)	0.4962 (3)	0.35087 (5)	0.0456 (4)
H7	0.7943	0.3690	0.3529	0.055*
C2	0.6424 (4)	0.5884 (3)	0.31602 (4)	0.0418 (4)
C6	0.5651 (4)	0.5936 (3)	0.38255 (4)	0.0434 (4)
H6	0.5952	0.5317	0.4059	0.052*

C9	−0.0652 (4)	1.0868 (2)	0.44833 (4)	0.0354 (4)
C5	0.4022 (4)	0.7803 (2)	0.38004 (4)	0.0373 (4)
C8	0.0994 (4)	1.0462 (2)	0.41147 (4)	0.0394 (4)
H8A	−0.0641	1.0315	0.3919	0.047*
H8B	0.2376	1.1643	0.4051	0.047*
C4	0.3656 (4)	0.8742 (3)	0.34537 (4)	0.0432 (4)
H4	0.2604	1.0029	0.3434	0.052*
H1	0.085 (6)	0.833 (3)	0.4716 (6)	0.060 (6)*
H2B	−0.073 (6)	1.041 (3)	0.5243 (5)	0.063 (6)*
H2A	−0.384 (6)	1.036 (3)	0.5048 (5)	0.059 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0747 (9)	0.0574 (7)	0.0404 (7)	0.0081 (7)	0.0097 (7)	−0.0019 (5)
O3	0.0573 (8)	0.0379 (6)	0.0523 (7)	0.0129 (6)	0.0001 (6)	0.0029 (5)
O2	0.0616 (8)	0.0476 (7)	0.0333 (6)	0.0157 (7)	0.0007 (6)	0.0033 (5)
N1	0.0445 (8)	0.0316 (7)	0.0364 (7)	0.0048 (6)	−0.0010 (6)	0.0002 (5)
N2	0.0459 (9)	0.0384 (8)	0.0385 (7)	−0.0022 (7)	0.0027 (7)	−0.0012 (6)
C1	0.0675 (14)	0.0622 (12)	0.0570 (12)	0.0038 (11)	0.0112 (11)	−0.0109 (9)
C3	0.0533 (11)	0.0464 (9)	0.0339 (8)	−0.0017 (9)	−0.0018 (8)	0.0082 (7)
C7	0.0549 (11)	0.0383 (8)	0.0437 (9)	0.0064 (8)	0.0028 (8)	0.0054 (7)
C2	0.0445 (10)	0.0438 (9)	0.0369 (9)	−0.0057 (8)	0.0030 (7)	−0.0010 (7)
C6	0.0536 (10)	0.0429 (9)	0.0337 (8)	0.0032 (9)	−0.0010 (7)	0.0079 (7)
C9	0.0363 (8)	0.0298 (7)	0.0401 (8)	−0.0019 (7)	−0.0087 (7)	−0.0011 (7)
C5	0.0396 (9)	0.0370 (8)	0.0354 (8)	−0.0015 (7)	−0.0014 (7)	0.0010 (6)
C8	0.0430 (9)	0.0361 (8)	0.0390 (8)	0.0026 (7)	−0.0032 (7)	0.0037 (7)
C4	0.0495 (10)	0.0386 (8)	0.0416 (9)	0.0032 (8)	−0.0021 (7)	0.0069 (7)

Geometric parameters (Å, º)

O1—C2	1.3701 (19)	C3—C2	1.367 (2)
O1—C1	1.412 (2)	C3—C4	1.377 (2)
O3—C9	1.2329 (18)	C3—H3	0.9300
O2—C5	1.3714 (19)	C7—C6	1.379 (2)
O2—C8	1.410 (2)	C7—C2	1.384 (2)
N1—C9	1.314 (2)	C7—H7	0.9300
N1—N2	1.413 (2)	C6—C5	1.368 (2)
N1—H1	0.88 (2)	C6—H6	0.9300
N2—H2B	0.91 (2)	C9—C8	1.498 (2)
N2—H2A	0.89 (2)	C5—C4	1.380 (2)
C1—H1A	0.9600	C8—H8A	0.9700
C1—H1B	0.9600	C8—H8B	0.9700
C1—H1C	0.9600	C4—H4	0.9300
C2—O1—C1	117.82 (13)	C3—C2—C7	119.18 (15)
C5—O2—C8	117.75 (11)	O1—C2—C7	124.33 (16)
C9—N1—N2	121.34 (14)	C5—C6—C7	120.86 (14)
C9—N1—H1	121.3 (13)	C5—C6—H6	119.6
N2—N1—H1	117.2 (14)	C7—C6—H6	119.6

N1—N2—H2B	104.8 (14)	O3—C9—N1	123.78 (15)
N1—N2—H2A	107.4 (13)	O3—C9—C8	118.28 (13)
H2B—N2—H2A	107.8 (19)	N1—C9—C8	117.92 (13)
O1—C1—H1A	109.5	C6—C5—O2	116.09 (13)
O1—C1—H1B	109.5	C6—C5—C4	119.31 (14)
H1A—C1—H1B	109.5	O2—C5—C4	124.59 (14)
O1—C1—H1C	109.5	O2—C8—C9	110.77 (12)
H1A—C1—H1C	109.5	O2—C8—H8A	109.5
H1B—C1—H1C	109.5	C9—C8—H8A	109.5
C2—C3—C4	120.96 (14)	O2—C8—H8B	109.5
C2—C3—H3	119.5	C9—C8—H8B	109.5
C4—C3—H3	119.5	H8A—C8—H8B	108.1
C6—C7—C2	119.79 (16)	C3—C4—C5	119.86 (15)
C6—C7—H7	120.1	C3—C4—H4	120.1
C2—C7—H7	120.1	C5—C4—H4	120.1
C3—C2—O1	116.49 (14)		

C4—C3—C2—O1	178.88 (17)	C7—C6—C5—C4	−1.7 (3)
C4—C3—C2—C7	−0.8 (3)	C8—O2—C5—C6	−175.24 (14)
C1—O1—C2—C3	177.62 (16)	C8—O2—C5—C4	5.8 (2)
C1—O1—C2—C7	−2.7 (3)	C5—O2—C8—C9	167.00 (14)
C6—C7—C2—C3	0.9 (3)	O3—C9—C8—O2	176.64 (14)
C6—C7—C2—O1	−178.80 (17)	N1—C9—C8—O2	−4.9 (2)
C2—C7—C6—C5	0.4 (3)	C2—C3—C4—C5	−0.5 (3)
N2—N1—C9—O3	4.3 (2)	C6—C5—C4—C3	1.7 (3)
N2—N1—C9—C8	−174.01 (14)	O2—C5—C4—C3	−179.35 (17)
C7—C6—C5—O2	179.31 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O3^{i}	0.89 (2)	2.51 (2)	3.155 (2)	130.4 (16)
N1—H1···N2^{ii}	0.88 (2)	2.18 (2)	2.984 (2)	152.2 (18)
N2—H2*B*···O3^{iii}	0.91 (2)	2.13 (2)	3.027 (2)	167.5 (18)

Symmetry codes: (i) *x*−1/2, −*y*+5/2, −*z*+1; (ii) *x*+1/2, −*y*+3/2, −*z*+1; (iii) *x*+1/2, −*y*+5/2, −*z*+1.