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Crystal structure of 2-(5-methoxy-1-benzofuran-3-yl)acetic acid

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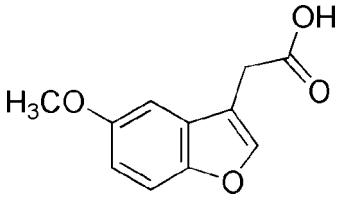
The benzofuran residue in the title compound, $C_{11}H_{10}O_4$, is essentially planar (the r.m.s. deviation for the nine non-H atoms = 0.011 Å). While the methoxy group is coplanar with the fused ring system [C—C—O—C torsion angle = 3.1 (3)°], the acetic acid residue occupies a position almost prime [C—C—C—C = 77.0 (2)°]. In the crystal, centrosymmetrically related molecules are linked by O—H···O hydrogen bonds to form eight-membered $\{\cdots HOCO\}_2$ synthons. The dimeric aggregates assemble into supramolecular layers in the *ab* plane *via* benzene-C—H···O(ring) interactions.

Keywords: crystal structure; benzofuran; hydrogen bonding.

CCDC reference: 1401314

1. Related literature

For a related structures and background to benzofurans and their applications, see: Dawood (2013); Khanam & Shamsuzzaman (2015); Radadiya & Shah (2015); Naik *et al.* (2015); Nevagi *et al.* (2015). For the synthesis, see: Basanagouda *et al.* (2015).



2. Experimental

2.1. Crystal data

$C_{11}H_{10}O_4$
M_r = 206.19
Monoclinic, $P2_1/c$
a = 5.8096 (3) Å
b = 13.2034 (5) Å
c = 12.5738 (6) Å
β = 97.641 (3)°
V = 955.93 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.35 × 0.30 × 0.25 mm

2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.961, T_{max} = 0.979
12813 measured reflections
2094 independent reflections
1621 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.110
S = 1.12
2094 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.82	2.6357 (17)	174
C2—H2···O4^{ii}	0.93	2.55	3.4629 (19)	169

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL2014*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5414).

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supporting information

Acta Cryst. (2015). E**71**, o1053–o1054 [https://doi.org/10.1107/S2056989015023609]

Crystal structure of 2-(5-methoxy-1-benzofuran-3-yl)acetic acid

Ramakrishna Gowda, K. V. Arjuna Gowda, M. Keshava Reddy and Mahantesha Basanagouda

S1. Comment

Benzofuran scaffolds have drawn considerable attention due to their physiological and chemotherapeutic properties as well as their widespread occurrence in nature. They display potent biological properties including antihyperglycemic, analgesic, antiparasitic, antimicrobial, antitumor and kinase inhibitor activities (Dawood, 2013; Khanam & Shamsuzzaman, 2015; Radadiya & Shah, 2015; Naik *et al.* 2015; Nevagi *et al.* 2015). In addition, substituted benzofurans find application such as fluorescent sensors, oxidant, antioxidants and brightening agents. The derivatives of 2,3-dihydro-benzofuranyl-3-acetic acid have been reported to be potent, selective and orally bioavailable G protein-coupled receptor 40 (GPR40) and free fatty acid receptor 1 agonists (FFA1) (Basanagouda *et al.*, 2015). A perspective view of the molecule is shown in Fig. 1 and geomtric data for the intermolecular interactions are listed in Table 1.

S2. Experimental

6-Methoxy-4-bromomethylcoumarin (10 mM) was refluxed in 1 M NaOH (100 mL) for 2 h (monitored by TLC). The reaction mixture was cooled, neutralized with 1 M HCl and the obtained product was filtered off and dried. Colourless blocks were obtained by recrystallization from ethanol and ethyl acetate mixture by slow evaporation.

S3. Refinement

The carbon-bound H-atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2–1.5U_{equiv}(C). The oxygen-bound H-atom was also placed in a calculated position (O—H = 0.82 Å) with U_{iso}(H) set to 1.5U_{equiv}(O).

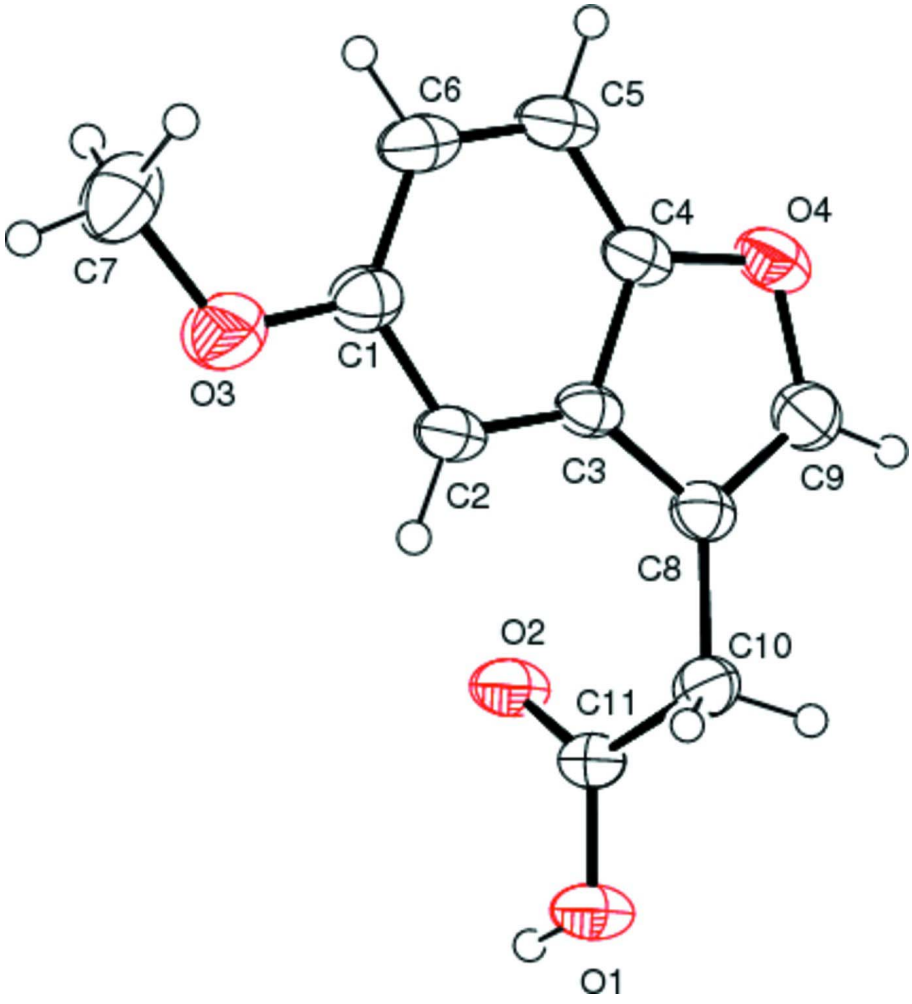

Figure 1

Molecular structure of the title compound showing atom labelling and 40% probability displacement ellipsoids.

2-(5-Methoxy-1-benzofuran-3-yl)acetic acid

Crystal data

$C_{11}H_{10}O_4$
$M_r = 206.19$
Monoclinic, $P2_1/c$
$a = 5.8096$ (3) Å
$b = 13.2034$ (5) Å
$c = 12.5738$ (6) Å
$\beta = 97.641$ (3)°
$V = 955.93$ (8) Å^3
$Z = 4$
$F(000) = 432$
$D_x = 1.433$ Mg m^{-3}
Melting point: 413 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5229 reflections
$\theta = 2.2$–28.6°
$\mu = 0.11$ mm^{-1}
$T = 296$ K
Block, colourless
0.35 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.961$, $T_{max} = 0.979$

12813 measured reflections
2094 independent reflections
1621 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.3°$
$h = -7 \rightarrow 7$
$k = -16 \rightarrow 16$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.110$
$S = 1.12$
2094 reflections
137 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.4069P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.017 (3)

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4010 (3)	0.61606 (13)	0.80077 (14)	0.0432 (4)
C2	0.2178 (3)	0.67578 (12)	0.82316 (13)	0.0389 (4)
H2	0.1770	0.6787	0.8922	0.047*
C3	0.0964 (3)	0.73116 (11)	0.74025 (12)	0.0349 (4)
C4	0.1631 (3)	0.72515 (13)	0.63818 (13)	0.0398 (4)
C5	0.3460 (3)	0.66724 (14)	0.61521 (14)	0.0477 (5)
H5	0.3882	0.6653	0.5464	0.057*
C6	0.4647 (3)	0.61208 (14)	0.69782 (15)	0.0479 (5)
H6	0.5890	0.5716	0.6848	0.057*
C7	0.7098 (4)	0.50545 (17)	0.8728 (2)	0.0646 (6)
H7A	0.7685	0.4733	0.9394	0.097*
H7B	0.6680	0.4547	0.8190	0.097*
H7C	0.8272	0.5488	0.8506	0.097*
C8	−0.0997 (3)	0.79821 (12)	0.73082 (13)	0.0378 (4)
C9	−0.1369 (3)	0.82596 (14)	0.62760 (14)	0.0476 (4)
H9	−0.2559	0.8692	0.5995	0.057*
C10	−0.2391 (3)	0.82719 (13)	0.81742 (14)	0.0421 (4)
H10A	−0.2708	0.7666	0.8566	0.051*
H10B	−0.3869	0.8541	0.7845	0.051*
C11	−0.1270 (3)	0.90353 (12)	0.89552 (13)	0.0367 (4)
O1	−0.2484 (2)	0.92135 (9)	0.97334 (10)	0.0491 (4)
H1	−0.1813	0.9636	1.0141	0.074*
O2	0.0578 (2)	0.94412 (10)	0.88700 (10)	0.0514 (4)
O3	0.5123 (3)	0.56354 (12)	0.88677 (12)	0.0665 (4)

O4	0.0193 (2)	0.78381 (10)	0.56745 (9)	0.0503 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0431 (9)	0.0419 (9)	0.0459 (10)	−0.0026 (7)	0.0101 (8)	−0.0053 (7)
C2	0.0428 (9)	0.0434 (9)	0.0328 (8)	−0.0051 (7)	0.0133 (7)	−0.0068 (7)
C3	0.0381 (8)	0.0356 (8)	0.0329 (8)	−0.0099 (7)	0.0113 (6)	−0.0089 (6)
C4	0.0456 (9)	0.0428 (9)	0.0325 (8)	−0.0113 (7)	0.0114 (7)	−0.0072 (7)
C5	0.0537 (11)	0.0543 (10)	0.0394 (9)	−0.0101 (9)	0.0218 (8)	−0.0140 (8)
C6	0.0464 (10)	0.0477 (10)	0.0535 (11)	−0.0024 (8)	0.0215 (8)	−0.0139 (8)
C7	0.0515 (12)	0.0578 (12)	0.0832 (15)	0.0092 (10)	0.0038 (11)	−0.0052 (11)
C8	0.0383 (9)	0.0399 (8)	0.0360 (8)	−0.0087 (7)	0.0075 (7)	−0.0069 (7)
C9	0.0477 (10)	0.0514 (10)	0.0439 (10)	−0.0038 (8)	0.0065 (8)	−0.0018 (8)
C10	0.0363 (9)	0.0472 (9)	0.0438 (9)	−0.0026 (7)	0.0093 (7)	−0.0071 (7)
C11	0.0408 (9)	0.0362 (8)	0.0349 (8)	0.0018 (7)	0.0118 (7)	−0.0002 (6)
O1	0.0558 (8)	0.0503 (7)	0.0461 (7)	−0.0115 (6)	0.0248 (6)	−0.0119 (6)
O2	0.0507 (8)	0.0599 (8)	0.0476 (7)	−0.0158 (6)	0.0207 (6)	−0.0172 (6)
O3	0.0661 (9)	0.0760 (10)	0.0590 (9)	0.0257 (8)	0.0144 (7)	0.0081 (7)
O4	0.0604 (8)	0.0598 (8)	0.0322 (6)	−0.0064 (6)	0.0114 (6)	−0.0009 (5)

Geometric parameters (Å, º)

C1—O3	1.372 (2)	C7—H7A	0.9600
C1—C2	1.383 (2)	C7—H7B	0.9600
C1—C6	1.394 (2)	C7—H7C	0.9600
C2—C3	1.387 (2)	C8—C9	1.338 (2)
C2—H2	0.9300	C8—C10	1.491 (2)
C3—C4	1.391 (2)	C9—O4	1.374 (2)
C3—C8	1.435 (2)	C9—H9	0.9300
C4—C5	1.371 (2)	C10—C11	1.495 (2)
C4—O4	1.375 (2)	C10—H10A	0.9700
C5—C6	1.377 (3)	C10—H10B	0.9700
C5—H5	0.9300	C11—O2	1.217 (2)
C6—H6	0.9300	C11—O1	1.3014 (18)
C7—O3	1.410 (2)	O1—H1	0.8200
O3—C1—C2	115.00 (15)	O3—C7—H7C	109.5
O3—C1—C6	123.86 (17)	H7A—C7—H7C	109.5
C2—C1—C6	121.13 (17)	H7B—C7—H7C	109.5
C1—C2—C3	118.41 (15)	C9—C8—C3	105.85 (15)
C1—C2—H2	120.8	C9—C8—C10	127.22 (17)
C3—C2—H2	120.8	C3—C8—C10	126.89 (15)
C2—C3—C4	119.14 (15)	C8—C9—O4	112.94 (17)
C2—C3—C8	134.93 (14)	C8—C9—H9	123.5
C4—C3—C8	105.92 (15)	O4—C9—H9	123.5
C5—C4—O4	126.81 (15)	C8—C10—C11	114.92 (14)
C5—C4—C3	123.03 (17)	C8—C10—H10A	108.5

O4—C4—C3	110.16 (15)	C11—C10—H10A	108.5
C4—C5—C6	117.44 (15)	C8—C10—H10B	108.5
C4—C5—H5	121.3	C11—C10—H10B	108.5
C6—C5—H5	121.3	H10A—C10—H10B	107.5
C5—C6—C1	120.83 (17)	O2—C11—O1	123.98 (15)
C5—C6—H6	119.6	O2—C11—C10	123.47 (14)
C1—C6—H6	119.6	O1—C11—C10	112.55 (14)
O3—C7—H7A	109.5	C11—O1—H1	109.5
O3—C7—H7B	109.5	C1—O3—C7	118.88 (16)
H7A—C7—H7B	109.5	C9—O4—C4	105.13 (13)
O3—C1—C2—C3	−179.94 (15)	C4—C3—C8—C9	0.53 (18)
C6—C1—C2—C3	0.7 (3)	C2—C3—C8—C10	−1.0 (3)
C1—C2—C3—C4	−0.3 (2)	C4—C3—C8—C10	178.12 (15)
C1—C2—C3—C8	178.71 (17)	C3—C8—C9—O4	−0.6 (2)
C2—C3—C4—C5	−0.5 (2)	C10—C8—C9—O4	−178.15 (15)
C8—C3—C4—C5	−179.78 (15)	C9—C8—C10—C11	−105.9 (2)
C2—C3—C4—O4	178.93 (14)	C3—C8—C10—C11	77.0 (2)
C8—C3—C4—O4	−0.33 (17)	C8—C10—C11—O2	4.0 (3)
O4—C4—C5—C6	−178.48 (16)	C8—C10—C11—O1	−175.80 (15)
C3—C4—C5—C6	0.9 (3)	C2—C1—O3—C7	−176.25 (17)
C4—C5—C6—C1	−0.4 (3)	C6—C1—O3—C7	3.1 (3)
O3—C1—C6—C5	−179.65 (17)	C8—C9—O4—C4	0.38 (19)
C2—C1—C6—C5	−0.3 (3)	C5—C4—O4—C9	179.42 (17)
C2—C3—C8—C9	−178.54 (18)	C3—C4—O4—C9	−0.01 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.82	2.6357 (17)	174
C2—H2···O4^{ii}	0.93	2.55	3.4629 (19)	169

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