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3-Methyl-4*H*-chromen-4-one

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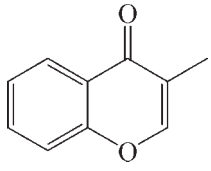
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.116; data-to-parameter ratio = 12.6.

In the title chromenone derivative, $C_{10}H_8O_2$, the two fused six-membered rings are coplanar, with a mean deviation of 0.0261 (1) Å from the plane through the non-H atoms of the rings. The carbonyl and methyl substituents of the pyran ring also lie close to that plane, with the O and C atoms deviating by 0.0557 (1) and 0.1405 (1) Å, respectively. In the crystal, weak C—H···O contacts form chains along the *a* axis.

Related literature

For the pharmaceutical applications of chromanone compounds, see: Shi *et al.* (2004). For related structures, see: Takikawa & Suzuki (2007); Patonay *et al.* (2002); Alaniz & Rovis, (2005).



Experimental

Crystal data

$C_{10}H_8O_2$
M_r = 160.16
Triclinic, $P\overline{1}$
a = 6.5284 (13) Å
b = 7.2210 (14) Å
c = 8.9834 (18) Å
α = 75.137 (2)°
β = 78.169 (2)°
γ = 80.895 (2)°
V = 398.12 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.989, T_{max} = 0.993
2771 measured reflections
1394 independent reflections
1143 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.00
1394 reflections
111 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.93	2.70	3.4374 (19)	137
C7—H7···O2^{ii}	0.93	2.69	3.3820 (19)	132

Symmetry codes: (i) $x+1, y, z$; (ii) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5009).

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supporting information

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3-Methyl-4*H*-chromen-4-one

Lujiang Hao, Jiangkui Chen and Xiaofei Zhang

S1. Comment

The synthesis of chromanone derivatives has attracted continuous research interest due to their applications as vasodilator, anti-hypertensive, bronchodilator, heptaprotective, anti-tumor, anti-mutagenic, geroprotective and anti-diabetic agents (Shi *et al.*, 2004). Here, we describe the cystallization and structural characterization of the title compound.

As shown in Fig 1. the two fused six membered rings are coplanar with a mean deviation of 0.0261 (1) Å from the plane through the non-hydrogen atoms of the rings. The carbonyl and methyl substituents of the pyran ring also lie close to that plane with deviations of 0.0557 (1) and 0.1405 (1) Å, respectively. The C=O and C—O bond distances, 1.367 (2) and 1.231 (2)—1.355 (2) Å, respectively, are in the normal range compared to reported chromanone derivatives (Takikawa & Suzuki, 2007; Patonay *et al.*, 2002; Alaniz & Rovis, 2005). In the crystal structure, chains along the *a* axis are formed *via* the weak C—H···O contacts.

S2. Experimental

3-methyl-4*H*-chromen-4-one powder (10 mmoL, 1.60 g) was purchased from Jinan Henghua Science & Technology Co. Ltd., dissolved in 20 ml ethanol and evaporated in an open flask at room temperature. One week later, colorless block like crystals of the title compound suitable for the X-ray analysis were obained. Anal. $C_{10}H_8O_2$: C, 74.93; H, 5.00%. Found: C, 74.86; H, 4.89%.

S3. Refinement

Hydrogen atoms were placed in geometrically calculated positions (C—H 0.95 Å for aromatic and formyl, 0.99 Å for methylene and 0.98 Å for methyl) and included in the refinement in a riding motion approximation with U_{iso}(H) = 1.2Ueq(C) [for methyl groups U_{iso}(H) = 1.5Ueq(C)].

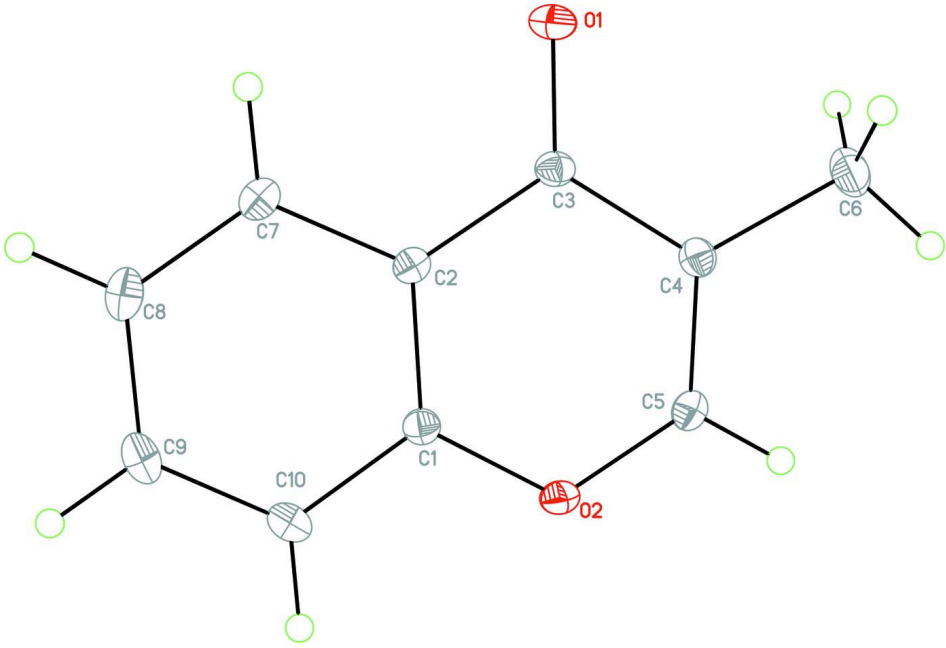

Figure 1

Structure of the title compound showing the atom numbering with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radius.

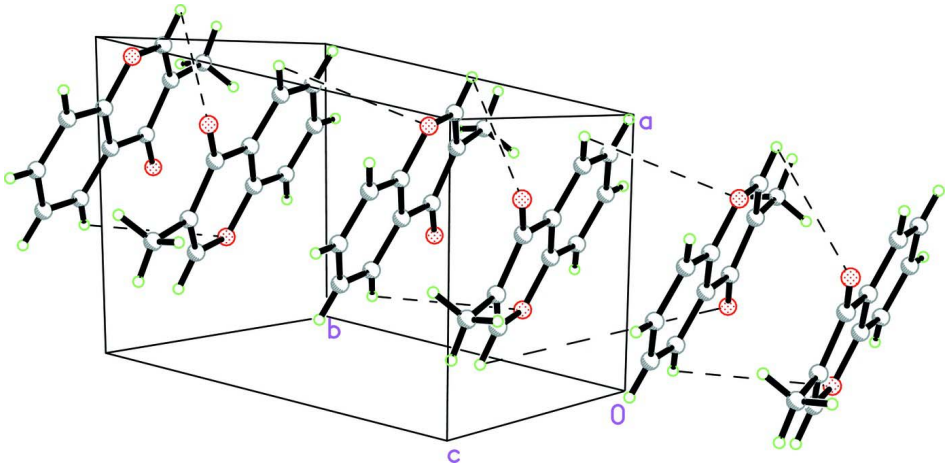

Figure 2

Crystal packing showing chains formed along the *a* axis *via* weak C—H···O contacts.

3-Methyl-4*H*-chromen-4-one

Crystal data

$C_{10}H_8O_2$
$M_r = 160.16$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.5284\ (13)$ Å
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$c = 8.9834\ (18)$ Å
$\alpha = 75.137\ (2)°$
$\beta = 78.169\ (2)°$
$\gamma = 80.895\ (2)°$
$V = 398.12\ (14)$ Å^3
$Z = 2$
$F(000) = 168$
$D_x = 1.336$ Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1573 reflections
θ = 2.4–28.4°
μ = 0.09 mm^{-1}
T = 296 K
Block, colorless
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.989, T_{max} = 0.993
2771 measured reflections
1394 independent reflections
1143 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −7→7
k = −8→8
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
S = 1.00
1394 reflections
111 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
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.067P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.032 (10)

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}
C1	0.5883 (2)	0.71757 (18)	1.05339 (16)	0.0417 (3)
C2	0.4277 (2)	0.76708 (17)	0.96592 (15)	0.0390 (3)
C3	0.4728 (2)	0.76636 (18)	0.79936 (15)	0.0427 (4)
C4	0.6928 (2)	0.71855 (19)	0.73797 (16)	0.0455 (4)
C5	0.8332 (2)	0.6710 (2)	0.83389 (17)	0.0503 (4)
H5	0.9726	0.6398	0.7905	0.060*
C6	0.7581 (3)	0.7246 (3)	0.56727 (18)	0.0700 (5)
H6A	0.9074	0.6903	0.5445	0.105*
H6B	0.7222	0.8524	0.5078	0.105*
H6C	0.6864	0.6350	0.5400	0.105*
C7	0.2263 (2)	0.8210 (2)	1.04176 (18)	0.0506 (4)

H7	0.1150	0.8533	0.9864	0.061*
C8	0.1897 (3)	0.8271 (2)	1.19601 (19)	0.0602 (4)
H8	0.0549	0.8646	1.2443	0.072*
C9	0.3541 (3)	0.7771 (2)	1.28035 (18)	0.0607 (5)
H9	0.3291	0.7818	1.3851	0.073*
C10	0.5524 (3)	0.7212 (2)	1.21027 (17)	0.0554 (4)
H10	0.6621	0.6859	1.2671	0.066*
O1	0.33452 (17)	0.80490 (17)	0.71782 (12)	0.0648 (4)
O2	0.79069 (14)	0.66418 (15)	0.98916 (11)	0.0522 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0424 (7)	0.0398 (7)	0.0441 (7)	−0.0053 (5)	−0.0089 (6)	−0.0103 (5)
C2	0.0379 (7)	0.0336 (6)	0.0444 (7)	−0.0056 (5)	−0.0078 (5)	−0.0057 (5)
C3	0.0444 (8)	0.0392 (7)	0.0440 (7)	−0.0064 (6)	−0.0133 (6)	−0.0031 (5)
C4	0.0487 (8)	0.0439 (7)	0.0421 (7)	−0.0055 (6)	−0.0062 (6)	−0.0080 (6)
C5	0.0397 (8)	0.0574 (9)	0.0522 (8)	−0.0016 (6)	−0.0028 (6)	−0.0162 (7)
C6	0.0782 (12)	0.0787 (12)	0.0445 (9)	−0.0009 (9)	−0.0016 (8)	−0.0108 (8)
C7	0.0418 (8)	0.0482 (8)	0.0594 (9)	−0.0046 (6)	−0.0063 (6)	−0.0106 (6)
C8	0.0552 (9)	0.0551 (9)	0.0635 (10)	−0.0085 (7)	0.0104 (7)	−0.0168 (7)
C9	0.0803 (12)	0.0573 (9)	0.0437 (8)	−0.0141 (8)	0.0018 (8)	−0.0164 (7)
C10	0.0673 (10)	0.0573 (9)	0.0461 (8)	−0.0084 (7)	−0.0180 (7)	−0.0129 (7)
O1	0.0559 (7)	0.0849 (8)	0.0544 (7)	−0.0039 (6)	−0.0253 (5)	−0.0076 (5)
O2	0.0403 (6)	0.0681 (7)	0.0517 (6)	0.0017 (5)	−0.0162 (4)	−0.0184 (5)

Geometric parameters (Å, º)

C1—O2	1.3668 (17)	C6—H6A	0.9600
C1—C2	1.3854 (19)	C6—H6B	0.9600
C1—C10	1.387 (2)	C6—H6C	0.9600
C2—C7	1.3967 (19)	C7—C8	1.368 (2)
C2—C3	1.4657 (19)	C7—H7	0.9300
C3—O1	1.2312 (16)	C8—C9	1.388 (2)
C3—C4	1.450 (2)	C8—H8	0.9300
C4—C5	1.332 (2)	C9—C10	1.366 (2)
C4—C6	1.4961 (19)	C9—H9	0.9300
C5—O2	1.3548 (17)	C10—H10	0.9300
C5—H5	0.9300		
O2—C1—C2	121.70 (12)	H6A—C6—H6B	109.5
O2—C1—C10	116.53 (12)	C4—C6—H6C	109.5
C2—C1—C10	121.77 (14)	H6A—C6—H6C	109.5
C1—C2—C7	117.46 (13)	H6B—C6—H6C	109.5
C1—C2—C3	120.18 (13)	C8—C7—C2	121.23 (14)
C7—C2—C3	122.34 (13)	C8—C7—H7	119.4
O1—C3—C4	122.69 (13)	C2—C7—H7	119.4
O1—C3—C2	122.50 (13)	C7—C8—C9	119.91 (15)

C4—C3—C2	114.81 (11)	C7—C8—H8	120.0
C5—C4—C3	119.62 (13)	C9—C8—H8	120.0
C5—C4—C6	121.16 (14)	C10—C9—C8	120.34 (14)
C3—C4—C6	119.22 (13)	C10—C9—H9	119.8
C4—C5—O2	125.65 (13)	C8—C9—H9	119.8
C4—C5—H5	117.2	C9—C10—C1	119.28 (14)
O2—C5—H5	117.2	C9—C10—H10	120.4
C4—C6—H6A	109.5	C1—C10—H10	120.4
C4—C6—H6B	109.5	C5—O2—C1	117.89 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.93	2.70	3.4374 (19)	137
C7—H7···O2^{ii}	0.93	2.69	3.3820 (19)	132

Symmetry codes: (i) $x+1, y, z$; (ii) $x-1, y, z$.