# organic compounds

# 3-Methyl-4H-chromen-4-one

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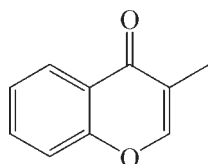Correspondence e-mail: lujianghao001@yahoo.com.cn

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

| | |
|---|---|
| $C_{10}H_8O_2$ | $c$ = 8.9834 (18) Å |
| $M_r$ = 160.16 | $\alpha$ = 75.137 (2)° |
| Triclinic, $P\bar{1}$ | $\beta$ = 78.169 (2)° |
| $a$ = 6.5284 (13) Å | $\gamma$ = 80.895 (2)° |
| $b$ = 7.2210 (14) Å | $V$ = 398.12 (14) Å$^3$ |

| | |
|---|---|
| $Z$ = 2 | $T$ = 296 K |
| Mo $K\alpha$ radiation | 0.12 × 0.10 × 0.08 mm |
| $\mu$ = 0.09 mm$^{-1}$ | |

### Data collection

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

### Refinement

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

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

## References

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**supplementary materials**

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

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### 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.

### 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%.

### 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 $U_{iso}(H) = 1.2U_{eq}(C)$ [for methyl groups $U_{iso}(H) = 1.5U_{eq}(C)$].
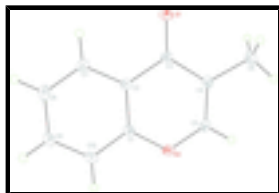
### Figures



Fig. 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.
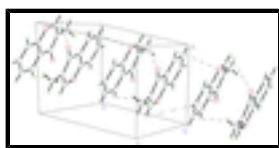


Fig. 2. Crystal packing showing chains formed along the *a* axis *via* weak C—H···O contacts.

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

*Crystal data*

| | |
|---|---|
| $C_{10}H_8O_2$ | $Z = 2$ |
| $M_r = 160.16$ | $F(000) = 168$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.336$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 6.5284$ (13) Å | Cell parameters from 1573 reflections |
| $b = 7.2210$ (14) Å | $\theta = 2.4–28.4°$ |
| $c = 8.9834$ (18) Å | $\mu = 0.09$ mm$^{-1}$ |
| $\alpha = 75.137$ (2)° | $T = 296$ K |
| $\beta = 78.169$ (2)° | Block, colorless |
| $\gamma = 80.895$ (2)° | $0.12 \times 0.10 \times 0.08$ mm |
| $V = 398.12$ (14) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 1394 independent reflections |
| Radiation source: fine-focus sealed tube | 1143 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.014$ |
| $\varphi$ and $\omega$ scans | $\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2001) | $h = -7\rightarrow7$ |
| $T_{min} = 0.989$, $T_{max} = 0.993$ | $k = -8\rightarrow8$ |
| 2771 measured reflections | $l = -10\rightarrow10$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | H-atom parameters constrained |
| $wR(F^2) = 0.116$ | $w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.067P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.00$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 1394 reflections | $\Delta\rho_{max} = 0.18$ e Å$^{-3}$ |
| 111 parameters | $\Delta\rho_{min} = -0.14$ e Å$^{-3}$ |
| 0 restraints | Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | 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 ($Å^2$)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, °)*

| | | | |
|---|---|---|---|
| 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, °)*

| $D$—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) $x−1, y, z$.

**Fig. 1**

**Fig. 2**