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4,6-Dimethyl-2*H*-chromen-2-one

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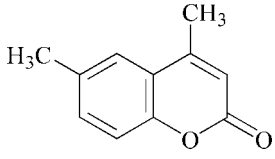
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.156; data-to-parameter ratio = 12.5.

In the title compound, $C_{11}H_{10}O_2$, the whole molecule apart from the H atoms possesses a planar structure with an r.m.s. deviation of 0.0202 (3) Å.

Related literature

For related literature, see: Alexander *et al.* (2005); Chavan *et al.* (2002); Smitha & Reddy (2004).



Experimental

Crystal data

$C_{11}H_{10}O_2$
M_r = 174.19
Monoclinic, $P2_1/c$
a = 7.056 (4) Å
b = 8.854 (4) Å
c = 13.976 (6) Å
β = 104.80 (2)°
V = 844.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.16 × 0.14 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.985, T_{max} = 0.993
4292 measured reflections
1500 independent reflections
788 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.156
S = 1.01
1500 reflections
120 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected bond and torsion angles (°).

O2—C9—O1	116.3 (2)	O2—C9—C8	126.5 (3)
C2—C3—C4—C10	179.2 (2)	C1—C6—C7—C11	−178.7 (2)
C10—C4—C5—C6	−179.3 (2)	C11—C7—C8—C9	−179.6 (3)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: AT2334).

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supplementary materials

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4,6-Dimethyl-2*H*-chromen-2-one

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Comment

Coumarins and their derivatives form an important class of compounds which are widely used as additives in food, perfumes, cosmetics, pharmaceuticals and optical brighteners (Chavan *et al.*, 2002; Alexander *et al.*, 2005; Smitha *et al.*, 2004). We report here the crystal structure of the title compound (I).

In the molecule of (I), the torsion angles of C10—C4—C5—C6 and C11—C7—C8—C9 are 179.3 (2)° and 179.6 (3)°, repectively, indicating that the two C atoms of methyl groups don't significantly deviate from the coumarin moiety. So the whole molecule except the H atoms assumes a planar structrue with an r.m.s deviation of 0.0202 (3) Å. C9 atom of the carbonyl group has a distorted trigonal geometry with O2—C9—O1 [116.3 (2)°] and O2—C9—C8 [126.5 (3)°] deviating significantly from the ideal sp^2 value of 120°.

Experimental

The title compound was prepared by solvent free pechmann reaction with sulfuric acid as catalyst. To a solution of *p*-cresol (2.3 g, 20 mmol) and ethyl acetoacetate (2.6 g, 20 mmol), the 75% sulfuric acid(50 ml) was slowly added at 283 K with stirring for 1 h. Then the mixture was moved to oil-bath and continuously stirred for 18 h at 318 K. The reaction mixture was poured into ice-water. The solid obtained was filtered off, washed with 5% sodium hydroxide solution until no color appears in the aqueous layer and dried at room temperature. The products were further purified by recrystallizing the crude product with methanol. Colourless crystals of (I) suitable for X-ray structure analysis were obtained by slowly evaporating from dichloromethane and petroleum ether.

Refinement

All H atoms were positioned geometrically and refined using riding on their parent atoms, with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq} for Csp^2—H, and C—H = 0.96Å and U_{iso}(H) = 1.5U_{eq} for Csp^3—H.

Figures

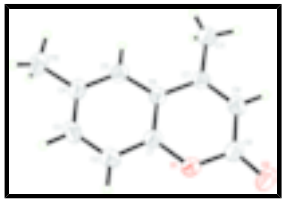

Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

4,6-Dimethyl-2*H*-chromen-2-one

Crystal data

$C_{11}H_{10}O_2$	F_{000} = 368
M_r = 174.19	D_x = 1.371 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 428 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.056 (4) Å	Cell parameters from 786 reflections
b = 8.854 (4) Å	θ = 2.8–25.6º
c = 13.976 (6) Å	μ = 0.09 mm^{-1}
β = 104.80 (2)º	T = 293 (2) K
V = 844.2 (7) Å^3	Needle, colourless
Z = 4	0.16 × 0.14 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1500 independent reflections
Radiation source: fine-focus sealed tube	788 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
T = 293(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −8→5
T_{min} = 0.985, T_{max} = 0.993	k = −10→8
4292 measured reflections	l = −16→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.156	$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.2401P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.003
1500 reflections	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
120 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.3485 (3)	0.56831 (19)	1.16838 (12)	0.0500 (5)
O2	0.4079 (3)	0.4494 (2)	1.30820 (13)	0.0703 (7)
C1	0.2949 (4)	0.5693 (3)	1.06742 (17)	0.0413 (7)
C2	0.2896 (4)	0.7070 (3)	1.02378 (19)	0.0522 (8)
H2	0.3227	0.7939	1.0618	0.063*
C3	0.2351 (4)	0.7149 (3)	0.9238 (2)	0.0540 (8)
H3	0.2297	0.8088	0.8934	0.065*
C4	0.1873 (4)	0.5878 (3)	0.86554 (18)	0.0465 (7)
C5	0.1987 (4)	0.4517 (3)	0.91231 (17)	0.0451 (7)
H5	0.1682	0.3647	0.8742	0.054*
C6	0.2538 (3)	0.4381 (3)	1.01418 (16)	0.0377 (6)
C7	0.2727 (4)	0.2988 (3)	1.06670 (18)	0.0417 (7)
C8	0.3269 (4)	0.3024 (3)	1.16491 (18)	0.0483 (7)
H8	0.3413	0.2113	1.1992	0.058*
C9	0.3641 (4)	0.4381 (3)	1.21995 (19)	0.0481 (7)
C10	0.1255 (4)	0.5999 (4)	0.75576 (18)	0.0650 (9)
H10A	0.1319	0.5022	0.7270	0.098*
H10B	0.2112	0.6683	0.7337	0.098*
H10C	−0.0065	0.6372	0.7357	0.098*
C11	0.2342 (5)	0.1527 (3)	1.01272 (19)	0.0608 (9)
H11A	0.2636	0.0708	1.0592	0.091*
H11B	0.3153	0.1452	0.9673	0.091*
H11C	0.0988	0.1477	0.9768	0.091*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0636 (13)	0.0453 (11)	0.0393 (10)	−0.0017 (9)	0.0098 (9)	−0.0044 (8)
O2	0.0945 (17)	0.0780 (15)	0.0352 (11)	−0.0032 (12)	0.0107 (10)	−0.0027 (9)
C1	0.0390 (16)	0.0451 (16)	0.0401 (14)	0.0025 (12)	0.0104 (12)	0.0000 (12)
C2	0.061 (2)	0.0418 (16)	0.0529 (17)	−0.0006 (14)	0.0129 (14)	−0.0025 (13)
C3	0.0587 (19)	0.0419 (17)	0.0617 (18)	0.0080 (14)	0.0160 (15)	0.0149 (14)

C4	0.0431 (16)	0.0553 (18)	0.0416 (14)	0.0045 (13)	0.0116 (12)	0.0106 (13)
C5	0.0422 (16)	0.0501 (17)	0.0413 (14)	0.0005 (12)	0.0072 (12)	−0.0029 (12)
C6	0.0336 (14)	0.0408 (15)	0.0384 (14)	0.0009 (11)	0.0085 (11)	0.0017 (11)
C7	0.0418 (16)	0.0412 (16)	0.0427 (15)	0.0000 (12)	0.0118 (12)	−0.0005 (11)
C8	0.0542 (18)	0.0424 (16)	0.0479 (16)	0.0012 (13)	0.0125 (13)	0.0078 (12)
C9	0.0499 (17)	0.0533 (18)	0.0404 (15)	0.0012 (13)	0.0104 (13)	0.0023 (13)
C10	0.063 (2)	0.085 (2)	0.0449 (17)	0.0104 (17)	0.0100 (15)	0.0186 (15)
C11	0.081 (2)	0.0426 (17)	0.0579 (17)	−0.0051 (15)	0.0167 (15)	−0.0018 (13)

Geometric parameters (Å, °)

O1—C9	1.349 (3)	C5—H5	0.9300
O1—C1	1.364 (3)	C6—C7	1.425 (3)
O2—C9	1.197 (3)	C7—C8	1.328 (3)
C1—C2	1.359 (3)	C7—C11	1.487 (3)
C1—C6	1.370 (3)	C8—C9	1.415 (3)
C2—C3	1.353 (3)	C8—H8	0.9300
C2—H2	0.9300	C10—H10A	0.9600
C3—C4	1.379 (4)	C10—H10B	0.9600
C3—H3	0.9300	C10—H10C	0.9600
C4—C5	1.363 (3)	C11—H11A	0.9600
C4—C10	1.488 (3)	C11—H11B	0.9600
C5—C6	1.382 (3)	C11—H11C	0.9600
C9—O1—C1	121.4 (2)	C8—C7—C11	120.8 (2)
C2—C1—O1	116.0 (2)	C6—C7—C11	120.7 (2)
C2—C1—C6	122.6 (2)	C7—C8—C9	123.2 (2)
O1—C1—C6	121.4 (2)	C7—C8—H8	118.4
C3—C2—C1	118.5 (3)	C9—C8—H8	118.4
C3—C2—H2	120.7	O2—C9—O1	116.3 (2)
C1—C2—H2	120.7	O2—C9—C8	126.5 (3)
C2—C3—C4	122.0 (3)	O1—C9—C8	117.2 (2)
C2—C3—H3	119.0	C4—C10—H10A	109.5
C4—C3—H3	119.0	C4—C10—H10B	109.5
C5—C4—C3	117.6 (2)	H10A—C10—H10B	109.5
C5—C4—C10	121.6 (3)	C4—C10—H10C	109.5
C3—C4—C10	120.8 (3)	H10A—C10—H10C	109.5
C4—C5—C6	122.5 (2)	H10B—C10—H10C	109.5
C4—C5—H5	118.7	C7—C11—H11A	109.5
C6—C5—H5	118.7	C7—C11—H11B	109.5
C1—C6—C5	116.8 (2)	H11A—C11—H11B	109.5
C1—C6—C7	118.4 (2)	C7—C11—H11C	109.5
C5—C6—C7	124.8 (2)	H11A—C11—H11C	109.5
C8—C7—C6	118.4 (2)	H11B—C11—H11C	109.5
C9—O1—C1—C2	−178.2 (2)	C4—C5—C6—C1	0.8 (4)
C9—O1—C1—C6	0.3 (3)	C4—C5—C6—C7	−178.4 (2)
O1—C1—C2—C3	−179.2 (2)	C1—C6—C7—C8	0.8 (4)
C6—C1—C2—C3	2.3 (4)	C5—C6—C7—C8	180.0 (2)
C1—C2—C3—C4	−0.7 (4)	C1—C6—C7—C11	−178.7 (2)
C2—C3—C4—C5	−0.7 (4)	C5—C6—C7—C11	0.5 (4)

C2—C3—C4—C10	179.2 (2)	C6—C7—C8—C9	1.0 (4)
C3—C4—C5—C6	0.6 (4)	C11—C7—C8—C9	−179.6 (3)
C10—C4—C5—C6	−179.3 (2)	C1—O1—C9—O2	−178.4 (2)
C2—C1—C6—C5	−2.3 (4)	C1—O1—C9—C8	1.5 (4)
O1—C1—C6—C5	179.3 (2)	C7—C8—C9—O2	177.8 (3)
C2—C1—C6—C7	177.0 (2)	C7—C8—C9—O1	−2.1 (4)
O1—C1—C6—C7	−1.4 (4)		

Fig. 1