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4-Chloro-2-phenyl-2*H*-chromene-3-carbaldehyde

B. Punithavalli and A. Therasa Alphonsa*

Department of Chemistry, Annamalai University, Annamalai Nagar-608002, Tamilnadu, India. *Correspondence e-mail: princykenisha@gmail.com

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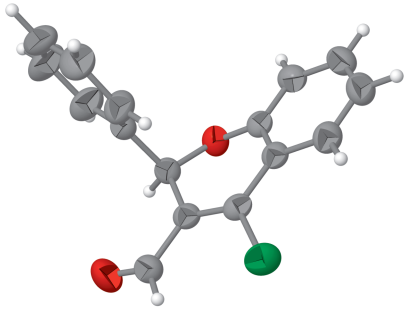
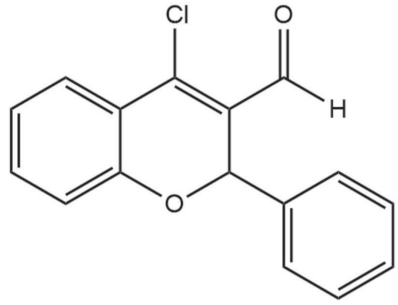
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, 4-chloro-2-phenyl-2*H*-chromene-3-carbaldehyde (PCC), $C_{16}H_{11}ClO_2$, was obtained in good yield by a standard one-pot method. The molecule has the following substituents: a chlorine atom at the 4-position, a phenyl group at the 2-position, and an aldehyde (–CHO) group at the 3-position of the 2*H*-chromene ring system.

3D view



Chemical scheme



Structure description

Heterocyclic compounds containing nitrogen and oxygen have attracted a lot of interest because of their diverse pharmacological activities (Swamy & Agasimundin, 2008; Tanaka & Sugino, 2001). The basic flavonoid structure is a flavone nucleus, which consists of 15 carbon atoms arranged in rings and is available as flavones, flavonols, flavanones, isoflavones, chalcones and their derivatives. In organic chemistry, 4-chloro-2-phenyl-2*H*-chromene-3-carbaldehyde is a noteworthy compound that is especially well-known for being synthesized from flavanone. This substance is a member of the chromene class, which includes a range of physiologically active compounds with uses in drug development and medicinal chemistry. The chromene ring with a phenyl substituent and an aldehyde functional group is part of the structural framework of 4-chloro-2-phenyl-2*H*-chromene-3-carbaldehyde (PCC), which makes it useful in a variety of chemical reactions, including nucleophilic interactions and electrophilic substitutions (Najmanová *et al.*, 2020).

Single crystal X-ray analysis confirmed that the 4-chloro-2-phenyl-2*H*-chromene-3-carbaldehyde crystallizes in the triclinic system in space group $P\overline{1}$. The title chromene derivative has the following substituents: a chlorine atom at the 4-position, a phenyl group at the 2-position, and an aldehyde (–CHO) group at the 3-position of the 2*H*-chromene ring system. The molecular structure is shown in Fig. 1 and the unit-cell contents in Fig. 2.

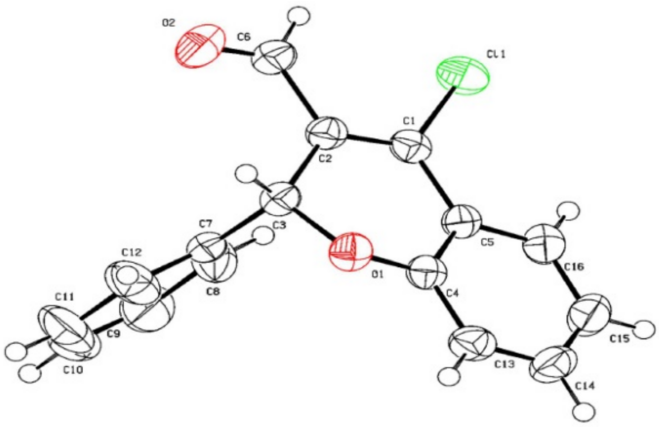


Figure 1
The molecular structure of 4-chloro-2-phenyl-2*H*-chromene-3-carbaldehyde. Displacement ellipsoids are at the 50% probability level.

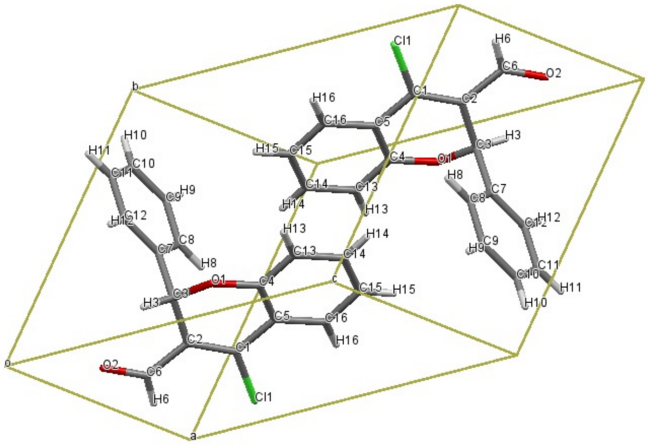


Figure 2
Packing of 4-chloro-2-phenyl-2*H*-chromene-3-carbaldehyde.

Synthesis and crystallization

The starting materials 2-phenylchroman-4-one, phosphoryl trichloride and dimethyl furan were purchased from Sigma-Aldrich chemical company with a stated purity and were used as such without further purification. The title compound was synthesized according to Fig. 3. In a round-bottom flask, flavanone (0.1 g) was added with phosphorus oxychloride (16 ml) and stirred well for 6-7 h. The completion of the reaction was monitored by TLC. After that, the reaction mixture was poured into ice-cold water. The resulting precipitate was washed with water and dried. The crude product was recrystallized from ethanol solution.

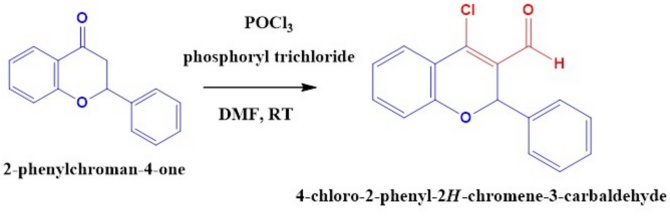


Figure 3
Reaction scheme for the synthesis of the title compound.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{11}ClO_2$
M_r	270.70
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	300
a, b, c (Å)	7.0108 (4), 8.7716 (5), 11.1285 (6)
α, β, γ (°)	75.127 (2), 83.188 (2), 73.584 (2)
V (Å^3)	633.68 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.30
Crystal size (mm)	0.30 × 0.20 × 0.13
Data collection	
Diffractometer	Bruker D8 QUEST diffractometer with PHOTON II detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.702, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24536, 3133, 2488
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.105, 1.03
No. of reflections	3133
No. of parameters	172
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.21

Computer programs: *APEX4* and *SAINT* (Bruker, 2021), *SHELXT2019/1* (Sheldrick, 2015*a*), *SHELXL2019/1* (Sheldrick, 2015*b*) and *SHELXTL* (Sheldrick, 2008).

Refinement

The crystal data and structure refinement parameters are listed in Table 1.

References

Bruker (2021). *APEX4* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Najmanová, M., Vopršalová, L., Saso, P. & Mladěnka, P. (2020). *Crit. Rev. Food Sci. Nutr.* **60**, 3155–3171.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Swamy, P. M. G. & Agasimundin, Y. S. (2008). *Rasayan J. Chem.* **1**, 421–428.
Tanaka, K. & Sugino, T. (2001). *Green Chem.* **3**, 133–134.

full crystallographic data

IUCrData (2025). **10**, x250657 [https://doi.org/10.1107/S2414314625006571]

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Crystal data

$C_{16}H_{11}ClO_2$
M_r = 270.70
Triclinic, $P\overline{1}$
a = 7.0108 (4) Å
b = 8.7716 (5) Å
c = 11.1285 (6) Å
α = 75.127 (2)°
β = 83.188 (2)°
γ = 73.584 (2)°
V = 633.68 (6) Å^3
Z = 2
$F(000)$ = 280
D_x = 1.419 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9898 reflections
θ = 2.5–27.4°
μ = 0.30 mm^{-1}
T = 300 K
Block, yellow
0.30 × 0.20 × 0.13 mm

Data collection

Bruker D8 QUEST diffractometer with PHOTON II detector
Radiation source: i-mu-s microfocus source
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.702, T_{max} = 0.746
24536 measured reflections
3133 independent reflections
2488 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.3°, θ_{min} = 2.5°
h = −9→9
k = −11→11
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 1.03
3133 reflections
172 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 0.2009P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-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.

Refinement. Hydrogen atoms were located in a difference map and refined as riding on their parent atoms with U(H)=1.2U_{eq}(C) and with $C_{tertiary}$-H=0.98Å or with C-H=0.93Å.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.15627 (6)	0.98500 (5)	0.71969 (4)	0.05455 (15)
O1	0.77862 (15)	0.76830 (13)	0.58422 (10)	0.0452 (3)
O2	0.6807 (2)	0.95248 (17)	0.89832 (13)	0.0695 (4)
C1	0.8078 (2)	0.60085 (18)	0.79480 (14)	0.0432 (3)
C2	1.0062 (3)	0.5239 (2)	0.81560 (18)	0.0655 (5)
H2	1.102219	0.579734	0.782252	0.079*
C3	1.0636 (4)	0.3651 (3)	0.8853 (2)	0.0828 (7)
H3	1.197400	0.315453	0.899833	0.099*
C4	0.9247 (4)	0.2807 (2)	0.93297 (19)	0.0754 (6)
H4	0.963825	0.173161	0.978827	0.090*
C5	0.7274 (4)	0.3548 (2)	0.9131 (2)	0.0747 (6)
H5	0.632676	0.297137	0.945091	0.090*
C6	0.6681 (3)	0.5158 (2)	0.84521 (17)	0.0592 (5)
H6	0.533599	0.566230	0.833782	0.071*
C7	0.7540 (2)	0.77322 (18)	0.71423 (14)	0.0407 (3)
H7	0.850791	0.827483	0.728683	0.049*
C8	0.5509 (2)	0.87461 (17)	0.74512 (14)	0.0400 (3)
C9	0.3969 (2)	0.88283 (17)	0.68077 (14)	0.0390 (3)
C10	0.4248 (2)	0.80733 (17)	0.57576 (13)	0.0394 (3)
C11	0.6219 (2)	0.74966 (17)	0.53280 (13)	0.0395 (3)
C12	0.5371 (3)	0.9571 (2)	0.84591 (15)	0.0506 (4)
H12	0.412489	1.015614	0.870651	0.061*
C13	0.2713 (2)	0.7949 (2)	0.51259 (16)	0.0487 (4)
H13	0.139474	0.833098	0.539225	0.058*
C14	0.3141 (3)	0.7262 (2)	0.41102 (17)	0.0573 (4)
H14	0.211223	0.717625	0.369606	0.069*
C15	0.5087 (3)	0.6702 (2)	0.37072 (16)	0.0565 (4)
H15	0.536306	0.624245	0.301928	0.068*
C16	0.6630 (3)	0.68122 (19)	0.43080 (15)	0.0489 (4)
H16	0.794096	0.642888	0.402954	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0411 (2)	0.0541 (3)	0.0653 (3)	−0.00800 (17)	0.00581 (18)	−0.0173 (2)
O1	0.0397 (5)	0.0553 (6)	0.0401 (6)	−0.0157 (5)	0.0023 (4)	−0.0085 (5)
O2	0.0744 (9)	0.0788 (9)	0.0638 (8)	−0.0161 (7)	−0.0156 (7)	−0.0305 (7)
C1	0.0508 (8)	0.0403 (8)	0.0374 (7)	−0.0065 (6)	−0.0038 (6)	−0.0124 (6)
C2	0.0532 (10)	0.0599 (11)	0.0650 (12)	0.0034 (8)	0.0055 (9)	−0.0064 (9)
C3	0.0729 (14)	0.0676 (13)	0.0742 (14)	0.0201 (11)	0.0018 (11)	−0.0031 (11)
C4	0.1089 (18)	0.0433 (10)	0.0546 (11)	0.0067 (11)	−0.0072 (11)	−0.0059 (8)
C5	0.1052 (18)	0.0531 (11)	0.0657 (13)	−0.0318 (12)	−0.0130 (12)	0.0022 (9)
C6	0.0670 (11)	0.0474 (9)	0.0620 (11)	−0.0193 (8)	−0.0173 (9)	0.0004 (8)
C7	0.0415 (8)	0.0406 (8)	0.0419 (8)	−0.0128 (6)	−0.0034 (6)	−0.0098 (6)
C8	0.0449 (8)	0.0339 (7)	0.0398 (7)	−0.0111 (6)	−0.0009 (6)	−0.0057 (6)

C9	0.0386 (7)	0.0326 (7)	0.0418 (8)	−0.0099 (6)	0.0028 (6)	−0.0033 (6)
C10	0.0435 (8)	0.0342 (7)	0.0384 (7)	−0.0120 (6)	−0.0019 (6)	−0.0030 (6)
C11	0.0449 (8)	0.0341 (7)	0.0368 (7)	−0.0128 (6)	−0.0014 (6)	−0.0012 (6)
C12	0.0591 (10)	0.0465 (9)	0.0454 (9)	−0.0100 (7)	−0.0048 (7)	−0.0129 (7)
C13	0.0455 (8)	0.0484 (9)	0.0515 (9)	−0.0138 (7)	−0.0068 (7)	−0.0068 (7)
C14	0.0677 (11)	0.0553 (10)	0.0543 (10)	−0.0213 (9)	−0.0161 (8)	−0.0105 (8)
C15	0.0762 (12)	0.0515 (10)	0.0451 (9)	−0.0179 (9)	−0.0050 (8)	−0.0147 (7)
C16	0.0570 (10)	0.0440 (8)	0.0425 (8)	−0.0118 (7)	0.0034 (7)	−0.0088 (7)

Geometric parameters (Å, º)

Cl1—C9	1.7343 (15)	C7—C8	1.504 (2)
O1—C11	1.3641 (18)	C7—H7	0.9800
O1—C7	1.4470 (18)	C8—C9	1.341 (2)
O2—C12	1.207 (2)	C8—C12	1.464 (2)
C1—C6	1.378 (2)	C9—C10	1.453 (2)
C1—C2	1.381 (2)	C10—C13	1.397 (2)
C1—C7	1.515 (2)	C10—C11	1.402 (2)
C2—C3	1.381 (3)	C11—C16	1.381 (2)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.364 (3)	C13—C14	1.377 (2)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.369 (3)	C14—C15	1.376 (3)
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.390 (3)	C15—C16	1.375 (2)
C5—H5	0.9300	C15—H15	0.9300
C6—H6	0.9300	C16—H16	0.9300
C11—O1—C7	116.95 (11)	C9—C8—C7	118.92 (13)
C6—C1—C2	118.58 (16)	C12—C8—C7	116.38 (13)
C6—C1—C7	122.85 (15)	C8—C9—C10	121.45 (13)
C2—C1—C7	118.54 (15)	C8—C9—Cl1	121.05 (12)
C3—C2—C1	120.8 (2)	C10—C9—Cl1	117.50 (11)
C3—C2—H2	119.6	C13—C10—C11	118.49 (14)
C1—C2—H2	119.6	C13—C10—C9	124.97 (14)
C4—C3—C2	120.2 (2)	C11—C10—C9	116.48 (13)
C4—C3—H3	119.9	O1—C11—C16	117.44 (14)
C2—C3—H3	119.9	O1—C11—C10	121.73 (13)
C3—C4—C5	119.78 (19)	C16—C11—C10	120.70 (14)
C3—C4—H4	120.1	O2—C12—C8	122.83 (16)
C5—C4—H4	120.1	O2—C12—H12	118.6
C4—C5—C6	120.3 (2)	C8—C12—H12	118.6
C4—C5—H5	119.8	C14—C13—C10	120.32 (16)
C6—C5—H5	119.8	C14—C13—H13	119.8
C1—C6—C5	120.26 (19)	C10—C13—H13	119.8
C1—C6—H6	119.9	C15—C14—C13	120.12 (16)
C5—C6—H6	119.9	C15—C14—H14	119.9
O1—C7—C8	111.67 (12)	C13—C14—H14	119.9

O1—C7—C1	109.74 (12)	C16—C15—C14	120.88 (16)
C8—C7—C1	114.24 (12)	C16—C15—H15	119.6
O1—C7—H7	106.9	C14—C15—H15	119.6
C8—C7—H7	106.9	C15—C16—C11	119.49 (16)
C1—C7—H7	106.9	C15—C16—H16	120.3
C9—C8—C12	124.70 (14)	C11—C16—H16	120.3

C6—C1—C2—C3	0.0 (3)	C7—C8—C9—Cl1	175.11 (10)
C7—C1—C2—C3	−178.08 (18)	C8—C9—C10—C13	172.68 (14)
C1—C2—C3—C4	1.2 (3)	Cl1—C9—C10—C13	−7.6 (2)
C2—C3—C4—C5	−1.0 (3)	C8—C9—C10—C11	−10.2 (2)
C3—C4—C5—C6	−0.4 (3)	Cl1—C9—C10—C11	169.61 (10)
C2—C1—C6—C5	−1.4 (3)	C7—O1—C11—C16	−154.86 (13)
C7—C1—C6—C5	176.64 (16)	C7—O1—C11—C10	29.37 (18)
C4—C5—C6—C1	1.6 (3)	C13—C10—C11—O1	175.26 (13)
C11—O1—C7—C8	−42.03 (16)	C9—C10—C11—O1	−2.10 (19)
C11—O1—C7—C1	85.70 (15)	C13—C10—C11—C16	−0.4 (2)
C6—C1—C7—O1	−95.72 (17)	C9—C10—C11—C16	−177.74 (13)
C2—C1—C7—O1	82.32 (17)	C9—C8—C12—O2	−176.79 (16)
C6—C1—C7—C8	30.6 (2)	C7—C8—C12—O2	3.7 (2)
C2—C1—C7—C8	−151.40 (15)	C11—C10—C13—C14	0.5 (2)
O1—C7—C8—C9	30.37 (18)	C9—C10—C13—C14	177.57 (14)
C1—C7—C8—C9	−94.90 (16)	C10—C13—C14—C15	−0.4 (3)
O1—C7—C8—C12	−150.09 (13)	C13—C14—C15—C16	0.2 (3)
C1—C7—C8—C12	84.64 (16)	C14—C15—C16—C11	−0.1 (3)
C12—C8—C9—C10	175.37 (13)	O1—C11—C16—C15	−175.62 (14)
C7—C8—C9—C10	−5.1 (2)	C10—C11—C16—C15	0.2 (2)
C12—C8—C9—Cl1	−4.4 (2)		