Crystal structure of 6-bromo-3-(4'-chlorophenyl)-4-methylcoumarin, $C_{16}H_{10}BrClO_2$

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Abstract

$C_{16}H_{10}BrClO_2$, monoclinic, $C12/c1$ (No. 15), $a = 21.984(7)$ Å, $b = 10.819(2)$ Å, $c = 18.168(2)$ Å, $\beta = 138.03(2)^\circ$, $V = 2889.9$ Å³, $Z = 8$, $R_{gt}(F) = 0.065$, $wR_{obs}(F) = 0.079$, $T = 293$ K.

Source of material

Purchased from Indofine Chemical Company. Crystals grown from ethyl acetate, mp 490 K – 492 K.

Discussion

The coumarin moiety is planar with an average deviation of the atoms from the least-squares plane of 0.043(5) Å. The phenyl ring attached at the C3 atom is twisted out of the coumarin plane with C2'–C1'–C3–C4 torsion angle of 69(2)°. In the coumarin compounds, the O1–C9 bond length is longer than the O1–C2 bond distance [1,2]. However, in the case of the title compound, these two bond lengths are the same due to the existence of an intramolecular H-bond with $d(O2 \cdots H6') = 2.42$ Å.

Table 1. Data collection and handling.

Crystal:	colorless prism, size $0.3 \times 0.3 \times 0.5$ mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	30.3 cm^{-1}
Diffraction, scan mode:	CAD4, $\omega/2\theta$
$2\theta_{\text{max}}$:	49.94°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	5682, 2543
Criterion for F_{obs} , $N(hkl)_{\text{gt}}$:	$F_{\text{obs}} > 3 \sigma(F_{\text{obs}})$, 1609
$N(\text{param})_{\text{refined}}$:	221
Program:	xtal [3]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{iso}
H(6')	8f	0.502(7)	0.15(1)	0.517(8)	0.06(3)
H(8)	8f	0.378(7)	−0.03(1)	0.086(8)	0.06(3)
H(5)	8f	0.377(7)	0.40(1)	0.116(9)	0.05(4)
H(3')	8f	0.234(7)	0.38(1)	0.387(8)	0.08(3)
H(7)	8f	0.395(8)	0.07(1)	−0.00(1)	0.13(4)
H(2')	8f	0.250(7)	0.33(1)	0.274(6)	0.11(4)
H(5')	8f	0.496(8)	0.20(1)	0.63(1)	0.07(4)
H(441)	8f	0.320(7)	0.45(1)	0.23(1)	0.16(7)
H(442)	8f	0.408(8)	0.45(2)	0.340(6)	0.29(7)
H(443)	8f	0.35(1)	0.47(1)	0.20(1)	0.20(5)

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br	8f	0.37016(9)	0.3690(2)	−0.0451(1)	0.0714(8)	0.115(1)	0.0534(7)	0.0119(9)	0.0456(7)	0.0060(9)
C(3)	8f	0.3767(7)	0.193(1)	0.3045(8)	0.035(6)	0.058(8)	0.041(6)	0.003(5)	0.023(5)	0.001(5)
C(7)	8f	0.3740(8)	0.134(2)	0.029(1)	0.051(7)	0.09(1)	0.063(8)	−0.002(8)	0.040(7)	−0.021(9)
C(9)	8f	0.3772(7)	0.106(1)	0.1625(9)	0.035(6)	0.065(9)	0.051(6)	0.003(6)	0.026(5)	−0.007(6)
C(5)	8f	0.3750(8)	0.311(1)	0.1106(9)	0.043(6)	0.064(9)	0.040(6)	0.011(6)	0.025(5)	−0.002(6)
C(2)	8f	0.3774(7)	0.062(1)	0.291(1)	0.033(6)	0.058(9)	0.052(7)	0.004(6)	0.023(6)	0.001(6)
C(6)	8f	0.3712(7)	0.259(1)	0.0382(9)	0.032(6)	0.078(9)	0.053(7)	0.004(6)	0.029(6)	−0.002(6)
O(1)	8f	0.3793(5)	0.0229(7)	0.2212(7)	0.057(5)	0.052(5)	0.072(5)	0.003(4)	0.047(5)	−0.000(4)
C(10)	8f	0.3761(7)	0.231(1)	0.1731(8)	0.033(6)	0.059(8)	0.045(6)	0.007(5)	0.025(5)	−0.002(6)
C(4)	8f	0.3771(7)	0.277(1)	0.2501(8)	0.040(6)	0.061(8)	0.038(5)	0.006(6)	0.025(5)	−0.001(6)

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Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(5')	8f	0.4485(9)	0.236(1)	0.567(1)	0.056(8)	0.08(1)	0.048(7)	0.008(7)	0.032(7)	0.014(7)
O(2)	8f	0.3743(6)	−0.0193(8)	0.3338(7)	0.069(6)	0.060(6)	0.066(5)	0.000(5)	0.044(5)	0.007(5)
C(2')	8f	0.2968(9)	0.283(1)	0.343(1)	0.066(8)	0.069(9)	0.055(7)	0.018(7)	0.040(7)	0.010(7)
C(1')	8f	0.3759(7)	0.228(1)	0.3835(9)	0.045(6)	0.054(7)	0.058(7)	0.007(6)	0.039(6)	0.010(6)
C(6')	8f	0.4507(8)	0.203(1)	0.4958(9)	0.050(7)	0.076(9)	0.051(7)	0.011(7)	0.036(6)	0.015(6)
C(44)	8f	0.380(1)	0.415(1)	0.266(1)	0.11(1)	0.044(8)	0.064(9)	0.015(8)	0.07(1)	0.010(7)
C(3')	8f	0.2931(9)	0.316(1)	0.414(1)	0.077(9)	0.08(1)	0.068(8)	0.023(8)	0.057(8)	0.015(7)
C(8)	8f	0.3763(9)	0.055(1)	0.091(1)	0.060(8)	0.064(9)	0.077(9)	−0.002(7)	0.049(8)	−0.016(8)
C(4')	8f	0.371(1)	0.291(1)	0.526(1)	0.09(1)	0.067(9)	0.074(9)	−0.005(8)	0.070(9)	−0.006(7)
Cl	8f	0.3684(3)	0.3323(4)	0.6166(3)	0.135(4)	0.099(3)	0.085(2)	0.015(3)	0.091(3)	0.006(2)

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