Crystal structure of 6-bromochromone, $C_9H_5BrO_2$

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Abstract

$C_9H_5BrO_2$, monoclinic, $P12_11$ (no. 4), $a = 3.922(1)$ Å, $b = 5.723(2)$ Å, $c = 17.208(5)$ Å, $\beta = 95.447(6)^\circ$, $V = 384.5$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.038$, $wR_{\text{ref}}(F^2) = 0.106$, $T = 193$ K.

Source of material

The title compound was purchased from Aldrich and crystals were grown from a solution of dichloromethane which was layered with hexanes. A mixture of 3-bromochromone and 6-bromochromone was dissolved in dichloromethane and layered with hexanes. The result was two crystal types, plates and needles.

Discussion

In the course of studying crystallization properties of substituted chromones [1], the title compound, 6-bromochromone, was crystallized in the same manner as 3-bromochromone. It was hoped

that the two compounds would crystallize in the same crystal system or even in the same space group. This was not the case, 6-bromochromone crystallized as large plate-like crystals in monoclinic, where 3-bromochromone forms needles in orthorhombic crystal system. Co-crystallization resulted in two crystal types, plates and needles, both having cell dimensions consistent with the previously solved corresponding compounds.

Table 1. Data collection and handling.

Crystal:	colorless plate, size $0.02 \times 0.12 \times 0.12$ mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	52.91 cm^{-1}
Diffraction, scan mode:	Bruker SMART CCD, ω/ϕ
$2\theta_{\text{max}}$:	55.78°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	2588, 1670
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1592
$N(\text{param})_{\text{refined}}$:	129
Programs:	SHELXS-97 [2], SHELXL-97 [3], SHELXTL [4]

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

Atom	Site	x	y	z	U_{iso}
H(1)	2a	0.93(1)	0.01(2)	0.577(4)	0.03(2)
H(2)	2a	0.64(1)	0.30(1)	0.517(4)	0.03(2)
H(5)	2a	0.43(1)	0.69(1)	0.753(3)	0.03(2)
H(7)	2a	0.91(2)	0.31(1)	0.929(4)	0.04(2)
H(8)	2a	1.02(2)	0.04(1)	0.823(4)	0.03(2)

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(1)	2a	0.55602(9)	0.7295(2)	0.93012(2)	0.0318(2)	0.0329(2)	0.0222(2)	0.0007(2)	0.0042(1)	−0.0033(2)
O(1)	2a	0.948(1)	0.0659(7)	0.6832(2)	0.037(2)	0.023(2)	0.037(2)	0.003(1)	0.006(2)	−0.005(2)
O(2)	2a	0.402(1)	0.6499(7)	0.6089(2)	0.055(2)	0.033(2)	0.024(2)	0.006(2)	0.001(2)	0.002(1)
C(1)	2a	0.852(2)	0.108(1)	0.6062(4)	0.039(3)	0.029(3)	0.038(3)	−0.006(2)	0.015(2)	−0.009(2)
C(2)	2a	0.676(2)	0.2932(9)	0.5791(3)	0.044(3)	0.031(3)	0.024(2)	−0.010(2)	0.009(2)	−0.007(2)
C(3)	2a	0.569(1)	0.4745(8)	0.6309(3)	0.031(2)	0.025(2)	0.024(2)	−0.006(2)	0.004(2)	−0.000(2)
C(4)	2a	0.671(1)	0.4272(8)	0.7139(3)	0.024(2)	0.020(2)	0.026(2)	−0.004(2)	0.003(2)	−0.001(2)
C(5)	2a	0.588(1)	0.5824(8)	0.7724(3)	0.026(2)	0.021(2)	0.021(2)	0.002(2)	0.004(2)	0.004(2)
C(6)	2a	0.680(1)	0.5268(8)	0.8495(3)	0.022(2)	0.022(2)	0.028(2)	−0.004(2)	0.003(2)	−0.001(2)
C(7)	2a	0.857(1)	0.3229(9)	0.8709(3)	0.028(2)	0.027(2)	0.023(2)	−0.003(2)	0.001(2)	0.004(2)
C(8)	2a	0.949(1)	0.1719(8)	0.8150(3)	0.030(2)	0.020(3)	0.036(3)	0.001(1)	−0.004(2)	0.007(2)
C(9)	2a	0.8520(9)	0.226(1)	0.7362(2)	0.026(2)	0.022(2)	0.028(2)	−0.002(3)	0.004(1)	−0.006(3)

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