Crystal structure of 4'-hydroxy-5,7-dimethoxyflavanone, C₁₇H₁₆O₅

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Received June 29, 1996, CSD-No. 402552

Source of material: Indofine Chemical Co.

The reported structure is the continuation in the systematic study of the conformational preferences of the flavanones using single crystal X-ray techniques (see ref. 1). Lorentz and polarization corrections were applied. The structure was solved and refined by Xtal3.4 programs for PC (see ref. 2). All hydrogens, except HO5 and HO(25), were generated by BONDAT (see ref. 3). None of the hydrogens were refined. The methoxy groups of the title compound are slightly twisted. The Chromon ring system has distorted half-chair conformation. The two molecules in the asymmetric unit differ in the dihedral angle between the planes of rings A and C, 36.3(7)° and 121.1(8)° in molecules (I) and (II), respectively.

C₁₇H₁₆O₅, orthorhombic, *Pbca* (No. 61), *a* = 15.50(1) Å, *b* = 21.980(3) Å, *c* = 17.280(2) Å, *V* = 5887.1 Å³, *Z* = 16, ρ_m = 1.300 g·cm⁻³, *R*(*F*) = 0.070, *R*_w(*F*) = 0.051.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless, clear prism, size 0.2 x 0.2 x 0.3 mm
Wavelength:	Cu K α radiation (1.5418 Å)
μ :	8.4 cm ⁻¹
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	$\omega/2\theta$
<i>T</i> _{measurement} :	293 K
$2\theta_{max}$:	119.9°
<i>N</i> (<i>hkl</i>) _{unique} :	1771
Criterion for <i>F</i> _o :	<i>F</i> _o > 3 σ (<i>F</i> _o)
<i>N</i> (<i>param</i>) _{refined} :	397
Program:	Xtal3.4

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(2')	8c	0.4830	0.2936	0.5603	0.038
H(3')	8c	0.5357	0.2199	0.4740	0.038
H(5')	8c	0.7347	0.1800	0.6227	0.038
H(6')	8c	0.6846	0.2576	0.7080	0.038
H(2)	8c	0.4831	0.3171	0.7089	0.038
H(13)	8c	0.6442	0.3425	0.7624	0.038
H(23)	8c	0.5781	0.2988	0.8006	0.038
H(6)	8c	0.4231	0.5786	0.7893	0.038
H(8)	8c	0.4820	0.4825	0.5906	0.038
H(111)	8c	0.3729	0.5492	0.9081	0.038
H(211)	8c	0.4612	0.5824	0.9099	0.038
H(311)	8c	0.4291	0.5474	0.9809	0.038
H(112)	8c	0.4446	0.6546	0.6962	0.038
H(212)	8c	0.3501	0.6317	0.7012	0.038
H(312)	8c	0.3797	0.6703	0.6324	0.038
H(32)	8c	0.8747	0.4137	0.3844	0.038
H(33)	8c	0.9174	0.3728	0.2650	0.038
H(35)	8c	0.8019	0.2094	0.3206	0.038
H(36)	8c	0.7572	0.2521	0.4415	0.038
H(22)	8c	0.7293	0.3360	0.5152	0.038
H(123)	8c	0.8945	0.3601	0.5520	0.038
H(223)	8c	0.8429	0.3015	0.5710	0.038
H(26)	8c	0.6871	0.5460	0.7387	0.038
H(28)	8c	0.6781	0.5207	0.5013	0.038
H(137)	8c	0.6780	0.4824	0.8427	0.038
H(237)	8c	0.7678	0.5136	0.8402	0.038
H(337)	8c	0.7523	0.4583	0.8923	0.038
H(138)	8c	0.5734	0.5900	0.5203	0.038
H(238)	8c	0.6619	0.6221	0.5105	0.038
H(338)	8c	0.5834	0.6575	0.5395	0.038

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(1)	8c	0.5400(4)	0.3868(3)	0.6531(3)	0.072(5)	0.039(4)	0.032(5)	-0.002(4)	0.001(4)	0.000(4)
O(2)	8c	0.4719(5)	0.4933(3)	0.8856(4)	0.081(6)	0.046(4)	0.055(6)	0.013(4)	0.004(5)	-0.005(4)
O(3)	8c	0.4242(5)	0.5799(3)	0.6335(4)	0.067(6)	0.059(5)	0.100(7)	0.004(4)	-0.022(5)	0.026(5)
O(4)	8c	0.5515(5)	0.3874(3)	0.8901(4)	0.109(7)	0.056(4)	0.026(5)	0.022(4)	0.000(5)	-0.007(4)
O(5)	8c	0.6691(4)	0.1496(3)	0.4893(3)	0.062(5)	0.046(4)	0.058(5)	0.006(4)	0.012(4)	-0.019(4)
C(1')	8c	0.5795(7)	0.2821(4)	0.6403(6)	0.064(8)	0.041(6)	0.041(9)	0.007(6)	0.012(7)	-0.006(6)
C(2)	8c	0.5445(7)	0.3303(4)	0.6960(6)	0.10(1)	0.051(7)	0.047(9)	0.017(6)	-0.002(7)	0.002(7)
C(2')	8c	0.5355(7)	0.2702(5)	0.5729(6)	0.071(8)	0.071(8)	0.034(9)	0.028(7)	-0.017(7)	-0.008(6)
C(3')	8c	0.5641(7)	0.2265(5)	0.5222(6)	0.076(9)	0.065(7)	0.042(8)	0.014(7)	-0.014(7)	-0.007(6)
C(3)	8c	0.5802(7)	0.3370(4)	0.7722(6)	0.10(1)	0.053(7)	0.031(8)	0.014(7)	-0.011(7)	0.010(6)
C(4)	8c	0.5455(6)	0.3878(4)	0.8202(6)	0.045(7)	0.035(5)	0.054(8)	0.002(5)	0.012(6)	-0.005(6)
C(4')	8c	0.6378(7)	0.1934(4)	0.5404(6)	0.061(8)	0.047(7)	0.043(9)	-0.021(6)	0.006(7)	0.004(6)
C(5)	8c	0.4742(6)	0.4922(4)	0.8073(7)	0.047(7)	0.046(7)	0.044(9)	-0.013(5)	-0.002(6)	0.008(6)
C(5')	8c	0.6808(7)	0.2047(4)	0.6096(6)	0.064(8)	0.051(7)	0.057(9)	0.009(6)	-0.013(7)	-0.003(6)
C(6)	8c	0.4449(7)	0.5404(4)	0.7630(7)	0.057(8)	0.041(6)	0.049(9)	0.002(6)	-0.002(7)	0.001(7)
C(6')	8c	0.6528(7)	0.2492(5)	0.6588(5)	0.065(8)	0.061(7)	0.035(7)	0.005(7)	-0.016(6)	-0.016(6)
C(7)	8c	0.4500(6)	0.5351(4)	0.6848(7)	0.040(7)	0.042(7)	0.09(1)	-0.002(6)	-0.017(7)	0.029(7)
C(8)	8c	0.4802(7)	0.4827(5)	0.6469(5)	0.055(8)	0.053(7)	0.038(8)	-0.002(6)	-0.015(6)	0.018(6)
C(9)	8c	0.5082(6)	0.4350(4)	0.6907(6)	0.043(7)	0.052(7)	0.025(9)	-0.007(6)	-0.005(6)	0.001(6)
C(10)	8c	0.5085(6)	0.4373(4)	0.7728(7)	0.035(6)	0.028(5)	0.07(1)	0.000(5)	0.002(6)	-0.004(5)
C(11)	8c	0.4329(7)	0.5447(5)	0.9258(6)	0.09(1)	0.057(8)	0.060(9)	0.017(7)	0.010(7)	-0.020(6)
C(12)	8c	0.3989(8)	0.6376(4)	0.6631(7)	0.09(1)	0.045(7)	0.14(1)	0.007(7)	-0.028(9)	0.016(8)
O(21)	8c	0.7562(4)	0.4204(3)	0.4959(3)	0.076(5)	0.047(4)	0.018(5)	0.022(4)	-0.005(4)	-0.003(4)
O(22)	8c	0.7607(4)	0.4409(3)	0.7714(4)	0.077(5)	0.063(5)	0.010(6)	0.002(4)	-0.002(4)	-0.009(4)
O(23)	8c	0.6395(4)	0.5964(3)	0.6175(4)	0.063(5)	0.046(4)	0.057(5)	0.019(4)	0.001(4)	-0.002(4)
O(24)	8c	0.8337(5)	0.3470(3)	0.7036(4)	0.106(6)	0.053(4)	0.023(6)	0.009(4)	-0.019(4)	-0.001(4)
O(25)	8c	0.8872(4)	0.2664(3)	0.2120(4)	0.081(5)	0.054(4)	0.027(5)	-0.001(4)	0.009(4)	-0.009(4)
C(22)	8c	0.7834(9)	0.3588(5)	0.5029(7)	0.17(2)	0.063(8)	0.04(1)	0.044(9)	-0.02(1)	-0.009(7)
C(23)	8c	0.8364(8)	0.3447(4)	0.5660(7)	0.12(1)	0.066(7)	0.03(1)	0.031(7)	-0.011(8)	0.000(7)
C(24)	8c	0.8121(7)	0.3719(4)	0.6431(7)	0.066(8)	0.047(7)	0.03(1)	-0.005(6)	-0.013(7)	-0.004(6)
C(25)	8c	0.7420(6)	0.4638(4)	0.7011(7)	0.053(7)	0.057(7)	0.003(9)	-0.017(6)	-0.009(6)	0.010(6)
C(26)	8c	0.7008(6)	0.5203(4)	0.6931(6)	0.043(7)	0.046(6)	0.040(9)	0.003(5)	0.002(6)	-0.004(5)
C(27)	8c	0.6789(6)	0.5407(4)	0.6194(7)	0.046(7)	0.050(7)	0.044(9)	-0.011(6)	0.005(6)	0.000(7)
C(28)	8c	0.6965(6)	0.5064(4)	0.5542(5)	0.067(8)	0.043(6)	0.022(8)	-0.006(6)	-0.004(6)	0.008(5)
C(29)	8c	0.7393(6)	0.4497(4)	0.5638(7)	0.045(6)	0.040(6)	0.020(9)	-0.003(5)	0.001(6)	0.000(6)
C(30)	8c	0.7631(6)	0.4282(4)	0.6365(6)	0.057(7)	0.040(6)	0.001(9)	-0.001(5)	-0.004(6)	0.003(6)
C(31)	8c	0.8097(8)	0.3348(5)	0.4240(6)	0.10(1)	0.065(8)	0.008(8)	0.024(7)	-0.003(7)	0.001(6)
C(32)	8c	0.8581(8)	0.3694(4)	0.3728(8)	0.08(1)	0.036(6)	0.07(1)	0.007(6)	-0.014(8)	-0.007(7)
C(33)	8c	0.8824(7)	0.3464(4)	0.3031(6)	0.058(8)	0.042(6)	0.048(8)	0.001(6)	0.015(6)	0.003(6)
C(34)	8c	0.8622(6)	0.2875(4)	0.2824(6)	0.049(7)	0.034(5)	0.039(8)	-0.008(5)	-0.013(6)	0.005(5)
C(35)	8c	0.8156(6)	0.2530(4)	0.3338(6)	0.062(8)	0.038(6)	0.033(7)	-0.002(6)	-0.004(6)	-0.003(6)
C(36)	8c	0.7895(6)	0.2760(4)	0.4029(6)	0.063(8)	0.046(6)	0.038(8)	0.001(6)	0.005(6)	0.010(5)
C(37)	8c	0.7390(7)	0.4726(5)	0.8390(5)	0.083(9)	0.086(8)	0.001(8)	-0.003(7)	-0.009(6)	-0.006(6)
C(38)	8c	0.6128(7)	0.6197(4)	0.5455(6)	0.083(9)	0.050(6)	0.053(8)	0.030(6)	-0.021(7)	0.012(6)

References

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