Crystal structure of 8-methyl-8-phenyl-[8H]-pyrano[3,2-f]quinoline, $C_{19}H_{15}NO$

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Source of material: The compound $C_{19}H_{15}NO$ was obtained by condensation of β -methylcinnamaldehyde with 6-hydroxyquinoline in presence of tetraethyl orthotitanate using toluene as solvent (see ref. 1). Crystals were obtained from heptane solution.

$C_{19}H_{15}NO$, monoclinic, $P12_1/a1$ (No. 14), $a = 21.741(4)$ Å, $b = 7.584(2)$ Å, $c = 8.802(2)$ Å, $\beta = 97.30(3)^\circ$, $V = 1439.5$ Å³, $Z = 4$, $R(F) = 0.038$, $R_w(F^2) = 0.116$.

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

Crystal:	colorless needle, size 0.10 x 0.16 x 0.43 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.78 cm ⁻¹
Diffractometer:	KM-4
Scan mode:	θ
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	54.04°
$N(hkl)_{\text{unique}}$:	2937
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	251
Programs:	SHELXS-86, SHELXL-93

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

Atom	Site	x	y	z	U_{iso}
H(3)	4e	0.3322(8)	1.004(3)	-0.052(2)	0.077(5)
H(4)	4e	0.4132(9)	1.150(3)	0.092(2)	0.082(6)
H(7)	4e	0.5211(7)	0.522(3)	0.149(2)	0.070(5)
H(8)	4e	0.5995(8)	0.645(2)	0.339(2)	0.066(4)
H(11)	4e	0.4740(9)	1.252(3)	0.294(2)	0.078(5)
H(12)	4e	0.5550(9)	1.349(3)	0.483(2)	0.087(6)
H(13)	4e	0.6374(9)	1.155(2)	0.566(2)	0.072(5)
H(16)	4e	0.390(1)	0.460(3)	0.176(2)	0.099(6)
H(17)	4e	0.336(1)	0.342(4)	0.376(3)	0.121(8)
H(18)	4e	0.247(1)	0.480(3)	0.441(3)	0.108(7)
H(19)	4e	0.207(1)	0.726(3)	0.319(2)	0.102(7)
H(20)	4e	0.2624(9)	0.858(3)	0.124(2)	0.082(5)
H(211)	4e	0.2895(9)	0.702(2)	-0.161(2)	0.076(5)
H(212)	4e	0.352(1)	0.718(3)	-0.231(3)	0.095(6)
H(213)	4e	0.3356(9)	0.534(3)	-0.141(2)	0.091(6)

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)	4e	0.42625(4)	0.6764(1)	0.0192(1)	0.0464(5)	0.0644(6)	0.0590(6)	0.0063(4)	0.0119(4)	-0.0089(4)
C(2)	4e	0.36316(6)	0.7433(2)	0.0062(2)	0.0448(6)	0.0625(8)	0.0539(8)	0.0072(5)	0.0077(5)	0.0034(6)
C(3)	4e	0.36507(7)	0.9417(2)	0.0097(2)	0.0565(8)	0.0636(9)	0.069(1)	0.0113(6)	0.0050(7)	0.0148(7)
C(4)	4e	0.41203(7)	1.0262(2)	0.0881(2)	0.0601(8)	0.0500(7)	0.0689(9)	0.0077(6)	0.0134(6)	0.0131(6)
C(5)	4e	0.46403(5)	0.9280(2)	0.1674(2)	0.0480(6)	0.0477(7)	0.0530(8)	0.0029(5)	0.0174(5)	0.0076(5)
C(6)	4e	0.46889(6)	0.7533(2)	0.1265(2)	0.0435(6)	0.0541(7)	0.0498(7)	0.0033(5)	0.0155(5)	0.0005(5)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(7)	4e	0.51975(6)	0.6489(2)	0.1857(2)	0.0484(7)	0.0525(7)	0.0655(9)	0.0086(5)	0.0165(6)	-0.0016(6)
C(8)	4e	0.56491(6)	0.7185(2)	0.2893(2)	0.0452(6)	0.0608(8)	0.0661(9)	0.0083(6)	0.0123(6)	0.0041(6)
C(9)	4e	0.56167(6)	0.8946(2)	0.3391(2)	0.0448(6)	0.0607(7)	0.0531(8)	-0.0022(5)	0.0165(5)	0.0038(6)
C(10)	4e	0.51063(6)	1.0006(2)	0.2773(2)	0.0481(6)	0.0498(7)	0.0546(8)	-0.0028(5)	0.0213(5)	0.0049(5)
C(11)	4e	0.50907(7)	1.1746(2)	0.3339(2)	0.0620(8)	0.0499(7)	0.072(1)	-0.0037(6)	0.0222(7)	0.0031(6)
C(12)	4e	0.55550(8)	1.2317(2)	0.4408(2)	0.072(1)	0.0632(9)	0.075(1)	-0.0169(7)	0.0271(8)	-0.0102(8)
C(13)	4e	0.60389(8)	1.1179(3)	0.4936(2)	0.0618(9)	0.083(1)	0.062(1)	-0.0201(8)	0.0182(7)	-0.0081(8)
N(14)	4e	0.60802(5)	0.9544(2)	0.4461(1)	0.0507(6)	0.0793(9)	0.0613(8)	-0.0079(6)	0.0132(5)	-0.0002(6)
C(15)	4e	0.33104(6)	0.6671(2)	0.1359(2)	0.0446(6)	0.0558(7)	0.0489(7)	0.0020(5)	0.0047(5)	-0.0034(5)
C(16)	4e	0.35160(8)	0.5145(2)	0.2114(2)	0.0630(8)	0.0618(8)	0.072(1)	0.0047(7)	0.0104(7)	0.0087(7)
C(17)	4e	0.3205(1)	0.4444(3)	0.3260(2)	0.087(1)	0.083(1)	0.076(1)	-0.017(1)	0.0023(9)	0.021(1)
C(18)	4e	0.26858(9)	0.5247(3)	0.3649(2)	0.071(1)	0.117(2)	0.064(1)	-0.033(1)	0.0124(8)	0.003(1)
C(19)	4e	0.24718(8)	0.6751(3)	0.2901(2)	0.0536(8)	0.113(2)	0.075(1)	-0.0098(9)	0.0207(7)	-0.016(1)
C(20)	4e	0.27806(7)	0.7460(2)	0.1769(2)	0.0478(7)	0.077(1)	0.069(1)	0.0071(7)	0.0111(6)	-0.0039(8)
C(21)	4e	0.33242(9)	0.6721(3)	-0.1465(2)	0.0626(9)	0.102(1)	0.053(1)	-0.0032(9)	0.0057(7)	-0.0010(9)

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