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Crystal structure of 1-(2-chloro-1-phenyl)-2,6,6,-trimethyl-3-(1-oxo-3-hydroxy-5,5-dimethyl-2-cyclohexen-2-yl)-4-oxo-4,5,6,7-tetrahydroindole, $C_{25}H_{28}ClNO_3$

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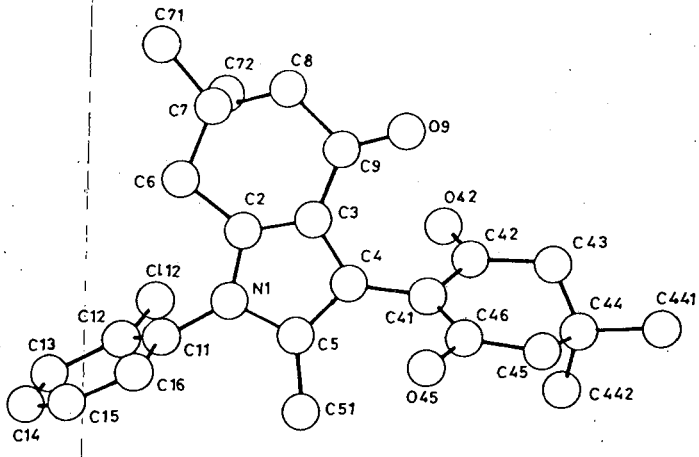

Source of material: see ref. 2.

$C_{25}H_{28}ClNO_3$, monoclinic, *C2/c* (No. 15), a =34.307(5) Å, b =6.829(2) Å, c =20.208(3) Å, β =101.615(2)°, V =4637.5 Å^3, Z =8, $R(F)$ =0.089, $R_w(F)$ =0.096.

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

Crystal:	colorless needles, size 0.4 x 0.125 x 0.075 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	1.86 cm^{-1}
Diffractometer:	Enraf Nonius CAD4
Scan mode:	ω-2θ
$T_{measurement}$:	295 K
$2\theta_{max}$:	80°
$N(hkl)_{unique}$:	2169
Criterion for F_o:	$F_o > 5\,\sigma\,(F_o)$
$N(param)_{refined}$:	330
Program:	SHELXTL-plus

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

Atom	Site	Occ.	x	y	z	B_{eq}
C(72)	8*f*	0.5	0.4380(7)	0.191(3)	0.104(1)	11.8(4)
C(72')	8*f*	0.5	0.4944(9)	–0.223(5)	0.112(2)	11.8(4)
Cl(12)	8*f*	0.8	0.3613(1)	0.0310(6)	0.2390(2)	11.8(4)
Cl(16)	8*f*	0.2	0.4295(6)	–0.618(3)	0.237(1)	11.8(4)

Table 3. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	8*f*	0.3867(3)	–0.306(1)	0.1710(5)	0.076(8)	0.059(7)	0.041(7)	–0.040(6)	0.012(6)	–0.013(6)
C(2)	8*f*	0.4107(3)	–0.218(2)	0.1345(6)	0.065(9)	0.07(1)	0.041(8)	–0.050(8)	0.019(7)	–0.006(7)
C(3)	8*f*	0.3957(4)	–0.240(2)	0.0684(5)	0.069(9)	0.068(9)	0.019(7)	–0.039(8)	0.018(7)	–0.002(7)
C(4)	8*f*	0.3613(3)	–0.356(2)	0.0612(5)	0.046(8)	0.025(7)	0.047(9)	–0.009(6)	0.006(7)	–0.003(7)
C(5)	8*f*	0.3551(4)	–0.394(2)	0.1256(6)	0.066(9)	0.019(7)	0.054(8)	–0.007(7)	0.012(8)	0.000(7)
C(51)	8*f*	0.3245(3)	–0.508(2)	0.1477(5)	0.063(8)	0.062(9)	0.038(7)	–0.026(8)	0.024(6)	0.001(7)
C(6)	8*f*	0.4484(4)	–0.111(3)	0.1706(8)	0.10(1)	0.16(2)	0.12(1)	–0.08(1)	0.04(1)	–0.02(1)
C(7)	8*f*	0.4670(4)	–0.016(2)	0.1176(6)	0.067(9)	0.11(1)	0.036(8)	–0.05(1)	0.004(7)	–0.002(8)
C(71)	8*f*	0.5048(4)	0.101(3)	0.1404(8)	0.09(1)	0.17(2)	0.12(1)	–0.07(1)	0.01(1)	–0.00(1)
C(8)	8*f*	0.4532(6)	–0.039(4)	0.0455(8)	0.21(2)	0.28(3)	0.08(1)	–0.15(2)	–0.01(1)	–0.03(2)
C(9)	8*f*	0.4164(4)	–0.169(2)	0.0195(7)	0.10(1)	0.08(1)	0.050(9)	–0.051(9)	0.019(9)	–0.019(9)
O(9)	8*f*	0.4077(2)	–0.192(1)	–0.0417(4)	0.097(7)	0.093(8)	0.046(5)	–0.033(6)	0.018(5)	–0.008(6)
C(11)	8*f*	0.3911(3)	–0.317(2)	0.2419(5)	0.064(8)	0.086(9)	0.027(6)	–0.029(7)	0.025(6)	–0.028(7)
C(12)	8*f*	0.3810(3)	–0.170(2)	0.2774(7)	0.051(8)	0.08(1)	0.052(9)	–0.022(8)	0.007(7)	0.025(9)

Table 3. (Continued)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(13)	8*f*	0.3877(4)	−0.180(3)	0.3525(9)	0.06(1)	0.10(1)	0.10(1)	−0.01(1)	0.024(9)	−0.02(1)
C(14)	8*f*	0.4027(5)	−0.339(4)	0.3802(8)	0.08(1)	0.16(2)	0.07(1)	−0.00(1)	0.01(1)	0.03(1)
C(15)	8*f*	0.4128(4)	−0.496(3)	0.3428(8)	0.07(1)	0.17(2)	0.14(1)	0.00(1)	0.013(9)	0.01(1)
C(16)	8*f*	0.4071(4)	−0.493(3)	0.2746(6)	0.10(1)	0.20(2)	0.040(8)	−0.01(1)	−0.009(8)	0.07(1)
C(41)	8*f*	0.3351(3)	−0.419(2)	−0.0030(5)	0.033(7)	0.030(8)	0.044(7)	0.006(6)	−0.005(6)	0.012(7)
C(42)	8*f*	0.3183(3)	−0.270(2)	−0.0509(5)	0.08(1)	0.025(8)	0.044(8)	−0.022(7)	0.005(7)	−0.013(7)
O(42)	8*f*	0.3216(2)	−0.093(1)	−0.0349(4)	0.109(7)	0.019(5)	0.079(6)	−0.006(5)	−0.006(5)	−0.005(5)
C(43)	8*f*	0.2958(3)	−0.330(2)	−0.1207(6)	0.071(9)	0.041(8)	0.070(9)	−0.006(8)	−0.011(7)	0.007(7)
C(44)	8*f*	0.2728(3)	−0.509(2)	−0.1199(5)	0.044(8)	0.033(7)	0.036(7)	−0.000(7)	−0.011(6)	0.001(6)
C(441)	8*f*	0.2542(4)	−0.574(2)	−0.1918(5)	0.10(1)	0.065(9)	0.052(8)	−0.023(8)	−0.008(7)	−0.002(7)
C(442)	8*f*	0.2373(4)	−0.469(2)	−0.0829(6)	0.070(9)	0.01(1)	0.076(9)	0.001(9)	0.003(8)	−0.013(8)
C(45)	8*f*	0.2985(3)	−0.668(2)	−0.0843(5)	0.051(8)	0.030(7)	0.051(7)	−0.011(7)	−0.006(6)	−0.010(7)
O(45)	8*f*	0.3435(2)	−0.750(1)	0.0210(3)	0.066(5)	0.021(4)	0.058(5)	−0.004(4)	−0.013(4)	0.002(4)
C(46)	8*f*	0.3257(3)	−0.607(2)	−0.0212(5)	0.043(8)	0.005(7)	0.055(8)	0.000(6)	0.006(6)	0.009(7)

References

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