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[2-(*N*,*N*-Dimethylamino)-5-methylphenyl]-diphenylmethanol

Louise B. Kranholm, Andrew D. Bond* and Christine J. McKenzie

University of Southern Denmark, Department of Chemistry, Campusvej 55, 5230 Odense M, Denmark

Correspondence e-mail: adb@chem.sdu.dk

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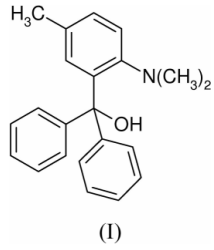
The crystal structure of (2-(*N*,*N*-dimethylamino)-5-methylphenyl)diphenylmethanol, $C_{22}H_{23}NO$, (I), at 180 K contains an intramolecular N—H···O hydrogen bond.



(I)

Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.153
Data-to-parameter ratio = 19.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Experimental

The compound was prepared according to a literature procedure (Ludt *et al.*, 1970). Crystals suitable for X-ray analysis were prepared by evaporation of an ethyl acetate/hexane solution.

Crystal data

$C_{22}H_{23}NO$
M_r = 317.41
Monoclinic, $P2_1/n$
a = 8.9287 (4) Å
b = 13.2618 (6) Å
c = 15.1880 (8) Å
β = 98.505 (1)°
V = 1778.64 (15) Å^3
Z = 4
D_x = 1.185 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3897 reflections
θ = 2.7–28.1°
μ = 0.07 mm^{-1}
T = 180 (2) K
Block, colourless
0.40 × 0.32 × 0.24 mm

Data collection

Bruker–Nonius X8APEXII CCD diffractometer
Thin-slice ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.820, T_{max} = 0.983
10423 measured reflections
4347 independent reflections
3398 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 28.3°
$h = -11 \rightarrow 11$
$k = -17 \rightarrow 9$
$l = -19 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.153
S = 1.08
4347 reflections
224 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0959P)^2 + 0.1677P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.88 (2)	1.87 (2)	2.6683 (14)	150.6 (18)

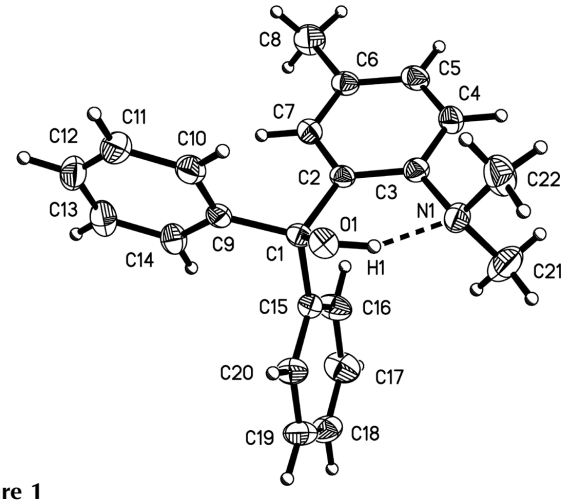


Figure 1
A view of the molecular structure, with displacement ellipsoids drawn at the 50% probability level for non-H atoms. H atoms are shown as spheres of arbitrary radius. The dashed line denotes the intramolecular hydrogen bond.

H atoms bound to C were positioned geometrically and allowed to ride during subsequent refinement: C—H = 0.95 Å, U_{iso}(H) = 1.2 U_{eq}(C) for H atoms bound to the phenyl rings; C—H = 0.98 Å, U_{iso}(H) = 1.5 U_{eq}(C) for H atoms of the methyl groups. The methyl groups were allowed to rotate about their local threefold axes. H1, associated with the hydroxyl group, was located in a difference Fourier map and refined freely with an isotropic displacement parameter.

Data collection: *APEX*2 (Bruker–Nonius, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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