Crystal structure of 2-[2,6-bis(1-methylethyl)phenyl]-2,3-dihydro-1*H*-isoindol-1-one, $C_{20}H_{23}NO$, *at 193K*

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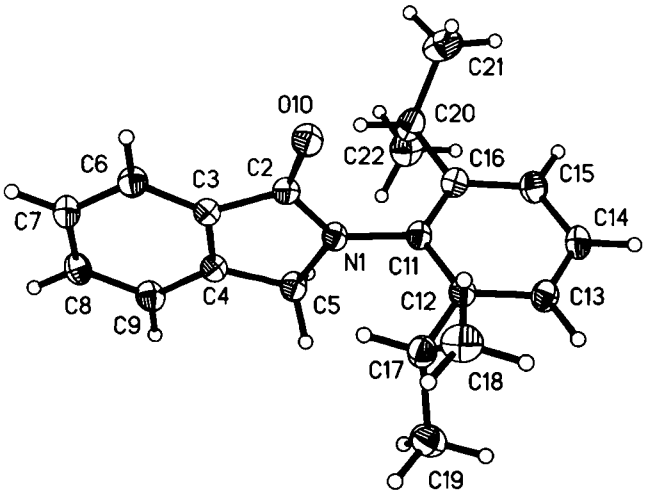

Abstract

$C_{20}H_{23}NO$, monoclinic, $C12/c1$ (No. 15), $a = 18.402(4)$ Å, $b = 14.897(3)$ Å, $c = 12.318(3)$ Å, $\beta = 95.09(3)°$, $V = 3363.5$ Å^3, $Z = 8$, $R_{gt}(F) = 0.053$, $wR_{ref}(F^2) = 0.150$, $T = 193$ K.

Source of material

A solution of phthaldialdehyde and 2,6-di(1-methylethyl)aniline in toluene was refluxed overnight under a Dean-Stark trap [1]. The title compound was crystallised from ethanol.

Discussion

The title compound adopts the structure as expected. The plane of aryl ring is perpenticular to isoindole plane. The nitrogen is sp^2-hybridized, and the sum of angles at N1 is 360.0°. The N1—C(11) bond is only slightly longer than N1—C2.

Table 1. Data collection and handling.

Crystal:	colourless prismatic, size 0.30 × 0.40 × 0.45 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.71 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC7S, $\omega/2\theta$
$2\theta_{max}$:	50.02°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5757, 2905
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2577
$N(param)_{refined}$:	200
Programs:	SHELXS-86 [2], SHELXL-97 [3], SHELXTL-NT [4], teXsan [5]

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

Atom	Site	x	y	z	U_{iso}
H(5A)	8*f*	0.1533	–0.1084	–0.0331	0.046
H(5B)	8*f*	0.2041	–0.0406	–0.0901	0.046
H(6A)	8*f*	0.0793	0.1768	0.1379	0.049
H(7A)	8*f*	–0.0132	0.2075	0.0020	0.053
H(8A)	8*f*	–0.0264	0.1205	–0.1538	0.054
H(9A)	8*f*	0.0534	0.0038	–0.1791	0.051
H(13A)	8*f*	0.3251	–0.2701	0.2242	0.047
H(14A)	8*f*	0.4379	–0.2233	0.1805	0.050
H(15A)	8*f*	0.4520	–0.0860	0.0996	0.053
H(17A)	8*f*	0.1598	–0.1424	0.1830	0.051
H(18A)	8*f*	0.2182	–0.1492	0.3614	0.084
H(18B)	8*f*	0.2338	–0.2517	0.3462	0.084
H(18C)	8*f*	0.1533	–0.2177	0.3487	0.084
H(19A)	8*f*	0.1644	–0.2663	0.0660	0.083
H(19B)	8*f*	0.1199	–0.2903	0.1649	0.083
H(19C)	8*f*	0.2004	–0.3242	0.1626	0.083
H(20A)	8*f*	0.3094	0.0726	0.0306	0.061
H(21A)	8*f*	0.4028	0.1036	0.1669	0.107
H(21B)	8*f*	0.4163	0.1543	0.0590	0.107
H(21C)	8*f*	0.4606	0.0671	0.0918	0.107
H(22A)	8*f*	0.3778	0.0845	–0.1212	0.098
H(22B)	8*f*	0.3322	–0.0045	–0.1270	0.098
H(22C)	8*f*	0.4159	–0.0073	–0.0905	0.098

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Table 3. 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*	0.21354(7)	-0.02913(9)	0.0751(1)	0.0378(7)	0.0371(7)	0.0254(7)	0.0056(6)	-0.0013(5)	-0.0005(5)
C(2)	8*f*	0.18493(9)	0.0396(1)	0.1298(1)	0.0360(8)	0.0349(8)	0.0261(8)	-0.0012(6)	0.0023(6)	0.0017(6)
C(3)	8*f*	0.12135(8)	0.0728(1)	0.0583(1)	0.0338(8)	0.0356(8)	0.0281(8)	-0.0009(6)	0.0036(6)	0.0021(6)
C(4)	8*f*	0.11419(9)	0.0211(1)	-0.0354(1)	0.0375(8)	0.0384(8)	0.0277(8)	-0.0001(7)	0.0015(6)	0.0018(7)
C(5)	8*f*	0.17330(9)	-0.0481(1)	-0.0308(1)	0.0442(9)	0.0429(9)	0.0274(8)	0.0063(7)	-0.0028(7)	-0.0039(7)
C(6)	8*f*	0.07416(9)	0.1427(1)	0.0745(1)	0.0421(9)	0.0440(9)	0.0355(9)	0.0038(7)	0.0035(7)	-0.0051(7)
C(7)	8*f*	0.01896(9)	0.1604(1)	-0.0065(2)	0.0394(9)	0.047(1)	0.046(1)	0.0084(7)	0.0022(7)	0.0012(8)
C(8)	8*f*	0.01132(9)	0.1081(1)	-0.1005(1)	0.0386(9)	0.055(1)	0.0390(9)	0.0045(8)	-0.0050(7)	0.0041(8)
C(9)	8*f*	0.0587(1)	0.0384(1)	-0.1160(1)	0.0451(9)	0.051(1)	0.0301(8)	0.0019(8)	-0.0026(7)	-0.0034(8)
O(10)	8*f*	0.20808(7)	0.06766(8)	0.21973(9)	0.0522(7)	0.0503(8)	0.0300(6)	0.0072(6)	-0.0057(5)	-0.0080(5)
C(11)	8*f*	0.27735(9)	-0.0804(1)	0.1116(1)	0.0369(8)	0.0375(8)	0.0254(7)	0.0062(7)	0.0005(6)	-0.0017(6)
C(12)	8*f*	0.26837(9)	-0.1614(1)	0.1660(1)	0.0387(9)	0.0380(9)	0.0276(8)	0.0033(7)	0.0002(6)	-0.0013(6)
C(13)	8*f*	0.32978(9)	-0.2149(1)	0.1902(1)	0.0457(9)	0.0407(9)	0.0314(8)	0.0056(7)	0.0017(7)	0.0042(7)
C(14)	8*f*	0.39741(9)	-0.1867(1)	0.1643(1)	0.0405(9)	0.049(1)	0.0345(8)	0.0123(8)	0.0004(7)	0.0017(8)
C(15)	8*f*	0.40578(9)	-0.1048(1)	0.1146(2)	0.0373(9)	0.051(1)	0.044(1)	0.0037(8)	0.0081(7)	0.0010(8)
C(16)	8*f*	0.34580(9)	-0.0498(1)	0.0867(1)	0.0418(9)	0.0415(9)	0.0347(8)	0.0037(7)	0.0067(7)	0.0017(7)
C(17)	8*f*	0.19507(9)	-0.1904(1)	0.2017(1)	0.0396(9)	0.042(1)	0.046(1)	0.0029(7)	0.0051(7)	0.0066(8)
C(18)	8*f*	0.2006(1)	-0.2035(2)	0.3262(2)	0.059(1)	0.064(1)	0.049(1)	-0.007(1)	0.0227(9)	-0.0057(9)
C(19)	8*f*	0.1674(1)	-0.2757(1)	0.1434(2)	0.053(1)	0.061(1)	0.051(1)	-0.0105(9)	-0.0017(9)	0.0020(9)
C(20)	8*f*	0.3556(1)	0.0398(1)	0.0309(2)	0.047(1)	0.045(1)	0.064(1)	0.0055(8)	0.0177(9)	0.0118(9)
C(21)	8*f*	0.4143(1)	0.0964(2)	0.0928(2)	0.079(2)	0.048(1)	0.090(2)	-0.009(1)	0.023(1)	-0.005(1)
C(22)	8*f*	0.3719(1)	0.0269(2)	-0.0881(2)	0.072(1)	0.068(1)	0.058(1)	-0.001(1)	0.016(1)	0.024(1)

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