Crystal structure of 4-*N*-phenylisoindolinone, $C_{14}H_{11}NO$

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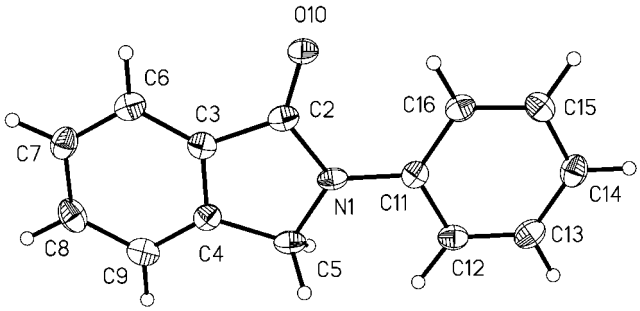

Abstract

$C_{14}H_{11}NO$, monoclinic, $P12_1/n1$ (No. 14), a = 5.925(4) Å, b = 7.556(2) Å, c = 23.11(1) Å, β = 94.67(5)°, V = 1031.3 Å^3, Z = 4, $R_{gt}(F)$ = 0.055, $wR_{ref}(F^2)$ = 0.140, T = 193 K.

Source of material

Phthaldialdehyde and aniline in toluene solution was refluxed overnight under a Dean-Stark trap [1]. The title compound was crystallised from ethanol.

Discussion

The title compound, 4-*N*-phenylisoindolinone, has a slightly distorted sp^2-hybridised nitrogen, the sum of angles at N1 is 359.1°. Since the phenyl ring is almost co-planar to the isoindolinone plane, 9.4(1)°, a reasonable π-interaction could be expected. The bond length of N1—C11 is slightly shorter, 1.421(3) Å, than in 2-[2,6-bis(1-methylethyl)phenyl]-2,3-dihydro-1*H*-isoindol-1-one [2], 1.428(2) Å, in which π-interaction can not exist because the aryl ring adopts perpendicular orientation to the isoindolinone part of the molecule. The π-interaction of the nitrogen to the phenyl ring might also explain the weaker interaction of the nitrogen to the carbonyl group; N1—C2 bond is 1.376(3) Å, whereas in 2-[2,6-bis(1-methylethyl)phenyl]-2,3-dihydro-1*H*-isoindol-1-one bond length is 1.358(2) Å.

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.20 × 0.30 × 0.45 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.85 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC7S, $\omega/2\theta$
$2\theta_{max}$:	50.06°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	7640, 1809
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1250
$N(param)_{refined}$:	145
Programs:	SHELXS-97 [3] SHELXL-97 [4], SHELXTL-NT [5]

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

Atom	Site	x	y	z	U_{iso}
H(5A)	4*e*	0.8331	0.3642	0.2822	0.045
H(5B)	4*e*	0.7066	0.1809	0.2731	0.045
H(6A)	4*e*	0.1207	0.5094	0.3717	0.047
H(7A)	4*e*	0.2537	0.4222	0.4642	0.052
H(8A)	4*e*	0.5970	0.2740	0.4786	0.057
H(9A)	4*e*	0.8110	0.2141	0.4009	0.051
H(12A)	4*e*	0.8416	0.2644	0.1857	0.046
H(13A)	4*e*	0.8638	0.2292	0.0880	0.054
H(14A)	4*e*	0.5729	0.3207	0.0229	0.053
H(15A)	4*e*	0.2574	0.4533	0.0567	0.049
H(16A)	4*e*	0.2277	0.4886	0.1544	0.044

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)	4*e*	0.5175(3)	0.3888(3)	0.24255(9)	0.024(1)	0.026(1)	0.047(1)	0.0030(9)	0.0034(9)	–0.0001(9)
C(2)	4*e*	0.3347(4)	0.4499(3)	0.2698(1)	0.031(1)	0.027(1)	0.047(2)	–0.003(1)	0.004(1)	–0.001(1)
C(3)	4*e*	0.3858(4)	0.4126(3)	0.3325(1)	0.036(2)	0.026(1)	0.041(2)	–0.005(1)	0.001(1)	0.001(1)
C(4)	4*e*	0.5905(4)	0.3259(3)	0.3405(1)	0.035(2)	0.027(1)	0.041(2)	–0.008(1)	0.006(1)	–0.004(1)
C(5)	4*e*	0.6881(4)	0.3048(3)	0.2826(1)	0.028(1)	0.029(1)	0.056(2)	0.001(1)	–0.000(1)	0.000(1)
C(6)	4*e*	0.2581(5)	0.4502(3)	0.3779(1)	0.038(2)	0.030(1)	0.050(2)	–0.000(1)	0.006(1)	–0.003(1)
C(7)	4*e*	0.3375(5)	0.3983(4)	0.4328(1)	0.049(2)	0.039(2)	0.042(2)	–0.007(1)	0.014(1)	–0.003(1)

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Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(8)	4*e*	0.5445(5)	0.3093(4)	0.4414(1)	0.063(2)	0.040(2)	0.038(2)	–0.007(2)	–0.005(1)	0.008(1)
C(9)	4*e*	0.6731(5)	0.2728(3)	0.3951(1)	0.041(2)	0.031(2)	0.056(2)	–0.000(1)	–0.004(1)	0.002(1)
O(10)	4*e*	0.1624(3)	0.5193(3)	0.24709(8)	0.033(1)	0.049(1)	0.044(1)	0.0150(9)	0.0028(8)	0.0038(9)
C(11)	4*e*	0.5289(4)	0.3763(3)	0.1815(1)	0.036(1)	0.021(1)	0.038(2)	–0.006(1)	0.006(1)	–0.001(1)
C(12)	4*e*	0.7219(4)	0.3010(3)	0.1600(1)	0.032(1)	0.034(2)	0.050(2)	–0.001(1)	0.001(1)	0.001(1)
C(13)	4*e*	0.7356(5)	0.2808(4)	0.1015(1)	0.042(2)	0.038(2)	0.055(2)	0.001(1)	0.014(1)	–0.003(1)
C(14)	4*e*	0.5631(5)	0.3358(4)	0.0626(1)	0.054(2)	0.039(2)	0.039(2)	–0.006(1)	0.012(1)	–0.004(1)
C(15)	4*e*	0.3740(5)	0.4142(3)	0.0830(1)	0.045(2)	0.035(2)	0.043(2)	0.000(1)	–0.003(1)	0.002(1)
C(16)	4*e*	0.3556(4)	0.4351(3)	0.1415(1)	0.033(1)	0.032(1)	0.046(2)	0.001(1)	0.007(1)	–0.003(1)

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