Crystal structure of 2-[2,6-di(methylethyl)phenylamino]pyridine, $C_{17}H_{22}N_2$

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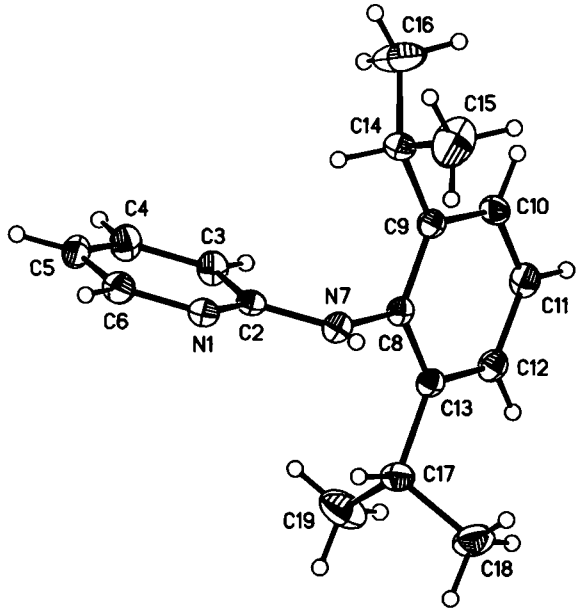

Abstract

$C_{17}H_{22}N_2$, monoclinic, $C12/c1$ (no. 15), a = 10.705(2) Å, b = 14.654(3) Å, c = 19.558(4) Å, β = 94.74(3)°, V = 3057.6 Å^3, Z = 8, $R_{gt}(F)$ = 0.079, $wR_{ref}(F^2)$ = 0.196, T = 173 K.

Source of material

The title compound was obtained in a one-step procedure [1,2]. 2-Chloropyridine and 2,6-di(methylethyl)aniline hydrochloride were heated at 180 °C for 90 minutes. The hydrochlorous raw product was suspended to aqueous sodium carbonate and then extracted with dichloromethane. The dichloromethane solution was dried over anhydrous sodium sulfate, then filtered and the solvent was removed. Recrystallization from diethylether/heptane yielded large colorless mosaic crystals.

Discussion

The crystal structure reported here is similar to 2-(2,6-dimethylphenylamino)pyridine [3]. 2-(2,6-Di(methylethyl)phenylamino)-pyridine crystallizes with two similar N7–H7···N1′ interactions that form dimeric structure. The N7–H7···N1′ angle is 167 (2)°, where the N1···H7′ distance is 2.13(3) Å and this results in a donor-acceptor distance of 2.998(3) Å.

Table 1. Data collection and handling.

Crystal:	colorless plate, size 0.20 × 0.25 × 0.35 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.65 cm^{-1}
Diffractometer, scan mode:	Nonius 95 mm KappaCCD, ω
$2\theta_{max}$:	53°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	26983, 3161
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2470
$N(param)_{refined}$:	175
Programs:	SHELXS-97 [4], SHELXL-97 [5], SHELXTL [6]

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

Atom	Site	x	y	z	U_{iso}
H(3A)	8*f*	0.3908	0.1666	0.2536	0.044
H(4A)	8*f*	0.4432	0.1692	0.1416	0.052
H(5A)	8*f*	0.2848	0.1705	0.0518	0.049
H(6A)	8*f*	0.0803	0.1660	0.0789	0.045
H(7)	8*f*	0.082(3)	0.175(2)	0.298(1)	0.036
H(10)	8*f*	0.4078	0.3364	0.4419	0.044
H(11)	8*f*	0.4563	0.2144	0.5138	0.046
H(12)	8*f*	0.3739	0.0717	0.4880	0.043
H(14)	8*f*	0.2512	0.3251	0.2763	0.047
H(15A)	8*f*	0.0764	0.3463	0.3388	0.122
H(15B)	8*f*	0.1169	0.4394	0.3079	0.122
H(15C)	8*f*	0.1505	0.4181	0.3857	0.122
H(16A)	8*f*	0.4430	0.3917	0.3108	0.118
H(16B)	8*f*	0.3807	0.4468	0.3677	0.118
H(16C)	8*f*	0.3426	0.4667	0.2900	0.118
H(17)	8*f*	0.1605	0.0164	0.3434	0.045
H(18A)	8*f*	0.0827	0.0199	0.4517	0.089
H(18B)	8*f*	0.2037	−0.0296	0.4836	0.089
H(18C)	8*f*	0.1103	−0.0810	0.4309	0.089
H(19A)	8*f*	0.3654	−0.0337	0.3312	0.110
H(19B)	8*f*	0.2836	−0.1140	0.3562	0.110
H(19C)	8*f*	0.3791	−0.0637	0.4084	0.110

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*	0.1090(2)	0.1666(1)	0.17886(9)	0.0247(9)	0.031(1)	0.036(1)	0.0000(8)	−0.0021(7)	0.0004(7)
C(2)	8*f*	0.2002(2)	0.1674(1)	0.2305(1)	0.023(1)	0.025(1)	0.033(1)	−0.0004(8)	0.0003(8)	−0.0002(8)
C(3)	8*f*	0.3285(2)	0.1674(2)	0.2175(1)	0.021(1)	0.051(2)	0.038(1)	−0.004(1)	0.0012(8)	−0.005(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(4)	8*f*	0.3594(2)	0.1686(2)	0.1509(1)	0.030(1)	0.057(2)	0.043(1)	–0.007(1)	0.009(1)	–0.009(1)
C(5)	8*f*	0.2658(2)	0.1690(2)	0.0974(1)	0.045(1)	0.047(2)	0.032(1)	–0.005(1)	0.007(1)	–0.002(1)
C(6)	8*f*	0.1434(2)	0.1671(2)	0.1145(1)	0.040(1)	0.038(1)	0.034(1)	0.002(1)	–0.0061(9)	0.0017(9)
N(7)	8*f*	0.1631(2)	0.1682(1)	0.29510(9)	0.0165(8)	0.040(1)	0.0342(9)	–0.0014(8)	0.0004(7)	0.0011(8)
C(8)	8*f*	0.2464(2)	0.1807(2)	0.3557(1)	0.0176(9)	0.034(1)	0.030(1)	0.0000(8)	0.0043(7)	–0.0005(8)
C(9)	8*f*	0.2973(2)	0.2684(2)	0.3704(1)	0.027(1)	0.033(1)	0.035(1)	–0.0007(9)	0.0086(8)	–0.0017(9)
C(10)	8*f*	0.3748(2)	0.2792(2)	0.4306(1)	0.035(1)	0.037(1)	0.040(1)	–0.010(1)	0.0062(9)	–0.007(1)
C(11)	8*f*	0.4035(2)	0.2060(2)	0.4741(1)	0.030(1)	0.053(2)	0.032(1)	–0.009(1)	–0.0011(9)	–0.003(1)
C(12)	8*f*	0.3537(2)	0.1204(2)	0.4586(1)	0.032(1)	0.042(1)	0.033(1)	0.000(1)	0.0023(9)	0.0038(9)
C(13)	8*f*	0.2736(2)	0.1063(2)	0.3995(1)	0.023(1)	0.034(1)	0.032(1)	–0.0025(9)	0.0044(8)	0.0007(8)
C(14)	8*f*	0.2645(2)	0.3493(2)	0.3231(1)	0.048(1)	0.027(1)	0.042(1)	0.001(1)	0.007(1)	0.0003(9)
C(15)	8*f*	0.1405(4)	0.3923(3)	0.3405(2)	0.091(3)	0.078(3)	0.079(2)	0.048(2)	0.028(2)	0.025(2)
C(16)	8*f*	0.3671(4)	0.4201(2)	0.3229(2)	0.091(3)	0.052(2)	0.092(3)	–0.029(2)	–0.008(2)	0.026(2)
C(17)	8*f*	0.2196(2)	0.0117(2)	0.3842(1)	0.038(1)	0.034(1)	0.041(1)	–0.005(1)	–0.002(1)	0.003(1)
C(18)	8*f*	0.1473(3)	–0.0230(2)	0.4431(2)	0.058(2)	0.057(2)	0.063(2)	–0.025(2)	0.006(1)	0.009(1)
C(19)	8*f*	0.3213(3)	–0.0562(2)	0.3685(2)	0.068(2)	0.045(2)	0.109(3)	0.003(2)	0.016(2)	–0.022(2)

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