Crystal structure of 2-(2,6-dimethylphenylamino)pyridine, C₁₃H₁₄N₂

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Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.25 × 0.35 × 0.40 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.70 cm ⁻¹
Diffractometer, scan mode:	Rigaku AFC7S, $\omega/2\theta$
$2\theta_{\max}$:	50.04°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	8271, 1997
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1433
$N(\text{param})_{\text{refined}}$:	192
Programs:	SHELXS-86 [2], SHELXL-97 [3], SHELXTL-NT [4], teXsan [5]

Abstract

C₁₃H₁₄N₂, monoclinic, $P12_1/c1$ (No. 14), $a = 12.65(2)$ Å, $b = 7.185(2)$ Å, $c = 13.87(2)$ Å, $\beta = 116.40(3)^\circ$, $V = 1129.5$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.043$, $wR_{\text{ref}}(F^2) = 0.103$, $T = 193$ K.

Source of material

The title compound was obtained in one-step synthesis. 2-Chloropyridine and 2,6-dimethylaniline hydrochloride were heated at 450 K for two hours. Resulting hydrochlorous raw product was suspended to sodium carbonate solution. Product was extracted into dichloromethane [1]. The title compound was crystallised from diethylether-heptane.

Discussion

Title compound crystallizes as a centrosymmetric dimer with two similar N–H–H interactions. Donor-acceptor distances are 3.054(2) Å. According to previously published studies, the formation of the centrosymmetric pairs seems to be typical for 2-aminopyridines. Also donor-acceptor distances are similar to previous data ([1] and references therein).

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(3)	4e	0.207(2)	0.150(2)	0.207(1)	0.036(4)
H(4)	4e	0.235(2)	−0.001(2)	0.070(2)	0.047(5)
H(5)	4e	0.415(2)	−0.171(2)	0.120(2)	0.045(5)
H(6)	4e	0.552(2)	−0.187(2)	0.304(1)	0.039(5)
H(7)	4e	0.407(2)	0.120(3)	0.479(2)	0.052(6)
H(101)	4e	0.384(4)	0.529(4)	0.386(3)	0.14(1)
H(102)	4e	0.264(3)	0.654(4)	0.302(2)	0.106(9)
H(103)	4e	0.310(3)	0.473(4)	0.274(2)	0.10(1)
H(11)	4e	0.086(2)	0.602(3)	0.311(2)	0.061(6)
H(12)	4e	−0.038(2)	0.450(3)	0.376(2)	0.082(7)
H(13)	4e	0.019(2)	0.154(3)	0.451(2)	0.072(7)
H(151)	4e	0.152(3)	−0.115(4)	0.503(2)	0.093(8)
H(152)	4e	0.280(3)	−0.042(3)	0.569(2)	0.093(8)
H(153)	4e	0.232(2)	−0.128(3)	0.449(2)	0.077(7)

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
N(1)	4e	0.4659(1)	-0.0275(2)	0.3606(1)	0.0322(8)	0.0346(7)	0.0341(7)	0.0056(6)	0.0167(6)	0.0018(5)
C(2)	4e	0.3656(1)	0.0705(2)	0.3329(1)	0.0296(8)	0.0271(7)	0.0313(8)	-0.0019(6)	0.0155(7)	0.0016(6)
C(3)	4e	0.2782(2)	0.0828(2)	0.2252(1)	0.0298(9)	0.0314(8)	0.0328(9)	-0.0004(7)	0.0138(7)	0.0001(7)
C(4)	4e	0.2963(2)	-0.0072(2)	0.1462(1)	0.040(1)	0.0332(8)	0.0319(9)	-0.0048(7)	0.0149(8)	-0.0015(7)
C(5)	4e	0.3996(2)	-0.1070(2)	0.1736(1)	0.050(1)	0.0339(9)	0.039(1)	-0.0029(8)	0.0253(9)	-0.0065(7)
C(6)	4e	0.4803(2)	-0.1128(2)	0.2812(1)	0.038(1)	0.0347(9)	0.044(1)	0.0050(7)	0.0229(8)	-0.0008(7)
N(7)	4e	0.3561(1)	0.1588(2)	0.4165(1)	0.0324(8)	0.0442(8)	0.0276(7)	0.0094(6)	0.0138(6)	0.0014(6)
C(8)	4e	0.2474(1)	0.2393(2)	0.4041(1)	0.0299(8)	0.0381(8)	0.0256(8)	0.0058(7)	0.0104(7)	-0.0025(6)
C(9)	4e	0.2146(2)	0.4156(2)	0.3565(1)	0.050(1)	0.0392(9)	0.0285(8)	0.0085(8)	0.0169(8)	0.0028(7)
C(10)	4e	0.2937(2)	0.5259(3)	0.3239(2)	0.088(2)	0.045(1)	0.067(2)	0.009(1)	0.051(1)	0.012(1)
C(11)	4e	0.1057(2)	0.4871(3)	0.3430(2)	0.058(1)	0.048(1)	0.037(1)	0.023(1)	0.0138(9)	0.0042(8)
C(12)	4e	0.0357(2)	0.3918(3)	0.3784(2)	0.037(1)	0.068(1)	0.055(1)	0.016(1)	0.017(1)	-0.009(1)
C(13)	4e	0.0707(2)	0.2214(3)	0.4268(2)	0.035(1)	0.060(1)	0.058(1)	-0.0020(9)	0.0238(9)	-0.0061(9)
C(14)	4e	0.1761(2)	0.1413(2)	0.4397(1)	0.0333(9)	0.0391(9)	0.0385(9)	-0.0004(7)	0.0166(8)	-0.0042(7)
C(15)	4e	0.2133(2)	-0.0469(3)	0.4919(2)	0.065(1)	0.041(1)	0.070(2)	-0.002(1)	0.041(1)	0.007(1)

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