Crystal structure of 2-(2,3-dimethylphenylamino)pyridine, C₁₃H₁₄N₂

M. Polamo* and M. Talja

University of Helsinki, Department of Chemistry, Laboratory of Inorganic Chemistry, P.O. Box 55 (A. I. Virtasen aukio 1), FIN-00014 Helsinki, Finland

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Table 1. Data collection and handling.

Crystal:	colorless, prismatic, size 0.20 × 0.35 × 0.35 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.73 cm ⁻¹
Diffractometer, scan mode:	Rigaku AFC7S, $\omega/2\theta$
$2\theta_{\max}$:	50.06°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	3618, 1863
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1625
$N(\text{param})_{\text{refined}}$:	193
Programs:	SHELXS-86 [2], SHELXL-97 [3], SHELXTL-NT [4], teXsan [5]

Abstract

C₁₃H₁₄N₂, monoclinic, $P12_1/n1$ (no. 14),
 $a = 11.304(8)$ Å, $b = 7.775(8)$ Å, $c = 13.451(9)$ Å,
 $\beta = 113.98(5)^\circ$, $V = 1080.2$ Å³, $Z = 4$,
 $R_{\text{gt}}(F) = 0.050$, $wR_{\text{ref}}(F^2) = 0.112$, $T = 193$ K.

Source of material

The title compound was obtained in one-step procedure. 2-chloropyridine and corresponding amine hydrochloride were heated at 180 °C for 90 minutes. The hydrochlorous raw product was suspended to aqueous sodium carbonate and then extracted with dichloromethane. Drying over anhydrous sodium sulfate, filtering and evaporation yielded the desired product. The white solid was crystallized from diethyl ether/heptane solution to afford a white crystalline solid.

Discussion

The structure obtained is highly similar to those reported for 2-phenylaminopyridines [1]. The title compound crystallizes as centrosymmetric dimer with two identical linear N7–H7···N1' interactions. The N7–H7···N1' angle is 173.9(2)° where the N(1)···H(7)' distance is fairly long 2.16(2) Å. This leads to long donor acceptor distance of 3.057(2) Å. Amino nitrogen, N7, has a nearly planar environment (the sum of angles is 355.02°).

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	0.466(2)	−0.197(2)	0.207(1)	0.041(4)
H(4)	4e	0.523(2)	−0.495(3)	0.238(1)	0.049(5)
H(5)	4e	0.626(2)	−0.595(3)	0.424(1)	0.045(5)
H(6)	4e	0.652(2)	−0.394(3)	0.565(1)	0.043(4)
H(7)	4e	0.483(2)	0.089(3)	0.409(2)	0.062(6)
H(101)	4e	0.696(2)	0.037(3)	0.308(2)	0.051(5)
H(102)	4e	0.661(2)	−0.028(3)	0.186(2)	0.072(6)
H(103)	4e	0.719(2)	0.158(3)	0.224(2)	0.075(7)
H(121)	4e	0.493(2)	0.311(3)	−0.046(2)	0.063(6)
H(122)	4e	0.634(2)	0.312(3)	0.065(2)	0.064(6)
H(123)	4e	0.574(2)	0.136(4)	0.008(2)	0.065(6)
H(13)	4e	0.309(2)	0.366(3)	−0.007(2)	0.055(5)
H(14)	4e	0.195(2)	0.348(3)	0.100(1)	0.055(5)
H(15)	4e	0.280(2)	0.184(3)	0.266(1)	0.049(5)

* Correspondence author (e-mail: mika.polamo@helsinki.fi)

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

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
N(1)	4e	0.5817(1)	−0.1917(2)	0.47263(9)	0.0455(7)	0.0356(8)	0.0303(6)	0.0023(6)	0.0179(6)	0.0005(5)
C(2)	4e	0.5311(1)	−0.1342(2)	0.3691(1)	0.0375(7)	0.0330(9)	0.0288(7)	−0.0016(7)	0.0179(6)	−0.0005(6)
C(3)	4e	0.5084(2)	−0.2450(2)	0.2805(1)	0.0458(8)	0.0333(9)	0.0305(7)	−0.0028(7)	0.0190(7)	−0.0015(6)
C(4)	4e	0.5429(2)	−0.4141(2)	0.3002(1)	0.0507(9)	0.0330(9)	0.0420(8)	−0.0045(8)	0.0255(7)	−0.0069(7)
C(5)	4e	0.5993(2)	−0.4737(2)	0.4064(1)	0.0519(9)	0.032(1)	0.0501(9)	0.0032(8)	0.0262(8)	0.0034(8)
C(6)	4e	0.6148(2)	−0.3579(2)	0.4886(1)	0.0508(9)	0.037(1)	0.0375(8)	0.0052(8)	0.0212(7)	0.0073(7)
N(7)	4e	0.5024(1)	0.0388(2)	0.35686(9)	0.0545(8)	0.0316(8)	0.0267(6)	0.0033(7)	0.0211(6)	−0.0020(5)
C(8)	4e	0.4508(1)	0.1248(2)	0.2548(1)	0.0409(8)	0.0277(8)	0.0267(7)	−0.0028(7)	0.0144(6)	−0.0042(6)
C(9)	4e	0.5251(1)	0.1421(2)	0.1928(1)	0.0410(7)	0.0270(8)	0.0289(7)	−0.0033(7)	0.0156(6)	−0.0046(6)
C(10)	4e	0.6606(2)	0.0727(3)	0.2327(1)	0.0442(8)	0.043(1)	0.0413(9)	0.0007(9)	0.0202(7)	0.0003(8)
C(11)	4e	0.4710(2)	0.2308(2)	0.0935(1)	0.0527(9)	0.0294(9)	0.0285(7)	−0.0059(8)	0.0163(7)	−0.0041(6)
C(12)	4e	0.5463(2)	0.2498(3)	0.0233(2)	0.081(1)	0.044(1)	0.0424(9)	−0.007(1)	0.037(1)	0.0007(8)
C(13)	4e	0.3499(2)	0.3059(2)	0.0611(1)	0.0563(9)	0.040(1)	0.0298(7)	−0.0012(9)	0.0071(7)	0.0027(8)
C(14)	4e	0.2797(2)	0.2929(3)	0.1244(1)	0.0407(9)	0.048(1)	0.0437(8)	0.0072(9)	0.0082(7)	−0.0019(8)
C(15)	4e	0.3294(2)	0.2003(2)	0.2202(1)	0.0403(8)	0.042(1)	0.0394(8)	−0.0008(8)	0.0167(7)	−0.0053(7)

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