Crystal structure of *N*-(4-nitrophenyl)quinoline-2-carboxamide, $C_{16}H_{11}N_3O_3$

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Abstract

$C_{16}H_{11}N_3O_3$, monoclinic, $P12_1/c1$ (no. 14), $a = 7.2928(3)$ Å, $b = 13.6807(6)$ Å, $c = 13.3131(7)$ Å, $\beta = 91.349(1)^\circ$, $V = 1327.9$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.035$, $wR_{\text{ref}}(F^2) = 0.103$, $T = 153$ K.

Source of material

The title compound was synthesized from 2-quinolinecarboxylic acid and *p*-nitrophenylamine according to the general procedure [1]. Colorless single crystals suitable for X-ray diffraction were obtained by recrystallization from dimethylsulfoxide.

Experimental details

N-bound H atom was located in a Fourier difference map and refined isotropically ($d(\text{N—H}) = 0.89(2)$ Å). C-bound H atoms were placed in calculated positions, with $d(\text{C—H}) = 0.95$ Å, and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Discussion

Quinoline-2-carboxamide compounds are a class of important materials as metal ligands [2] and as potential radioligands for visualization of peripheral benzodiazepine receptors [3]. Here, we have synthesized the title compound and determined its crystal structure.

In the crystal structure, the significant shorter bonds of N2—C11 (1.358(2) Å) and N2—C12 (1.397(1) Å) indicate the electron delocalization. Nitrogen atom N2 has effectively planar coordination. The quinoline ring system is planar within 0.016(1) Å. The dihedral angle between the C2/C3/C4/C9/C10/N1 and C2/C11/O1/N2 planes is 2.21(4)°, that between C2/C11/O1/N2 and C12→C27 planes is 2.62(4)° and that between C12→C27 and C15/N3/O2/O3 planes is 5.03(5)°. There are two types of intramolecular hydrogen bonds. The first type is an N—H···N bond (N2—H2N···N1, $d(\text{H2N} \cdots \text{N1}) = 2.13(1)$ Å). The other type is a C—H···O bond (C13—H13···O1, $d(\text{H13} \cdots \text{O1}) = 2.28$ Å). Furthermore, there are intramolecular hydrogen bonds (C5—H5···O1, $d(\text{H5} \cdots \text{O1}) = 2.41$ Å; C17—H17···O2, $d(\text{H17} \cdots \text{O2}) = 2.55$ Å and C17—H17···O3, $d(\text{H17} \cdots \text{O3}) = 2.57$ Å).

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.20 × 0.59 × 0.62 mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	1.05 cm ^{−1}
Diffractometer, scan mode:	Rigaku R-Axis RAPID, ω
$2\theta_{\text{max}}$:	54.96°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	20792, 3042
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 2811
$N(\text{param})_{\text{refined}}$:	204
Programs:	SHELXS-97 [4], SHELXL-97 [5]

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	0.0707	0.4792	0.2542	0.029
H(4)	4e	0.0065	0.3144	0.2268	0.029
H(5)	4e	0.0180	0.1407	0.2931	0.029
H(6)	4e	0.0882	0.0350	0.4240	0.031
H(7)	4e	0.1966	0.0956	0.5799	0.031
H(8)	4e	0.2410	0.2615	0.6036	0.028
H(13)	4e	0.2848	0.7656	0.4365	0.027
H(14)	4e	0.3835	0.9079	0.5193	0.028
H(16)	4e	0.4999	0.7511	0.7715	0.027
H(17)	4e	0.4036	0.6087	0.6894	0.026
H(2N)	4e	0.290(2)	0.530(1)	0.549(1)	0.032(3)

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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
O(1)	4e	0.1776(1)	0.62973(6)	0.35478(6)	0.0421(4)	0.0226(4)	0.0217(4)	−0.0041(3)	−0.0057(3)	0.0030(3)
O(2)	4e	0.4993(1)	1.00816(6)	0.65747(7)	0.0652(6)	0.0177(4)	0.0379(5)	−0.0004(4)	−0.0127(4)	−0.0018(3)
O(3)	4e	0.5843(1)	0.92228(6)	0.78689(6)	0.0474(5)	0.0278(4)	0.0281(4)	−0.0036(3)	−0.0118(3)	−0.0051(3)
N(1)	4e	0.1971(1)	0.40071(6)	0.47587(6)	0.0205(4)	0.0200(4)	0.0186(4)	−0.0017(3)	−0.0002(3)	−0.0009(3)
N(2)	4e	0.2820(1)	0.58446(6)	0.51201(6)	0.0266(4)	0.0173(4)	0.0202(4)	−0.0025(3)	−0.0025(3)	0.0005(3)
N(3)	4e	0.5147(1)	0.92958(6)	0.70222(7)	0.0316(5)	0.0204(4)	0.0257(4)	0.0007(3)	−0.0030(3)	−0.0038(3)
C(2)	4e	0.1649(1)	0.46112(7)	0.40056(7)	0.0209(4)	0.0203(5)	0.0186(4)	−0.0008(3)	0.0005(3)	−0.0010(3)
C(3)	4e	0.0930(1)	0.43237(8)	0.30568(7)	0.0318(5)	0.0237(5)	0.0177(4)	−0.0004(4)	−0.0024(4)	0.0018(4)
C(4)	4e	0.0561(1)	0.33567(8)	0.28966(7)	0.0285(5)	0.0264(5)	0.0162(4)	−0.0024(4)	−0.0024(4)	−0.0028(3)
C(5)	4e	0.0646(1)	0.16570(7)	0.35519(8)	0.0253(5)	0.0231(5)	0.0230(5)	−0.0047(4)	0.0007(4)	−0.0044(4)
C(6)	4e	0.1048(1)	0.10334(8)	0.43291(8)	0.0278(5)	0.0197(5)	0.0295(5)	−0.0041(4)	0.0019(4)	−0.0016(4)
C(7)	4e	0.1708(1)	0.13965(8)	0.52632(8)	0.0285(5)	0.0237(5)	0.0257(5)	−0.0016(4)	−0.0012(4)	0.0046(4)
C(8)	4e	0.1979(1)	0.23778(8)	0.54024(7)	0.0257(5)	0.0249(5)	0.0201(4)	−0.0020(4)	−0.0031(4)	0.0008(4)
C(9)	4e	0.1620(1)	0.30373(7)	0.46058(7)	0.0181(4)	0.0207(5)	0.0190(4)	−0.0016(3)	0.0004(3)	−0.0013(3)
C(10)	4e	0.0924(1)	0.26751(7)	0.36729(7)	0.0194(4)	0.0215(5)	0.0186(4)	−0.0022(3)	0.0009(3)	−0.0023(3)
C(11)	4e	0.2080(1)	0.56772(7)	0.41903(7)	0.0222(4)	0.0207(5)	0.0190(4)	−0.0015(3)	0.0004(3)	−0.0004(3)
C(12)	4e	0.3363(1)	0.67329(7)	0.55508(7)	0.0183(4)	0.0187(4)	0.0201(4)	−0.0011(3)	0.0003(3)	−0.0009(3)
C(13)	4e	0.3291(1)	0.76266(7)	0.50409(7)	0.0263(5)	0.0211(5)	0.0191(4)	−0.0006(4)	−0.0016(3)	0.0013(3)
C(14)	4e	0.3871(1)	0.84676(7)	0.55317(8)	0.0274(5)	0.0184(5)	0.0233(5)	0.0005(4)	−0.0005(4)	0.0017(3)
C(15)	4e	0.4502(1)	0.84128(7)	0.65173(8)	0.0221(4)	0.0186(5)	0.0234(5)	−0.0003(4)	−0.0005(4)	−0.0036(4)
C(16)	4e	0.4568(1)	0.75337(7)	0.70367(7)	0.0245(5)	0.0230(5)	0.0196(4)	0.0003(4)	−0.0032(3)	−0.0004(3)
C(17)	4e	0.3998(1)	0.66948(7)	0.65492(7)	0.0242(5)	0.0194(5)	0.0216(5)	0.0000(4)	−0.0019(4)	0.0025(3)

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