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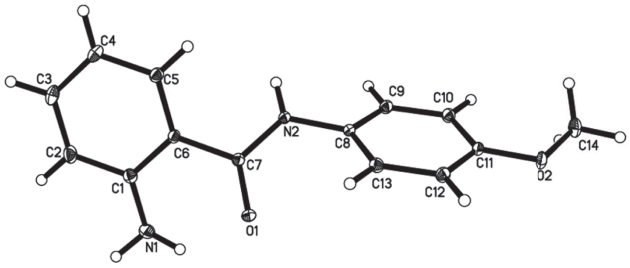
Crystal structure of 2-amino-N-(4-methoxyphenyl) benzamide, $C_{14}H_{14}N_2O_2$



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Abstract

$C_{14}H_{14}N_2O_2$, $P2_1/n$ (no. 14), $a = 13.5536(9)$ Å, $b = 5.0730(3)$ Å, $c = 17.6641(12)$ Å, $\beta = 100.448(2)°$, $V = 1194.40(13)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.046$, $wR(F^2) = 0.125$, $T = 100$ K.

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The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The reagents (isatoic anhydride and *p*-anisidine) and solvents used in this study are commercially available. The synthesis of 2-amino-*N*-(4-methoxyphenyl)benzamide was carried out according to procedures describes previously [1–3]. The compound was obtained as colorless crystals (ethanol). M.p. 121°C [3]; All other analytical data in accordance with the literature [3].

Table 1: Data collection and handling.

Crystal:	Brown, plate, size 0.115×0.365×0.458 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.92 cm^{-1}
Diffractometer, scan mode:	D8 Venture area detector, φ and ω scans
$2\theta_{max}$:	66.3°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	27499, 4542
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3515
$N(param)_{refined}$:	176
Programs:	SHELX [6], BRUKER SHELXTL [7]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2A)	4*e*	0.9033	0.5429	0.3591	0.020
H(3A)	4*e*	0.9684	0.2269	0.4496	0.021
H(4A)	4*e*	0.8610	−0.0388	0.5073	0.018
H(5A)	4*e*	0.6880	0.0313	0.4773	0.015
H(9A)	4*e*	0.3929	−0.1331	0.3088	0.015
H(10A)	4*e*	0.2171	−0.1415	0.2911	0.015
H(12A)	4*e*	0.2239	0.5089	0.4256	0.015
H(13A)	4*e*	0.3990	0.5142	0.4442	0.015
H(14A)	4*e*	−0.0256	0.0021	0.3135	0.026
H(14B)	4*e*	0.0692	−0.1854	0.3408	0.026
H(14C)	4*e*	0.0565	−0.0365	0.2597	0.026
H(1N2)	4*e*	0.545(1)	0.018(3)	0.3888(8)	0.023(4)
H(2N1)	4*e*	0.762(1)	0.781(3)	0.2941(9)	0.029(4)
H(1N1)	4*e*	0.656(1)	0.726(3)	0.3073(9)	0.027(4)

Discussion

2-Aminobenzamide derivatives have been identified as a precursor for the synthesis of a divergent of heterocyclic compounds, such as quinazolones, quinazolinones, phthalimides, benzimidazolones, pyrroloquinazolones, and quinazolinediones [4, 5]. The title crystal structure contains one molecule in the asymmetric unit. There is a dihedral

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Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	4*e*	0.54796(5)	0.6149(1)	0.37478(4)	0.0114(3)	0.0082(3)	0.0232(4)	0.0014(2)	0.0018(3)	0.0013(3)
O(2)	4*e*	0.10136(5)	0.1964(2)	0.34968(4)	0.0080(3)	0.0173(4)	0.0186(3)	0.0002(3)	0.0026(2)	−0.0018(3)
N(1)	4*e*	0.71804(7)	0.6602(2)	0.30501(5)	0.0159(4)	0.0164(4)	0.0203(4)	−0.0007(3)	0.0052(3)	0.0062(3)
N(2)	4*e*	0.52000(6)	0.1784(2)	0.38958(5)	0.0080(3)	0.0076(3)	0.0195(4)	0.0009(3)	0.0016(3)	0.0005(3)
C(1)	4*e*	0.75525(7)	0.4849(2)	0.36367(5)	0.0126(4)	0.0121(4)	0.0132(4)	−0.0005(3)	0.0030(3)	−0.0012(3)
C(2)	4*e*	0.85896(8)	0.4407(2)	0.38313(6)	0.0105(4)	0.0201(5)	0.0209(5)	−0.0016(4)	0.0051(4)	0.0000(4)
C(3)	4*e*	0.89783(8)	0.2509(2)	0.43662(6)	0.0095(4)	0.0241(5)	0.0197(5)	0.0026(4)	0.0022(3)	−0.0018(4)
C(4)	4*e*	0.83432(7)	0.0945(2)	0.47166(6)	0.0117(4)	0.0187(5)	0.0152(4)	0.0050(4)	0.0008(3)	0.0006(4)
C(5)	4*e*	0.73160(7)	0.1368(2)	0.45353(5)	0.0108(4)	0.0127(4)	0.0139(4)	0.0019(3)	0.0021(3)	0.0002(3)
C(6)	4*e*	0.69097(7)	0.3320(2)	0.40089(5)	0.0085(4)	0.0098(4)	0.0120(4)	0.0005(3)	0.0011(3)	−0.0013(3)
C(7)	4*e*	0.58114(7)	0.3881(2)	0.38729(5)	0.0094(4)	0.0094(4)	0.0115(4)	0.0001(3)	0.0011(3)	−0.0003(3)
C(8)	4*e*	0.41307(7)	0.1899(2)	0.37815(5)	0.0082(4)	0.0088(4)	0.0144(4)	0.0003(3)	0.0018(3)	0.0020(3)
C(9)	4*e*	0.35854(7)	−0.0030(2)	0.33277(6)	0.0107(4)	0.0098(4)	0.0167(4)	0.0013(3)	0.0022(3)	−0.0012(3)
C(10)	4*e*	0.25386(7)	−0.0082(2)	0.32189(6)	0.0109(4)	0.0110(4)	0.0152(4)	−0.0008(3)	0.0011(3)	−0.0014(3)
C(11)	4*e*	0.20407(7)	0.1839(2)	0.35659(5)	0.0077(4)	0.0120(4)	0.0131(4)	0.0006(3)	0.0023(3)	0.0025(3)
C(12)	4*e*	0.25832(7)	0.3781(2)	0.40201(6)	0.0117(4)	0.0116(4)	0.0154(4)	0.0010(3)	0.0038(3)	−0.0015(3)
C(13)	4*e*	0.36239(7)	0.3816(2)	0.41301(5)	0.0118(4)	0.0103(4)	0.0150(4)	−0.0007(3)	0.0028(3)	−0.0018(3)
C(14)	4*e*	0.04602(8)	−0.0231(2)	0.31302(6)	0.0096(4)	0.0219(5)	0.0203(5)	−0.0032(4)	0.0009(3)	−0.0028(4)

angle between the ring I (C1—C6) and ring II (C8—C13) equal to 78.0°. The molecules packing in the crystal structure is stabilized by two intermolecular hydrogen bonds, of which O1 work as hydrogen bond acceptors and N2, and C9 work as hydrogen bond donors. The distance of the interactions between N2—H1N2···O1 is 2.062 (15) Å, C9—H9A···O1 is 2.55 (1) Å and the angles are 159° and 125°, respectively.

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References

1. Mabkhot, Y. N.; Al-Har, M. S.; Barakat, A.; Al-Showiman, S. S.: Diversity oriented design of various hydrazides and amides derived from isatoic anhydride and their antimicrobial activity evaluation. Dig. J. Nanomater. Biostruct. **8** (2013) 1345–1355.
2. Mabkhot, Y. N.; Al-Majid, A. M.; Barakat, A.; Al-Showiman, S. S.; Al-Har, M. S.; Radi, S.; Naseer, M. M.; Hadda, T. B.: Synthesis and biological evaluation of 2-aminobenzamide derivatives as antimicrobial agents: opening/closing pharmacophore site. Int. J. Mol. Sci. **15** (2014) 5115–5127.
3. Mabkhot, Y. N.; Al-Har, M. S.; Barakat, A.; Aldawsari, F. D.; Aldalbahi, A.; Ul-Haq, Z.: Synthesis, anti-microbial and molecular docking studies of quinazolin-4(3H)-one derivatives. Molecules **19** (2014) 8725–8739.
4. Khan, I.; Ibrar, A.; Ahmed, W.; Saeed, A.: Synthetic approaches, functionalization and therapeutic potential of quinazoline and quinazolinone skeletons: the advances continue. Europ. J. Med. Chem. **90** (2015) 124–169.
5. Ma, Y.-G.; Zhang, Y.; Feng, B.-B.; Wang, X.-S. Synthesis of 6-aryl-5H-quinazolino[4,3-b]quinazolin-8(6H)-one derivatives in ionic liquids catalyzed by iodine. Res. Chem. Intermediat. (2015) 1–11, DOI 10.1007/s11164–015-2072–8.
6. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112–122.
7. Brucker. APEX2, SAINT and SADABS. Brucker AXS Inc., Madison, Wisconsin, USA, 2009.