Crystal structure of 3-(pyrazin-2-ylamino)-2-benzo- furan-1(3*H*)-one, $C_{12}H_9N_3O_2$

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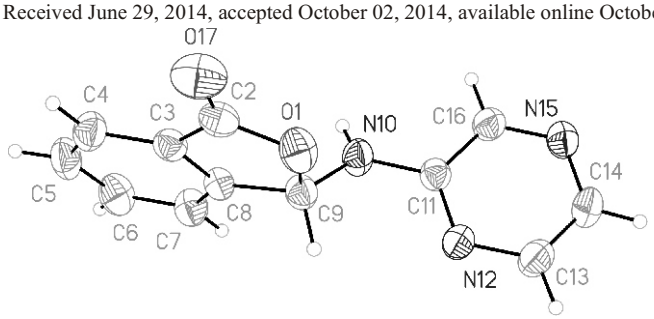

Abstract

$C_{12}H_9N_3O_2$, monoclinic, $P2_1/c$ (no. 14), a = 7.524(1) Å, b = 7.981(1) Å, c = 17.622(2) Å, β = 98.31(1)°, V = 1047.0 Å^3, Z = 4, $R_{gt}(F)$ = 0.0581, $wR_{ref}(F^2)$ = 0.1337, T = 293 K.

Table 1. Data collection and handling.

Crystal:	white chunks, size 0.1 0.2 0.3 mm
Wavelength:	Mo K radiation (0.71073 Å)
μ:	1.02 cm^{-1}
Diffractometer, scan mode:	Xcalibur, Eos, ω
$2\theta_{max}$:	52.58°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4672, 2115
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1275
$N(param)_{refined}$:	155
Programs:	SHELX [9], Crysalis PRO [10]

Source of material

For the preparation of the title compound, a solution of 2-carboxybenzaldehyde (1 mmol) in methanol (30 ml) was added to a solution of pyrazin-2-amine (1 mmol) in methanol (10 ml) at room temperature. The mixture was refluxed for one hour, the mixture was left to cool to RT. Crystals suitable for X-ray diffraction analysis were obtained by evaporated of methanol from the mixture after two days (yield, 88%).

Discussion

Pharmaceutical chemistry is a very important sector of pharmaceutical science dealing with determination of the influence of chemical structures on biological activity. In the practice of pharmaceutical chemistry the organic synthesis of new compounds is based on the modification of structure and the identification of their biological activities [1, 2]. Benzofuranones are an important class of synthetic and naturally occurring products exhibiting diverse biological and pharmacological properties [3]. Pyrazines form an important class of analogues, which occupy a special role in natural and synthetic compounds [4]. Pyrazine derivatives are well known for their anticancer, antinociceptive, antimycobacterial, antiinflammatory activities [5–8]. In this work we coupled benzofuranone with pyrazine ligands to produce the title compound 3-(pyrazin-2-ylamino)-2-benzofuran-1(3*H*)-one in good yield. In the molecule of the title compound, $C_{12}H_9N_3O_2$, the essentially planar phthalide group is oriented at a dihedral angle of 89.47° with respect to the substituted aromatic ring. In the crystal structure, molecules are primarily linked by N–H N hydrogen bonds (N N = 3.07 Å) to form chains in the b direction.

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

Atom	Site	x	y	z	U_{iso}
H(16A)	4*e*	0.0068	0.5630	0.2575	0.045
H(10A)	4*e*	0.1131	0.3358	0.3429	0.046
H(14A)	4*e*	0.3420	0.8755	0.1968	0.051
H(13A)	4*e*	0.5565	0.7635	0.2860	0.054
H(9A)	4*e*	0.4376	0.3725	0.4252	0.042
H(7A)	4*e*	0.3364	0.0242	0.3744	0.049
H(4A)	4*e*	0.1615	0.0541	0.6173	0.050
H(5A)	4*e*	0.2003	0.2025	0.5607	0.056
H(6A)	4*e*	0.2826	0.2166	0.4407	0.057

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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}
O(1)	4*e*	0.2625(2)	0.4638(2)	0.4923(1)	0.054(1)	0.029(1)	0.046(1)	0.0013(8)	0.0014(9)	0.0031(9)
N(15)	4*e*	0.1430(3)	0.7310(3)	0.2182(1)	0.044(1)	0.038(1)	0.041(1)	0.001(1)	0.005(1)	0.007(1)
N(12)	4*e*	0.4083(2)	0.5930(3)	0.3268(1)	0.034(1)	0.043(1)	0.045(1)	0.004(1)	0.004(1)	0.013(1)
C(11)	4*e*	0.2425(3)	0.5329(3)	0.3164(1)	0.034(1)	0.031(1)	0.030(1)	0.001(1)	0.006(1)	0.001(1)
C(16)	4*e*	0.1094(3)	0.6054(3)	0.2623(1)	0.033(1)	0.040(2)	0.038(2)	0.003(1)	0.004(1)	0.004(1)
N(10)	4*e*	0.2042(2)	0.3976(2)	0.3593(1)	0.037(1)	0.036(1)	0.040(1)	0.010(1)	0.005(1)	0.008(1)
O(17)	4*e*	0.1613(2)	0.4293(2)	0.6051(1)	0.054(1)	0.063(1)	0.050(1)	0.005(1)	0.009(1)	0.022(1)
C(3)	4*e*	0.2286(3)	0.1911(3)	0.5287(1)	0.028(1)	0.033(2)	0.035(2)	0.000(1)	0.001(1)	0.000(1)
C(14)	4*e*	0.3118(3)	0.7881(3)	0.2274(2)	0.050(2)	0.039(2)	0.039(2)	0.006(1)	0.008(1)	0.009(1)
C(13)	4*e*	0.4408(3)	0.7198(4)	0.2811(2)	0.039(1)	0.049(2)	0.047(2)	0.009(1)	0.005(1)	0.010(2)
C(9)	4*e*	0.3104(3)	0.3569(3)	0.4297(1)	0.036(1)	0.036(2)	0.033(2)	0.001(1)	0.002(1)	0.004(1)
C(8)	4*e*	0.2814(3)	0.1827(3)	0.4574(1)	0.033(1)	0.031(2)	0.034(2)	0.002(1)	0.003(1)	0.004(1)
C(2)	4*e*	0.2108(3)	0.3678(3)	0.5496(2)	0.030(1)	0.043(2)	0.039(2)	0.000(1)	0.002(1)	0.002(2)
C(7)	4*e*	0.3020(3)	0.0305(3)	0.4230(2)	0.049(2)	0.039(2)	0.034(2)	0.004(1)	0.008(1)	0.001(1)
C(4)	4*e*	0.1968(3)	0.0478(3)	0.5690(2)	0.043(1)	0.047(2)	0.033(2)	0.004(1)	0.004(1)	0.007(1)
C(5)	4*e*	0.2194(3)	0.1040(3)	0.5348(2)	0.051(2)	0.035(2)	0.052(2)	0.004(1)	0.002(1)	0.014(2)
C(6)	4*e*	0.2699(3)	0.1123(3)	0.4629(2)	0.058(2)	0.030(2)	0.053(2)	0.002(1)	0.003(1)	0.002(2)

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