Crystal structure of 4,6-dimethoxypyrimidin-2-amine-1-(4-nitrophenyl)-piperazine (1:1), $C_{10}H_{14}N_3O_2{\cdot}C_6H_8N_3O_2$, $C_{16}H_{23}N_6O_4$

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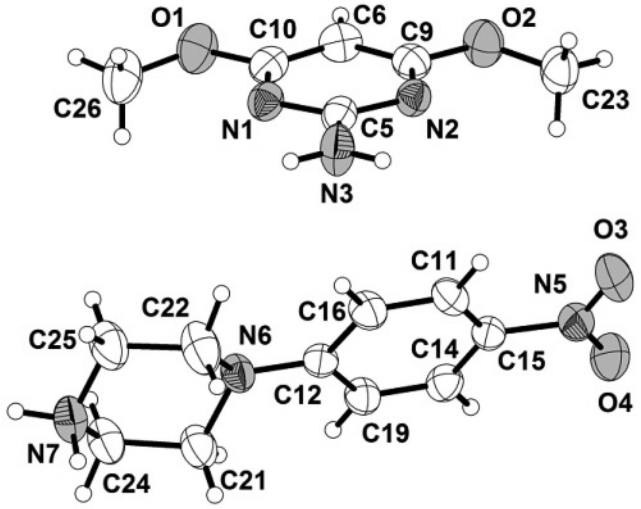

Abstract

$C_{16}H_{22}N_6O_4$, triclinic, $P\bar{1}$ (no. 2), a = 7.4257(7) Å, b = 11.390(1) Å, c = 11.998(1) Å, α = 65.648(3)°, β = 89.905(3)°, γ = 74.090(3)°, V = 881.9 Å^3, Z = 2, $R_{gt}(F)$ = 0.0478, $wR_{ref}(F^2)$ = 0.1439, T = 273 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.18×0.21×0.21 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.31 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, ω
$2\theta_{max}$:	50.38°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8540, 3163
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2047
$N(param)_{refined}$:	237
Programs:	SHELX [6], DIAMOND [7]

Source of material

4,6-Dimethoxypyrimidin-2-amine (0.20 g, 1 mmol) and 1-(4-nitrophenyl)piperazine (0.18 g, 1 mmol) were mixed in acetonitrile (20 mL) and refluxed for 10 hours. After extraction and drying, the title compound was obtained of which 10 mg was dissolved in 10 ml acetone, and the solution was kept at room temperature for 4 d. Colourless block-shaped crystals were obtained by slow evaporation of the solution containing the compound in air.

Experimental details

All H atoms were constrained to ideal geometries, with C–H = 0.93-0.97 Å, and with U_{iso}(H) = 2.0U_{eq}(C).

Discussion

Pyrimidine and their derivatives as an integral part of nucleic acids in DNA and RNA, playing an important role in several biological processes [1-3]. Pyrimidine possesses a wide spectrum of biological activities like antitubercular, antibacterial, antifungal, antiviral, anti-inflammatory, antimalarial activity, anticancer, antineoplastic activity, and anti-HIV activity [4]. Also, piperazine derivatives display antimicrobial, antituberculosis, anticancer, antiviral and antimalarial activities [5]. In our attempt to attach the two compounds, the title compound was unexpectedly obtained. In the title co-crystal structure the asymmetric unit comprises one 4,6-dimethoxypyrimidin-2-amine molecule and one 1-(4-nitrophenyl)piperazine molecule. Two 4,6-dimethoxypyrimidin-2-amine and 1-(4-nitrophenyl)piperazine molecules are connected by strong intermolecular N–H···N^i hydrogen bonds (N3···N2: 3.208(3) Å, N3–H3A···N2: 159°; symmetry code ii: $-x$, $2-y$, $-z$; N3···N7: 2.990(3) Å, N3–H3B···N7: 152°; symmetry code ii: $1-x$, $1-y$, $-z$; N7···N3: 2.990(3) Å, N7–H7···N3: 127°; symmetry code: ii: $1-x$, $1-y$, $-z$) to form supramolecular adducts consisting of one 4,6-dimethoxypyrimidin-2-amine and one 1-(4-nitrophenyl)piperazine molecule.

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

Atom	Site	x	y	z	U_{iso}
H(6)	2*i*	0.6673	0.8798	0.2482	0.063
H(7A)	2*i*	0.5269	0.1736	0.2015	0.071
H(7B)	2*i*	0.7277	0.1574	0.1944	0.071
H(11)	2*i*	0.0738	0.7578	0.3163	0.061
H(14)	2*i*	0.2379	0.4481	0.6495	0.058
H(16)	2*i*	0.2428	0.6253	0.2284	0.061
H(3A)	2*i*	0.0627	0.9152	–0.0309	0.079
H(3B)	2*i*	0.2139	0.8335	–0.0740	0.079
H(19)	2*i*	0.4097	0.3150	0.5637	0.055
H(21A)	2*i*	0.3896	0.1994	0.3956	0.075
H(21B)	2*i*	0.5396	0.1997	0.4872	0.075
H(22A)	2*i*	0.4209	0.5153	0.1613	0.087
H(22B)	2*i*	0.3089	0.4123	0.1764	0.087
H(23A)	2*i*	0.0844	1.1291	0.1994	0.103
H(23B)	2*i*	0.1330	1.0838	0.3410	0.103
H(23C)	2*i*	0.0828	0.9852	0.2945	0.103
H(24A)	2*i*	0.7743	0.1669	0.3708	0.074
H(24B)	2*i*	0.6719	0.0575	0.3919	0.074
H(25A)	2*i*	0.5531	0.3704	0.0701	0.088
H(25B)	2*i*	0.6981	0.3648	0.1680	0.088
H(26A)	2*i*	0.7935	0.5942	0.0908	0.122
H(26B)	2*i*	0.9802	0.6342	0.0638	0.122
H(26C)	2*i*	0.7934	0.7244	–0.0264	0.122

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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}
N(2)	2*i*	0.2504(2)	0.9401(2)	0.1197(2)	0.047(1)	0.051(1)	0.044(1)	–0.0152(8)	0.0097(8)	–0.0228(9)
N(1)	2*i*	0.4896(2)	0.8068(2)	0.0493(2)	0.043(1)	0.048(1)	0.046(1)	–0.0084(8)	0.0065(8)	–0.0160(8)
N(6)	2*i*	0.4541(2)	0.3734(2)	0.3339(2)	0.057(1)	0.040(1)	0.039(1)	–0.0082(8)	0.0079(8)	–0.0173(8)
O(2)	2*i*	0.3395(2)	1.0006(2)	0.2680(2)	0.065(1)	0.080(1)	0.062(1)	–0.0203(9)	0.0070(8)	–0.0432(9)
C(5)	2*i*	0.3099(3)	0.8749(2)	0.0493(2)	0.046(1)	0.049(1)	0.045(1)	–0.014(1)	0.010(1)	–0.019(1)
C(6)	2*i*	0.5746(3)	0.8771(2)	0.1981(2)	0.050(1)	0.054(1)	0.045(1)	–0.015(1)	–0.004(1)	–0.013(1)
N(7)	2*i*	0.6248(3)	0.1975(2)	0.2199(2)	0.056(1)	0.064(1)	0.063(1)	–0.0073(9)	0.0090(9)	–0.039(1)
O(1)	2*i*	0.8003(2)	0.7459(2)	0.1278(2)	0.0456(9)	0.073(1)	0.069(1)	–0.0003(8)	–0.0012(8)	–0.0254(9)
C(9)	2*i*	0.3865(3)	0.9385(2)	0.1931(2)	0.057(1)	0.043(1)	0.042(1)	–0.015(1)	0.005(1)	–0.015(1)
C(10)	2*i*	0.6165(3)	0.8108(2)	0.1231(2)	0.041(1)	0.043(1)	0.044(1)	–0.0071(9)	0.002(1)	–0.005(1)
C(11)	2*i*	0.1411(3)	0.6682(2)	0.3657(2)	0.055(1)	0.038(1)	0.057(2)	–0.009(1)	0.005(1)	–0.020(1)
C(12)	2*i*	0.3478(3)	0.4534(2)	0.3850(2)	0.041(1)	0.041(1)	0.041(1)	–0.0140(9)	0.0039(9)	–0.017(1)
N(5)	2*i*	0.0251(3)	0.6970(2)	0.5462(2)	0.053(1)	0.060(1)	0.077(2)	–0.023(1)	0.019(1)	–0.042(1)
C(14)	2*i*	0.2395(3)	0.4833(2)	0.5646(2)	0.053(1)	0.055(1)	0.041(1)	–0.020(1)	0.010(1)	–0.022(1)
C(15)	2*i*	0.1383(3)	0.6155(2)	0.4908(2)	0.042(1)	0.048(1)	0.057(1)	–0.019(1)	0.012(1)	–0.031(1)
C(16)	2*i*	0.2430(3)	0.5887(2)	0.3135(2)	0.061(1)	0.043(1)	0.041(1)	–0.011(1)	0.005(1)	–0.015(1)
N(3)	2*i*	0.1800(3)	0.8745(2)	–0.0277(2)	0.042(1)	0.093(2)	0.081(1)	–0.011(1)	0.006(1)	–0.062(1)
O(4)	2*i*	0.0205(3)	0.6470(2)	0.6581(2)	0.086(1)	0.086(1)	0.073(1)	–0.031(1)	0.031(1)	–0.052(1)
C(19)	2*i*	0.3419(3)	0.4041(2)	0.5129(2)	0.051(1)	0.041(1)	0.041(1)	–0.0091(9)	0.0052(9)	–0.014(1)
O(3)	2*i*	–0.0638(3)	0.8148(2)	0.4786(2)	0.090(1)	0.056(1)	0.104(2)	–0.008(1)	0.030(1)	–0.042(1)
C(21)	2*i*	0.5013(4)	0.2263(2)	0.4009(2)	0.078(2)	0.043(1)	0.056(1)	–0.006(1)	0.016(1)	–0.019(1)
C(22)	2*i*	0.4276(4)	0.4205(2)	0.2007(2)	0.102(2)	0.055(2)	0.041(1)	0.003(1)	0.008(1)	–0.018(1)
C(23)	2*i*	0.1437(3)	1.0541(3)	0.2764(2)	0.069(2)	0.084(2)	0.073(2)	–0.023(1)	0.019(1)	–0.052(2)
C(24)	2*i*	0.6571(3)	0.1536(2)	0.3510(2)	0.068(2)	0.050(1)	0.061(2)	–0.003(1)	0.005(1)	–0.027(1)
C(25)	2*i*	0.5845(4)	0.3421(2)	0.1576(2)	0.106(2)	0.059(2)	0.052(2)	–0.014(1)	0.023(1)	–0.028(1)
C(26)	2*i*	0.8456(4)	0.6683(3)	0.0583(3)	0.057(2)	0.085(2)	0.089(2)	0.001(1)	0.011(1)	–0.038(2)

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