Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N^6-(4-Methoxybenzoyl)adenine

Yang Bo, Kun Cheng, Sai Bi and Shu-Sheng Zhang*

College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China

Correspondence e-mail: shushzhang@126.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.120
Data-to-parameter ratio = 13.5

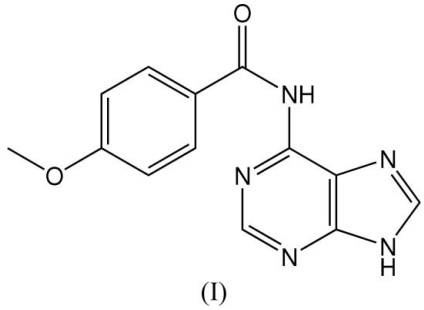
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 23 August 2006
Accepted 24 August 2006

The molecules of the title compound, $C_{13}H_{11}N_5O_2$, are linked into chains along the *c* axis by N—H···O and C—H···O hydrogen-bond contacts. N—H···N interactions connect the chains into two-dimensional layers. The packing is further stabilized by π–π interactions involving the purine system.

Comment

The purines are very important organic compounds, having pyrimidine and imidazole units. They are an important constituent in the structure of ribonucleic acid (RNA) and deoxyribonucleic acid (DNA). Purine derivatives are important pharmaceutical intermediates of extensive function, for example, 6-(*N*-benzoylamino)purine is a competitive inhibitor of xanthine oxidase (Pierre *et al.*, 2003). Purine rings substituted at positions 2, 6 or 8 are present in anticancer and hypotensive drugs (Van Aerschot *et al.*, 1993). As part of our ongoing research on purine derivatives, the title compound, (I), was synthesized.



(I)

The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The purine system is essentially planar, with a dihedral angle of 3.40 (1)° between the pyrimidine ring (*A*, atoms N3/N4/C1/C2/C4/C5) and the imidazole ring (*B*, atoms N1/N2/C2–C4). The dihedral angle between the mean plane of the purine system and benzene ring (C, atoms C7–C12) is 44.65 (1)°. There exists an intramolecular N2—H2*A*···O1 hydrogen contact, forming a seven-membered ring.

In the crystal structure, molecules of (I) are linked into chains along the *c* axis by N5—H5*A*···O1^{ii} and C8—H8*A*···O1^{ii} hydrogen-bond contacts (see Table 2 for details). In addition, N2—H2*A*···N1^{i} interactions connect the chains into two-dimensional layers (Fig. 2 and Table 2). The packing is further stabilized by π–π interactions involving the purine system, the distances being *Cg*1···*Cg*2^{iii} = 3.493 Å and *Cg*2···*Cg*2^{iii} = 3.739 Å [*Cg*1 and *Cg*2 denote the centroids of rings *A* and *B*, respectively; symmetry code: (iii) 1 − *x*, 1 − *y*, 1 − *z*].

Experimental

Adenine (13.5 g, 0.1 mol) was suspended in dry pyridine (250 ml). 4-Methoxybenzoyl chloride (17.1 g, 0.1 mol) was added dropwise using a syringe. The mixture was stirred for 3 h at 378 K and allowed to stand overnight at room temperature. The reaction solution was treated with methanol (50 ml), and the solvent was subsequently evaporated *in vacuo*. The residue was evaporated twice with toluene and then stirred with hot 2-propanol. The mixture was allowed to cool slowly, and the product which precipitated out was filtered off and dried *in vacuo* to give the title compound, (I) (yield 87.5%, m.p. 485–487 K). Compound (I) was dissolved in MeOH–$CHCl_3$ (1:3 *v*/*v*). After filtration, the colourless filtrate was left at room temperature. Single crystals of (I) suitable for X-ray crystallographic analysis were obtained.

Crystal data

$C_{13}H_{11}N_5O_2$
M_r = 269.27
Monoclinic, $P2_1/c$
a = 12.398 (3) Å
b = 10.045 (3) Å
c = 10.079 (3) Å
β = 98.804 (4)°
V = 1240.5 (6) Å^3
Z = 4
D_x = 1.442 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colourless
0.32 × 0.17 × 0.05 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.995
6725 measured reflections
2446 independent reflections
1634 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.121
S = 1.02
2446 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2 + 0.1439P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	2.45	2.809 (2)	106
N2—H2A···N1^{i}	0.86	2.09	2.935 (3)	166
N5—H5A···O1^{ii}	0.86	2.13	2.961 (2)	163
C8—H8A···O1^{ii}	0.93	2.30	3.209 (3)	165

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with N—H = 0.86 Å, C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

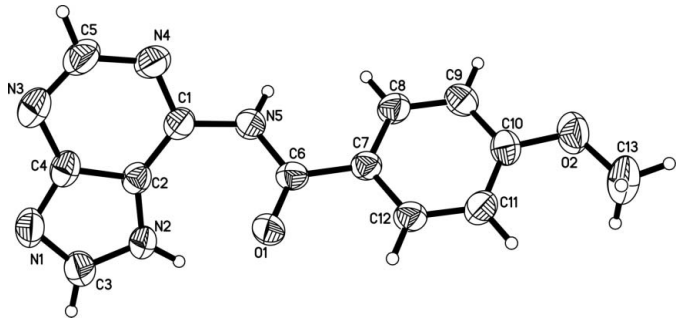


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

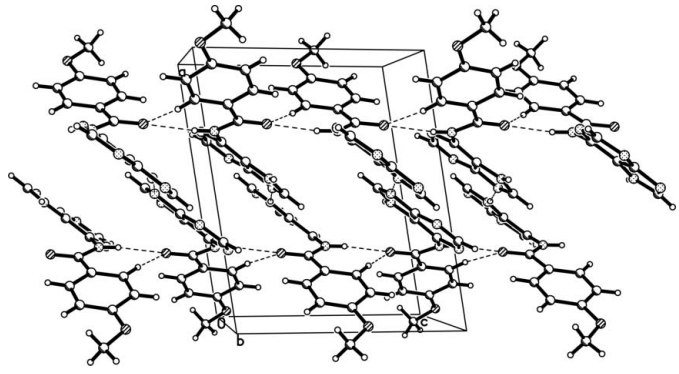


Figure 2
Packing diagram of (I) showing the intermolecular hydrogen-bond contacts (dashed lines), viewed down the *b* axis,

This project was supported by the Special Project of Qingdao for Leadership of Science and Technology (No. 05–2-JC-80) and the Outstanding Adult-Young Scientific Research Encouraging Foundation of Shandong Province (No. 2005BS04007).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Pierre, R., Claire, L. & Christian, M. (2003). *Eur. J. Med. Chem.* **38**, 199.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Van Aerschot, A., Petros, M. & Piet, A. (1993). *J. Med. Chem.* **36**, 2938–2942.