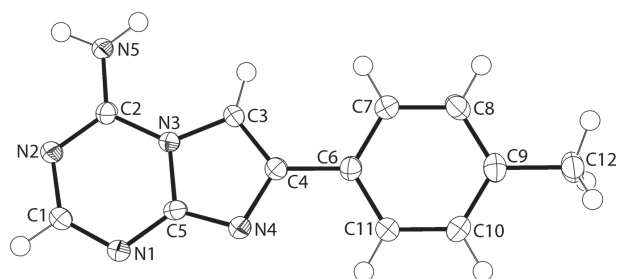


Felicia Phei Lin Lim, Anton V. Dolzhenko, Nathan R. Halcovitch and Edward R.T. Tiekink*

Crystal structure of 7-(4-methylphenyl)imidazo[1,2-*a*][1, 3, 5]triazin-4-amine, C₁₂H₁₁N₅



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Abstract

C₁₂H₁₁N₅, monoclinic, $P2_1/n$ (no. 14), $a = 7.3455(1)$ Å, $b = 12.2470(1)$ Å, $c = 12.1689(1)$ Å, $\beta = 103.505(1)^\circ$, $V = 1064.45(2)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0365$, $wR_{\text{ref}}(F^2) = 0.0987$, $T = 100$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The compound was prepared and characterised as described in the literature [5]. Crystals for the crystallographic study were obtained from the slow evaporation of a very dilute methanol solution.

Experimental details

The C-bound H atoms were geometrically placed ($C-H = 0.98-0.99$ Å) and refined as riding with $U_{\text{iso}}(H) = 1.2-1.5U_{\text{eq}}(C)$. The N-bound hydrogen atoms were located in difference Fourier maps, but were refined with a distance

Table 1: Data collection and handling.

Crystal:	Block, colourless
Size:	$0.44 \times 0.16 \times 0.09$ mm
Wavelength:	Cu $K\alpha$ radiation (1.54184 Å)
μ :	0.73 mm^{-1}
Diffractometer, scan mode:	SuperNova, φ and ω -scans
θ_{max} , completeness:	76.5° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	18249, 2225, 0.026
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2132
$N(\text{param})_{\text{refined}}$:	163
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3], WinGX and ORTEP [4]

restraint of $N-H = 0.88 \pm 0.01$ Å, and with unconstrained $U_{\text{iso}}(H)$.

Discussion

The 5-aza-7-deaza-isostere (imidazo[1,2-*a*][1, 3, 5]triazine) of the purine system is an important scaffold for the construction of various drugs. Such compounds have been developed as inhibitors for enzymes, e.g. focal adhesion kinase [6]. Further, these compounds display anti-viral activity [7], are agonists of opioid m-receptors [8] and function as ligands for adenosine receptors [9]. A hindrance to the embellishment of this class of compound has been the difficulty in their synthesis. Very recently, a new procedure for the synthesis of 5-aza-7-deaza-isosteres was developed, i.e. through the reaction of 2-aminoimidazoles, triethylorthoformate and cyanamide under microwave irradiation [5]. The title compound was one of the new compounds synthesised in the course of that study.

The title molecule is shown in the figure (70% displacement ellipsoids) and comprises a six- and five-membered fused ring system connected to the 4-methylphenyl group at C4. The r.m.s. deviation of the nine atoms of the imidazo-triazine group is 0.0218 Å with the maximum deviations being 0.0399(7) Å for the C2 atom and to the other side of the least-squares plane, 0.0273(7) Å for the C3 atom. The amino-N5 atom lies 0.1258(13) Å out of the plane in the direction of the C2 atom. There is a twist between this plane and that through the appended 4-methylphenyl group as seen in the dihedral angle of $12.39(4)^\circ$ formed between them. The overall molecular geometry resembles that reported for the 4-methoxyphenyl derivative [5].

*Corresponding author: Edward R.T. Tiekink, Research Centre for Crystalline Materials, School of Science and Technology, Sunway University, 47500 Bandar Sunway, Selangor Darul Ehsan, Malaysia, e-mail: edwardt@sunway.edu.my

Felicia Phei Lin Lim and Anton V. Dolzhenko: School of Pharmacy, Monash University Malaysia, Jalan Lagoon Selatan, Bandar Sunway, Selangor Darul Ehsan 47500, Malaysia

Nathan R. Halcovitch: Department of Chemistry, Lancaster University, Lancaster LA1 4YB, UK

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
N1	0.65755(12)	0.76747(7)	0.76013(7)	0.0160(2)
N2	0.56271(12)	0.90789(7)	0.62085(7)	0.0152(2)
N3	0.43165(12)	0.73441(7)	0.58693(7)	0.0135(2)
N4	0.51177(12)	0.59379(7)	0.70583(7)	0.0153(2)
N5	0.35748(13)	0.86947(7)	0.44944(7)	0.0167(2)
H1N	0.2954(19)	0.8213(10)	0.4000(11)	0.027(4)*
H2N	0.382(2)	0.9366(8)	0.4286(12)	0.026(4)*
C1	0.65857(14)	0.86774(8)	0.72106(8)	0.0158(2)
H1	0.7367	0.9183	0.7696	0.019*
C2	0.45045(14)	0.83930(8)	0.55095(8)	0.0137(2)
C3	0.32629(14)	0.64623(8)	0.53665(8)	0.0145(2)
H3	0.2379	0.6448	0.4659	0.017*
C4	0.37712(14)	0.56166(8)	0.61100(8)	0.0143(2)
C5	0.54085(14)	0.69780(8)	0.68995(8)	0.0139(2)
C6	0.30889(14)	0.44836(8)	0.59856(8)	0.0147(2)
C7	0.20768(15)	0.40938(9)	0.49422(9)	0.0175(2)
H7	0.1760	0.4576	0.4315	0.021*
C8	0.15305(15)	0.30053(9)	0.48163(9)	0.0184(2)
H8	0.0847	0.2754	0.4100	0.022*
C9	0.19638(14)	0.22754(8)	0.57174(9)	0.0172(2)
C10	0.29339(15)	0.26757(8)	0.67647(9)	0.0186(2)
H10	0.3222	0.2196	0.7395	0.022*
C11	0.34874(15)	0.37631(8)	0.69031(9)	0.0172(2)
H11	0.4140	0.4018	0.7625	0.021*
C12	0.14124(16)	0.10914(9)	0.55662(9)	0.0212(2)
H12A	0.0357	0.0951	0.5912	0.032*
H12B	0.2476	0.0633	0.5930	0.032*
H12C	0.1045	0.0919	0.4758	0.032*

As anticipated, the molecular packing features a number of conventional hydrogen-bonding interactions. Thus, centrosymmetrically related molecules associate *via* amine-N—H...N(triazine) hydrogen bonds and eight-membered {...HNCN}₂ synthons [N5—H2n...N2: 2.066(11) Å and 179.6(17)° for symmetry operation 1−*x*, 2−*y*, 1−*z*]. The dimeric aggregates are connected into twisted, one-dimensional supramolecular chains, parallel to [1 0 1], *via* amine-H...amine-N—H...N(triazine) hydrogen bonds, involving the other amine-H and triazine-N atoms [N5—H1n...N1:

2.074(13) Å and 168.2(12)° for symmetry operation −1/2 + *x*, 3/2−*y*, −1/2 + *z*].

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