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2-Amino-4-(4-methoxyphenyl)-1,3-thiazole

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.009 Å
R factor = 0.068
wR factor = 0.187
Data-to-parameter ratio = 8.1

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

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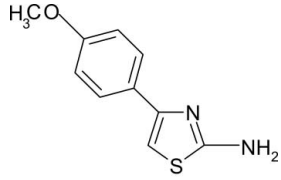
The molecule of the title compound, $C_{10}H_{10}N_2OS$, is not planar, with a dihedral angle of 14.8 (2)° between the planes of the benzene and thiazole rings. Molecules are linked by intermolecular N—H···O and N—H···N hydrogen bonds between the amino H atoms and O and N atoms of the methoxy group and thiazole ring, respectively, forming an infinite chain.

Comment

Heterocycles containing the 1,3-thiazole ring system exhibit a wide spectrum of biological activities, including antiviral and antifungal. The 1,3-thiazole ring has been identified as a central structural element of a number of biologically active natural products (Zabriskie *et al.*, 1988; Hara *et al.*, 1988; Crews *et al.*, 1988) and of pharmacologically active compounds (Metzger, 1979, 1984). The bioactivity of *S*,*N*-thiazoles is mainly due to their structural similarities with protein imidazolyl entities (Kornis, 1984) as well as their biological, structural, electronic and spectroscopic properties (Comba, 1993; Brown & Lee, 1993). Their existence may modify the bioactive and pharmaceutical characteristics of the adducts (Chohan *et al.*, 2002; Nakamura *et al.*, 1995; Boden & Pattanden, 1994). This study was undertaken in order to ascertain the crystal structure of (I).



(I)

Compound (I) (Fig. 1) is a 2-aminothiazole, (II) (Caranoni & Capella, 1982), and/or a 2-amino-4-phenylthiazole, (III) (Au-Alvarez *et al.*, 1999), derivative.

Comparing (I) with (III) reveals that all bond lengths and angles of the thiazole ring in (I) are nearly the same. The C2—S1—C5 [88.4 (3)°] bond angle in (I) is smaller than the corresponding one [90.17°] in 2-amino-4-phenylthiazole hydrobromide monohydrate, (IV) (Form *et al.*, 1974), while it is nearly the same as that [88.7 (2)°] in (III).

An examination of the deviations from the least-squares planes through individual rings shows that the thiazole and benzene rings are both planar. The dihedral angle between the two rings is 14.8 (2)°. The thiazole ring has a pseudo-twofold axis running through S1 and the mid-point of the N3—C4 bond (Table 1).

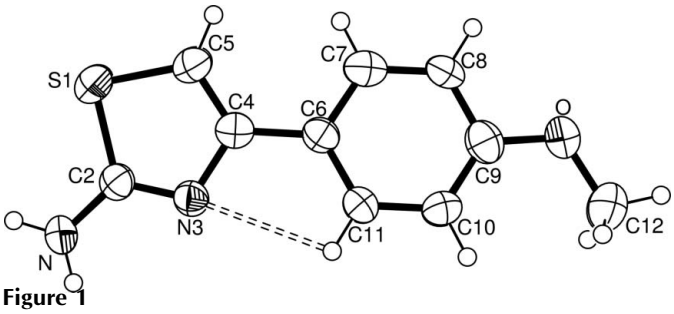


Figure 1
An *ORTEP-3* (Farrugia, 1997) drawing of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular C—H···N hydrogen bond is shown as dashed lines.

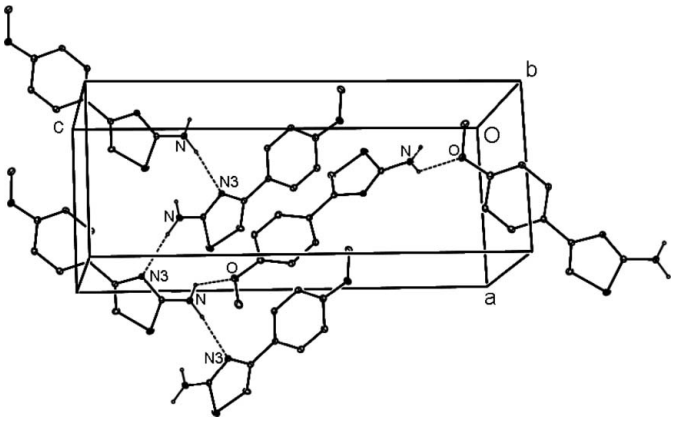


Figure 2
Packing diagram of (I). Intermolecular N—H···O and N—H···N hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

It is claimed that the planarity of the molecule in (III) is related to the shortness of the C4—C6 bond length (Au-Alvarez *et al.*, 1999). The C4—C6 bond lengths are 1.477 (8), 1.473 (5) and 1.505 Å, while the dihedral angles between the planes of the benzene and thiazole rings are 14.8 (2), 6.2 (3) and 19.23° in (I), (III) and (IV), respectively. The C4—C6 bond length in (III) is 0.004 and 0.029 Å shorter than those in (I) and (IV), respectively. Thus, the C4—C6 bonds may be assumed as nearly the same in (I) and (III). However, the differences between the dihedral angles are 8.6° [for (I) and (III)] and 13.03° [for (III) and (IV)]. As a result, there is no clear relationship between the coplanarity of the benzene and thiazole rings and the shortness of the C4—C6 bonds.

The crystal packing is stabilized by intramolecular and intermolecular hydrogen bonds, forming a chain (Table 2 and Fig. 2).

Experimental

For preparing the title compound, (I), a mixture of 4-methoxyacetophenone (0.150 g, 0.001 mmol), thiourea (0.152 g, 0.002 mmol) and iodine (0.254 g, 0.001 mmol) in methanol (40 ml) was heated on a steam bath for 5 h. The hydroiodide separated; the product was filtered off, washed with diethyl ether and then dried. It was dissolved in hot water, the solution was filtered while hot and the clear solution was neutralized with an aqueous solution of ammonia (1.0 ml, 25%). The resulting solid was filtered off and recrystallized from ethanol (yield 0.2 g, 97%; m.p. 484 K).

Crystal data

$C_{10}H_{10}N_2OS$
M_r = 206.26
Orthorhombic, $Pn2_1a$
a = 7.181 (2) Å
b = 7.750 (2) Å
c = 17.994 (3) Å
V = 1001.4 (4) Å^3
Z = 4
D_x = 1.368 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 2.6–28.3°
μ = 2.61 mm^{-1}
T = 296 (2) K
Plate, colorless
0.35 × 0.25 × 0.10 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Non–profiled ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.475, T_{max} = 0.768
1034 measured reflections
1034 independent reflections
847 reflections with $I > 2\sigma(I)$
θ_{max} = 70.8°
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 9$
$l = -22 \rightarrow 0$
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.187
S = 1.05
1034 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1346P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), no Friedel pairs
Flack parameter: −0.01 (7)

Table 1
Selected geometric parameters (Å, °).

S1—C5	1.728 (7)	N3—C4	1.395 (7)
S1—C2	1.733 (6)	C4—C5	1.336 (8)
N—C2	1.353 (8)	C6—C4	1.477 (8)
N3—C2	1.310 (7)		
C5—S1—C2	88.4 (3)	N3—C2—S1	115.0 (4)
C2—N3—C4	110.2 (5)	N—C2—S1	120.7 (4)
N3—C2—N	124.3 (6)	C5—C4—N3	114.9 (5)
C2—S1—C5—C4	1.0 (5)	C4—N3—C2—S1	−3.1 (6)
C5—S1—C2—N3	1.3 (5)	N3—C4—C5—S1	−3.0 (7)
C2—N3—C4—C5	3.9 (7)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N—H1···O^{i}	0.86	2.39	3.040 (9)	133
N—H2···N3^{ii}	0.86	2.11	2.968 (7)	175
C11—H11···N3	0.93	2.60	2.913 (7)	100

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

H atoms were positioned geometrically, with N—H = 0.86 and C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, and constrained to ride on their parent atoms with U_{iso}(H) = xU_{eq}(C,N),

where x = 1.2 for aromatic H, x = 1.5 for methyl H and x = 1.6 for amino H.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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