

3-(4-Methoxyphenyl)-6-methyl-1,2,4,5-tetrazine

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In the title compound, $C_{10}H_{10}N_4O$, the tetrazine ring is twisted with respect to the benzene ring, with a dihedral angle of $14.8(4)^\circ$.

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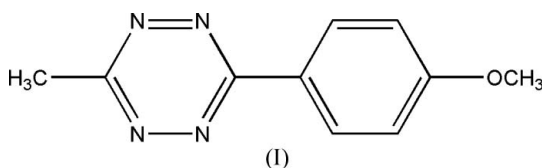
Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.059
 wR factor = 0.181
Data-to-parameter ratio = 15.5

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

Comment

1,2,4,5-Tetrazine derivatives have been widely used in pesticides and herbicides (Sauer, 1996). In continuation of our investigation on the structures of 1,2,4,5-tetrazine derivatives (Hu *et al.*, 2004, 2005), we present here the structure of the title compound, (I).



The molecular structure of (I) is illustrated in Fig. 1. The tetrazine ring is twisted with respect to the benzene ring, with a dihedral angle of $14.8(4)^\circ$. The methoxy group is coplanar with the benzene ring.

Experimental

Hydrazine hydrate (18 ml, 85%) was added dropwise to an anhydrous ethanol solution (35 ml) of acetamidine hydrochloride (54 ml) and ethyl 4-methoxybenzimidate hydrochloride (18 ml) at 263 K over 1 h. The solution was then stirred for 30 min at room temperature. The resulting red solution was poured into water (100 ml) and extracted with chloroform (100 ml). The chloroform solution was oxidized by adding sodium nitrite (58 mmol) followed by dropwise addition of acetic acid (58 mmol). The reaction mixture was filtered and the solvent was evaporated to obtain the purple crude product which was purified by chromatography on silica gel with dichloromethane as the eluent. Recrystallization from a tetrahydrofuran-ethanol solution (4:1 *v/v*) afforded single crystals of (I).

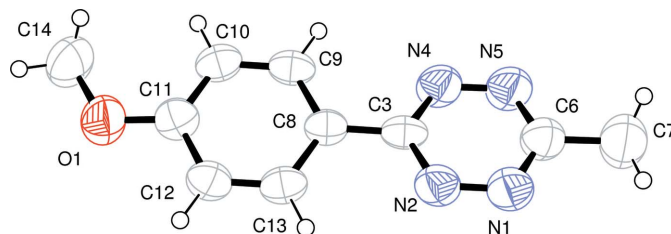


Figure 1

The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Crystal data

C₁₀H₁₀N₄O
M_r = 202.22
 Monoclinic, *P*2₁/*c*
a = 11.861 (5) Å
b = 7.111 (3) Å
c = 11.996 (5) Å
 β = 96.987 (7)°
V = 1004.3 (7) Å³

Z = 4
D_x = 1.337 Mg m⁻³
 Mo *K*α radiation
 μ = 0.09 mm⁻¹
T = 293 (2) K
 Prism, red
 0.18 × 0.15 × 0.12 mm

Data collection

Bruker SMART CCD area-detector
 diffractometer
 φ and ω scans
 Absorption correction: none
 4732 measured reflections

2161 independent reflections
 972 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.057
 θ_{\max} = 27.0°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.059
wR (*F*²) = 0.181
S = 0.93
 2161 reflections
 139 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0862P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.15 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.20 \text{ e } \text{Å}^{-3}$
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.019 (5)

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and torsion angles were refined to fit the electron density

[*U*_{iso}(H) = 1.5*U*_{eq}(C)]. Other H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined in riding mode, with *U*_{iso}(H) = 1.2*U*_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; 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, 1999); software used to prepare material for publication: *SHELXL97*.

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