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# 4-(4-Methoxyphenyl)-3-methyl-5-(2-pyridyl)-4*H*-1,2,4-triazole dihydrate

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**Key indicators**

Single-crystal X-ray study
*T* = 295 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.048
*wR* factor = 0.115
Data-to-parameter ratio = 15.1

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



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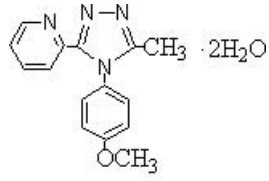
In the title compound, $C_{15}H_{14}N_4O\cdot 2H_2O$, the 1,2,4-triazole, pyridine and benzene rings do not share a common plane. The crystal structure is stabilized by O—H···N and O—H···O intermolecular hydrogen-bond interactions.

## Comment

Substituted 1,2,4-triazoles have attracted considerable attention in recent years (Bencini *et al.*, 1987; Koningsbruggen *et al.*, 1997; Moliner *et al.*, 1998; Klingele & Brooker, 2003). This is mainly because of the fact that their ligand strength is in the appropriate region to give spin-crossover complexes with iron(II) salts, which could be used as molecular-based memory devices, displays and optical switches (Garcia *et al.*, 1997; Kahn & Martinez, 1998). We have synthesized a new compound, 4-(*p*-methoxyphenyl)-3-methyl-5-(2-pyridyl)-1,2,4-triazole, and we report here the crystal structure of its dihydrate, (I).



(I)

The three rings of (I) do not share a common plane. The dihedral angle between the 1,2,4-triazole and pyridine rings is 38.22 (9)°, and that between the 1,2,4-triazole and substituted benzene rings is 82.25 (6)°.

Two N atoms of the 1,2,4-triazole ring form intermolecular hydrogen bonds with the water molecules (Table 2). An additional strong hydrogen-bond interaction involving the water molecules is observed.

## Experimental

The title compound was synthesized by the reaction of 4,4′-dimethoxyphenylphosphazoanilide with *N*-acetyl-*N*′-(2-pyridoyl)hydrazine in *o*-dichlorobenzene at 463–473 K (Grimmel *et al.*, 1946; Klingsberg, 1958). Single crystals suitable for X-ray diffraction were obtained by recrystallization from water.

*Crystal data*

$C_{15}H_{14}N_4O\cdot 2H_2O$
$M_r$ = 302.33
Monoclinic, $P2_1/c$
$a$ = 11.629 (3) Å
$b$ = 9.927 (2) Å
$c$ = 14.019 (3) Å
$\beta$ = 106.897 (4)°
$V$ = 1548.5 (6) Å$^3$
$Z$ = 4
$D_x$ = 1.297 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 793 reflections
$\theta$ = 3.1–25.1°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 295 (2) K
Block, yellow
0.31 × 0.22 × 0.20 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.97, $T_{max}$ = 0.98
7967 measured reflections
3038 independent reflections
2217 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027
$\theta_{max}$ = 26.0°
$h = -14 \rightarrow 14$
$k = -6 \rightarrow 12$
$l = -17 \rightarrow 16$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.115
$S$ = 0.97
3038 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.0126P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.13 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C6—N2 | 1.295 (2) | C11—O1 | 1.361 (2) |
| C6—N1 | 1.379 (2) | C15—O1 | 1.414 (2) |
| C7—N3 | 1.278 (2) | N2—N3 | 1.396 (2) |
| C7—N1 | 1.374 (2) | | |
| N2—C6—N1 | 110.48 (14) | C7—N1—C6 | 103.61 (14) |
| N2—C6—C1 | 122.70 (15) | C7—N1—C8 | 126.22 (14) |
| N1—C6—C1 | 126.79 (15) | C6—N1—C8 | 130.10 (14) |
| N3—C7—N1 | 111.19 (15) | C6—N2—N3 | 107.09 (14) |
| N3—C7—C14 | 126.65 (15) | C7—N3—N2 | 107.60 (14) |
| N1—C7—C14 | 122.04 (15) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2$D$···N3$^{i}$ | 0.85 | 2.43 | 2.906 (2) | 116 |
| O3—H3$B$···N2$^{i}$ | 0.85 | 2.29 | 2.848 (2) | 124 |
| O2—H2$C$···O3$^{ii}$ | 0.85 | 2.06 | 2.783 (2) | 143 |

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

All H atoms were located in a difference Fourier map and allowed to ride on their parent atoms at distances of 0.85 (O—H), 0.93 (C—H aromatic) and 0.96 Å (C—H methyl), with $U_{iso}$(H) values of 1.2–1.5 times $U_{eq}$ of the parent atoms.

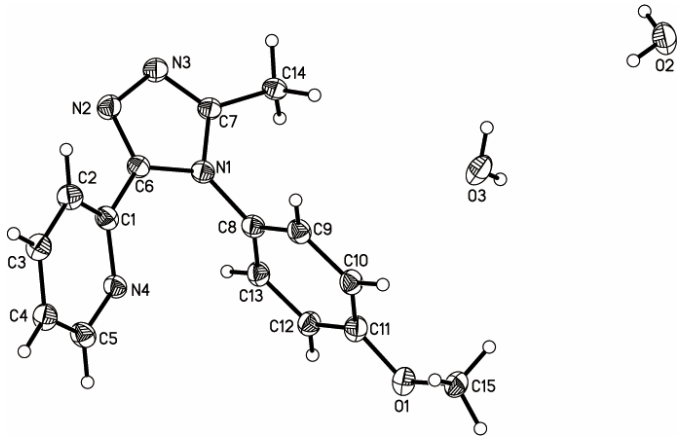



**Figure 1**
The molecular structure of the title compound, with the atom-labelling scheme. Displacement ellipsoids are shown at the 67% probability level.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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