

3-Ethyl-4-phenyl-5-(2-pyridyl)-1,2,4-triazole

Chun-Yi Liu, Zuo-Xiang Wang,
An-Yu Zhou, Lu-Tong Yuan and
Yan Lan*Department of Chemistry and Chemical
Engineering, Southeast University, Nanjing
210096, People's Republic of ChinaCorrespondence e-mail:
wangzx0908@yahoo.com.cn

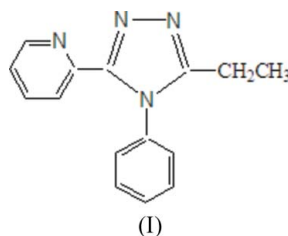
Key indicators

Single-crystal X-ray study
 $T = 273$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
Disorder in main residue
 R factor = 0.057
 wR factor = 0.122
Data-to-parameter ratio = 13.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the crystal structure of the title compound, $\text{C}_{15}\text{H}_{14}\text{N}_4$, all three aromatic rings, *viz.* 1,2,4-triazole, pyridine and benzene. The crystal structure shows that all three rings are not coplanar.

Comment

The coordination chemistry of substituted 1,2,4-triazoles has gained considerable attention in recent years (Bencini *et al.*, 1987; Koningsbruggen *et al.*, 1997; Moliner *et al.*, 1998; Moliner *et al.*, 2001; Klingele & Brooker, 2003). This is mainly because of the fact that their ligand strength is in the 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). Recently, we have prepared some new substituted 1,2,4-triazole derivatives and their transition-metal complexes, and we report here the crystal structure analysis of 3-ethyl-4-phenyl-5-(2-pyridyl)-1,2,4-triazole, (I).



In the title structure, all three aromatic rings, *viz.* 1,2,4-triazole, pyridine, and benzene. All three aromatic rings are not coplanar. The dihedral angle between the 1,2,4-triazole and the pyridine rings is $11.71(15)^\circ$, and that between the 1,2,4-triazole and the benzene rings is $84.61(7)^\circ$. The ethyl group is disordered.

Experimental

The title compound was synthesized by reaction of diphenylphosphazoanilide with *N*-propionyl-*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 recrystallized from ethyl acetate.

Crystal data

$\text{C}_{15}\text{H}_{14}\text{N}_4$
 $M_r = 250.30$
Monoclinic, $P2_1/n$
 $a = 10.4365(14)$ Å
 $b = 9.0713(12)$ Å
 $c = 14.1861(18)$ Å
 $\beta = 94.107(3)^\circ$
 $V = 1339.6(3)$ Å³
 $Z = 4$

$D_x = 1.241$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 1381 reflections
 $\theta = 2.3$ – 20.0°
 $\mu = 0.08$ mm⁻¹
 $T = 273(2)$ K
Rhombhedron, colorless
 $0.30 \times 0.24 \times 0.22$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.98$, $T_{\max} = 0.98$
 7002 measured reflections

2625 independent reflections
 1547 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$
 $\theta_{\text{max}} = 26.0^\circ$
 $h = -8 \rightarrow 12$
 $k = -11 \rightarrow 11$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.122$
 $S = 1.07$
 2625 reflections
 194 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.12 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97
 Extinction coefficient: 0.0071 (18)

Table 1

Selected geometric parameters (\AA , $^\circ$).

C1–N2	1.307 (3)	C2–N3	1.277 (3)
C1–N1	1.357 (3)	C2–N1	1.356 (3)
C1–C3	1.454 (3)	N1–C8	1.432 (3)
N2–C1–N1	110.2 (2)	C2–N1–C8	124.4 (2)
N2–C1–C3	123.4 (2)	C1–N1–C8	130.7 (2)
N1–C1–C3	126.4 (2)	C1–N2–N3	106.35 (19)
N3–C2–N1	110.69 (19)	C2–N3–N2	107.93 (17)
C2–N1–C1	104.85 (19)		

All H atoms were located in a difference Fourier map and allowed to ride on their parent atoms at C–H distances of 0.93 (aromatic), 0.96 (methyl) and 0.97 \AA (methylene), with $U_{\text{iso}}(\text{H})$ values of 1.2–1.5 times U_{eq} of the parent atom.

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.

We are grateful to Southeast University, Nanjing, for financial assistance though project No. 913–9207041142.

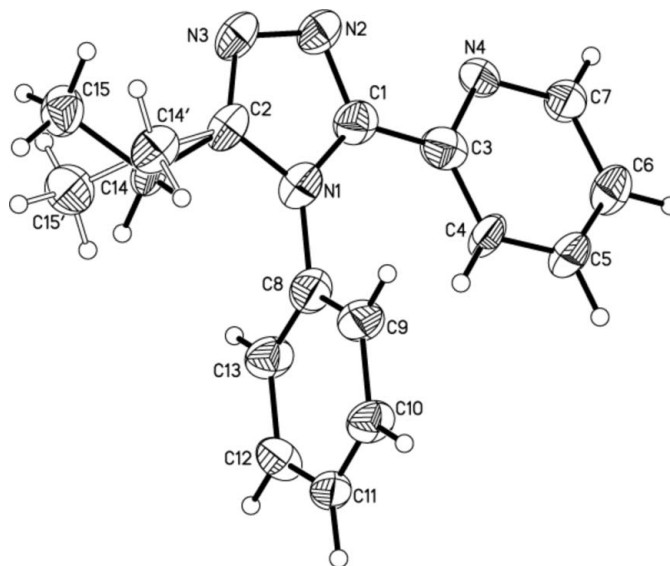


Figure 1

The molecular structure of the title compound, with the atomic labelling. Displacement ellipsoids are drawn at the 50% probability level. Both disorder components are shown.

References

Bencini, A., Gatteschi, D., Zanchini, C., Haasnoot, J. G., Prins, R. & Reedijk, J. (1987). *J. Am. Chem. Soc.* **109**, 2926–2931.
 Bruker (2000). SMART (Version 5.625), SAINT (Version 6.01), SHELXTL (Version 6.10) and SADABS (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
 Garcia, Y., Koningsbruggen, P. J., Codjovi, E., Lapouyade, R., Kahn, O. & Rabardel, L. (1997). *J. Mater. Chem.* **7**, 857–858.
 Grimm, H. W., Guenther, A. & Morgan, J. F. (1946). *J. Am. Chem. Soc.* **68**, 539–542.
 Kahn, O. & Martinez, C. J. (1998). *Science*, **279**, 44–48.
 Klingele, M. H. & Brooker, S. (2003). *Coord. Chem. Rev.* **241**, 119–132.
 Klingsberg, E. (1958). *J. Org. Chem.* **23**, 1086–1087.
 Koningsbruggen, P. J., Haasnoot, J. G., Kooijman, H., Reedijk, J. & Spek, A. L. (1997). *JOURNAL NAME?* **36**, 2487–2489.
 Moliner, N., Gaspar, A. B., Munoz, M. C., Niel, V., Cano, J. & Real, J. A. (2001). *Inorg. Chem.* **40**, 3986–3991.
 Moliner, N., Munoz, M. C., Koningsbruggen, P. J. & Real, J. A. (1998). *Inorg. Chim. Acta*, **274**, 1–6.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.