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4,4,5,5-Tetramethyl-2-(4-pyridyl)imidazolin-1-oxyl 3-oxide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.079
wR factor = 0.206
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.

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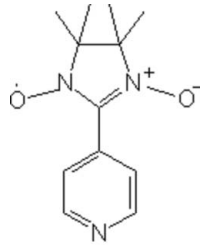
The molecular structure of the title radical compound, $C_{12}H_{16}N_3O_2$, has crystallographic C_2 symmetry. The dihedral angle between the pyridine and imidazole rings is 25.66 (15)°.

Comment

Nitroxide radicals are widely used to prepare molecule-based magnetic materials (Vostrikova *et al.*, 2000; Oshio *et al.*, 2002). We report here the synthesis and crystal structure of the title radical compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The molecule has crystallographic C_2 symmetry, the C3—C4 bond, atom N1 and the mid-point of the C5—C5*A* bond being located on a twofold axis. The pyridine ring is twisted with respect to the imidazole ring with a dihedral angle of 25.66 (15)°.

Experimental

The title compound was prepared according to the method reported by Ullman *et al.* (1974). 2,3-Dimethyl-2,3-bis(hydroxylamino)butane and 4-pyridinecarbaldehyde were dissolved in a methanol solution which was stirred for 1 h at room temperature, and then filtered. Single crystals of (I) were obtained from the filtrate.

Crystal data

$C_{12}H_{16}N_3O_2$
M_r = 234.28
Monoclinic, $C2/c$
a = 11.205 (7) Å
b = 10.452 (7) Å
c = 11.031 (8) Å
β = 108.051 (11)°
V = 1228.3 (14) Å^3
Z = 4
D_x = 1.267 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, blue
0.24 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector detector diffractometer
φ and ω scans
Absorption correction: none
3365 measured reflections
1258 independent reflections
655 reflections with $I > 2\sigma(I)$
R_{int} = 0.088
θ_{max} = 26.5°

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.079$	$w = 1/[\sigma^2(F_o^2) + (0.09P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.206$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.03$	$\Delta\rho_{max} = 0.23$ e Å^{-3}
1258 reflections	$\Delta\rho_{min} = -0.26$ e Å^{-3}
81 parameters	

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and torsion angles were refined to fit the electron density, $U_{iso}(H) = 1.5U_{eq}(C)$. Aromatic H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$.

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

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References

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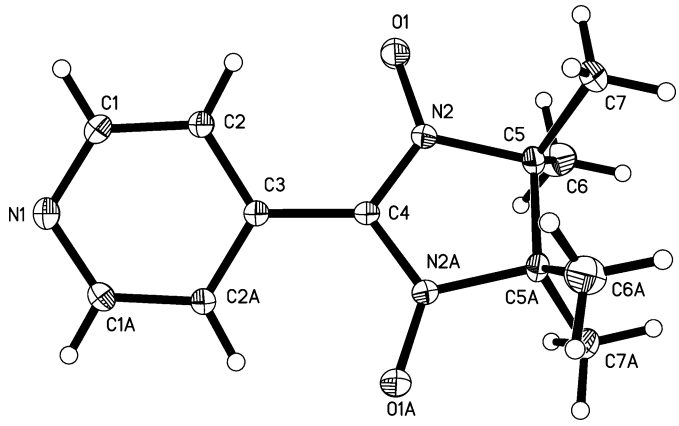

Figure 1
The molecular structure of (I) with 15% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry code: (A) $-x$, y, $-z + \frac{1}{2}$].

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