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2,2-Dimethyl-6-(4-nitrophenyl)-4-phenyl-1,3-diazabicyclo[3.1.0]hex-3-ene

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In the crystal structure of the title compound, $C_{18}H_{17}N_3O_2$, the imidazoline ring has a very flattened envelope conformation, with a twisted endocyclic C=N double bond.

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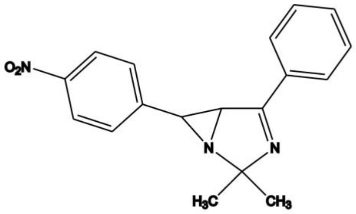
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.067
wR factor = 0.198
Data-to-parameter ratio = 10.1

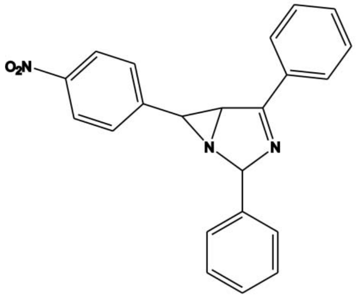
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

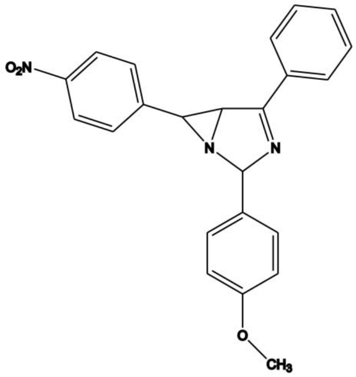
Bicyclic aziridines represent a very interesting class of organic compounds, possessing unique photochromic properties. It has been demonstrated that these compounds form deeply colored, fairly stable materials under UV radiation (Orlov *et al.*, 1988). This property allows us to consider bicyclic aziridines as possible candidates in the search for radiochromic materials. Among these compounds, 2,2-dimethyl-6-(4-nitrophenyl)-4-phenyl-1,3-diazabicyclo[3.1.0]hex-3-ene, (I), is one of the most interesting, and we have carried out an X-ray diffraction study of it.



(I)



(II)



(III)

The imidazoline ring has a very flattened envelope conformation. The deviation of atom N2 from the mean plane of the remaining ring atoms is 0.09 (1) Å. This conformation of the five-membered ring results in a slight twisting of the C=N double bond, the C3—N2—C2—C1 torsion angle being 5.8 (2)°. There is a similar twisting of the C=N double bond in compounds (II) (3.2°; Orlov *et al.*, 1991) and (III) (2.7°; Kaluski *et al.*, 1994). The C1—C2 bond is shortened, to 1.488 (3) Å, compared with the average value of 1.512 Å (Bürgi & Dunitz, 1994).

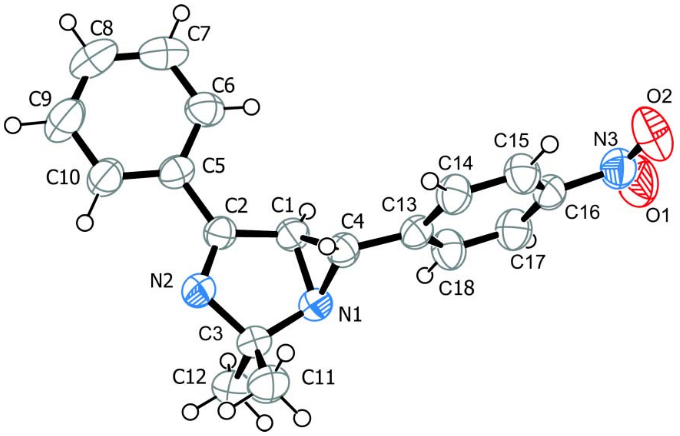


Figure 1
View of the title compound. The non-H atoms are shown with displacement ellipsoids drawn at the 50% probability level.

The aziridine and imidazoline rings are *cis*-fused, the H1—C1—N1—Lp (where Lp is the N lone pair) torsion angle being 2°. The angle between the two ring planes is 113 (2)°. The same conformation is observed for compounds (II) and (III).

The phenyl substituent is rotated with respect to the N2═C2 double bond, the N2—C2—C5—C10 torsion angle being 14.2 (3)°. In turn, the *p*-nitrophenyl substituent is rotated with respect to the aziridine plane, the N1—C4—C13—C18 torsion angle being 19.5 (3)°; this compares with a value of 29.1° in compound (II). In (III), however, the corresponding angle is 113.9°. The nitro group is coplanar with the attached aromatic ring, the O2—N3–C16—C15 torsion angle being 1.8 (3)°.

Experimental

The title compound was prepared according to the procedure of Heine *et al.* (1968).

Crystal data

$C_{18}H_{17}N_3O_2$
$M_r = 307.35$
Triclinic, $P\bar{1}$
$a = 9.535\ (3)$ Å
$b = 9.539\ (3)$ Å
$c = 10.093\ (3)$ Å
$\alpha = 103.89\ (2)°$
$\beta = 92.05\ (3)°$
$\gamma = 113.50\ (2)°$
$V = 808.3\ (5)$ Å^3
$Z = 2$
$D_x = 1.263$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
$\theta = 10$–$14°$
$\mu = 0.08$ mm^{-1}
$T = 294\ (2)$ K
Block, blue
0.4 × 0.2 × 0.2 mm

Data collection

Siemens P3/PC diffractometer
θ–2θ scans
Absorption correction: none
2960 measured reflections
2786 independent reflections
2425 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.038$
$\theta_{\rm max} = 25.1°$
$h = 0 \rightarrow 11$
$k = -11 \rightarrow 10$
$l = -12 \rightarrow 11$
2 standard reflections every 98 reflections intensity decay: 5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.198$
$S = 1.08$
2786 reflections
276 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.1417P)^2 + 0.1312P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.42$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.25$ e Å^{-3}
Extinction correction: none

Table 1
Selected interatomic distances (Å).

N1—C1	1.470 (2)	C1—C4	1.506 (3)
N1—C4	1.476 (3)	C2—C5	1.475 (3)
N1—C3	1.487 (3)	C3—C11	1.516 (3)
N2—C2	1.283 (3)	C3—C12	1.527 (3)
N2—C3	1.479 (3)	C4—C13	1.479 (3)
C1—C2	1.488 (3)		

The H atom parameters were freely refined and the C—H distances lie in the range 0.86 (3)–1.02 (3) Å.

Data collection: *P3* (Siemens,1989); cell refinement: *P3*; data reduction: *XDISK* (Siemens, 1991); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1991); software used to prepare material for publication: *SHELXL97*.

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