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5-(4-Chlorophenyl)-3-oxa-4-azatricyclo[5.2.1.0^{2,6}]-dec-4-ene

A. Thiruvalluvar,[a]* V. Parthasarathi,[b] V. Kabaleeswaran,[c] S. S. Rajan,[c] A. Nagarajan[d] and M. Krishna Pillay[d]

[a]Department of Physics, Rajah Serfoji Govt College, Thanjavur 613 005, Tamilnadu, India, [b]Department of Physics, Bharathidasan University, Tiruchirapalli 620 024, India, [c]Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, and [d]Department of Chemistry, Bharathidasan University, Tiruchirapalli 620 024, India

Correspondence e-mail: athiru@eth.net

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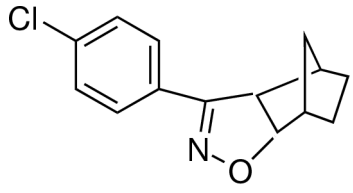
The asymmetric unit of the title compound, $C_{14}H_{14}ClNO$, contains two crystallographically independent molecules related by a pseudo-inversion centre at (1.00, 0.65, 0.25). The isoxazoline rings of these two molecules are planar and the structure analysis confirms the *exo*-orientation of the isoxazole ring to norbornane. The two molecules in the asymmetric unit differ in the conformation of the chlorophenyl rings.



(I)

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.144
Data-to-parameter ratio = 15.0

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

Experimental

The title compound was obtained employing Torssell's one-pot synthesis (Larsen & Torssell, 1984) by the cycloaddition of norbornene with 4-chlorobenzonitrile oxide (Nagarajan & Krishna Pillay, 1993). Recrystallization from ethanol afforded the crystals. The yield of isolated product was 75%.

Crystal data

$C_{14}H_{14}ClNO$
M_r = 247.73
Monoclinic, $P2_1/n$
a = 11.782 (4) Å
b = 10.288 (3) Å
c = 20.461 (3) Å
β = 100.20 (2)°
V = 2440.9 (11) Å^3
Z = 8
D_x = 1.348 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 7–32°
μ = 2.62 mm^{-1}
T = 298 (2) K
Block, colourless
0.20 × 0.12 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
4716 measured reflections
4622 independent reflections
3767 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 69.9°
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 12$
$l = -24 \rightarrow 24$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.144
S = 1.05
4622 reflections
308 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0849P)^2 + 0.5370P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0027 (3)

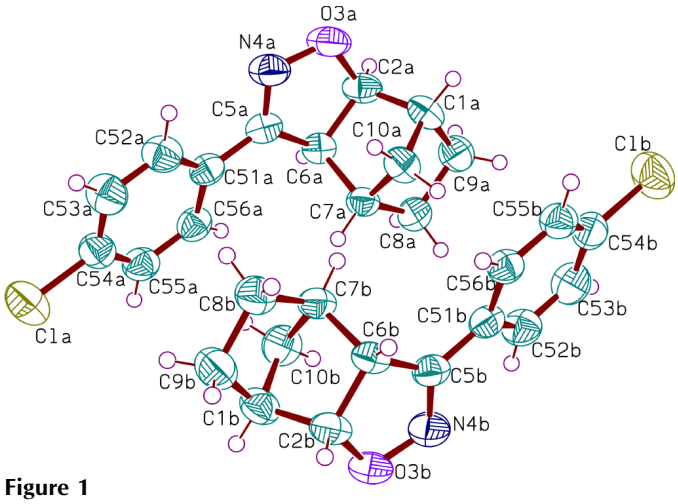


Figure 1
View of the asymmetric unit of (I), with displacement ellipsoids shown at the 50% probability level (Farrugia, 1997).

Table 1
Selected geometric parameters (Å, °).

O3*A*—N4*A*	1.411 (2)	O3*B*—N4*B*	1.413 (2)
N4*A*—C5*A*	1.279 (2)	N4*B*—C5*B*	1.283 (2)
C6*A*—C5*A*—C51*A*—C56*A*	−16.4 (3)	C6*B*—C5*B*—C51*B*—C56*B*	22.3 (3)
N4*A*—C5*A*—C51*A*—C52*A*	−12.8 (3)	N4*B*—C5*B*—C51*B*—C52*B*	20.6 (3)

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *MolEN* (Fair, 1990); data reduction: *MolEN*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997).

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