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***N*-(*p*-Chlorobenzylidene)phenylamine *N*-oxide**

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***N*-(*p*-Chlorobenzylidene)phenylamine
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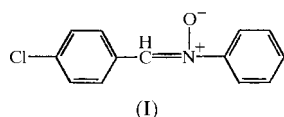
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The crystal structure of the title compound, C₁₃H₁₀ClNO, confirms that it exists as a nitron. The geometry about C=N is *Z*. The relevant torsion angles indicate *trans* and *cis* conformations around the nitron bond.

Comment

The title compound, (I), has been analysed as part of crystallographic studies on substituted *N*-phenylnitrones. There are two independent molecules in the asymmetric unit. The molecule exists as a nitron. The average C=N distance of 1.307 (2) Å is within 3σ of the value of 1.279 (8) Å reported by Allen *et al.* (1987) and is also comparable with the value of 1.304 (3) Å reported in a similar situation (Vijayalakshmi *et al.*, 1997). The dihedral angles between planes C8/N7/C7 and N7/C7/C1 is 0.29 (3)° (molecule 1) and between C8A/N7A/C7A and N7A/C7A/C1A is 0.30 (3)° (molecule 2). This indicates that the nitron groups formed by atoms C8/N7/C7/C1 in molecule 1 and by C8A/N7A/C7A/C1A in molecule 2 attached to two phenyl rings are nearly planar. The C1–C7 and C1A–C7A distances of 1.442 (2) and 1.443 (2) Å, respectively, are nearly equal to the value of 1.438 (4) Å reported by Bedford *et al.* (1991). The C–Cl distance of 1.740 (2) Å in molecules 1 and 2 is comparable with the distance of 1.736 (10) Å reported by Allen *et al.* (1987). The phenyl bond lengths and angles for both molecules are in agreement with the expected values reported by Allen *et al.* (1987). The angles between the least-squares planes of the two phenyl rings in molecule 1 and 2 are 125.8 (6) and 126.1 (6)°, respectively. A short intermolecular contact is observed, C7···O7ⁱ 3.379 (1) Å and C7A···O7Aⁱ 3.386 (1) Å [symmetry code: (i) *x*, *y*, *z* – 1].

**Experimental**

A solution of 4-chlorobenzaldehyde (1.40 g) in ethanol (25 ml) was added dropwise with stirring to a solution of *N*-phenylhydroxylamine (1.09 g) in ethanol (10 ml). The mixture was warmed for about 1 h at 333 K. On cooling, crude crystals of the title compound separated and were crystallized from ethanol [m.p. 426 K; yield 1.90 g (82%)]. The title compound was prepared in the Department of Industrial Chemistry, Alagappa University, Karaikudi, India.

Crystal data

C₁₃H₁₀ClNO
M_r = 231.67
 Triclinic, *P* $\bar{1}$
a = 13.594 (2) Å
b = 14.808 (3) Å
c = 5.6110 (15) Å
 α = 90.089 (17)°
 β = 98.130 (18)°
 γ = 83.505 (14)°
V = 1110.8 (4) Å³

Z = 4
D_x = 1.385 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 25 reflections
 θ = 2–25°
 μ = 0.319 mm⁻¹
T = 293 (2) K
 Rectangular block, yellow
 0.20 × 0.20 × 0.15 mm

Data collection

Rigaku AFC-7S diffractometer
 ω –2θ scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 T_{\min} = 0.927, T_{\max} = 0.990
 4199 measured reflections
 3914 independent reflections
 2936 reflections with *I* > 2σ(*I*)
R_{int} = 0.044

θ_{\max} = 24.86°
h = 0 → 16
k = –17 → 17
l = –6 → 6
 3 standard reflections
 every 100 reflections
 frequency: 150 min
 intensity decay: none

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.036
wR(*F*²) = 0.115
S = 1.020
 3914 reflections
 291 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0540P)^2 + 0.3079P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.028$
 $\Delta\rho_{\max} = 0.20 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e \AA}^{-3}$
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.0105 (17)

Table 1

Selected geometric parameters (Å, °).

C11–C4	1.7398 (19)	N7A–O7A	1.2980 (19)
O7–N7	1.2976 (18)	N7A–C7A	1.307 (2)
C1–C2	1.398 (2)	N7A–C8A	1.453 (2)
N7–C7	1.307 (2)	C8A–C9A	1.381 (3)
N7–C8	1.451 (2)	C8A–C13A	1.387 (3)
C8–C9	1.377 (3)	C7A–C1A	1.443 (2)
C8–C13	1.393 (2)	C6A–C5A	1.374 (3)
C11–C12	1.380 (3)	C6A–C1A	1.407 (2)
C11–C10	1.381 (3)	C1A–C2A	1.398 (3)
C6–C5	1.375 (3)	C13A–C12A	1.377 (3)
C10–C9	1.380 (3)	C2A–C3A	1.375 (3)
C2–C3	1.371 (3)	C10A–C9A	1.382 (3)
C3–C4	1.385 (3)	C10A–C11A	1.383 (3)
C4–C5	1.382 (3)	C12A–C11A	1.381 (3)
C13–C12	1.378 (3)	C4A–C5A	1.380 (3)
C11A–C4A	1.7402 (19)	C4A–C3A	1.389 (3)
O7–N7–C7	124.13 (15)	O7A–N7A–C7A	124.61 (16)
O7–N7–C8	115.32 (14)	O7A–N7A–C8A	115.50 (14)
C7–N7–C8	120.52 (14)	C7A–N7A–C8A	119.86 (15)
C9–C8–N7	118.13 (16)	C9A–C8A–N7A	118.24 (16)
C13–C8–N7	120.91 (16)	C13A–C8A–N7A	120.76 (16)
C3–C4–C11	119.31 (15)	N7A–C7A–C1A	126.93 (16)

O7–N7–C7–C1	–2.2 (3)
C8–N7–C7–C1	179.65 (16)
C2–C1–C7–N7	162.77 (18)
C6–C1–C7–N7	–18.6 (3)
O7–N7–C8–C9	–33.4 (2)
C7–N7–C8–C9	144.82 (18)
O7–N7–C8–C13	144.82 (18)
C7–N7–C8–C13	–36.9 (3)
N7–C8–C13–C12	–179.26 (17)
N7–C8–C9–C10	179.66 (17)
O7A–N7A–C8A–C9A	34.9 (2)
C7A–N7A–C8A–C9A	–143.41 (19)
O7A–N7A–C8A–C13A	–143.76 (19)
C7A–N7A–C8A–C13A	37.9 (3)
O7A–N7A–C7A–C1A	1.7 (3)
C8A–N7A–C7A–C1A	179.87 (16)
N7A–C7A–C1A–C2A	–164.33 (18)
N7A–C7A–C1A–C6A	17.7 (3)
N7A–C8A–C13A–C12A	179.28 (18)
N7A–C8A–C9A–C10A	–179.92 (17)

All H atoms were located from difference Fourier maps and were included in the structure-factor calculations with isotropic displacement parameters equal to $1.1U_{\text{eq}}$ of the carrier atom, but the parameters were not refined.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structures Corporation, 1995a); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structures Corporation, 1995b); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine

structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1983).

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