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N-(4-Cyanophenyl)-*α*-(4-methoxyphenyl)nitrone

Jun-Gill Kang,[a]* Jung-Pyo Hong[a] and Il-Hwan Suh[b]

[a]Department of Chemistry, Chungnam National University, Taejon, 305-764, Korea, and [b]Department of Physics, Chungnam National University, Taejon, 305-764, Korea
Correspondence e-mail: jgkang@hanbat.chungnam.ac.kr

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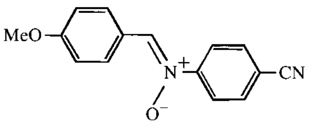
In the crystal structure of the title compound, 4-cyano-*N*-(4-methoxybenzylidene)phenylamine *N*-oxide, $C_{15}H_{12}N_2O_2$, the 4-methoxyphenyl is approximately coplanar with the nitrone moiety but significantly rotated with respect to the 4-cyanophenyl moiety. The extent of this rotation is significantly different for the two crystallographically independent molecules of the asymmetric unit [dihedral angles of 19.4 (1) and 26.5 (1)°]. The geometry about the C=N bond is *Z*. The two molecules are related to one another by a pseudo inversion centre.

Comment

The title compound, (I), was synthesized for use as a photobleachable material. The crystal structure of (I) confirms that it exists as a nitrone.



(I)

The asymmetric unit of (I) consists of two crystallographically independent molecules, *A* (unprimed labels) and *B* (primed labels), as shown in Fig. 1. The nitrone units in each molecule are closely planar, with displacements of −0.016 (2) [−0.022 (2)], 0.0329 (2) [0.039 (2)], 0.012 (2) [0.019 (2)], 0.000 (2) [0.000 (2)] and −0.015 (2) [−0.021 (2)] Å, respectively, for atoms C5, C8, N1, O2 and C9 (values for molecule *B*, here and elsewhere, are given in square brackets). The nitrone unit is closely coplanar with the 4-methoxyphenyl group: the dihedral angle is 5.2 (1) [3.0 (1)]°. The 4-cyanophenyl unit is substantially twisted with respect to the nitrone unit and the 4-methoxyphenyl group, with dihedral angles of 24.2 (1) [27.1 (1)] and 19.4 (1) [26.5 (1)]°, respectively. Similar planarity of the nitrone moiety is found in *N*-methyl benzaldehyde nitrone (Bedford *et al.*, 1991) and *N*-(*p*-hydroxybenzylidene)phenylamine *N*-oxide (Vijayalakshmi *et al.*, 1997).

Both molecule *A* and molecule *B* adopt the more commonly observed *Z* isomer. The torsion angle about the C=N bond, O2—N1—C8—C5, is 3.3 (4) [3.3 (4)]°. The N1—O2 bond lengths are nearly equal to the value of 1.293 (3) Å reported by Bedford *et al.* (1991). The phenyl bond lengths and angles are in agreement with the expected values reported by Allen *et al.* (1987).

As is apparent from Fig. 1, the two molecules are related to each other by a pseudo inversion centre. Deviations are manifest in different intramolecular dihedral angles between the 4-cyanophenyl and 4-methoxymethyl groups and in intermolecular dihedral angles of 6.4 (1) and 4.4 (1)° between pseudo-symmetrically related 4-cyanomethyl and 4-methoxyphenyl groups.

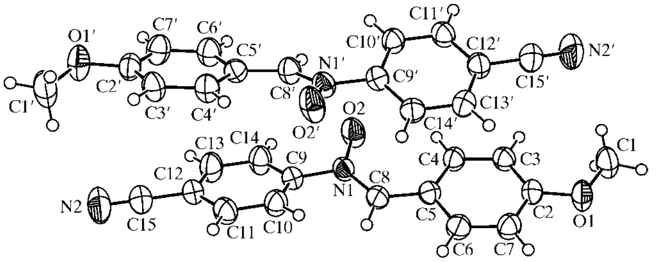


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms are shown as spheres of an arbitrary radius.

Experimental

The title compound was prepared by condensing *p*-methoxybenzenealdehyde with freshly prepared *p*-cyanophenylhydroxylamine in absolute ethanol at room temperature for 48 h. Evaporation of the solvent yielded a red oil, which was twice crystallized from ethanol. A yellow single crystal of (I) was coated with lacquer prior to mounting on the diffractometer, because of its instability in air.

Crystal data

$C_{15}H_{12}N_2O_2$
$M_r = 252.27$
Triclinic, $P\bar{1}$
$a = 7.5821\ (16)$ Å
$b = 7.613\ (2)$ Å
$c = 22.270\ (3)$ Å
$\alpha = 99.469\ (16)°$
$\beta = 96.999\ (12)°$
$\gamma = 94.79\ (2)°$
$V = 1251.5\ (5)$ Å^3
$Z = 4$
$D_x = 1.339$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 11.28–14.24°$
$\mu = 0.091$ mm^{-1}
$T = 293$ K
Plate, yellow
0.50 × 0.30 × 0.13 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Non-profiled $\omega/2\theta$ scans
4490 measured reflections
4370 independent reflections
2688 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.054$
$\theta_{\rm max} = 24.97°$
$h = -9 \rightarrow 8$
$k = -9 \rightarrow 8$
$l = 0 \rightarrow 26$
3 standard reflections
frequency: 300 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.177$
$S = 1.009$
4370 reflections
415 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.0037P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.24$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—O2	1.297 (3)	N1′—O2′	1.299 (3)
N1—C8	1.309 (3)	N1′—C8′	1.314 (3)
N1—C9	1.454 (3)	N1′—C9′	1.450 (3)
N2—C15	1.139 (3)	N2′—C15′	1.137 (4)
O1—C2	1.360 (3)	O1′—C2′	1.364 (3)
O1—C1	1.432 (3)	O1′—C1′	1.427 (4)
O2—N1—C8	122.8 (2)	O2′—N1′—C8′	122.6 (2)
O2—N1—C9	116.3 (2)	O2′—N1′—C9′	116.3 (2)
C2—O1—C1	118.5 (2)	C2′—O1′—C1′	118.5 (2)
N1—C8—C5	129.0 (2)	N1′—C8′—C5′	127.5 (2)
N2—C15—C12	178.4 (4)	N2′—C15′—C12′	178.6 (4)
O2—N1—C8—C5	3.3 (4)	O2′—N1′—C8′—C5′	3.3 (4)
C9—N1—C8—C5	−176.0 (2)	C9′—N1′—C8′—C5′	−175.0 (2)
C4—C5—C8—N1	−6.8 (5)	C4′—C5′—C8′—N1′	−2.4 (4)
C6—C5—C8—N1	173.6 (3)	C6′—C5′—C8′—N1′	177.3 (3)
O2—N1—C9—C10	−154.1 (2)	O2′—N1′—C9′—C10′	−150.9 (2)
C8—N1—C9—C10	25.3 (4)	C8′—N1′—C9′—C10′	27.4 (4)
O2—N1—C9—C14	23.3 (3)	O2′—N1′—C9′—C14′	25.9 (3)
C8—N1—C9—C14	−157.4 (3)	C8′—N1′—C9′—C14′	−155.8 (2)
N1—C9—C14—C13	−179.0 (3)	N1′—C9′—C14′—C13′	−177.3 (2)

All non-H atoms were refined anisotropically. The positions of the H atoms were refined, but their isotropic *U* values were constrained.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1998).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: JA1009). Services for accessing these data are described at the back of the journal.

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