

Related literature. Several 1-aryl-4-(β -2-quinolyl/1-isoquinolyethyl)piperazines and related compounds have been synthesized and evaluated for their hypotensive activity (Murti, Bhandari, Ram, Prabhakar, Saxena, Jain, Gulati, Srimal, Dhawan, Nityanand & Anand, 1989). Most of the compounds exhibited prominent hypotensive activity and weak diuretic, antiinflammatory and CNS depressant activities. Among them, the centrally acting title compound, centhaquin, was found to possess the most suitable profile of hypotensive activity.

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(E)-1,2-Bis(2,3,5,6-tetrafluoro-4-pyridyl)diazene 1,2-Dioxide*

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Abstract. $C_{10}F_8N_4O_2$, $M_r = 360.12$, monoclinic, $P2_1/n$, $a = 6.012$ (2), $b = 5.653$ (2), $c = 18.174$ (3) Å, $\beta = 97.74$ (2)°, $V = 612.0$ Å³, $Z = 2.0$, $D_x = 1.95$ Mg m⁻³, $F(000) = 352.0$, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 0.161$ mm⁻¹, $T = 293$ K, $R = 0.042$ for 776 unique reflexions [$F \geq 3\sigma(F)$]. The structure is composed of centrosymmetric *trans*-dimers of 2,3,5,6-tetrafluoro-4-nitrosopyridine [N—N 1.320 (4) Å]. This contrasts with the benzene analogue, where *cis*-dimer coexists with monomer [Prout, Coda, Forder & Kamenar (1974). *Cryst. Struct. Commun.* **3**, 39-40].

Experimental. Initial sample preparation employed the method of Banks, Du Boisson, Marraccini, Sekhri & Tipping (1987). However, purification of the green mixture thus produced relied on flash column chromatography (silica eluted with light petroleum). The first (blue-green) fraction was distilled to remove most of the eluent and the stillpot residue cooled to 195 K to afford white crystals suitable for X-ray investigation.

Crystal size 0.30 × 0.40 × 0.40 mm, Enraf-Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation, unit-cell dimensions from setting angles of 25 accurately centred reflexions ($7.6 \leq \theta \leq 8.7^\circ$), ω - 2θ scan mode, ω -scan width ($0.70 + 0.35 \tan \theta$)° and scan speed ranging from 1.4 to

5.0° min⁻¹ according to the intensity gathered in a pre-scan, $-7 \leq h \leq 7$, $0 \leq k \leq 6$, $0 \leq l \leq 21$, $0 \leq \theta \leq 25^\circ$, 1321 reflexions measured, 931 unique ($R_{\text{int}} = 0.010$), 776 observed ($F \geq 3\sigma(F)$), intensity standards ($\bar{1}1\bar{6}$; $\bar{1}1\bar{5}$; $2\bar{1}0$) measured every 2.5 h, 15% decay, Lp and decomposition corrections applied, absorption ignored. *MULTAN80* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) used to solve the phase problem, all atoms found in Fourier map, full-matrix least squares based on F using *SHELX76* (Sheldrick, 1976), final $R = 0.042$, $wR = 0.045$, $w = 2.6449/[\sigma^2(F) + 0.0005F^2]$, anisotropic thermal parameters for all atoms. Maximum fluctuation in final ΔF map in range -0.2 to 0.2 e Å⁻³, maximum Δ/σ 0.004. Scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV), computation carried out on the Amdahl 5890 system of the University of Manchester Computing Centre. Literature surveyed via the Cambridge Structural Database using the Crystal Structure Search and Retrieval interactive system (CSSR, 1984). Fractional atomic coordinates and vibrational parameters are presented in Table 1† and selected bond lengths and angles in Table 2. The molecule including atomic labelling is displayed in Fig. 1.

† Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53272 (6 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

* Alternative name: 2,2',3,3',5,5',6,6'-octafluoro-4,4'-azopyridine *N,N'*-dioxide.

Table 1. Fractional atomic coordinates and vibrational parameters (Å²)

	x	y	z	U _{eq} *
C(1)	0.3781 (5)	0.6505 (4)	0.4142 (1)	0.0419 (6)
C(2)	0.1818 (5)	0.7695 (4)	0.4195 (1)	0.0474 (6)
C(3)	0.1129 (5)	0.9351 (5)	0.3656 (2)	0.0512 (6)
N(4)	0.2233 (4)	0.9842 (4)	0.3107 (1)	0.0520 (6)
C(5)	0.4099 (5)	0.8725 (5)	0.3069 (1)	0.0505 (7)
C(6)	0.4954 (5)	0.7000 (5)	0.3568 (1)	0.0476 (6)
N(1)	0.4554 (4)	0.4656 (4)	0.4665 (1)	0.0462 (5)
O(1)	0.4432 (4)	0.2522 (3)	0.4485 (1)	0.0784 (7)
F(2)	0.0636 (3)	0.7284 (3)	0.47497 (9)	0.0720 (5)
F(3)	-0.0757 (3)	1.0550 (3)	0.3693 (1)	0.0789 (5)
F(5)	0.5231 (3)	0.9302 (3)	0.25177 (8)	0.0783 (5)
F(6)	0.6853 (3)	0.5877 (3)	0.35010 (9)	0.0745 (5)

$$*U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

Table 2. Bonds (Å) and angles (°)

C(1)—C(2)	1.373 (4)	C(1)—C(6)	1.365 (3)
C(1)—N(1)	1.447 (3)	C(2)—C(3)	1.378 (4)
C(2)—F(2)	1.330 (3)	C(3)—N(4)	1.300 (3)
C(3)—F(3)	1.330 (3)	N(4)—C(5)	1.298 (4)
C(5)—C(6)	1.384 (4)	C(5)—F(5)	1.325 (3)
C(6)—F(6)	1.326 (3)	N(1)—O(1)	1.250 (3)
N(1)—N(1)'	1.320 (4)		
C(6)—C(1)—C(2)	119.4 (2)	N(1)—C(1)—C(2)	120.7 (2)
N(1)—C(1)—C(6)	119.8 (2)	C(3)—C(2)—C(1)	117.5 (2)
F(2)—C(2)—C(1)	121.3 (2)	F(2)—C(2)—C(3)	121.2 (3)
N(4)—C(3)—C(2)	123.7 (3)	F(3)—C(3)—C(2)	119.1 (2)
F(3)—C(3)—N(4)	117.1 (2)	C(5)—N(4)—C(3)	118.1 (2)
C(6)—C(5)—N(4)	123.7 (2)	F(5)—C(5)—N(4)	117.2 (2)
F(5)—C(5)—C(6)	119.1 (3)	C(5)—C(6)—C(1)	117.5 (3)
F(6)—C(6)—C(1)	120.8 (2)	F(6)—C(6)—C(5)	121.7 (2)
O(1)—N(1)—C(1)	121.5 (2)		

A prime denotes an atom generated by 1 - x, 1 - y, 1 - z.

Related literature. Absence of monomer indicates that the title molecule is analogous to 4-bromo-2,3,5,6-tetrafluoronitrosobenzene (Castellano, Green

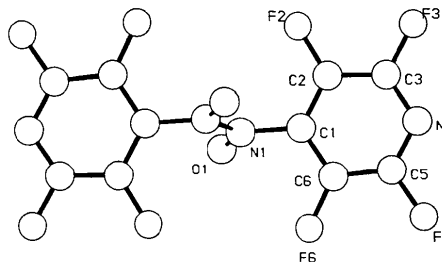


Fig. 1. The title molecule including labelling scheme drawn using *PLUTO* (Motherwell & Clegg, 1978).

& Kauffman, 1966) and not pentafluoronitrosobenzene.

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N-(4-Fluorophenyl)-C,C-diphenylnitronium*

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Abstract. C₁₉H₁₄FNO, *M_r* = 291.33, orthorhombic, *Pbca*, *a* = 17.851 (3), *b* = 8.783 (1), *c* = 18.686 (3) Å, *V* = 2929.7 Å³, *Z* = 8, *D_x* = 1.32 Mg m⁻³, λ(Mo *K*α)

= 0.71069 Å, μ = 0.053 mm⁻¹, *F*(000) = 1216, *T* = 293 K, *R* = 0.049 for 1511 unique reflexions [*F* ≥ 3σ(*F*)]. The nitronium and bonded C atoms are nearly planar [O=N=C—Ph = 3.1 (1)°]. However all the aromatic rings are twisted [C—N—C—C = 67.4 (3), N—C—C—C = 33.0 (3), 57.8 (3)°]. The molecular

* IUPAC name: *N*-(diphenylmethylene)-*p*-fluoroaniline *N*-oxide.