Littérature associée. Structure cristalline du *N*-(4,6-diméthylpyridin-2-yl)benzamide (Rodier, Piessard, Le Baut & Michelet, 1986). Structure cristalline du *N*-éthyl-*N*-(4,6-pyridin-2-yl)benzamide (Rodier, Piessard, Le Baut & Brion, 1987).

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Structure of *N*,*N*-Bis(2,3,4,5,6-Pentafluorophenyl)oxamide

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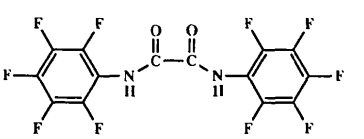
Abstract. $C_{14}H_2F_{10}N_2O_2$, $M_r = 420.16$, monoclinic, $P2_1/n$, $a = 14.206$ (1), $b = 4.990$ (1), $c = 10.964$ (3) Å, $\beta = 111.68$ (1)°, $V = 722.3$ (1) Å^3, $Z = 2$, $D_x = 1.932$ Mg m^{-3}, λ(Cu $K\alpha_1$) = 1.54050 Å, $\mu = 1.974$ mm^{-1}, $F(000) = 412$, $T = 295$ K, final $R = 0.040$ for 971 reflections. The midpoint of the oxamide carbon chain lies on a crystallographic inversion center. An intermolecular hydrogen bond, N—H···O [N(1)—O(3) 2.877 (2) Å], was observed.

Experimental. (I) was obtained by the reaction of pentafluoroaniline with oxalyl chloride in C_6H_6. Recrystallization from $CH_3(CH_2)_4CH_3/CH_3COOC_2H_5$ gave colorless prisms (0.30 × 0.30 × 0.45 mm) having m.p. 515.5–517.0 K. The combustion analysis of this compound was consistent with the structure. Rigaku AFC-5 four-circle diffractometer used with ω–2θ-scan method, ω-scan width $(1.3 + 0.14 \tan\theta)°$ and scan speed 16° min^{-1}. Lattice parameters obtained from least-squares analysis of 20 reflections with 2θ values ranging from 55 to 61°. Of 1323 reflections scanned within index range h −15–15, k 0–5, l 0–12 up to $\sin\theta/\lambda < 0.56$ Å^{-1}, $R_{int} = 0.018$ for 69 reflections, 1072 unique reflections [$F > \sigma(F)$] classified as observed. Three standard reflections measured every 150 reflections, intensity variation <3%. Intensities corrected for Lorentz and polarization factors, but absorption correction not applied. Structure solved using program package *SAPI*85 (Yao, Zheng, Qian, Han, Gu & Fan, 1985), a version of *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). The refinement was carried out by the full-matrix least-squares method with anisotropic temperature factors for non-H atoms. The function minimized was $\sum w[|(|F_o|)^2 - (|F_c|)^2|]^2$ with $w = 1/[\sigma^2(F_o) + 0.016(F_c)]$; $\sigma(F_o)$ was determined from counting statistics. All H atoms located from a difference map and theoretical calculations were refined, initial thermal parameters set at equivalent isotropic thermal parameters of each bonded atom. Final discrepancy indices $R = 0.040$, $wR = 0.042$, $S = 2.018$ for 136 variables and 971 reflections with $F > 3\sigma(F)$. Maximum $\Delta/\sigma = 0.27$ in final least-squares cycle. Final difference Fourier excursions 0.19 and −0.23 e Å^{-3}. All major computations performed on a PANAFACOM computer with the *RCRYSTAN* (Rigaku Corporation, 1985) X-ray analysis program system. The atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV).



(I)

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Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = \frac{1}{3}\sum_i\sum_j B_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq} (Å^2)
N(1)	0.9503 (1)	0.3442 (3)	0.3423 (1)	3.15 (4)
C(2)	0.9736 (1)	0.5469 (3)	0.4289 (1)	3.29 (5)
O(3)	0.9561 (1)	0.7815 (2)	0.4018 (1)	4.59 (4)
C(4)	0.9003 (1)	0.3854 (3)	0.2065 (1)	3.02 (5)
C(5)	0.9328 (1)	0.5723 (4)	0.1375 (1)	3.64 (5)
C(6)	0.8804 (1)	0.6168 (4)	0.0058 (1)	4.18 (6)
C(7)	0.7962 (1)	0.4688 (4)	−0.0612 (1)	4.07 (6)
C(8)	0.7652 (1)	0.2749 (4)	0.0035 (1)	3.81 (6)
C(9)	0.8157 (1)	0.2373 (3)	0.1362 (1)	3.28 (5)
F(10)	1.0184 (1)	0.7110 (2)	0.1966 (1)	5.45 (4)
F(11)	0.9131 (1)	0.8025 (3)	−0.0576 (1)	6.32 (5)
F(12)	0.7454 (1)	0.5122 (3)	−0.1887 (1)	6.16 (4)
F(13)	0.6848 (1)	0.1209 (3)	−0.0618 (1)	5.79 (4)
F(14)	0.7816 (1)	0.0533 (2)	0.1977 (1)	4.46 (3)

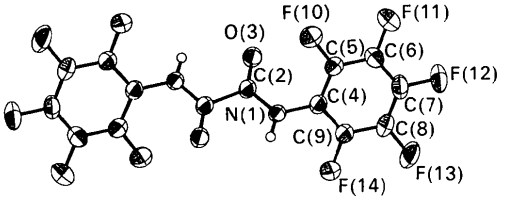

Fig. 1. *ORTEP*II drawing of (I). Ellipsoids are drawn at the 50% probability level while isotropic H thermal parameters are represented by spheres of arbitrary size.

Final atomic parameters are listed in Table 1.* Bond lengths and angles are listed in Table 2. Fig. 1 shows an *ORTEP*II drawing (Johnson, 1976) of the molecule with its atom labels.

* Tables of H-atom coordinates, anisotropic thermal parameters and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54496 (5 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS0521]

Table 2. *Bond lengths* (Å) *and angles* (°)

N(1)—C(2)	1.342 (2)	N(1)—C(4)	1.408 (2)
C(2)—O(3)	1.211 (2)	C(4)—C(5)	1.383 (3)
C(5)—F(10)	1.339 (2)	C(5)—C(6)	1.376 (2)
C(6)—F(11)	1.340 (2)	C(6)—C(7)	1.366 (2)
C(7)—F(12)	1.333 (2)	C(7)—C(8)	1.365 (3)
C(8)—F(13)	1.343 (2)	C(8)—C(9)	1.377 (2)
C(9)—F(14)	1.333 (2)	C(9)—C(4)	1.378 (2)
C(2)—C(2^i)	1.533 (4)		

C(2)—N(1)—C(4)	122.3 (1)	O(3)—C(2)—N(1)	125.5 (1)
C(9)—C(4)—C(5)	117.0 (1)	C(9)—C(4)—N(1)	120.5 (1)
C(5)—C(4)—N(1)	122.5 (1)	F(10)—C(5)—C(6)	117.8 (1)
F(10)—C(5)—C(4)	120.7 (1)	C(6)—C(5)—C(4)	121.4 (1)
F(11)—C(6)—C(7)	119.8 (1)	F(11)—C(6)—C(5)	119.9 (1)
C(7)—C(6)—C(5)	120.3 (2)	F(12)—C(7)—C(8)	120.5 (1)
F(12)—C(7)—C(6)	120.2 (2)	C(8)—C(7)—C(6)	119.3 (1)
F(13)—C(8)—C(7)	120.2 (1)	F(13)—C(8)—C(9)	119.6 (2)
C(7)—C(8)—C(9)	120.2 (1)	F(14)—C(9)—C(8)	119.0 (1)
F(14)—C(9)—C(4)	119.4 (1)	C(8)—C(9)—C(4)	121.6 (1)
N(1)—C(2)—C(2^i)	112.9 (2)	O(3)—C(2)—C(2^i)	121.5 (2)

Symmetry code: (i) $2-x, 1-y, 1-z$.

Related literature. The crystallographic studies of several urea cytokinins have been carried out in order to provide the basis for consideration of the stereochemical structure–activity relationships (Yamaguchi & Shudo, 1991).

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Structure of *N*-(2,3,5,6-Tetrafluoropyridyl)-*N'*-phenylurea

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Abstract. $C_{12}H_7F_4N_3O$, $M_r = 285.20$, monoclinic, $P2_1/n$, $a = 7.594$ (1), $b = 24.316$ (4), $c = 6.298$ (4) Å, $\beta = 96.47$ (1)°, $V = 1155.7$ (3) Å^3, $Z = 4$, $D_x = 1.639$ Mg m^{-3}, λ(Cu $K\alpha_1$) = 1.54050 Å, $\mu = 1.322$ mm^{-1}, $F(000) = 576$, $T = 295$ K, final $R = 0.055$ for 1194 reflections. The phenyl ring lies at

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