corrections were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 71, 148). All computer programs were from the *TEXSAN* package (Molecular Structure Corporation, 1985). Table 1 lists the final atomic coordinates and equivalent isotropic temperature factors; Table 2 presents selected interatomic distances and angles.* Fig. 1 shows the atom-numbering scheme and the thermal motion of the molecule; Fig. 2 illustrates the molecular packing.

Related literature. Equilibrium acidity data [pK_a values in dimethyl sulfoxide (DMSO) solution] for five variously *G*-substituted aryl-1,3-propanedinitriles (where G = 3-CN, 4-Cl, 4-H, 4-CH_3, 4-OCH_3) as well as the title compound (G = 4-NH_2) are 1.9, 3.14, 4.24, 4.85, 5.68 (Arnett, Chawla, Amarnath & Whitesell, 1987) and 7.24 (Jirka, 1989), respectively. These acidity data plot linearly with Hammett σ. It is therefore likely that the title compound is deprotonated at C(2), rather than at N(4), in DMSO solution. The X-ray structure for the title compound indicates that an H atom is bound at C(2).

Two of us (MJB and GPJ) are grateful to the donors of the Petroleum Research Fund, administered by the American Chemical Society, for support of this work.

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* Lists of structure factors, anisotropic thermal parameters, intermolecular distances, torsion angles and selected least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54580 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR0366]

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N-(4,6-Diméthylpyridin-2-yl)benzènethiocarboxamide

Par N. Rodier

Laboratoire de Chimie minérale, Faculté des Sciences pharmaceutiques et biologiques, 5 Rue J.-B. Clément, 92296 Châtenay-Malabry CEDEX, France

et J.-M. Robert et G. Le Baut

Laboratoire de Chimie thérapeutique, Faculté de Pharmacie, 1 Rue Gaston-Veil, 44035 Nantes CEDEX, France

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Abstract. $C_{14}H_{14}N_2S$, M_r = 242.3, monoclinic, $C2/c$, a = 20.004 (2), b = 7.997 (1), c = 15.954 (1) Å, β = 90.40 (1)°, V = 2552.2 (7) Å^3, Z = 8, D_x = 1.261 Mg m^{-3}, λ(Cu $K\overline{\alpha}$) = 1.5418 Å, μ = 2.0 mm^{-1}, F(000) = 1024, T = 295 (1) K, R = 0.039 for 1807 independent observed reflections. There is a delocalized orbital over the N—C═S thioamide group. The pyridinyl and the phenyl rings are approximately planar and the dihedral angles between their least-squares planes and the NCS thioamide plane are 25.2 (2) and 44.2 (2)° respectively. The molecules form pairs in which they are linked to each other by two weak N(7)—H(7)···N(1$^{\rm i}$) hydrogen bonds [3.192 (3) Å, 177 (3)°] (i: $-x$, y, $\frac{3}{2}-z$). The title compound shows only a very moderate anti-inflammatory activity, even though it is the thio analog of *N*-(4,6-dimethylpyridin-2-yl)benzamide which is a non-acidic compound exhibiting a potent anti-inflammatory activity.

Partie expérimentale. Cristal parallélépipédique: 0,13 × 0,22 × 0,26 mm. Dimensions de la maille déterminées avec 25 réflexions pour lesquelles 17,55 ≤ θ ≤ 32,40°. Diffractomètre Enraf–Nonius CAD-4, balayage $\theta/2\theta$, $0{,}023 \le (\sin\theta)/\lambda \le 0{,}573$ Å^{-1}; $0 \le h \le 22$, $0 \le k \le 9$, $-18 \le l \le 17$. Réflexions de contrôle de l'intensité: $10,\bar{2},1$, $11\bar{7}$ et $\bar{5}\bar{1}7$. Variations non significatives de I au cours des mesures. 2007 réflex-

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Tableau 1. *Coordonnées atomiques relatives, facteurs de température isotropes équivalents et écarts-type*

$B_{\text{éq}} = (4/3)[\beta_{11}a^2 + \beta_{22}b^2 + \beta_{33}c^3 + \beta_{12}ab(\cos\gamma) + \beta_{13}ac(\cos\beta) + \beta_{23}bc(\cos\alpha)]$.

	x	y	z	$B_{\text{éq}}$(Å^2)
N(1)	−0,03001 (9)	0,3848 (2)	0,6449 (1)	3,32 (4)
C(2)	0,0184 (1)	0,2898 (3)	0,6126 (1)	3,03 (4)
C(3)	0,0179 (1)	0,2288 (3)	0,5309 (1)	3,41 (5)
C(4)	−0,0352 (1)	0,2751 (3)	0,4791 (1)	3,65 (5)
C(5)	−0,0834 (1)	0,3797 (3)	0,5105 (2)	3,93 (5)
C(6)	−0,0803 (1)	0,4314 (3)	0,5937 (2)	3,70 (5)
N(7)	0,06890 (8)	0,2550 (3)	0,6726 (1)	3,16 (4)
C(8)	0,1329 (1)	0,2059 (3)	0,6634 (1)	2,94 (4)
C(9)	0,1668 (1)	0,1694 (3)	0,7447 (1)	3,01 (4)
C(10)	0,1338 (1)	0,0773 (3)	0,8059 (1)	3,68 (5)
C(11)	0,1653 (1)	0,0436 (4)	0,8817 (2)	4,84 (6)
C(12)	0,2283 (1)	0,1024 (4)	0,8975 (2)	5,47 (7)
C(13)	0,2615 (1)	0,1931 (5)	0,8371 (2)	5,74 (7)
C(14)	0,2313 (1)	0,2248 (4)	0,7599 (2)	4,32 (6)
S(15)	0,17410 (3)	0,1851 (1)	0,57479 (4)	4,61 (1)
C(16)	−0,0377 (1)	0,2132 (4)	0,3894 (2)	5,14 (6)
C(17)	−0,1320 (1)	0,5440 (4)	0,6309 (2)	5,32 (6)

Tableau 2. *Longueurs* (Å) *et angles des liaisons* (°) *et écarts-type*

N(1)—C(2)	1,337 (3)	N(7)—C(8)	1,348 (3)
N(1)—C(6)	1,344 (3)	C(8)—C(9)	1,487 (3)
C(2)—C(3)	1,391 (3)	C(8)—S(15)	1,650 (2)
C(2)—N(7)	1,415 (3)	C(9)—C(10)	1,393 (3)
C(3)—C(4)	1,391 (3)	C(9)—C(14)	1,384 (3)
C(4)—C(5)	1,374 (3)	C(10)—C(11)	1,386 (3)
C(4)—C(16)	1,515 (4)	C(11)—C(12)	1,368 (4)
C(5)—C(6)	1,392 (3)	C(12)—C(13)	1,379 (4)
C(6)—C(17)	1,498 (4)	C(13)—C(14)	1,392 (4)
C(2)—N(1)—C(6)	117,6 (2)	C(2)—N(7)—C(8)	131,2 (2)
N(1)—C(2)—C(3)	124,0 (2)	N(7)—C(8)—C(9)	113,0 (2)
N(1)—C(2)—N(7)	111,5 (2)	N(7)—C(8)—S(15)	127,0 (2)
C(3)—C(2)—N(7)	124,4 (2)	C(9)—C(8)—S(15)	120,0 (2)
C(2)—C(3)—C(4)	117,6 (2)	C(8)—C(9)—C(10)	120,0 (2)
C(3)—C(4)—C(5)	118,7 (2)	C(8)—C(9)—C(14)	120,6 (2)
C(3)—C(4)—C(16)	119,7 (2)	C(10)—C(9)—C(14)	119,4 (2)
C(5)—C(4)—C(16)	121,6 (2)	C(9)—C(10)—C(11)	120,0 (2)
C(4)—C(5)—C(6)	120,1 (2)	C(10)—C(11)—C(12)	120,4 (2)
N(1)—C(6)—C(5)	121,8 (2)	C(11)—C(12)—C(13)	120,0 (2)
N(1)—C(6)—C(17)	116,2 (2)	C(12)—C(13)—C(14)	120,4 (3)
C(5)—C(6)—C(17)	122,0 (2)	C(9)—C(14)—C(13)	119,8 (2)

ions indépendantes mesurées, 200 réflexions inobservées [$I < 3\sigma(I)$]. Programme *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). Affinement basé sur les *F*. Programme à matrice complète. Facteurs de diffusion des *International Tables for X-ray Crystallography* (1974, Tome IV, pp. 99, 149). Paramètres affinés: x, y, z de tous les atomes et β_{ij} de C, N et S. B de chaque H pris égal à ($B_{\text{éq}}$ de l'atome lié à H) × 1,3. $R = 0{,}039$, $wR = 0{,}038$, $w = 1$ pour toutes les réflexions, $S = 1{,}31$, g (coefficient d'extinction secondaire isotrope) = $1{,}33\,(7) \times 10^{-6}$, $(\Delta/\sigma)_{\max} = 0{,}05$, $\Delta\rho_{\max} = 0{,}26\,(4)$, $\Delta\rho_{\min} = -0{,}32\,(4)$ e Å^{-3}. Les valeurs maximale et minimale de la densité électronique résiduelle s'observent au voisinage de l'atome de soufre. Programmes de calcul du système *SDP* (B. A. Frenz & Associates, Inc. 1982). Figs. 1 et 2: *ORTEP*II (Johnson, 1976).

Les coordonnées atomiques relatives et les facteurs de température isotrope équivalents sont rapportés dans le Tableau 1, les principales distances interatomiques et les angles des liaisons dans le Tableau 2.[*] La Fig. 1 représente la molécule vue en perspective et la Fig. 2 la projection de la structure sur la face (010). Les noms des atomes sont indiqués sur la Fig. 1.

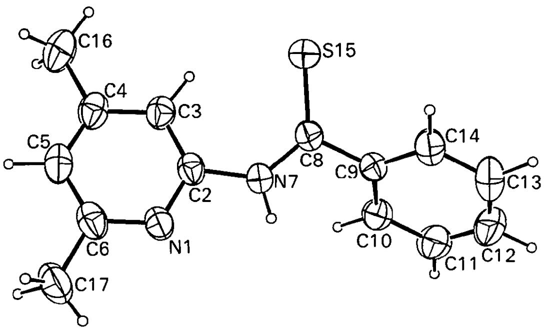

Fig. 1. Dessin de la molécule vue en perspective et noms des atomes.

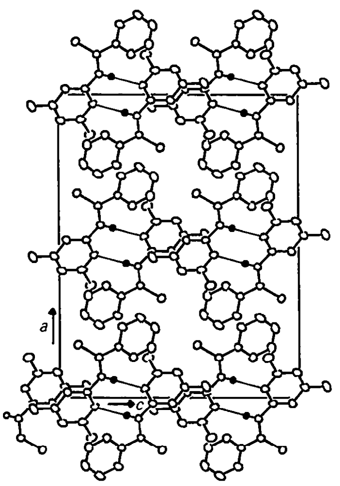

Fig. 2. Dessin de la structure vue selon [010]. Les cercles noirs représentent les atomes H(7) et les traits les plus fins les liaisons hydrogène N(7)—H(7)···N(1^{i}).

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[*] Les listes des facteurs de structure, des coefficients d'agitation thermique anisotrope des 'atomes lourds', des coordonnées des atomes d'hydrogène, des distances C—H et N—H, des angles de torsion, des distances des atomes aux plans moyens et des distances interatomiques intermoléculaires ont été déposées aux archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 54527 (14 pp.). On peut en obtenir des copies en s'adressant à: The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre. [Référence de CIF: PA0251]

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

By Kentaro Yamaguchi and Go Matsumura

School of Pharmaceutical Sciences, Showa University, 1-5-8 Hatanodai, Shinagawa-ku, Tokyo 142, Japan

and Naoki Haga and Koichi Shudo

Faculty of Pharmaceutical Sciences, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113, Japan

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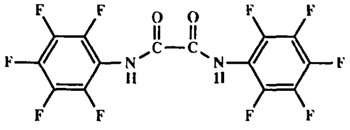
Abstract. $C_{14}H_2F_{10}N_2O_2$, $M_r = 420.16$, monoclinic, $P2_1/n$, $a = 14.206$ (1), $b = 4.990$ (1), $c = 10.964$ (3) Å, $\beta = 111.68$ (1)°, $V = 722.3$ (1) Å^3, $Z = 2$, $D_x = 1.932$ Mg m^{-3}, λ(Cu $K\alpha_1$) = 1.54050 Å, $\mu = 1.974$ mm^{-1}, $F(000) = 412$, $T = 295$ K, final $R = 0.040$ 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}, $R_{\text{int}} = 0.018$ 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 *SAPI85* (Yao, Zheng, Qian, Han, Gu & Fan, 1985), a version of *MULTAN80* (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).



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