$w = 1/\sigma^2(F)$, $(\Delta/\sigma)_{max} = 0{,}02$, $|\Delta\rho|_{max} = 0{,}16$ (4) e Å^{-3}. Facteurs de diffusion des *International Tables for X-ray Crystallography* (1974). Programmes de calcul du système *SDP* (B. A. Frenz & Associates, Inc., 1982). Angles de torsion: *ORFFE* (Busing, Martin & Levy, 1964). Fig. 1 et 2: *ORTEP*II (Johnson, 1976).

Les coordonnées atomiques relatives sont rapportées dans le Tableau 1.* Les longueurs et les angles des liaisons dans le Tableau 2. Les quatre molécules de *N*-(diméthyl-4,6 pyridyl-2) phényl-3 propènamide-(*E*) présentes dans l'unité asymétrique sont désignées respectivement par molécule 1, molécule 2, molécule 3 et molécule 4. Les numéros utilisés pour nommer leurs atomes s'obtiennent en ajoutant aux numéros indiqués sur la Fig. 1, les nombres 100, 200, 300 ou 400. Le premier chiffre du numéro obtenu désigne ainsi la molécule á laquelle appartient l'atome. La Fig. 1 représente la molécule 1 et la Fig. 2 une vue de la structure en perspective.

Littérature associée. Structure de l'acide (isobutyl-4 phényl)-2 propionique (McConnell, 1974). Ce composé, dénommé aussi ibuprofen ou prufen, est un antipyrétique et un antiinflammatoire. Etude spectrale de quelques *N*-(pyridinyl-2) benzamides et structure cristalline du *N*-éthyl *N*-(diméthyl-4,6 pyridinyl-2) benzamide (Rodier, Piessard, Le Baut & Brion, 1987). Synthèse et effets dopaminergiques centraux des *N*-(diméthyl-4,6 pyridinyl-2) benzamides (Bouhayat, Piessard, Le Baut, Sparfel, Petit, Piriou & Welin, 1985). Structure cristalline du *N*-(diméthyl-4,6 pyridinyl-2) benzamide (Rodier, Piessard, Le Baut & Michelet, 1986). Composés anti-inflammatoires non acides: activité des *N*-(diméthyl-4,6 pyridinyl-2) benzamides et de composés dérivés (Robert-Piessard, Le Baut, Courant, Brion, Sparfel, Bouhayat, Petit, Sanchez, Juge, Grimaud & Welin, 1990).

* Les listes des facteurs de structure observés et calculés, des coefficients d'agitation thermique anisotrope, des paramètres (non affinés) des atomes d'hydrogène, des distances C—H, N—H et O—H, des distances des atomes aux plans moyens, des angles de torsion et des distances interatomiques intermoléculaires ont été déposées au dépôt d'archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 52847: 44 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.

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Acta Cryst. (1990). C**46**, 1749–1751

Structure of a Thiadiazole

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(*Received* 7 *February* 1990; *accepted* 26 *March* 1990)

Abstract. 3-Amino-4-azido-1,2,5-thiadiazole, $C_2H_2N_6S$, $M_r = 142{\cdot}1$, monoclinic, $P2_1/a$, $a = 9{\cdot}018$ (1), $b = 10{\cdot}975$ (1), $c = 5{\cdot}5305$ (1) Å, $\beta = 99{\cdot}17$ (1)°, $U = 540{\cdot}4$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}747$ Mg m^{-3}, λ(Cu $K\alpha_1$) = 1·54050 Å, $\mu = 4{\cdot}423$ mm^{-1}, $F(000) = 288$, $T = 293$ K, final $R = 0{\cdot}058$ for 761 reflexions. The azido group adopts an extended *trans* conformation. The amino N atom, with sp^2 character, participates in two N···N intermolecular hydrogen bonds, 3·264 (5) and 3·125 (5) Å.

Experimental. A pale-yellow prism, 0·30 × 0·15 × 0·55 mm, by recrystallization from C_2H_5OH. Rigaku AFC-5 four-circle diffractometer used with θ–2θ

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Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters with e.s.d.'s in parentheses*

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

	x	y	z	B_{eq} (Å^2)
S(1)	0·8881 (1)	0·2643 (1)	0·2640 (1)	4·38 (3)
N(2)	0·9271 (3)	0·1300 (2)	0·1596 (5)	4·14 (8)
C(3)	0·8599 (3)	0·0459 (3)	0·2750 (5)	3·53 (8)
C(4)	0·7772 (3)	0·1002 (2)	0·4500 (5)	3·30 (8)
N(5)	0·7846 (3)	0·2184 (2)	0·4646 (5)	3·73 (8)
N(6)	0·8663 (3)	−0·0736 (2)	0·2298 (6)	4·56 (10)
N(7)	0·6973 (3)	0·0246 (2)	0·5885 (5)	4·32 (8)
N(8)	0·6320 (3)	0·0798 (2)	0·7377 (5)	3·86 (9)
N(9)	0·5703 (4)	0·1174 (3)	0·8791 (7)	5·85 (11)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

S(1)—N(2)	1·641 (3)	C(4)—N(7)	1·404 (5)
N(2)—C(3)	1·323 (5)	N(7)—N(8)	1·244 (4)
C(3)—N(6)	1·338 (5)	N(8)—N(9)	1·109 (5)
C(3)—C(4)	1·441 (5)	N(5)—S(1)	1·638 (3)
C(4)—C(5)	1·301 (4)		
S(1)—N(2)—C(3)	108·4 (2)	N(5)—C(4)—N(7)	125·5 (3)
N(2)—C(3)—C(4)	111·2 (3)	C(4)—N(5)—S(1)	107·1 (2)
N(2)—C(3)—N(6)	123·8 (3)	N(5)—S(1)—N(2)	98·0 (1)
C(4)—C(3)—N(6)	124·9 (3)	C(4)—N(7)—N(8)	114·3 (2)
C(3)—C(4)—N(5)	115·2 (3)	N(7)—N(8)—N(9)	172·7 (3)
C(3)—C(4)—N(7)	119·1 (2)		

scan method, ω scan width $(1{\cdot}3 + 0{\cdot}41\tan\theta)°$ and scan speed 16° min^{-1}. Lattice parameters obtained from least-squares analysis of 20 reflexions with 2θ values ranging from 56 to 61°. Out of 977 reflexions scanned within the index range h −10 to 10, k 0 to 12, l 0 to 6 up to $\sin\theta/\lambda \le 0{\cdot}56$ Å^{-1} including 95 equivalent reflexions ($R_{int} = 0{\cdot}042$), 761 unique reflexions classified as observed with $F > 3\sigma(F)$. Three standard reflexions measured every 150 reflexions, no significant intensity variation. 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) 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 $\sum w[|(|F_o|)^2 - (|F_c|)^2|]^2$ with $w = 1/[\sigma^2(F_o) + 0{\cdot}02(F_o)^2]$, $\sigma(F_o)$ determined from counting statistics. All H atoms located from the difference map and refined, the initial thermal parameters set at the equivalent isotropic thermal parameter of each bonded atom. Final discrepancy indices $R = 0{\cdot}058$, $wR = 0{\cdot}064$, $S = 1{\cdot}719$ for 761 reflexions. Maximum $\Delta/\sigma = 0{\cdot}13$ in final least-squares cycle. Final difference Fourier map showed no residuals greater than 0·32 e Å^{-3}. All calculations performed using a PANAFACOM computer with *RCRYSTAN* (Rigaku Corporation, 1985) X-ray analysis program system. The atomic scattering factors were those from *International Tables for X-ray Crystallography* (1974).

Final atomic parameters are listed in Table 1.* The bond lengths and angles are listed in Table 2. Fig. 1 shows a thermal-ellipsoid plot of the molecule with atomic labelling. Fig. 2 presents the crystal structure.

Related literature. The title compound is an isomerization product of 5-amino-1,2,3-thiadiazolo[4,5-c]-

* Lists of structure amplitudes, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52882 (4 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

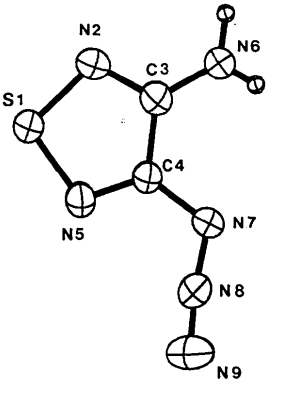

Fig. 1. Thermal-ellipsoid plot. Ellipsoids are drawn at the 50% probability level while isotropic hydrogen thermal parameters are represented by spheres of arbitrary size.

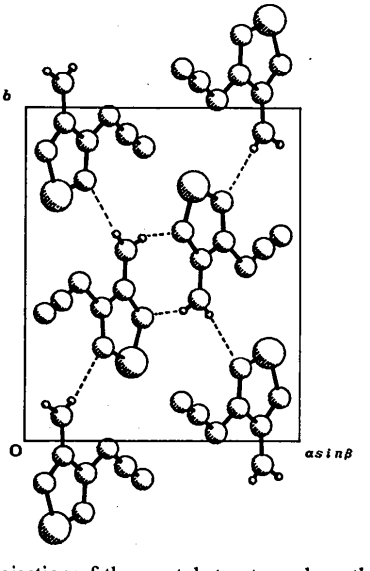

Fig. 2. Projection of the crystal structure along the c axis.

1,2,5-thiadiazole obtained from 3,4-diamino-1,2,5-thiadiazole (Komin & Carmack, 1976).

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Acta Cryst. (1990). C**46**, 1751–1752

Structure of a Pyrazine Derivative

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(*Received* 7 *February* 1990; *accepted* 26 *March* 1990)

Abstract. 2-Phenyl-1,2,3-triazolo[4,5-*b*]pyrazine, $C_{10}H_7N_5$, $M_r = 197{\cdot}2$, orthorhombic, $P2_1nb$, $a = 9{\cdot}975\ (1)$, $b = 24{\cdot}238\ (1)$, $c = 3{\cdot}921\ (1)$ Å, $U = 930{\cdot}8\ (1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}407$ Mg m^{-3}, λ(Cu $K\alpha_1$) $= 1{\cdot}54050$ Å, $\mu = 0{\cdot}772$ mm^{-1}, $F(000) = 408$, $T = 293$ K, final $R = 0{\cdot}046$ for 699 reflexions. The dihedral angle between the triazolopyrazine and phenyl rings is 2·3 (4)°.

Experimental. A colorless prism $0{\cdot}30 \times 0{\cdot}55 \times 0{\cdot}50$ mm, recrystallization from C_2H_5OH/CH_2Cl_2. Rigaku AFC-5 four-circle diffractometer used with θ–2θ scan method, ω scan width $(1{\cdot}3 + 0{\cdot}41\tan\theta)°$ and scan speed 16° min^{-1}. Lattice parameters obtained from least-squares analysis of 20 reflexions with 2θ values ranging from 59 to 61°. Out of 973 reflexions scanned within index range h 0 to 11, k 0 to 27, l 0 to 4 up to $\sin\theta/\lambda \le 0{\cdot}56$ Å^{-1}, 699 unique reflexions classified as observed with $F > 3\sigma(F)$. Three standard reflexions measured every 150 reflexions, no significant intensity variation. 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) 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 $\sum w[(|F_o|)^2 - (|F_c|)^2]^2$ with $w = 1/[\sigma^2(F_o) + 0{\cdot}02(F_o)^2]$, $\sigma(F_o)$ determined from counting statistics. All H atoms are located from the difference map and refined. Final discrepancy indices, $R = 0{\cdot}046$, $wR = 0{\cdot}041$, $S = 1{\cdot}431$ for 699 reflexions. Maximum $\Delta/\sigma = 0{\cdot}11$ in final least-squares cycle. Final difference Fourier maps showed no residuals greater than $0{\cdot}36$ e Å^{-3}. All calculations performed using a PANAFACOM computer with *RCRYSTAN* (Rigaku Corporation, 1985) X-ray analysis program system. The atomic scattering factors were those from *International Tables for X-ray Crystallography* (1974). Final atomic parameters are listed in Table 1.* The bond lengths and angles are listed in Table 2. Fig. 1 shows a thermal-ellipsoid plot of the molecule with atomic labelling.

* Lists of structure amplitudes, anisotropic thermal parameters, H-atom coordinates and deviations from the least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52883 (4 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters with e.s.d.'s in parentheses*

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

	x	y	z	B_{eq}(Å^2)
N(1)	0·0589 (3)	0·6777 (1)	0·6545 (4)	3·68 (20)
N(2)	0·0721 (3)	0·6292 (1)	0·8170 (3)	3·17 (20)
N(3)	0·1975 (4)	0·6089 (1)	0·8500 (5)	3·96 (21)
C(4)	0·2738 (4)	0·6480 (1)	0·6951 (6)	3·44 (22)
C(5)	0·1885 (4)	0·6898 (1)	0·5767 (7)	3·32 (21)
N(6)	0·4106 (4)	0·6477 (1)	0·6532 (8)	5·25 (22)
C(7)	0·4537 (6)	0·6920 (2)	0·4864 (9)	5·22 (24)
C(8)	0·3665 (6)	0·7341 (2)	0·3682 (8)	4·73 (23)
N(9)	0·2331 (3)	0·7351 (1)	0·4075 (6)	4·58 (22)
C(10)	−0·0452 (4)	0·5998 (1)	0·9365 (6)	3·18 (21)
C(11)	−0·1726 (4)	0·6201 (1)	0·8744 (6)	4·06 (22)
C(12)	−0·2851 (6)	0·5893 (2)	0·9771 (9)	5·34 (24)
C(13)	−0·2670 (6)	0·5390 (2)	1·1379 (9)	5·68 (26)
C(14)	−0·1379 (6)	0·5203 (2)	1·2046 (8)	5·11 (25)
C(15)	−0·0243 (4)	0·5499 (1)	1·1082 (8)	4·07 (22)

0108-2701/90/091751-02$03.00