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

References

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

KOMIN, A. P. & CARMACK, M. (1976). *J. Heterocycl. Chem.* **13**, 13–22.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

Rigaku Corporation (1985). *RCRYSTAN. X-ray Analysis Program System.* Rigaku Corporation, Tokyo, Japan.

YAO, J.-X., ZHENG, C.-D., QIAN, J.-Z., HAN, F.-S., GU, Y.-X. & FAN, H.-F. (1985). *SAPI 85. A Computer Program for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Institute of Physics, Academia Sinica, Beijing, People's Republic of China.

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

Structure of a Pyrazine Derivative

BY KENTARO YAMAGUCHI, AKIO OHSAWA AND CHIKAKO KAWABATA

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

(*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

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

N(1)—N(2)	1·343 (4)	C(8)—N(9)	1·316 (7)
N(1)—C(5)	1·338 (5)	C(10)—C(11)	1·363 (6)
N(2)—C(10)	1·431 (5)	C(11)—C(12)	1·390 (7)
N(2)—N(3)	1·330 (6)	C(12)—C(13)	1·384 (9)
N(3)—C(4)	1·351 (6)	C(13)—C(14)	1·368 (8)
C(4)—C(5)	1·393 (6)	C(14)—C(15)	1·377 (7)
C(4)—N(6)	1·350 (6)	C(15)—C(10)	1·398 (6)
C(5)—N(9)	1·356 (5)		
N(6)—C(7)	1·327 (7)		
C(7)—C(8)	1·409 (8)		

N(1)—N(2)—N(3)	117·3 (3)	N(1)—N(2)—C(10)	120·9 (3)
N(2)—N(3)—C(4)	101·9 (3)	N(3)—N(2)—C(10)	121·6 (3)
N(3)—C(4)—C(5)	109·1 (3)	N(2)—C(10)—C(11)	119·7 (3)
N(3)—C(4)—N(6)	126·8 (4)	N(2)—C(10)—C(15)	118·1 (3)
C(4)—C(5)—N(1)	109·5 (3)	C(10)—C(11)—C(12)	118·7 (4)
C(4)—C(5)—N(9)	123·9 (3)	C(11)—C(12)—C(13)	120·1 (5)
N(6)—C(4)—C(5)	123·9 (3)	C(12)—C(13)—C(14)	119·8 (5)
C(4)—N(6)—C(7)	111·8 (4)	C(13)—C(14)—C(15)	121·4 (4)
N(6)—C(7)—C(8)	123·7 (5)	C(14)—C(15)—C(10)	117·6 (4)
C(7)—C(8)—N(9)	125·2 (4)	C(15)—C(10)—C(11)	122·0 (4)
C(8)—N(9)—C(5)	111·2 (3)		
N(9)—C(5)—N(1)	126·5 (3)		
C(5)—N(1)—N(2)	102·0 (3)		

Related literature. The title compound was prepared by the condensation of 4,5-diamino-2-phenyl-1,2,3-triazole with 1,2-dicarbonyl. See Satoh & Adachi (1978) for the preparation of related compounds.

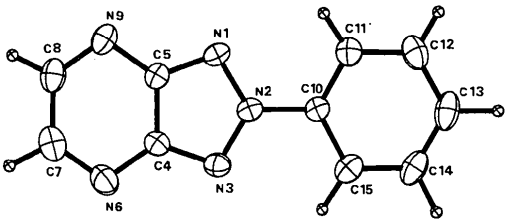

Fig. 1. Thermal-ellipsoid plot. Ellipsoids are drawn at the 50% probability level while isotropic hydrogen thermal parameters are represented by spheres of arbitrary size.

References

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

Rigaku Corporation (1985). *RCRYSTAN. X-ray Analysis Program System.* Rigaku Corporation, Tokyo, Japan.

SATOH, N. & ADACHI, J. (1978). *J. Org. Chem.* **43**, 314–340.

YAO, J.-X., ZHENG, C.-D., QIAN, J.-Z., HAN, F.-S., GU, Y.-X. & FAN, H.-F. (1985). *SAPI*85. *A Computer Program for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Institute of Physics, Academia Sinica, Beijing, People's Republic of China.

SHORT COMMUNICATION

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

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

Crystal studies of musk compounds. I. 4-*tert*-Butyl-3-methoxy-2,6-dinitrotoluene (musk ambrette). Erratum.

By DIRK J. A. DE RIDDER, KEES GOUBITZ and HENK SCHENK, *Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht* 166, 1018 *WV Amsterdam, The Netherlands*

(*Received* 14 *May* 1990)

Abstract. In the paper by De Ridder, Goubitz & Schenk [*Acta Cryst.* (1990), C**46**, 468–470], the equation given for the weighting scheme is in error. The correct weighting scheme is $w^{-1} = 4{\cdot}86 + F_{obs} + 0{\cdot}009F_{obs}^2$.

All relevant information is given in the *Abstract.*

0108-2701/90/091752-01$03.00