The crystal structures viewed along each *a* axis are shown in Fig. 3. In both crystals the coumarin moieties are stacked along the *a* axes. In U, the hydrogen bond O(12)—H···O(11) forms a ribbon along the *c* axis. The O(12)···O(11) distance and O(12)—H···O(11) angle are 2·746 (2) Å and 175 (1)° respectively.

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References

BEDDARD, G. S., CARLIN, M. S. & DAVIDSON, R. S. (1977). *J. Chem. Soc. Perkin Trans.* 2, pp. 262–267.

DEAN, F. M. (1973). *Naturally Occurring Oxygen Ring Compounds*, ch. 6, pp. 176–191. London: Butterworths.

GAVUZZO, E., MAZZA, F. & GIGLIO, E. (1974). *Acta Cryst.* B**30**, 1351–1357.

International Tables for X-ray Crystallography (1974). Vol. IV, pp. 72–73. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

JOHNSON C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee.

MORIYA, T. (1983). *Bull. Chem. Soc. Jpn*, **56**, 6–14.

SATO, M. & HASEGAWA, M. (1971). *Phytochemistry*, **10**, 2367–2372.

SATO, M. & HASEGAWA, M. (1972). *Phytochemistry*, **11**, 657–662.

SHELDRICK, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.

UENO, K. & SAITO, N. (1976). *Acta Cryst.* B**32**, 946–948.

UENO, K. & SAITO, N. (1977). *Acta Cryst.* B**33**, 283–285.

UENO, K., SAITO, N. & SATO, M. (1978). *Bull. Chem. Soc. Jpn*, **51**, 3170–3174.

UENO, K., SATO, M. & SAITO, N. (1983). *Bull. Chem. Soc. Jpn*, **56**, 1577–1580.

UENO, K., SHIRAKI, M., SATO, M. & SAITO, N. (1985). *Bull. Chem. Soc. Jpn*, **58**, 230–235.

Acta Cryst. (1985). C**41**, 1789–1790

Structure of 3-Phenyl-4-(1-phenylethyl)-5-(2-thienyl)-4,5-dihydro-1,2,4-oxadiazole

BY C. RUIZ-VALERO, A. MONGE* AND E. GUTIÉRREZ-PUEBLA

Instituto de Química Inorgánica 'Elhuyar', Serrano 113, 28006 *Madrid, Spain and Departamento de Química Inorgánica, Facultad de Químicas, Universidad Complutense,* 28040 *Madrid, Spain*

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Abstract. $C_{20}H_{18}N_2OS$, $M_r = 334·4$, monoclinic, $P2_1/n$, $a = 8·84$ (1), $b = 12·235$ (1), $c = 15·903$ (3) Å, $\beta = 91·90$ (5)°, $V = 1719$ (2) Å^3, $Z = 4$, $D_x = 1·29$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 1·872$ cm^{-1}, $F(000) = 704$, $T = 290$ K, $R = 0·052$ for 1750 observed reflexions. The configuration of the title compound has been established. Bond lengths and angles are normal. The dihydrooxadiazole ring is not planar, maximum deviation 0·098 (4) Å from the least-squares plane.

Introduction. The title compound has been prepared and studied by spectroscopy by Arjona, Plumet, Ossorio & Carreiro (1985).

In order to establish unequivocally the configuration of this compound, which was difficult to resolve by conventional techniques such as ^{1}H NMR and ^{13}C NMR spectroscopy, its crystal structure has been determined.

Experimental. Colourless, prismatic crystal 0·4 × 0·2 × 0·6 mm. Enraf–Nonius CAD-4*F* automatic diffractometer; cell dimensions refined by least-squares fitting of θ values of 25 reflexions; intensities of 3742 unique reflexions, $1 < \theta < 27°$, *hkl* −11,0,0 to 11,15,20, monochromatic Mo $K\alpha$ radiation, $\omega/2\theta$ scans; three reflexions monitored periodically during data collection showed no crystal decomposition; intensities corrected for Lorentz and polarization effects; 1750 considered observed [$I > 2\sigma(I)$]. Scattering factors for neutral atoms from *International Tables for X-ray Crystallography* (1974). Structure solved with *MULTAN*77 (Main, Lessinger, Woolfson, Germain & Declercq, 1977); best *E* map revealed all non-H atoms. An empirical absorption correction (Walker & Stuart, 1983) was applied at the end of the isotropic refinement; anisotropic full-matrix least-squares refinement, $\sum w(|F_o| - |F_c|)^2$ minimized; unit weights; a difference synthesis calculated with reflexions having $\sin\theta/\lambda < 0·5$ Å^{-1} showed all H atoms as highest peaks; final refinement with fixed isotropic temperature factors for H atoms led to $R = 0·052$; max. and average Δ/σ in final LS cycle 0·018 and 0·005; final difference synthesis had no electron density >0·21 or <−0·18 e Å^{-3}. No correction for secondary extinction. Most of the calculations performed with *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976). Least-squares planes computed with *PARST*5 (Nardelli, Musatti, Domiano & Andreetti, 1965).

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* Author for correspondence.

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Discussion. Table 1* contains the final atomic parameters. Fig. 1 (Johnson, 1965) shows the geometry of the structure and the atom labelling. Bond lengths and angles together with their e.s.d.'s are in Table 2.

Table 1. *Coordinates and equivalent isotropic thermal parameters* (Å² × 10⁴)

$$U_{\text{eq}} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a^*_ia^*_j\mathbf{a}_i.\mathbf{a}_j\cos(a_i,a_j).$$

	x	y	z	U_{eq}
S	0·88620 (17)	0·16196 (13)	0·52613 (9)	924 (7)
O	0·86204 (38)	0·16512 (24)	0·73857 (18)	789 (13)
N(1)	0·97190 (42)	0·25237 (32)	0·74337 (22)	694 (14)
N(2)	0·77288 (33)	0·31319 (24)	0·66500 (19)	490 (11)
C(1)	0·91155 (42)	0·33407 (34)	0·70499 (22)	502 (13)
C(2)	0·74462 (47)	0·19680 (33)	0·67708 (25)	574 (15)
C(3)	0·83215 (57)	0·05659 (44)	0·46422 (29)	789 (20)
C(4)	0·72034 (58)	−0·00012 (41)	0·49605 (32)	811 (20)
C(5)	0·67313 (47)	0·03992 (38)	0·57400 (25)	637 (16)
C(6)	0·75619 (42)	0·13228 (31)	0·59850 (23)	504 (14)
C(7)	0·99405 (40)	0·43728 (33)	0·69747 (22)	499 (13)
C(8)	1·09946 (45)	0·46877 (35)	0·76038 (25)	604 (15)
C(9)	1·18346 (48)	0·56258 (40)	0·75169 (30)	710 (18)
C(10)	1·16518 (49)	0·62617 (39)	0·68121 (34)	743 (19)
C(11)	1·06068 (51)	0·59678 (40)	0·61894 (29)	735 (19)
C(12)	0·97547 (45)	0·50276 (37)	0·62675 (25)	614 (15)
C(13)	0·64270 (41)	0·38969 (30)	0·67184 (23)	499 (13)
C(14)	0·52770 (41)	0·36239 (31)	0·60186 (24)	495 (14)
C(15)	0·57161 (46)	0·36613 (37)	0·51973 (27)	639 (16)
C(16)	0·47302 (56)	0·33989 (43)	0·45380 (28)	770 (19)
C(17)	0·32734 (60)	0·31116 (45)	0·46907 (34)	851 (22)
C(18)	0·28159 (51)	0·30877 (48)	0·54941 (39)	927 (23)
C(19)	0·37980 (47)	0·33493 (41)	0·61675 (28)	716 (18)
C(20)	0·58160 (50)	0·39067 (37)	0·76033 (26)	687 (17)

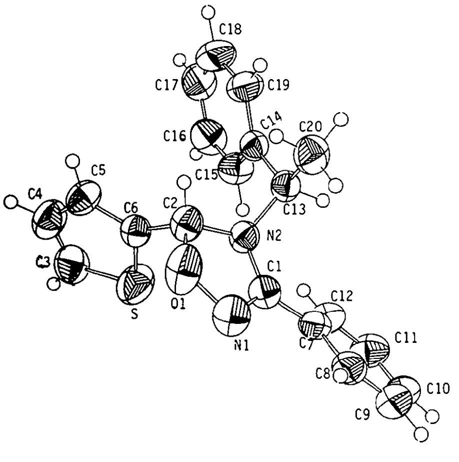

Fig. 1. *ORTEP* (Johnson, 1965) drawing of the molecule showing the atom numbering.

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

S—C(3)	1·682 (5)	C(7)—C(12)	1·386 (6)
S—C(6)	1·693 (4)	C(8)—C(9)	1·376 (6)
O—N(1)	1·444 (5)	C(9)—C(10)	1·370 (7)
O—C(2)	1·455 (5)	C(10)—C(11)	1·380 (7)
N(1)—C(1)	1·279 (5)	C(11)—C(12)	1·383 (7)
N(2)—C(1)	1·386 (5)	C(13)—C(14)	1·518 (5)
N(2)—C(2)	1·460 (5)	C(13)—C(20)	1·524 (6)
N(2)—C(13)	1·490 (5)	C(14)—C(15)	1·377 (6)
C(1)—C(7)	1·465 (6)	C(14)—C(19)	1·378 (6)
C(2)—C(6)	1·485 (6)	C(15)—C(16)	1·379 (6)
C(3)—C(4)	1·323 (7)	C(16)—C(17)	1·365 (7)
C(4)—C(5)	1·408 (7)	C(17)—C(18)	1·352 (8)
C(5)—C(6)	1·397 (6)	C(18)—C(19)	1·393 (7)
C(7)—C(8)	1·398 (5)		
C(3)—S—C(6)	92·7 (2)	C(1)—C(7)—C(8)	120·1 (4)
N(1)—O—C(2)	107·6 (3)	C(8)—C(7)—C(12)	118·6 (4)
O—N(1)—C(1)	106·5 (4)	C(7)—C(8)—C(9)	120·5 (4)
C(2)—N(2)—C(13)	117·8 (3)	C(8)—C(9)—C(10)	120·4 (5)
C(1)—N(2)—C(13)	121·6 (3)	C(9)—C(10)—C(11)	119·9 (5)
C(1)—N(2)—C(2)	105·8 (3)	C(10)—C(11)—C(12)	120·4 (4)
N(1)—C(1)—N(2)	115·1 (4)	C(7)—C(12)—C(11)	120·3 (4)
N(2)—C(1)—C(7)	123·9 (4)	N(2)—C(13)—C(20)	111·7 (3)
N(1)—C(1)—C(7)	120·7 (4)	N(2)—C(13)—C(14)	108·0 (3)
O—C(2)—N(2)	103·1 (3)	C(14)—C(13)—C(20)	115·4 (4)
N(2)—C(2)—C(6)	113·0 (3)	C(13)—C(14)—C(19)	123·0 (4)
O—C(2)—C(6)	110·9 (4)	C(13)—C(14)—C(15)	119·0 (4)
S—C(3)—C(4)	112·3 (4)	C(15)—C(14)—C(19)	118·0 (4)
C(3)—C(4)—C(5)	113·7 (5)	C(14)—C(15)—C(16)	121·6 (4)
C(4)—C(5)—C(6)	111·0 (4)	C(15)—C(16)—C(17)	120·1 (4)
C(2)—C(6)—C(5)	127·9 (4)	C(16)—C(17)—C(18)	119·2 (5)
S—C(6)—C(5)	110·3 (3)	C(17)—C(18)—C(19)	121·5 (5)
S—C(6)—C(2)	121·7 (3)	C(14)—C(19)—C(18)	119·7 (5)
C(1)—C(7)—C(12)	121·2 (4)		

The structure consists of individual molecules of the title compound held together by van der Waals forces. C(13) is anticlinal to C(6) and synperiplanar to H(2). The relevant torsion angles are C(6)—C(2)—N(2)—C(13) = 110·7 (4)° and H(2)—C(2)—N(2)—C(13) = −13·0 (3)°.

The dihydrooxadiazole ring is not planar, maximum deviation from the least-squares plane, 0·098 (4) Å. The thienyl and phenyl rings are essentially planar.

References

Arjona, O., Plumet, J., Ossorio, R. P. & Carreiro, C. (1985). Private communication. Departamento de Quimica Orgánica, Univ. Complutense.

International Tables for X-ray Crystallography (1974). Vol. IV, pp. 72–98. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.

Main, P., Lessinger, L., Woolfson, M. M., Germain, G. & Declercq, J.-P. (1977). *MULTAN77. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

Nardelli, M., Musatti, A., Domiano, P. & Andreetti, G. D. (1965). *Ric. Sci.* **35**, 807–810.

Stewart, J. M., Machin, P. A., Dickinson, C. W., Ammon, H. L., Heck, H. & Flack, H. (1976). The *XRAY76* system. Tech. Rep. TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland.

Walker, N. & Stuart, D. (1983). *Acta Cryst.* A**39**, 158–166.

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[*] Lists of structure amplitudes, anisotropic thermal parameters, H-atom parameters and bond lengths and angles involving H atoms have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42425 (29 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.