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Crystal Studies of Heterocyclic Compounds Containing One Oxygen and Two Nitrogen Atoms. III. Bis[2-(5-phenyl-1,3,4-oxadiazolyl)methyl] Ether

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Abstract. $C_{18}H_{14}N_4O_3$, $M_r = 334{\cdot}3$, monoclinic, $P2_1/c$, $a = 17{\cdot}881\ (3)$, $b = 11{\cdot}285\ (2)$, $c = 7{\cdot}697\ (1)$ Å, $\beta = 95{\cdot}18\ (1)°$, $V = 1546{\cdot}8\ (7)$ Å^3, $Z = 4$, $D_x = 1{\cdot}435$ g cm^{-3}, $\mu = 8{\cdot}04$ cm^{-1}. Diffractometer data measured at room temperature [λ(Cu $K\alpha$) = 1·54178 Å]. $F(000) = 696$; final $R = 0{\cdot}0362$ for 1766 independent reflections with $I > 3\sigma(I)$. All four rings of the molecule are planar and nearly coplanar.

Introduction. The title compound was obtained by condensation of diglycolic acid chloride with dibenzoylhydrazine (Krakowiak & Kotełko, 1983). The formula was confirmed by IR, NMR and MS analyses. The compound shows anticancer and antivirus activity.

Table 1. *Final fractional coordinates* (×10^4) *and equivalent isotropic temperature factors* (×10^4) *with e.s.d.'s in parentheses*

$U_{eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33} + 2U_{13}\cos\beta)$.

	x	y	z	U_{eq}(Å^2)
O1	2464 (1)	5116 (1)	7544 (2)	466 (8)
N1	3892 (1)	8381 (2)	7197 (3)	517 (11)
N2	3209 (1)	8023 (2)	7808 (3)	517 (11)
N3	539 (1)	7440 (2)	5670 (3)	512 (11)
N4	1276 (1)	7161 (2)	5333 (3)	511 (11)
C3	3240 (1)	6894 (2)	7943 (3)	409 (11)
C4	2665 (1)	6102 (2)	8620 (3)	455 (12)
C5	2105 (1)	5415 (2)	5871 (3)	465 (12)
C6	1407 (1)	6119 (2)	5948 (3)	418 (11)
C1	293 (1)	6536 (2)	6472 (3)	394 (10)
C11	−446 (1)	6374 (2)	7104 (3)	384 (10)
C12	−961 (1)	7302 (2)	6914 (3)	440 (12)
C13	−1663 (1)	7169 (2)	7495 (3)	487 (12)
C14	−1861 (1)	6120 (2)	8244 (3)	539 (13)
C15	−1350 (1)	5198 (2)	8440 (3)	541 (14)
C16	−642 (1)	5322 (2)	7877 (3)	465 (12)
O3	812 (1)	5651 (1)	6692 (2)	417 (8)
C2	4268 (1)	7423 (2)	7002 (3)	393 (11)
C21	5013 (1)	7309 (2)	6379 (2)	404 (11)
C22	5396 (1)	8329 (2)	5952 (3)	528 (14)
C23	6101 (1)	8232 (3)	5369 (4)	604 (15)
C24	6426 (1)	7136 (3)	5206 (3)	608 (16)
C25	6053 (1)	6130 (3)	5637 (3)	600 (16)
C26	5348 (1)	6211 (2)	6225 (3)	512 (13)
O2	3891 (1)	6437 (1)	7456 (2)	416 (8)

Experimental. Colourless crystals from ethanol, room temperature, $\mu r = 0{\cdot}17$, r being about 0·2 mm, CAD-4 diffractometer, θ–2θ scan technique; lattice parameters by least-squares method using 25 reflections with $\theta \leq 16°$, total of 3197 independent reflections measured to $(\sin\theta)/\lambda = 0{\cdot}63$ Å^{-1}, data not corrected for

Table 2. *Selected bond lengths* (Å) *and angles* (°)

O1–C4	1·415 (3)	O1–C5	1·426 (3)
C3–C4	1·490 (3)	C5–C6	1·485 (3)
N2–C3	1·280 (3)	N4–C6	1·281 (3)
N1–N2	1·407 (3)	N3–N4	1·403 (3)
N1–C2	1·289 (3)	C1–N3	1·290 (3)
C2–O2	1·363 (2)	C1–O3	1·363 (2)
O2–C3	1·357 (2)	O3–C6	1·360 (2)
C2–C21	1·461 (3)	C1–C11	1·459 (3)
C21–C22	1·394 (3)	C11–C12	1·394 (3)
C22–C23	1·380 (4)	C12–C13	1·379 (3)
C23–C24	1·377 (4)	C13–C14	1·377 (3)
C24–C25	1·373 (4)	C14–C15	1·383 (3)
C25–C26	1·379 (3)	C15–C16	1·382 (3)
C21–C26	1·386 (3)	C11–C16	1·387 (3)
C11–C12–C13	119·8 (2)	C21–C22–C23	119·6 (2)
C12–C13–C14	120·4 (2)	C22–C23–C24	120·4 (2)
C13–C14–C15	120·0 (2)	C23–C24–C25	120·1 (2)
C14–C15–C16	120·3 (2)	C24–C25–C26	120·2 (3)
C15–C16–C11	119·7 (2)	C25–C26–C21	120·1 (2)
C16–C11–C12	119·8 (2)	C26–C21–C22	119·5 (2)
C1–C11–C12	118·7 (2)	C2–C21–C22	119·1 (2)
C1–C11–C16	121·5 (2)	C2–C21–C26	121·4 (2)
C11–C1–N3	128·1 (2)	C21–C2–N1	127·8 (2)
C11–C1–O3	119·6 (2)	C21–C2–O2	119·9 (2)
N3–C1–O3	112·4 (2)	N1–C2–O2	112·3 (2)
C1–O3–C6	102·3 (2)	C2–O2–C3	102·5 (2)
O3–C6–N4	112·8 (2)	O2–C3–N2	112·8 (2)
C6–N4–N3	106·3 (2)	C3–N2–N1	106·3 (2)
N4–N3–C1	106·1 (2)	N2–N1–C2	106·0 (2)
C5–C6–O3	120·1 (2)	C4–C3–O2	120·3 (2)
C5–C6–N4	127·0 (2)	C4–C3–N2	126·8 (2)
C6–C5–O1	113·7 (2)	C3–C4–O1	114·5 (2)
C5–O1–C4	114·4 (2)		

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absorption, maximum values of h,k,l were 21,13,9 respectively, standard reflection 212 with mean variation 0·6%, solution by direct methods using *SHELX*76 (Sheldrick, 1976), H atoms found on difference map, refinement by full-matrix least squares (F magnitudes, 282 parameters), final $R = 0{\cdot}0362$ for 1766 reflections with $I > 3\sigma(I)$, $wR = 0{\cdot}0403$ where $w = 1{\cdot}0000\sigma^2(F) + 0{\cdot}0054(F^2)$; max. shift/e.s.d. = 0·20, largest peak on final difference map was 0·17 e Å^{-3}. Atomic scattering factors those of *SHELX*.

Discussion. The final positional parameters are listed in Table 1, bond lengths and bond angles in Table 2.*

The molecules are in general positions (the numbering of the atoms is shown in Fig. 1). All the rings of the molecule are planar [the maximum distance from the plane is 0·006 (4) Å]. The oxadiazole and the neighbouring phenyl rings are almost coplanar [2·7 (3) and 0·9 (3)°]. The oxadiazole rings form an angle of 18·7 (3)°. Therefore, the whole molecule is nearly planar. The distances and angles between the C4, O1 and C5 atoms are typical for ethers. The distances between the middles of the rings are within the limits of 3·85–4·37 Å. Hence, it seems that all four rings of the molecule can take part in intermolecular charge-transfer interactions, though this is not confirmed by the colour of the crystals.

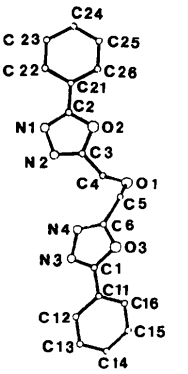

Fig. 1. The atom-numbering scheme.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44146 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

KRAKOWIAK, K. & KOTEŁKO, B. (1983). *Acta Pol. Pharm.* **40**, 685–688.

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

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Crystal Studies of Heterocyclic Compounds Containing One Oxygen and Two Nitrogen Atoms. IV. *N,N'*-Ditosylperhydro-1,4,6-oxadiazocine

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Abstract. $C_{19}H_{24}N_2O_5S_2$, $M_r = 424{\cdot}6$, monoclinic, $P2_1/n$ (non-standard group), $a = 12{\cdot}523$ (4), $b = 5{\cdot}374$ (1), $c = 30{\cdot}128$ (9) Å, $\beta = 100{\cdot}49$ (3)°, $V = 1993{\cdot}8$ (16) Å^3, $Z = 4$, $\mu = 25{\cdot}8$ cm^{-1}, $D_x = 1{\cdot}414$ g cm^{-3}. Diffractometer data at room temperature, λ(Cu $K\alpha$) = 1·54178 Å. $F(000) = 896$; final

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