Table 3. *Selected bond lengths (Å), angles (°) and torsion angles (°) involving non-H atoms*

	(A)	(B)	(C) (a)	(b)
O(1)—C(1)	1·366 (3)	1·371 (3)	1·364 (4)	1·374 (5)
O(1)—C(9)	1·444 (3)	1·435 (3)	1·438 (4)	1·436 (6)
N—C(7)	1·464 (2)	1·469 (4)	1·475 (4)	1·467 (4)
N—C(11)	1·485 (3)	1·458 (3)	1·462 (4)	1·481 (4)
C(1)—C(6)	1·401 (3)	1·384 (4)	1·389 (5)	1·389 (5)
C(6)—C(7)	1·495 (3)	1·523 (3)	1·518 (4)	1·513 (5)
C(7)—C(8)	1·523 (3)	1·525 (4)	1·538 (5)	1·519 (5)
C(8)—C(9)	1·498 (4)	1·505 (5)	1·526 (4)	1·508 (5)
C(8)—C(10)	1·523 (3)	1·546 (4)	1·541 (5)	1·536 (4)
C(10)—C(11)	1·621 (3)	1·569 (4)	1·578 (4)	1·592 (5)
C(1)—O(1)—C(9)	119·9 (2)	113·6 (3)	114·4 (3)	115·1 (3)
C(7)—N—C(11)	104·7 (2)	108·0 (2)	109·5 (2)	108·8 (2)
O(1)—C(1)—C(6)	124·2 (2)	122·7 (2)	122·4 (3)	123·6 (3)
C(1)—C(6)—C(7)	116·6 (2)	121·6 (2)	121·2 (3)	120·8 (3)
N—C(7)—C(6)	118·4 (2)	114·5 (2)	112·1 (2)	110·5 (3)
N—C(7)—C(8)	104·5 (2)	101·8 (2)	107·5 (2)	106·0 (2)
C(6)—C(7)—C(8)	108·9 (1)	111·7 (2)	113·6 (3)	111·8 (2)
C(7)—C(8)—C(9)	109·1 (2)	111·7 (2)	111·8 (2)	111·8 (3)
C(7)—C(8)—C(10)	102·2 (1)	105·8 (2)	104·3 (3)	104·1 (3)
C(9)—C(8)—C(10)	118·5 (2)	113·7 (3)	110·9 (2)	114·1 (3)
O(1)—C(9)—C(8)	110·4 (2)	111·7 (2)	112·0 (2)	111·9 (3)
C(8)—C(10)—C(11)	101·8 (2)	104·8 (2)	102·1 (2)	104·4 (2)
N—C(11)—C(10)	106·4 (2)	102·4 (2)	105·0 (2)	105·7 (2)
C(1)—O(1)—C(9)—C(8)	−27·2 (3)	−54·9 (3)	−55·6 (3)	48·7 (4)
C(11)—N—C(7)—C(6)	−162·0 (2)	−78·1 (2)	123·4 (3)	92·2 (3)
C(11)—N—C(7)—C(8)	−40·6 (2)	42·6 (2)	−2·0 (3)	−29·1 (3)
C(7)—N—C(11)—C(10)	19·4 (2)	−38·3 (2)	22·1 (3)	12·1 (3)
N—C(7)—C(8)—C(9)	172·4 (2)	−152·6 (2)	100·6 (3)	157·6 (3)
C(6)—C(7)—C(8)—C(9)	−60·1 (2)	−30·0 (3)	−24·0 (4)	37·1 (4)
N—C(7)—C(8)—C(10)	46·1 (2)	−28·4 (3)	−19·3 (3)	34·0 (3)
C(6)—C(7)—C(8)—C(10)	173·6 (2)	94·2 (3)	−144·0 (3)	−86·5 (3)
C(7)—C(8)—C(9)—O(1)	58·0 (2)	58·4 (3)	52·8 (3)	−57·8 (4)
C(10)—C(8)—C(9)—O(1)	174·3 (2)	−61·2 (3)	168·8 (2)	59·9 (4)
C(7)—C(8)—C(10)—C(11)	−31·7 (2)	6·4 (3)	31·3 (3)	−25·7 (3)
C(9)—C(8)—C(10)—C(11)	−151·6 (2)	129·4 (2)	−89·2 (3)	−147·8 (3)
C(8)—C(10)—C(11)—N	8·4 (2)	18·2 (2)	−33·1 (3)	9·0 (3)

hindrance between the methylene C(9) of the benzopyran ring system and H(C8) in the course of the cycloaddition. Thus, the chances of cycloaddition are considerably reduced as shown by the low yield (15%) (Tuge, Ueno & Ueda, 1981). The resultant

isomer (*A*) shows an abnormally long bond length for C(10)—C(11) [1·621 (3) Å] due to the steric hindrance between the methoxycarbonyl group and the phenyl ring bonded to C(10).

Isomer (*B*) has a *cis* juncture at C(7)—C(8) and causes a fair approach of the methoxycarbonyl group to the benzopyran ring system. Isomer (*C*) also has a *cis* juncture at C(7)—C(8). Isomer (*C*) is composed of two pairs of racemic molecules. The conformations of these pairs are considerably different as shown in Table 3 and Fig. 1. The difference is mainly caused by inversions of C(9) and O(1) of the benzopyran rings and C(10) and C(11) of the pyrrole rings. Such different conformations of the two pairs are related to the high yield (30%) and the increased chance of cycloaddition. The bond lengths C(10)—C(11) for isomers the increased (*B*) and (*C*) are also unusually long as shown in Table 3. However, these lengths are shorter than that of isomer (*A*).

The variations of torsion angles of the benzopyran and pyrrole rings are remarkable (Table 3). These variations are caused by stress or strain in the pyrrole rings in the course of cycloaddition and by steric hindrances between the two phenyl rings and methoxycarbonyl moieties.

References

FRENZ, B. A. (1985). *Enraf–Nonius SDP-Plus Structure Determination Package*. Version 3.0. Enraf–Nonius, Delft, The Netherlands.

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

SAKURAI, T. & KOBAYASHI, K. (1979). *Rika Gaku Kenkyusho Hokoku*, **55**, 69–77. (In Japanese.)

TUGE, O., UENO, K. & UEDA, I. (1981). *Heterocycles*, **16**, 1503–1508.

Structure of 3-Benzoyl-2-phenylquinoxaline 1,4-Dioxide

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Abstract. $C_{21}H_{14}N_2O_3$, $M_r = 342·36$, monoclinic, $P2_1/c$, $a = 7·520$ (3), $b = 36·048$ (7), $c = 12·801$ (3) Å, $\beta = 100·51$ (2)°, $V = 3415·5$ Å^3, $Z = 8$, $D_x = 1·332$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0·71073$ Å, $\mu = 0·846$ cm^{-1}, $F(000) = 1424$, $T = 295$ (1) K, $R = 0·045$ for 2796 unique observed reflections with $I > 3·0\sigma(I)$.

The two independent molecules in the asymmetric unit have different conformations with respect to the orientation of phenyl ring and the benzoyl group. The dihedral angles between the phenyl ring and the pyrazine ring in the quinoxaline moiety are 68·6 and 107·2° for molecules A and B. There are also differences in the torsion angle about the C—C bond linking the benzene and keto groups, C(16)—C(15)—C(3)—C(2): $-103\cdot0$ (A) and $103\cdot7°$ (B).

Introduction. The extensive interest in the chemistry of quinoxaline 1,4-dioxide and over a thousand of its derivatives is prompted by their antibacterial and animal growth-promoting activities. In the last decade, quinoxaline 1,4-dioxide and some of its derivatives have also been extensively examined for mutagenicity (Negishi, Tanaka & Hayatsu, 1980; Beutin, Preller & Kowalski, 1981). As a part of a systematic investigation we previously reported photochemical reactions (Yan, Feng, Wang, Zhao, Tan & Xue, 1985; Lin & Wang, 1986a) and crystal structures (Lin & Cong, 1987; Cong, Lin & Wang, 1989; Wang, Wang & Wang, 1990) of several 2,3-substituted quinoxaline 1,4-dioxides. In the present work we describe the crystal structure of 2-phenyl-3-benzoylquinoxaline 1,4-dioxide (PBQO).

Experimental. The title compound was synthesized by a method reported previously (Issidorides & Haddadin, 1966; Lin & Wang, 1986b). A yellow crystal (thin rectangular plate) recrystallized by slow evaporation from a solution of chloroform-acetonitrile with dimensions $0\cdot4 \times 0\cdot1 \times 0\cdot8$ mm. Enraf–Nonius CAD-4 diffractometer with graphite-monochromated Mo $K\alpha$ radiation. Lattice parameters from least-squares refinement of 25 reflections with $9 < \theta < 14°$. 6560 reflections measured, 5956 unique ($R_{int} = 0\cdot032$), using ω–2θ scan technique within the ranges $1 \le \theta \le 25°$, $0 \le h \le 8$, $0 \le k \le 40$, $-15 \le l \le 15$, $\sin\theta/\lambda = 0\cdot5942$ Å^{-1}. Three standard reflections were measured every hour and showed a variation of less than $1\cdot0\%$. 2796 independent reflections with $I > 3\cdot0\sigma(I)$ considered observed. Data corrected for Lorentz and polarization factors, and absorption effects using ψ scans (from 0·909 to 0·999 on I).

The structure was solved by direct methods using *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). All non-H atoms were refined anisotropically by full-matrix least squares on F, minimizing $\Sigma w(|F_o| - |F_c|)^2$. A difference Fourier synthesis calculated at this stage of the refinement revealed all H atoms; these were included at the difference-map positions with arbitrary isotropic temperature factors, $B = 4\cdot0$ Å^2 in the

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *with e.s.d.'s in parentheses*

	x	y	z	B_{eq}
Molecule A				
N(1)	0·0055 (5)	0·13879 (9)	0·2991 (3)	3·85 (8)
N(2)	0·0510 (5)	0·1986 (1)	0·1701 (3)	4·28 (8)
O(1)	−0·0270 (4)	0·11225 (8)	0·3606 (2)	5·12 (8)
O(2)	0·0633 (5)	0·22682 (8)	0·1096 (3)	5·98 (9)
O(3)	−0·2443 (4)	0·1726 (1)	−0·0196 (3)	7·5 (1)
C(1)	0·0861 (5)	0·1716 (1)	0·3443 (3)	3·60 (9)
C(2)	−0·0361 (5)	0·1356 (1)	0·1915 (3)	3·60 (9)
C(3)	−0·0158 (5)	0·1662 (1)	0·1294 (3)	3·8 (1)
C(4)	0·1089 (5)	0·2016 (1)	0·2802 (3)	3·8 (1)
C(5)	0·1859 (6)	0·2346 (1)	0·3243 (4)	4·7 (1)
C(6)	0·2400 (7)	0·2366 (1)	0·4319 (4)	5·4 (1)
C(7)	0·2191 (7)	0·2065 (1)	0·4958 (4)	5·4 (1)
C(8)	0·1443 (6)	0·1744 (1)	0·4545 (3)	4·6 (1)
C(9)	−0·0964 (6)	0·0991 (1)	0·1474 (3)	4·3 (1)
C(10)	0·0201 (7)	0·0699 (1)	0·1533 (4)	5·7 (1)
C(11)	−0·0304 (9)	0·0355 (1)	0·1161 (5)	7·6 (2)
C(12)	−0·204 (1)	0·0295 (2)	0·0673 (5)	8·4 (2)
C(13)	−0·3241 (8)	0·0581 (2)	0·0572 (5)	8·7 (2)
C(14)	−0·2737 (7)	0·0929 (2)	0·0970 (4)	6·4 (1)
C(15)	−0·0838 (6)	0·1670 (1)	0·0103 (3)	4·6 (1)
C(16)	0·0449 (6)	0·1626 (1)	−0·0619 (3)	3·8 (1)
C(17)	0·2251 (6)	0·1542 (2)	−0·0243 (4)	5·3 (1)
C(18)	0·3419 (7)	0·1523 (2)	−0·0946 (4)	7·1 (1)
C(19)	0·2841 (4)	0·1588 (2)	−0·2008 (4)	6·9 (1)
C(20)	0·1056 (7)	0·1664 (1)	−0·2387 (3)	5·2 (1)
C(21)	−0·0120 (6)	0·1681 (1)	−0·1700 (3)	4·1 (1)
Molecule B				
O(1)	0·4323 (4)	0·12693 (8)	0·2188 (2)	4·99 (8)
O(2)	0·7044 (5)	0·18106 (9)	0·6041 (2)	5·81 (8)
O(3)	0·4549 (4)	0·1087 (1)	0·6316 (3)	6·7 (1)
N(1)	0·5106 (4)	0·13877 (9)	0·3108 (3)	3·54 (8)
N(2)	0·6517 (5)	0·1670 (1)	0·5102 (3)	3·92 (8)
C(1)	0·5768 (5)	0·1749 (1)	0·3200 (3)	3·43 (9)
C(2)	0·5292 (5)	0·1167 (1)	0·3978 (3)	3·36 (9)
C(3)	0·5969 (5)	0·1320 (1)	0·4970 (3)	3·60 (9)
C(4)	0·6502 (5)	0·1896 (1)	0·4205 (3)	3·7 (1)
C(5)	0·7167 (6)	0·2255 (1)	0·4306 (4)	4·9 (1)
C(6)	0·7100 (7)	0·2464 (1)	0·3420 (4)	5·9 (1)
C(7)	0·6378 (7)	0·2327 (1)	0·2416 (4)	5·5 (1)
C(8)	0·5717 (6)	0·1974 (1)	0·2306 (3)	4·5 (1)
C(9)	0·4839 (6)	0·0771 (1)	0·3834 (3)	4·3 (1)
C(10)	0·5948 (8)	0·0543 (1)	0·3407 (4)	6·9 (2)
C(11)	0·557 (1)	0·0177 (2)	0·3276 (5)	10·4 (2)
C(12)	0·410 (1)	0·0025 (2)	0·3546 (6)	12·2 (3)
C(13)	0·2972 (9)	0·0248 (2)	0·3950 (5)	10·0 (2)
C(14)	0·3303 (7)	0·0617 (2)	0·4110 (4)	6·7 (1)
C(15)	0·5968 (6)	0·1110 (1)	0·5997 (3)	4·3 (1)
C(16)	0·7674 (6)	0·0948 (1)	0·6569 (3)	3·70 (9)
C(17)	0·9116 (6)	0·0880 (1)	0·6058 (3)	4·6 (1)
C(18)	1·0666 (7)	0·0720 (2)	0·6615 (4)	6·2 (1)
C(19)	1·0783 (7)	0·0636 (2)	0·7667 (4)	6·8 (1)
C(20)	0·9386 (8)	0·0706 (1)	0·8186 (4)	6·0 (1)
C(21)	0·7812 (7)	0·0856 (1)	0·7634 (3)	4·9 (1)

The thermal parameters given for anisotropically refined atoms are the equivalent isotropic thermal parameters defined as: $4/3[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ac(\cos\beta)B(1,3)]$, where a, b, c are real-cell parameters and $B(i,j)$ are anisotropic β's.

subsequent calculations, but not refined. Final $R = 0\cdot045$ and $wR = 0\cdot047$ for 469 variables with $w = 1/\sigma^2(F_o)$ and $S = 1\cdot438$, $(\Delta/\sigma)_{max} = 0\cdot02$ in final refinement cycle, the difference electron density map was essentially featureless with $\Delta\rho = 0\cdot40$ e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). All calculations on a PDP 11/44 computer using Enraf–Nonius *Structure Determination Package* (B. A. Frenz & Associates Inc., 1982) and *ORTEP*II (Johnson, 1976).

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

	Molecule A	Molecule B
N(1)—O(1)	1·291 (5)	1·291 (4)
N(2)—O(2)	1·291 (5)	1·298 (4)
N(1)—C(2)	1·361 (5)	1·355 (5)
N(1)—C(1)	1·404 (5)	1·393 (5)
N(2)—C(3)	1·341 (5)	1·330 (5)
N(2)—C(4)	1·403 (5)	1·406 (5)
C(2)—C(3)	1·384 (6)	1·394 (5)
C(4)—C(5)	1·389 (6)	1·386 (6)
C(5)—C(6)	1·367 (7)	1·356 (7)
C(6)—C(7)	1·385 (7)	1·392 (7)
C(7)—C(8)	1·350 (7)	1·364 (7)
C(1)—C(8)	1·403 (6)	1·398 (6)
C(2)—C(9)	1·472 (6)	1·471 (6)
C(9)—C(10)	1·361 (7)	1·355 (8)
C(10)—C(11)	1·365 (7)	1·352 (8)
C(11)—C(12)	1·358 (9)	1·340 (12)
C(12)—C(13)	1·365 (9)	1·338 (11)
C(13)—C(14)	1·380 (9)	1·363 (8)
C(14)—C(9)	1·390 (7)	1·385 (8)
C(3)—C(15)	1·518 (6)	1·517 (6)
C(15)—O(3)	1·216 (5)	1·213 (6)
C(15)—C(16)	1·464 (7)	1·478 (6)
C(16)—C(17)	1·387 (6)	1·387 (7)
C(17)—C(18)	1·369 (8)	1·378 (6)
C(18)—C(19)	1·371 (7)	1·368 (8)
C(19)—C(20)	1·370 (7)	1·365 (8)
C(20)—C(21)	1·357 (7)	1·375 (7)
C(21)—C(16)	1·387 (5)	1·389 (6)
O(1)—N(1)—C(1)	119·2 (3)	118·9 (3)
O(1)—N(1)—C(2)	121·4 (3)	121·3 (3)
C(1)—N(1)—C(2)	119·5 (3)	119·8 (3)
N(1)—C(1)—C(4)	120·2 (3)	120·2 (4)
N(1)—C(1)—C(8)	120·6 (3)	121·1 (4)
C(8)—C(1)—C(4)	119·2 (4)	118·7 (4)
C(1)—C(4)—N(2)	119·0 (4)	118·3 (4)
N(2)—C(4)—C(5)	120·2 (4)	120·9 (4)
C(1)—C(4)—C(5)	120·8 (4)	120·8 (4)
C(4)—C(5)—C(6)	118·5 (4)	118·8 (4)
C(5)—C(6)—C(7)	120·7 (4)	121·6 (5)
C(6)—C(7)—C(8)	121·5 (4)	120·1 (5)
C(7)—C(8)—C(1)	119·3 (4)	120·0 (4)
C(4)—N(2)—O(2)	120·0 (3)	119·2 (3)
C(4)—N(2)—C(3)	118·9 (4)	119·3 (3)
O(2)—N(2)—C(3)	121·1 (3)	121·5 (3)
N(2)—C(3)—C(2)	123·0 (4)	123·0 (4)
N(2)—C(3)—C(15)	114·0 (4)	114·4 (3)
C(2)—C(3)—C(15)	122·8 (4)	122·4 (4)
N(1)—C(2)—C(3)	119·0 (4)	119·0 (4)
N(1)—C(2)—C(9)	117·6 (4)	118·6 (3)
C(3)—C(2)—C(9)	123·4 (4)	122·4 (4)
C(2)—C(9)—C(10)	120·9 (4)	119·6 (4)
C(2)—C(9)—C(14)	121·6 (4)	122·9 (4)
C(10)—C(9)—C(14)	117·5 (4)	117·5 (5)
C(9)—C(10)—C(11)	122·8 (5)	120·8 (6)
C(10)—C(11)—C(12)	119·7 (6)	122·1 (7)
C(11)—C(12)—C(13)	119·2 (5)	117·7 (6)
C(12)—C(13)—C(14)	121·3 (5)	122·3 (7)
C(13)—C(14)—C(9)	119·6 (5)	119·5 (6)
C(3)—C(15)—O(3)	117·0 (4)	117·7 (4)
C(3)—C(15)—C(16)	119·5 (4)	119·4 (4)
O(3)—C(15)—C(16)	123·5 (4)	123·0 (4)
C(15)—C(16)—C(17)	121·4 (4)	121·3 (4)
C(15)—C(16)—C(21)	119·7 (4)	119·0 (4)
C(17)—C(16)—C(21)	118·9 (4)	119·8 (4)
C(16)—C(17)—C(18)	119·1 (4)	119·3 (4)
C(17)—C(18)—C(19)	121·2 (5)	120·0 (5)
C(18)—C(19)—C(20)	120·0 (5)	121·4 (5)
C(19)—C(20)—C(21)	119·4 (4)	119·3 (4)
C(20)—C(21)—C(16)	121·4 (4)	120·1 (5)
C(16)—C(15)—C(3)—C(2)	−103·0	103·7
N(1)—C(2)—C(9)—C(10)	−68·8	72·2

Discussion. Final atomic coordinates and equivalent isotropic temperature factors are listed in Table 1* and bond lengths and bond angles are given in Table 2. Fig. 1 shows the conformation of the two crystallographically independent molecules, A and B, with the atom-labeling system. The two independent molecules in the asymmetric unit have different conformations with respect to the orientation of phenyl ring and the benzoyl group. The phenyl rings in both molecules are planar. The dihedral angles between the phenyl ring and the pyrazine ring in the quinoxaline moiety are 68·6 and 107·2° for molecules A and B; the torsion angles are $-103·0$ (A) and 103·7° (B) for C(16)—C(15)—C(3)—C(2) and $-68·8$ (A) and 72·2° (B) for N(1)—C(2)—C(9)—C(10).

Although the molecules have different conformations, the corresponding bond distances and angles for molecules A and B are very similar, the mean differences are 0·008 (7) Å and 0·6 (5)° respectively. Bond lengths involving the C(12) atom in molecule B are shorter than usual [C(11)—C(12) = 1·340 (12), C(12)—C(13) = 1·338 (1) Å].
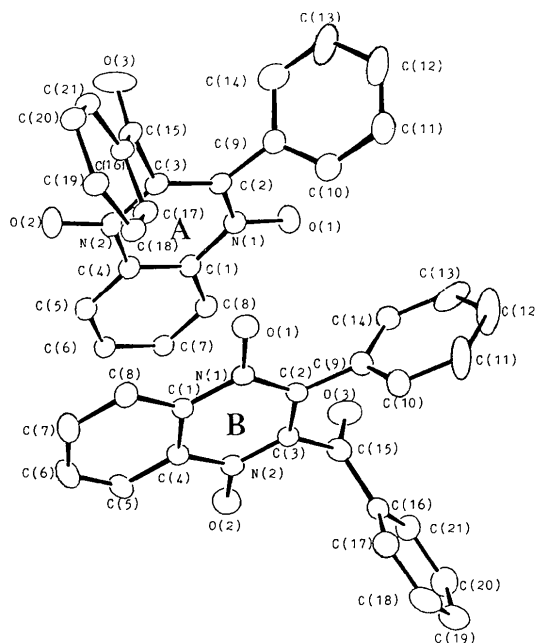

Fig. 1. Molecular conformation of 2-phenyl-3-benzoylquinoxaline 1,4-dioxide (molecules A and B) with the atom-labeling system. Thermal ellipsoids are drawn at the 50% probability level.

The bond distances in the heterocyclic ring are similar to the values found in other substituted quinoxaline di-*N*-oxides like 6-chloro-3-ethoxy-carbonyl-2-methylquinoxaline 1,4-dioxide (Mac-Donald & Arora, 1981), 2-methylcarboethoxy-quinoxaline 1,4-dioxide (Lin & Cong, 1987), 2-[*N*-(2-hydroxyethyl)carboxamide]-3-methylquinoxaline 1,4-dioxide (Bartczak, Galdecki, Wolf & Mak, 1988), quinoxaline 1,4-dioxide and 2,3-dimethylquinoxaline 1,4-dioxide (Cong, Lin & Wang, 1989), and 2-me-thyl-3-phenylacryloylquinoxaline 1,4-dioxide (Wang, Wang & Wang, 1990). The dihedral angles between the benzene ring and the pyrazine ring are 1·7 and 2·1° for molecules *A* and *B* respectively, which indicates that the quinoxaline parts are essentially planar.

The packing diagram of PBQO is illustrated in Fig. 2. The crystal structure of PBQO is stabilized by
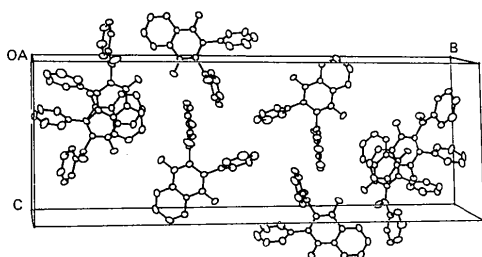
van der Waals interactions. There are no inter-molecular distances between non-H atoms less 3·127 Å.

Fig. 2. Unit-cell packing diagram.

References

B. A. FRENZ & ASSOCIATES INC. (1982). *SDP Structure Determination Package.* College Station, Texas, USA.

BARTCZAK, T. J., GALDECKI, Z., WOLF, W. & MAK, T. C. W. (1988). *J. Cryst. Spectrosc. Res.* **18**, 165–174.

BEUTIN, L., PRELLER, E. & KOWALASKI, B. (1981). *Antimicrob. Agents Chemother.* **20**, 336–343.

CONG, Q.-Z., LIN, S.-K. & WANG, H.-Q. (1989). *Jiegou Huaxue,* **8**, 31–36.

ISSIDORIDES, C. H. & HADDADIN, M. J. (1966). *J. Org. Chem.* **31**, 4067–4068.

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

LIN, S.-K. & CONG, Q.-Z. (1987). *J. Mol. Struct.* **159**, 279–286.

LIN, S.-K. & WANG, H.-Q. (1986*a*). *Heterocycles,* **24**, 659–664.

LIN, S.-K. & WANG, H.-Q. (1986*b*). *Youji Huaxue,* **4**, 298–300. (In Chinese).

MACDONALD, L. & ARORA, S. K. (1981). *Acta Cryst.* B37, 1445–1446.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1982). *MULTAN*11/82. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

NEGISHI, T., TANAKA, K. & HAYATSU, H. (1980). *Chem. Pharm. Bull.* **28**, 1347–1349.

WANG, Y., WANG, M. & WANG, H.-Q. (1990). *Jiegou Huaxue,* **9**, 203–206.

YAN, R.-Z., FENG, L.-B., WANG, H.-Q., ZHAO, R.-C., TAN, P.-Z. & XUE, F.-Q. (1985). *Acta Chim. Sin.* **43**, 498–501. (In Chinese.)