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Three Stereoisomeric Methyl 8-Bromo-2,3-diphenyl-2,3,3a,9b-tetrahydro-1*H*,4*H*-[1]benzopyrano[4,3-*b*]pyrrole-2-carboxylates

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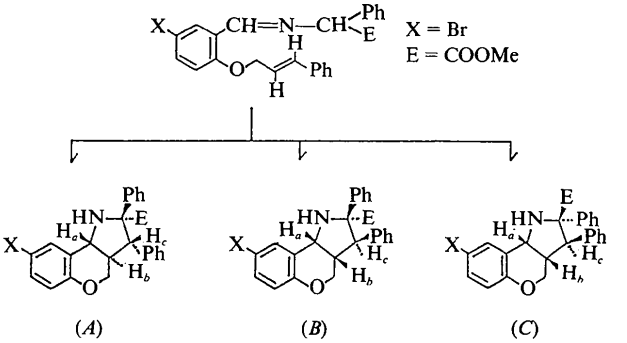
Abstract. $C_{25}H_{22}BrNO_3$, $M_r = 464{\cdot}4$, Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 2{\cdot}88$ mm^{-1}, $T = 298$ K. (*A*) Monoclinic, $P2_1/c$, $a = 9{\cdot}848$ (2), $b = 12{\cdot}935$ (2), $c = 16{\cdot}549$ (2) Å, $\beta = 92{\cdot}81$ (1)°, $V = 2105{\cdot}5$ (5) Å^3, $Z = 4$, $D_m = 1{\cdot}456$, $D_x = 1{\cdot}464$ Mg m^{-3}, $F(000) = 952$, $R = 0{\cdot}0363$ for 2880 observed reflections. (*B*) Monoclinic, $C2/c$, $a = 48{\cdot}06$ (1), $b = 6{\cdot}159$ (1), $c = 14{\cdot}829$ (3) Å, $\beta = 103{\cdot}76$ (2)°, $V = 4263$ (2) Å^3, $Z = 8$, $D_m = 1{\cdot}452$, $D_x = 1{\cdot}446$ Mg m^{-3}, $F(000) = 1904$, $R = 0{\cdot}0426$ for 2834 observed reflections. (*C*) Monoclinic, $P2_1/c$, $a = 11{\cdot}664$ (2), $b = 22{\cdot}979$ (3), $c = 15{\cdot}985$ (3) Å, $\beta = 101{\cdot}37$ (1)°, $V = 4200$ (1) Å^3, $Z = 8$, $D_m = 1{\cdot}477$, $D_x = 1{\cdot}468$ Mg m^{-3}, $F(000) = 1904$, $R = 0{\cdot}0436$ for 5176 observed reflections. These isomers consist of three pairs of racemic and configurational isomers which are caused by the asymmetric C atoms in the pyrrole rings, and isomer (*C*) consists of two pairs of conformational isomers caused by torsions between the benzopyrano and pyrrole rings. Isomers (*A*) and (*C*) have intramolecular O···HN hydrogen bonds between the carbonyl and pyrrole moieties.

Introduction. During the course of studies on the intramolecular 1,3-dipolar cycloaddition of imines of glycine esters to carbon–carbon multiple bonds, methyl 2-[2-(cinnamyloxy)benzylideneamino]-2-phenylacetates were found to give thermally three stereoisomeric cycloadducts (Tuge, Ueno & Ueda, 1981) as shown in (I). The X-ray analyses were carried out to reveal the conformations of isomeric cycloadducts (*A*), (*B*) and (*C*) in order to know the stereochemical course in the intramolecular cycloaddition of the bromine-substituted imine.



(I)

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Table 1. *Experimental and refinement data*

	(*A*)	(*B*)	(*C*)
Radius of crystal r (mm) and μr	0·12, 0·35	0·13, 0·37	0·12, 0·34
Range of h, k and l	$\bar{1}1$, 11; 0, 14; $\bar{1}8$,0	0, 53; 6, 6; $\bar{1}6$, 16	$\bar{1}3$, 13; 0, 25; 0, 17
θ range ( )	$0 \le 2\theta \le 120$	$0 \le 2\theta \le 120$	$0 \le 2\theta \le 120$
Standard reflections	$\bar{1}4\bar{1}$; 223; $2\bar{1}3$	11,$\bar{1}$,1; 604; 204	$\bar{1}15$; 154; 024
Number of reflections measured	3495	6624	6785
Number of unique reflections	2880	2834	5176
	$I \ge 2{\cdot}33[\sigma(I)]$	$I \ge 2{\cdot}33[\sigma(I)]$	$I \ge 2{\cdot}33[\sigma(I)]$
Final wR	0·0427	0·0451	0·0426
S	0·885	1·037	0·875
F_1, F_2*	7·73, 28·17	16·44, 67·02	15·36, 66·01
a_1, b_1, c_2*	−0·037, 0·269, 1·53	0·001, 0·028, 0·449	0·025, 0·020, 0·480
a_3, b_3, c_3*	2·00, −0·097, 0·0021	9·49, −0·263, 0·0025	10·24, −0·391, 0·0039
Maximum shift/e.s.d.†	0·46	0·27	0·64
Maximum height in final difference Fourier synthesis (eÅ^{-3})	0·18	0·27	0·43

* $w = a_1 + b_1 F_o$ for $|F_o| < F_1$, $w = c_2$ for $F_1 \le |F_o| \le F_2$ and $w = (a_3 + b_3|F_o| + c_3 F_o^2)^{-1}$ for $|F_o| > F_2$.
† For non-H atoms.

Experimental. Experimental and refinement data are shown in Table 1. Density measured by flotation in KI solution. Colorless prisms of these crystals were ground manually to spheres of diameter of about 0·25 mm. Enraf–Nonius CAD-4 diffractometer with graphite-monochromatized Cu $K\alpha$ radiation. Cell dimensions derived from least-squares treatment of the setting angles for 25 reflections, $15 \le 2\theta \le 40°$. ω–2θ scan technique, $0 \le 2\theta \le 120°$. Three standard reflections measured every 2 h exposure time, no significant variation in intensities. Lorentz and polarization corrections applied, but absorption ignored. Structures for all compounds solved by the heavy-atom method. All coordinates, anisotropic thermal parameters for non-H and isotropic ones for H atoms refined by block-diagonal least squares, $\sum w(|F_o| - |F_c|)^2$ minimized. Atomic scattering factors and anomalous-dispersion factors f', f'' from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 72–98). Calculation performed on a VAX11/750 using the Enraf–Nonius *Structure Determination Package* (Frenz, 1985) and *UNICS*III program system (Sakurai & Kobayashi, 1979).

Discussion. The atomic parameters for the non-H atoms are given in Table 2.* The selected bond lengths, angles and torsion angles are listed in Table 3. A stereoscopic view of stereoisomers (*A*), (*B*) and (*C*) are shown in Fig. 1 with the atom-numbering schemes (*ORTEP*; Johnson, 1965). The isomers (*A*) and (*C*) have intramolecular NH···O hydrogen bonds between the pyrrole and carbonyl groups. H···O distances are respectively 2·20 (3), 2·26 (3) and 2·09 (3) Å for isomer (*A*), molecules (*a*) and (*b*) of isomer (*C*). On the other hand, isomer (*B*) has no

* 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 53414 (63 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Fractional atomic coordinates with their estimated standard deviations in parentheses*

$B_{eq} = (4/3)\sum_i\sum_j \beta_{ij} \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
(*A*)				
Br	0·14135 (3)	0·17728 (3)	−0·14487 (2)	5·99 (1)
O(1)	0·7275 (2)	0·0446 (2)	−0·1093 (1)	4·23 (4)
O(2)	0·6856 (2)	0·4211 (1)	0·0966 (1)	5·26 (5)
O(3)	0·8300 (2)	0·3784 (1)	0·1992 (1)	4·00 (4)
N	0·5872 (2)	0·2273 (2)	0·0801 (1)	3·15 (4)
C(1)	0·5950 (2)	0·0763 (2)	−0·1123 (1)	3·27 (5)
C(2)	0·5220 (3)	0·0591 (2)	−0·1850 (2)	3·91 (6)
C(3)	0·3873 (3)	0·0877 (2)	−0·1947 (2)	4·11 (6)
C(4)	0·3265 (3)	0·1356 (2)	−0·1312 (2)	3·77 (6)
C(5)	0·3972 (2)	0·1536 (2)	−0·0585 (2)	3·34 (6)
C(6)	0·5322 (2)	0·1241 (2)	−0·0480 (1)	2·96 (5)
C(7)	0·6177 (2)	0·1395 (2)	0·0282 (1)	2·82 (5)
C(8)	0·7647 (2)	0·1563 (2)	0·0067 (1)	2·83 (5)
C(9)	0·8131 (2)	0·0632 (2)	−0·0374 (2)	3·57 (6)
C(10)	0·8334 (2)	0·1831 (2)	0·0885 (1)	2·83 (5)
C(11)	0·7119 (2)	0·2412 (2)	0·1331 (1)	2·83 (5)
C(12)	0·7388 (2)	0·3574 (2)	0·1401 (2)	3·37 (6)
C(13)	0·9694 (2)	0·2366 (2)	0·0843 (1)	3·02 (5)
C(14)	0·9851 (3)	0·3269 (2)	0·0415 (2)	3·90 (6)
C(15)	1·1121 (3)	0·3739 (2)	0·0385 (2)	5·07 (8)
C(16)	1·2232 (3)	0·3308 (3)	0·0787 (2)	5·94 (9)
C(17)	1·2090 (3)	0·2394 (3)	0·1192 (2)	5·92 (9)
C(18)	1·0832 (3)	0·1933 (2)	0·1224 (2)	4·38 (7)
C(19)	0·6932 (2)	0·1955 (2)	0·2171 (1)	3·11 (5)
C(20)	0·5655 (3)	0·1869 (2)	0·2467 (2)	3·72 (6)
C(21)	0·5474 (3)	0·1446 (2)	0·3228 (2)	4·71 (7)
C(22)	0·6563 (4)	0·1103 (2)	0·3692 (2)	5·08 (8)
C(23)	0·7845 (4)	0·1201 (3)	0·3415 (2)	5·36 (8)
C(24)	0·8036 (3)	0·1630 (2)	0·2661 (2)	4·20 (7)
C(25)	0·8731 (4)	0·4851 (2)	0·2076 (2)	5·62 (9)
(*B*)				
Br	0·01106 (1)	−0·00450 (8)	−0·16376 (3)	8·27 (1)
O(1)	0·09184 (4)	−0·6100 (4)	0·0889 (1)	5·30 (6)
O(2)	0·10317 (4)	−0·7117 (3)	−0·1321 (1)	4·62 (5)
O(3)	0·09435 (3)	−0·3874 (3)	−0·1999 (1)	4·08 (4)
N	0·12956 (4)	−0·1898 (3)	−0·0458 (1)	3·20 (5)
C(1)	0·07437 (5)	−0·4652 (5)	0·0317 (2)	4·18 (7)
C(2)	0·04573 (6)	−0·5254 (5)	−0·0017 (3)	5·35 (9)
C(3)	0·02732 (6)	−0·3918 (6)	−0·0590 (2)	5·45 (9)
C(4)	0·03683 (6)	−0·1938 (5)	−0·0835 (2)	4·93 (8)
C(5)	0·06493 (5)	−0·1327 (5)	−0·0519 (2)	4·13 (7)
C(6)	0·08427 (5)	−0·2701 (4)	0·0051 (2)	3·49 (6)
C(7)	0·11590 (5)	−0·2099 (4)	0·0325 (2)	3·44 (6)
C(8)	0·13382 (5)	−0·3880 (5)	0·0902 (2)	3·80 (6)
C(9)	0·11693 (6)	−0·5122 (6)	0·1466 (2)	5·15 (8)
C(10)	0·14498 (5)	−0·5304 (4)	0·0205 (2)	2·99 (6)
C(11)	0·13550 (5)	−0·4078 (4)	−0·0746 (2)	2·82 (5)
C(12)	0·10908 (5)	−0·5236 (4)	−0·1365 (2)	3·21 (6)
C(13)	0·17673 (5)	−0·5787 (4)	0·0502 (2)	2·79 (5)
C(14)	0·19670 (5)	−0·4169 (4)	0·0792 (2)	4·04 (7)
C(15)	0·22564 (6)	−0·4621 (5)	0·1028 (2)	4·90 (8)
C(16)	0·23517 (5)	−0·6695 (5)	0·0966 (2)	4·36 (7)
C(17)	0·21583 (6)	−0·8315 (4)	0·0683 (2)	4·19 (7)
C(18)	0·18658 (5)	−0·7875 (4)	0·0459 (2)	3·36 (6)

Table 2 (*cont.*)

	x	*y*	*z*	B_{eq}(Å^2)
C(19)	0·15820 (4)	−0·4067 (4)	−0·1314 (2)	2·81 (5)
C(20)	0·17409 (5)	−0·2239 (4)	−0·1386 (2)	3·73 (6)
C(21)	0·19622 (6)	−0·2313 (5)	−0·1844 (2)	4·44 (7)
C(22)	0·20242 (6)	−0·4198 (5)	−0·2236 (2)	4·39 (7)
C(23)	0·18647 (6)	−0·6010 (5)	−0·2189 (2)	4·32 (7)
C(24)	0·16465 (5)	−0·5954 (4)	−0·1731 (2)	3·62 (6)
C(25)	0·06896 (6)	−0·4761 (6)	−0·2626 (2)	5·48 (9)
(*Ca*)				
Br	0·59359 (4)	−0·03265 (2)	0·40522 (3)	6·16 (1)
O(1)	0·1187 (2)	−0·0614 (1)	0·1815 (1)	4·10 (6)
O(2)	0·4690 (2)	−0·0605 (1)	−0·0909 (2)	4·27 (6)
O(3)	0·3123 (2)	−0·1071 (1)	−0·1622 (1)	3·27 (5)
N	0·3837 (2)	−0·0557 (1)	0·0553 (2)	3·01 (6)
C(1)	0·2293 (3)	−0·0573 (1)	0·2288 (2)	3·43 (9)
C(2)	0·2441 (3)	−0·0701 (2)	0·3155 (2)	4·3 (1)
C(3)	0·3516 (4)	−0·0632 (2)	0·3674 (2)	4·7 (1)
C(4)	0·4459 (3)	−0·0444 (2)	0·3336 (2)	4·1 (1)
C(5)	0·4324 (3)	−0·0335 (1)	0·2473 (2)	3·49 (9)
C(6)	0·3235 (3)	−0·0393 (1)	0·1940 (2)	2·98 (8)
C(7)	0·3076 (3)	−0·0219 (1)	0·1008 (2)	2·80 (8)
C(8)	0·1813 (3)	−0·0287 (1)	0·0511 (2)	3·03 (8)
C(9)	0·1133 (3)	−0·0734 (1)	0·0925 (2)	3·46 (9)
C(10)	0·1948 (3)	−0·0489 (1)	−0·0384 (2)	2·82 (7)
C(11)	0·3122 (3)	−0·0849 (1)	−0·0181 (2)	2·55 (7)
C(12)	0·3749 (3)	−0·0826 (1)	−0·0934 (2)	2·74 (7)
C(13)	0·2008 (3)	0·0002 (1)	−0·1008 (2)	2·95 (8)
C(14)	0·1387 (3)	−0·0034 (2)	−0·1835 (2)	3·92 (9)
C(15)	0·1512 (4)	0·0372 (2)	−0·2451 (2)	5·0 (1)
C(16)	0·2263 (3)	0·0829 (2)	−0·2242 (2)	4·5 (1)
C(17)	0·2868 (4)	0·0889 (2)	−0·1422 (3)	5·0 (1)
C(18)	0·2743 (3)	0·0480 (2)	−0·0811 (2)	4·5 (1)
C(19)	0·2940 (3)	−0·1498 (1)	0·0017 (2)	2·53 (7)
C(20)	0·3653 (3)	−0·1761 (1)	0·0712 (2)	3·51 (9)
C(21)	0·3526 (3)	−0·2346 (2)	0·0878 (2)	4·5 (1)
C(22)	0·2701 (4)	−0·2678 (2)	0·0357 (3)	4·6 (1)
C(23)	0·1984 (3)	−0·2419 (2)	−0·0330 (2)	4·4 (1)
C(24)	0·2104 (3)	−0·1835 (1)	−0·0488 (2)	3·47 (9)
C(25)	0·3552 (4)	−0·1019 (2)	−0·2412 (2)	4·9 (1)
(*Cb*)				
Br	−0·12046 (5)	0·06843 (2)	0·49037 (3)	7·19 (1)
O(1)	0·3478 (2)	0·1590 (1)	0·4437 (2)	5·04 (7)
O(2)	0·1257 (3)	0·1180 (1)	0·0710 (2)	5·92 (9)
O(3)	0·1146 (2)	0·2140 (1)	0·0722 (1)	3·83 (6)
N	0·1185 (2)	0·1048 (1)	0·2334 (2)	3·21 (7)
C(1)	0·2419 (3)	0·1360 (2)	0·4520 (2)	3·92 (9)
C(2)	0·2023 (4)	0·1496 (2)	0·5264 (2)	5·1 (1)
C(3)	0·0959 (4)	0·1308 (2)	0·5385 (2)	5·3 (1)
C(4)	0·0284 (4)	0·0966 (2)	0·4764 (2)	4·5 (1)
C(5)	0·0657 (3)	0·0826 (1)	0·4027 (2)	3·82 (9)
C(6)	0·1721 (3)	0·1027 (1)	0·3894 (2)	3·42 (9)
C(7)	0·2105 (3)	0·0891 (1)	0·3065 (2)	3·32 (8)
C(8)	0·3176 (3)	0·1241 (1)	0·2968 (2)	3·54 (9)
C(9)	0·4018 (3)	0·1313 (2)	0·3808 (3)	4·9 (1)
C(10)	0·2671 (3)	0·1816 (1)	0·2564 (2)	2·82 (8)
C(11)	0·1390 (3)	0·1651 (1)	0·2071 (2)	2·73 (7)
C(12)	0·1263 (3)	0·1626 (1)	0·1093 (2)	3·24 (8)
C(13)	0·3479 (3)	0·2141 (1)	0·2097 (2)	3·33 (8)
C(14)	0·3881 (3)	0·2693 (2)	0·2376 (2)	4·4 (1)
C(15)	0·4461 (4)	0·2994 (2)	0·1994 (3)	6·4 (1)
C(16)	0·5041 (4)	0·2756 (2)	0·1319 (3)	7·3 (2)
C(17)	0·4671 (4)	0·2215 (2)	0·1017 (3)	6·7 (2)
C(18)	0·3879 (3)	0·1902 (2)	0·1409 (3)	5·0 (1)
C(19)	0·0494 (3)	0·2074 (1)	0·2313 (2)	2·74 (7)
C(20)	−0·0521 (3)	0·1876 (1)	0·2548 (2)	3·51 (9)
C(21)	−0·1314 (3)	0·2267 (2)	0·2763 (2)	4·5 (1)
C(22)	−0·1132 (3)	0·2855 (2)	0·2752 (2)	4·3 (1)
C(23)	−0·0118 (3)	0·3059 (2)	0·2532 (2)	4·0 (1)
C(24)	0·0685 (3)	0·2672 (1)	0·2314 (2)	3·33 (8)
C(25)	0·1020 (4)	0·2132 (2)	−0·0205 (2)	5·9 (1)

such hydrogen bond because of the anti-bonding conformations of these groups. For all isomers, the molecules are held together by van der Waals forces.

The asymmetric four C atoms in the pyrrole rings cause the three configurational isomers (*A*), (*B*) and (*C*) as shown in (I). Isomer (*A*) has a *trans* juncture at C(7)—C(8). The configuration causes great steric

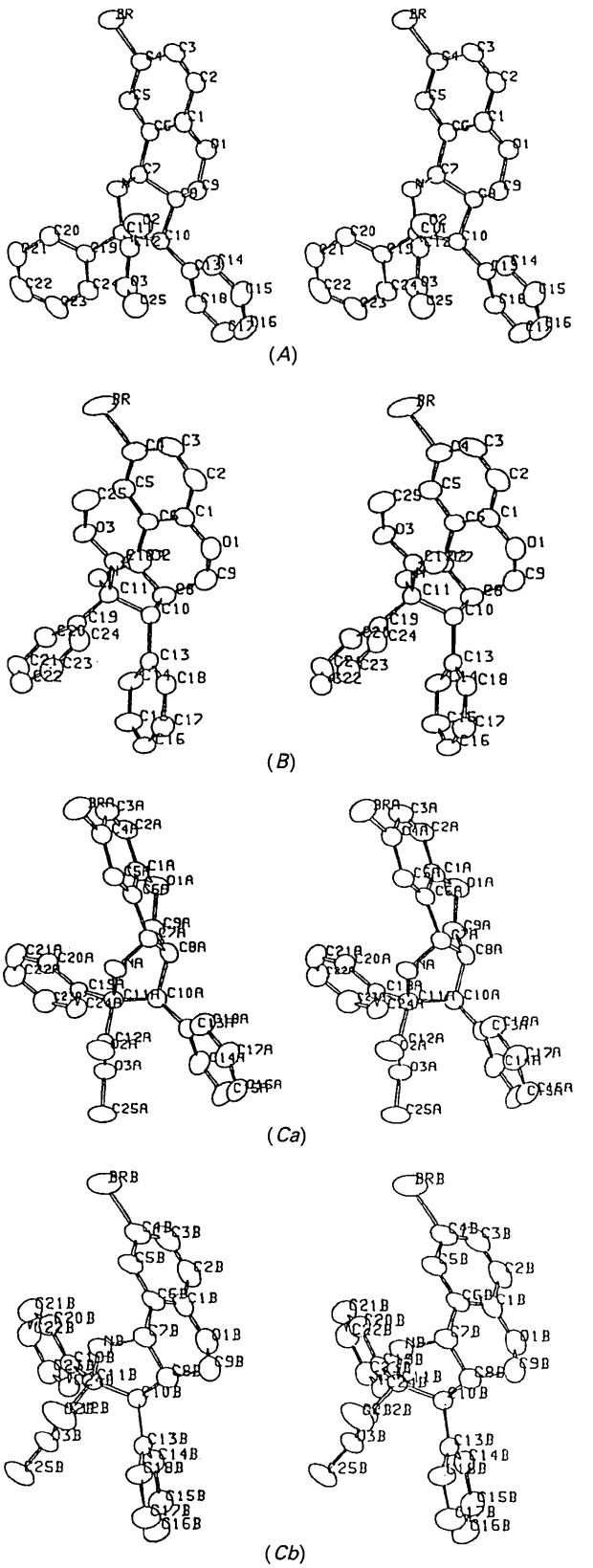

Fig. 1. Stereoviews of the three stereoisomers.

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

			(C)	
	(*A*)	(*B*)	(*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 (3)	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.

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

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

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