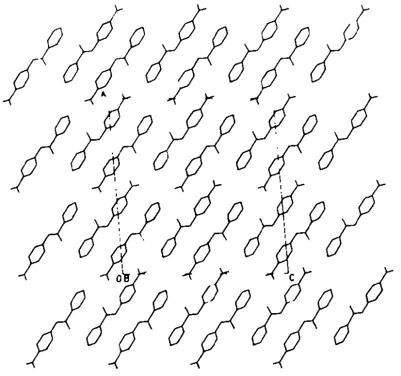

Fig. 2. Projection of the structure down **b**.

indicating that C(sp^2) has a stronger resistance against out-of-plane bending than the N^1 atom. The value of τ shows that the twist around C(1)—N(1) is minimal. As a result of molecular overcrowding, the *p*-nitrophenyl and phenyl rings are twisted from the amidine plane by 78·9 (4) and 21·2 (4)°, respectively, showing lack of conjugation. The nitro group is twisted by 4·8 (4)° relative to the C(2)—C(7) ring.

Molecular packing is shown in Fig. 2. The shortest intermolecular contact is O(2)···H(15)($-x$, $-y$, $-z$) 2·43 (4) Å. Molecules linked by these contacts are situated around a symmetry centre forming 'dimers', but the O···H distance is rather long for a hydrogen bond.

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Conformational Study of Optically Active Oxaziridines. Structures of (I) *N*-Isopropyl-, (II) *N-tert*-Butyl- and (III) *N*-Methylsulfonyldiphenyloxaziridine

By Gabriele Bocelli, Paolo Sgarabotto* and Franco Ugozzoli

Istituto di Strutturistica Chimica, Università degli Studi di Parma, Centro di Studio per la Strutturistica Diffrattometrica del CNR, Viale delle Scienze, I-43100 Parma, Italy

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Abstract. (I) $C_{16}H_{17}NO$, $M_r = 239{\cdot}3$, orthorhombic, $P2_12_12_1$, $a = 14{\cdot}330\,(4)$, $b = 10{\cdot}502\,(3)$, $c = 9{\cdot}251\,(2)$ Å, $V = 1392{\cdot}2\,(6)$ Å^3, $Z = 4$, $D_x = 1{\cdot}14$ g cm^{-3}, $\lambda(\text{Cu } K\alpha) = 1{\cdot}5418$ Å, $\mu = 5{\cdot}2$ cm^{-1}, $F(000) = 512$, $T = 293$ K, final conventional R 0·041 for 1259 symmetry-independent observed reflections. (II) $C_{17}H_{19}NO$, $M_r = 253{\cdot}3$, orthorhombic, $P2_12_12_1$, $a = 14{\cdot}110\,(4)$, $b = 10{\cdot}805\,(3)$, $c = 9{\cdot}498\,(2)$ Å, $V = 1448{\cdot}1\,(7)$ Å^3, $Z = 4$, $D_x = 1{\cdot}16$ g cm^{-3}, $\lambda(\text{Cu } K\alpha) = 1{\cdot}5418$, $\mu = 5{\cdot}3$ cm^{-1}, $F(000) = 544$, $T = 293$ K, final conventional R 0·035 for 1492 symmetry-independent observed reflections. (III) $C_{14}H_{13}NO_3S$, $M_r = 275{\cdot}3$, monoclinic, $P2_1/c$, $a = 5{\cdot}591\,(2)$, $b = 18{\cdot}704\,(6)$, $c = 12{\cdot}585\,(4)$ Å, $\beta = 100{\cdot}2\,(1)°$, $V = 1295{\cdot}3\,(9)$ Å^3, $Z = 4$, $D_x = 1{\cdot}41$ g cm^{-3}, $\lambda(\text{Cu } K\alpha) = 1{\cdot}5418$ Å, $\mu = 22{\cdot}1$ cm^{-1}, $F(000) = 576$, $T = 293$ K, final conventional R 0·046 for 1326 symmetry-independent observed reflections. The conformational geometry of the diphenyloxaziridine moiety is similar for the three compounds and seems not to be influenced by substituents at N. A small but significant shortening of the N—O distance in the oxaziridine ring is observed

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* To whom all correspondence should be addressed.

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associated with the presence, in compound (III), of the $-SO_2-$ group substituent at the N and interpreted in terms of lone-pair–*d*-orbital interactions.

Introduction. Structural studies of etherocyclic systems containing a stable chiral N atom are of fundamental importance to clarify some aspects of the correlations between chirooptical properties and chemical and pharmacological activities. Previous studies (Bucciarelli, Moretti, Torre, Andreetti, Bocelli & Sgarabotto, 1976; Forni, Garuti, Moretti, Torre, Andreetti, Bocelli & Sgarabotto, 1978) undertaken in this laboratory concerned the assignment of the absolute configuration of optically active oxaziridines containing a stable chiral N atom. In order to correlate the chirooptical properties with the conformation of the substituents at the asymmetric N we have determined the crystal and molecular structure of *N*-isopropyldiphenyloxaziridine (I), *N-tert*-butyldiphenyloxaziridine (II) and *N*-methylsulfonyldiphenyloxaziridine (III).

Experimental. Crystals of compounds (I) and (II) colourless prisms elongated on [001], of compound (III) yellow prisms elongated on [100]. The specimen dimensions 0·19 × 0·14 × 0·38; 0·20 × 0·25 × 0·30; 0·50 × 0·27 × 0·31 mm respectively. Siemens AED diffractometer on line to a General Automation Jumbo 220 microcomputer, Ni-filtered Cu *Kα* radiation, θ–2θ scan, scan width from $(\theta - 0{\cdot}60)^\circ$ to $(\theta + 0{\cdot}60 + 0{\cdot}142\tan\theta)^\circ$; scan speed 3·0° min^{-1}. Cell dimensions based on 29 $(\theta,\chi,\varphi)_{hkl}$ measured intensities. (I) 1538 ($0 \le h \le 17$, $0 \le k \le 12$, $0 \le l \le 11$); (II) 1615 ($0 \le h \le 17$, $0 \le k \le 13$, $0 \le l \le 11$); (III) 2819 ($0 \le h \le 6$, $0 \le k \le 22$, $-15 \le l \le 15$) symmetry-independent reflections ($3 \le \theta \le 70^\circ$) collected at $T = 293$ K with a modified version (Belletti, Ugozzoli, Cantoni & Pasquinelli, 1979) of the Lehmann & Larsen (1974) procedure. One standard reflection every 50, no significant variation. Corrections for Lorentz and polarization, no correction for absorption effects. Structures solved by direct methods (*SHELX*76; Sheldrick, 1976). (I) 1259, (II) 1492, (III) 1326 symmetry-independent observed reflections $[I > 2\sigma(I)]$, in full-matrix least-squares refinement; (I) 231, (II) 248, (III) 224 parameters; all H atoms located in the difference-Fourier map refined isotropically. $\sum w(F_o - F_c)^2$ minimized with $w = [\sigma^2(F_o) + 0{\cdot}005F_o^2]^{-1}$; *SHELX*76 system (Sheldrick, 1976); maximum shift of parameters 0·8σ for S, 0·6 for O and N, 0·4 for C, 1·2 for H. $\Delta\rho_{\max}$ and $\Delta\rho_{\min}$ (I) 0·11, −0·14; (II) 0·12, −0·16; (III) 0·18, −0·32 e Å^{-3}. Final refinement converged to R and wR (I) 0·041, 0·047; (II) 0·036, 0·039; (III) 0·046, 0·047. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Table 1. *Fractional atomic coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (× 10^4 Å^2) *for non-hydrogen atoms with e.s.d.'s in parentheses*

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

	x	y	z	$U_{\rm eq}$
(I) *N*-Isopropyldiphenyloxaziridine				
O(1)	709 (1)	7136 (2)	4477 (2)	726 (6)
N(1)	1729 (2)	6958 (2)	4860 (3)	674 (7)
C(1)	1196 (1)	8063 (2)	5296 (3)	537 (6)
C(2)	924 (1)	8077 (2)	6881 (3)	539 (6)
C(3)	926 (2)	6944 (3)	7668 (3)	688 (8)
C(4)	624 (3)	6925 (4)	9094 (4)	862 (11)
C(5)	312 (3)	8020 (4)	9745 (3)	865 (11)
C(6)	308 (2)	9145 (4)	8983 (4)	816 (11)
C(7)	614 (2)	9174 (3)	7547 (3)	642 (8)
C(8)	1333 (2)	9325 (2)	4573 (3)	548 (7)
C(9)	2012 (2)	10156 (3)	5073 (3)	663 (8)
C(10)	2152 (2)	11317 (3)	4397 (4)	799 (10)
C(11)	1614 (3)	11662 (4)	3233 (4)	833 (11)
C(12)	928 (3)	10864 (4)	2740 (3)	825 (11)
C(13)	784 (2)	9688 (3)	3409 (3)	671 (8)
C(14)	2285 (2)	7048 (3)	3511 (4)	811 (10)
C(15)	3283 (3)	7261 (6)	3999 (6)	1058 (17)
C(16)	2154 (4)	5825 (5)	2677 (6)	1132 (20)
(II) *N-tert*-Butyldiphenyloxaziridine				
O(1)	5662 (1)	7064 (2)	4645 (2)	505 (7)
N(1)	6684 (2)	6880 (2)	5108 (3)	500 (8)
C(1)	6166 (2)	8023 (3)	5367 (3)	406 (8)
C(2)	5866 (2)	8153 (3)	6892 (3)	405 (8)
C(3)	5780 (2)	7101 (3)	7714 (3)	505 (10)
C(4)	5447 (3)	7186 (3)	9091 (4)	618 (12)
C(5)	5201 (3)	8313 (4)	9641 (4)	648 (13)
C(6)	5286 (3)	9365 (4)	8840 (4)	630 (13)
C(7)	5621 (3)	9288 (3)	7459 (3)	518 (12)
C(8)	6301 (2)	9202 (3)	4572 (3)	426 (9)
C(9)	7043 (2)	9991 (3)	4901 (3)	532 (10)
C(10)	7149 (3)	11096 (3)	4189 (4)	641 (14)
C(11)	6521 (3)	11422 (4)	3156 (4)	692 (14)
C(12)	5777 (3)	10656 (4)	2834 (4)	646 (13)
C(13)	5654 (3)	9541 (3)	3540 (3)	512 (10)
C(14)	7332 (2)	6656 (4)	3891 (4)	600 (12)
C(15)	8314 (3)	6887 (8)	4489 (7)	1007 (26)
C(16)	7191 (5)	5266 (5)	3590 (7)	965 (22)
C(17)	7182 (4)	7370 (5)	2536 (5)	821 (19)
(III) *N*-Methylsulfonyldiphenyloxaziridine				
S(1)	3578 (2)	8870 (1)	581 (1)	562 (4)
O(1)	2398 (4)	9662 (1)	2156 (2)	617 (11)
O(2)	5842 (5)	8791 (1)	230 (3)	702 (11)
O(3)	2590 (5)	8298 (1)	1098 (3)	726 (11)
N(1)	4003 (5)	9641 (2)	1324 (3)	528 (12)
C(1)	4967 (6)	9599 (2)	2480 (3)	517 (14)
C(2)	6215 (6)	10277 (2)	2906 (3)	498 (13)
C(3)	5143 (9)	10932 (2)	2620 (4)	631 (18)
C(4)	6303 (8)	11555 (2)	2970 (4)	690 (20)
C(5)	8532 (8)	11538 (2)	3612 (4)	681 (19)
C(6)	9600 (9)	10898 (2)	3906 (5)	692 (17)
C(7)	8448 (7)	10267 (2)	3568 (4)	603 (17)
C(8)	5865 (6)	8912 (2)	3018 (3)	526 (14)
C(9)	7863 (7)	8568 (2)	2776 (4)	573 (16)
C(10)	8679 (8)	7946 (2)	3316 (4)	642 (18)
C(11)	7523 (8)	7678 (2)	4087 (4)	668 (17)
C(12)	5555 (9)	8020 (2)	4344 (4)	658 (18)
C(13)	4708 (8)	8639 (2)	3821 (4)	589 (16)
C(18)	1402 (10)	9173 (3)	−479 (5)	646 (18)

Discussion. Final atomic coordinates and equivalent isotropic thermal parameters are given in Table 1.* The arbitrary numbering scheme used in the crystal analysis is shown in Figs. 1, 2 and 3, which represent perspective views of the *N*-isopropyl-, *N-tert*-butyl- and *N*-methyl-

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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 44743 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

sulfonyldiphenyloxaziridines, respectively. Bond distances and angles and selected torsion angles are reported in Table 2.

The bond lengths in the oxaziridine ring, considerably different from those expected from the hybridization of the atoms involved, are in agreement with those found in related compounds with highly strained three-membered rings previously studied. A comparison of the dimensions of all monophenyl *cis-* and *trans-* and diphenyl substituted oxaziridine rings

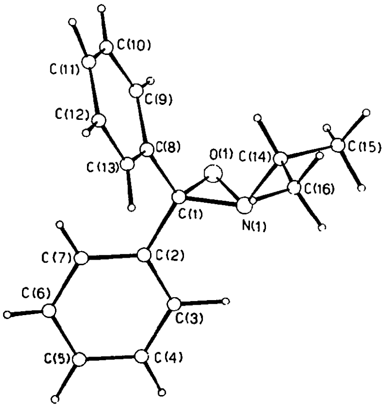

Fig. 1. Perspective view of *N*-isopropyldiphenyloxaziridine with the atomic numbering scheme.

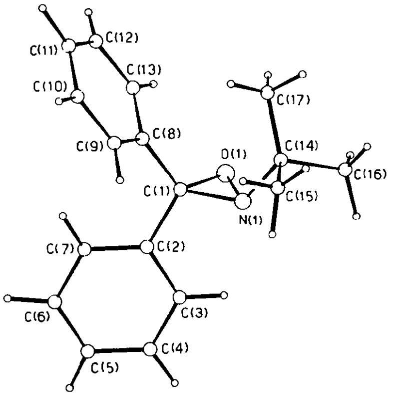

Fig. 2. Perspective view of *N-tert*-butyldiphenyloxaziridine with the atomic numbering scheme.

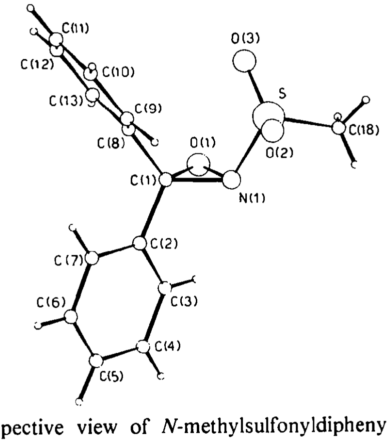

Fig. 3. Perspective view of *N*-methylsulfonyldiphenyloxaziridine with the atomic numbering scheme.

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

	(I)	(II)	(III)
O(1)–N(1)	1·516 (3)	1·521 (3)	1·495 (5)
O(1)–C(1)	1·417 (3)	1·432 (4)	1·427 (4)
N(1)–C(1)	1·447 (3)	1·456 (4)	1·461 (5)
N(1)–C(14)	1·484 (5)	1·494 (5)	
C(1)–C(2)	1·517 (4)	1·516 (4)	1·498 (5)
C(1)–C(8)	1·498 (3)	1·493 (5)	1·497 (5)
C(2)–C(3)	1·395 (4)	1·384 (4)	1·383 (5)
C(2)–C(7)	1·380 (4)	1·383 (5)	1·373 (5)
C(3)–C(4)	1·389 (5)	1·393 (5)	1·368 (6)
C(4)–C(5)	1·373 (6)	1·370 (5)	1·360 (6)
C(5)–C(6)	1·376 (6)	1·373 (6)	1·359 (6)
C(6)–C(7)	1·399 (5)	1·397 (5)	1·375 (6)
C(8)–C(9)	1·386 (4)	1·385 (4)	1·369 (6)
C(8)–C(13)	1·387 (4)	1·389 (5)	1·390 (6)
C(9)–C(10)	1·385 (5)	1·380 (5)	1·383 (6)
C(10)–C(11)	1·373 (5)	1·368 (6)	1·354 (7)
C(11)–C(12)	1·370 (6)	1·371 (6)	1·360 (7)
C(12)–C(13)	1·396 (5)	1·389 (5)	1·374 (6)
C(14)–C(15)	1·516 (5)	1·518 (6)	
C(14)–C(16)	1·510 (6)	1·542 (7)	
C(14)–C(17)		1·515 (6)	
S(1)–O(2)			1·420 (4)
S(1)–O(3)			1·414 (3)
S(1)–N(1)			1·712 (4)
S(1)–C(18)			1·734 (6)
N(1)–O(1)–C(1)	59·0 (1)	59·0 (1)	60·0 (2)
O(1)–N(1)–C(1)	57·1 (1)	57·4 (1)	57·7 (2)
O(1)–N(1)–C(14)	108·3 (2)	112·2 (2)	
C(1)–N(1)–C(14)	117·8 (2)	125·1 (2)	
O(1)–C(1)–N(1)	63·9 (1)	63·6 (1)	62·4 (2)
O(1)–C(1)–C(2)	113·4 (1)	112·7 (2)	114·4 (3)
O(1)–C(1)–C(8)	115·7 (2)	116·0 (2)	116·1 (3)
N(1)–C(1)–C(2)	114·4 (1)	112·4 (2)	112·1 (3)
N(1)–C(1)–C(8)	121·1 (1)	125·0 (2)	122·1 (3)
C(2)–C(1)–C(8)	117·2 (2)	116·1 (2)	117·8 (3)
C(1)–C(2)–C(3)	119·7 (2)	119·2 (2)	120·2 (3)
C(1)–C(2)–C(7)	121·5 (2)	121·6 (2)	121·4 (3)
C(3)–C(2)–C(7)	118·7 (2)	119·1 (2)	118·4 (3)
C(2)–C(3)–C(4)	120·5 (3)	120·3 (3)	120·8 (4)
C(3)–C(4)–C(5)	120·4 (3)	120·1 (3)	120·2 (3)
C(4)–C(5)–C(6)	119·7 (3)	120·2 (3)	119·6 (4)
C(5)–C(6)–C(7)	120·2 (3)	120·0 (3)	120·8 (4)
C(2)–C(7)–C(6)	120·4 (3)	120·2 (3)	120·1 (4)
C(1)–C(8)–C(9)	120·0 (2)	120·4 (2)	121·6 (3)
C(1)–C(8)–C(13)	121·0 (2)	119·9 (2)	118·8 (3)
C(9)–C(8)–C(13)	119·0 (2)	119·6 (2)	119·5 (3)
C(8)–C(9)–C(10)	120·3 (2)	120·2 (2)	119·8 (4)
C(9)–C(10)–C(11)	120·3 (3)	120·3 (3)	120·4 (4)
C(10)–C(11)–C(12)	120·2 (3)	120·0 (3)	120·4 (4)
C(11)–C(12)–C(13)	119·9 (3)	120·7 (3)	120·5 (4)
C(8)–C(13)–C(12)	120·2 (2)	119·2 (3)	119·5 (4)
N(1)–C(14)–C(15)	105·4 (3)	104·0 (3)	
N(1)–C(14)–C(16)	108·0 (3)	102·9 (3)	
N(1)–C(14)–C(17)		119·3 (3)	
C(15)–C(14)–C(16)	113·3 (3)	110·3 (4)	
C(15)–C(14)–C(17)		111·2 (3)	
C(16)–C(14)–C(17)			108·7 (4)
O(2)–S(1)–O(3)			120·4 (2)
O(2)–S(1)–N(1)			102·3 (2)
O(2)–S(1)–C(18)			109·7 (2)
O(3)–S(1)–N(1)			114·4 (2)
O(3)–S(1)–C(18)			108·9 (2)
N(1)–S(1)–C(18)			98·9 (2)
S(1)–N(1)–O(1)			111·2 (2)
S(1)–N(1)–C(1)			119·3 (2)
C(2)–C(1)–N(1)–C(14)	−160·1 (2)	−159·2 (3)	
C(8)–C(1)–N(1)–C(14)	−11·0 (4)	−8·8 (5)	
C(1)–N(1)–C(14)–C(15)	101·7 (3)	98·4 (4)	
C(1)–N(1)–C(14)–C(16)	−137·0 (3)	−146·5 (4)	
C(1)–N(1)–C(14)–C(17)		−26·2 (5)	
C(2)–C(1)–N(1)–S(1)			155·2 (3)
C(8)–C(1)–N(1)–S(1)			7·1 (5)
C(1)–N(1)–S(1)–O(2)			−90·6 (4)
C(1)–N(1)–S(1)–O(3)			41·4 (4)

reported in the literature is shown in Table 3. A small but significant shortening of the N—O distance is observed with the presence of the SO_2 group substituent at the N and interpreted in terms of lone-pair–*d*-orbital interactions. In this case, consequently, the other bond dimensions of the heterocyclic ring not being influenced, the endocyclic angle at the carbon also undergoes a small decrease.

The conformational geometry of the diphenyloxaziridine moiety is similar for the three compounds and seems not to be influenced by the substituents at the N. In fact the dihedral angle formed by the oxaziridine ring with the C(Ph)—C(1)—N(1) plane, when the C(Ph) is *trans*, is 74·8 (2)° in both (I) and (II), and 73·1 (4)° in (III). When the C(Ph) and the substituents at the N are *cis* with respect to the oxaziridine ring, these angles are 74·4 (2), 75·6 (2) and 75·1 (4)° in derivatives (I), (II), (III) respectively. This geometry is consistent with that reported in the literature for other oxaziridine derivatives (Kimura, Watson, Davis, Lamendola & Nadir, 1979; Chen, Watson, Davis, Lamendola & Nadir, 1978): a comparison can be made by the analysis of the C(Ph)—C—N—C(or S) torsion angle which ranges from 7·1 to 12·8° for *cis* and from 149·0 to 161·0° for *trans* conformations (see Table 3).

The orientation of the phenyl rings with respect to the oxaziridine ring can be described by the mutual dihedral angles they form. An analysis of the planarity is reported in Table 4. These reciprocal orientations correlate quite well with those observed in the other diphenyl derivatives previously studied: 55·0 and 59·2° are the dihedral angles of the mean plane of the benzene ring *cis* and 91·8 and 100·1° of that *trans* with respect to the oxaziridine plane, the dihedral angles between the phenyl rings in the (−) and (+) epimers being 114·1 and 105·8° respectively.

The dimensions of the isopropyl and of the *tert*-butyl moieties are consistent with those reported in the literature (Cannon, Daly, Silverton, Boyd & Jerina, 1972, and references therein). The orientations of these groups with respect to the oxaziridine ring, deduced from the torsion angles reported in Table 2, are quite similar. The position adopted by the SO_2 group with respect to the oxaziridine ring is comparable with that found in analogous derivatives in which the N lone pair lies opposite to the sulfonyl O atoms as shown by the values of the torsion angles C(1)—N(1)—S(1)—O(2) −90·6 and C(1)—N(1)—S(1)—O(3) 41·4° [−117 and 12° in 2-(*p*-toluenesulfonyl)-3-(*p*-chlorophenyl)oxaziridine (Kimura, Watson, Davis, Lamendola & Nadir, 1979); −101 and 27° in 2-(*p*-toluenesulfonyl)-3-(*m*-nitrophenyl)oxaziridine (Chen, Watson, Davis, Lamendola & Nadir, 1978)]. Molecular packings are consistent with van der Waals interactions.

We thank Professor G. Torre and coworkers who suggested this research and prepared the crystals.

Table 3. *Comparison of dimensions of the oxaziridine moiety*

Reference	C—N (Å)	C—O (Å)	N—O (Å)	$\hat{C}$ (°)	$\hat{N}$ (°)	$\hat{O}$ (°)
(I) **	1·447 (3)	1·417 (3)	1·516 (3)	63·9 (1)	57·1 (1)	59·0 (2)
(II) **	1·456 (4)	1·432 (4)	1·521 (3)	63·6 (2)	57·5 (2)	59·0 (2)
(III) **	1·461 (5)	1·427 (4)	1·495 (5)	62·4 (3)	57·7 (2)	60·0 (3)
(*a*) **	1·473 (3)	1·433 (4)	1·544 (3)	64·2 (2)	56·7 (2)	59·2 (2)
(*a*) **	1·464 (5)	1·419 (4)	1·519 (4)	63·6 (2)	56·8 (2)	59·7 (2)
(*b*) *	1·440 (12)	1·438 (11)	1·508 (10)	63·2 (5)	58·4 (5)	58·4 (5)
(*c*) *	1·434 (6)	1·405 (5)	1·500 (6)	63·8 (3)	57·2 (3)	59·0 (2)
(*d*) *	1·450	1·415	1·494	62·8	57·5	59·7
(*e*) *	1·443 (6)	1·414 (5)	1·487 (6)	62·7 (3)	57·7 (3)	59·6 (3)

(*a*) Forni, Garuti, Moretti, Torre, Andreetti, Bocelli & Sgarabotto (1978); (*b*) Jerslev (1967); (*c*) Cannon, Daly, Silverton, Boyd & Jerina (1972); (*d*) Kimura, Watson, Davis, Lamendola & Nadir (1979); (*e*) Chen, Watson, Davis, Lamendola & Nadir (1978).

* Monophenyl derivatives.

** Diphenyl derivatives.

Table 4. *Distances* (Å × 10^3) *of relevant atoms from the mean plane with e.s.d.'s in parentheses, and angles* (°) *between planes*

	(I)	(II)	(III)
Plane *A*: O(1), N(1), C(1)			
Plane *B*: C(2)—C(7)			
C(2)	0 (2)	2 (3)	6 (4)
C(3)	1 (3)	−1 (3)	−5 (5)
C(4)	−4 (4)	−1 (4)	−3 (5)
C(5)	3 (4)	2 (4)	3 (5)
C(6)	0 (3)	0 (4)	−4 (6)
C(7)	−1 (3)	−2 (4)	−9 (5)
Plane *C*: C(8)—C(13)			
C(8)	7 (3)	9 (3)	6 (4)
C(9)	−6 (3)	0 (4)	−5 (5)
C(10)	0 (3)	0 (4)	−2 (5)
C(11)	8 (4)	7 (4)	5 (5)
C(12)	−4 (4)	−2 (4)	−1 (5)
C(13)	−4 (3)	−7 (4)	−6 (5)
A–*B*	94·2	93·1	91·5
A–*C*	59·9	52·2	53·1
B–*C*	109·8	104·6	105·4

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