2·98, and C(3*)···C(5*) 3·09 Å. These intermolecular contacts are only little affected by variations of the three Euler angles (≤ 5°) with a fixed position of *B* in the unit cell. Therefore we assume that only by conformational variation can an optimal packing be achieved. Fig. 2 shows the packing arrangement in the unit cell. The central segments of both conformations are nearly parallel to each other and approximately related by a 180° rotation about [001] followed by a $\frac{1}{2}$, $\frac{1}{2}$, 0 translation.

This work was supported by the Deutsche Forschungsgemeinschaft.

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Structures of *N*,*N*′-Dimethyl-2,2′-dithiodibenzamide and 2-(Benzylsulfinyl)-*N*-methylbenzamide. Intramolecular Nonbonding S···O Interaction

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(*Received* 16 *December* 1988; *accepted* 29 *March* 1989)

Abstract. $C_{16}H_{16}N_2O_2S_2$ (I), $M_r = 332{\cdot}45$, monoclinic, $C2/c$, $a = 18{\cdot}680\ (4)$, $b = 4{\cdot}9246\ (7)$, $c = 18{\cdot}733\ (5)$ Å, $\beta = 112{\cdot}43\ (2)°$, $V = 1593{\cdot}0\ (6)$ Å^3, $Z = 4$, $D_x = 1{\cdot}386$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}327$ mm^{-1}, $F(000) = 696$, $T = 293$ K, $R = 0{\cdot}036$ for 1625 observed reflections. $C_{15}H_{15}NO_2S$ (II), orthorhombic, $Pcab$, $a = 16{\cdot}148\ (3)$, $b = 12{\cdot}428\ (2)$, $c = 14{\cdot}233\ (2)$ Å, $V = 2857{\cdot}5\ (7)$ Å^3, $Z = 8$, $D_x = 1{\cdot}271$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}213$ mm^{-1}, $F(000) = 1152$, $T = 293$ K, $R = 0{\cdot}055$ for 2292 observed reflections. Molecule (I) with a crystallographic twofold axis shows short intramolecular S···O contacts of 2·896 (1) Å. The molecules form ribbon-like intermolecular hydrogen bonds between amide groups. The N···O distance is 2·818 (2) Å. For molecule (II) the intramolecular S···O distance is 2·717 (3) Å. The molecules are linked by the hydrogen bonds between the sulfinyl oxygen and the N—H of the amide group, forming a zigzag chain. The N···O length is 2·851 (4) Å.

Introduction. It is well known that some S atoms in compounds such as σ-sulfuranes and thiathiophthenes show hypervalency (Musher, 1969). The characteristic features of the hypervalent bonds in these compounds are as follows:

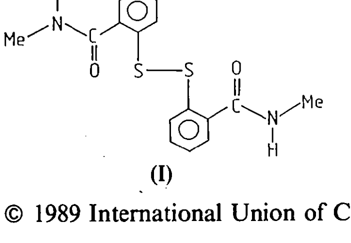
(1) A tetravalent or divalent S atom forms an *X*···S···*Y* bond system with electronegative groups *X* and *Y*, where *X* = *Y* or not.

(2) These S···*X* and S···*Y* bonds are longer than usual S—*X* and S—*Y* single-bond distances, respectively, but they are much shorter than the sum of the van der Waals radii.

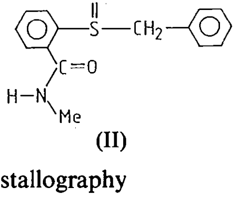
(3) These bonds correspond to Pauling's bond order 0·5 and are more liable to changes in bond length if the molecule is perturbed to some degree.

(4) The *X*···S···*Y* arrangement is almost linear.

Besides such typical hypervalent bonds, S···O, S···N or S···halogen nonbonding intramolecular contacts are often observed in some organic sulfur compounds (Iwasaki & Akiba, 1985; Iwasaki, 1986; Iwasaki & Masuko, 1986). For the title compounds the electron-attracting benzamide group is expected to have a short intramolecular contact with the S atom. We determined the crystal structures of these two compounds in order to study hypervalency of the S atoms.



(I)



(II)

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Experimental. Details of data collection and structure refinement are shown in Table 1. Intensity data were collected using a Rigaku AFC-4 diffractometer with graphite monochromator. Structures were solved by the program *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). H atoms were found from the difference maps. Block-diagonal least squares with anisotropic temperature factors for non-H atoms and isotropic ones for H. $\sum w(|F_c| - k^{-1}|F_o|)^2$ was minimized, $w = 1/(1{\cdot}858 - 0{\cdot}1308|F_o| + 0{\cdot}0026|F_o|^2)$ for (I), $w = 1/(1{\cdot}550 - 0{\cdot}0104|F_o| + 0{\cdot}0004|F_o|^2)$ for (II). Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). All computations were performed on a HITAC M260 computer of the Data Processing Center with the programs *UNICS*III (Sakurai & Kobayashi, 1979), *MULTAN*78 and *ORTEP*II (Johnson, 1976). The final atomic parameters are given in Table 2.*

Table 1. *Details of data collection and structure refinement*

	(I)	(II)
Color	Colorless	Colorless
Crystal shape	Needles	Plates
Crystal size (mm)	0·40 × 0·65 × 0·50	0·30 × 0·35 × 0·60
2θ range (°) and No. of reflections for cell parameters	30–35, 25	29·5–35, 25
Scan range, 2θ (°)	2–55	2–55
Scan width, $\Delta\omega$ (°)	$1{\cdot}5 + 0{\cdot}4\tan\theta$	$1{\cdot}3 + 0{\cdot}3\tan\theta$
Scan speed, 2θ (° min^{-1})	4	4
Scan mode	2θ–ω	2θ–ω
Monitored refections (every 50 reflections)	10,0,2, $80\bar{8}$, 420	801, 540, 207
Variation of intensities	1·014–0·989	1·030–0·944
Ranges of h, k, l	0–24, 0–6, −24–24	0–21, 0–16, 0–18
Time for background (s)	10	10
No. of reflections:		
measured	2015	3542
unique	1836	3335
observed [$\lvert F_o\rvert > 3\sigma(F)$]	1625	2292
R	0·035	0·054
wR	0·034	0·062
$\Delta\rho_{\max}$ (e Å^{-3})	0·227	0·316
$(\Delta/\sigma)_{\max}$	0·187 (C8, y)	0·417 (C15, y)
S	1·044	1·084

Table 2. *Positional parameters and equivalent isotropic temperature factors* (Å^2) *for non*-H *atoms*

$$B_{\rm eq} = \tfrac{4}{3}\textstyle\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
(*a*) *N*,*N*′-Dimethyl-2,2′-dithiodibenzamide (× 10^5)				
S(1)	3044 (2)	10863 (8)	30830 (2)	3·12 (1)
O(1)	10488 (7)	6129 (20)	47458 (6)	3·62 (3)
N(1)	10614 (8)	−37864 (25)	50598 (7)	3·13 (4)
C(1)	10385 (8)	−14450 (28)	32398 (8)	2·63 (4)
C(2)	13873 (7)	−26125 (27)	39773 (7)	2·46 (4)
C(3)	19718 (8)	−45236 (31)	41122 (8)	3·03 (4)
C(4)	22155 (9)	−53024 (36)	35320 (10)	3·69 (5)
C(5)	18671 (10)	−41735 (38)	28083 (10)	3·96 (5)
C(6)	12853 (10)	−22715 (37)	26593 (9)	3·60 (5)
C(7)	11491 (8)	−17854 (26)	46265 (8)	2·49 (3)
C(8)	8474 (11)	−32768 (38)	57162 (10)	4·02 (5)
(*b*) 2-(Benzylsulfinyl)-*N*-methylbenzamide (× 10^4, for S × 10^5)				
S(1)	36999 (5)	5555 (6)	5895 (5)	2·99 (2)
O(1)	3540 (1)	736 (2)	1619 (1)	4·10 (6)
O(2)	3890 (1)	109 (2)	−1267 (2)	3·91 (6)
N(1)	2869 (2)	57 (3)	−2330 (2)	4·43 (8)
C(1)	2909 (2)	1336 (2)	−7 (2)	2·78 (6)
C(2)	2718 (2)	1197 (2)	−958 (2)	2·78 (7)
C(3)	2075 (5)	1812 (3)	−1340 (2)	3·65 (8)
C(4)	1643 (2)	2534 (3)	−789 (3)	4·25 (9)
C(5)	1833 (2)	2656 (3)	146 (3)	4·43 (9)
C(6)	2459 (2)	2044 (3)	546 (2)	3·65 (8)
C(7)	3205 (2)	413 (2)	−1538 (2)	3·02 (7)
C(8)	3311 (3)	−673 (4)	−2945 (3)	6·04 (13)
C(9)	4608 (2)	1405 (3)	333 (2)	3·31 (8)
C(11)	4550 (2)	2495 (3)	749·(2)	3·27 (7)
C(12)	4770 (2)	2689 (4)	1673 (3)	5·13 (11)
C(13)	4694 (3)	3736 (4)	2048 (3)	6·69 (15)
C(14)	4403 (3)	4550 (4)	1505 (4)	6·57 (14)
C(15)	4190 (3)	4384 (4)	601 (4)	6·10 (13)
C(16)	4262 (2)	3364 (3)	225 (3)	4·61 (10)

Discussion. The molecular structures with the atomic numbering are shown in Fig. 1. Bond distances and angles are listed in Table 3.

Structure of (I). The molecule has a twofold symmetry coincident with the crystallographic twofold axis perpendicular to the *ac* plane. The S(1)—S(1$^{\rm i}$) bond length (i = $-x$, y, $\frac{1}{2}-z$) of 2·042 (1) Å and the C(1)—S(1)—S(1$^{\rm i}$)—C(1$^{\rm i}$) torsion angle of 88·04 (7)° are normal in disulfides. The intramolecular S···O length is 2·896 (1) Å; this is longer than the expected value (2·4–2·7 Å), but still shorter than the van der Waals contact (3·35 Å). The O(1)···S(1)—S(1$^{\rm i}$) angle is 173·52 (4)°. Such a linear O···S—S arrangement with a short S···O distance is a characteristic feature of the hypervalent sulfur compounds. This S···O interaction is so weak that the S(1)—C(1) and S(1)—S(1$^{\rm i}$) bonds are not affected. Intramolecular interactions of a linear O···S—S···O type have been reported in 3,5-diacetamido-1,2-dithiolium bromide (Hordvik & Kjoge, 1966), bis(*o*-nitrophenyl) disulfide (Ricci & Bernal, 1970) and dimethyl 2,2′-dithiodibenzoate (Kucsman, Kapovits, Párkányi, Argay & Kálmán, 1984). The S···O distances of these compounds are 2·52–2·69 Å. The dihedral angle between the phenyl ring and the plane defined by the four atoms of the amide group is 44·3 (1)°.

Fig. 2 shows the crystal structure viewed along the *a* axis. The molecules form a long ribbon along the *b* axis *via* intermolecular hydrogen bonds between amide groups. The O(1)···N(1$^{\rm ii}$) (ii = x, $y+1$, z) distance is 2·818 (2) Å. The O atom is shared between the intramolecular S···O interaction and the N—H···O hydrogen bonding. Dimensions of hypervalent intramolecular contacts and intermolecular hydrogen bonds are summarized in Table 4.

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* Lists of structure factors, anisotropic temperature factors for non-H atoms and atomic parameters for H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52091 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 3. *Bond distances* (Å) *and angles* (°)

(*a*) *N*,*N*′-Dimethyl-2,2′-dithiodibenzamide

S(1)—S(1$^{\text{i}}$)	2·042 (1)	C(1)—C(6)	1·394 (2)
S(1)—C(1)	1·792 (2)	C(2)—C(3)	1·390 (2)
O(1)—C(7)	1·230 (2)	C(2)—C(7)	1·502 (2)
N(1)—C(7)	1·326 (2)	C(3)—C(4)	1·383 (2)
N(1)—C(8)	1·452 (2)	C(4)—C(5)	1·377 (3)
C(1)—C(2)	1·406 (2)	C(5)—C(6)	1·380 (3)
S(1$^{\text{i}}$)—S(1)—C(1)	104·74 (5)	C(2)—C(3)—C(4)	121·1 (1)
C(7)—N(1)—C(8)	121·9 (1)	C(3)—C(4)—C(5)	119·2 (2)
S(1)—C(1)—C(2)	119·0 (1)	C(4)—C(5)—C(6)	120·9 (2)
S(1)—C(1)—C(6)	122·4 (1)	C(1)—C(6)—C(5)	120·6 (2)
C(2)—C(1)—C(6)	118·7 (1)	O(1)—C(7)—N(1)	122·7 (1)
C(1)—C(2)—C(3)	119·5 (1)	O(1)—C(7)—C(2)	121·4 (1)
C(1)—C(2)—C(7)	121·0 (1)	N(1)—C(7)—C(2)	116·0 (1)
C(3)—C(2)—C(7)	119·4 (1)		

Symmetry code: (i) $-x, y, \frac{1}{2}-z$.

(*b*) 2-(Benzylsulfinyl)-*N*-methylbenzamide

S(1)—O(1)	1·504 (3)	C(3)—C(4)	1·381 (5)
S(1)—C(1)	1·814 (3)	C(4)—C(5)	1·374 (6)
S(1)—C(9)	1·843 (3)	C(5)—C(6)	1·387 (5)
O(2)—C(7)	1·232 (4)	C(9)—C(11)	1·481 (5)
N(1)—C(7)	1·327 (5)	C(11)—C(12)	1·384 (6)
N(1)—C(8)	1·450 (6)	C(11)—C(16)	1·392 (5)
C(1)—C(2)	1·398 (4)	C(12)—C(13)	1·411 (7)
C(1)—C(6)	1·387 (4)	C(13)—C(14)	1·357 (7)
C(2)—C(3)	1·399 (4)	C(14)—C(15)	1·348 (7)
C(2)—C(7)	1·499 (4)	C(15)—C(16)	1·380 (7)
O(1)—S(1)—C(1)	104·8 (1)	C(1)—C(6)—C(5)	119·9 (3)
O(1)—S(1)—C(9)	104·1 (1)	O(2)—C(7)—N(1)	122·1 (3)
C(1)—S(1)—C(9)	99·3 (1)	O(2)—C(7)—C(2)	119·9 (3)
C(7)—N(1)—C(8)	121·4 (3)	N(1)—C(7)—C(2)	118·1 (3)
S(1)—C(1)—C(2)	122·8 (2)	S(1)—C(9)—C(11)	113·3 (2)
S(1)—C(1)—C(6)	116·3 (2)	C(9)—C(11)—C(12)	121·5 (3)
C(2)—C(1)—C(6)	120·8 (3)	C(9)—C(11)—C(16)	121·1 (3)
C(1)—C(2)—C(3)	118·2 (3)	C(12)—C(11)—C(16)	117·4 (3)
C(1)—C(2)—C(7)	119·8 (3)	C(11)—C(12)—C(13)	119·8 (4)
C(3)—C(2)—C(7)	122·0 (3)	C(12)—C(13)—C(14)	120·2 (5)
C(2)—C(3)—C(4)	120·6 (3)	C(13)—C(14)—C(15)	121·2 (5)
C(3)—C(4)—C(5)	120·6 (4)	C(14)—C(15)—C(16)	119·3 (5)
C(4)—C(5)—C(6)	119·9 (4)	C(11)—C(16)—C(15)	122·2 (4)

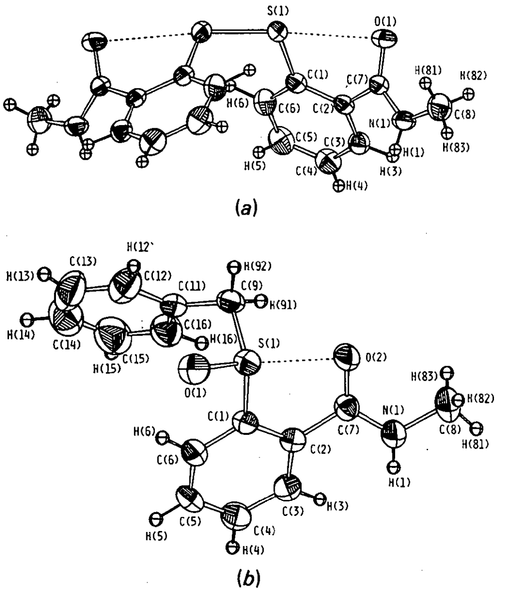

Fig. 1. The molecular structures with atomic numbering. The thermal ellipsoids for non-H atoms are drawn at 50% probability. (*a*) (I), (*b*) (II).

Table 4. *Dimensions* (Å *and* °) *of* S···O *intramolecular contacts and intermolecular hydrogen bonds.*

(I)		(II)	
S(1)···O(1)	2·896 (1)	S(1)···O(2)	2·717 (3)
S(1$^{\text{i}}$)—S(1)···O(1)	173·52 (4)	O(1)—S(1)···O(2)	175·4 (1)
C(1)—S(1)···O(1)	75·19 (6)	C(1)—S(1)···O(2)	74·6 (1)
C(7)—O(1)···S(1)	85·74 (9)	C(7)—O(2)···S(1)	98·1 (2)
O(1)···N(1$^{\text{ii}}$)	2·818 (2)	O(1)···N(1$^{\text{i}}$)	2·851 (4)
O(1)···H(1$^{\text{ii}}$)	2·03 (2)	O(1)···H(1$^{\text{i}}$)	2·04 (4)
O(1)···H(1$^{\text{ii}}$)—N(1$^{\text{ii}}$)	163 (2)	O(1)···H(1$^{\text{i}}$)—N(1$^{\text{i}}$)	161 (4)
C(7)—O(1)···H(1$^{\text{ii}}$)	167·7 (6)	S(1)—O(1)···H(1$^{\text{i}}$)	132 (1)
C(7)—O(1)···N(1$^{\text{ii}}$)	171·2 (1)	S(1)—O(1)···N(1$^{\text{i}}$)	127·2 (2)

Symmetry codes. For (I): (i) $-x, y, \frac{1}{2}-z$; (ii) $x, 1+y, z$. For (II): (i) $\frac{1}{2}-x, y, \frac{1}{2}+z$.

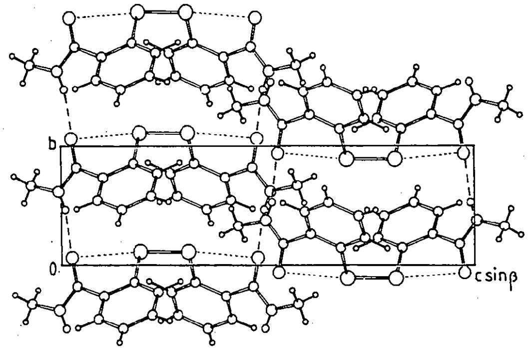

Fig. 2. The projection of the crystal structure of (I) viewed along the *a* axis. The molecules with the symmetry operation involving $x+\frac{1}{2}$ are omitted. Broken lines show the hydrogen bonding and dotted lines show the intramolecular S···O interactions.

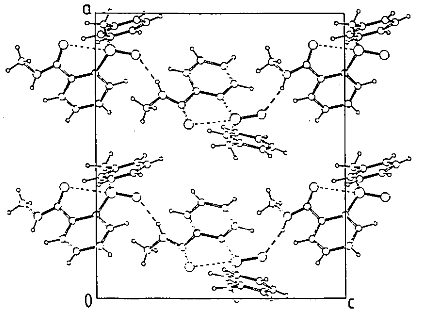

Fig. 3. The projection of the crystal structure of (II) viewed along the *b* axis within the range from $y = 0{\cdot}0$ to $0{\cdot}5$. Broken lines show the hydrogen bonding and dotted lines show intramolecular S···O interactions.

Structure of (II). The bond distances and angles of the sulfinyl group show normal values. The dihedral angle between the two phenyl groups is 145·8 (1)°. The dimensions of the amide groups for both (I) and

(II) are close to those of benzamide (Blake & Small, 1972). A short intramolecular S···O contact was also observed between S(1) and O(2) of the amide group. The S(1)···O(2) distance is 2·717 Å, which is shorter than the corresponding value of (I). In this case, O(2), S(1) and O(1) are also arranged linearly. The dihedral angle between the phenyl group, C(1)–C(6), and the amide plane is 20·0 (1)°.

Molecules are linked by the hydrogen bonds between O(1) of the sulfoxide and the N—H of the amide group at (i) = $\frac{1}{2}-x$, y, $\frac{1}{2}+z$, forming a zigzag chain along the c axis as shown in Fig. 3. The O(1)···N(1^{i}) distance is 2·851 Å and the O atom of the amide group is not bifurcated.

We thank Professor Sigeru Oae from the Okayama Science University for supplying the samples. This work was supported in part by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture.

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Structures of 5-Bromo-6-ethoxy-5,6-dihydrouridine and -thymidine Derivatives, a Class of Potential Antitumoral and Antiviral *N*-Nucleosides

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(*Received* 6 *December* 1988; *accepted* 29 *March* 1989)

Abstract. (I): (+)-(5*R*,6*R*)-5-Bromo-6-ethoxy-5,6-dihydro-2′,3′-isopropylidene-β-D-ribofuranosyluracil, $C_{14}H_{21}BrN_2O_7$, m.p. 408·7–409·6 K, $[\alpha]_D^{23\,^\circ C} = +31·1^\circ$ (c = 1·2% in MeOH), $M_r = 409·2$, monoclinic, $P2_1$, $a = 9·218\,(2)$, $b = 9·6619\,(11)$, $c = 10·4938\,(14)$ Å, $\beta = 99·305\,(8)^\circ$, $V = 922·4\,(2)$ Å^3, $Z = 2$, $D_x = 1·47$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 2·24$ mm^{-1}, $F(000) = 420$, room temperature, R (= wR) = 0·046 for 2595 observed reflections [$|F_o| > 4\sigma(F_o)$ and $|F_o| > 8·0$]. (II): (+)-(5*R*,6*R*)-5-Bromo-2′-deoxy-6-ethoxy-5,6-dihydro-β-D-ribofuranosylthymine, $C_{12}H_{19}BrN_2O_6$, m.p. 376·1–376·5 K, $[\alpha]_D^{23\,^\circ C} = +58·8^\circ$ (c = 1·02% in MeOH), $M_r = 367·2$, monoclinic, $P2_1$, $a = 6·0428\,(9)$, $b = 8·5270\,(15)$, $c = 14·589\,(2)$ Å, $\beta = 96·80\,(1)^\circ$, $V = 746·4\,(1)$ Å^3, $Z = 2$, $D_x = 1·63$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 2·75$ mm^{-1}, $F(000) = 376$, room temperature, $R = 0·053$ ($wR = 0·040$) for 1579 observed reflections [$|F_o| > 4\sigma(F_o)$]. Both furanose rings adopt an envelope conformation with C(4′)-*exo* and C(1′)-*exo* for (I) and (II) respectively. The orientation of the dihydropyrimidine base relative to the sugar ring shows an unusual *syn* conformation [$\chi_{CN} = 62·5\,(6)^\circ$] for (I) whereas the glycosyl linkage of compound (II) shows an *anti* conformation [$\chi_{CN} = -134·0\,(8)^\circ$]. In both compounds the pyrimidine ring displays a half-chair form. The conformation of the hydroxymethyl group at C(4′) is *gauche–gauche* for (I) [$\varphi_{OO} = -68·2\,(7)^\circ$, $\varphi_{OC} = 50·1\,(8)^\circ$] and *trans–gauche* for (II) [$\varphi_{OO} = 180\,(1)^\circ$, $\varphi_{OC} = -61\,(1)^\circ$]. The absolute configuration of (I) was confirmed by least-squares refinement of x [$x = 0·008\,(16)$] [Bernardinelli & Flack (1985). *Acta Cryst.* **A41**, 500–511] and that of compound (II) deduced from the starting material.

0108-2701/89/121917-05$03.00