Table 2. *Bond lengths* (Å) *and angles* (°)

C(2)–N(1)	1·377 (2)	C(5)–N(1)	1·379 (2)
C(3)–C(2)	1·524 (2)	O(2)–C(2)	1·210 (2)
C(4)–C(3)	1·536 (2)	C(31)–C(3)	1·533 (2)
C(5)–C(4)	1·510 (2)	C(41)–C(4)	1·525 (3)
O(5)–C(5)	1·217 (2)	C(32)–C(31)	1·514 (3)
O(33)–C(31)	1·434 (2)	C(34)–O(33)	1·426 (2)

C(5)–N(1)–C(2)	113·8 (1)	C(3)–C(2)–N(1)	107·9 (1)
O(2)–C(2)–N(1)	123·8 (2)	O(2)–C(2)–C(3)	128·3 (2)
C(4)–C(3)–C(2)	104·6 (1)	C(31)–C(3)–C(2)	110·4 (1)
C(31)–C(3)–C(4)	113·7 (1)	C(5)–C(4)–C(3)	104·5 (1)
C(41)–C(4)–C(3)	114·3 (2)	C(41)–C(4)–C(5)	109·7 (1)
C(4)–C(5)–N(1)	108·4 (1)	O(5)–C(5)–N(1)	124·3 (1)
O(5)–C(5)–C(4)	127·3 (1)	C(32)–C(31)–C(3)	114·0 (2)
O(33)–C(31)–C(3)	104·5 (1)	O(33)–C(31)–C(32)	112·9 (2)
C(34)–O(33)–C(31)	115·0 (2)		

parameters were refined freely with individual isotropic temperature factors. The terminal value of R_w was 0·050 with $R = 0·050$.* Weights were given by $w = k[\sigma^2(F_o) + g(F_o^2)]^{-1}$, where g refined to 0·000380. Complex neutral-atom scattering factors were employed (Cromer & Waber, 1965; Cromer & Liberman, 1970). Table 1 lists the final non-hydrogen atom coordinates, Table 2 the bond lengths and angles. Calculations were carried out with *SHELX* (Sheldrick, 1976) and local programs. Fig. 1 was drawn with *RSPLOT* (W. S. Sheldrick).

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* Lists of structure factors, anisotropic thermal parameters and H atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35609 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. Molecules of (1*b*) build centrosymmetric dimers through N(1)–H···O(5) hydrogen bonds of length 2·88 (1) Å. N(1), C(2), C(3) and C(4) are coplanar: distances from the least-squares plane are N(1) 0·002, C(2) −0·002, C(3) 0·001, C(5) −0·001 Å. C(4) is displaced −0·134, O(2) −0·008 and O(5) −0·055 Å from this plane. Bond angles at C(2) and C(3) are similar to those at C(5) and C(4) respectively. The torsion angles H(31)–C(3)–C(4)–C(41) and H(41)–C(4)–C(3)–C(31) are respectively 3(1) and 3(1)°. A torsion angle of 127·6 (2)° is observed for C(31)–C(63)–C(4)–C(41). It may, therefore, be concluded that the five-membered ring is relatively non-strained for C(31) and C(41) in a *trans* position to one another. A similar observation was made for the model compound (RRS–SSR)-2-[1-(ethylsulphonyl)-ethyl]-3-methylsuccinimide (Lotter, Klein, Rüdiger & Scheer, 1977), in which C(31) and C(41) are likewise *trans* to one another. A comparison of the geometry of (1*b*) with that of (1*c*), for which C(31) and C(41) are *cis* to one another, is made in the following paper (Sheldrick, 1981).

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(SRS–RSR)-2-(1-Methoxyethyl)-3-methylsuccinimide

By W. S. Sheldrick

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Abstract. $C_8H_{13}NO_3$, monoclinic, $P2_1/c$, $a = 12·984$ (4), $b = 7·559$ (3), $c = 9·734$ (3) Å, $\beta = 97·77$ (4)°, $M_r = 171·2$, $Z = 4$, $D_x = 1·20$ Mg m^{-3}; $R = 0·057$ and $R_w = 0·051$ for 1420 observed reflexions. The relative configuration of the three chiral centres is SRS or RSR. The molecules build centrosymmetric dimers through N–H···O hydrogen bonds of length 2·91 (1) Å. The five-membered ring is markedly twisted with C(3) and C(4) displaced respectively −0·114 and 0·180 Å from the plane of the remaining ring atoms. A torsion angle of 23·3 (2)° is observed between the *cis*-substituted C(3) and C(4).

Introduction. In order to elucidate the configurations of methanol adducts of the bile pigment phycocyanobilin dimethyl ester, all four racemic stereoisomers (1*a*)–(1*d*) of 2-(1-methoxyethyl)-3-methylsuccinimide were synthesized by Gossauer & Hinze (1981). The previous paper (Sheldrick, 1981) reported the structure of (1*b*), an isomer with *trans*-substituted C(3) and C(4). This paper reports the structure of the *cis* isomer (1*c*), for which pronounced ring strain would be expected, as a result of steric contacts between the *cis* substituents.

(1*a*)   (1*b*)   (1*c*)   (1*d*)
(*RRR–SSS*)   (*RRS–SSR*)   (*SRS–RSR*)   (*SRR–RSS*)
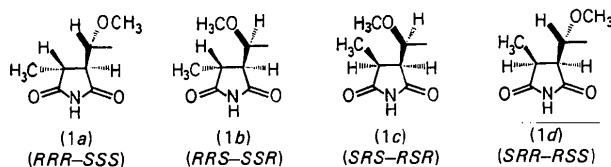
Cell dimensions were determined by a least-squares fit to settings for 15 reflexions $\pm(hkl)$ on a Syntex $P2_1$ diffractometer (Cu $K\alpha$ radiation, $\lambda = 1\cdot54178$ Å). Data collection was carried out in the θ–2θ mode ($2\theta \leq 135°$) with graphite-monochromated Cu $K\alpha$ radiation. No absorption correction was applied [μ(Cu $K\alpha$) = 0·68 mm^{-1}]. After application of the observation criterion $F \geq 2\cdot5\sigma(F)$, 1420 unique reflexions were retained for use in the analysis. The structure was solved by direct methods and refined by full-matrix least squares with anisotropic temperature factors for the non-hydrogen atoms. The H atom positional parameters were refined freely and, with the exception of the methyl protons of C(34), were assigned individual isotropic temperature factors. The terminal value of R_w was 0·051 with $R = 0\cdot057$.* Weights were given by the counting statistics. Complex neutral-atom

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* Lists of structure factors, anisotropic thermal parameters and H atom parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35610 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Positional parameters and equivalent isotropic thermal parameters*

	x	y	z	U_{eq} (Å$^2 \times 10^3$)†
N(1)	0·3771 (1)	0·5565 (2)	0·3921 (2)	62
C(2)	0·2792 (2)	0·6089 (3)	0·3388 (2)	64
O(2)	0·2185 (1)	0·6807 (2)	0·4042 (1)	91
C(3)	0·2626 (2)	0·5580 (3)	0·1846 (2)	64
C(31)	0·1842 (2)	0·4061 (4)	0·1607 (3)	76
C(32)	0·0736 (3)	0·4556 (9)	0·1827 (5)	127
O(33)	0·2246 (1)	0·2662 (2)	0·2484 (1)	81
C(34)	0·1866 (4)	0·0933 (5)	0·2051 (5)	128
C(4)	0·3727 (2)	0·5147 (3)	0·1542 (2)	57
C(41)	0·3885 (2)	0·3636 (4)	0·0552 (3)	76
C(5)	0·4348 (2)	0·4877 (3)	0·2963 (2)	58
O(5)	0·5208 (1)	0·4247 (2)	0·3230 (1)	75

$$\dagger\ U_{eq} = \tfrac{1}{3}\Sigma_i \Sigma_j a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

Table 2. *Bond lengths (Å) and angles (°)*

|			
C(2)–N(1)	1·365 (3)	C(5)–N(1)	1·375 (3)
O(2)–C(2)	1·207 (3)	C(3)–C(2)	1·536 (3)
C(31)–C(3)	1·531 (4)	C(4)–C(3)	1·534 (3)
C(32)–C(31)	1·526 (5)	O(33)–C(31)	1·415 (3)
C(34)–O(33)	1·440 (4)	C(41)–C(4)	1·526 (3)
C(5)–C(4)	1·518 (3)	O(4)–C(5)	1·209 (3)
C(5)–N(1)–C(2)	114·6 (2)	O(2)–C(2)–N(1)	124·9 (2)
C(3)–C(2)–N(1)	107·4 (2)	C(3)–C(2)–O(2)	127·8 (3)
C(31)–C(3)–C(2)	109·8 (2)	C(4)–C(3)–C(2)	103·4 (2)
C(4)–C(3)–C(31)	115·4 (2)	C(32)–C(31)–C(3)	114·5 (3)
O(33)–C(31)–C(3)	106·5 (2)	O(33)–C(31)–C(32)	112·2 (3)
C(34)–O(33)–C(31)	114·7 (3)	C(41)–C(4)–C(3)	119·3 (2)
C(5)–C(4)–C(3)	104·3 (2)	C(5)–C(4)–C(41)	112·0 (2)
C(4)–C(5)–N(1)	107·2 (2)	O(5)–C(5)–N(1)	125·1 (2)
O(5)–C(5)–C(4)	127·6 (2)		
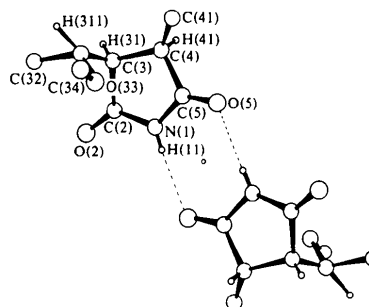
Fig. 1. The dimer of (1*c*).

scattering factors were employed (Cromer & Waber, 1965; Cromer & Liberman, 1970). Table 1 lists the final non-hydrogen atom coordinates, Table 2 the bond lengths and angles. Calculations were carried out with *SHELX* (Sheldrick, 1976) and local programs. Fig. 1 was drawn by *RSPLOT* (W. S. Sheldrick).

Discussion. As was observed for (1*b*), molecules of (1*c*) build centrosymmetric dimers through N(1)—H$\cdots$O(5) hydrogen bonds. The N(1)$\cdots$O(5) distance of 2·91 (1) Å in (1*c*) is 0·03 Å longer than that in (1*b*). A marked twisting of the five-membered ring is observed for (1*c*). Distances from the least-squares plane through N(1), C(2) and C(5) are: C(3) −0·114, C(4) 0·180, O(2) 0·069 and O(5) −0·076 Å. This ring twisting is further evidenced by the torsion angle C(31)—C(3)—C(4)—C(41) for the *cis*-substituted C(31) and C(41), which has a value of 23·3 (2)°. For comparison, torsion angles of 3 (1)° were observed for the *cis*-substituted H and C atoms at C(3) and C(4) in (1*b*). The exocyclic bond angles at C(3) and C(4) in (1*c*) are markedly different from one another. Although, as a result of steric contacts, both C(31)—C(3)—C(4) and C(41)—C(4)—C(3) are significantly wider than the equivalent bond angles in (1*b*), the degree of widening is more pronounced for the latter, which is 119·3 (2)°. C(41)—C(4)—C(5) is 112·0 (2)°, 2·3° wider than the equivalent angle in (1*b*), whereas C(31)—C(3)—C(2) is 0·6° smaller.

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SHORT COMMUNICATION

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Racemic 3-[benzyl(phenyl)phosphinyl]-2-butenoic acid: errata. By M. L. GŁOWKA, *Institute of General Chemistry, Technical University of Łódź, 36 Żwirki, 90–924 Łódź, Poland*

Abstract

E.s.d.'s for bond lengths and angles, the y coordinate for C(3) [new value 0·7156 (9)], and the bond length C(16)–C(11) [new value 1·415 (10) Å] in the paper by Głowka [*Acta Cryst.* (1978), B34, 3089–3091] are revised and a missing hydrogen-bond distance is added [O(1)···O(2) 2·587 (7) Å].

The y coordinate of C(3) is 0·7156 (9). The remaining corrections are given in Table 1.

The author thanks Professor G. Ferguson for pointing out the errors.

Table 1. *Bond lengths* (Å) *and angles* (°)

P—O(1)	1·493 (4)	C(3)–C(4)	1·415 (14)	C(8)–C(9)	1·510 (9)	C(13)–C(14)	1·379 (13)	
P—C(1)	1·796 (6)	C(4)–C(5)	1·402 (14)	C(9)–O(2)	1·310 (8)	C(14)–C(15)	1·402 (13)	
P—C(7)	1·827 (7)	C(5)–C(6)	1·405 (10)	C(9)–O(3)	1·194 (8)	C(15)–C(16)	1·409 (10)	
P—C(10)	1·827 (8)	C(6)–C(1)	1·402 (10)	C(10)–C(11)	1·520 (8)	C(16)–C(11)	1·415 (10)	
C(1)–C(2)	1·410 (11)	C(7)–C(8)	1·333 (8)	C(11)–C(12)	1·404 (10)			
C(2)–C(3)	1·431 (10)	C(7)–C(17)	1·525 (8)	C(12)–C(13)	1·434 (10)	O(1)···O(2)	2·587 (7)	
P—C(7)–C(8)	113·6 (5)	O(1)–P–C(7)	113·2 (3)	C(6)–C(1)–C(2)	121·2 (6)	C(12)–C(13)–C(14)	120·0 (7)
P—C(7)–C(17)	117·1 (5)	O(1)–P–C(10)	112·9 (3)	C(7)–C(8)–C(9)	127·5 (6)	C(13)–C(14)–C(15)	121·7 (7)
P—C(10)–C(11)	109·9 (5)	C(7)–P–C(10)	106·6 (3)	C(8)–C(7)–C(17)	129·3 (6)	C(14)–C(15)–C(16)	118·9 (8)
P—C(1)–C(2)	116·3 (5)	C(1)–C(2)–C(3)	119·1 (7)	C(8)–C(9)–O(2)	117·5 (5)	C(15)–C(16)–C(11)	120·4 (7)
P—C(1)–C(6)	122·5 (5)	C(2)–C(3)–C(4)	119·5 (8)	C(8)–C(9)–O(3)	119·5 (6)	C(16)–C(11)–C(12)	120·1 (6)
C(1)–P–O(1)	112·5 (3)	C(3)–C(4)–C(5)	119·9 (7)	O(2)–C(9)–O(3)	122·9 (7)	C(16)–C(11)–C(10)	120·7 (6)
C(1)–P–C(7)	105·0 (3)	C(4)–C(5)–C(6)	121·1 (7)	C(10)–C(11)–C(12)	119·2 (6)	C(9)–O(2)–H(1)	107 (3)
C(1)–P–C(10)	106·1 (3)	C(5)–C(6)–C(1)	119·2 (7)	C(11)–C(12)–C(13)	118·9 (7)	P–O(1)···H(1)	140 (2)

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