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Structure of (4*S*,4′*S*,5′*S*) 3-(5′-Benzyloxy-5′-methyl-2′-oxo-2′,3′,4′,5′-tetrahydro-4′-furyl)-4-phenyl-1,3-oxazolidin-2-one

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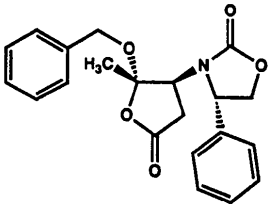
Abstract. $C_{21}H_{21}NO_5$, $M_r = 367{\cdot}4$, orthorhombic, $P2_12_12_1$, $a = 5{\cdot}656\ (1)$, $b = 10{\cdot}765\ (2)$, $c = 31{\cdot}631\ (7)$ Å, $V = 1925{\cdot}9\ (5)$ Å^3, $Z = 4$, $D_x = 1{\cdot}27$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 7{\cdot}1$ cm^{-1}, $F(000) = 776$, $T = 298$ K, $R = 0{\cdot}070$ ($wR = 0{\cdot}109$) for 1376 unique observed reflections. The known stereochemistry from a synthetic precursor gave the relative stereochemistries and fixed the enantiomorph.

Experimental. Crystals (colorless prisms) of $C_{21}H_{21}NO_5$ [hereafter (1)] obtained by Dr Roderick W. Bates and Professor Louis S. Hegedus (Colorado State University). Crystal size 0·34 × 0·38 × 0·45 mm. Nicolet *R*3*m* diffractometer, unit-cell constants from least-squares fit of setting angles for 25 reflections ($2\theta_{av} = 50{\cdot}41°$). Data collected ($\theta/2\theta$ scans) to $(\sin\theta)/\lambda = 0{\cdot}5992$ Å^{-1}, $0 \le h \le 7$, $0 \le k \le 13$, $0 \le l \le 38$. Three standard reflections (200, 040, 0,0,10) measured every 97; Lorentz and polarization corrections; no absorption correction applied due to low absorption coefficient; 1706 unique reflections, 1376 reflections with $F_o > 2{\cdot}5\sigma(F_o)$ observed.



(1)

Structure solved by direct methods (*SOLV*); block-diagonal (maximum 103 parameters/block, 247 parameters total, data/parameters = 5·6) weighted {$w = [\sigma^2(F) + gF]^{-1}$, $g = 5{\cdot}95 \times 10^{-3}$} least-squares refinement on *F*. H atoms in idealized positions [C—H = 0·96 Å, $U(H) = 1{\cdot}2 \times U_{iso}(C)$]. Non-H atoms refined with anisotropic thermal parameters. At convergence [$(\Delta/\sigma)_{max} = -0{\cdot}057$, $(\Delta/\sigma)_{mean} = 0{\cdot}009$ for last four cycles] $R = 0{\cdot}070$, $wR = 0{\cdot}109$, $S = 1{\cdot}192$, slope of normal probability plot = 0·989, $(\Delta\rho) = 0{\cdot}21$ e Å^{-3}, 1·14 Å from H(5), $(\Delta\rho)_{min} = -0{\cdot}23$ e Å^{-3}. The known stereochemistry at C(4) (*S*) (Bates, 1990) from a synthetic precursor gave the relative stereochemistries at C(4′) (*S*) and C(5′) (*S*) and fixed the enantiomorph. Neutral-atom scattering factors and anomalous-disperson corrections used (*International Tables for X-ray Crystallography*, 1974, Vol. IV); all calculations performed using *SHELXTL* program library (Sheldrick, 1983). Table 1 gives atomic coordinates and Table 2 gives bond lengths and angles.† Fig. 1. shows the structure of (1), as well as the numbering scheme used.

Table 1. *Atomic coordinates and isotropic thermal parameters* (Å^2 × 10^3)

Equivalent isotropic U_{eq} defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
C(1)	−0·2576 (10)	0·1727 (5)	0·0453 (2)	69 (2)
C(2)	−0·0801 (11)	0·0380 (5)	0·0007 (2)	73 (2)
C(3)	0·0881 (9)	0·0557 (5)	0·0376 (2)	62 (2)
C(4)	−0·1146 (10)	0·1830 (6)	0·1441 (2)	73 (2)
C(5)	0·0347 (9)	0·1877 (4)	0·1040 (2)	56 (2)
C(6)	0·0725 (14)	0·3251 (5)	0·0978 (2)	83 (2)
C(7)	−0·1364 (16)	0·3830 (7)	0·1206 (3)	105 (3)
C(8)	−0·3024 (13)	0·0843 (7)	0·1487 (2)	92 (3)
C(9)	−0·0256 (17)	0·1849 (9)	0·2197 (2)	115 (3)
C(10)	0·1657 (15)	0·2304 (8)	0·2461 (2)	98 (3)
C(11)	0·3009 (18)	0·3351 (8)	0·2357 (3)	103 (3)
C(12)	0·4801 (22)	0·3726 (8)	0·2620 (3)	120 (4)
C(13)	0·5231 (21)	0·3102 (11)	0·3002 (3)	126 (4)
C(14)	0·3952 (26)	0·2117 (11)	0·3110 (3)	144 (5)
C(15)	0·2115 (19)	0·1668 (8)	0·2832 (3)	120 (4)
C(16)	0·1741 (8)	−0·0669 (5)	0·0551 (2)	63 (2)
C(17)	0·0475 (15)	−0·1349 (6)	0·0833 (2)	91 (3)
C(18)	0·1264 (21)	−0·2533 (6)	0·0950 (2)	128 (4)
C(19)	0·3309 (17)	−0·3001 (7)	0·0795 (2)	120 (4)
C(20)	0·4557 (16)	−0·2318 (7)	0·0519 (4)	160 (6)
C(21)	0·3811 (11)	−0·1154 (8)	0·0405 (3)	121 (4)
N	−0·0665 (7)	0·1250 (4)	0·0675 (1)	58 (1)
O(1)	−0·3992 (8)	0·2448 (4)	0·0594 (2)	95 (2)
O(2)	−0·2696 (8)	0·1264 (4)	0·0070 (1)	83 (2)
O(3)	−0·2071 (16)	0·4866 (5)	0·1190 (2)	166 (3)
O(4)	−0·2367 (9)	0·3005 (4)	0·1459 (1)	91 (2)
O(5)	0·0570 (8)	0·1791 (4)	0·1768 (1)	86 (2)

† Lists of anisotropic thermal parameters, H-atom coordinates and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54264 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

C(1)—N	1·387 (7)	C(1)—O(1)	1·201 (7)
C(1)—O(2)	1·312 (8)	C(2)—C(3)	1·518 (8)
C(2)—O(2)	1·447 (8)	C(3)—C(16)	1·512 (7)
C(3)—N	1·487 (6)	C(4)—C(5)	1·524 (8)
C(4)—C(8)	1·510 (10)	C(4)—O(4)	1·442 (8)
C(4)—O(5)	1·418 (7)	C(5)—C(6)	1·507 (7)
C(5)—N	1·455 (6)	C(6)—C(7)	1·518 (11)
C(7)—O(3)	1·187 (9)	C(7)—O(4)	1·322 (9)
C(9)—C(10)	1·451 (12)	C(9)—O(5)	1·438 (8)
C(10)—C(11)	1·401 (12)	C(10)—C(15)	1·383 (11)
C(11)—C(12)	1·373 (14)	C(12)—C(13)	1·402 (13)
C(13)—C(14)	1·329 (17)	C(14)—C(15)	1·444 (16)
C(16)—C(17)	1·359 (9)	C(16)—C(21)	1·363 (9)
C(17)—C(18)	1·400 (10)	C(18)—C(19)	1·354 (14)
C(19)—C(20)	1·341 (13)	C(20)—C(21)	1·371 (12)

N—C(1)—O(1)	124·8 (6)	N—C(1)—O(2)	111·6 (5)
O(1)—C(1)—O(2)	123·6 (6)	C(3)—C(2)—O(2)	106·0 (4)
C(2)—C(3)—C(16)	111·9 (4)	C(2)—C(3)—N	100·6 (4)
C(16)—C(3)—N	113·3 (4)	C(5)—C(4)—C(8)	119·6 (5)
C(5)—C(4)—O(4)	105·6 (5)	C(8)—C(4)—O(4)	106·1 (5)
C(5)—C(4)—O(5)	103·2 (4)	C(8)—C(4)—O(5)	112·9 (5)
O(4)—C(4)—O(5)	109·0 (5)	C(4)—C(5)—C(6)	102·7 (4)
C(4)—C(5)—N	115·3 (4)	C(6)—C(5)—N	114·0 (4)
C(5)—C(6)—C(7)	103·3 (5)	C(6)—C(7)—O(3)	128·9 (8)
C(6)—C(7)—O(4)	110·2 (6)	O(3)—C(7)—O(4)	120·8 (8)
C(10)—C(9)—O(5)	108·3 (7)	C(9)—C(10)—C(11)	122·9 (7)
C(9)—C(10)—C(15)	117·4 (8)	C(11)—C(10)—C(15)	119·7 (8)
C(10)—C(11)—C(12)	119·8 (7)	C(11)—C(12)—C(13)	120·6 (9)
C(12)—C(13)—C(14)	120·6 (10)	C(13)—C(14)—C(15)	120·2 (9)
C(10)—C(15)—C(14)	119·1 (9)	C(3)—C(16)—C(17)	122·8 (5)
C(3)—C(16)—C(21)	119·1 (5)	C(17)—C(16)—C(21)	118·0 (6)
C(16)—C(17)—C(18)	119·7 (7)	C(17)—C(18)—C(19)	121·0 (8)
C(18)—C(19)—C(20)	118·8 (7)	C(19)—C(20)—C(21)	120·7 (9)
C(16)—C(21)—C(20)	121·6 (8)	C(1)—N—C(3)	108·8 (4)
C(1)—N—C(5)	122·5 (4)	C(3)—N—C(5)	120·4 (4)
C(1)—O(2)—C(2)	109·7 (5)	C(4)—O(4)—C(7)	111·1 (5)
C(4)—O(5)—C(9)	117·7 (5)		

Related literature. Two compounds have been structurally characterized that contain a 4-phenyl-1,3-oxazolidin-2-one substructure: 8-chloro-5,6-dihydro-3-(*o*-fluorophenyl)-6-(4-phenyl-2-oxo-oxazolidin-3-yl-carbonyl)furo[3,2-*f*]-1,2-benzisoxazole (Plattner *et al.*, 1984) and (*R*)-3-[(*R*)-(6,7-dichloro-2,3-dihydrobenzofuran-2-yl)carbonyl]-4-phenyl-2-oxazolidone (Nakai, 1988). The title compound (1) differs from these related compounds in that the N atom is bound to the C atom of a five-membered ring rather than a carbonyl C atom.

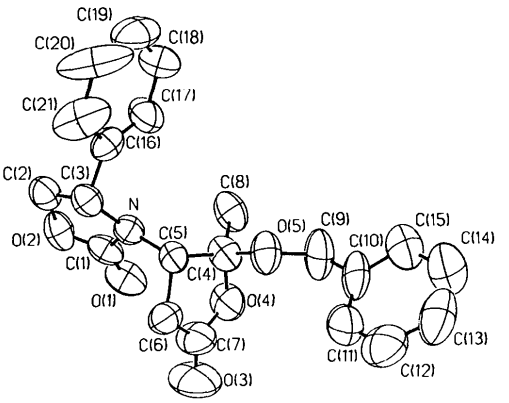

Fig. 1. The structure of (1) (50% probability thermal ellipsoids). H atoms have been omitted for clarity.

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Structure of 2-Ethoxycarbonyl-4,6-diphenylpyridine 1-(4-Bromobenzoyl)imide

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Abstract. [*N*-(2-Ethoxycarbonyl-4,6-diphenyl)-pyridinio]-3-bromobenzamidate, $C_{27}H_{21}BrN_2O_3$, M_r = 501·38, monoclinic, $P2_1/c$, a = 13·1959 (4), b = 8·0449 (2), c = 22·0192 (12) Å, β = 96·303 (3)°, V = 2323·4 (2) Å^3, Z = 4, D_x = 1·433 g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ = 26·65 cm^{-1}, $F(000)$ = 1024, T = 293 K, R = 0·055 for 2068 observed reflexions. The structure includes a stacking zone, in which the

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