Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^4$) *for* $[ZnCl_2(C_5H_5NO)_2]$

	x	y	z	U_{eq}*
Zn	0	0	0	357 (3)
Cl	1492 (1)	187 (1)	1535 (2)	512 (5)
O	388 (2)	−542 (1)	−1634 (4)	517 (12)
N	−389 (2)	−798 (1)	−2448 (4)	360 (10)
C(1)	−337 (3)	−1275 (1)	−2269 (5)	436 (16)
C(2)	−1059 (3)	−1558 (1)	−3168 (6)	485 (17)
C(3)	−1863 (3)	−1357 (1)	−4249 (5)	531 (18)
C(4)	−1917 (3)	−871 (1)	−4377 (5)	494 (18)
C(5)	−1178 (3)	−596 (1)	−3471 (5)	435 (16)

* $U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}\mathbf{a}_i.\mathbf{a}_j a_i^* a_j^*$.

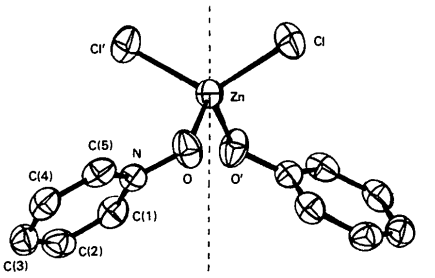

Fig. 1. An *ORTEP* plot of the $[ZnCl_2(C_5H_5NO)_2]$ molecule viewed perpendicular to [001]. Ellipsoids are at the 50% probability level.

Table 2. *Bond distances* (Å) *and angles* (°) *in dichlorobis(pyridine N-oxide)zinc*(II)

Zn–O	1·992 (2)	Zn–Cl	2·214 (1)
	O–N	1·338 (4)	
N–C(1)	1·353 (4)	N–C(5)	1·350 (4)
C(1)–C(2)	1·360 (5)	C(4)–C(5)	1·365 (5)
C(2)–C(3)	1·384 (5)	C(3)–C(4)	1·375 (6)
O–Zn–O'	106·8 (2)	Cl–Zn–Cl'	119·5 (1)
O–Zn–Cl	106·4 (1)	O–Zn–Cl'	108·5 (1)
	Zn–O–N	120·4 (1)	
O–N–C(1)	117·4 (3)	O–N–C(5)	122·1 (2)
N–C(1)–C(2)	120·2 (3)	N–C(5)–C(4)	120·4 (3)
C(1)–C(2)–C(3)	120·1 (3)	C(5)–C(4)–C(3)	120·1 (3)
C(2)–C(3)–C(4)	118·6 (3)	C(1)–N–C(5)	120·5 (3)

(') denotes twofold-related atoms.

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Structure of Methyl Tetrahydro-3,4-dihydroxy-2,4,5-trimethyl-2-furancarboxylate at 163 K

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(*Received* 16 *January* 1986; *accepted* 28 *February* 1986)

Abstract. $C_9H_{16}O_5$, $M_r = 204·22$, monoclinic, $P2_1$, $a = 10·5910$ (14), $b = 18·908$ (3), $c = 7·9060$ (8) Å, $\beta = 100·849$ (13)°, $V = 1554·9$ (3) Å^3, $Z = 6$, $D_x = 1·308$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0·997$ cm^{-1}, $F(000) = 660$, $R = 0·0389$ for 3978 reflections ($F \geq 4\sigma_F$). The asymmetric unit is a trimer linked through three hydrogen bonds [O···H distances 1·91 (3), 1·97 (3), 2·09 (4) Å] and a bifurcated hydrogen bond [O···H distances 2·32 (4), 2·37 (4) Å]. In addition, trimers are linked along **a** and along **b** by hydrogen bonds [O···H distances 1·94 (4), 2·05 (3) Å, respectively].

Experimental. Title compound prepared from D-ribonic acid. Absolute configuration correct as shown [m.p. 408 K; $[\alpha]_D^{25°C} = -32°$ ($CHCl_3$, 0·92 g dm^{-3})]. Transparent, colorless crystals obtained from ethyl acetate/hexane solution. Crystal for data collection cut from a large plate having a corrugated surface. Summary of data collection and structural refinement in Table 1.

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0108-2701/86/081095-03$01.50

Table 1. *Summary of data collection and structural refinement for* $C_9H_{16}O_5$

Data collection (163 K)*†	
Mode	ω scan
Scan range	Symmetrically over 1·0° about $K\alpha_{1,2}$ maximum
Background	Offset 1·0 and −1·0° in ω from $K\alpha_{1,2}$ maximum
Scan rate (° min^{-1})	3·0–6·0
Exposure time (h)	61·9
Stability analysis†	
Check reflections	200; 020; 003; 1$\bar{1}$2
Computed s	−0·00024 (16)
t	0·000004 (3)
Correction range (on I)	0·999–1·004
2θ range (°)	4·0–60·0
Range in hkl, min.	0,0,−11
max.	14,25,11
Reflections measured; total, unique	4658, 4658
Crystal dimensions (mm)	0·50 × 0·24 × 0·24
Crystal volume (mm^3)	0·0429
Crystal faces	All sides were cut
Transmission-factor range	0·964–0·983
Structure refinement‡	
Instability factor p†	0·04
Reflections used ($F \geq 4\sigma_F$)	3978
Number of variables	570
Goodness of fit, S	1·224
R, wR	0·0389, 0·0413
R for all data	0·0501
Max. shift/e.s.d.	0·0094
Max., min. in difference map (e Å^{-3})	0·28, −0·21

* Unit-cell parameters were obtained by least-squares refinement of the setting angles of 45 reflections with $21 \cdot 1 < 2\theta < 29 \cdot 2°$.

† Syntex $P2_1$ autodiffractometer with a graphite monochromator and a Syntex LT-1 inert-gas (N_2) low-temperature delivery system. Data reduction was carried out as described by Riley & Davis (1976). Crystal and instrument stability were monitored by remeasurement of four check reflections after every 96 reflections. As detailed by Henslee & Davis (1975), these data were analyzed to relate intensity to exposure time by the equation $y = 1 \cdot 0 + sx + tx^2$, where x is exposure time (h), y is fractional intensity relative to $x = 0$, and s and t are coefficients determined by least-squares fit.

‡ Function minimized was $\sum w(F_o - F_c)^2$, where $w = \sigma_F^{-2}$, $\sigma_F = F\sigma_I/2I$, $\sigma_I = [N_{pk} + N_{bg1} + N_{bg2} + (pI)^2]^{1/2}$.

Table 2. *Positional and equivalent isotropic thermal parameters for nonhydrogen atoms in three molecules of* $C_9H_{16}O_5$

For anisotropic atoms, the U value is U_{eq}, calculated as $U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}(Å^2)
O(1*A*)	0·76957 (15)	0·644808	0·6136 (2)	0·0269 (5)
C(2*A*)	0·6905 (2)	0·66179 (13)	0·7353 (3)	0·0225 (6)
C(3*A*)	0·5529 (2)	0·66038 (12)	0·6308 (3)	0·0211 (6)
C(4*A*)	0·5738 (2)	0·69368 (12)	0·4608 (3)	0·0214 (6)
C(5*A*)	0·7011 (2)	0·65920 (13)	0·4406 (3)	0·0238 (6)
C(6*A*)	0·7310 (2)	0·73495 (13)	0·8108 (3)	0·0252 (6)
O(7*A*)	0·8314 (2)	0·76281 (11)	0·8039 (3)	0·0372 (6)
O(8*A*)	0·6444 (2)	0·76094 (10)	0·8987 (2)	0·0296 (5)
C(9*A*)	0·6776 (3)	0·8282 (2)	0·9839 (4)	0·0374 (9)
C(10*A*)	0·7176 (3)	0·60865 (15)	0·8821 (4)	0·0319 (8)
O(11*A*)	0·5087 (2)	0·58937 (10)	0·6081 (2)	0·0280 (5)
O(12*A*)	0·5963 (2)	0·76713 (9)	0·4908 (2)	0·0261 (5)
C(13*A*)	0·4672 (3)	0·6813 (2)	0·3055 (3)	0·0312 (8)
C(14*A*)	0·7837 (3)	0·7026 (2)	0·3444 (4)	0·0398 (10)
O(1*B*)	0·28228 (13)	0·58947 (10)	0·7232 (2)	0·0227 (4)
C(2*B*)	0·1573 (2)	0·58797 (13)	0·6146 (3)	0·0202 (6)
C(3*B*)	0·0623 (2)	0·59216 (13)	0·7403 (3)	0·0226 (6)
C(4*B*)	0·1350 (2)	0·54749 (13)	0·8911 (3)	0·0233 (6)
C(5*B*)	0·2725 (2)	0·57401 (13)	0·9007 (3)	0·0227 (6)
C(6*B*)	0·1346 (2)	0·51874 (13)	0·5148 (3)	0·0220 (6)
O(7*B*)	0·0286 (2)	0·50265 (10)	0·4391 (2)	0·0307 (5)
O(8*B*)	0·2399 (2)	0·48215 (11)	0·5086 (2)	0·0355 (6)
C(9*B*)	0·2179 (5)	0·4142 (2)	0·4218 (6)	0·0653 (15)
C(10*B*)	0·1481 (3)	0·64793 (15)	0·4860 (3)	0·0298 (8)
O(11*B*)	0·0493 (2)	0·66235 (11)	0·7956 (2)	0·0340 (6)
O(12*B*)	0·1318 (2)	0·47525 (10)	0·8384 (2)	0·0288 (5)
C(13*B*)	0·0880 (3)	0·5560 (2)	1·0587 (3)	0·0395 (10)
C(14*B*)	0·3776 (3)	0·5234 (2)	0·9770 (4)	0·0343 (8)
O(1*C*)	0·36249 (15)	0·83253 (9)	0·5315 (2)	0·0220 (4)
C(2*C*)	0·3243 (2)	0·89089 (12)	0·4145 (3)	0·0190 (6)
C(3*C*)	0·3085 (2)	0·95402 (12)	0·5314 (3)	0·0207 (6)
C(4*C*)	0·2581 (2)	0·91651 (12)	0·6766 (3)	0·0198 (6)
C(5*C*)	0·3492 (2)	0·85340 (12)	0·7055 (3)	0·0204 (6)
C(6*C*)	0·1971 (2)	0·87523 (13)	0·2927 (3)	0·0217 (6)
O(7*C*)	0·1289 (2)	0·92187 (10)	0·2213 (2)	0·0302 (5)
O(8*C*)	0·1773 (2)	0·80696 (10)	0·2616 (2)	0·0327 (6)
C(9*C*)	0·0628 (3)	0·7896 (2)	0·1368 (5)	0·0481 (11)
C(10*C*)	0·4241 (2)	0·90138 (15)	0·3009 (3)	0·0267 (7)
O(11*C*)	0·4283 (2)	0·98512 (10)	0·6020 (2)	0·0304 (5)
O(12*C*)	0·1344 (2)	0·88818 (10)	0·6097 (2)	0·0253 (5)
C(13*C*)	0·2577 (3)	0·96191 (15)	0·8346 (3)	0·0291 (7)
C(14*C*)	0·3048 (3)	0·79209 (14)	0·8006 (3)	0·0294 (8)

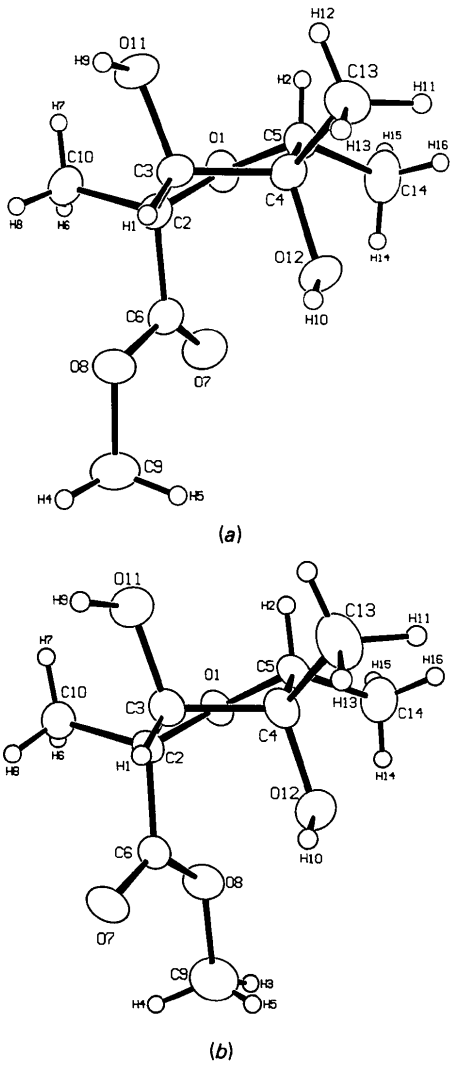

Fig. 1. (*a*) View of molecule *A* showing atom labeling. (*b*) View of molecule *B* showing atom labeling. The conformation of molecule *C* is very similar to that of molecule *B*.

A single five-membered ring obtained with *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978); remaining 37 atoms obtained from five electron-density maps. H atoms located in an electron density difference map at $R = 0.068$ as peaks of 0·27–0·56 e Å^{-3}. All positions and thermal parameters (isotropic H atoms) were refined by full-matrix least squares (*SHELX*76, Sheldrick, 1976) in three blocks of two molecules per block. Scattering factors and anomalous-dispersion corrections for C and O from *International Tables for X-ray Crystallography* (1974); H scattering factors from Stewart, Davidson & Simpson (1965). Atomic parameters in Table 2.* Bond lengths and bond angles in Table 3; atom labeling in Fig. 1 and packing in Fig. 2. Least-squares-planes program from Cordes (1983); principal computer programs are given by Gadol & Davis (1982).

Related literature. Structures of related compounds have been reported by Hirata, Sakabe & Goto (1977), Kruger, Steyn, Vleggaar & Rabie (1979), and Norrestam (1978).

* Lists of H-atom parameters, anisotropic thermal parameters, torsion angles, least-squares planes and structure factor amplitudes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42882 (32 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

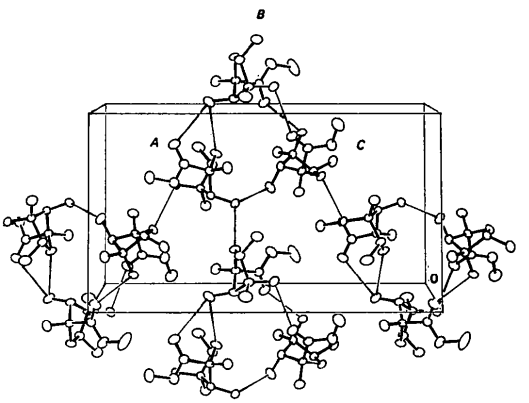

Fig. 2. Packing diagram viewed approximately along **c***. The trimeric units are hydrogen bonded along both the *a* and *b* axes. Molecules *A*, *B* and *C* have been labeled in one trimer.

Table 3. *Bond lengths* (Å) *and bond angles* (°) *for nonhydrogen atoms in* $C_9H_{16}O_5$

	A	*B*	*C*
C(2)–O(1)	1·425 (3)	1·436 (2)	1·448 (3)
C(5)–O(1)	1·448 (3)	1·456 (3)	1·463 (3)
C(3)–C(2)	1·535 (3)	1·544 (3)	1·538 (3)
C(6)–C(2)	1·536 (3)	1·524 (3)	1·530 (3)
C(10)–C(2)	1·521 (4)	1·513 (4)	1·524 (4)
C(4)–C(3)	1·538 (3)	1·544 (3)	1·529 (3)
O(11)–C(3)	1·422 (3)	1·412 (3)	1·414 (3)
C(5)–C(4)	1·533 (3)	1·528 (3)	1·524 (3)
O(12)–C(4)	1·421 (3)	1·427 (3)	1·423 (3)
C(13)–C(4)	1·521 (3)	1·510 (4)	1·516 (3)
C(14)–C(5)	1·506 (4)	1·505 (4)	1·505 (4)
O(7)–C(6)	1·197 (3)	1·208 (3)	1·210 (3)
O(8)–C(6)	1·344 (3)	1·321 (3)	1·323 (3)
C(9)–O(8)	1·451 (3)	1·455 (5)	1·450 (4)
C(2)–O(1)–C(5)	110·0 (2)	110·3 (2)	109·3 (2)
C(3)–C(2)–C(6)	113·1 (2)	108·6 (2)	110·3 (2)
C(3)–C(2)–C(10)	115·0 (2)	115·2 (2)	114·8 (2)
C(3)–C(2)–O(1)	104·6 (2)	104·7 (2)	104·9 (2)
C(6)–C(2)–C(10)	107·4 (2)	108·2 (2)	106·3 (2)
C(6)–C(2)–O(1)	108·0 (2)	111·4 (2)	111·2 (2)
C(10)–C(2)–O(1)	108·4 (2)	108·8 (2)	109·5 (2)
C(4)–C(3)–O(11)	112·0 (2)	109·8 (2)	108·1 (2)
C(4)–C(3)–C(2)	100·7 (2)	100·3 (2)	100·6 (2)
O(11)–C(3)–C(2)	109·9 (2)	111·2 (2)	111·7 (2)
C(5)–C(4)–O(12)	108·1 (2)	107·4 (2)	105·9 (2)
C(5)–C(4)–C(13)	112·6 (2)	113·0 (2)	114·8 (2)
C(5)–C(4)–C(3)	101·0 (2)	101·0 (2)	100·1 (2)
O(12)–C(4)–C(13)	111·1 (2)	111·4 (2)	112·0 (2)
O(12)–C(4)–C(3)	107·5 (2)	108·5 (2)	108·8 (2)
C(13)–C(4)–C(3)	115·8 (2)	114·9 (2)	114·3 (2)
C(14)–C(5)–O(1)	110·2 (2)	109·4 (2)	110·9 (2)
C(14)–C(5)–C(4)	115·2 (2)	115·9 (2)	115·5 (2)
O(1)–C(5)–C(4)	106·0 (2)	105·0 (2)	103·9 (2)
O(7)–C(6)–O(8)	124·2 (2)	124·2 (2)	124·4 (2)
O(7)–C(6)–C(2)	124·4 (2)	120·9 (2)	122·0 (2)
O(8)–C(6)–C(2)	111·2 (2)	114·6 (2)	113·3 (2)
C(9)–O(8)–C(6)	115·5 (2)	114·8 (3)	115·4 (2)

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