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Structures of Three α-Chloro-γ-lactones

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Abstract. 4-Chloro-2-oxatricyclo[4.2.1.0^{4,8}]nonan-3-one, (2), $C_8H_9ClO_2$, $M_r = 172 \cdot 61$, monoclinic, $P2_1/c$, $a = 6 \cdot 442$ (4), $b = 10 \cdot 063$ (1), $c = 11 \cdot 758$ (2) Å, $\beta = 95 \cdot 82$ (3)°, $V = 758 \cdot 3$ (7) Å^3, $Z = 4$, $D_x = 1 \cdot 51$ Mg m^{-3}, $\lambda(Mo\ K\alpha) = 0 \cdot 71073$ Å, $\mu = 0 \cdot 442$ mm^{-1}, $F(000) = 360$, $T = 293$ K, $R = 0 \cdot 035$ for 1815 reflections with $I > 3\sigma(I)$. 4-Chloro-2-oxatricyclo[5.2.1.0^{4,9}]decan-3-one, (4), $C_9H_{11}ClO_2$, $M_r = 186 \cdot 64$, monoclinic, $P2_1/n$, $a = 6 \cdot 148$ (1), $b = 11 \cdot 150$ (4), $c = 12 \cdot 577$ (2) Å, $\beta = 100 \cdot 95$ (1)°, $V = 846 \cdot 5$ (6) Å^3, $Z = 4$, $D_x = 1 \cdot 46$ Mg m^{-3}, $\lambda(Mo\ K\alpha) = 0 \cdot 71073$ Å, $\mu = 0 \cdot 401$ mm^{-1}, $F(000) = 392$, $T = 293$ K, $R = 0 \cdot 045$ for 1321 reflections with $I > 3\sigma(I)$. (±)-2aα-Chloro-3,4,4aα,5,6,7,7aα,7bα-octahydro-2a*H*-indeno[7,1-*b,c*]furan-2-one, (6), $C_{10}H_{13}ClO_2$, $M_r = 200 \cdot 67$, monoclinic, $P2_1/n$, $a = 8 \cdot 120$ (2), $b = 9 \cdot 454$ (3), $c = 12 \cdot 624$ (4) Å, $\beta = 97 \cdot 26$ (2)°, $V = 961 \cdot 3$ (9) Å^3, $Z = 4$, $D_x = 1 \cdot 39$ Mg m^{-3}, $\lambda(Mo\ K\alpha) = 0 \cdot 71073$ Å, $\mu = 0 \cdot 358$ cm^{-1}, $T = 293$ K, $F(000) = 424$, $R = 0 \cdot 036$ for 1018 reflections with $I > 3\sigma(I)$. In all three compounds, the bond lengths are unexceptional, the angles in the five-membered rings are significantly smaller than tetrahedral values and the angles in the six-membered rings [(4) and (6)] are somewhat enlarged. In (2), the three five-membered rings all have envelope conformations. In (4), the five-membered rings have envelope conformations and the six-membered ring is in a twist boat conformation. In (6), the five-membered rings also have envelope conformations while the six-membered ring is a chair which is slightly distorted owing to its fusion to two five-membered rings.

Introduction. Recently we reported methodology for the selective formation of carbocyclic α,γ-dichloroesters and/or annulated α-chloro-γ-lactones *via* transition-metal-promoted intramolecular radical cyclizations of olefinic α,α-dichloroesters and acids (Hayes, Freyer, Parvez & Weinreb, 1986). Several γ-lactones have been produced using this methodology, including simple cyclopentane and cyclohexane derivatives, along with bridged and fused tricyclic systems. X-ray studies have been carried out on some of these α-chloro-γ-lactones to confirm structural assignments made by NMR, and to establish unambiguously stereochemical relationships. Cyclization of 3-(3-cyclopentenyl)-2,2-dichloropropionic acid (1) with 1·2 mol% of RuCl$_2$-(PPh$_3$)$_3$ gave bridged lactone (2) in 88% yield. Likewise, lactone (4) was synthesized (88% yield) from 3-(3-cyclohexenyl)-2,2-dichloropropionic acid (3) and 2·2 mol% of catalyst. The fused bicyclic lactone (6) was prepared from 4-(2-cyclohexenyl)-2,2-dichlorobutyric acid (5) using 1·5 mol% of RuCl$_2$(PPh$_3$)$_3$ in 46% yield.
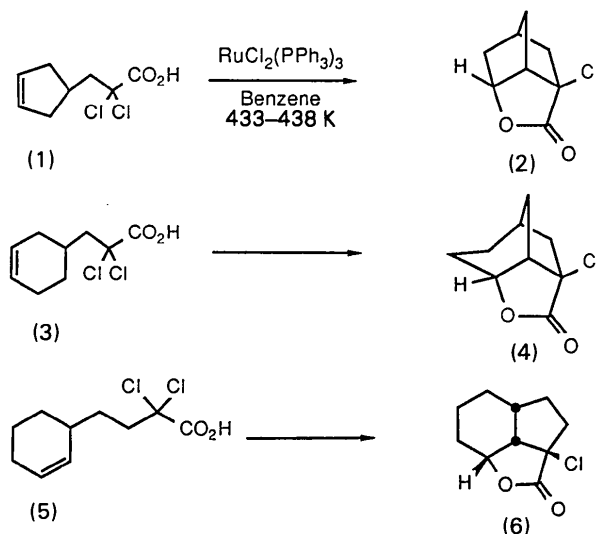
Table 1. *Summary of data collection and structure refinement parameters*

	(2)	(4)	(6)
Crystal size (mm)	0·35×0·45×0·90	0·30×0·40×0·55	0·18×0·27×0·36
Reflections used for cell constants			
number	25	25	25
θ range (°)	10–18	10–15	10–20
Scan type	$\omega/2\theta$	$\omega/2\theta$	$\omega/2\theta$
Scan width (°)	(0·80+0·35tanθ)	(1·00+0·35tanθ)	(1·00+0·35tanθ)
Variable scan speed (min⁻¹)	0·6–5·5	1·0–5·5	0·8–5·5
Max. scan time per reflection (s)	60	100	100
Range for data collection			
θ (°)	2–30	2–25	2–25
h	0/9	0/7	0/9
k	0/14	0/13	0/11
l	−16/16	−14/14	−15/15
Crystal decay (%)	9·9	1·9	27·7
Empirical absorption correction			
max. transmission coefficient	0·9975	0·9988	0·9994
min. transmission coefficient	0·9014	0·9244	0·9318
Reflections measured			
total	2503	1724	1919
unique	2197	1480	1688
observed [$I > 3\sigma(I)$]	1819	1321	1018
Reflection-averaging agreement on F	0·008	0·016	0·022
R, wR	0·035, 0·051	0·045, 0·082	0·036, 0·048
Data/parameter ratio	13·3	8·6	6·0
Weighting scheme	$w=1/(\sigma^2F+0.01F^2)^{1/2}$	$w=1/(\sigma^2F+0.01F^2)^{1/2}$	$w=1/(\sigma^2F+0.04F^2)^{1/2}$
Max. shift/e.s.d. ratio (Δ/σ)	<0·1	<0·02	<0·01
Min./max. height in final $\Delta\rho$ (e Å⁻³)	−0·25/0·26	−0·20/0·27	−0·25/0·30
Goodness of fit, S	1·92	0·86	1·73

Table 2. *Final fractional coordinates and B_{eq}'s with e.s.d.'s in parentheses*

	x	y	z	B_{eq}*(Å²)
Compound (2)				
Cl	0·24253 (7)	0·09294 (4)	0·93930 (3)	4·363 (8)
O(1)	0·5897 (2)	0·3691 (1)	0·8422 (1)	4·62 (2)
O(2)	0·6367 (2)	0·2567 (2)	1·0066 (1)	5·59 (3)
C(1)	0·5271 (2)	0·2884 (2)	0·9226 (1)	3·83 (3)
C(2)	0·3016 (2)	0·2531 (1)	0·8879 (1)	2·90 (2)
C(3)	0·2780 (2)	0·2655 (1)	0·7575 (1)	3·09 (2)
C(4)	0·4218 (2)	0·3860 (2)	0·7491 (1)	3·78 (3)
C(5)	0·2831 (2)	0·5042 (2)	0·7705 (1)	4·14 (3)
C(6)	0·0917 (2)	0·4374 (2)	0·8129 (1)	3·50 (3)
C(7)	0·0594 (2)	0·3218 (2)	0·7295 (1)	3·49 (3)
C(8)	0·1566 (2)	0·3650 (2)	0·9252 (1)	3·40 (2)
Compound (4)				
Cl	0·37960 (9)	0·05645 (5)	0·36293 (4)	5·26 (1)
O(1)	0·5541 (2)	0·3606 (1)	0·2832 (1)	3·81 (2)
O(2)	0·2793 (3)	0·3261 (1)	0·3710 (1)	5·77 (3)
C(1)	0·4018 (3)	0·2904 (2)	0·3144 (1)	3·56 (3)
C(2)	0·4083 (3)	0·1674 (1)	0·2642 (1)	3·22 (3)
C(3)	0·6306 (2)	0·1617 (1)	0·2261 (1)	3·17 (3)
C(4)	0·6824 (2)	0·2956 (2)	0·2149 (1)	3·45 (3)
C(5)	0·6226 (3)	0·3412 (2)	0·1001 (1)	4·38 (4)
C(6)	0·4063 (3)	0·2906 (2)	0·0362 (1)	4·40 (4)
C(7)	0·3589 (3)	0·1609 (2)	0·0673 (1)	3·75 (3)
C(8)	0·5759 (3)	0·0993 (1)	0·1166 (1)	3·58 (3)
C(9)	0·2313 (3)	0·1530 (2)	0·1602 (2)	3·91 (4)
Compound (6)				
Cl	0·38760 (9)	0·91217 (8)	0·83351 (7)	6·12 (2)
O(1)	0·6795 (2)	0·6727 (2)	0·7579 (1)	5·09 (4)
O(2)	0·4371 (3)	0·5861 (2)	0·7881 (2)	7·70 (6)
C(1)	0·5432 (3)	0·6731 (3)	0·8062 (2)	4·68 (6)
C(2)	0·5488 (3)	0·7916 (3)	0·8850 (2)	3·90 (5)
C(3)	0·7240 (3)	0·8508 (3)	0·8897 (2)	3·88 (5)
C(4)	0·7829 (3)	0·7963 (3)	0·7880 (2)	4·40 (6)
C(5)	0·9608 (4)	0·7529 (3)	0·7953 (3)	5·79 (7)
C(6)	1·0163 (3)	0·6674 (4)	0·8939 (3)	5·73 (7)
C(7)	0·9938 (4)	0·7501 (3)	0·9923 (3)	6·15 (8)
C(8)	0·8153 (4)	0·7949 (3)	0·9960 (2)	5·22 (7)
C(9)	0·7017 (4)	0·6819 (4)	1·0306 (2)	6·45 (8)
C(10)	0·5289 (4)	0·7375 (3)	0·9948 (2)	5·92 (8)

$* B_{eq} = \frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)].$

Experimental. For the three structures, accurate cell dimensions were obtained by least-squares refinement of the setting angles of 25 reflections measured on an Enraf–Nonius CAD-4 diffractometer using graphite-monochromatized Mo $K\alpha$ radiation. In each case intensities were collected by the $\omega/2\theta$ scanning procedure. The stability of each crystal was monitored by measurement of three reflections at regular intervals; the data were corrected for decay by appropriate scaling. All data were corrected for Lorentz and polarization effects and for absorption (North, Phillips & Mathews, 1968). A summary of data collection and structure refinement parameters for the three structures is given in Table 1.

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

	(2)	(4)	(6)
Cl–C(2)	1·776 (1)	1·785 (2)	1·794 (3)
O(1)–C(1)	1·339 (1)	1·335 (3)	1·330 (3)
O(1)–C(4)	1·468 (1)	1·464 (3)	1·461 (3)
O(2)–C(1)	1·198 (1)	1·198 (3)	1·192 (3)
C(1)–C(2)	1·511 (1)	1·514 (3)	1·495 (4)
C(2)–C(3)	1·531 (1)	1·533 (3)	1·523 (3)
C(2)–C(8)	1·554 (1)		
C(2)–C(9)		1·543 (3)	
C(2)–C(10)			1·505 (4)
C(3)–C(4)	1·535 (1)	1·539 (3)	1·516 (4)
C(3)–C(7)	1·522 (1)		
C(3)–C(8)		1·522 (3)	1·542 (4)
C(4)–C(5)	1·523 (1)	1·509 (3)	1·493 (4)
C(5)–C(6)	1·531 (1)	1·525 (4)	1·505 (4)
C(6)–C(7)	1·523 (1)	1·541 (3)	1·497 (5)
C(6)–C(8)	1·529 (1)		
C(7)–C(8)		1·524 (3)	1·517 (4)
C(7)–C(9)		1·529 (3)	
C(8)–C(9)			1·511 (5)
C(9)–C(10)			1·513 (4)
C(1)–O(1)–C(4)	110·15 (5)	111·6 (2)	111·3 (2)
C(1)–C(1)–O(2)	123·30 (7)	122·4 (3)	122·2 (3)
O(1)–C(1)–C(2)	107·58 (6)	109·4 (2)	110·5 (2)
O(2)–C(1)–C(2)	129·09 (7)	128·2 (2)	127·3 (3)
Cl–C(2)–C(1)	110·76 (5)	108·9 (1)	106·0 (2)
Cl–C(2)–C(3)	114·32 (4)	113·6 (1)	114·6 (2)
Cl–C(2)–C(8)	113·93 (4)		
Cl–C(2)–C(9)		111·7 (2)	
Cl–C(2)–C(10)			113·0 (2)
C(1)–C(2)–C(3)	104·28 (5)	105·3 (2)	104·6 (2)
C(1)–C(2)–C(8)	110·04 (5)		
C(1)–C(2)–C(9)		112·2 (2)	
C(1)–C(2)–C(10)			111·1 (2)
C(3)–C(2)–C(8)	102·85 (5)		
C(3)–C(2)–C(9)		105·0 (2)	
C(3)–C(2)–C(10)			107·3 (2)
C(2)–C(3)–C(4)	97·40 (5)	101·6 (2)	103·6 (2)
C(2)–C(3)–C(7)	104·05 (5)		
C(2)–C(3)–C(8)		104·2 (2)	104·6 (2)
C(4)–C(3)–C(7)	104·09 (6)		
C(4)–C(3)–C(8)		112·0 (2)	116·9 (2)
O(1)–C(4)–C(3)	105·35 (6)	106·4 (2)	105·1 (2)
O(1)–C(4)–C(5)	111·59 (7)	109·5 (2)	108·4 (2)
C(3)–C(4)–C(5)	103·77 (5)	113·4 (2)	116·6 (2)
C(4)–C(5)–C(6)	102·50 (6)	114·2 (2)	112·6 (3)
C(5)–C(6)–C(7)	100·79 (6)	113·7 (2)	110·5 (3)
C(5)–C(6)–C(8)	109·39 (6)		
C(7)–C(6)–C(8)	101·52 (6)		
C(3)–C(7)–C(6)	94·70 (5)		
C(6)–C(7)–C(8)		109·5 (2)	112·9 (2)
C(6)–C(7)–C(9)		113·4 (2)	
C(8)–C(7)–C(9)		101·5 (2)	
C(2)–C(8)–C(6)	102·75 (5)		
C(3)–C(8)–C(7)		100·9 (2)	115·2 (2)
C(3)–C(8)–C(9)			104·5 (2)
C(7)–C(8)–C(9)			115·6 (3)
C(2)–C(9)–C(7)	105·1 (2)		
C(8)–C(9)–C(10)			104·2 (3)
C(2)–C(10)–C(9)			101·0 (2)

Table 3 (cont.)

	(2)	(4)	(6)
ClC(2)–C(1)O(2)	–31·8 (1)	–43·5 (2)	–69·0 (3)
C(4)O(1)–C(1)C(2)	–3·2 (1)	–2·2 (3)	–6·2 (3)
O(1)C(1)–C(2)C(3)	26·8 (1)	–16·6 (3)	–8·5 (3)
O(1)C(2)–C(3)C(4)	–36·7 (1)	–22·7 (3)	18·7 (3)
C(2)C(3)–C(4)O(1)	35·2 (1)	21·8 (3)	–22·3 (3)
C(3)C(4)–O(1)C(1)	–21·5 (1)	–13·0 (3)	18·4 (3)
C(7)C(3)–C(4)C(5)	24·4 (1)		
C(3)C(4)–C(5)C(6)	11·3 (1)		
C(4)C(5)–C(6)C(7)	–43·2 (1)		
C(5)C(6)–C(7)C(3)	56·6 (1)		
C(6)C(7)–C(3)C(4)	–49·6 (1)		
C(8)C(2)–C(3)C(7)	–28·4 (1)		
C(2)C(3)–C(7)C(6)	51·9 (1)		
C(3)C(7)–C(6)C(8)	–56·0 (1)		
C(7)C(6)–C(8)C(2)	39·9 (1)		
C(3)C(2)–C(8)C(6)	–7·0 (1)		
C(8)C(3)–C(4)C(5)		11·9 (3)	–28·0 (3)
C(3)C(4)–C(5)C(6)		39·3 (3)	43·7 (3)
C(4)C(5)–C(6)C(7)		–33·2 (3)	–59·0 (3)
C(5)C(6)–C(7)C(8)		–23·8 (3)	58·7 (3)
C(6)C(7)–C(8)C(3)		72·2 (3)	–42·8 (3)
C(4)C(3)–C(8)C(7)		–66·4 (3)	27·2 (3)
C(9)C(2)–C(3)C(8)		–20·6 (3)	
C(2)C(3)–C(8)C(7)		42·6 (3)	
C(3)C(8)–C(7)C(9)		–47·9 (3)	
C(8)C(7)–C(9)C(2)		35·3 (3)	
C(3)C(2)–C(9)C(7)		–9·2 (3)	
C(10)C(2)–C(3)C(8)			13·9 (3)
C(2)C(3)–C(8)C(9)			13·1 (3)
C(3)C(8)–C(9)C(10)			–35·3 (3)
C(8)C(9)–C(10)C(2)			43·2 (3)
C(3)C(2)–C(10)C(9)			–35·1 (3)

The structures were solved by the heavy-atom method. The structures were refined by full-matrix least-squares calculations on Fs, initially with isotropic and finally with anisotropic temperature factors for the non-H atoms. At intermediate stages in the refinements difference maps revealed all H atoms in the three structures which were included in the subsequent cycles with isotropic thermal parameters. Refinement converged with $R = 0.035$, 0·045 and 0·036 and $wR = 0.051$, 0·082 and 0·048 for (2), (4) and (6), respectively. In the refinement cycles, weights were derived from the counting statistics. Scattering factors were those of Cromer & Mann (1968) and Stewart, Davidson & Simpson (1965) and allowance was made for anomalous dispersion (Cromer & Liberman, 1970). The computer programs used were part of the Enraf–Nonius *Structure Determination Package* (B. A. Frenz & Associates, Inc., 1985). The final fractional coordinates with e.s.d.'s are given in Table 2* and molecular dimensions are in Table 3. Fig. 1 shows the *ORTEP* (Johnson, 1976) drawings of the molecular structures of (2), (4) and (6) with the crystallographic numbering schemes while the crystal structures are depicted in Figs. 2–4.

Discussion. The structure of (2) is comprised of three five-membered rings A, B and C which have C(3)-,

* Lists of strucutre factors, anisotropic temperature factors and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44479 (54 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

C(7)- and C(7)-envelope conformations, respectively. The structure of (4) consists of two five-membered rings, A and C, with C(3)- and C(8)-envelope conformations, respectively, and a six-membered ring B which adopts a twist boat conformation. The structure of (6) is also composed of two five-membered rings, A and C, which have C(3)- and C(9)-envelope conformations and a six-membered ring B which displays a distorted chair conformation.

The bond distances in the three structures are in excellent agreement and are within the limits expected for the corresponding bonds, e.g. C—Cl 1·776 (1)–1·794 (3), C=O 1·192 (3)–1·198 (1), C_{sp^2}—O 1·330 (3)–1·339 (1), and C_{sp^3}—O 1·461 (3)–1·468 (1) Å; C_{sp^2}—C_{sp^3} 1·495 (4) Å in (6) is, however,
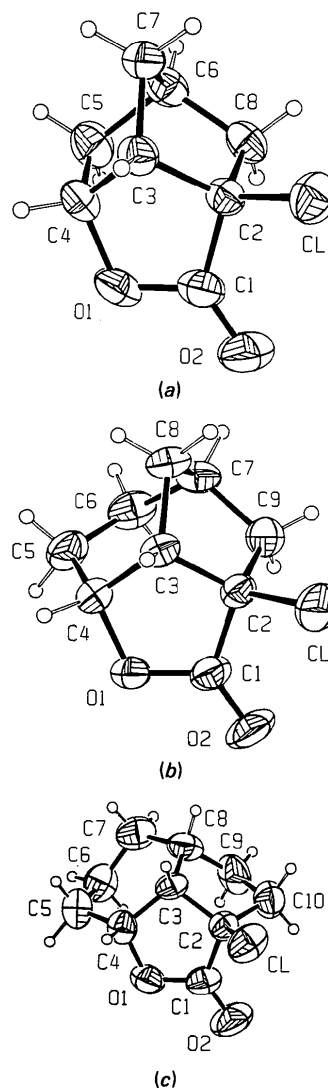

(a)

(b)

(c)

Fig. 1. *ORTEP* drawings of the molecular structures of (a) (2), (b) (4), and (c) (6) with crystallographic numbering schemes. The ellipsoids correspond to 50% probability contours of atomic displacement.
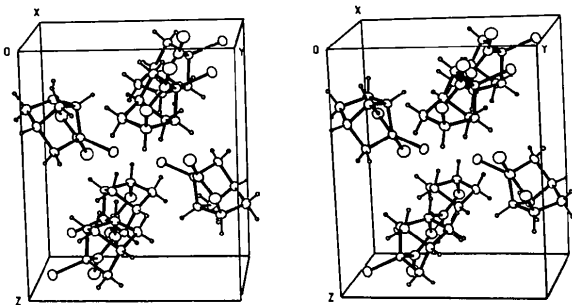
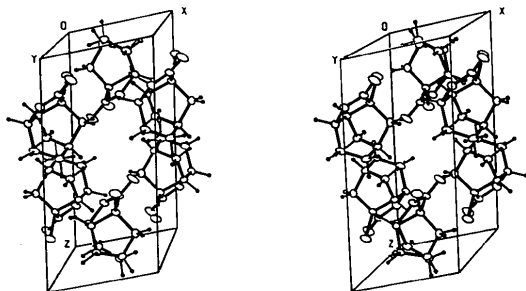Fig. 2. Stereoview of the crystal packing in the unit cell for (2).

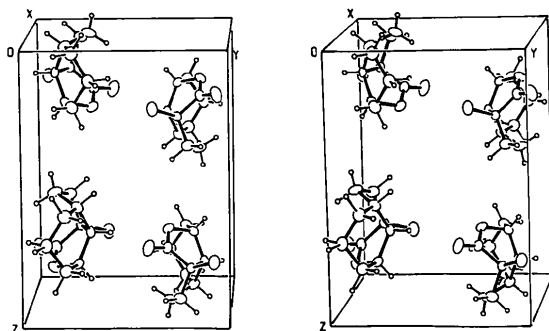Fig. 3. Stereoview of the crystal packing in the unit cell for (4).

Fig. 4. Stereoview of the crystal packing in the unit cell for (6).

significantly shorter than the corresponding bond in (2) and (4), 1·511 (1) and 1·514 (3) Å, respectively. The average C_{sp^3}—C_{sp^3} bond lengths in (2) [1·531 (1), range 1·522 (1)–1·544 (1) Å] and (4) [1·529 (3), range 1·509 (3)–1·543 (3) Å] agree very well while those in (6) [1·512 (4), range 1·493 (4)–1·542 (4) Å] are slightly shorter than those in the other two structures.

The endocyclic bond angles in the five-membered rings in all three structures are significantly smaller than their expected values. Ring A in (2) exhibits significantly smaller angles than the other two structures, e.g. angles C(1)–O(1)–C(4), O(1)–C(1)–C(2) and C(2)–C(3)–C(4) in the three structures are, respectively, 110·15 (5), 107·58 (6) and 97·40 (5)° in (2), 111·6 (2), 109·4 (2) and 101·6 (2)° in (4) and 111·3 (2), 110·5 (2) and 103·6 (2)° in (6). With the exception of C(3)–C(8)–C(7) [100·9 (2)°] in ring B in (4), the angles are in the range 109·5 (2)–114·2 (2)°. The angles in ring B of fused lactone (6) are larger [range 110·5 (3)–116·9 (2)°] than those observed in ring B in bridged lactone (4). The crystals of the three compounds consist of discrete molecules separated by normal van der Waals distances (Figs. 2–4).

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Structure of the Sodium Salt of Penicillanic Acid

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Abstract. $Na^+.C_8H_{10}NO_3S^-$, $M_r = 223·2$, orthorhombic, $P2_12_12_1$, $a = 10·640$ (16), $b = 15·093$ (25), $c = 5·982$ (26) Å, $V = 960·6$ Å^3, $Z = 4$, $D_x = 1·54$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1·54178$ Å, $\mu = 26·86$ cm^{-1}, $F(000) = 460·0$, $T = 293$ K, $R = 0·04$ for 522 observed reflexions. The conformation of this penicillin is C3, with the α-CH_3 in pseudo-equatorial, and the β-CH_3 and the C(3) substituent in pseudo-axial positions. This geometry is