Refinement

Refinement on F
$R = 0.046$
$wR = 0.065$
$S = 1.895$
2555 reflections
203 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o) + 0.00002|F_o|^2]$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Extinction correction: $I_{corr} = I_o(1 + gI_c)$
Extinction coefficient: $g = 1.11 \times 10^{-5}$
Scattering factors from *International Tables for Crystallography* (Vol. C)
Absolute configuration: Flack (1983)
Flack parameter = 0.02 (2)

Table 1. *Selected geometric parameters (Å, °)*

Cl1—C1	1.745 (3)	N3—C12	1.458 (4)
O1—C4	1.364 (4)	N3—C14	1.457 (4)
O1—C7	1.415 (4)	C3—C8	1.494 (4)
O2—C8	1.243 (3)	C9—C10	1.525 (4)
O3—C13	1.416 (4)	C9—C12	1.512 (4)
N1—C6	1.351 (4)	C10—C11	1.526 (4)
N2—C8	1.326 (4)	C11—C13	1.509 (4)
N2—C9	1.456 (4)	C14—C15	1.497 (6)
N3—C11	1.465 (4)		
C4—O1—C7	119.6 (3)	N2—C9—C10	113.2 (3)
C8—N2—C9	124.2 (2)	N2—C9—C12	109.7 (3)
C11—N3—C12	103.5 (2)	C10—C9—C12	103.4 (2)
C11—N3—C14	113.2 (3)	C9—C10—C11	105.8 (3)
C12—N3—C14	112.3 (3)	N3—C11—C10	103.4 (2)
O1—C4—C3	116.9 (3)	N3—C11—C13	113.1 (2)
O1—C4—C5	122.5 (3)	C10—C11—C13	113.7 (3)
C3—C4—C5	120.7 (3)	N3—C12—C9	103.9 (2)
O2—C8—N2	121.2 (3)	O3—C13—C11	111.3 (3)
O2—C8—C3	120.1 (3)	N3—C14—C15	113.6 (4)
N2—C8—C3	118.7 (3)		
O2—C8—N2—C9	−4.5 (4)	N3—C12—C9—C10	30.9 (3)
O2—C8—C3—C4	170.4 (3)	C8—N2—C9—C10	82.6 (3)
N2—C8—C3—C4	−9.9 (4)	C8—N2—C9—C12	−162.5 (3)
N3—C11—C10—C9	−20.6 (3)	C11—C10—C9—C12	−6.1 (3)

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2N···O1	0.946	1.892	2.628 (2)	132.8
O3—H3O···O2^{i}	1.07 (5)	1.78 (5)	2.847 (3)	173 (4)
N1—H1NA···O2^{ii}	0.949	2.184	2.951 (2)	137.1
N1—H1NB···O3^{iii}	0.950	2.135	2.944 (3)	142.3

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

Refinement was carried out using full-matrix least-squares methods. Anomalous-dispersion effects were included in F_c (Ibers & Hamilton, 1964); the values for $\Delta f'$ and $\Delta f''$ were those of Creagh & McAuley (1992). The values for the mass attenuation coefficients are those of Creagh & Hubbel (1992). All non-H atoms were refined anisotropically, and all H atoms, except for H3O, were placed in calculated positions and were not refined. Atom H3O was located in a difference Fourier map and refined isotropically.

Data collection: *Rigaku AFC Software* (Rigaku Corporation, 1990). Cell refinement: *Rigaku AFC Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1993). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985) and *DIRDIF*94 (Beurskens *et al.*, 1994). Program(s) used to refine structure: *TEXSAN*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *TEXSAN*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SX1037). Services for accessing these data are described at the back of the journal.

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Two Oxazolidinone Derivatives

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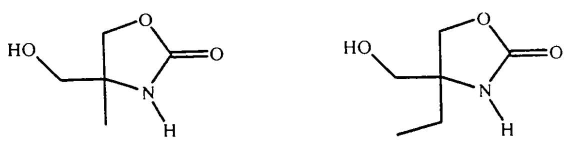
Abstract

The structures of two substituted oxazolidinones, namely, 4-hydroxymethyl-4-methyloxazolidin-2-one [$C_5H_9NO_3$, (1)] and 4-ethyl-4-hydroxymethyloxazolidin-2-one [$C_6H_{11}NO_3$, (2)], are reported. Bond distances in the two structures are almost identical. The oxazolidinone rings both adopt envelope conformations; the fold in (1) is significantly larger than that in (2). There is no

intramolecular hydrogen bonding in either structure and the intermolecular hydrogen-bonding schemes are very similar.

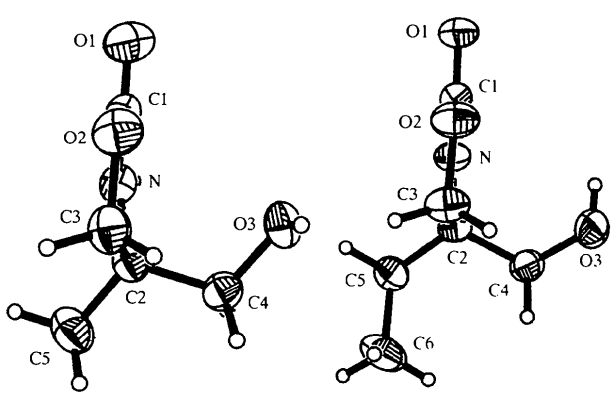
Comment

Several 4-alkyl-4-(hydroxymethyl)oxazolidinones, including (1) and (2), were synthesized as intermediates in a search for new stable *N*-halamine bactericides for treating aqueous solutions (Kohl *et al.*, 1980; Burkett *et al.*, 1981; Worley & Burkett, 1984; Barnela *et al.*, 1987; Worley *et al.*, 1987; Worley & Williams, 1988). Compound (2) proved to be soluble in many organic solvents, whereas (1) was soluble only in polar media. Furthermore, the hydroxyl moiety on (2) was much more reactive as a nucleophile than that on (1). Semi-empirical molecular-orbital calculations using the *AM*1 package (Dewar *et al.*, 1985; Dewar & Stewart, 1988) did not suggest a reason for these differences (such as an intramolecular hydrogen bond in one, but not the other). When suitable crystals became available, the structures were determined.



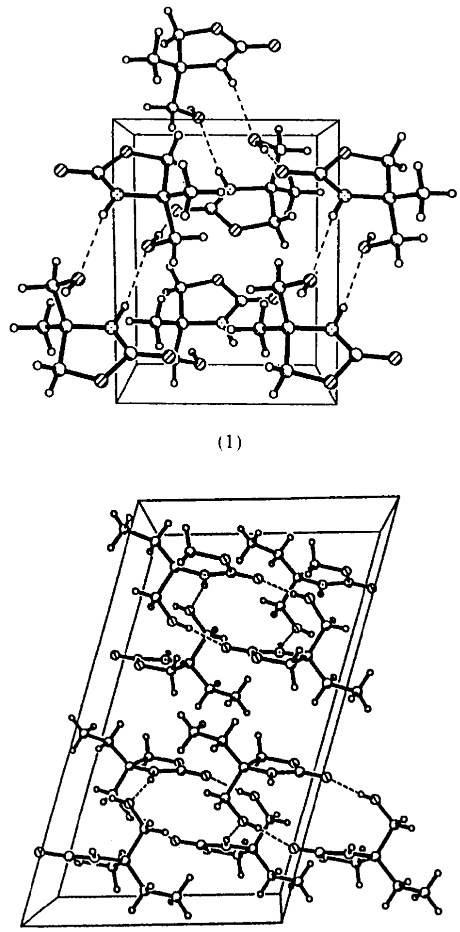
(1) (2)

The two structures are qualitatively and quantitatively quite similar. The rings in both structures adopt envelope conformations, with C2 out of the plane of the other four atoms, as depicted in Fig. 1. The largest structural difference between the two is the fold of the envelope (*i.e.* the angle between the N, C2, C3 and N, C1, C2, C3 planes); in (1), the fold is 19.5 (2)°, while in (2), it is 9.4 (1)°. There are no intramolecular hydrogen bonds in either structure; however, both structures feature intermolecular hydrogen-bonding networks which are qualitatively similar. In both cases, the hydroxyl group accepts a hydrogen bond from an amide hydrogen on another molecule and donates a hydrogen bond to a carbonyl oxygen on a third, as depicted in Fig. 2. It is possible that the difference in ring fold is a result of formation of the hydrogen-bonded networks in the two structures.



(1) (2)

Fig. 1. Views of the two title structures (50% probability ellipsoids) showing the conformations of the oxazolidinone rings.



(1)

(2)

Fig. 2. Views of the unit cells [projected down **a** with **b** horizontal in (1), and down **b** with **a** horizontal in (2)] showing the hydrogen-bonding scheme.

Experimental

For the preparation of 4-hydroxymethyl-4-methyloxazolidin-2-one, (1), 2-amino-2-methyl-1,3-propanediol (0.155 mol), diethyl carbonate (0.144 mol), sodium methoxide (0.00185 mol) and dry ethanol (100 ml) were added to a 200 ml round-bottomed flask. The mixture was heated with stirring at 383 K for 2 d. The ethanol was removed by fractional distillation. When ethyl acetate was mixed with the residue, a white solid precipitated. The product was recovered by vacuum filtration (70% yield). The data crystal was grown from acetone (m.p. 388–389 K). ^{1}H NMR (DMSO-d_6) δ: 1.15 (*s*, 3H), 3.24–3.27 (*m*, 2H), 3.85 (*d*, 1H, J = 5.0 Hz), 4.16 (*d*, 1H, J = 5.0 Hz), 5.07 (*t*, 1H, J = 5.0 Hz), 7.51 (*s*, 1H) p.p.m. (TMS); ^{13}C NMR (DMSO-d_6) δ: 22.5, 58.0, 66.3, 71.8, 158.2 p.p.m. (TMS); IR (KBr pellet): 3326, 3252, 2980, 1720 cm^{-1}; MS (*m/z*) 131. For the preparation of 4-ethyl-4-hydroxymethyloxazolidin-2-one, (2), 2-amino-2-ethyl-1,3-propanediol (0.155 mol), diethyl carbonate (0.144 mol), and sodium methoxide (0.00185 mol) were added to a 100 ml round-bottomed flask. The viscous mixture was heated with stirring at 383 K for 24 h. The ethanol and excess diethyl carbonate were removed by fractional distillation. When ethyl acetate (50 ml) was mixed with the residue, a white solid precipitated. The product was recovered by vacuum filtration (80% yield). The data crystal was grown from ethyl acetate (m.p. 348–350 K). ^{1}H NMR ($CDCl_3$) δ: 0.91 (*t*, 3H, J = 7.5 Hz), 1.53–1.65 (*m*, 2H), 3.32 (*s*, 2H), 4.08 (*d*, 1H, J = 5.0 Hz), 4.32 (*d*, 1H, J = 3.8 Hz), 5.83 (*s*, 1H), 7.46 (*s*, 1H) p.p.m. (TMS); ^{13}C NMR ($CDCl_3$) δ: 7.7, 28.2, 62.6, 66.2, 71.2, 160.8 p.p.m. (TMS); IR (KBr pellet): 3316, 3245, 2967, 1727 cm^{-1}; MS (*m/z*) 145.

Compound (1)

Crystal data

$C_5H_9NO_3$	Mo $K\alpha$ radiation
M_r = 131.13	λ = 0.71073 Å
Monoclinic	Cell parameters from 25 reflections
$P2_1/n$	θ = 7.5–15.0°
a = 9.004 (2) Å	μ = 0.116 mm^{-1}
b = 7.065 (2) Å	T = 295 (2) K
c = 9.851 (3) Å	Thick diamond-shaped plate
β = 97.96 (2)°	0.60 × 0.30 × 0.14 mm
V = 620.6 (3) Å^3	Colorless
Z = 4	
D_x = 1.403 Mg m^{-3}	
D_m not measured	

Data collection

Siemens *R3m/V* diffractometer	999 reflections with $I > 2\sigma(I)$
$2\theta-\omega$ scans	R_{int} = 0.058
Absorption correction: ψ scan of 6 reflections (*XEMP*; Siemens, 1990*a*)	θ_{max} = 27.55°
T_{min} = 0.856, T_{max} = 0.947	$h = 0 \rightarrow 11$
1523 measured reflections	$k = 0 \rightarrow 9$
1435 independent reflections	$l = -12 \rightarrow 12$
	2 standard reflections every 100 reflections intensity decay: <1%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.1099P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.122	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
S = 1.058	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
1435 reflections	Extinction correction: none
88 parameters	Scattering factors from *International Tables for Crystallography* (Vol. C)
H atoms: amido and hydroxyl H atoms refined, others riding	

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (1)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij}a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
O1	0.1765 (2)	−0.2455 (2)	0.9134 (2)	0.0569 (4)
C1	0.1845 (2)	−0.0748 (3)	0.9312 (2)	0.0408 (4)
N	0.2627 (2)	0.0215 (2)	1.03295 (15)	0.0379 (4)
C2	0.2702 (2)	0.2226 (3)	1.0014 (2)	0.0360 (4)
C3	0.1350 (2)	0.2354 (3)	0.8884 (2)	0.0437 (5)
O2	0.10522 (14)	0.0445 (2)	0.84186 (13)	0.0487 (4)
C4	0.4175 (2)	0.2673 (3)	0.9476 (2)	0.0400 (4)
O3	0.44969 (14)	0.1384 (2)	0.84515 (14)	0.0430 (4)
C5	0.2528 (2)	0.3471 (3)	1.1237 (2)	0.0547 (6)

Table 2. *Selected geometric parameters (Å, °) for (1)*

O1—C1	1.219 (2)	C2—C4	1.528 (2)
C1—N	1.330 (2)	C2—C3	1.535 (2)
C1—O2	1.349 (2)	C3—O2	1.438 (2)
N—C2	1.457 (2)	C4—O3	1.419 (2)
C2—C5	1.517 (3)		
O1—C1—N	129.0 (2)	N—C2—C3	99.02 (14)
O1—C1—O2	120.6 (2)	C5—C2—C3	112.52 (15)
N—C1—O2	110.4 (2)	C4—C2—C3	112.04 (15)
C1—N—C2	111.93 (15)	O2—C3—C2	105.67 (14)
N—C2—C5	112.5 (2)	C1—O2—C3	108.64 (14)
N—C2—C4	110.09 (14)	O3—C4—C2	112.76 (14)
C5—C2—C4	110.2 (2)		

Table 3. *Hydrogen-bonding geometry (Å, °) for (1)*

D—H···A	D—H	H···A	D···A	D—H···A
N—H1*A*···O3^{i}	0.84 (2)	2.12 (2)	2.926 (2)	162 (2)
O3—H3*C*···O1^{ii}	0.83 (2)	1.94 (2)	2.765 (2)	174 (2)

Symmetry codes: (i) $1 - x, -y, 2 - z$; (ii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$.

Compound (2)

Crystal data

$C_6H_{11}NO_3$	Mo $K\alpha$ radiation
M_r = 145.16	λ = 0.71073 Å
Monoclinic	Cell parameters from 25 reflections
$C2/c$	θ = 7.5–15.0°
a = 10.450 (3) Å	μ = 0.108 mm^{-1}
b = 8.198 (3) Å	T = 294 (2) K
c = 17.497 (7) Å	Thick plate
β = 106.85 (3)°	0.58 × 0.56 × 0.24 mm
V = 1434.6 (9) Å^3	White
Z = 8	
D_x = 1.344 Mg m^{-3}	
D_m not measured	

Data collection

Siemens *R3m/v* diffractometer	1073 reflections with $I > 2\sigma(I)$
$2\theta-\omega$ scans	R_{int} = 0.016
Absorption correction: ψ scan of 7 reflections (*XEMP*; Siemens, 1990*a*)	θ_{max} = 25.05°
T_{min} = 0.933, T_{max} = 0.974	$h = 0 \rightarrow 12$
1335 measured reflections	$k = 0 \rightarrow 9$
1263 independent reflections	$l = -20 \rightarrow 19$
	2 standard reflections every 100 reflections intensity decay: <1%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0470P)^2 + 0.9955P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.103$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
$S = 1.081$	$\Delta\rho_{min} = -0.14$ e Å^{-3}
1262 reflections	Extinction correction: none
97 parameters	Scattering factors from *International Tables for Crystallography* (Vol. C)
H atoms: amido and hydroxyl H atoms refined, others riding; fixed U	

Table 4. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (2)*

$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
O1	0.97411 (11)	0.1539 (2)	0.33620 (8)	0.0489 (4)
C1	1.0873 (2)	0.2071 (2)	0.34994 (9)	0.0347 (4)
N	1.19818 (13)	0.1292 (2)	0.34957 (8)	0.0350 (3)
C2	1.31517 (15)	0.2334 (2)	0.36361 (9)	0.0314 (4)
C3	1.2574 (2)	0.3919 (2)	0.38714 (11)	0.0431 (4)
O2	1.11566 (12)	0.36531 (15)	0.37009 (8)	0.0473 (4)
C4	1.3572 (2)	0.2524 (2)	0.28779 (10)	0.0399 (4)
O3	1.25899 (14)	0.3286 (2)	0.22437 (8)	0.0522 (4)
C5	1.4297 (2)	0.1625 (2)	0.43090 (10)	0.0440 (4)
C6	1.5566 (2)	0.2643 (3)	0.45442 (14)	0.0667 (6)

Table 5. *Selected geometric parameters (Å, °) for (2)*

O1—C1	1.218 (2)	C2—C5	1.530 (2)
C1—N	1.324 (2)	C2—C3	1.538 (2)
C1—O2	1.354 (2)	C3—O2	1.440 (2)
N—C2	1.453 (2)	C4—O3	1.420 (2)
C2—C4	1.522 (2)	C5—C6	1.519 (3)
O1—C1—N	128.8 (2)	N—C2—C3	99.55 (12)
O1—C1—O2	121.40 (15)	C4—C2—C3	112.45 (14)
N—C1—O2	109.75 (14)	C5—C2—C3	113.29 (14)
C1—N—C2	114.18 (14)	O2—C3—C2	106.04 (13)
N—C2—C4	110.75 (13)	C1—O2—C3	109.46 (12)
N—C2—C5	109.80 (13)	O3—C4—C2	113.59 (14)
C4—C2—C5	110.52 (13)	C6—C5—C2	115.2 (2)

Table 6. *Hydrogen-bonding geometry (Å, °) for (2)*

D—H···A	D—H	H···A	D···A	D—H···A
N—H1A···O3^{i}	0.84 (2)	2.06 (2)	2.878 (2)	164 (2)
O3—H3C···O1^{ii}	0.89 (2)	1.87 (2)	2.759 (2)	174 (2)

Symmetry codes: (i) $\frac{5}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $2 - x, y, \frac{1}{2} - z$.

For both compounds, data collection: *P*3 (Siemens, 1990*b*); cell refinement: *P*3; data reduction: *SHELXTL* (Siemens, 1994); program(s) used to solve structures: *SHELXS*86 (Sheldrick, 1985); program(s) used to refine structures: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *XP* in *SHELXTL*; software used to prepare material for publication: *XCIF* in *SHELXTL*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: BK1395). Services for accessing these data are described at the back of the journal.

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N-(3-Nitrobenzylidene)-*p*-phenylenediamine

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Abstract

The molecule of the title compound, $C_{13}H_{11}N_3O_2$, is nearly planar. There is an extended series of π bonds through the whole molecule. The molecules pack in a columnar manner with a 'ring-double-bond overlap' mode, in which the interplanar spacings are alternately 3.459 (5) and 3.526 (5) Å.

Comment

Conjugated organic molecules containing both donor and acceptor groups are of great interest for molecular electronics devices. The title compound, (I), was designed as a medium for high-density data storage. As an aid to understanding its optical and electronic properties, the crystal structure of (I) has been determined.

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