We thank A. Johansson MSc for preliminary synthesis of the title compound.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry, including H-atom geometry, have been deposited with the IUCr (Reference: AB1137). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Two Dimethylmorpholinium Bromides

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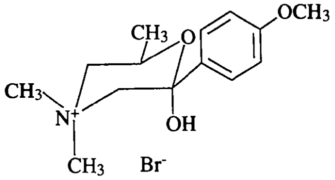
Abstract

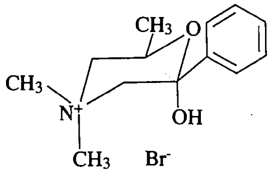
In the title compounds 2-hydroxy-2-(4-methoxyphenyl)-4,4,6-trimethylmorpholinium bromide, $C_{14}H_{22}NO_3^+.Br^-$, (1), and 2-hydroxy-4,4,6-trimethyl-2-phenylmorpholinium bromide hydrate, $C_{13}H_{20}NO_2^+.Br^-.xH_2O$, (2), the morpholinium rings adopt a chair conformation with the magnitudes of the endocyclic torsion angles in (1) and (2) in the ranges 50.5 (7)–60.1 (7) and 49.4 (4)–58.3 (4)°, respectively. The hydroxyl group is in the axial position of the morpholinium ring in both structures with C—OH bond distances of 1.410 (9) and 1.409 (4) Å. In (2), the hydroxy H atom points towards a Br ion [O···Br 3.246 (3), H···Br 2.55 (3) Å, O—H···Br 172 (3)°]. The OH···Br interaction in (1) is longer and nonlinear [O···Br 3.427 (5) Å, O—H···Br 123 (8)°].

Comment

As part of a larger study of structural changes in reactions involving tetrahedral intermediates and substituent effects in 2-substituted 2-hydroxy-4,4-dimethylmorpholinium bromides (Lee *et al.*, 1992), the syntheses of some morpholinium bromides (Garcia-Guajardo, Fronczek & Gandour, 1986; Altbach *et al.*, 1988; Garcia, Fronczek & Gandour, 1992*a*, 1993*a*) were performed. 2-Hydroxy-2-(4-methoxyphenyl)-4,4-dimethyl-6-methylmorpholinium bromide (1) was prepared by condensing 4-methoxy-2′-bromoacetophenone with 2-hydroxy-*N*,*N*-dimethylpropanol amine following the procedure described by Garcia (1986). Similarly, 2-hydroxy-4,4-dimethyl-6-methyl-2-phenylmorpholinium bromide hydrate (2) was prepared by condensing 2′-bromoacetophenone with 2-hydroxy-*N*,*N*-dimethylpropanol amine. Crystals of (1) (m.p. 443–445 K) and (2) (m.p. 480–482 K) were grown by slow cooling of methanol.



(1)



(2)

The average values of the O—CH_3 and C(aromatic)—O distances and the C(aromatic)—O—CH_3 angles in (1) [1.42 (1) and 1.372 (8) Å, 119.0 (6)°, respectively] are in agreement with those determined by X-ray crystallography by Nyburg & Faerman (1986) (1.425, 1.371 Å; 117.7°). Structural data for the title compounds are also in agreement with those for 2-(4-cyanophenyl)-2-hydroxy-4,4-dimethylmorpholinium bromide (Altbach *et al.*, 1988), 2-hydroxy-4,4-dimethyl-2-(4-tolyl)morpholinium bromide (Garcia, Fronczek & Gandour, 1992*a*), 2-hydroxy-2-(2-methylphenyl)-4,4-dimethylmorpholinium bromide (Garcia, Fronczek &

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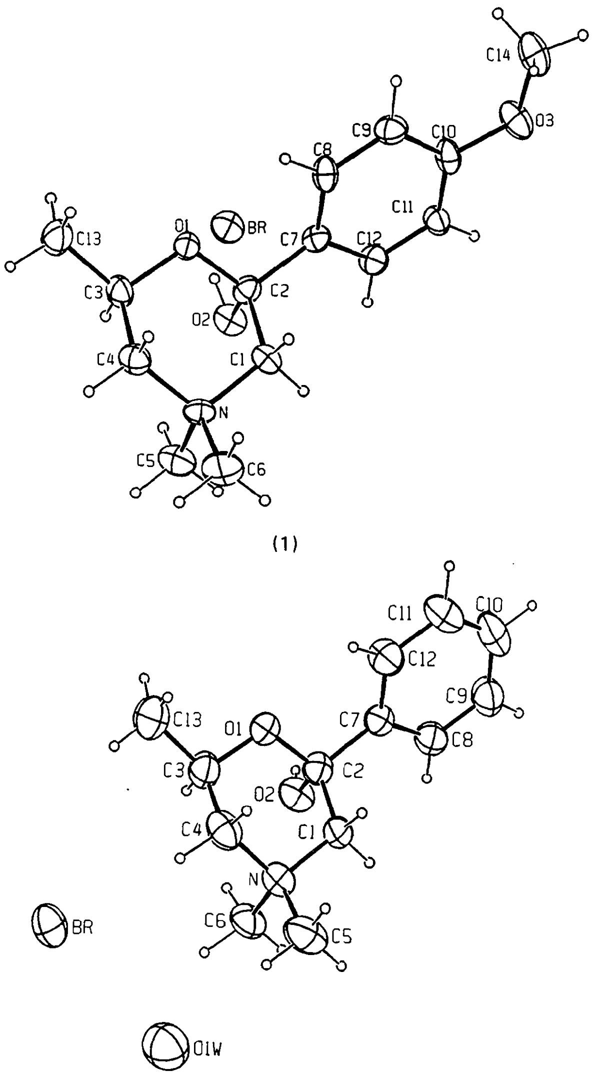
Gandour, 1993*a*), 2-hydroxy-6-methyl-2-(4-nitrophenyl)-4,4-dimethylmorpholinium bromide (Garcia, Fronczek & Gandour, 1993*b*), 4,4-dimethyl-2-oxomorpholinium bromide (Garcia-Guajardo, Fronczek & Gandour, 1986) and *N*-(3-hydroxypropyl)-*N*,*N*-dimethyl-*N*-[2-oxo-2-(4-phenylphenyl)ethyl]ammonium bromide (Garcia, Fronczek & Gandour, 1992*b*). The pharmacological activity of related compounds is reported by Anderson *et al.* (1966) and Lee *et al.* (1992).

The morpholinium rings in (1) and (2) adopt chair conformations with the following torsion angles: ω_1(O1—C2—C1—N) 52.6 (8), 49.4 (4); ω_2(C2—C1—N—C4) −50.5 (7), −50.5 (4); ω_3(C1—N—C4—C3) 52.5 (7), 54.0 (4); ω_4(N—C4—C3—O1) −58.2 (8), −58.3 (4); ω_5(C4—C3—O1—C2) 60.1 (7), 57.8 (4) and ω_6(C3—O1—C2—C1) −56.8 (7), −52.1 (4)°. They are distorted from the ideal D_{3d} chair conformation of cyclohexane (Hargittai & Hargittai, 1986) which has torsion angles ω_1, ω_2, ω_3, ω_4, ω_5 and ω_6 of ±54.4° (Hendrickson, 1967).

In (2), the partially populated water, O1*W*, is at a distance of 3.27 (1) Å from the bromide ion and 2.85 (1) Å from the morpholinium O atom O($x + \frac{1}{2}, \frac{3}{2} - y, z - \frac{1}{2}$).



(1)

(2)

Fig. 1. *ORTEP* drawing (Johnson, 1965) of molecules (1) and (2); heavy atoms are drawn as 40% probability ellipsoids and H atoms as circles of arbirtrary radii.

Experimental

Compound (1)

Crystal data

$C_{14}H_{22}NO_3^+.Br^-$
$M_r = 332.3$
Orthorhombic
$Pna2_1$
$a = 11.341$ (4) Å
$b = 15.692$ (6) Å
$c = 8.479$ (3) Å
$V = 1509$ (2) Å^3
$Z = 4$
$D_x = 1.462$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10\text{–}13°$
$\mu = 2.7$ mm^{-1}
$T = 295$ K
Prism
0.40 × 0.40 × 0.24 mm
Colorless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega\text{–}2\theta$ scans
Absorption correction: empirical
$T_{\min} = 0.738$, $T_{\max} = 0.999$
1604 measured reflections
1418 independent reflections

1159 observed reflections [$I > \sigma(I)$]
$\theta_{\max} = 25°$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 18$
$l = 0 \rightarrow 10$
3 standard reflections
frequency: 167 min
intensity variation: <2%

Refinement

Refinement on F
$R = 0.0464$
$wR = 0.0468$
$S = 2.176$
1159 reflections
176 parameters
$w = 4F_o^2[\sigma^2(I) + (0.02F_o^2)^2]^{-1}$
$(\Delta/\sigma)_{\max} = 0.03$

$\Delta\rho_{\max} = 0.87$ e Å^{-3}
$\Delta\rho_{\min} = -0.28$ e Å^{-3}
Extinction correction: $(1 + gI_c)^{-1}$ applied to F_c
Extinction coefficient: 8.7 (6) × 10^{-8}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

$$B_{\text{eq}} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Br	0.67054 (6)	0.88346 (5)	0.00000	4.16 (1)
O1	0.6600 (4)	0.5983 (3)	0.2187 (6)	2.5 (1)
O2	0.7691 (4)	0.6780 (3)	0.0378 (6)	3.0 (1)
O3	0.9940 (5)	0.8035 (3)	0.6793 (6)	3.5 (1)
N	0.8130 (4)	0.4881 (3)	0.0355 (7)	2.6 (1)
C1	0.8581 (6)	0.5544 (4)	0.1504 (8)	2.5 (2)
C2	0.7730 (6)	0.6288 (4)	0.1769 (9)	2.4 (1)
C3	0.6116 (7)	0.5414 (4)	0.1049 (9)	2.8 (2)
C4	0.6913 (6)	0.4635 (4)	0.0847 (9)	2.8 (2)
C5	0.8190 (7)	0.5174 (5)	−0.130 (1)	3.8 (2)

C6	0.8914 (7)	0.4098 (5)	0.052 (1)	4.2 (2)
C7	0.8227 (6)	0.6799 (4)	0.3151 (9)	2.2 (1)
C8	0.7861 (6)	0.6658 (4)	0.4669 (8)	2.7 (2)
C9	0.8372 (6)	0.7077 (5)	0.5932 (9)	2.9 (2)
C10	0.9322 (6)	0.7625 (4)	0.5626 (8)	2.7 (2)
C11	0.9681 (6)	0.7756 (5)	0.4108 (8)	2.6 (2)
C12	0.9148 (6)	0.7355 (4)	0.2890 (9)	2.8 (2)
C13	0.4909 (7)	0.5172 (5)	0.159 (1)	3.8 (2)
C14	0.9673 (7)	0.7852 (5)	0.839 (1)	4.0 (2)

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

O1—C2	1.414 (8)	C2—C7	1.53 (1)
O1—C3	1.425 (9)	C3—C4	1.53 (1)
O2—C2	1.410 (9)	C3—C13	1.49 (1)
O3—C10	1.372 (8)	C7—C8	1.37 (1)
O3—C14	1.42 (1)	C7—C12	1.38 (1)
N—C1	1.514 (9)	C8—C9	1.38 (1)
N—C4	1.493 (9)	C9—C10	1.40 (1)
N—C5	1.48 (1)	C10—C11	1.37 (1)
N—C6	1.522 (9)	C11—C12	1.35 (1)
C1—C2	1.53 (1)		
C2—O1—C3	113.1 (5)	O1—C3—C4	110.4 (6)
C10—O3—C14	119.0 (6)	O1—C3—C13	107.7 (6)
C1—N—C4	108.1 (5)	C4—C3—C13	111.9 (6)
C1—N—C5	112.4 (5)	N—C4—C3	111.8 (5)
C1—N—C6	107.4 (6)	C2—C7—C8	121.7 (6)
C4—N—C5	112.8 (5)	C2—C7—C12	119.2 (6)
C4—N—C6	107.9 (5)	C8—C7—C12	118.8 (7)
C5—N—C6	108.0 (6)	C7—C8—C9	121.6 (6)
N—C1—C2	114.0 (5)	C8—C9—C10	118.0 (7)
O1—C2—O2	111.5 (5)	O3—C10—C9	123.1 (6)
O1—C2—C1	110.4 (5)	O3—C10—C11	117.2 (6)
O1—C2—C7	108.7 (6)	C9—C10—C11	119.7 (6)
O2—C2—C1	108.3 (6)	C10—C11—C12	121.1 (7)
O2—C2—C7	111.5 (5)	C7—C12—C11	120.7 (7)
C1—C2—C7	106.3 (6)		
C2—O1—C3—C4	60.1 (7)	N—C1—C2—O2	−69.8 (7)
C4—N—C1—C2	−50.5 (7)	O2—C2—C7—C12	−38.5 (8)
N—C1—C2—O1	52.6 (8)	H2OH—O2—C2—O1	46 (6)

Compound (2)

Crystal data

$C_{13}H_{20}NO_2^+.Br^-.xH_2O$
(x = 1/3)
$M_r = 308.2$
Monoclinic
$P2_1/n$
$a = 8.451\ (3)$ Å
$b = 13.535\ (2)$ Å
$c = 12.915\ (2)$ Å
$\beta = 93.38\ (2)°$
$V = 1474.8\ (9)$ Å^3
$Z = 4$
$D_x = 1.388$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 1–25°$
$\mu = 2.8$ mm^{-1}
$T = 298$ K
Needle
0.38 × 0.10 × 0.06 mm
Colorless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega–2\theta$ scans
Absorption correction: empirical
$T_{min} = 0.914$, $T_{max} = 0.994$
2889 measured reflections
2583 independent reflections
1705 observed reflections [$I > \sigma(I)$]

$R_{int} = 0.024$
$\theta_{max} = 25°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 16$
$l = -15 \rightarrow 15$
3 standard reflections
frequency: 177 min
intensity variation: −3.4% (linear correction)

Refinement

Refinement on F
$R = 0.044$
$wR = 0.033$
$S = 1.388$
1705 reflections
244 parameters
$w = 4F_o^2[\sigma^2(I) + (0.02F_o^2)^2]^{-1}$

$(\Delta/\sigma)_{max} = 0.03$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (2)

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Br	0.71862 (5)	0.67662 (4)	0.09612 (3)	5.18 (1)
O1	0.7140 (3)	0.7343 (2)	0.5168 (2)	4.09 (6)
O2	0.5427 (3)	0.8658 (2)	0.4807 (2)	4.45 (6)
N	0.8453 (4)	0.8648 (2)	0.3673 (2)	4.00 (7)
C1	0.8171 (4)	0.8951 (3)	0.4766 (3)	3.48 (9)
C2	0.6897 (4)	0.8372 (3)	0.5285 (3)	3.51 (8)
C3	0.7317 (5)	0.7021 (3)	0.4127 (3)	4.6 (1)
C4	0.8676 (5)	0.7545 (3)	0.3667 (3)	4.5 (1)
C5	0.9943 (5)	0.9145 (4)	0.3358 (3)	5.8 (1)
C6	0.7126 (5)	0.8957 (3)	0.2918 (3)	4.9 (1)
C7	0.7016 (4)	0.8594 (3)	0.6434 (3)	3.27 (8)
C8	0.6472 (5)	0.9481 (3)	0.6793 (3)	4.4 (1)
C9	0.6632 (5)	0.9714 (3)	0.7836 (3)	5.3 (1)
C10	0.7313 (5)	0.9052 (4)	0.8530 (3)	5.8 (1)
C11	0.7885 (5)	0.8173 (3)	0.8184 (3)	5.4 (1)
C12	0.7741 (5)	0.7946 (3)	0.7142 (3)	4.5 (1)
C13	0.7581 (7)	0.5918 (3)	0.4170 (4)	7.9 (2)
O1*W*	0.949 (1)	0.8705 (8)	0.0874 (7)	7.6 (3)

Table 4. *Selected geometric parameters* (Å, °) *for* (2)

O1—C2	1.417 (4)	C3—C4	1.502 (6)
O1—C3	1.429 (5)	C3—C13	1.511 (6)
O2—C2	1.409 (4)	C7—C8	1.376 (5)
N—C1	1.502 (5)	C7—C12	1.384 (5)
N—C4	1.504 (5)	C8—C9	1.382 (6)
N—C5	1.505 (5)	C9—C10	1.369 (9)
N—C6	1.501 (5)	C10—C11	1.369 (7)
C1—C2	1.519 (5)	C11—C12	1.379 (5)
C2—C7	1.511 (5)		
C2—O1—C3	115.1 (3)	C1—C2—C7	108.9 (3)
C1—N—C4	107.6 (3)	O1—C3—C4	110.7 (3)
C1—N—C5	108.3 (3)	O1—C3—C13	106.8 (3)
C1—N—C6	112.4 (3)	C4—C3—C13	111.5 (4)
C4—N—C5	109.6 (3)	N—C4—C3	111.5 (3)
C4—N—C6	111.2 (3)	C2—C7—C8	120.0 (3)
C5—N—C6	107.8 (3)	C2—C7—C12	121.6 (3)
N—C1—C2	115.4 (3)	C8—C7—C12	118.3 (3)
O1—C2—O2	110.7 (3)	C7—C8—C9	120.8 (4)
O1—C2—C1	110.4 (3)	C8—C9—C10	120.1 (4)
O1—C2—C7	107.4 (3)	C9—C10—C11	119.8 (4)
O2—C2—C1	107.1 (3)	C10—C11—C12	120.0 (4)
O2—C2—C7	112.4 (3)	C7—C12—C11	120.9 (4)
C2—O1—C3—C4	57.8 (4)	N—C1—C2—O2	−71.2 (4)
C4—N—C1—C2	−50.5 (4)	O2—C2—C7—C8	−42.9 (5)
N—C1—C2—O1	49.4 (4)	H2OH—O2—C2—O1	76 (2)

R_{int} was not calculated for (1) as there were no redundant data. For (1), the hydroxyl H atom was refined isotropically. All other H atoms were placed in calculated positions with $B = 1.3 \times B_{eq}$ of the bonded C atom. Refinement of the inversion-related structure yielded $R = 0.0465$, $wR = 0.0471$ and $S = 2.187$.

For (2), the H atoms were refined, except for those of the water molecule which were not located. Refinement of the water molecule as fully occupied led to $B = 40$ Å^2. Refinement of the occupation factor for O1*W* led to $x = 0.334\,(5)$. The values quoted for the density *etc.* are for $x = 1/3$.

Programs used included *MolEN* (Fair, 1990) and *ORTEP* (Johnson, 1965).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and torsion angles have been deposited with the IUCr (Reference: CR1117). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2,2-Dimethyl-5-(dimethylamino)indan-1,3-dione

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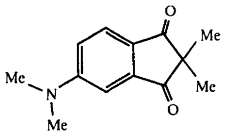
Abstract

The title compound, $C_{13}H_{15}NO_2$, lies on a crystallographic mirror plane. The indan-1,3-dione and the dimethylamino systems are therefore coplanar. The C—C—C angle formed by the *gem*-dimethyl groups is 110.3 (1)° and the C—C—C—O torsion angles which they form with the carbonyl O atoms have magnitudes of 61.6 (1) and 61.3 (1)°. The C=O distances are 1.217 (2) and 1.210 (2) Å. The *N*-methyl groups lying on the crystallographic mirror plane have their atoms disordered into half-populated positions. The N—C(methyl) distances are 1.432 (2) and 1.447 (2) Å.

Comment

As part of an ongoing study on nucleophilic aromatic substitution reactions with the fluoride ion, a number of substituted indan-1,3-diones were required (Enas, Garcia, Mathis & Gerdes, 1993). The crystal structures of a number of substituted indan-1,3-diones have been studied over the last 20 years on account of the well known anticoagulant activity of the parent compound in vitamin K-dependent biosynthesis (Ernster, Lind & Rase, 1972; Bravic, Gaultier & Hauw, 1974; Csöregh & Eckstein, 1979). The title compound, (I), was prepared in four steps from the known 2,2-dimethyl-1-indanone (Ohkata, Akiyama, Wada, Shun, Toda & Hanafusa, 1984), affording yellow needles when recrystallized by slow cooling and evaporation of ethanol.



(I)

The geometry about the N atom is perfectly planar, with angle magnitudes for C11—N—C5, C5—N—C12 and C11—N—C12 of 121.5 (1), 121.4 (1) and 117.1 (1)°, respectively. The *gem*-dimethyl groups are almost perfectly *gauche* to the carbonyl O atoms with magnitudes for C10—C9—C1—O1 and C10—C9—C8—O2 of 61.6 (1) and −61.3 (1)°, respectively, deviating only slightly from the perfect *gauche* conformation value of 60° (Klyne & Prelog, 1960).

Structural data for 2-ethyl-2-nitroindan-1,3-dione (Garcia, Enas, Chang & Fronczek, 1993), 5-amino-2,2-dimethylindan-1,3-dione and 2,2-dimethyl-5-nitroindan-1,3-dione (Garcia, Enas & Fronczek, 1993), 2-nitroindan-1,3-dione dihydrate (Selenius & Lundgren, 1980), and 2-(2-nitrobenzylidene)indan-1,3-dione (Varghese, Srinivasan, Ramadas & Padmanabhan, 1986) are in agreement with those of the title compound. Examples of planar dimethylamino-aromatic groups in agreement with that of the title compound are *trans*-1-(2-chloro-4-dimethylaminophenyl)-2-nitroethylene (Cameron, Cowley & Thompson, 1974), *N*,*N*-dimethyl-2,4-dinitro-3-toluidine (Maurin & Krygowski, 1987) and 9-(4-dimethylamino-2-methylphenyl)-10-methylacridinium chloride dihydrate (Reiss, Goubitz & Heijdenrijk, 1989).

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