turn, is slightly shorter (though not significantly) than that in (II) [1·486 (5) Å]. Allen & Kirby (unpublished results) have determined that the average length for a $C(sp^3)$—O bond of the type R_3C—OC(=O)— is 1·473 (2) Å so it can only be stated that the $C(sp^3)$—O length in (II) may be sufficiently elongated to be consistent with the reactivity of (II).

Molecule (I) packs as hydrogen-bonded dimers around centers of symmetry with O(11) to O(12) separations of 2·837 (2) Å (the molecule at x,y,z is hydrogen bonded to the molecule at $1-x$, $-y$, $1-z$). All other intermolecular distances in (I) and all in (II) correspond to normal van der Waals contacts.

References

BUCOURT, R. (1974). *Topics in Stereochemistry*, edited by E. L. ELIEL & N. L. ALLINGER, pp. 159–224. New York: John Wiley.
BUYS, H. R. & GEISE, H. J. (1970). *Tetrahedron Lett.* pp. 2991–2992.
CHADWICK, D. J. & DUNITZ, J. D. (1979). *J. Chem. Soc. Perkin Trans.* 2, pp. 276–284.
CROMER, D. T. & WABER, J. T. (1965). *Acta Cryst.* **18**, 104–109.
GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* A**27**, 368–376.
HARLOW, R. L. & SIMONSEN, S. H. (1976). *Acta Cryst.* B**32**, 2137–2144.
JEFFREY, G. A., ROSENSTEIN, R. D. & VLASSE, M. (1967). *Acta Cryst.* **22**, 725–733.
JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3974. Oak Ridge National Laboratory, Tennessee.
JONES, D. S. & KARLE, I. L. (1974). *Acta Cryst.* B**30**, 624–627.
JONES, P. G. & KIRBY, A. J. (1979). *J. Chem. Soc. Chem. Commun.* pp. 288–289.
MAYER, B. J., SPENCER, T. A. & ONAN, K. D. (1984). *J. Am. Chem. Soc.* In the press.
ONAN, K. D., MAYER, B. J. & SPENCER, T. A. (1984). *Acta Cryst.* C**40**, 1044–1047.
STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

Acta Cryst. (1984). C**40**, 1044–1047

The Structures of 9-Hydroxy-10-methyl-*trans*-2-decalone, $C_{11}H_{18}O_2$ (I), and 9-Acetoxy-10-methyl-*trans*-2-decalone, $C_{13}H_{20}O_3$ (II)[*]

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Abstract. (I): $M_r = 182{\cdot}3$, monoclinic, $P2_1/c$, $a = 12{\cdot}325$ (1), $b = 6{\cdot}357$ (1), $c = 14{\cdot}400$ (1) Å, $\beta = 116{\cdot}70$ (8)°, $U = 1008$ Å^3, $Z = 4$, D_m(flotation) = 1·19, $D_x = 1{\cdot}201$ g cm^{-3}, μ(Cu $K\alpha$) = 6·48 cm^{-1}, $F(000) = 400$, room temperature, final $R = 0{\cdot}059$ for 1199 reflections. (II): $M_r = 224{\cdot}3$, monoclinic, $P2_1/n$, $a = 7{\cdot}822$ (1), $b = 10{\cdot}731$ (1), $c = 15{\cdot}052$ (2) Å, $\beta = 101{\cdot}02$ (1)°, $U = 1240$ Å^3, $Z = 4$, D_m(flotation) = 1·19, $D_x = 1{\cdot}201$ g cm^{-3}, μ(Cu $K\alpha$) = 6·85 cm^{-1}, $F(000) = 488$, room temperature, final $R = 0{\cdot}069$ over 1424 reflections. Both molecules adopt relatively undistorted chair–chair conformations. In (II) the ester carbonyl group is synplanar to the $C(sp^3)$—O bond. All intermolecular separations for (I) and (II) appear to be normal van der Waals contacts apart from a weak O···O hydrogen bond of 2·938 (3) Å in (I).

Introduction. In the preceding communication (Onan, Mayer & Spencer, 1984) the structures of two *cis* decalones were described. This communication reports the structures of two *trans* decalones, 9-hydroxy-10-methyl-*trans*-2-decalone (I) and 9-acetoxy-10-methyl-*trans*-2-decalone (II), which were needed for comparison with the structures of the aforementioned *cis* decalones and for a projected comparison with the structures of *trans* decalones bearing an additional axial substituent at C(6). The latter compounds are being used in studies of intramolecular α-proton transfer (Jacobs, Nelson & Spencer, 1980; Gula, Vitale & Spencer, unpublished results).

Experimental. Pastille-shaped crystals of (I) were obtained by slow evaporation from a solution of ether and methanol, chunky crystals of (II) were grown from ether, crystal dimensions *ca* 0·16 × 0·24 × 0·40 mm (I) and 0·20 × 0·20 × 0·25 mm (II); Syntex $P2_1$ automated diffractometer, Cu $K\alpha$ radiation, cell

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[*] 8a-Hydroxy-4a-methyl-*trans*-decahydro-2-naphthalenone and 4a-methyl-2-oxo-*trans*-decahydro-8a-naphthyl acetate, respectively.
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Table 1. *Fractional atomic coordinates of the non-hydrogen atoms* ($\times 10^4$) *and equivalent isotropic temperature factors* ($\times 10^4$) *for* (I) *and* (II), *with estimated standard deviations in parentheses*

$$U_{eq} = \tfrac{1}{3}(U_{11} + U_{22} + U_{33} + 2U_{13}\cos\beta).$$

	x	*y*	*z*	U_{eq}
Compound I				
C(1)	4312 (2)	7206 (4)	5742 (2)	470
C(2)	4381 (2)	5197 (4)	6303 (1)	455
C(3)	3366 (2)	4773 (4)	6578 (2)	436
C(4)	2114 (2)	5220 (4)	5673 (2)	419
C(5)	808 (2)	7593 (4)	4199 (2)	469
C(6)	705 (2)	9574 (5)	3572 (2)	564
C(7)	1738 (2)	9705 (5)	3263 (2)	587
C(8)	2973 (2)	9493 (4)	4210 (2)	517
C(9)	3060 (2)	7475 (4)	4815 (1)	388
C(10)	2038 (2)	7366 (3)	5162 (1)	353
O(11)	5230 (1)	3976 (3)	6544 (1)	668
O(12)	2872 (1)	5679 (3)	4152 (1)	468
C(16)	2163 (2)	9097 (4)	5944 (2)	487
Compound II				
C(1)	6084 (4)	6368 (3)	4037 (2)	545
C(2)	4646 (4)	6577 (3)	4563 (2)	598
C(3)	2851 (4)	6720 (3)	4021 (2)	714
C(4)	2783 (4)	7621 (3)	3227 (2)	592
C(5)	4181 (4)	8449 (3)	1967 (2)	625
C(6)	5656 (5)	8373 (3)	1441 (2)	720
C(7)	7412 (4)	8245 (3)	2061 (2)	662
C(8)	7457 (4)	7203 (3)	2749 (2)	558
C(9)	5992 (3)	7337 (2)	3285 (2)	441
C(10)	4184 (4)	7377 (3)	2655 (2)	498
O(11)	4960 (4)	6600 (3)	5378 (2)	952
O(12)	6092 (2)	8577 (2)	3719 (1)	440
C(13)	7520 (4)	8982 (3)	4288 (2)	553
O(14)	8841 (3)	8394 (2)	4504 (2)	825
C(15)	7237 (5)	10279 (3)	4616 (2)	758
C(16)	3781 (4)	6140 (3)	2141 (2)	701

parameters by least squares from 2θ values of 13 reflections with $62 \leq 2\theta \leq 92°$ (I) and 15 reflections with $53 \leq 2\theta \leq 78°$ (II), $\theta/2\theta$ scans, variable-speed scan, $4 \leq 2\theta \leq 130°$, 1622 (I) and 1845 (II) independent reflections collected, 1199 with $I > 2\sigma(I)$ considered observed for (I), 1424 for (II); two check reflections measured every 98 reflections for (I) and every 48 reflections for (II) showed a maximum variation of 6% with no trend for (I) and a maximum variation of 10% with a diminution of *ca* 6% for (II); Lorentz–polarization and empirical absorption corrections applied, scattering factors for C and O from Cromer & Waber (1965), for H from Stewart, Davidson & Simpson (1965); structures solved by direct methods [*MULTAN*80 (Germain, Main & Woolfson, 1971)], full-matrix least-squares refinement minimizing $\sum w||F_o| - |F_c||^2$ with weights $w^{1/2} = 1$ for $|F_o| \leq 7{\cdot}0$ and $w^{1/2} = 7{\cdot}0/|F_o|$ for $|F_o| > 7{\cdot}0$ (program based on *FMLS* by P. K. Gantzel, R. A. Sparks and K. N. Truebloood, modified by A. T. McPhail); all H atoms for (I) located in a difference synthesis, as were all except the acetoxy methyl H atoms for (II), anisotropic temperature factors for non-hydrogen atoms, isotropic factors for H atoms; inspection of F_o *vs* F_c values for low-angle reflections of high intensity indicated secondary extinction and six reflections (002, $1\bar{1}0$, $1\bar{1}1$, $20\bar{2}$, 200, $40\bar{4}$) were removed from the data set for (I) and one reflection (012) was removed from the data set for (II); convergence for (I) at $R = 0{\cdot}059$, $wR = 0{\cdot}056$, $S = 0{\cdot}428$, $\Delta_{\text{mean}}/\sigma_{\text{max}} = 0{\cdot}060$ for non-hydrogen atoms, maximum $\Delta\rho$ peak 0·28 e Å^{-3}; for (II) $R = 0{\cdot}069$, $wR = 0{\cdot}068$, $S = 0{\cdot}543$, $\Delta_{\text{mean}}/\sigma_{\text{max}} = 0{\cdot}073$ for non-hydrogen atoms, maximum $\Delta\rho$ peak 0·32 e Å^{-3};[*] *ORTEP* (Johnson, 1965) was used for drawings of single molecules.

Discussion. Final atomic parameters for the non-hydrogen atoms of (I) and (II) are listed in Table 1. The molecular conformations of the *trans*-fused molecules are shown in Figs. 1 and 2, respectively, each with the numbering scheme employed. Bond lengths and angles for (I) and (II), and analogous atoms in 9-methoxycarbonyl-*trans*-2-decalone[†] (Chadwick & Dunitz, 1979) (III), are compared in Table 2. Endocyclic torsion angles for (I), (II) and (III) are given in Table 3.

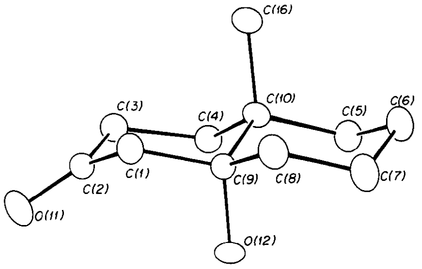

Fig. 1. View of 9-hydroxy-10-methyl-*trans*-2-decalone with the atom-numbering scheme.

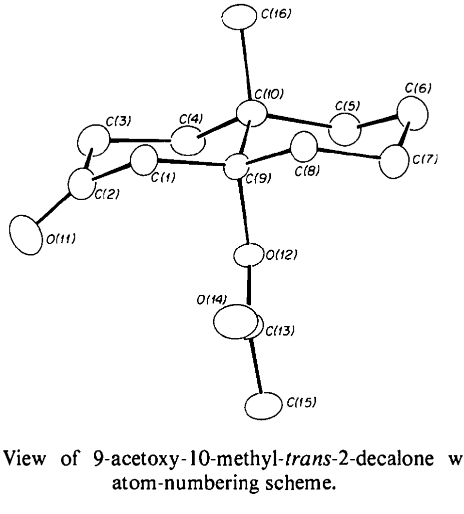

Fig. 2. View of 9-acetoxy-10-methyl-*trans*-2-decalone with the atom-numbering scheme.

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[*] Lists of structure factors, anisotropic thermal parameters and hydrogen-atom parameters and a complete table of torsion angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39229 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

[†] Methyl-2-oxo-*trans*-decahydro-8a-naphthalenecarboxylate.

Table 2. *Interatomic distances* (Å) *and valency angles* (°) *for* (I), (II) *and* (III), *with estimated standard deviations in parentheses*

	(I)	(II)	(III)*
C(1)—C(2)	1·493 (3)	1·511 (4)	1·504
C(1)—C(9)	1·531 (3)	1·529 (4)	1·541
C(2)—C(3)	1·497 (3)	1·491 (4)	1·509
C(2)—O(11)	1·222 (3)	1·205 (4)	1·214
C(3)—C(4)	1·534 (3)	1·530 (5)	1·521
C(4)—C(10)	1·532 (3)	1·541 (4)	1·530
C(5)—C(6)	1·521 (4)	1·521 (5)	1·522
C(5)—C(10)	1·534 (3)	1·548 (4)	1·524
C(6)—C(7)	1·528 (3)	1·512 (5)	1·526
C(7)—C(8)	1·527 (3)	1·521 (4)	1·525
C(8)—C(9)	1·527 (3)	1·528 (4)	1·539
C(9)—C(10)	1·552 (3)	1·546 (4)	1·558
C(9)—O(12)	1·439 (3)	1·478 (3)	
C(10)—C(16)	1·532 (3)	1·538 (4)	
O(12)—C(13)		1·344 (3)	
C(13)—O(14)		1·202 (4)	
C(13)—C(15)		1·507 (5)	
C(2)—C(1)—C(9)	111·0 (2)	110·7 (2)	114·9
C(1)—C(2)—C(3)	116·5 (2)	116·5 (2)	116·1
C(1)—C(2)—O(11)	122·0 (2)	120·6 (3)	121·6
C(3)—C(2)—O(11)	121·4 (2)	122·8 (3)	122·1
C(2)—C(3)—C(4)	112·5 (2)	112·4 (3)	113·9
C(3)—C(4)—C(10)	113·2 (2)	114·0 (2)	112·2
C(6)—C(5)—C(10)	113·5 (2)	113·8 (3)	110·8
C(5)—C(6)—C(7)	111·1 (2)	112·0 (3)	110·9
C(6)—C(7)—C(8)	111·2 (2)	112·8 (3)	111·6
C(7)—C(8)—C(9)	111·7 (2)	111·6 (2)	113·9
C(1)—C(9)—C(8)	112·1 (2)	113·1 (2)	110·4
C(1)—C(9)—C(10)	111·1 (2)	112·4 (2)	108·9
C(1)—C(9)—O(12)	106·8 (2)	107·1 (2)	107·7
C(8)—C(9)—C(10)	111·2 (2)	111·7 (2)	108·2
C(8)—C(9)—O(12)	109·8 (2)	109·7 (2)	108·9
C(10)—C(9)—O(12)	105·4 (2)	102·2 (2)	112·7
C(4)—C(10)—C(5)	109·9 (2)	109·7 (2)	113·7
C(4)—C(10)—C(9)	108·1 (2)	109·1 (2)	113·7
C(4)—C(10)—C(16)	108·8 (2)	109·2 (2)	
C(5)—C(10)—C(9)	108·7 (2)	108·4 (2)	111·0
C(5)—C(10)—C(16)	109·2 (2)	109·4 (2)	
C(9)—C(10)—C(16)	112·1 (2)	111·1 (2)	
C(9)—O(12)—C(13)		122·7 (2)	
O(12)—C(13)—O(14)		124·7 (3)	
O(12)—C(13)—C(15)		110·6 (2)	
O(14)—C(13)—C(15)		124·7 (3)	

* Chadwick & Dunitz (1979); estimated standard deviations are *ca* 0·003 Å for bond lengths and 0·2° for bond angles.

Table 3. *Endocyclic torsion angles* (°) *for* (I), (II) *and* (III), *with estimated standard deviations in parentheses*

	(I)	(II)*	(III)†
Ring *A*			
C(9)—C(1)—C(2)—C(3)	−49·4 (2)	−49·9 (3)	−45·9
C(1)—C(2)—C(3)—C(4)	45·4 (2)	46·7 (3)	43·6
C(2)—C(3)—C(4)—C(10)	−48·7 (2)	−48·2 (3)	−46·8
C(3)—C(4)—C(10)—C(9)	55·7 (2)	52·9 (2)	53·6
C(4)—C(10)—C(9)—C(1)	−59·5 (2)	−56·2 (2)	−53·8
C(10)—C(9)—C(1)—C(2)	56·2 (2)	54·4 (2)	49·2
Ring *B*			
C(10)—C(5)—C(6)—C(7)	55·1 (2)	52·5 (3)	57·6
C(5)—C(6)—C(7)—C(8)	−53·5 (2)	−50·9 (3)	−53·7
C(6)—C(7)—C(8)—C(9)	55·4 (2)	53·5 (2)	53·4
C(7)—C(8)—C(9)—C(10)	−57·1 (2)	−56·7 (3)	−53·7
C(8)—C(9)—C(10)—C(5)	55·7 (2)	56·0 (2)	56·5
C(9)—C(10)—C(5)—C(6)	−55·4 (2)	−54·4 (3)	−59·9

* The signs of the torsion angles for (II) are the reverse of those which would be calculated from the coordinates in Table 1.

† Chadwick & Dunitz (1979).

As expected, the *trans*-2-decalone systems of both (I) and (II) adopt chair–chair conformations. The cyclohexanone ring in each is flattened slightly beyond the accepted standard [mean endocyclic dihedral angles: 52·5 (5)° (I), 51·5 (4)° (II), cyclohexanone (Bucourt, 1974) 54·2°] while the cyclohexane-ring conformation in each is nearly ideal [mean endocyclic dihedral angles: 55·4 (12)° (I), 54·0 (22)° (II), cyclohexane (Buys & Geise, 1970) 55·9°].* The conformations of these rings are similar to those in (III) except that the *A* ring in (III) is flatter (mean dihedral angle 48·8°). This substantial closing of dihedral angles in (III) is due to the orientation of the bridgehead $-CO_2CH_3$ group. In (III) the bridgehead methoxycarbonyl is oriented in the preferred conformation for esters (Dunitz & Strickler, 1968), *i.e.* with the $-C{=}O$ group synplanar with respect to a $C^{\alpha}-C^{\beta}$ bond, in this case the C(8)—C(9) bond. This causes the transannular interactions which so substantially flatten the *A* ring in (III). In (II) there is no $C^{\alpha}-C^{\beta}$ bond. The O(12)—C(13) bond of the acetoxy group is *gauche* to both the C(1)—C(9) and C(8)—C(9) bonds and the $-C{=}O$ group is synplanar with the C(9)—O(12) bond [C(9)—O(12)—C(13)—O(14) 0·2 (3)°].

Comparison of the observed bond lengths and angles in Table 2 indicates only small differences between molecules and shows most parameters to lie within normal ranges. The main differences occur about the cyclohexanone carbonyl group. Though the sums of the C(1)—C(2) and C(2)—O(11) bond lengths are the same for both (I) and (II), in (II) the C(2)—O(11) bond is significantly shorter than that in (I). Also in (II), the C(1)—C(2)—O(11) angle is smaller than the C(3)—C(2)—O(11) angle while the opposite is true for (I). Although the mean $C(sp^3)-C(sp^3)$ bond length is 1·532 Å for (I) and 1·531 Å for (II), the C(9)—C(10) bond is slightly longer in each, 1·552 for (I) and 1·546 Å for (II). These values are very similar to those observed in a variety of *trans*-fused ring systems, *e.g.* in (III) 1·558 Å, in *trans*-2-decalone (Schubert, Schäfer & Pauli, 1974) (studied by electron diffraction) 1·548 Å, in 8a-*tert*-butyl-*trans*-decahydroquinoline picrate (Hargrave & Eliel, 1980) 1·549 Å, and in 5α-androstane-3,17-dione (Coiro, Giglio, Lucano & Puliti, 1973) 1·554 Å. This length in (I) is also identical to that in 9-hydroxy-10-methyl-*cis*-2-decalone (IV) (Onan, Mayer & Spencer, 1984). The C(9)—O(12) bond in (II), 1·478 (3) Å, is significantly longer than the 1·439 (3) Å distance in (I) and the 1·440 Å C(methyl)—O(carboxylate) bond in (III). The 1·439 (3) Å length in (I) is, however, essentially identical with that in its *cis* analogue, (IV) (1·434 (2) Å).

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* Standard deviations quoted for means are sample standard deviations; estimated standard deviations for individual torsion angles in (I) are *ca* 0·2° and in (II), *ca* 0·3°.

Molecules of alcohol (I) dimerize about a center of symmetry with rather weak hydrogen bonds, O(11)··· O(12) 2·938 (3) Å. All other intermolecular separations for (I) and all intermolecular separations for (II) appear to be normal van der Waals contacts.

References

BUCOURT, R. (1974). *Topics in Stereochemistry*, edited by E. L. ELIEL & N. L. ALLINGER, pp. 159–224. New York: John Wiley.

BUYS, H. R. & GEISE, H. J. (1970). *Tetrahedron Lett.* pp. 2991–2992.

CHADWICK, D. J. & DUNITZ, J. D. (1979). *J. Chem. Soc. Perkin Trans.* 2, pp. 276–284.

COIRO, V. M., GIGLIO, E., LUCANO, A. & PULITI, R. (1973). *Acta Cryst.* B**29**, 1404–1409.

CROMER, D. T. & WABER, J. T. (1965). *Acta Cryst.* **18**, 104–109.

DUNITZ, J. D. & STRICKLER, P. (1968). *Structural Chemistry and Molecular Biology*, edited by A. RICH & N. DAVIDSON, p. 443. San Francisco: Freeman.

GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* A**27**, 368–376.

HARGRAVE, K. D. & ELIEL, E. L. (1980). *Isr. J. Chem.* **20**, 127–132.

JACOBS, J. N., NELSON, J. A. & SPENCER, T. A. (1980). *J. Org. Chem.* **45**, 1645–1650.

JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.

ONAN, K. D., MAYER, B. J. & SPENCER, T. A. (1984). *Acta Cryst.* C**40**, 1041–1044.

SCHUBERT, W., SCHÄFER, L. & PAULI, G. H. (1974). *J. Mol. Struct.* **21**, 53–60.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

Acta Cryst. (1984). C**40**, 1047–1050

A 1:2 Complex between 1,4,7,10,13,16-Hexaoxacyclooctadecane (18-Crown-6) and 2-(2-Benzimidazolyl)guanidine, $C_{12}H_{24}O_6.2C_8H_9N_5$

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Abstract. $M_r = 614{\cdot}7$, monoclinic, $C2/c$, $a = 20{\cdot}894$ (4), $b = 8{\cdot}399$ (1), $c = 18{\cdot}330$ (3) Å, $\beta = 93{\cdot}09$ (2)°, $V = 3212$ (1) Å^3, $D_x = 1{\cdot}271$ Mg m^{-3}, $Z = 4$, $F(000) = 1312$, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}5418$ Å, $\mu(\mathrm{Cu}\,K\alpha) = 0{\cdot}77$ mm^{-1}, $T = 293$ K, $R = 0{\cdot}049$ for 1462 independent reflexions. The 18-crown-6 molecule lies at an inversion center and adopts the D_{3d} conformation. Two guest 2-(2-benzimidazolyl)guanidine molecules, related by the same center of symmetry, bind to the crown ether *via* (guanidine)N—H···O hydrogen bonds. Additional stabilization is provided by intramolecular N—H···N, as well as intermolecular base-pairing N—H···N hydrogen bonding involving guest molecules. The structure is compared with that of the known isomorphous analogue, (1,10-diaza-18-crown-6).[2-(2-benzimidazolyl)guanidine]$_2$.

Introduction. Molecular-mechanics calculations on 18-crown-6 (Bovill, Chadwick & Sutherland, 1980) indicate that the D_{3d} conformation lies 32·8 kJ mol^{-1} above the lowest-energy conformation. The lowest-energy conformation corresponds to that adopted in the crystalline state (Dunitz & Seiler, 1974). The D_{3d} conformation would be the lowest-energy conformation if it were not for the unfavorable dipolar interactions between the three O atoms on each face. The D_{3d} conformation becomes favored when the dipolar interactions are minimized by coordination to electron acceptors. Trigonal acceptors (—XH$_3$) or acceptors bridging alternate ether O atoms stabilize the D_{3d} conformation. Unfavorable or widely separated acceptor sites can lead to the stabilization of alternate conformations.

The replacement of ether O atoms by —NH— groups provides sites which can act as either electron or proton donors. In the 1:4 complex of 1,10-diaza-18-crown-6 with thiourea the aza-group H atom bonds intramolecularly to an adjacent ether O which aids in the stabilization of a biangular conformation (Weber, 1982). In the 1:2 complex of 1,10-diaza-18-crown-6 with 2-(2-benzimidazolyl)guanidine the crown adopts a D_{3d} conformation (Watson, Galloy, Grossie, Vögtle &

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