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A 1:1 Adduct Between the *trans–transoid–trans* Isomer of 2,3,11,12-Tetra-anisyl-18-crown-6 with the (*RRRR*)-Configuration and Ammonia–Borane

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Abstract. (2*R*,3*R*,11*R*,12*R*)-2,3,11,12-Tetrakis-4-methoxyphenyl-1,4,7,10,13,16-hexaoxacyclooctadecane–ammonia–borane–methanol (4/4/4/3), $C_{40}H_{48}O_{10}.BH_3NH_3.0\cdot75CH_3OH$, $M_r = 744$, triclinic, $P1$, $a = 7\cdot995$ (2), $b = 11\cdot035$ (2), $c = 13\cdot371$ (4) Å, $\alpha = 68\cdot34$ (2), $\beta = 74\cdot62$ (2), $\gamma = 82\cdot84$ (2)°, $V = 1057$ Å^3, $Z = 1$, $D_x = 1\cdot17$ Mg m^{-3}, $\lambda(\text{Cu } K\alpha) = 1\cdot54178$ Å, $\mu = 0\cdot65$ mm^{-1}, $F(000) = 399\cdot5$, room temperature, $R = 0\cdot044$ for 2765 unique observed reflections with $|F_o| > 3\sigma(|F_o|)$. One molecule of BH_3NH_3 is hydrogen bonded through its NH_3 group to the nearer triangle of O atoms on one of the two homotopic faces of the title chiral receptor (4). In adopting an all-*gauche* conformation, the macrocyclic ring carries a pair of vicinal diequatorial anisyl groups and a pair of vicinal diaxial anisyl groups, one *syn* and the other *anti* to the bound BH_3NH_3 substrate molecule: the latter anisyl substituent totally obscures the 'free' face of the macrocycle, thus preventing adduct formation with a second BH_3NH_3 molecule.

Introduction. The fact that enantioselective reductions of aromatic ketones can be performed (Allwood, Shahriari-Zavareh, Stoddart & Williams, 1984) using the ammonia–borane (BH_3NH_3) adducts of the chiral *trans–transoid–trans*-tetraphenyl-18-crown-6 derivatives (9)* gives added significance to a determination of the solid-state structure of these adducts. In this paper, we (*a*) describe the preparation of a 1:1 adduct between the *trans–transoid–trans* isomer (4) of (2*R*,3*R*,11*R*,12*R*)-tetra-anisyl-18-crown-6, (*b*) report on the determination of its crystal structure, and (*c*) compare the structural characteristics of [(4).BH_3NH_3] with those already reported (Allwood *et al.*, 1984) for [(9).BH_3NH_3].

Experimental. Addition of an excess of ammonia–borane to a solution of (+)-(4) in methanol gave a crystalline adduct on removal of the solvent under vacuum. Recrystallization from methanol with *n*-hexane as a precipitant afforded single crystals of

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[*] In order to avoid repetition in the presentation of configurational formulae, the reader is referred to Pears, Shahriari-Zavareh, Stoddart, Crosby, Allwood & Williams (1988*c*; paper VII) and to Fig. 1 of Pears, Shahriari-Zavareh, Stoddart, Crosby, Allwood, Slawin & Williams (1988*a*; paper I).

[(4).BH_3NH_3] as a methanol solvate that were suitable for X-ray structural analysis. Crystal size: 0·43 × 0·43 × 0·28 mm. Refined unit-cell parameters obtained from centring 15 reflections. Nicolet *R*3*m* diffractometer. 2810 independent reflections ($\theta \leq 58°$) measured, Cu *Kα* radiation (graphite monochromator), ω scan. 2765 [$|F_o| > 3\sigma(|F_o|)$] considered observed, index range *h* 0/8, *k* −11/11, *l* −13/14; two check reflections measured every 50 reflections, net count constant; Lorentz and polarization corrections, no absorption correction. Structure solved by direct methods and ΔE map recycling; a ΔF map revealed the presence of an included molecule of methanol of estimated occupancy 0·75; non-hydrogen atoms refined anisotropically; BH_3, NH_3 and CH_3 groups refined as rigid bodies; positions of H atoms calculated (B—H 1·08, C—H 0·96 Å); H atoms assigned isotropic thermal parameters, $U(\mathrm{H}) = 1{\cdot}2\,U_{\mathrm{eq}}(X)$ (X = C, N, B), and allowed to ride on parent X atoms. The hydroxy proton on the methanol was not located. An empirical extinction correction was applied ($g = 0{\cdot}0282$). Refinement using *F* magnitudes by block-cascade full-matrix least squares; $R = 0{\cdot}044$; $wR = 0{\cdot}053$ [$w^{-1} = \sigma^2(F) + 0{\cdot}0016F^2$]; residual electron density in difference map within −0·15 and 0·19 e Å^{-3}; atomic scattering factors and dispersion corrections from *International Tables for X-ray Crystallography* (1974). Computations carried out on an Eclipse S140 computer using the *SHELXTL* program system (Sheldrick, 1983).

Discussion. Table 1* lists the fractional atomic coordinates of the non-hydrogen atoms, Table 2 the bond lengths and angles and selected torsion angles.

The structure of [(4).BH_3NH_3] is illustrated in Fig. 1 which includes the atomic numbering scheme. Fig. 2 shows space-filling representations of the 1:1 adduct viewed from opposite sides of the macrocyclic ring.

On 1:1 adduct formation with BH_3NH_3, the conformation of (4) retains its all-*gauche* geometry but changes from one with local pseudo-C_2 symmetry to another with the typical local pseudo-D_{3d} symmetry (Wipff, Weiner & Kollman, 1982; Wipff, Kollman & Lehn, 1983) that characterizes the vast majority of all 18-crown-6 derivatives when they bind substrates. However, in the case of [(4).BH_3NH_3], there is considerable distortion of the all-*gauche* conformation of the macrocyclic ring in (4) away from being as highly symmetrical as implied by the D_{3d} point group. This distortion is reflected in the relative dispositions of the six O atoms, which, instead of alternating equally above and below their mean plane, are disposed relative to each other such that five of them are essentially coplanar (with a maximum standard deviation of 0·03 Å), leaving the sixth one [O(16)] lying 0·6 Å away from this plane directed towards the bound BH_3NH_3 molecule. The anisyl groups are oriented such that one vicinal pair [located at C(8) and C(9)] are pseudo-axial whilst the other vicinal pair [located at C(17) and C(18)] are pseudo-equatorial. The BH_3NH_3 is bound (Figs. 1 and 2*a*) in a perching mode (Trueblood, Knobler, Lawrence & Stevens, 1982) to one face of the macrocycle: it would appear that steric interactions between the bound substrate and the *syn* axial anisyl substituent could be responsible for inducing the *anti* anisyl substituent to obscure (Fig. 2*b*) the other face of the macrocycle, thus preventing the approach of a second BH_3NH_3 molecule to form a 1:2 adduct as in

Table 1. *Atom coordinates* (×10^4) *and equivalent isotropic temperature factors* (Å^2×10^3)

	x	*y*	*z*	U_{eq}*
O(1)	2626 (3)	13276 (2)	1462 (2)	72 (1)
C(2)	4167 (6)	13544 (4)	1641 (4)	90 (2)
C(3)	4149 (6)	12951 (3)	2856 (3)	84 (2)
O(4)	4771 (3)	11632 (2)	3108 (2)	76 (1)
C(5)	4856 (6)	11036 (3)	4234 (3)	86 (2)
C(6)	5284 (4)	9620 (4)	4492 (3)	79 (1)
O(7)	3955 (3)	9031 (2)	4352 (2)	69 (1)
C(8)	3476 (4)	7762 (3)	5114 (3)	65 (1)
C(9)	1556 (4)	7662 (3)	5184 (3)	69 (1)
O(10)	1393 (3)	7888 (2)	4106 (2)	70 (1)
C(11)	−172 (5)	7486 (3)	4031 (3)	84 (2)
C(12)	−284 (5)	8010 (4)	2860 (4)	88 (2)
O(13)	−493 (3)	9384 (2)	2516 (2)	77 (1)
C(14)	−861 (6)	9939 (4)	1455 (4)	96 (2)
C(15)	−972 (5)	11393 (4)	1123 (4)	91 (2)
O(16)	690 (3)	11860 (2)	929 (2)	77 (1)
C(17)	885 (4)	13215 (3)	287 (3)	68 (1)
C(18)	2643 (4)	13568 (3)	330 (3)	67 (1)
C(19)	4612 (4)	6698 (3)	4778 (3)	63 (1)
C(20)	5176 (5)	6785 (3)	3696 (3)	74 (1)
C(21)	6215 (5)	5823 (3)	3392 (3)	74 (1)
C(22)	6675 (4)	4726 (3)	4201 (3)	69 (1)
C(23)	6104 (5)	4606 (3)	5284 (3)	78 (1)
C(24)	5072 (5)	5581 (3)	5576 (3)	74 (1)
C(25)	458 (4)	8605 (3)	5697 (3)	71 (1)
C(26)	25 (5)	8311 (3)	6828 (3)	80 (1)
C(27)	−865 (6)	9181 (4)	7320 (3)	90 (2)
C(28)	−1350 (5)	10399 (4)	6647 (3)	82 (2)
C(29)	−967 (5)	10700 (3)	5515 (3)	83 (2)
C(30)	−68 (5)	9830 (3)	5035 (3)	77 (1)
C(31)	748 (4)	13496 (3)	−882 (3)	66 (1)
C(32)	−485 (4)	14384 (3)	−1337 (3)	72 (1)
C(33)	−628 (5)	14634 (3)	−2394 (3)	75 (1)
C(34)	477 (4)	14008 (3)	−3044 (3)	68 (1)
C(35)	1735 (5)	13127 (4)	−2615 (3)	79 (1)
C(36)	1823 (5)	12870 (3)	−1540 (3)	76 (1)
C(37)	3064 (4)	14974 (3)	−370 (3)	67 (1)
C(38)	4519 (5)	15264 (3)	−1280 (3)	74 (1)
C(39)	4919 (5)	16536 (4)	−1928 (3)	82 (1)
C(40)	3921 (5)	17553 (3)	−1712 (3)	79 (1)
C(41)	2496 (6)	17294 (4)	−832 (3)	89 (2)
C(42)	2087 (5)	16012 (4)	−170 (3)	84 (1)
O(43)	7724 (4)	3724 (3)	3973 (2)	91 (1)
C(44)	8693 (7)	3941 (5)	2898 (4)	106 (2)
O(45)	−2251 (4)	11345 (3)	7022 (3)	110 (1)
C(46)	−2553 (9)	11133 (6)	8163 (5)	123 (3)
O(47)	256 (4)	14335 (3)	−4090 (2)	87 (1)
C(48)	1364 (7)	13745 (5)	−4795 (4)	104 (2)
O(49)	4445 (4)	18764 (3)	−2420 (3)	103 (1)
C(50)	3489 (8)	19870 (4)	−2221 (5)	122 (3)
N	3271 (3)	10153 (3)	2031 (2)	66 (1)
B	4460 (7)	9852 (6)	1000 (4)	91 (2)
O(51)	7815 (8)	7625 (7)	424 (5)	142 (3)
C(52)	6852 (12)	6945 (8)	160 (7)	123 (4)

* Equivalent isotropic *U* defined as one third of the trace of the orthogonalized U_{ij} tensor.

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* Lists of structure-factor amplitudes, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44790 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å), *angles* (°) *and selected torsion angles* (°)

O(1)—C(2)	1·401 (6)	O(1)—C(18)	1·424 (4)
C(2)—C(3)	1·507 (6)	C(3)—O(4)	1·423 (4)
O(4)—C(5)	1·420 (5)	C(5)—C(6)	1·486 (5)
C(6)—O(7)	1·398 (5)	O(7)—C(8)	1·421 (3)
C(8)—C(9)	1·528 (5)	C(8)—C(19)	1·521 (4)
C(9)—O(10)	1·408 (5)	C(9)—C(25)	1·518 (5)
O(10)—C(11)	1·418 (5)	C(11)—C(12)	1·479 (7)
C(12)—O(13)	1·414 (4)	O(13)—C(14)	1·417 (5)
C(14)—C(15)	1·496 (6)	C(15)—O(16)	1·410 (5)
O(16)—C(17)	1·427 (4)	C(17)—C(18)	1·526 (5)
C(17)—C(31)	1·507 (5)	C(18)—C(37)	1·512 (4)
C(19)—C(20)	1·367 (5)	C(19)—C(24)	1·384 (4)
C(20)—C(21)	1·380 (5)	C(21)—C(22)	1·380 (4)
C(22)—C(23)	1·358 (5)	C(22)—O(43)	1·379 (4)
C(23)—C(24)	1·382 (5)	C(25)—C(26)	1·378 (5)
C(25)—C(30)	1·399 (4)	C(26)—C(27)	1·381 (6)
C(27)—C(28)	1·389 (5)	C(28)—C(29)	1·379 (6)
C(28)—O(45)	1·367 (6)	C(29)—C(30)	1·374 (6)
C(31)—C(32)	1·394 (5)	C(31)—C(36)	1·374 (5)
C(32)—C(33)	1·369 (5)	C(33)—C(34)	1·377 (5)
C(34)—C(35)	1·391 (5)	C(34)—O(47)	1·364 (5)
C(35)—C(36)	1·379 (6)	C(37)—C(38)	1·411 (4)
C(37)—C(42)	1·373 (5)	C(38)—C(39)	1·375 (5)
C(39)—C(40)	1·369 (6)	C(40)—C(41)	1·373 (5)
C(40)—O(49)	1·361 (4)	C(41)—C(42)	1·389 (5)
O(43)—C(44)	1·387 (5)	O(45)—C(46)	1·412 (7)
O(47)—C(48)	1·402 (6)	O(49)—C(50)	1·429 (6)
N—B	1·574 (6)	O(51)—C(52)	1·328 (14)

C(2)—O(1)—C(18)	114·6 (2)	O(1)—C(2)—C(3)	110·1 (3)
C(2)—C(3)—O(4)	109·4 (4)	C(3)—O(4)—C(5)	112·1 (3)
O(4)—C(5)—C(6)	110·0 (4)	C(5)—C(6)—O(7)	109·0 (3)
C(6)—O(7)—C(8)	117·9 (3)	O(7)—C(8)—C(9)	106·0 (2)
O(7)—C(8)—C(19)	112·2 (2)	C(9)—C(8)—C(19)	113·1 (3)
C(8)—C(9)—O(10)	107·4 (2)	C(8)—C(9)—C(25)	110·6 (3)
O(10)—C(9)—C(25)	113·1 (3)	C(9)—O(10)—C(11)	115·9 (2)
O(10)—C(11)—C(12)	109·0 (3)	C(11)—C(12)—O(13)	109·2 (4)
C(12)—O(13)—C(14)	112·3 (4)	O(13)—C(14)—C(15)	109·3 (4)
C(14)—C(15)—O(16)	109·3 (3)	C(15)—O(16)—C(17)	114·6 (3)
O(16)—C(17)—C(18)	106·3 (3)	O(16)—C(17)—C(31)	111·0 (3)
C(18)—C(17)—C(31)	112·4 (2)	O(1)—C(18)—C(17)	107·7 (2)
O(1)—C(18)—C(37)	112·4 (3)	C(17)—C(18)—C(37)	112·1 (3)
C(8)—C(19)—C(20)	122·0 (3)	C(8)—C(19)—C(24)	120·3 (3)
C(20)—C(19)—C(24)	117·7 (3)	C(19)—C(20)—C(21)	121·9 (3)
C(20)—C(21)—C(22)	119·3 (3)	C(21)—C(22)—C(23)	119·8 (3)
C(21)—C(22)—O(43)	123·3 (3)	C(23)—C(22)—O(43)	116·9 (3)
C(22)—C(23)—C(24)	120·2 (3)	C(19)—C(24)—C(23)	121·0 (3)
C(9)—C(25)—C(26)	121·0 (3)	C(9)—C(25)—C(30)	121·1 (3)
C(26)—C(25)—C(30)	117·8 (3)	C(25)—C(26)—C(27)	122·7 (3)
C(26)—C(27)—C(28)	118·6 (4)	C(27)—C(28)—C(29)	119·6 (4)
C(27)—C(28)—O(45)	124·8 (4)	C(29)—C(28)—O(45)	115·6 (3)
C(28)—C(29)—C(30)	121·2 (3)	C(25)—C(30)—C(29)	120·1 (3)
C(17)—C(31)—C(32)	121·7 (3)	C(17)—C(31)—C(36)	121·3 (3)
C(32)—C(31)—C(36)	117·0 (3)	C(31)—C(32)—C(33)	122·0 (3)
C(32)—C(33)—C(34)	120·1 (3)	C(33)—C(34)—C(35)	119·3 (3)
C(33)—C(34)—O(47)	115·9 (3)	C(35)—C(34)—O(47)	124·9 (3)
C(34)—C(35)—C(36)	119·5 (3)	C(31)—C(36)—C(35)	122·2 (3)
C(18)—C(37)—C(38)	119·8 (3)	C(18)—C(37)—C(42)	123·2 (3)
C(38)—C(37)—C(42)	117·0 (3)	C(37)—C(38)—C(39)	120·6 (3)
C(38)—C(39)—C(40)	121·1 (3)	C(39)—C(40)—C(41)	119·2 (3)
C(39)—C(40)—O(49)	115·4 (3)	C(41)—C(40)—O(49)	125·4 (3)
C(40)—C(41)—C(42)	120·0 (4)	C(37)—C(42)—C(41)	122·0 (3)
C(22)—O(43)—C(44)	118·7 (3)	C(28)—O(45)—C(46)	118·0 (4)
C(34)—O(47)—C(48)	118·4 (3)	C(40)—O(49)—C(50)	118·2 (3)

C(18)—O(1)—C(2)—C(3)	−168·4 (3)	C(14)—C(15)—O(16)—C(17)	161·4 (3)
O(1)—C(2)—C(3)—O(4)	86·1 (4)	C(15)—O(16)—C(17)—C(18)	171·1 (3)
C(2)—C(3)—O(4)—C(5)	177·5 (4)	O(16)—C(17)—C(18)—O(1)	−58·8 (3)
C(3)—O(4)—C(5)—C(6)	172·5 (3)	C(2)—O(1)—C(18)—C(17)	179·7 (3)
O(4)—C(5)—C(6)—O(7)	−62·7 (4)	O(7)—C(8)—C(9)—C(25)	−65·8 (3)
C(5)—C(6)—O(7)—C(8)	−142·1 (3)	C(19)—C(8)—C(9)—O(10)	−65·2 (3)
C(6)—O(7)—C(8)—C(9)	150·8 (3)	C(19)—C(8)—C(9)—C(25)	170·9 (2)
O(7)—C(8)—C(9)—O(10)	58·1 (3)	O(16)—C(17)—C(18)—C(37)	177·1 (3)
C(8)—C(9)—O(10)—C(11)	163·0 (3)	C(31)—C(17)—C(18)—O(1)	179·5 (3)
C(9)—O(10)—C(11)—C(12)	169·3 (3)	C(31)—C(17)—C(18)—C(37)	55·4 (4)
O(10)—C(11)—C(12)—O(13)	−67·6 (4)	C(9)—C(8)—C(19)—C(20)	81·7 (4)
C(11)—C(12)—O(13)—C(14)	−171·5 (3)	C(8)—C(9)—C(25)—C(26)	−79·6 (4)
C(12)—O(13)—C(14)—C(15)	−177·1 (3)	C(18)—C(17)—C(31)—C(36)	62·4 (4)
O(13)—C(14)—C(15)—O(16)	68·6 (4)	C(17)—C(18)—C(37)—C(42)	62·3 (5)

the case of the *cis–transoid–cis* (2) (Pears, Shahriari-Zavareh, Stoddart, Crosby, Allwood & Williams, 1988*b;* paper IV) and *trans–cisoid–trans* (3) (Pears, Shahriari-Zavareh, Stoddart, Crosby, Allwood, Slawin & Williams, 1988*b*; paper VI) isomers of 2,3,11,-12-tetra-anisyl-18-crown-6. The situation is reminiscent of the solid-state structures already noted for the 1:1 adducts formed between (*a*) *trans–transoid–trans*-2,3,11,12-tetraphenyl-18-crown-6 (8) and BH_3NH_3 (Allwood *et al.*, 1984) and (*b*) *cis–cisoid–cis*-2,3,-11,12-tetra-anisyl-18-crown-6 (1) and BH_3NH_3 (Pears, Shahriari-Zavareh, Stoddart, Crosby, Allwood & Williams, 1988*a*; paper II). Thus, it might be concluded that, in the absence of pseudo-axial substituents obscuring one of the faces of a 2,3,11,12-tetra-aryl-18-crown-6 derivative, these macrocyclic receptors

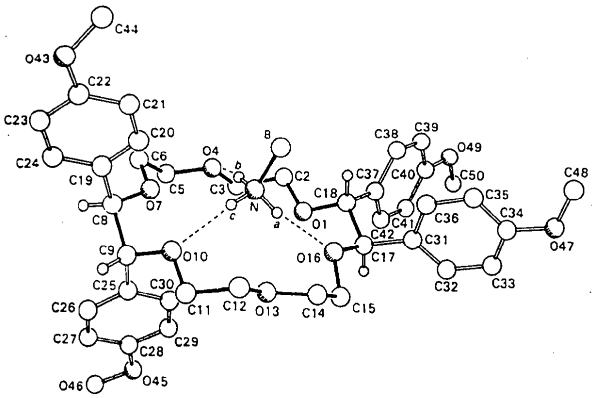

Fig. 1. Ball-and-stick representation of the structure of [(4).BH_3-NH_3] showing the atomic numbering scheme. The 18-crown-6 ring is highlighted with solid C—C and C—O bonds.

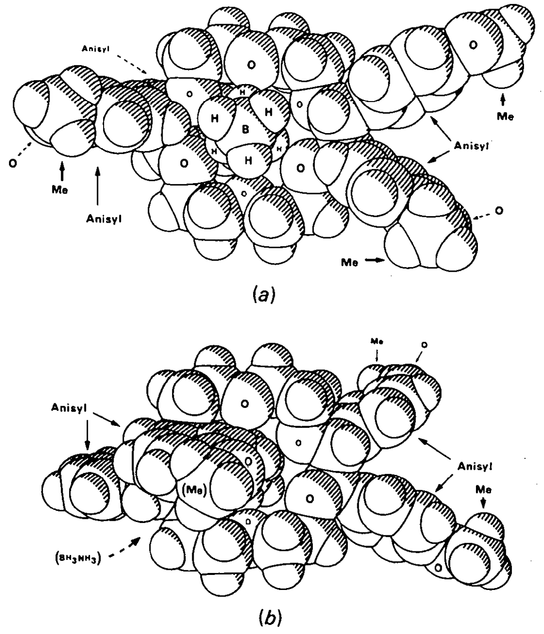

Fig. 2. Space-filling representations of [(4).BH_3NH_3] looking down on (*a*) the face of the macrocycle to which BH_3NH_3 is bound and (*b*) the 'free' face of the macrocycle which is obscured by an axial anisyl substituent.

prefer to bind two neutral BH_3NH_3 substrates simultaneously to their opposite faces.

The NH_3 and BH_3 groups in the substrate are staggered with respect to each other, the smallest H—N—B—H torsion angle being 54°. The NH_3 group in BH_3NH_3 is hydrogen bonded to O(4), O(10) and O(16) with N···O distances of 3·05 (1), 3·13 (1) and 2·93 (1) Å, respectively. Significantly, it is the out-of-plane O atom [O(16)] which is involved in the shortest hydrogen-bond contact. Whilst the N—H···O angles at H(*b*), H(*c*) and H(*a*) are all the same (165°), the angles between the COC planes and their HO vectors are 33, 19 and 11°, respectively. The N···O distances to the oxygen atoms on the opposite face, O(1), O(7) and O(13), are 3·25 (1), 3·01 (1) and 3·01 (1) Å, respectively. The N atom is displaced 1·27 (1) Å from the best mean plane of the six O atoms in the macrocycle and the B—N bond is inclined at 11·1° to the normal to this plane. These values compare closely with those of 1·24 Å and 13° already reported (Allwood *et al.*, 1984) for *trans–transoid–trans*-tetraphenyl-18-crown-6 (8). The similarity of the solid-state structures of these two 1:1 adducts is reassuring when one considers the potential roles (Stoddart, 1984, 1987*a,b,c*; Colquhoun, Stoddart & Williams, 1986) of (4) and (8) as chiral auxiliaries and catalysts.

There is one short intermolecular contact, namely of 3·37 (1) Å, between O(1) and C(44) in symmetry-related adducts. Not surprisingly, it involves a methoxy carbon atom of an anisyl substituent. There are no other contacts of less than normal van der Waals distances between symmetry-related adducts.

The crystal structures reported in this series of eight papers give considerable insight into the effect of changing the relative configurations of four substituents in a receptor molecule upon the noncovalent interactions involving one substrate (BH_3NH_3) and one receptor constitution (2,3,11,12-tetra-anisyl-18-crown-6). Together with the crystal structures also available for some of the diastereoisomers of 2,3,11,12-tetraphenyl-18-crown-6 (Weber, Sheldrick, Burgemeister, Dietl, Mannschreck & Merz, 1984; Blasius, Rausch, Andreetti & Rebizant, 1984) and their adducts with BH_3NH_3 (Allwood *et al.*, 1984), these data will provide a focal point for reference when we discuss (Allwood, Crosby, Koppenhöffer, Pears, Shahriari-Zavareh, Slawin, Stoddart & Williams, 1988) the physical and chemical properties of these receptors and their BH_3NH_3 adducts in solution.

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