Table 3. *Ring-puckering coordinates and asymmetry parameters*

Ring	Q (Å)	φ (°)	θ (°)	ΔC_s(°)	ΔC_2(°)
Six-membered					
A	0·373 (8)	203 (1)	128·5 (9)	17·7 [C(1)]	6·0 [C(1)—C(2)]
B	0·234 (6)	44 (1)	153·3 (7)	5·9 [C(6)]	7·5 [C(5)—C(6)]
C	0·075 (6)	69 (5)	172·5 (6)	1·8 [C(9)]	4·6 [C(9)—C(11)]
F	0·028 (8)	174 (15)	177·2 (8)	0·5 (N)	4·0 [N—C(22)]
Five-membered					
D	0·465 (5)	17·6 (7)	–	–	0·9 [C(16)]
E	0·419 (5)	317·3 (7)	–	6·5 (N)	14·4 [C(17)]

Table 4. *Torsion angles (°) in D, E and F rings*

Column I refers to the title compound, II to solanida-2,4,6-triene and III to 21,27-bisnordemissidine.

Ring D	I	II	III
C(17)—C(13)—C(14)—C(15)	47·5 (5)	47·2 (4)	45 (2)
C(13)—C(14)—C(15)—C(16)	−38·5 (5)	−36·5 (4)	−46 (2)
C(14)—C(15)—C(16)—C(17)	14·5 (5)	11·2 (4)	28 (2)
C(15)—C(16)—C(17)—C(13)	14·8 (5)	17·5 (4)	2 (2)
C(14)—C(13)—C(17)—C(16)	−37·3 (5)	−38·8 (4)	−26 (2)
Ring E			
C(16)—C(17)—C(20)—C(22)	4·9 (5)	3·6 (4)	3 (2)
C(17)—C(20)—C(22)—N	−29·8 (5)	−28·9 (4)	−43 (2)
C(20)—C(22)—N—C(16)	46·6 (5)	45·9 (4)	46 (2)
C(22)—N—C(16)—C(17)	−41·8 (5)	−42·6 (4)	−31 (2)
N—C(16)—C(17)—C(20)	21·4 (5)	22·9 (4)	24 (2)
Ring F			
N—C(22)—C(23)—C(24)	56·4 (7)	56·8 (5)	61 (2)
C(22)—C(23)—C(24)—C(25)	−54·0 (8)	−53·5 (5)	−54 (2)
C(23)—C(24)—C(25)—C(26)	53·7 (7)	52·4 (5)	52 (2)
C(24)—C(25)—C(26)—N	−55·9 (7)	−54·5 (5)	−51 (2)
C(25)—C(26)—N—C(22)	61·8 (6)	60·0 (5)	54 (2)
C(26)—N—C(22)—C(23)	−62·3 (7)	−61·6 (5)	−61 (2)

C(27) methyl group is equatorial [C(27)—C(25)—C(24)—C(23) = 176·6 (9)°], while C(21) assumes an α pseudo-equatorial position [C(21)—C(20)—C(17)—C(16) = 128·9 (8)°].

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Structures of Three Complexes with the Host Diaza-18-Crown-6*

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Abstract. Bis(*p*-nitrobenzaldehyde oxime)–diaza-18-crown-6 (2/1), $C_{12}H_{26}N_2O_4.2C_7H_6N_2O_3$, (1), $M_r = 594·63$, triclinic, $P\bar{1}$, $a = 4·657$ (1), $b = 11·197$ (2), $c = 15·418$ (3) Å, $\alpha = 104·49$, $\beta = 96·29$ (2), $\gamma = 98·51$ (2)°, $V = 760·7$ (3) Å³, $Z = 1$, $D_x = 1·298$ g cm⁻³, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0·94$ cm⁻¹, $F(000) = 316$, $T = 298$ K, $R = 0·0637$ for 947 reflections. Bis(*N*-hydroxybenzamide)–diaza-18-crown-6 (2/1), $C_{12}H_{26}N_2O_4.2C_7H_7NO_2$, (2), $M_r = 536·63$, monoclinic, $P2_1/c$, $a = 15·989$ (2) (supercell $A = 2a$), $b = 5·030$ (1), $c = 17·929$ (2) Å, $\beta = 100·88$ (1)°, $V = 1416·0$ (3) Å³, $Z = 2$, $D_x = 1·258$ g cm⁻³, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0·87$ cm⁻³, $F(000) = 576$, $T = 298$ K, $R = 0·0767$ for 1856 reflections. 2,6-Dihydroxynaphthalene–diaza-18-crown-6 (1/1), $C_{12}H_{26}N_2O_4.C_{10}H_8O_2$, (3), $M_r = 422·53$, triclinic, $P\bar{1}$, $a = 7·639$ (1), $b = 9·648$ (1), $c = 18·045$ (2) Å, $\alpha = 80·43$ (1), $\beta = 80·30$ (1), $\gamma = 67·84$ (1)°, $V = 1206·3$ (2) Å³, $Z = 2$, $D_x = 1·163$ g cm⁻³, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0·79$ cm⁻¹, $F(000) = 456$, $R = 0·060$ for 2582 reflections. In complexes (1) and (2), the diaza-18-crown-6 hosts lie on centers of symmetry with a guest molecule on each side of the molecular plane and

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* Diaza-18-crown-6 = 1,4,10,13-tetraoxa-7,16-diazacyclooctadecane.

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hydrogen bonded to an aza N atom. The host adopts a conformation similar to that of uncomplexed 18-crown-6. In (3) there are two independent host molecules and two independent guest molecules each of which lies on a center of symmetry. Each 2,6-dihydroxynaphthalene bridges two host molecules forming two independent hydrogen-bonded infinite chains throughout the solid. The host molecules adopt an approximate D_{3d} conformation.

Introduction. The interactions between crown macrocylces and uncharged organic host molecules have become of increasing interest during the past decade (Vögtle, Sieger & Müller, 1981; Vögtle, Müller & Watson, 1984; Goldberg, 1984; Watson, Vögtle & üller, 1988a). This is due primarily to the interest n and importance of weak interactions in some biochemical processes. Crown compounds not only provide cavities but also multiple electron donor enters that can act as binding sites for electrostatic dipole/dipole interactions and hydrogen bonding. Of particular interest is the multiplicity of these binding sites and their geometric arrangement (Watson, Galloy, Grossie, Vögtle & Müller, 1984). The stereochemical differences between host:guest complexes n the crystalline state and in solution are also of interest. In general, complexes between diaza-18-crown-6 and neutral organic molecules containing proton donors are stabilized by hydrogen bonds to the aza N atoms. In some complexes, the proton of the guest has been transferred to the basic N atom of the diaza-18-crown-6 host (Watson, Vögtle & Müller, 1988b) forming ionic host:guest complexes. In this paper, we report the structures of three new host:guest complexes.

Experimental. All complexes were prepared by mixing the appropriate stoichiometric ratios in a minimum of refluxing ethyl acetate. Useable crystals were obtained either by cooling to room temperature or recrystallization from ethyl acetate. All data were collected on a Nicolet $R3M/\mu$ update of a $P2_1$ diffractometer. Unit-cell parameters were obtained by a least-squares refinement of 25 reflections. Intensity data were collected in the ω mode with a variable scan rate of 4–29° min^{-1} using graphite-monochromated Mo $K\alpha$ radiation. Lorentz and polarization corrections were applied. A ψ-scan absorption correction was applied to (2) and (3). The intensities of standard reflections varied by a maximum of ± 2%. The structures were solved by direct methods and refined by a block-cascade least-squares technique. In (3), all H-atom positional parameters were refined, along with four refined isotropic thermal parameters. In (1), all H atoms were allowed to ride on the attached atoms except for the two H atoms participating in hydrogen bonding. The phenyl ring

Table 1. *Crystal and refinement data*

	(1)	(2)	(3)
Color	Colorless	Colorless	Colorless
Crystal size (mm)	0·03 × 0·13 × 0·52	0·10 × 0·25 × 0·43	0·38 × 0·43 × 0·45
2θ range for data collection (°)	3–40	3–45	3–45
Number of reflections for lattice parameters	25	25	25
2θ range for lattice parameters (°)	22·55–33·56	24·89–36·53	40·87–44·95
Space group	$P\bar{1}$	$P2_1/c$	$P\bar{1}$
Systematic extinctions	None	$h0l:l = 2n + 1$ $0k0:k = 2n + 1$	None
Monitored reflections	020,1$\bar{1}$1	3$\bar{1}$3,006	$\bar{3}$17,14$\bar{4}$
hkl range	−4,4;−10,10;0,14	−17,16;0,5;0,18	−18,8;−10,10;0,19
Number of reflections measured	1635	2123	3510
Number of unique reflections	1422	1856	3169
R_{int}	0·009	0·008	0·007
Number with $I \geq 3\sigma(I)$	947	1149	2582
Transmission factors	–	0·880–0·952	0·866–0·991
Number of parameters	200	243	377
R	0·0637	0·0767	0·0600
wR	0·0408	0·0859	0·0690
R (all data)	0·102	0·124	0·075
wR (all data)	0·045	0·103	0·089
S	1·583	1·328	1·834
$(\Delta/\sigma)_{max}$	0·020	0·006	0·028
Electron density max. (e Å^{-3})	0·17	0·63	0·21
min. (e Å^{-3})	−0·23	−0·32	−0·35
g (weight)	0·00061	0·00196	0·00116

Table 2. *Atomic coordinates* ($\times 10^4$) *and isotropic thermal parameters* ($\text{Å}^2 \times 10^3$) *for complex* (1)

	x	y	z	U
N(1)	7027 (10)	7879 (4)	567 (3)	50 (2)*
C(2)	5729 (12)	8774 (5)	1200 (4)	59 (3)
C(3)	7957 (14)	9660 (5)	1942 (4)	66 (3)
O(4)	9720 (8)	10475 (4)	1562 (2)	52 (2)
C(5)	11510 (14)	11483 (5)	2251 (4)	58 (3)
C(6)	13581 (13)	12230 (5)	1825 (4)	57 (3)
O(7)	11949 (8)	12857 (3)	1306 (3)	51 (2)
C(8)	13723 (13)	13664 (5)	915 (4)	65 (3)
C(9)	15156 (13)	12955 (5)	173 (4)	67 (3)
C(10)	4093 (12)	6517 (5)	3306 (3)	48 (3)
C(11)	5038 (12)	5680 (5)	3744 (4)	59 (3)
C(12)	7307 (13)	6058 (6)	4458 (4)	65 (3)
C(13)	8611 (14)	7286 (7)	4742 (4)	54 (3)
C(14)	7716 (14)	8150 (6)	4330 (4)	66 (3)
C(15)	5454 (14)	7764 (5)	3618 (4)	60 (3)
C(16)	1740 (12)	6054 (5)	2532 (4)	54 (3)
N(17)	933 (10)	6819 (4)	2103 (3)	53 (2)
O(18)	−1231 (9)	6229 (4)	1369 (3)	68 (2)
N(19)	11136 (14)	7714 (6)	5494 (4)	71 (3)
O(20)	11835 (11)	6932 (5)	5856 (3)	98 (3)
O(21)	12242 (11)	8815 (5)	5733 (3)	99 (3)

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

of the guest molecule in (2) appeared to be disordered and was refined as such; however, a few weak reflections are consistent with a doubling of the a axis and an ordered phenyl ring. The occupancy factor for the disordered structure refined to 0·51 (2). The H atoms of the phenyl ring were refined while the remainder were allowed to ride on the attached atoms. $\Sigma w(|F_o| - |F_c|)^2$ was minimized with $w = [\sigma^2(F_o) + gF_o^2]^{-1}$. Crystal and refinement data are presented in Table 1. All computer programs supplied by Nicolet (Nicolet Instrument Corporation,

Table 3. Atomic coordinates ($\times 10^4$) and isotropic thermal parameters ($\text{Å}^2 \times 10^3$) for complex (2)

	x	y	z	U
N(1)	6143 (3)	8122 (8)	4307 (2)	46 (2)*
C(2)	5518 (3)	10046 (12)	3918 (3)	61 (2)
C(3)	4829 (4)	8690 (12)	3356 (3)	63 (2)
O(4)	4357 (2)	7025 (9)	3749 (2)	63 (2)
C(5)	3616 (4)	5980 (12)	3274 (3)	64 (2)
C(6)	3232 (4)	3831 (14)	3695 (4)	88 (3)
O(7)	2969 (3)	4635 (10)	4239 (2)	81 (2)
C(8)	2604 (4)	2590 (13)	4696 (4)	73 (3)
C(9)	3215 (3)	560 (11)	5117 (3)	60 (2)
C(1)	956 (3)	2479 (11)	6423 (3)	45 (2)
C(2A)	458 (7)	773 (24)	5911 (7)	56 (4)
C(2B)	548 (7)	4424 (23)	5920 (6)	55 (4)
C(3A)	−400 (7)	1009 (28)	5752 (8)	74 (6)
C(3B)	−326 (8)	4612 (28)	5777 (8)	68 (6)
C(4)	−821 (4)	2950 (16)	6106 (5)	77 (3)
C(5A)	−311 (8)	4581 (29)	6619 (10)	82 (7)
C(5B)	−461 (7)	1135 (29)	6594 (9)	77 (6)
C(6A)	573 (7)	4386 (22)	6783 (7)	61 (5)
C(6B)	429 (8)	836 (23)	6755 (6)	59 (5)
C(7)	1897 (3)	2015 (10)	6589 (3)	40 (2)
N(8)	2375 (3)	4175 (9)	6659 (3)	48 (2)
O(9)	3250 (2)	4008 (7)	6839 (2)	53 (1)
O(10)	2206 (2)	−212 (6)	6628 (3)	64 (2)

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

Table 4. Atomic coordinates ($\times 10^4$) and isotropic thermal parameters ($\text{Å}^2 \times 10^3$) for complex (3)

	x	y	z	U
C(1)	4544 (4)	3335 (3)	5560 (1)	49 (1)*
C(2)	4959 (4)	3408 (3)	6252 (1)	50 (1)
O(2)	4839 (3)	2405 (2)	6870 (1)	71 (1)
C(3)	5545 (4)	4563 (3)	6361 (2)	53 (1)
C(4)	5707 (4)	5621 (3)	5785 (1)	52 (1)
C(4A)	5293 (3)	5580 (2)	5054 (1)	42 (1)
C(5)	2602 (4)	1251 (3)	385 (2)	57 (1)
C(6)	2509 (4)	669 (3)	1124 (2)	60 (2)
O(6)	984 (3)	1185 (2)	1650 (1)	86 (1)
C(7)	4067 (4)	−549 (3)	1388 (2)	59 (1)
C(8)	5647 (4)	−1166 (3)	905 (2)	57 (1)
C(8A)	5779 (3)	−618 (3)	132 (1)	49 (1)
N(9)	8025 (4)	3681 (3)	1170 (2)	97 (1)
C(10)	7265 (8)	4509 (5)	1786 (3)	145 (3)
C(11)	8737 (10)	4827 (5)	2072 (2)	141 (3)
O(12)	9408 (4)	5827 (3)	1489 (1)	97 (1)
C(13)	10886 (10)	6045 (7)	1652 (3)	143 (3)
C(14)	11362 (7)	7173 (7)	1093 (5)	152 (4)
O(15)	12072 (3)	6554 (3)	361 (2)	107 (1)
C(16)	12612 (7)	7500 (6)	−189 (4)	152 (3)
C(17)	13445 (5)	6713 (7)	−863 (4)	150 (3)
N(18)	5775 (4)	67 (3)	3392 (1)	63 (1)
C(19)	4365 (6)	1326 (3)	3006 (2)	76 (2)
C(20)	2415 (6)	1459 (4)	3349 (2)	81 (2)
O(21)	2149 (3)	1830 (2)	4094 (1)	67 (1)
C(22)	296 (5)	2006 (4)	4461 (2)	89 (2)
C(23)	106 (4)	2399 (4)	5231 (2)	90 (2)
O(24)	1250 (3)	1142 (2)	5691 (1)	76 (1)
C(25)	898 (5)	1360 (4)	6463 (2)	90 (2)
C(26)	2269 (6)	48 (4)	6879 (2)	88 (2)

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

1986) for Desktop 30 Microeclipse and NOVA 4/C configuration; atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974, Vol. IV). Tables 2, 3 and 4 give the atomic positional param-

Table 5. Bond distances (Å) for (1), (2) and (3)

	(1)	(2)	(3a)*	(3b)†
N(1)—C(2)	1·463 (7)	1·469 (7)	1·393 (6)	1·452 (4)
N(1)—C(9A)	1·462 (6)	1·470 (6)	1·521 (7)	1·460 (5)
C(2)—C(3)	1·495 (7)	1·508 (8)	1·461 (10)	1·480 (6)
C(3)—O(4)	1·414 (8)	1·404 (7)	1·468 (6)	1·412 (4)
O(4)—C(5)	1·422 (6)	1·423 (6)	1·310 (9)	1·418 (4)
C(5)—C(6)	1·495 (9)	1·513 (9)	1·464 (10)	1·470 (6)
C(6)—O(7)	1·421 (8)	1·346 (9)	1·473 (9)	1·426 (4)
O(7)—C(8)	1·422 (8)	1·406 (8)	1·354 (7)	1·408 (4)
C(8)—C(9)	1·501 (9)	1·512 (8)	1·464 (10)	1·488 (5)

Nitrobenzaldehyde oxime (1)

C(10)—C(11)	1·378 (9)	C(13)—N(19)	1·488 (8)
C(10)—C(15)	1·385 (7)	C(14)—C(15)	1·371 (8)
C(10)—C(16)	1·460 (7)	C(16)—N(17)	1·279 (9)
C(11)—C(12)	1·374 (7)	N(17)—O(18)	1·383 (6)
C(12)—C(13)	1·359 (9)	N(19)—O(20)	1·213 (9)
C(13)—C(14)	1·371 (11)	N(19)—O(21)	1·210 (8)

N-Hydroxybenzamide (2)

C(1)—C(2a)	1·391 (12)	C(3a)—C(4)	1·403 (17)
C(1)—C(6a)	1·365 (14)	C(4)—C(5a)	1·378 (16)
C(1)—C(7)	1·495 (17)	C(5a)—C(6)	1·391 (17)
N(8)—O(9)	1·378 (5)	C(7)—N(8)	1·320 (7)
C(2a)—C(3a)	1·354 (16)	C(7)—O(10)	1·222 (6)

2,6-Dihydroxynaphthalene (3)‡

C(1)—C(2)	1·359 (4)	C(5)—C(6)	1·360 (4)
C(1)—C(4c')	1·416 (3)	C(5)—C(8a')	1·415 (3)
C(2)—C(3)	1·399 (5)	C(6)—O(6)	1·316 (3)
C(2)—O(2)	1·365 (3)	C(6)—C(7)	1·404 (3)
C(3)—C(4)	1·355 (4)	C(7)—C(8)	1·359 (4)
C(4)—C(4c)	1·417 (4)	C(8)—C(8a)	1·409 (4)
C(4a)—C(4a')	1·405 (6)	C(8a)—C(8a')	1·414 (4)

* The labels N(1) to C(9) in this column correspond to N(9) to C(17) in Table 4.

† The labels N(1) to C(9) in this column correspond to N(18) to C(16) in Table 4 and in Fig. 3.

‡ C(1) to C(4a) and C(5) to C(8a) correspond to one half of the two independent 2,6-dihydroxynaphthalene molecules.

Table 6. Selected bond angles (°) for (1), (2) and (3)

	(1)	(2)	(3a)*	(3b)†
C(2)—N(1)—C(9')	112·5 (4)	111·0 (4)	112·8 (4)	113·5 (3)
N(1)—C(2)—C(3)	113·0 (5)	111·4 (5)	110·8 (4)	110·9 (3)
C(2)—C(3)—O(4)	108·6 (5)	109·2 (5)	108·3 (4)	108·9 (3)
C(3)—O(4)—C(5)	111·1 (4)	112·7 (4)	113·2 (4)	112·5 (3)
O(4)—C(5)—C(6)	109·1 (5)	109·6 (4)	110·7 (5)	109·9 (3)
C(5)—C(6)—O(7)	108·9 (5)	115·3 (6)	109·1 (5)	109·9 (3)
C(6)—O(7)—C(8)	113·8 (4)	113·5 (5)	113·6 (5)	112·7 (2)
O(7)—C(8)—C(9)	112·5 (5)	116·2 (5)	108·5 (5)	108·2 (3)
C(8)—C(9)—N(1')	111·5 (5)	110·2 (5)	110·9 (4)	110·8 (3)

* The labels N(1) to C(9) in this column correspond to N(9) to C(17) in Table 4.

† The labels N(1) to C(9) in this column correspond to N(18) to C(26) in Table 4.

eters for (1), (2) and (3), while Tables 5 and 6 list selected interatomic distances and valence angles. Figs. 1, 2 and 3 are drawings of the three complexes.*

Discussion. In complexes (1) and (2), the diaza-18-crown-6 molecules lie on centers of symmetry with the organic guest hydrogen bonded on each side to the aza N atoms. In complex (1), $O(18)\cdots N(1)$ ($-1 + x$, y, z) = 2·639 (6), $H(18)\cdots N(1)$ = 1·78 (4) Å and $O(18)$—$H(18)\cdots N(1)$ = 161 (3)°. In complex (2), $O(9)\cdots N(1)$ ($1-x$, $1-y$, $1-z$) = 2·658 (7), $H(9)\cdots H(1)$ = 1·74 (4) Å and $O(9)$—$H(9)\cdots N(1)$ = 173 (3)°. The diaza-18-crown-6 host adopts a conformation resembling the more flattened conformation of uncomplexed 18-crown-6 (Bovill, Chadwick, Sutherland &
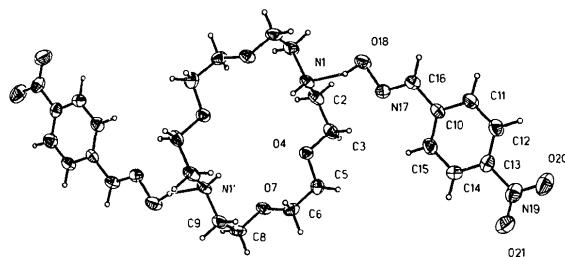
Fig. 1. Drawing of complex (1) with thermal ellipsoids drawn at the 30% probability level. H atoms are represented by spheres of arbitrary size. Hydrogen bonds are indicated as unshaded lines.
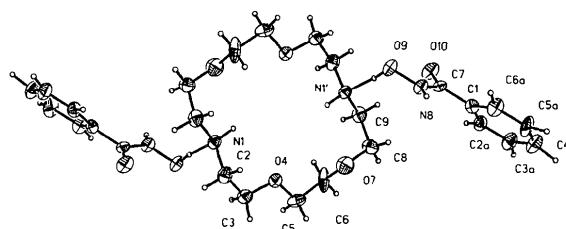

Fig. 2. Drawing of complex (2) with thermal ellipsoids drawn at the 30% probability level. H atoms are represented by spheres of arbitrary size. Hydrogen bonds are indicated as unshaded lines.
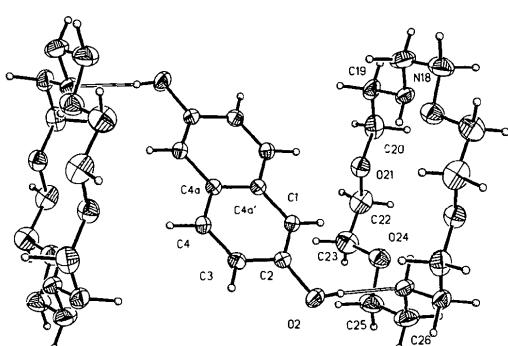

Fig. 3. Drawing of one molecular unit in complex (3). Thermal ellipsoids are drawn at the 30% probability level. H atoms are represented by spheres of arbitrary size. Hydrogen bonds are indicated by unshaded lines.

Table 7. *Torsion angles* (°) *for* (1), (2) *and* (3)

	(1)	(2)	(3a)	(3b)
N(1)—C(2)—C(3)—O(4)	68·8 (7)	65·2 (6)	65·7 (4)	65·5 (3)
C(2)—C(3)—O(4)—C(5)	169·1 (5)	171·0 (5)	−172·6 (4)	178·9 (2)
C(3)—O(4)—C(5)—C(6)	173·3 (5)	169·6 (5)	−173·9 (4)	−179·7 (3)
O(4)—C(5)—C(6)—O(7)	68·4 (6)	61·8 (6)	−68·1 (5)	−69·1 (4)
C(5)—C(6)—O(7)—C(8)	176·2 (4)	179·0 (5)	−177·9 (5)	−170·4 (3)
C(6)—O(7)—C(8)—C(9)	69·5 (6)	73·6 (6)	175·0 (4)	−175·3 (3)
O(7)—C(8)—C(9)—N(1')	60·4 (7)	57·7 (7)	63·5 (5)	61·4 (5)
C(8)—C(9)—N(1')—C(2')	−167·5 (6)	−177·2 (6)	−176·5 (5)	179·8 (4)
C(9)—N(1')—C(2')—C(3')	−178·0 (5)	−176·9 (5)	178·6 (4)	−175·2 (3)

Watson, 1980). The H atoms of the hydrogen bonds are not transferred from the guest molecules. The bond distances of the host molecules in (1) and (2) agree quite well except for C(6)—O(7) which is about 8σ shorter in (2) than in (1) or in literature values (Watson, Galloy, Grossie, Vögtle & Müller, 1984; Watson, Vögtle & Müller, 1988a,b).

The 1:1 complex (3) contains two independent host and two independent guest molecules each lying on a center of symmetry. The host molecules adopt an approximate D_{3d} conformation which is the most common observed for 18-crown-6 and diaza-18-crown-6 (Bovill, Chadwick, Sutherland & Watson, 1980; Watson, Galloy, Grossie, Vögtle & Müller, 1984; Watson, Vögtle & Müller, 1988a,b), with C—O—C—C and O—C—C—O torsion angles near 180 and 70° (see Table 7). This is the expected *gauche* conformation of the ethyleneoxy units (Goldberg, 1984). Molecule (3b) exhibits distances and angles which correspond closely to those reported in the literature; however, (3a) exhibits larger standard deviations and larger variations in distances. Each guest molecule hydrogen bonds to two host molecules forming two independent infinite chains in the solid, $N(9)\cdots O(6)$ ($1 + x$, y, z) = 2·742 (6), $N(9)\cdots H(6)$ = 1·90 (4) Å, $N(9)\cdots H(6)$—O(6) = 170 (3)° and $N(18)\cdots O(2)$ ($1-x$, $-y$, $1-z$) = 2·725 (4), $N(18)\cdots H(2)$ = 1·93 (3) Å, $N(18)\cdots H(2)$—O(2) = 172 (3)°.

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