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CYCLOPHANES—13[1a]

CRYSTAL AND MOLECULAR STRUCTURE OF [2.2][2,5]FURANO(1,4)NAPHTHALENOPHANE

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Abstract—The crystal and molecular structure of [2.2](2,5)furano(1,4)naphthalenophane (1) was determined by X-ray crystallography. The molecule exists in the *anti*-conformation and the study represents the first instance in which the structural features of a naphthalenoid ring within a cyclophane were determined. Crystals of cyclophane 1 are orthorhombic, space group *Pbca*, with $a = 7.859(2)$, $b = 11.482(3)$ and $c = 28.818(8)$ Å. While the nonbridged portion of the naphthalenoid ring is planar, the portion which is bridged to the furanoid ring through its 1 and 4 C atoms is puckered and boat-shaped. These C atoms are positioned 14° out of the plane of the other four C atoms of this ring. The furanoid ring is essentially planar but is not parallel to the naphthalenoid ring. It is inclined 22° to the least squares plane of the bridged portion of the naphthalenoid ring. This angle of inclination staggers the atoms of the furanoid and bridged naphthalenoid ring and positions the 3 and 4 C atoms, the 2 and 5 C atoms and the O atom of the furanoid ring 3.4, 2.9 and 2.6 Å, respectively, from the least squares plane of the bridged portion of the naphthalenoid ring. While the internal angles around the bridging C atoms α- to the naphthalenoid ring are 109°, those α- to the furanoid ring are 113°. In addition unusually large bond angles (~137°) at the 2 and 5 C atoms of the furanoid ring, external to the ring, are also observed. The distortions are considered with respect to the strain within the cyclophane macrocycle and are compared with other similar systems.

[2.2] Cyclophanes are an interesting class of highly strained molecules.[2] The accommodation of strain in these systems occurs through distortion of bridging carbon bond angles, puckering of constituent aromatic rings, and in some cases by the non-parallel orientation of these rings. Crystal structure information has provided insight into the relative importance of these factors in several cases, originally in cyclophanes consisting of benzenoid aromatic rings[3–6] and more recently in those containing heteroaromatic rings.[7,8] In this paper we describe the crystal structure of [2.2](2,5)-furano(1,4)naphthalenophane (1) and compare the restults with those obtained for other molecules of this class (Table 1). The synthesis[9] and conformational study of 1 has been previously described,[10] and nmr and electronic spectral data clearly favors the *anti*- over the *syn*-conformation (see Fig. 1).

1

Fig. 1.

EXPERIMENTAL

Crystals of 1 were obtained by recrystallization from 3:2 benzene:hexane solutions, and are orthorhombic, with $a = 7.859(2)$, $b = 11.482(3)$, $c = 28.818(8)$ Å. (CuK$_\alpha$ radiation).

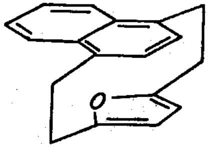
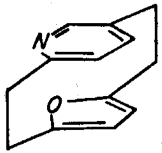
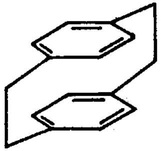
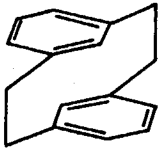
The density, 1.26 g-cm^{-3}, measured by flotation in NaNO$_3$aq, agrees well with that calculated for $z = 8$, 1.269 g-cm^{-3}. The space group was uniquely determined to be *Pbca* from systemtic absences (**Ok1**, **k**odd; **hO1**, **1**odd; **hkO**, **h**odd) observed on Weissenberg photographs. Unfortunately, even the best crystals obtained were of poor diffraction quality (Lauê photographs), and were needles elongated along the *c* direction, with small cross sections. A fragment cut from one of these needles, of approximate dimensions 0.05 × 0.08 × 0.34 mm in the a, b and c directions, respectively, was used for data collection.

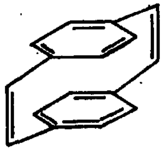
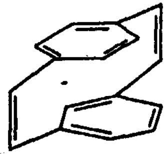
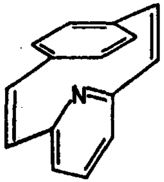
3-Dimensional intensity data were collected on a Syntex P2$_1$ automatic four-circle diffractometer, using Ni-filtered CuK$_\alpha$ (λ = 1.5418 Å) radiation. The diffracted intensities were collected by symmetric 2° $2\theta:\theta$ scans with the variable scan rate (1.95–3.91°/min.) determined in each case by a fast prescan. Intensities of 2224 reflections up to $\theta = 66°$ were measured, of which 1066 or 47.9% had intensity greater than $1.96\sigma(I)$ and were classified as observed. A set of three standard reflections, measured after every 50 reflections, showed less than statistical variation during data collection. The data were corrected for Lorentz and polarization factors, an assessment of the overall scale and temperature factors was obtained from a Wilson plot, and a list of normalized structure factors (E's) was produced. No absorption corrections were applied.

Phase determination was carried out using direct methods (MULTAN). With a 90% probability acceptance criterion, Σ_1 failed to determine unambiguously the sign of any of the reflections. According to the results of Σ_2 and Converge, three origin fixing reflections were used along with three other reflections for direct indication of the phases of 161 reflections with $E > 1.69$. An E-map computed using a solution obtained from these terms gave plausible positions for all non-hydrogen atoms in the structure. Three full-matrix least squares cycles with isotropic temperature parameters for these atoms reduced R$_1$ to 0.119, where $R_1 = \Sigma(|F_0| - |F_c|)/\Sigma|F_0|$. At this stage of refinement R$_2$, defined as $R_2 = (\Sigma\omega(|F_0| - |F_c|)^2/\Sigma\omega F_0^2)^{1/2}$ was 0.138 ($(1/\omega) = [\sigma(F)]^2 + 0.04\,F^2$).

A difference electron-density map was then computed to locate the H atoms, with three more least-squares cycles lowering R$_1$ to 0.101, and R$_2$ to 0.118. The data set was of insufficient size to complete refinement of the non-H atoms anisotropically. The effect of this paucity of data is reflected in the relatively high estimated standard deviations for the bond distances and angles: 0.012 Å and 0.8° respectively for non-H atoms; 0.094 Å for –C–H bonds, 5.6° for –C–C–H bond angles and 6.2° for H–C–H bond

Table 1. Structural parameters of selected [2.2]cyclophanes

Compound	Angle of Inclination of Aromatic Planes	Bridging Group	Bridge C-C Bond Length (Å)	Angles at Bridging Atoms[b]	D (Å)[c]	Reference
 1	22°	$-CH_2-CH_2-$	1.57 (3)	113.5° (16) 108.9° (16)	0.00 0.177	a
 2	23°	$-CH_2-CH_2-$	1.574 (5)	114.0° (5) 108.5° (5)	0.022 0.172	8
 3	0°	$-CH_2-CH_2-$	1.569	113.7°	0.157	3
 4	0°	$-CH_2-CH_2-$	1.568	110.3°	Central-0.143 Distant-0.042	4

 5	0°	-CH=CH-	1.336 (6)	118.8°	0.172	5
 6	41°	-CH=CH-	1.346 (4)	125.7° (5) 120.8°	Meta central -0.018 Meta distant -0.026 Para 0.235	6
 7	90°	-CH=CH-	1.33 (1)	128.2° (6) 119.5° (6)	0.00 0.222	7

[a] Data from this work.

[b] Angles at bridging atoms for bridging carbon nearest heteroaromatic ring (upper value) and for bridging carbon nearest benzenoid ring (lower value). Estimated standard deviations in parentheses.

[c] D is defined as the distance the 1,4-carbon atoms of a given aromatic ring lie out of the plane defined by the other atoms in the ring (upper value, hetero-ring; lower value, benzenoid ring).

angles. On the final cycle of least squares, no parameter shift was greater than 0.16 of the corresponding esd. A table of observed and calculated structure factors is available.[11] A final difference electron density map showed no peaks greater than 0.5–1.0 eÅ^{-3}. All computing was performed on a Syntex XTL Structure Determination System.[12]

RESULTS

In spite of the relatively high estimated standard deviations for the bond angles, a clear picture of the structure and conformation of **1** emerges. The furanoid ring is planar (plane B; Table 2) within experimental error, is oriented *anti* to the naphthalenoid ring, and, as shown in Fig. 2, is inclined at an angle of 22.2° to the least-squares plane of C atoms 1,2,7,8,9 and 10 composing the bridged half of the naphthalenoid ring (plane A). The least-squares plane of the four bridging C atoms (plane C), holding the two rings in that position, is inclined 83° to the latter plane (Table 2 and Fig. 2).

Interatomic distances are given in Table 3, and pertinent bond angles are given in Table 4. Final positional and thermal parameters are listed in Table 5.

Figure 3 illustrates some important intramolecular distances and angles, looking at the molecule through the molecular cavity in the direction of the long axis of the naphthalenoid ring. The three distances represented by vertical arrows are the perpendicular distances from atoms in the furanoid ring to the previously mentioned least-squares plane (A) of the naphthalenoid ring. Figure 4 shows a stereoscopic diagram of the crystal packing of the unit cell; intermolecular contacts are all normal and have not been tabulated here. Figure 5 shows a projection of **1** perpendicular to the naphthalenoid ring, and also shows the atom labeling scheme.

DISCUSSION

The key structural features of [2.2]cyclophanes as a molecular class can perhaps best be understood by considering these molecules to be composed of four fragments (two aromatic fragments and two two-carbon fragments bridging them) whose individual structural integrities must be compromised to afford minimum strain for the entire molecule. Difficulty arises in connecting electron-rich mutually repelling aromatic rings, which require planarity for aromaticity, with bridging C atoms whose bond angles are most stable at 109.5° for sp^3 and 120° for sp^2 hybridization. If the bridging bond angles are allowed to approach their optimum geometries, the aromatic rings would be relatively far apart from one another and transannular π-π interaction would be minimized. As a result, however, the aromatic rings would be significantly puckered and aromatic stabilization would be lost since intra-ring p-orbital overlap

Table 2. Least-squares plane calculations for **1**

Plane	Atoms	Equation
A	C1, C2, C7, C8, C9, C10	(-0.7659)X + (0.5139)Y - (0.3863)Z + 4.2462 = 0.
B	O, C15, C16, C17, C18	(-0.6067)X + (0.7791)Y - (0.1575)Z + 0.2008 = 0.
C	C11, C12, C13, C14	(-0.3635)X - (0.7441)Y - (0.5605)Z + 3.7000 = 0.
D	C1, C2, C7, C8	(-0.7272)X + (0.6088)Y - (0.3172)Z + 3.6796 = 0.

Interplanar angles	
AB	22.18°
BC	105.71°
AC	83.54°

Distances of atoms from planes (with standard deviation)(Å)

A		B		C	
C1	0.103(8)	O	0.005(5)	C11	0.007(11)
C2	-0.041(7)	C15	-0.006(8)	C12	-0.006(9)
C7	-0.046(7)	C16	0.000(11)	C13	-0.009(12)
C8	0.120(8)	C17	0.014(10)	C14	0.007(11)
C9	-0.087(10)	C18	-0.015(8)		
C10	-0.086(10)	C12	-0.193(9)		
		C14	-0.173(11)		
		D			
		C1	-0.003(8)		
		C2	0.006(7)		
		C7	-0.006(7)		
		C8	0.004(8)		
		C3	0.130(9)		
		C6	0.101(9)		

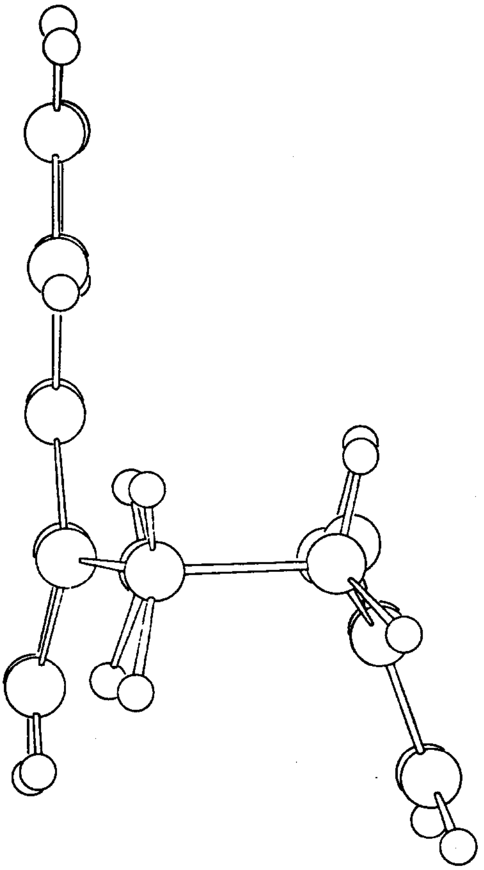


Fig. 2. Structure of [2.2](2,5)furano(1,4)naphthalenophane (1).

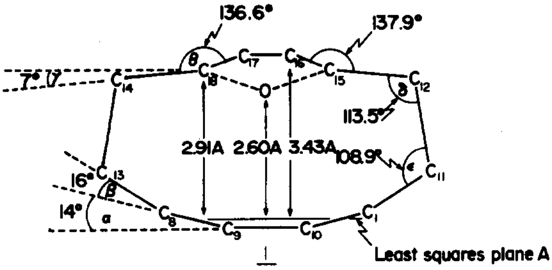


Fig. 3. Pertinent atomic distances and angles in 1.

would no longer be at a maximum. If, on the other hand, planarity of the aromatic rings were maintained the angles associated with the bridging atoms would be contracted relative to their standard values, causing an increase in angle strain and transannular π-π interaction. Rather than undergo the severe loss of aromatic stabilization or increased transannular π-π interaction and bridging angle strain, which these extreme orientations require, the system instead spreads the stresses and strains through all the fragments. In fact recent results have shown that a number of cyclophanes exist in which the aromatic moieties are not held parallel to one another,[6-8] thus allowing yet another avenue for reduction of transannular π-π interaction.[14]

All of the features described above and others are evident in the structure of 1. It is obvious from Figs. 2 and 5 that (a) the location of the furanoid O atom centrally above the bridged portion of the naphthalenoid ring, and (b) the staggered location of the furanoid C atoms with respect to those of the bridged naphthalenoid ring are not mere coincidence. Along with the 22° in-

Table 3. Interatomic distances (Å) and their estimated standard deviations in 1

C1-C2	1.435(11)	C1-C11	1.499(13)
C2-C3	1.427(11)	C11-C12	1.561(14)
C3-C4	1.359(13)	C8-C13	1.489(15)
C4-C5	1.380(14)	C13-C14	1.587(16)
C5-C6	1.366(13)	C14-C18	1.481(13)
C6-C7	1.429(12)	C15-C12	1.498(11)
C7-C2	1.430(10)	C15-C16	1.370(12)
C7-C8	1.426(11)	C16-C17	1.392(14)
C8-C9	1.358(13)	C17-C18	1.362(13)
C9-C10	1.394(14)	O - C15	1.386(9)
C1-C10	1.375(12)	O - C18	1.378(9)
O-C1	2.81	O-C8	2.82
O-C2	2.86	O-C7	2.87
O-C10	3.04	O-C9	3.05
C1-C8	2.82	C15-C18	2.24
C5-H5	0.91(11)	C4-H4	1.10(13)
C6-H6	0.98(8)	C3-H3	0.81(9)
C9-H9	0.79(9)	C10-H10	0.84(10)
C13-H13A	1.10(8)	C11-H11A	0.91(5)
C13-H13B	0.82(10)	C11-H11B	1.08(9)
C14-H14A	1.18(11)	C12-H12A	1.02(6)
C14-H14B	0.96(8)	C12-H12B	1.14(11)
C17-H17	1.00(14)	C16-H16	0.65(10)

Table 4. Selected bond angles (and their estimated standard deviations)

C2-C1-C10	117.4(7)	C14-C18-C17	136.6(8)
C2-C1-C11	122.1(7)	C17-C18-O	108.6(7)
C10-C1-C11	117.7(7)	C14-C18-O	114.5(7)
C1-C2-C3	121.8(7)	C15-O-C18	108.6(6)
C1-C2-C7	118.3(7)	C8-C9-C10	121.4(9)
C2-C3-C4	120.4(8)	C1-C10-C9	121.4(9)
C3-C4-C5	120.6(9)	C1-C11-C12	109.1(8)
C4-C5-C6	121.1(9)	C11-C12-C15	113.4(8)
C5-C6-C7	121.5(8)	C8-C13-C14	108.7(9)
C2-C7-C6	116.6(7)	C13-C14-C18	113.7(9)
C2-C7-C8	120.0(7)	C12-C15-C16	137.9(8)
C6-C7-C8	123.2(7)	C12-C15-O	115.1(6)
C7-C8-C9	117.3(8)	C15-C16-C17	109.9(9)
C7-C8-C13	121.1(8)	C16-C17-C18	106.4(9)
C9-C8-C13	119.1(9)		

Table 5. Final positional and thermal parameters for 1

	X/a σ	Y/b σ	Z/$\bar{c}$ σ	B
C1	.3824 (10)	.0067 (7)	.1690 (3)	4.15 (17)
C2	.4922 (9)	.1055 (6)	.1749 (2)	3.31 (14)
C3	.4890 (12)	.1746 (8)	.2160 (3)	4.47 (19)
C4	.5889 (12)	.2707 (8)	.2197 (3)	4.98 (20)
C5	.6929 (12)	.3041 (9)	.1835 (3)	5.33 (21)
C6	.6955 (11)	.2433 (8)	.1428 (3)	4.86 (19)
C7	.5972 (9)	.1397 (6)	.1367 (3)	3.68 (16)
C8	.5881 (10)	.0778 (7)	.0939 (3)	4.63 (18)
C9	.5157 (12)	-.0295 (9)	.0948 (4)	4.94 (21)
C10	.4129 (12)	-.0648 (9)	.1316 (3)	5.13 (22)
C11	.2107 (12)	-.0002 (9)	.1915 (4)	5.63 (22)
C12	.0883 (12)	.0880 (8)	.1673 (3)	4.80 (19)
C13	.6067 (16)	.1392 (11)	.0487 (4)	6.54 (28)
C14	.4386 (13)	.2118 (9)	.0390 (4)	5.43 (22)
C15	.1182 (10)	.0986 (7)	.1161 (2)	3.62 (15)
C16	.0600 (13)	.0481 (9)	.0761 (3)	5.39 (24)
C17	.1593 (12)	.0836 (7)	.0387 (4)	5.31 (21)
C18	.2819 (10)	.1548 (7)	.0564 (3)	4.34 (17)
O	.2552 (6)	.1667 (4)	.1037 (2)	3.62 (10)
H3	.415 (11)	.150 (7)	.233 (3)	5.8 (22)
H4	.587 (15)	.318 (11)	.253 (5)	14.7 (40)
H5	.756 (15)	.371 (10)	.183 (4)	11.4 (35)
H6	.754 (12)	.255 (8)	.113 (3)	7.8 (23)
H9	.505 (1)	-.069 (8)	.073 (3)	7.3 (26)
H10	.357 (14)	-.127 (10)	.127 (3)	10.5 (34)
H11A	.212 (6)	.025 (5)	.221 (2)	1.4 (12)
H11B	.180 (10)	-.091 (8)	.187 (3)	6.9 (22)
H12A	.105 (8)	.168 (6)	.181 (2)	3.3 (14)
H12B	-.041 (12)	.049 (7)	.176 (3)	7.2 (22)
H13A	.601 (10)	.067 (7)	.024 (2)	5.9 (20)
H13B	.671 (11)	.195 (8)	.052 (3)	7.2 (27)
H14A	.418 (12)	.220 (8)	-.001 (4)	10.5 (29)
H14B	.454 (10)	.284 (7)	.055 (3)	5.5 (19)
H16	.011 (9)	.014 (6)	.088 (2)	2.9 (18)
H17	.169 (16)	.074 (11)	.004 (5)	15.5 (44)

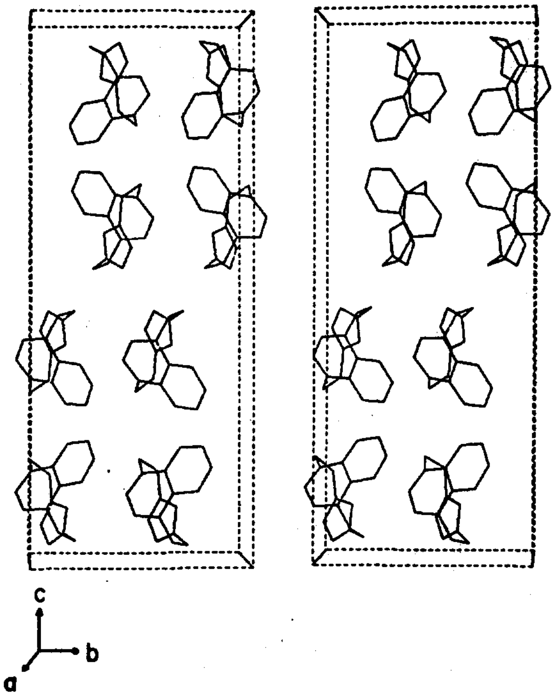


Fig. 4. The crystal packing of a unit cell of 1.

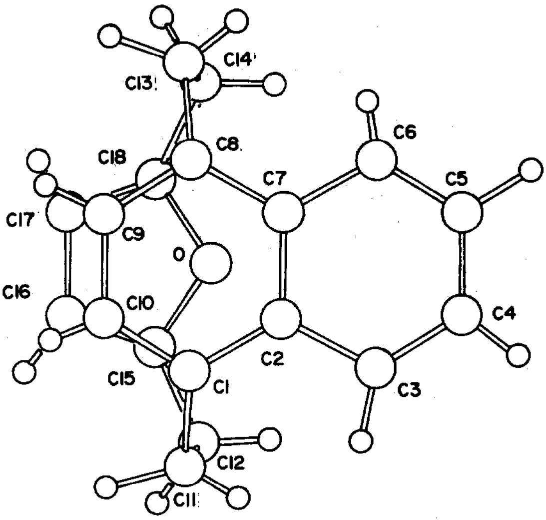


Fig. 5. Projection of 1 perpendicular to the naphthalenoid ring.

clination of planes A and B (Table 2) this off-center positioning of the two rings allows for a minimum of transannular π-π interaction between the two aromatic π-clouds. In fact the distance between C atoms 17 and 16 of the furanoid ring is 3.4 Å away from plane A. This value is identical to that found in graphite[2] between aromatic planes and is considered to be the best distance for minimal transannular π-π repulsion and maximum transannular π-π interaction. This distance is maintained at the expense of forcing the O atom, centrally, into the π-cloud of the bridged portion of the naphthalenoid ring. While this result is probably due to the lower steric requirement of the O atom (a fact which is substantiated by conformational behavior in similar systems)[10], it is possible that the orbital associated with the O atom (normally hydridized sp^2 in furan) finds this central region an area of minimum interaction with the π-cloud of the naphthalenoid ring.[10]

With the above considerations it becomes obvious why the molecule exists in the *anti*- rather than the *syn*-conformation. The flipping behavior of the furanoid ring around its 2,5-C atom axis is rather facile in [2.2]cyclophanes.[10] However, for the *syn*-conformation of 1, even if the O atom were centrally positioned above the bridged portion of the naphthalenoid ring, there would be a much larger degree of transannular π-π repulsion. Everything else being equal, the molecule thus finds less severe transannular interaction in the *anti*-conformation.

Even with the reduction of transannular π-π interaction described above, the rings are close to one another (Fig. 3) and the π-clouds still repel one another to a significant extent. This can be seen in distortions of angles α and β associated with the puckering of the bridged portion of the naphthalenoid ring, angle γ associated with the furanoid ring and angle δ associated with the bridging C atoms once removed from the furanoid ring. As in other 1,4-bridged cyclophanes much of the transannular π-π repuslion is taken up by bending angles α and β. In our case these angles are 14° and 16° respectively and are similar to those found in previous studies on similar systems (Table 1). Interestingly, since the furanoid ring is planar, there is no angle comparable to α. Angle γ is found to be 7°, which brings C12 and C14 an average of 0.18 (1) Å out of the furanoid plane. This value (7°) is less than half the corresponding value for angle β (16°) and implies, at least in these systems, that at these positions, angle strain is better accommodated adjacent to the naphthalenoid rather than the furanoid ring.

The accommodation of angle strain at the bridge C atoms (angles δ and ϵ) is however reversed. In similar cyclophanes angle ϵ is usually 114°. Here it is found to be 108.9° (average), very close to the normal value of 109.5°. In contrast angle δ is 113°, significantly expanded from normal values.

Along with the above we note with interest some unusual structural features in 1 with regard to the naphthalenoid and furanoid rings. For the furanoid ring the C14-C18-C17 and C12-C15-C16 angles (θ) are among the largest observed for such angles in similar furanoid systems.[15] Large values are also observed in 2,[8] and it is possible that overall conformations of 1 and 2 are a result of a delicate balance of minimizing transannular π-π interactions, as well as minimizing strain at angles exocyclic to the furanoid ring. In [2.2](2,5)thiophenophane,[16] the thiophenoid rings are parallel to one another and are somewhat puckered. The angles related to the C-C-C angles described above are 134.3°, 134.7°, 135.8° and 126.5°. While the furanoid ring in 2 is somewhat puckered, in 1 the ring is planar, presumably a consequence of the macrocycle's ability to accommodate the strain.

It seems reasonable that angles δ and θ are closely coupled with the angle of inclination of the two aromatic moieties and as the angle of inclination increases form 0°–90° angles δ and θ will also increase. This structural relationship is of considerable interest since furanoid rings in [2.2]cyclophanes undergo conformational flipping which involves increasing and decreasing the angle of inclination.

For the naphthalenoid ring there are three interesting features, two of which are noted for the first time. First, the naphthalene C–C bonds associated with the puckered portion of the ring (av. 1.429(10) Å) are significantly longer than the other C–C bonds (av. 1.372(10) Å). Second, there are two pairs of chemically equivalent hydrogen atoms which show unusual distortions, *viz*, (H3, H6) and (H9, H10). The H3, H6 pair have an average C–C–H angle of 131.8(55)°[17], while the H9, H10 pair are found out of the C1-C8-C9-C10 plane by an average of 0.17(10) Å. While neither of these deviations are highly significant, we wish to call attention to them since the out-of-plane deviations have been observed earlier in **3**.[3] We do plan to examine these distortions carefully in related molecules, if crystals of sufficient quality can be obtained.

Thirdly, in comparing H9 and H10 with the comparable position in **3**, the atoms bound to C2 and C7 in **1** should also show this out-of-plane distortion. We note here that this is also observed since the least squares plane of C2, C3, C4, C5, C6 and C7 is not coplanar with C1, C2, C7 and C8. C3 and C6 are found out of that plane by an average of 0.12(1) Å, slightly less than the comparable H atoms on C9 and C10. It is probable that all these deviations are derived from the loss of aromaticity of the naphthalenoid ring caused by the transannular π-π interaction.

The accommodation of strain in **1** occurs somewhat analogously to that previously documented for the mixed heterocyclophane **2**, ([2.2(2,5)furano(2,6)pyridinophane) which exists in the *syn*-conformation (i.e., the O and N atoms are *syn*- with respect to one another). The aromatic rings in this molecule are inclined 23° to one another. The furanoid O again is located nearly directly above the center of the pyridinoid ring. There exists about the same degree of puckering of the pyridinoid ring as in the bridged half of naphthalenoid ring in **1**. The authors of the study state that lone-pair repulsion of O and N is small, causing little additional distortion. There are, however, *trends* in nonbonded contacts and angle distortions (see δ angles and O–N, O–C8 distances in Fig. 6) which suggest that O–N repulsion may indeed be important in that system. The answer to this question awaits the determination of related heteroaromatic cyclophane structures.

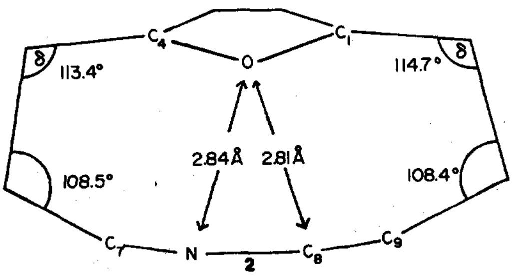


Fig. 6.

At this point it seems clear that the position of the hetero-atom and the π-cloud of the heteroaromatic ring with respect to the other aromatic moiety in **1** and other cyclophanes containing hetero-atoms, are very important factors in determining the structures and conformations of these systems. Of course the role that angle distortion and aromatic ring puckering plays in reducing strain is also of great importance. It seems that all these factors are not mutually exclusive. We hope to examine more closely the relative strength of these factors by determining structures of a series of molecules in which the heteroatom in **1** is changed (e.g. **8** and **9**) and in which the naphthalenoid moiety in **1** is replaced (e.g. **10** and **11**; see Fig. 7).

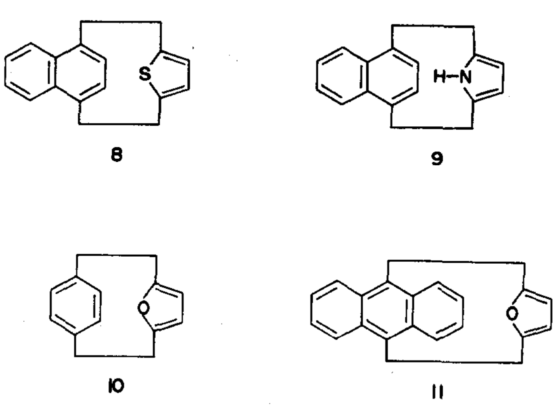


Fig. 7.

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[13] Many of these molecules, though relatively rigid, display conformational behavior which allows one or more of the aromatic rings to flip[1a,10] through the cavity defined by the cyclophane macrocycle, albeit, in some instances, with relatively high activation energies. The question then arises, when these molecules pack with rings non-parallel to one another and thus destroying some crystallographic symmetry, whether the structure as determined by crystallographic techniques truly reflects the structure of the molecular system. It should be noted, however, that while one might expect the packing process to exert its own requirements upon structure, it has been pointed out previously[7] that molecules which are intrinsically asymmetric in solution would not have symmetry imposed by the crystallization process (see A. I. Kitaigorodskii, *Organic Chemical Crystallography*. Consultants Bureau, New York, 1961).

[14] There is another possible way for these cyclophanes to ac-

commodate strain which involves twisting one aromatic ring with respect to the other around an axis normal to the bridged portion of the rings[3] We thank one referree for pointing this out.

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[17] This distortion has also been observed in *syn*[2.2](1,4)naphthalenophane. Unpublished results, Albert Fratini, University of Dayton. We thank Dr. Fratini for communicating these results prior to publication.