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Crystal Structures of Inclusion Complexes of Cholic Acid with Aniline, Mono- and Difluorinated Anilines: Guest Information Expressed by Molecular Assembly

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Abstract. The crystal structures of cholic acid (CA), a naturally occurring bile acid, complexed with aniline, and its mono- and difluorinated derivatives were elucidated by X-ray crystallography. Comparison of the structures obtained shows that the molecular assembly pattern and the related structural change of the CA molecule vary among different complexes. These structural changes are the molecular information of the guests.

Key words: Multimolecular inclusion complex, molecular assembly, cholic acid, molecular information.

Supplementary Data relating to this article are deposited with the British Library as Supplementary Publication No. SUP 82197 (27 pages).

1. Introduction

Much effort has been made to construct organized structures having desired architectural features in the solid state [1–6]. A typical method is to design molecular components to suit the particular purpose required. This method is based on a concept that the nature of the molecular crystals obtained results from that of the components. For example, Lehn *et al.* [2] reported molecular complex systems consisting of a substituted triaminopyrimidine and barbituric derivative, where the nature of the carbonyl and amino groups appeared in a supramolecular strand. Thus molecular information of the components such as functional group, complementarity and molecular size, must be well known in advance in order to achieve successful molecular design.

Here we present our view regarding the relationship between molecular assembly and its components, which is different from the concept mentioned above:

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the assembly pattern and related structural changes are the molecular information of the components. In this paper, we report on the molecular information of the guests expressed by the molecular assembly pattern using our host–guest systems. For this purpose cholic acid (CA), a naturally occurring bile acid, is used as the host. This compound has the property of 'isostructurality' [7] when cocrystallized with analogous guests. Aniline and its fluorinated derivatives are used as guests. From the crystal structure, we found that a slight difference in the guest structure markedly affects the assembly pattern as well as the side chain conformation of CA. These structural changes contain information on the property of small molecules, although the precise meaning of the changes has not been analyzed in terms of intermolecular forces. Some of the results have been reported in a preceding paper [8].

2. Experimental

2.1. PREPARATION OF INCLUSION COMPLEXES

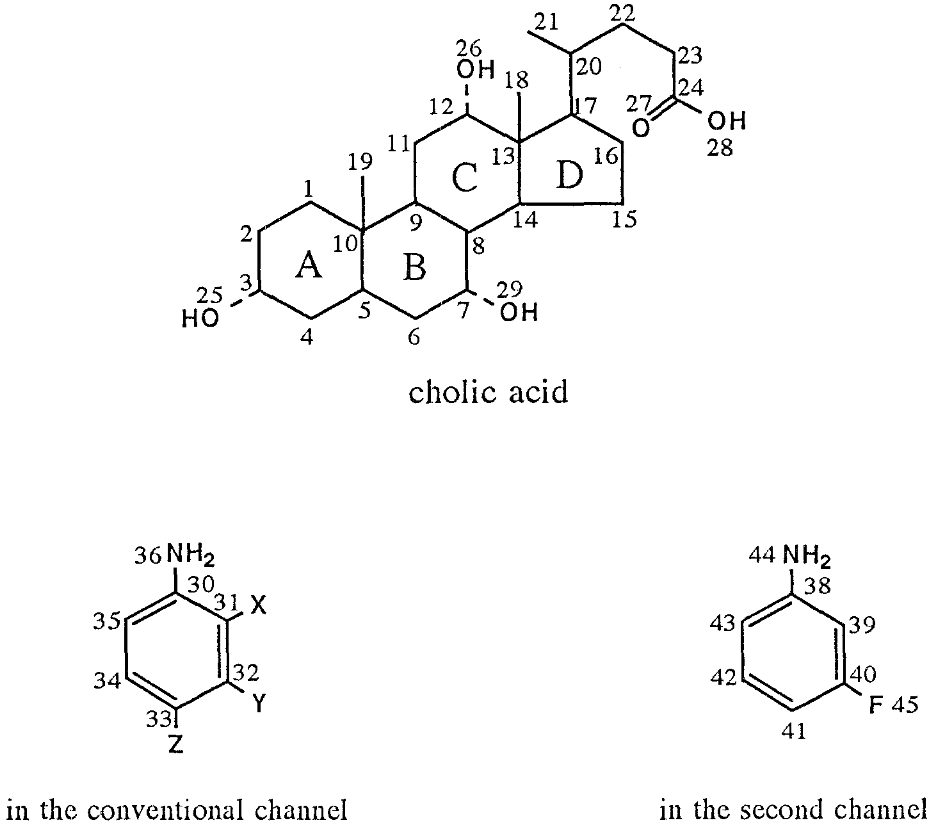
Solutions of CA (0.3 g) in aniline, 2-, 3- and 4-fluoroaniline (2-FA, 3-FA and 4-FA, respectively) and 3,4-difluoroaniline (34-DFA) (2 cm^3) were kept at room temperature for about 12 h and crystals of the inclusion complex with a host–guest ratio of 1 : 1 or 1 : 2 were obtained as colorless needles.

2.2. X-RAY STRUCTURAL ANALYSES AND REFINEMENT

X-ray diffraction measurements were performed on a Rigaku AFC7R diffractometer with graphite-monochromated Cu K_α ($\lambda = 1.54178$ Å) radiation at 293 K. Data were corrected for Lorentz and polarization effects. An empirical absorption correction using the program DIFABS [9] and a correction for secondary extinction were applied. The structures were solved by direct methods: SAPI91 [10] and DIRDIF92 [11] for CA–2-FA and SHELXS86 [12] and DIRDIF92 for CA–4-FA and CA–34-DFA. Some hydroxyl hydrogen atoms were located from the difference Fourier map. Other hydrogen atoms were placed at calculated positions. Non-hydrogen atoms were refined anisotropically, whereas hydrogen atoms were included but not refined. The weighting scheme used was $w = 1/\sigma^2(F_o) = 4F_o^2/\sigma^2(F_o^2)$. The absolute configurations conformed to a previously reported structure of CA [8]. All calculations were performed using the TEXSAN crystallographic software package [13].

2.3. VAN DER WAALS SURFACE AREA AND MOLECULAR VOLUME CALCULATIONS

van der Waals surface area and molecular volume calculations were performed with the MOL-MOLIS/CRYS of Daikin Industries Co., Ltd. on an IRIS Indigo R4000 XS24 Silicon Graphics workstation.



aniline : X=Y=Z=H
2-fluoroaniline : X=F,Y=Z=H
3-fluoroaniline : X=Z=H, Y=F
4-fluoroaniline : X=Y=H, Z=F
3,4-difluoroaniline : X=H, Y=Z=F

Structure I.

3. Results and Discussion

3.1. STRUCTURES OF CA INCLUSION COMPLEXES

The measurement conditions and structural details are listed in Table I. The positional parameters and temperature factors for non-hydrogen atoms of CA–2-FA, –4-FA and –34-DFA are given in Tables II, III and IV, respectively. Figure 1 shows an ORTEP [14] drawing of CA and 4-FA. The crystal structures drawn with CHARON [15] of the inclusion complexes of CA with aniline and monofluorinated aniline, i.e., 2-FA, 3-FA and 4-FA are depicted in Figure 2. CA molecules are arranged in such a way that the OH and CH_3 groups associate to form hydrophilic and

TABLE I. Crystal data for CA inclusion complexes.

Complex	CA–aniline[a]	CA–2-FA	CA–3-FA[a]	CA–4-FA	CA–34-DFA
Mol. formula	$C_{30}H_{47}NO_5$	$C_{30}H_{46}FNO_5$	$C_{36}H_{52}F_2N_2O_5$	$C_{30}H_{46}FNO_5$	$C_{30}H_{45}F_2NO_5$
M	501.71	519.70	630.81	519.70	523.68
Space group	$P2_1$	$P2_1$	$P2_1$	$P2_1$	$P2_1$
Z	2	2	2	2	2
a/Å	13.801(3)	13.613(3)	14.326(3)	13.834(4)	13.928(2)
b/Å	8.066(3)	8.147(4)	7.847(3)	8.109(4)	8.135(3)
c/Å	14.094(3)	14.034(2)	16.125(3)	13.993(3)	14.029(2)
β/deg	116.01(1)	113.71(1)	106.58(1)	115.54(2)	115.94(1)
V/Å^3	1409.9(7)	1425.0(9)	1737.4(7)	1416.2(9)	1429.5(6)
D_{calc}/g cm^{-3}	1.182	1.211	1.206	1.219	1.217
μ/cm^{-1}	5.94	6.92	6.75	6.62	7.35
$F(000)$	548	564	680	564	566
Crystal size/mm	0.30 × 0.25 × 0.25	0.25 × 0.25 × 0.35	0.20 × 0.20 × 0.10	0.20 × 0.10 × 0.30	0.20 × 0.05 × 0.25
2θ limit/deg	120.3	120.1	120.2	120.2	120.2
No. of observed reflctns.[b]	1448	1214	1925	1466	1117
No. of variables	325	334	406	334	343
R	0.050	0.069	0.060	0.050	0.068
R_w	0.038	0.096	0.035	0.029	0.103
Goodness of fit indicator	2.19	1.48	3.21	2.14	1.95

[a] Reference [8].
[b] Criterion for F_{obs} exclusion: $I > 3\sigma(I)$.

hydrophobic layers, respectively. Conventional channel-like spaces are observed in the hydrophobic layers. Channels consist of steroidal A rings and side chains, and are parallel to the *b* axis. Another type of channel, i.e., 'the second channel' is formed in the hydrophobic layers of the CA–3-FA structure, the details of which have been described in a previous paper [8]. The guest molecules are accommodated inside these channels. Details of the CA–34-DFA structure will be discussed below.

X-ray measurements of CA inclusion complexes have hitherto shown that hydrogen bond networks are formed between components and play an important role in stabilizing the crystal lattice [8, 16–29]. In the present structures, it can be seen that an F atom affects the hydrogen bond network pattern. As shown in Figure 3, there are at least two patterns in the present CA inclusion complexes. One is a bridged bicyclic system and the other is a single cyclic system. In the structures of CA–aniline, –3-FA and –4-FA, the amino group is hydrogen bonded to O(26) and O(27) or O(28) atoms and forms a bridged bicyclic system. The hydrogen bond pat-

TABLE II. Positional parameters and temperature factors [$B_{(\mathrm{eq})}$] for non-hydrogen atoms of CA–2-FA.

Atom	x	y	z	$B_{(\mathrm{eq})}$[a]
F(37)	0.527(2)	0.0854	0.679(2)	28(1)
O(25)	1.0919(6)	0.207(1)	0.6221(5)	5.3(2)
O(26)	0.8187(5)	0.518(1)	0.1935(4)	4.3(2)
O(27)	0.3441(7)	0.271(2)	−0.1546(8)	8.3(3)
O(28)	0.3019(6)	0.526(1)	−0.1946(7)	7.2(2)
O(29)	0.9110(5)	−0.020(1)	0.2713(4)	3.9(1)
N(36)	0.398(3)	−0.082(5)	0.753(3)	23(1)
C(1)	1.1805(8)	0.396(2)	0.4240(7)	4.4(3)
C(2)	1.1316(8)	0.387(1)	0.5056(7)	3.9(2)
C(3)	1.1466(8)	0.215(1)	0.5516(7)	3.6(2)
C(4)	1.1013(8)	0.090(1)	0.4688(7)	3.6(2)
C(5)	1.1486(8)	0.097(1)	0.3856(7)	3.8(2)
C(6)	1.1001(8)	−0.035(1)	0.3012(7)	3.8(2)
C(7)	0.9871(7)	−0.002(1)	0.2239(6)	3.2(2)
C(8)	0.9767(7)	0.169(1)	0.1770(6)	3.2(2)
C(9)	1.0196(7)	0.301(1)	0.2617(7)	2.9(2)
C(10)	1.1393(7)	0.275(1)	0.3373(7)	3.6(2)
C(11)	1.0011(8)	0.473(1)	0.2114(6)	4.0(2)
C(12)	0.8832(7)	0.510(1)	0.1337(7)	3.4(2)
C(13)	0.8450(7)	0.377(1)	0.0496(6)	3.2(2)
C(14)	0.8617(7)	0.210(1)	0.1053(6)	3.1(2)
C(15)	0.8031(8)	0.090(1)	0.0192(7)	4.0(2)
C(16)	0.7050(8)	0.186(1)	−0.0529(7)	3.9(2)
C(17)	0.7192(7)	0.368(1)	−0.0164(6)	3.1(2)
C(18)	0.9063(8)	0.393(2)	−0.0198(7)	4.0(2)
C(19)	1.2122(8)	0.280(2)	0.2778(8)	4.7(3)
C(20)	0.6655(8)	0.491(1)	−0.1061(7)	3.9(2)
C(21)	0.6853(8)	0.671(2)	−0.0743(9)	4.6(3)
C(22)	0.5449(8)	0.456(1)	−0.1677(7)	4.2(2)
C(23)	0.4819(9)	0.458(2)	−0.1005(7)	5.5(3)
C(24)	0.369(1)	0.412(2)	−0.1529(8)	5.0(3)
C(30)	0.387(3)	−0.106(4)	0.670(3)	21(1)
C(31)	0.471(2)	−0.020(3)	0.636(2)	12.4(7)
C(32)	0.461(2)	−0.050(4)	0.537(3)	18(1)
C(33)	0.432(4)	−0.123(6)	0.475(3)	23(2)
C(34)	0.353(2)	−0.210(4)	0.497(3)	19(1)
C(35)	0.333(2)	−0.223(3)	0.581(3)	15.3(9)

[a] $B_{(\mathrm{eq})} = (8/3)\pi^2\{U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos a\}$.

TABLE III. Positional parameters and temperature factors [$B_{(\mathrm{eq})}$] for non-hydrogen atoms of CA–4-FA.

Atom	x	y	z	$B_{(\mathrm{eq})}$[a]
F(36)	0.4127(6)	0.6171	0.3932(5)	12.5(3)
O(25)	−0.0896(4)	0.456(1)	0.3776(3)	4.5(1)
O(26)	0.1785(3)	0.768(1)	0.8098(3)	4.0(1)
O(27)	0.6598(5)	0.518(1)	1.1591(5)	6.7(2)
O(28)	0.7009(4)	0.785(1)	1.1951(4)	5.4(2)
O(29)	0.0899(3)	0.225(1)	0.7336(3)	3.7(1)
N(36)	0.3895(7)	0.661(2)	0.7703(6)	10.9(4)
C(1)	−0.1803(5)	0.647(1)	0.5710(6)	4.2(2)
C(2)	−0.1303(6)	0.632(1)	0.4918(5)	3.9(2)
C(3)	−0.1454(6)	0.464(1)	0.4443(5)	3.8(2)
C(4)	−0.1002(5)	0.334(1)	0.5298(5)	3.3(2)
C(5)	−0.1465(5)	0.343(1)	0.6113(5)	3.6(2)
C(6)	−0.0989(5)	0.205(1)	0.6951(5)	3.6(2)
C(7)	0.0144(5)	0.242(1)	0.7781(5)	3.2(2)
C(8)	0.0264(5)	0.415(1)	0.8257(5)	2.8(2)
C(9)	−0.0190(5)	0.551(1)	0.7409(5)	2.7(2)
C(10)	−0.1394(5)	0.517(1)	0.6614(5)	3.3(2)
C(11)	0.0001(5)	0.723(1)	0.7920(5)	3.4(2)
C(12)	0.1172(6)	0.757(1)	0.8711(5)	3.7(2)
C(13)	0.1599(5)	0.622(1)	0.9564(5)	3.0(2)
C(14)	0.1415(5)	0.456(1)	0.9001(5)	2.8(2)
C(15)	0.2024(5)	0.334(1)	0.9886(5)	3.6(2)
C(16)	0.3012(6)	0.434(1)	1.0631(6)	4.1(2)
C(17)	0.2838(5)	0.615(1)	1.0239(5)	3.0(2)
C(18)	0.1010(5)	0.638(1)	1.0288(5)	4.1(2)
C(19)	−0.2148(5)	0.526(1)	0.7155(5)	4.6(2)
C(20)	0.3401(6)	0.738(1)	1.1144(5)	3.7(2)
C(21)	0.3195(6)	0.918(1)	1.0821(6)	4.4(2)
C(22)	0.4625(5)	0.701(1)	1.1714(5)	3.9(2)
C(23)	0.5189(5)	0.717(1)	1.1002(5)	5.0(2)
C(24)	0.6337(6)	0.661(2)	1.1547(6)	4.7(2)
C(30)	0.3940(9)	0.646(2)	0.6764(9)	6.7(3)
C(31)	0.3424(8)	0.524(2)	0.604(1)	7.1(3)
C(32)	0.352(1)	0.512(2)	0.512(1)	8.1(4)
C(33)	0.411(1)	0.629(2)	0.491(1)	7.7(4)
C(34)	0.4616(9)	0.753(2)	0.557(1)	9.1(4)
C(35)	0.4547(9)	0.759(2)	0.651(1)	8.2(4)

[a] $B_{(\mathrm{eq})} = (8/3)\pi^2\{U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos \gamma + 2U_{13}aa^*cc^* \cos \beta + 2U_{23}bb^*cc^* \cos a\}$.

TABLE IV. Positional parameters and temperature factors [$B_{(\mathrm{eq})}$] for non-hydrogen atoms of CA–34-DFA.

Atom	x	y	z	$B_{(\mathrm{eq})}$[a]
F(37)	0.091(1)	0.6343	0.676(1)	16.9(6)
F(38)	0.075(2)	0.407(4)	0.543(2)	23(1)
O(25)	1.1240(6)	0.647(3)	1.0920(8)	6.9(3)
O(26)	0.6854(6)	0.336(2)	0.8178(6)	5.8(2)
O(27)	0.343(1)	0.592(3)	0.342(1)	9.3(4)
O(28)	0.3072(9)	0.330(3)	0.2974(8)	8.2(3)
O(29)	0.7629(6)	0.878(2)	0.9089(6)	5.3(2)
N(36)	−0.252(2)	0.488(4)	0.642(3)	21(1)
C(1)	0.927(1)	0.456(3)	1.174(1)	6.4(4)
C(2)	1.005(1)	0.465(3)	1.127(1)	6.1(4)
C(3)	1.053(1)	0.638(3)	1.142(1)	5.9(4)
C(4)	0.969(1)	0.761(3)	1.101(1)	5.1(3)
C(5)	0.887(1)	0.755(3)	1.143(1)	5.1(3)
C(6)	0.803(1)	0.889(3)	1.099(1)	6.4(4)
C(7)	0.720(1)	0.855(3)	0.985(1)	5.1(4)
C(8)	0.671(1)	0.690(3)	0.971(1)	4.8(4)
C(9)	0.757(1)	0.549(3)	1.014(1)	5.3(4)
C(10)	0.835(1)	0.583(3)	1.133(1)	5.1(4)
C(11)	0.704(1)	0.380(3)	0.993(1)	6.0(4)
C(12)	0.624(1)	0.344(3)	0.875(1)	5.2(4)
C(13)	0.5408(9)	0.479(3)	0.8377(9)	4.5(3)
C(14)	0.599(1)	0.646(3)	0.857(1)	5.6(4)
C(15)	0.507(1)	0.769(3)	0.793(1)	6.0(4)
C(16)	0.434(1)	0.672(3)	0.695(1)	5.7(4)
C(17)	0.473(1)	0.493(3)	0.711(1)	5.6(4)
C(18)	0.4657(9)	0.461(3)	0.890(1)	5.7(3)
C(19)	0.777(1)	0.569(3)	1.205(1)	6.6(4)
C(20)	0.381(1)	0.363(3)	0.655(1)	6.0(4)
C(21)	0.412(1)	0.185(3)	0.673(1)	6.6(4)
C(22)	0.326(1)	0.407(3)	0.533(1)	5.4(4)
C(23)	0.400(1)	0.394(3)	0.482(1)	6.1(4)
C(24)	0.348(1)	0.456(4)	0.369(1)	6.5(5)
C(30)	−0.167(3)	0.474(5)	0.629(2)	12(1)
C(31)	−0.074(2)	0.573(4)	0.666(2)	10.7(8)
C(32)	0.001(2)	0.539(4)	0.635(2)	9.1(7)
C(33)	−0.009(3)	0.422(5)	0.567(2)	13(1)
C(34)	−0.094(5)	0.333(6)	0.534(3)	20(2)
C(35)	−0.171(2)	0.368(6)	0.560(3)	15(1)

[a] $B_{(\mathrm{eq})} = (8/3)\pi^2\{U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos\gamma + 2U_{13}aa^*cc^* \cos\beta + 2U_{23}bb^*cc^* \cos a\}$.

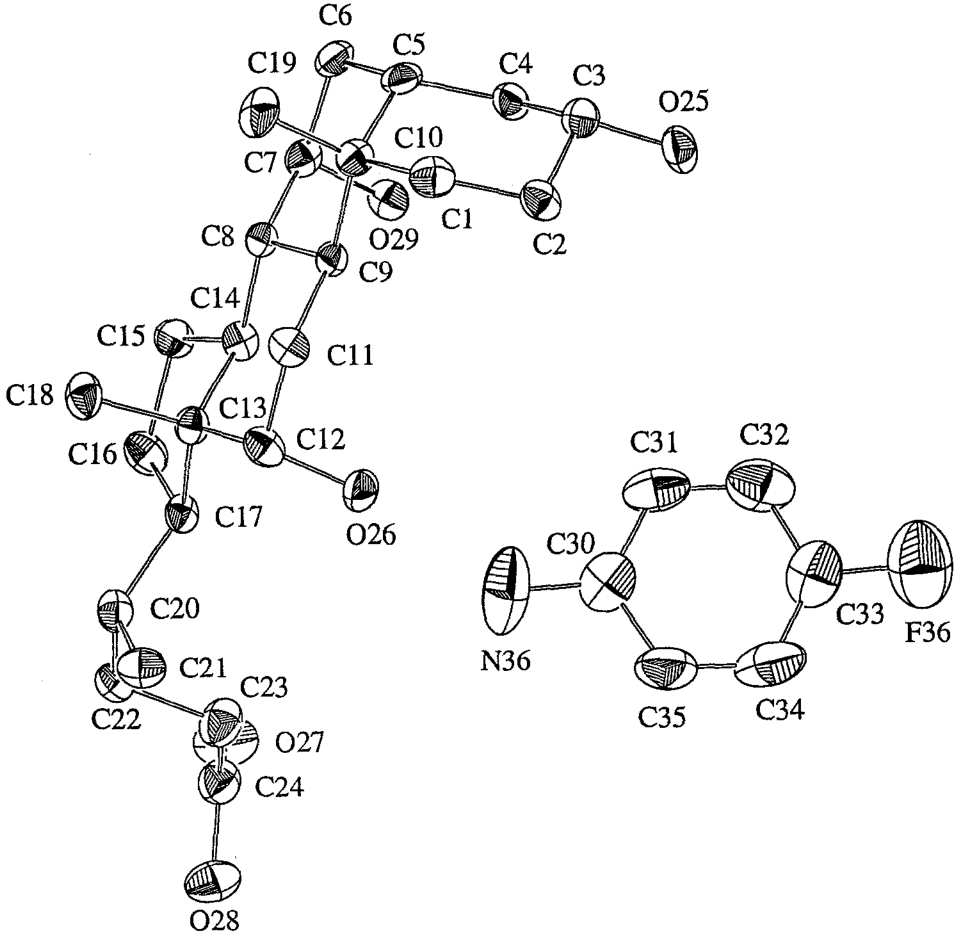


Fig. 1. ORTEP drawing of the molecular structures of CA and 4-FA in the CA—4-FA inclusion complex. All the atoms are represented by thermal ellipsoids with 30% probability levels. H atoms are omitted for clarity.

tern, however, is ambiguous. For example, the interatomic distance between N(36) and O(26) [N(36)···O(26)] is 3.23(1) Å, while N(36)···O(27) and N(36)···O(28) are 3.37(1) and 3.26(2) Å, respectively, in the CA–34-DFA structure. Because of the similarity in value, it is difficult to determine conclusively which of the O atoms is hydrogen bonded to the N(36) atom. Similar ambiguity is seen in the CA–aniline, –3-FA and –4-FA inclusion complexes. In contrast, a conspicuous difference is observed in the hydrogen bond network of the CA–2-FA structure. The amino group of 2-FA does not form any intermolecular hydrogen bonds and, consequently, a single cyclic system is formed. Instead, an intramolecular hydrogen bond may be formed judging from a N(36)···F(37) distance of 2.74(5) Å.

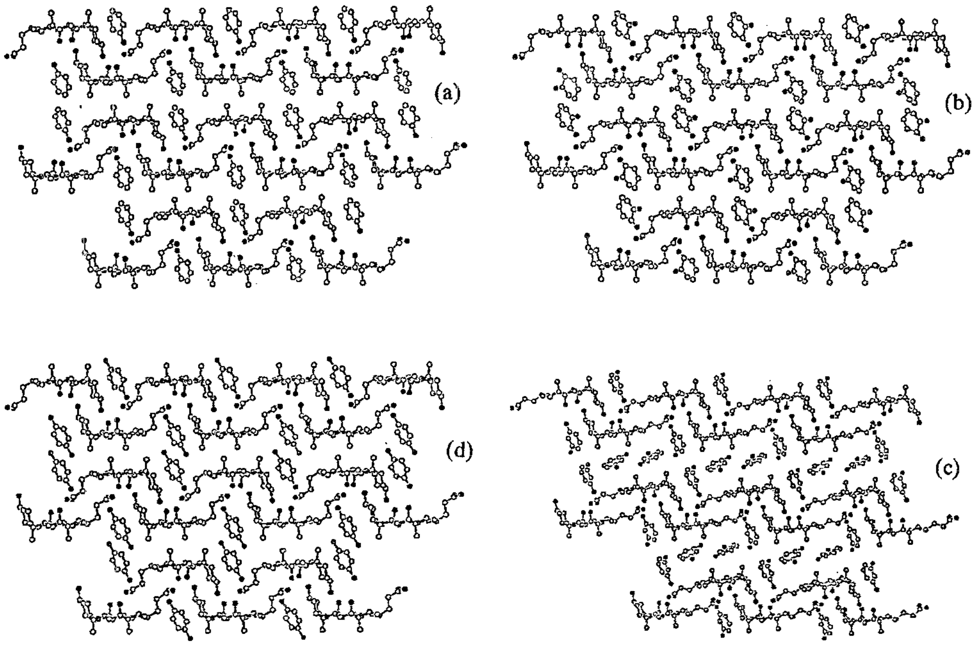


Fig. 2. CHARON drawings of the packing diagrams of the CA inclusion complexes as viewed along the *b* axis. Clockwise from top left: (a) CA–aniline [8], (b) CA–2-FA, (c) CA–3-FA [8], and (d) CA–4-FA. C and F atoms are represented by empty and half-filled circles, respectively. O and N atoms are represented by filled circles. H atoms are omitted for clarity.

3.2. GUEST INFORMATION EXPRESSED BY MOLECULAR ASSEMBLY AND RELATED STRUCTURAL CHANGES

In the present study we consider that the molecular assembly pattern and related structural changes are the molecular information of the guest. Our hypothesis is based on the fact that the structural features of the molecular assembly essentially result from the interaction between components. First, we examine the guest information expressed by molecular assembly. Comparison of the structures shows that the most notable difference is the presence of the second channels in the hydrophobic layers of the CA–3-FA structure. To confirm our assumption that the appearance of the second channels is induced by the *meta*-F atom, we further investigated the crystal structure of the inclusion complex of CA with 34-DFA containing *meta*- and *para*-F atoms. This crystal structure is depicted in Figure 4. The hydrogen bond network pattern is similar to those of CA–aniline, –3-FA and – 4-FA. It is noteworthy that the structure does not contain the second channels and is essentially the same as those of the CA–aniline, –2-FA and –4-FA inclusion complexes. A comparison between the CA–3-FA and –34-DFA structures, therefore, indicates that the *meta*-F atom does not always induce the appearance of the second channels. Also, the results prove that the ability of the *meta*-F atom to induce the appearance of the second channel is inactivated by the *para*-F atom. The mechanism of the

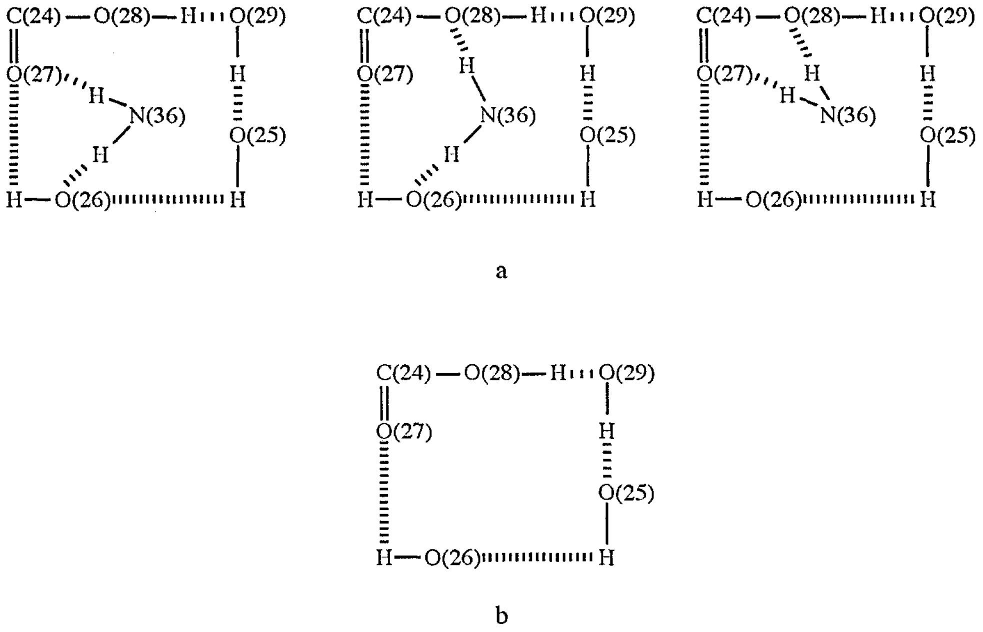


Fig. 3. Schematic representations of the hydrogen bond network observed in (a) CA–aniline, –3-FA, –4-FA and –34-DFA, (b) CA–2-FA. The distinction among the three patterns in (a) is unclear.

channel disappearance induced by the *para*-F atom, however, is not clear. We have examined the guest size effect on the appearance of the second channel. Table V shows the surface areas and volumes of the guest molecules. It is obvious that both the area and volume of 3-FA are quite similar to those of the other monofluorinated anilines. 34-DFA has the largest area and volume among the five molecules. Consequently, the appearance of the second channel is not simply related to the size of the guest molecule. Although the reason for this unique structure remains unclear, the 'double-channel-type structure' in the CA–3-FA complex clearly reflects the molecular information of 3-FA. The absence of the second channels in the other structures is definitely a piece of guest information.

Another notable structural difference is the host–guest ratio; namely, the CA–3-FA complex has the ratio of 1 : 2 while the others have the ratio of 1 : 1. This difference in stoichiometry results from the *meta*-F atom, as mentioned above. We may consider the 1 : 2 ratio as a piece of molecular information about 3-FA.

Because of the 1 : 2 ratio, a large difference is observed in the lattice constants of the CA–3-FA complex compared with those of the other complexes. Thus the *a* and *c* lattice constants of the CA–3-FA complex are somewhat larger as compared with the others: at least 0.398 and 2.031 Å longer along the *a* and *c* axes, respectively. This is naturally due to the double-channel-type structure. Slight differences in the lattice constants are observed in the other complexes; these are within 0.315, 0.081

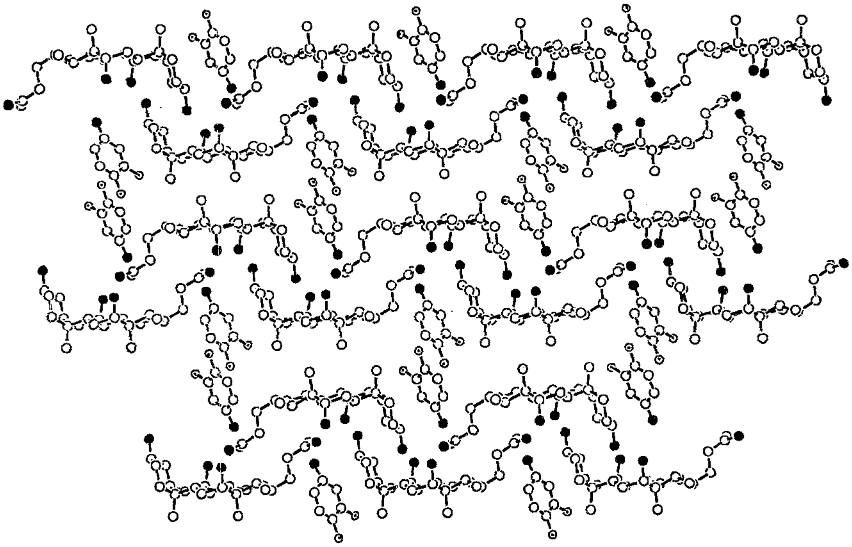


Fig. 4. CHARON drawing of the packing diagrams of CA–34-DFA as viewed along the *b* axis. C and F atoms are represented by empty and half-filled circles, respectively. O and N atoms are represented by filled circles. H atoms are omitted for clarity.

TABLE V. Van der Waals surface areas (in Å^2) and molecular volumes (in Å^3) of the guests.

Guest	Surface area	Molecular volume
Aniline	94.6	125.2
2-FA	100.0	131.5
3-FA	100.1	132.5
4-FA	100.3	132.5
34-DFA	105.8	139.7

and 0.101 Å along the *a*, *b* and *c* axes, respectively. It remains unknown whether these differences could be regarded as significant. However, the lattice constants definitely reflect some properties of each guest molecule. It was found that only 3-FA has significant guest information that can be expressed by the lattice constant changes among the guests studied here.

X-ray analyses have shown that the side chain of CA takes various conformations in the molecular complexes. The importance of the side chain conformation in the stabilization of the crystal lattice was reported by Miyata *et al.* [21]. They found that the side chain employs its conformational freedom to accommodate different guest species, i.e., ‘guest-dependent conformation’. Contrary to their concept, we wish to regard these conformational changes as molecular information related to the guests. Table VI shows several torsion angles of the CA side chain. It is understandable that the angles observed in CA–3-FA differ from those of others, since

TABLE VI. Torsion angles for CA molecules (in degrees).

Inclusion complex	CA–aniline[a]	CA–2-FA	CA–3-FA[a]	CA–4-FA	CA–34DFA
C(13)—C(17)—C(20)—C(21)	−55.1(9)	−55(1)	−58(1)	55.3(9)	−54(1)
C(17)—C(20)—C(22)—C(23)	61.2(8)	58(1)	−166.1(8)	−61.8(9)	62(1)
C(20)—C(22)—C(23)—C(24)	−170.6(7)	−174(1)	176.7(9)	173.4(8)	−173(1)
C(22))—C(23)—C(24)—O(27)	80(1)	89(1)	−43(1)	−83(1)	83(2)

[a] Reference [8].

this complex has a unique crystal structure as described above. The torsion angles of the other complexes also differ markedly from each other, although their structures are quite similar. The results suggest that guest information represented by conformational changes is rather sensitive compared to the molecular assembly and the lattice constants mentioned above.

4. Conclusion

Until now, X-ray crystallography has been exclusively used to elucidate crystal structures. Little attention has therefore been given to information provided by the molecular assembly. In this paper, we assessed the significance of the molecular assembly pattern and related changes in the host molecule from the viewpoint of molecular information and attached great importance to them.

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