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Self-organization of adenine and thymine derivatives in thermotropic liquid crystal

Toshio Itahara [a,*], Yukiko Yokogawa [b]

[a] *Faculty of Engineering, Kagoshima University, Korimoto, Kagoshima 890-0065, Japan*
[b] *Faculty of Science, Kagoshima University, Korimoto, Kagoshima 890-0065, Japan*

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Abstract

Self-organization of adenine and thymine derivatives was studied by comparison of IR spectra of these compounds in crystal, liquid crystal, and isotropic liquid states. The adenine derivative mainly formed weaker hydrogen-bonded assemblies in the liquid crystal state, compared with assemblies in crystal state. The thymine derivative existed as a component of a network of prolonged hydrogen bonds interconnecting thymine rings in the liquid crystal state. The mixing of the adenine and thymine derivatives at a molar ratio of 1:1 resulted in a formation of base pair between adenine and thymine rings. The structures of hydrogen-bonded assemblies in the liquid crystal state were presumed on the basis of the temperature-dependent IR spectra.

Keywords: Temperature-dependent IR; Liquid crystal; Self-organization; Adenine; Thymine; 3-Methyluracil

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1. Introduction

Since the pioneering work of Kato and Frēcht [1] and Lehn and co-workers [2], hydrogen-bonded liquid crystals have been studied by several groups of workers [3]. The presence of hydrogen bond in liquid crystal state has been determined by IR spectroscopy [4] or the other methods. On the other hand, it is well known that the nucleic bases associate to form the hydrogen-bonded assemblies [5]. We previously reported the liquid crystallinity of the adenine derivative (**1**) and the thymine derivative (**2**) as a communication [6]. Although the temperature-dependent IR and Raman spectra of the nucleic acid-related molecules are known [7], the IR study of the nucleic base derivatives in liquid crystal state has not been reported. It is expected that the nucleic base derivatives can be ordered in liquid crystal state, compared in isotropic liquid state. Therefore it appeared of interest to investigate the self-organization of the nucleic base derivatives in liquid crystal state by means of temperature-dependent IR spectroscopy. Furthermore a 3-methyluracil derivative (**3**) was synthesized. IR spectra of **3** were compared with those of **2**, because **3** cannot form a hydrogen-bonded assembly as a result of the methylation of NH at the 3-position (see Scheme 1).

2. Experimental

2.1. General

The elemental analysis was performed in the Analytical Center of Kyoto University. The ^{1}H NMR spectrum (400 MHz) and ^{13}C NMR spectrum (100 MHz) were obtained with a JEOL GSX 400 spectrometer. The chemical shifts (δ-values) were measured in parts per million (ppm) down-field from tetramethylsilane as an internal reference. The IR spectra were recorded with a JASCO FT/IR-420 spectrometer. The samples at various temperatures were sandwiched between two KBr crystal plates with a 0.05 mm spacer. The sandwiched samples were held on a hot stage (JASCO HC-500/H), equipped with a temperature controller (JASCO TC-1000). Differential scanning

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[*] Corresponding author. Tel./fax: +81 99 285 8208.
E-mail address: itahara@be.kagoshima-u.ac.jp (T. Itahara).

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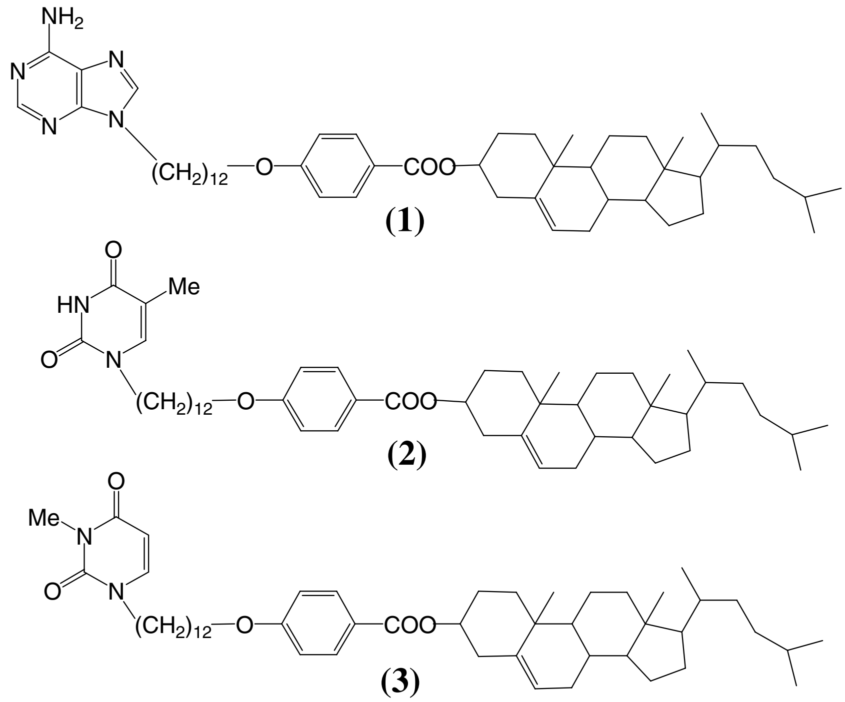


Scheme 1.

calorimetry (DSC) measurements were carried out with a Shimadzu DSC-60. Microscopy observations were performed under a Nikon Eclipse E600 POL equipped with a hot stage (Tokai Hit ThermoPlate or Linkam LK-600PH).

2.2. Synthesis of adenine, thymine, and 3-methyluracil derivatives

A solution of cholesteryl *p*-hydroxybenzoate [8] (1 mmol) and 1,12-dibromododecane (1 mmol) in acetone (150 ml) containing K_2CO_3 (1 mmol) was heated at reflux temperature for 24 h under nitrogen atmosphere. The reaction mixture was evaporated to give a residue, which was chromatographed on silica gel. Elution by a mixture of chloroform and hexane (2:1) gave cholesteryl *p*-(12-bromododecyloxy)benzoate (0.56 mmol): mp 75–76 °C; IR ($CDCl_3$) ν 1703, 1606, 1510, 1468, 1369, 1317, 1277, 1254, 1169, 1120, 1009 cm^{-1}; ^{1}H NMR ($CDCl_3$) δ 7.98 (d, 2H, $J = 8.8$ Hz), 6.89 (d, 2H, $J = 8.8$ Hz), 5.42 (d, 1H, $J = 3.6$ Hz, Chol-6), 4.82 (m, 1H, Chol-3), 4.00 (t, 2H, $J = 6.4$ Hz), 3.41 (t, 2H, $J = 6.4$ Hz), 2.45 (d, 2H, $J = 7.6$ Hz, Chol-4), 1.06 (s, 3H, Chol-19 or 18), 0.92 (d, 3H, $J = 6.4$ Hz, Chol-21), 0.87 (dd, 6H, $J = 6.4$ Hz, $J = 1.6$ Hz, Chol-26,27), 0.69 (s, 3H, Chol-18 or 19) 2.10–0.90 (m, 46H). Anal. Calcd for $C_{46}H_{73}BrO_3$: C, 73.28; H, 9.76. Found: C, 73.22; H, 9.48.

A mixture of cholesteryl *p*-(12-bromododecyloxy)benzoate (0.5 mmol) with adenine, thymine, or 3-methyluracil (0.6 mmol) in *N*,*N*-dimethylformamide (70 ml) containing K_2CO_3 (0.5 mmol) was stirred at room temperature for 24 h under nitrogen atmosphere. The reaction mixture was evaporated to give a residue, which was chromatographed on silica gel. By monitoring at 254 nm, elution by chloroform or a mixture of chloroform and methanol gave **1** (0.15 mmol), **2** (0.14 mmol), or **3** (0.17 mmol).

2.2.1. Cholesteryl p-[12-(adenin-9-yl)dodecyloxy]benzoate (*1*)

^{1}H NMR ($CDCl_3$) δ 8.38 (s, 1H, A-2), 7.97 (d, 2H, $J = 8.8$ Hz), 7.79 (s, 1H, A-8), 6.89 (d, 2H, $J = 8.8$ Hz), 5.53 (s, 2H, Ade-NH_2), 5.41 (d, 1H, $J = 3.6$ Hz, Chol-6), 4.82 (m, 1H, Chol-3), 4.19 (t, 2H, $J = 7.2$ Hz), 4.00 (t, 2H, $J = 6.4$ Hz), 2.45 (d, 2H, $J = 7.6$ Hz, Chol-4), 1.06 (s, 3H, Chol-19 or 18), 0.92 (d, 3H, $J = 6.4$ Hz, Chol-21), 0.87 (dd, 6H, $J = 6.4$, $J = 1.6$ Hz, Chol-26,27), 0.69 (s, 3H, Chol-18 or 19) 2.10–0.90 (m, 46H); ^{13}C NMR ($CDCl_3$) δ 165.79, 162.81, 155.63, 152.94, 150.11, 140.36, 139.78, 131.50, 123.02, 122.64, 119.69, 113.96, 74.18, 68.17, 56.70, 56.16, 50.06, 43.95, 42.33, 39.76, 39.52, 38.31, 37.07, 36.66, 36.20, 35.80, 31.93, 31.89, 30.08, 29.48, 29.47, 29.45, 29.40, 29.33, 29.11, 29.04, 28.24, 28.01, 27.96, 26.66, 25.97, 24.29, 23.84, 22.82, 22.57, 21.06, 19.38, 18.73, 11.87. Found: C, 75.49; H, 9.45; N, 8.41. Calcd for $C_{51}H_{77}N_5O_3$: C, 75.79; H, 9.60; N, 8.67.

2.2.2. Cholesteryl p-[12-(thymin-1-yl)dodecyloxy]benzoate (*2*)

^{1}H NMR ($CDCl_3$) δ 8.18 (s, 1H, T3-NH), 7.98 (d, 2H, $J = 8.8$ Hz), 6.97 (s, 1H, T6), 6.89 (d, 2H, $J = 8.8$ Hz), 5.42 (d, 1H, $J = 3.6$ Hz), 4.84 (m, 1H), 4.00 (t, 2H, $J = 6.4$ Hz), 3.68 (t, 2H, $J = 6.8$ Hz), 2.45 (d, 2H, $J = 7.2$ Hz, Chol-4), 1.92 (d, 3H, $J = 1.0$ Hz, T5-Me), 1.06 (s, 3H, Chol-19 or 18), 0.92 (d, 3H, $J = 6.4$ Hz, Chol-21), 0.87 (dd, 6H, $J = 6.4$, $J = 1.6$ Hz, Cho-26,27), 0.69 (s, 3H, Chol-18 or 19) 2.10–0.90 (m, 46H); ^{13}C NMR ($CDCl_3$) δ 165.84, 164.09, 162.82, 150.73, 140.42, 139.80, 131.51, 123.04, 122.67, 113.98, 110.50, 74.21, 68.18, 56.72, 56.16, 50.08, 48.58, 42.34, 39.77, 39.53, 38.31, 37.08, 36.68, 36.20, 35.81, 31.95, 31.91, 29.50, 29.50, 29.49, 29.43, 29.34, 29.19, 29.11, 29.10, 28.24, 28.02, 27.97, 26.45, 25.98, 24.31, 23.85, 22.83, 22.57, 21.07, 19.40, 18.73, 12.33, 11.88. Found: C, 76.60; H, 9.70; N, 3.44. Calcd for $C_{51}H_{78}N_2O_5$: C, 76.65; H, 9.84; N, 3.51.

2.2.3. *Cholesteryl p-[12-(3-methyluracil-1-yl) dodecyloxy]benzoate (**3**)*

^{1}H NMR ($CDCl_3$) δ 7.97 (d, 2H, $J=8.0$Hz), 7.11 (d, 1H, $J=7.6$ Hz, U6), 6.89 (d, 2H, $J=8.0$ Hz), 5.73 (d, 1H, $J=7.6$ Hz, U5), 5.41 (d, 1H, $J=3.6$ Hz), 4.81 (m, 1H), 4.00 (t, 2H, $J=6.4$ Hz), 3.73 (t, 2H, $J=6.8$ Hz), 3.34 (s, 3H, U3-Me), 2.45 (d, 2H, $J=7.2$ Hz, Chol-4), 1.06 (s, 3H, Chol-19 or 18), 0.92 (d, 3H, $J=6.4$ Hz, Chol-21), 0.87 (dd, 6H, $J=6.4$, $J=1.6$ Hz, Cho-26,27), 0.69 (s, 3H, Chol-18 or 19) 2.10–0.90 (m, 46H); ^{13}C NMR ($CDCl_3$) δ 165.74, 163.29, 162.76, 151.56, 142.05, 139.73, 131.45, 122.98, 122.61, 113.92, 101.25, 74.15, 68.12, 56.66, 56.11, 50.01, 49.90, 42.28, 39.71, 39.48, 38.26, 37.02, 36.62, 36.15, 35.75, 31.89, 31.85, 29.45, 29.44, 29.44 29.37, 29.28, 29.11, 29.06, 28.98, 28.19, 27.96, 27.91, 27.72, 26.42, 25.92, 24.25, 23.79, 22.77, 22.52, 21.01, 19.34, 18.69, 11.82. Anal. Calcd for $C_{51}H_{78}N_2O_5$: C, 76.65; H, 9.84; N, 3.51. Found: C, 76.35; H, 9.77; N, 3.50.

3. Results and discussion

The thermal mesomorphic phases of the nucleic base derivatives and their mixtures were analyzed by differential scanning calorimetry (DSC) and polarizing microscopy. The polarizing microscopy observation showed the cholesteric liquid crystallinity of **1**, **2**, and **3**. The thermodynamic data are summarized in Table 1. Equimolecular amounts of **1** and **2** were dissolved in chloroform and the solvent was allowed to evaporate slowly, leaving a white solid behind. The clearing point of the mixture of **1** and **2** was 190 °C, and those of **1** and **2** alone were 168 and 185 °C, respectively. Therefore the mixing of **1** and **2** resulted in a stabilization of the liquid crystalline phase. This may be caused by a formation of base-paired assembly between **1** and **2**. On the other hand, the clearing point of a mixture of **1** and **3** at a molar ratio of 1:1 was lower than those of the individual components, because **1** and **3** did not associate to form an assembly.

Table 1
Thermal behavior of the nucleic base derivatives

Compounds	Phase behavior[a] (°C)								
	Heating				Cooling				
1	C	152	N*	168	I	162	N*	143	C
2	C	162	N*	185	I	180	N*	113	C
3	C	153[b]	N*	170[c]	I	160	N*	141	C
1+**2** (1:1)[d]	C	138	N*	190	I	180	N*	70	G
1+**3** (1:1)[d]	C	136	N*	160	I	154	N*	132	G

[a] The thermal mesomorphic phases were determined by polarizing microscopy and differential scanning calorimetry upon heating and cooling at a rate of 5 °C. C, crystal; N*, cholesteric liquid crystal; I, isotropic liquid; G, glass solid.

[b] $\Delta H = 28.6$ kJ/mol.

[c] $\Delta H = 1.1$ kJ/mol.

[d] A molar ratio.

The existence of hydrogen bonds of the nucleic base derivatives was studied by comparison of IR spectra of these compounds in the crystal, in the liquid crystal, and in the isotropic liquid states. Fig. 1 shows the IR spectra of **1**. Four NH_2 stretching bands were found at 3481 (non-H-bond: non-hydrogen-bonded bands), 3403 (non-H-bond), 3327 (H-bond), and 3180 cm^{-1} (H-bond) in isotropic liquid at 180 °C. On the other hand, a smaller band at 3481 cm^{-1} (non-H-bond) and larger bands at 3334 and 3178 cm^{-1} (H-bond) were found in liquid crystal state at 160 °C. This suggests that **1** mainly existed as a hydrogen-bonded form in the liquid crystal. Furthermore NH_2 scissoring vibrations were observed at 1670 cm^{-1} in crystal at 20 °C, at 1651 cm^{-1} in liquid crystal at 160 °C, and at 1628 cm^{-1} in isotropic liquid at 180 °C. In the classic IR study for 9-ethyladenine, the band at 1675 cm^{-1} is assigned to the NH_2 scissoring in the spectrum of the solid and the band at 1629 cm^{-1} is assigned to that in the solution [9]. For reference the IR spectrum of **1** in $CDCl_3$ at room temperature showed the band at 1630 cm^{-1}. These assignments are consistent with the data reported in the recent study [10]. The scissoring vibrations are expected to be higher in crystal because of stronger hydrogen bond [9]. On the basis of these data, it can be presumed that **1** mainly formed weaker hydrogen-bonded assemblies in the liquid crystal state, compared with assemblies in the crystal state. It is well known that rod-like molecules or molecular aggregates tend to show a liquid crystalline behavior. Therefore the hydrogen-bonded assemblies in the liquid crystal state may be shown as (**A**) and/or (**B**) as given in Scheme 2, although there are several types of molecular assemblies for adenine itself [5,11].

Fig. 2 shows the IR spectra of **2**. Two NH stretching bands of **2** were found at 3413 (non-H-bond) and 3205 cm^{-1} (H-bond) in isotropic liquid state at 200 °C, suggesting that **2** existed in both non-hydrogen-bonded and hydrogen-bonded forms at 200 °C. However the non-hydrogen-

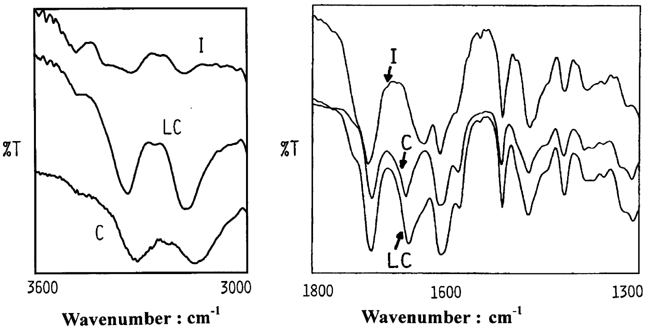
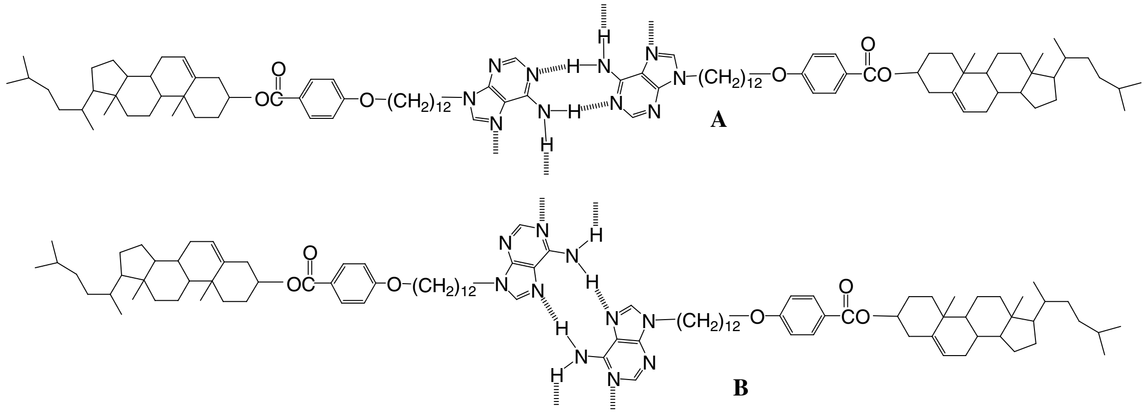


Fig. 1. IR spectra of **1** in crystal, in liquid crystal, and in isotropic liquid states. C (crystal at room temperature, 20 °C): 3311, 3149, 2929, 2852, 1709, 1670, 1606, 1574, 1510, 1468, 1417 cm^{-1}. LC (liquid crystal at 160 °C upon heating): 3481, 3334, 3178, 2931, 2852, 1709, 1651, 1601, 1574, 1508, 1468, 1414 cm^{-1}. I (isotropic liquid at 180 °C upon heating): 3481, 3403, 3327, 3180, 2929, 2856, 1712, 1628, 1603, 1576, 1508, 1466, 1414 cm^{-1}. For reference in ($CDCl_3$) at room temperature: 3519, 3408, 2935, 2856, 1701, 1630, 1604, 1580, 1510, 1469, 1414 cm^{-1}.



Scheme 2.

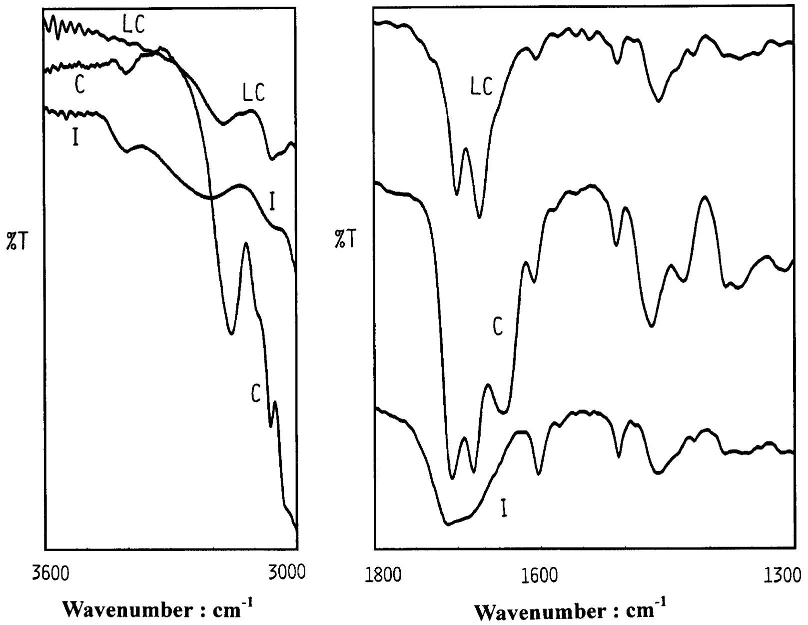
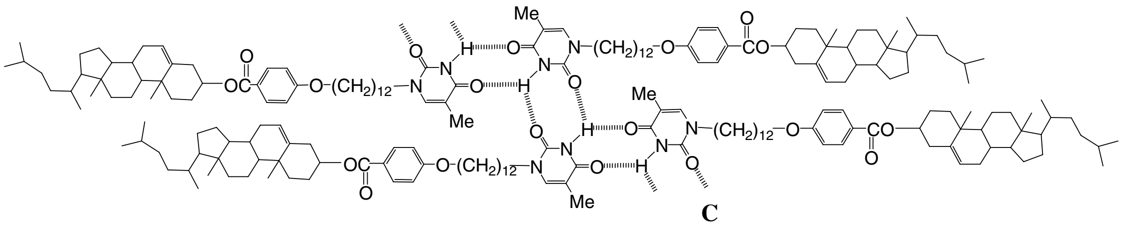


Fig. 2. IR spectra of **2** in crystal, in liquid crystal, and in isotropic liquid states. C (crystal at 30 °C upon heating): 3155, 3062, 2931, 2852, 1707, 1682, 1651, 1608, 1510, 1468, 1429 cm^{-1}. LC (liquid crystal at 170 °C upon heating): 3180, 3059, 2933, 2854, 1701, 1673, 1604, 1508, 1464, 1417 cm^{-1}. I (isotropic liquid at 200 °C upon heating): 3413, 3205, 3062, 2929, 2856, 1712(broad), 1603, 1508, 1464, 1419 cm^{-1}. For reference, in (CDCl$_3$) at room temperature: 3392, 3170, 3035, 2931, 2856, 1700, 1682, 1606, 1510, 1468 cm^{-1}.

bonded NH stretching vibration was little found in liquid crystal state at 170 °C and in crystal state at 30 °C. This suggests that **2** primarily existed as a hydrogen-bonded form in not only the crystal state but also the liquid crystal state. Interestingly three bands of the carbonyl stretching at 1707 (cholesteryl benzoate), 1682 (thymine at 2-position), and 1651 cm^{-1} (thymine at 4-position) in the crystal state were replaced by two bands at 1701 (cholesteryl benzoate) and 1673 cm^{-1} (thymine at 2- and 4-positions) in the liquid crystal state. For reference the IR spectrum of **2** in CDCl$_3$ at room temperature showed the bands at 1700 (cholesteryl benzoate) and 1682 cm^{-1} (thymine at 2- and 4-positions, a broad band). From a consideration of the IR data, it can be concluded that **2** existed in a network of prolonged hydrogen bonds interconnecting thymine rings in the liquid crystal state. Therefore we picture the structure as (**C**) in Scheme 3 that has the bifurcated system of hydrogen bonds [12].

Fig. 3 shows the IR spectra of **3**. The carbonyl stretching bands of **3** were found at 1711 (cholesteryl benzoate) and 1668 cm^{-1} (thymine at 2- and 4-positions) in crystal state at 25 °C, at 1711 and 1670 cm^{-1} in liquid crystal state at 160 °C, and at 1712 and 1672 cm^{-1} in isotropic liquid state at 180 °C. The carbonyl stretching bands were little shifted by the increase in temperature. As we would expect, this suggests that **3** cannot form a hydrogen-bonded assembly. As a result, the spectra in the crystal, in the liquid crystal, and in the isotropic liquid states were similar to one another.

Fig. 4 shows the IR spectra of a mixture of **1** and **2** at a molar ratio of 1:1. The NH$_2$ and NH stretching bands of the mixture were found at 3332 (H-bond: hydrogen-bonded bands) and 3186 cm^{-1} (H-bond) in crystal state at 25 °C, at 3481 (non-H-bond, a small band), 3327 (H-bond) and 3195 cm^{-1} (H-bond) in liquid crystal state at 160 °C, and at 3483 (non-H-bond), 3404 (non-H-bond), 3332 (H-bond)



Scheme 3.

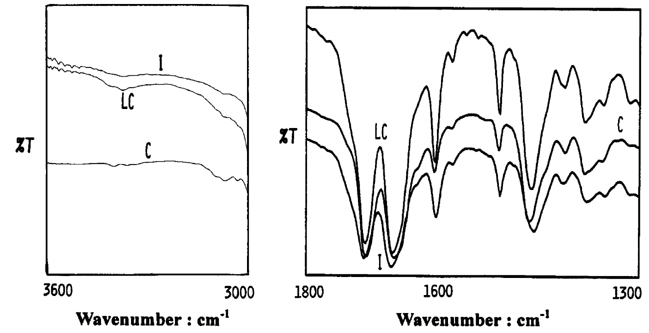


Fig. 3. IR spectra of **3** in crystal, in liquid crystal, and in isotropic liquid states. C (crystal at 25 °C upon heating): 2929, 2854, 1711, 1668, 1606, 1510, 1463, 1412, 1383 cm^{-1}. LC (liquid crystal at 160 °C upon heating): 2930, 2855, 1711, 1670, 1604, 1508, 1462, 1412, 1381 cm^{-1}. I (isotropic liquid at 180 °C upon heating): 2931, 2856, 1712, 1672, 1603, 1508, 1458, 1414, 1379 cm^{-1}.

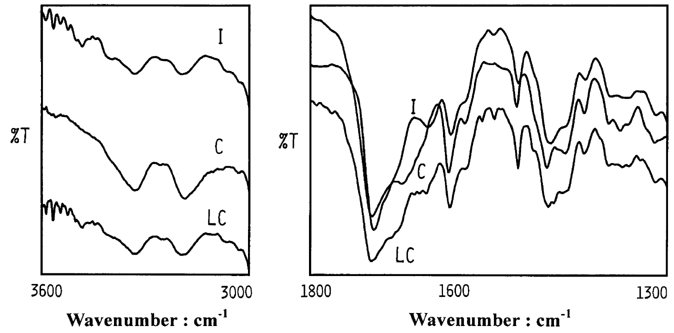
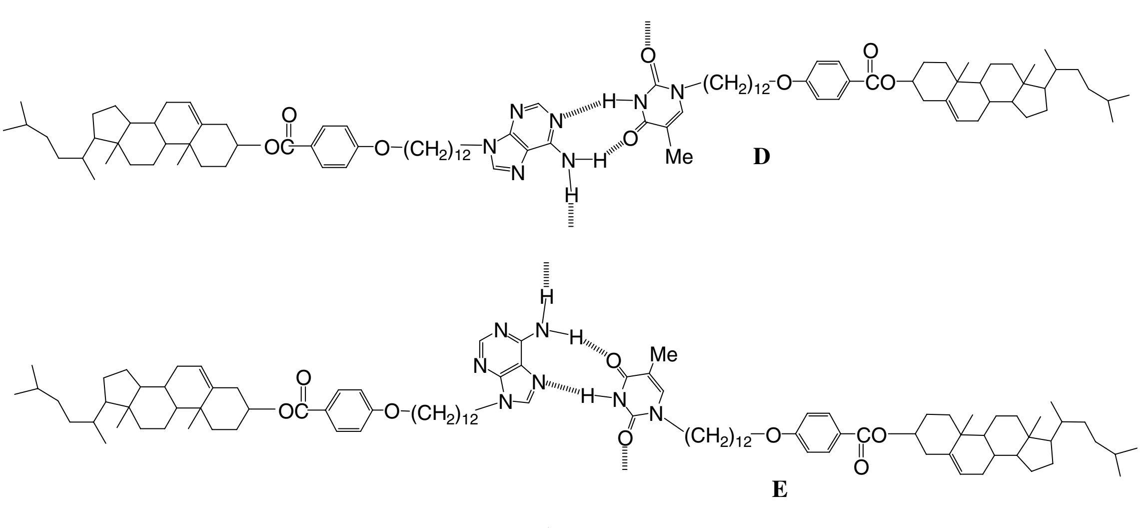


Fig. 4. IR spectra of a mixture of **1** and **2** at a molar ratio of 1:1 in crystal, in liquid crystal, and in isotropic liquid states. C (crystal at 25 °C upon heating): 3332, 3186, 2931, 2852, 1711 (broad), 1672, 1606, 1510, 1442, 1416, 1365, 1317 cm^{-1}. LC (liquid crystal at 160 °C upon heating): 3481, 3327, 3195, 2929, 2854, 1714(broad), 1660 (sh), 1605, 1508, 1441, 1417, 1363, 1317 cm^{-1}. I (isotropic liquid at 195 °C upon heating): 3483, 3404, 3332, 3195, 2931, 2856, 1712(broad), 1635, 1603, 1508, 1441, 1416, 1358, 1315 cm^{-1}.

and 3195 cm^{-1} (H-bond) in isotropic liquid state at 195 °C. The hydrogen-bonded bands of the mixture were similar in the crystal, in the liquid crystal, and in the isotropic liquid states. It is known that a mixture of adenine and thymine exists as the base-paired form in the solid state [13]. Therefore it can be assumed that **1** and **2** were primarily associated to form a base pair between adenine and thymine rings not only in the solid state but also in the liquid crystal and isotropic liquid states. We were not able to analyze the carbonyl stretching bands because of broad spectra, but NH_2 scissoring vibrations were observed at 1672 cm^{-1} in the crystal state, at ca. 1660 cm^{-1} (a shoulder-band) in the liquid crystal state, and at 1635 cm^{-1} in the isotropic liquid state. Although there are several types of base pairs between adenine and thymine rings [5,11], the hydrogen-bonded assemblies in the liquid crystal state may be shown as (**D**) and/or (**E**) in Scheme 4.

Fig. 5 shows the IR spectra of a mixture of **1** and **3** at a molar ratio of 1:1. The NH_2 stretching bands of **1** were found at 3327 (H-bond) and 3153 cm^{-1} (H-bond) in crystal state at 21 °C, while the bands were found at 3481 (non-H-bond), 3400 (non-H-bond), 3331 (H-bond) and 3182 cm^{-1}



Scheme 4.

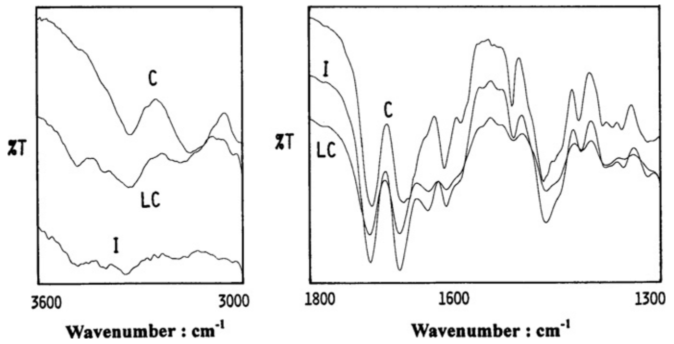


Fig. 5. IR spectra of a mixture of **1** and **3** at a molar ratio of 1:1 in crystal, in liquid crystal, and in isotropic liquid states. C (crystal at room temperature, 21 °C): 3327, 3153, 2929, 2852, 1711, 1664, 1655(sh), 1606, 1583, 1510, 1466, 1416, 1383, 1367, 1354, 1317 $\mathrm{cm^{-1}}$. LC (liquid crystal at 150 °C upon heating): 3481, 3400, 3331, 3182, 2931, 2854, 1713, 1670, 1630, 1603, 1583(sh), 1508, 1462, 1414, 1379, 1352, 1317 $\mathrm{cm^{-1}}$. I (isotropic liquid at 190 °C upon heating): 3481, 3398, 3342, 3188, 2929, 2858, 1714, 1670, 1628, 1603, 1583(sh), 1508, 1462, 1412, 1377, 1352, 1317 $\mathrm{cm^{-1}}$.

(H-bond) in liquid crystal state at 150 °C, and at 3481 (non-H-bond), 3398 (non-H-bond), 3342 (H-bond) and 3188 $\mathrm{cm^{-1}}$ (H-bond) in isotropic liquid state at 190 °C. In comparison with Fig. 4, the NH_2 stretching bands in Fig. 5 were remarkably dependent on the increase in temperature, because **1** and **3** did not associate to form an assembly. This presents further evidence in support of the base pairing between **1** and **2** in Fig. 4.

4. Conclusion

Although the literature contains a lot of references to the self-organization of nucleic base derivatives [5], we report for the first time the self-organization of adenine and thymine derivatives in thermotropic liquid crystal on the basis of the temperature-dependent IR spectra. The adenine derivative, the thymine derivative, and the mixture of adenine and thymine derivatives in a molar ratio of 1:1 primarily existed as hydrogen-bonded assemblies in liquid crystal state. It is well known that rod-like molecules or molecular aggregates tend to show a liquid crystalline behavior. Therefore, it is conceivable that the nucleic base derivatives form rod-like assemblies in the liquid crystal state. From a consideration of the present IR data, it seems most reasonable to conclude that the self-organization of the nucleic base derivatives results in a formation of a network of prolonged hydrogen bonds interconnecting the nucleic bases in liquid crystal state, and as a result, the order of the rod-like assemblies is kept dynamically.

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