Thermochimica Acta, 181 (1991) 155–166
Elsevier Science Publishers B.V., Amsterdam

ANALYSIS OF A MODEL SYSTEM FOR THE INTERACTION BETWEEN DNA AND HISTONE H1

AKIHIRO KAGEMOTO *, HIDETAKA IRIE, MASAFUMI ARAMATA and YOSHIHIRO BABA

Laboratory of Chemistry, Department of General Education, Osaka Institute of Technology, Asahi-ku, Osaka 535 (Japan)

(Received 7 September 1990)

ABSTRACT

In order to obtain information about the interaction between base pairs of DNA and amino acid residues containing histone H1, the heats of mixing ($\Delta_{mix}H$) of (adenosine 5′-monophosphate)–(uridine 5′-monophosphate), i.e. AMP–UMP duplex (duplex I), and/or (guanosine 5′-monophosphate)–(cytidine 5′-monophosphate), i.e. GMP–CMP duplex (duplex II), and L-lysine (Lys) and/or L-glutamic acid (Glu) monomer systems were measured at 298.15 ± 0.005 K by means of an automatic compensated flow microcalorimeter equipped with a computer. The heats of interaction (ΔH) for these systems were estimated to be about -58 kJ for duplex I–Lys, -56 kJ for duplex II–Lys, -42 kJ for duplex I–Glu and -29 kJ for duplex II–Glu systems, per mole of amino acid.

Furthermore, in order to confirm the ΔH estimated from $\Delta_{mix}H$, *ab initio* molecular orbital calculation for these systems was carried out using the IMSPACK and GAUSSIAN 80 programs with the STO-3G minimal basis set. The interaction energies (ΔE) obtained were estimated to be about -15.7 kJ mol^{-1} for duplex I–Lys, -23.7 kJ mol^{-1} for duplex II–Lys, -8.8 kJ mol^{-1} for duplex I–Glu and -13.2 kJ mol^{-1} for duplex II–Glu systems.

The signs of ΔH obtained for all systems were in good agreement with those of ΔE, suggesting that amino acid molecules interact with the bases of DNA. However, the absolute values of ΔH and ΔE for each system do not agree. It is suggested that for duplex I and/or II and Lys systems, an electrostatic interaction between the negative charge of the nucleotide phosphate and the positive charge of Lys, and the interaction between the base of the nucleotide and the amino acid play an important role in forming duplex–amino acid complex systems.

INTRODUCTION

Interaction between nucleic acid and protein occurs at all levels of replication, transcription and regulatory processes. In particular, deoxyribonucleic acid (DNA), when complexed with histones in the form of

* Author for correspondence.

0040-6031/91/$03.50

nucleohistone, is not available for transcription. The DNA–histone complex is, therefore, of interest and very important for life. Moreover, it is well known that histone interacts with DNA and makes an important contribution in the control of hereditary genetic information. Histone is a basic protein consisting of five major histone species including H1, H2A, H2B, H3 and H4. Of these species, histone H1, known as lysine-rich protein, differs from the other histones. Bustin and Cole [1] recognised that histone H1 consists of three domains in sequence and Hartman et al. [2] also reported that histone H1 has three distinct structures in aqueous solution: a random coil "nose" having 35–40 residues from the N-terminal end; a global "head" involving the next approximately 80 residues; and a random coil "tail" of the remainder of the histone H1 molecule.

Many studies on the interactions between DNA and histone H1 have been carried out using spectral measurements such as circular dichroism [3] and proton nuclear resonance [3–5]. However, because histone H1 has a complicated nose-head-tail structure with 213 amino acid residues, it is very difficult to determine to what position the histone H1 and the base pair of DNA bind.

No information, however, is available on the position of the bond between amino acid and DNA. One approach is to analyse this problem using a simple model such as the interaction between nucleotide monomer duplex and amino acid monomer: in this paper, we have studied the interactions between (adenosine 5′-monophosphate)–(uridine 5′-monophosphate) and/or (guanosine 5′-monophosphate)–(cytidine 5′-monophosphate) duplexes and *N*-acetyl-L-lysine-*N*-methylamide, as the model for lysine, and/or *N*-acetyl-L-glutamic acid, as the model for glutamic acid, containing histone H1, using calorimetry and *ab initio* molecular orbital calculation of these systems.

EXPERIMENTAL

The nucleotide monomers used in this study were adenosine 5′-monophosphate (AMP) and uridine 5′-monophosphate (UMP), which were purchased from Sigma Chemical Co. Ltd., U.S.A., and guanosine 5′-monophosphate (GMP) and cytidine 5′-monophosphate (CMP), purchased from Yamasa Shouyu Co. Ltd., Japan; these samples were used without any purification. *N*-Acetyl-L-lysine-*N*-methylamide (Lys) and *N*-acetyl-L-glutamic acid (Glu), used as models of lysine and glutamic acid, were also purchased from Sigma Chemical Co. Ltd., U.S.A. These samples were prepared from equimolar mixtures of AMP and UMP and/or GMP and CMP; the formation of the duplexes was confirmed by means of high-performance liquid chromatography. Duplexes prepared as an equimolar mixture of AMP and UMP and/or GMP and CMP are abbreviated to duplex I

and duplex II, respectively. The buffer solution used to adjust to pH 7.60 was 0.1 mol dm^{-3} tris-HCl(tris(hydroxymethyl)aminomethane hydrochloride). The water used to prepare the buffer solution was passed through an inverse osmotic membrane, and distilled and deionized by ion-exchange resin.

APPARATUS AND PROCEDURE

The calorimeter used for measurements of the heats of mixing of nucleotide duplexes and amino acid monomers was similar to the automatic compensated flow microcalorimeter described in a previous paper [6]. It was positioned in a water bath kept at 298.15 ± 0.005 K.

For the calorimetric measurements, the duplexes (AMP–UMP) (duplex I) and/or (GMP–CMP) (duplex II) formed by an equimolar mixture of their components at a given concentration (5.0×10^{-4} mol dm^{-3}), were mixed with amino acid solutions at various flow concentrations.

Ab initio molecular orbital (MO) calculations were carried out using the IMSPACK [7] and GAUSSIAN 80 [8] programs with the STO-3G [9] minimal basis set to obtain information concerning the interaction energies between the base pairs of the nucleotide duplex and the amino acid.

Structures for the hydrated methylammonium ion, instead of *N*-acetyl-L-lysine-*N*-methylamide in aqueous solution, and for acetate ion, instead of *N*-acetyl-L-glutamic acid in aqueous solution, were optimised using the STO-3G minimal basis set. Also, structures for the hydrated adenine–uracil (Ade–Ura) base pair, as a model for duplex I, and the hydrated guanine–cytosine (Gua–Cyt) base pair, as a model for duplex II, were compared with the calculated values from the same basis set as reported in previous papers [10,11]. The structure of water was referred to the experimental value [12].

The interaction energy, ΔE, between base pair and amino acid was calculated using the following equation

$$\Delta E = E_{\text{prod}} - E_{\text{react}} \tag{1}$$

where E_{prod} and E_{react} are the total electronic energies of product and reactant, respectively.

The reason for using the methylammonium ion instead of *N*-acetyl-L-lysine-*N*-methylamide and/or the acetate ion instead of *N*-acetyl-L-glutamic acid in the *ab initio* MO calculation is as follows: because, as mentioned above, the amino acid molecule is large, *ab initio* MO calculations can be inapplicable to these molecules. Therefore methylammonium and acetate ions, which bond with the base of the nucleotide duplex, were used to carry out the *ab initio* MO calculations for these systems.

RESULTS AND DISCUSSION

Heats of mixing of nucleotide duplex with amino acid monomer

The heats of mixing of duplex I and/or duplex II and Lys and/or Glu systems were measured over the various concentrations of amino acid monomer using compensated flow microcalorimetry at 298.15 ± 0.005 K.

All systems were exothermic, demonstrating that interactions between duplex I and/or duplex II and Lys and/or Glu may exist. The results obtained are summarised in Table 1 and are shown in Fig. 1a and b, where the heats of mixing, $\Delta_{mix}H$ per mole of phosphorus of nucleotide, are plotted against the molar ratio, r, of amino acid to the phosphorus of the nucleotide.

As seen in Fig. 1a, the absolute values of $\Delta_{mix}H$ for duplex I–and/or duplex II–Lys systems increase at first, and then reach constant values at $r = 0.25$ for duplex I–Lys and $r = 0.20$ for duplex II–Lys systems. These

TABLE 1

Heats of mixing, $\Delta_{mix}H$, between nucleotide duplexes and amino acid for various molar ratios, r, at 298.15 ± 0.005 K

r [a]	$\Delta_{mix}H$ (kJ mol^{-1}) [b]	r [a]	$\Delta_{mix}H$ (kJ mol^{-1}) [b]
Duplex I–Lys system		Duplex II–Lys system	
0.100	−4.5	0.025	−2.0
0.125	−5.2	0.050	−3.6
0.150	−5.8	0.100	−4.8
0.200	−6.0	0.125	−6.0
0.225	−6.4	0.200	−7.2
0.250	−7.5	0.225	−9.6
0.325	−7.6	0.250	−10.6
0.375	−7.7	0.350	−10.0
0.400	−7.3	0.400	−10.8
0.475	−7.4	0.450	−10.6
0.500	−7.6	0.500	−10.0
Duplex I–Glu system		Duplex II–Glu system	
0.050	−1.2	0.100	−2.0
0.075	−3.6	0.140	−2.2
0.150	−4.6	0.150	−2.3
0.250	−4.6	0.250	−2.8
0.300	−5.0	0.300	−3.3
0.350	−4.8	0.350	−3.6
0.400	−5.1	0.400	−3.5
0.450	−4.9	0.450	−3.8
0.500	−5.2	0.500	−3.6

[a] r is the molar ratio of amino acid to the phosphorus content of the nucleotide.
[b] mol here means mole of nucleotide phosphorus.

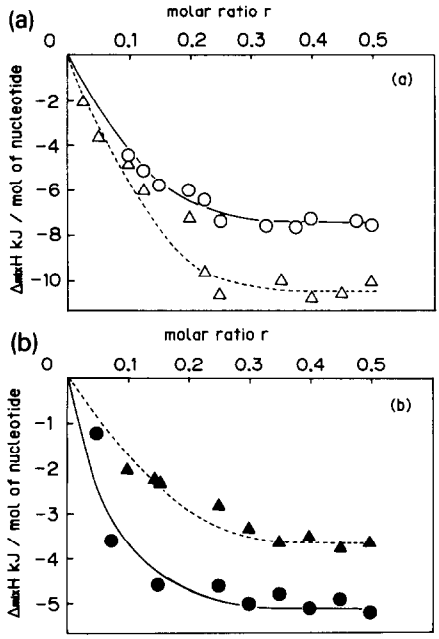

Fig. 1. Plots of heats of mixing, $\Delta_{mix}H$, against molar ratio, r, between Lys and/or Glu and nucleotide: a, duplex I, ——(○)——; duplex II, - - - - - -(△)- - - - -; and b, duplex I, ——(●)——; duplex II, - - - - - -(▲)- - - - -.

constant values of $\Delta_{mix}H$ for each system may indicate the termination of the interactions between duplex I and/or duplex II and Lys; they are estimated to be about -7.5 kJ mol^{-1} for duplex I–Lys and -10.3 kJ mol^{-1} for duplex II–Lys systems. These values correspond to the net heats of interaction, assuming that the heat of dilution for each system is negligibly small. The results obtained are listed in Table 2.

However, as seen in Fig. 1b, $\Delta_{mix}H$ values for duplex I–and/or duplex II–Glu systems are exothermic, demonstrating that interactions for both

TABLE 2

The value of $\Delta_{mix}H$ and r determined graphically from Fig. 1a and b for each duplex–amino acid system

System	r [a]	$\Delta_{mix}H$ (kJ mol^{-1}) [b]
Duplex I–Lys	0.25	−7.5
Duplex II–Lys	0.20	−10.3
Duplex I–Glu	0.15	−5.0
Duplex II–Glu	0.25	−3.6

[a] Here r is the molar ratio of amino acid to the phosphorus content in the nucleotide.
[b] mol means mole of nucleotide phosphorus.

systems may exist. The absolute values of $\Delta_{mix}H$ increase at first and reach constant values at $r = 0.15$ for duplex I–Glu and $r = 0.25$ for duplex II–Glu systems. This behaviour is similar to that of the Lys systems. The values of $\Delta_{mix}H$ in these systems are estimated to be about -5.0 kJ mol^{-1} for duplex I–Glu and -3.6 kJ mol^{-1} for duplex II–Glu and are listed in Table 2.

Thermodynamic quantities of duplex–amino acid systems

It is assumed that the complex between duplex and amino acid monomer is formed according to the reaction process

duplex + amino acid $\rightleftharpoons$ (duplex–amino acid) complex (2)

The thermodynamic quantities of all the systems were determined using the following equation, as reported previously [13]

$$\Delta_{mix}H = \frac{\Delta H}{2}\left[n + r + \frac{1}{KP} - \sqrt{\left(n + r + \frac{1}{KP}\right)^2 - 4nr}\right] \quad (3)$$

where ΔH is the heat of interaction between nucleotide duplex and amino acid, corresponding to the enthalpy change per mole of amino acid, n is the number of binding sites per mole of phosphorus of nucleotide duplex, K is the binding constant in this reaction process as shown in eqn. (2), P is the concentration of phosphorus of nucleotide duplex which is fixed in this experiment and r is the molar ratio of amino acid to phosphate of the nucleotide.

Assuming that eqn. (3) can be applied to the present study, the value of $\Delta_{mix}H$ can be calculated at a given value of r. The values of ΔH, n and K are variable functions, and the values of ΔH, K and n calculated using eqn. (3) which give the best fit to the observed values can be determined by optimisation of eqn. (3). The estimated values of ΔH, K and n for duplexes I and II are listed in Table 3, together with the values of the free energy change, ΔG, and the entropy change, ΔS, accompanying complex forma-

TABLE 3

Thermodynamic quantities for the interaction between nucleotide duplexes and amino acids determined from eqn. (3)

Nucleotide duplex	Amino acid	K (dm^{-3} mol^{-1}) [a]	ΔG (kJ mol^{-1}) [a]	ΔH (kJ mol^{-1}) [a]	ΔS (J mol^{-1} K^{-1}) [a]	n [b]	ΔH_{inf} [c] (kJ mol^{-1})
Duplex I	Lys	5.4×10^4	-27	-58	-104	0.14	-57
Duplex II	Lys	8.0×10^4	-28	-56	-94	0.20	-55
Duplex I	Glu	4.0×10^5	-32	-42	-34	0.12	-49
Duplex II	Glu	1.6×10^4	-24	-29	-17	0.15	-34

[a] mol here means mole of amino acid.

[b] n is the number of binding sites per mole of phosphorus of duplex.

[c] ΔH_{inf} is the heat of binding per mole of amino acid determined by extrapolating to infinite dilution as shown in Fig. 2a and b; mol here means mole of amino acid.

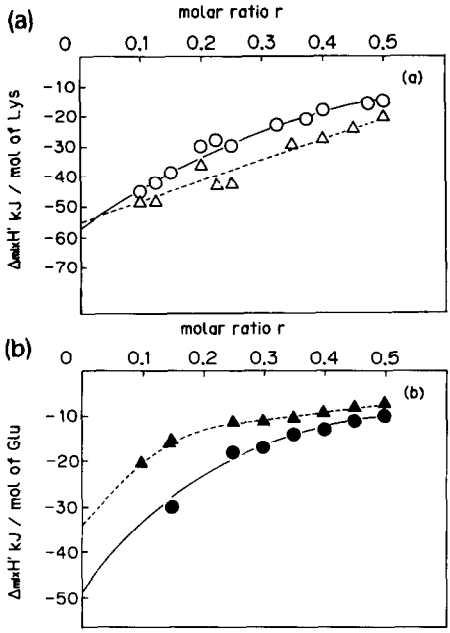

Fig. 2. Plots of heats of mixing, $\Delta_{mix}H'$, converted per mole of amino acid against molar ratio, r, between Lys and/or Glu and nucleotide: a, duplex I, ——(○)——; duplex II, - - - - - -(△)- - - - -; and b, duplex I, ——(●)——; duplex II, - - - - - -(▲)- - - - -.

tion, where the ΔG and ΔS values were calculated from $\Delta G = -RT \ln K$ and $\Delta S = (\Delta H - \Delta G)/T$, respectively. As seen in Table 3, the absolute value of ΔG for duplex I–Lys is small compared with that for duplex II–Lys, suggesting that the complex between duplex II and Lys is more stable than that of duplex I and Lys.

On the other hand, as seen in Table 3, the absolute value of ΔG for duplex II–Glu is smaller than that for duplex I–Glu, suggesting that the duplex II–Glu system is also more stable than the duplex I–Glu system. From these results for the thermodynamic quantities as shown in Tables 2 and 3, the binding mode may demonstrate the existence of the different interactions, such as the electrostatic interaction between the $-PO_4^-$ group of the nucleotide duplex and the $-NH_3^+$ group of the Lys molecule, and the interaction between the base of the nucleotide and the amino acid. These interactions play an important role in the formation of complexes between duplex I and/or duplex II and amino acid.

Figure 2a and b shows the plots of $\Delta_{mix}H'$ converted per mole of amino acid against r. ΔH_{inf} values determined by extrapolating the calculated value per mole of amino acid to infinite dilution are also listed in the last column of Table 3. As seen in Table 3, the ΔH values estimated from eqn. (3) are reasonable when compared with ΔH_{inf}, and also the r value for each system, determined graphically from Fig. 1a and b, compares favourably with the n values which give the best fit to the experimental data.

Ab initio MO calculation

In order to confirm the interaction between the base of the nucleotide and the amino acid noted above and in order to obtain further information on the binding position of the amino acid for duplex I and/or II accompanying interactions between the base pair of nucleotide and amino acids, *ab initio* MO calculation was carried out for these systems. In these cases, adenine–uracil (Ade–Ura) and guanine–cytosine (Gua–Cyt) duplexes were substituted for duplex I and duplex II, respectively and methylammonium ion and acetate ion were used instead of Lys and Glu, respectively, as described in the experimental section of this paper.

The interaction of these systems has been assumed to occur according to the following reaction processes

$$\begin{array}{l} (\text{Ade}-\text{Ura}) \\ \quad | \quad | \\ \text{H}_2\text{O} \quad \text{H}_2\text{O} \end{array} + \text{Lys}-\text{H}_2\text{O} \longrightarrow \begin{array}{l} (\text{Ade}-\text{Ura}) \\ \quad | \quad | \\ \text{H}_2\text{O} \quad \text{Lys} \end{array} + 2\text{H}_2\text{O} \qquad (4)$$

$$\begin{array}{l} (\text{Gua}-\text{Cyt}) \\ \quad | \quad | \\ 2\text{H}_2\text{O} \quad \text{H}_2\text{O} \end{array} + \text{Lys}-\text{H}_2\text{O} \longrightarrow \begin{array}{l} (\text{Gua}-\text{Cyt}) \\ \quad | \quad | \\ \text{Lys} \quad \text{H}_2\text{O} \end{array} + 3\text{H}_2\text{O} \qquad (5)$$

$$\begin{array}{l} (\text{Ade}-\text{Ura}) \\ \quad | \quad | \\ \text{H}_2\text{O} \quad \text{H}_2\text{O} \end{array} + \text{Glu}-\text{H}_2\text{O} \longrightarrow \begin{array}{l} (\text{Ade}-\text{Ura}) \\ \quad | \quad | \\ \text{Glu} \quad \text{H}_2\text{0} \end{array} + 2\text{H}_2\text{O} \qquad (6)$$

$$\begin{array}{l} (\text{Gua}-\text{Cyt}) \\ \quad | \quad | \\ 2\text{H}_2\text{O} \quad \text{H}_2\text{O} \end{array} + \text{Glu}-\text{H}_2\text{O} \longrightarrow \begin{array}{l} (\text{Gua}-\text{Cyt}) \\ \quad | \quad | \\ 2\text{H}_2\text{O} \quad \text{Glu} \end{array} + 2\text{H}_2\text{O} \qquad (7)$$

The geometrical structures accompanying the interaction between base pair and amino acid according to these reaction processes are shown in Figs. 3a and b, and 4a and b, respectively.

The (Ade–Ura)– and/or (Gua–Cyt)–Lys systems

The most likely interaction between the Lys molecule and the hydrated Ade–Ura base pair is considered to be the binding structure shown in Fig. 3a because of the evidence of the net charge, as previously reported [10]; the Lys molecule probably binds to the O_6 of uracil in the hydrated Ade–Ura base pair, as shown in Fig. 3a. Assuming this binding mode, the E_{react} and E_{prod} values were calculated by using *ab initio* MO calculation and the results obtained are summarised in Table 4; ΔE, according to the eqn. (1) was estimated to be -15.7 kJ mol^{-1}, see Table 4.

On the other hand, from the net charge of the hydrated Gua–Cyt base pair [11], Lys is considered to adopt the binding structure shown in Fig. 3b, and the binding position of the Lys molecule seems to be the N_7 of the guanine base in the hydrated Gua–Cyt base pair. The E_{react} and E_{prod}

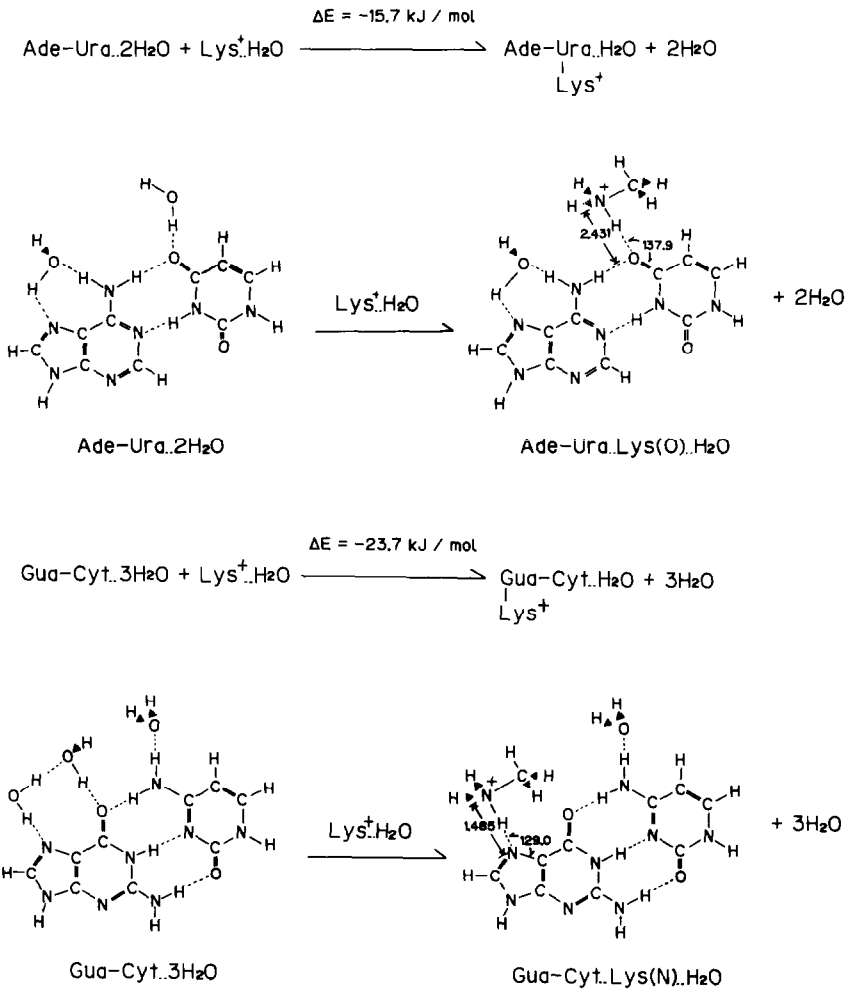

Fig. 3. The reaction processes and geometrical structures between: a, Ade–Ura; and/or b, Gua–Cyt duplexes and Lys. Units are ångströms and degrees.

values were also calculated and ΔE was estimated to be -23.7 kJ mol^{-1}; the results obtained are listed in Table 4.

The (Ade–Ura)– and/or (Gua–Cyt)–Glu systems

In order to obtain information concerning the interactions between the hydrated Ade–Ura and/or Gua–Cyt base pairs and Glu, *ab initio* MO calculation was also carried out. For the hydrated (Ade–Ura)–Glu system, it seems likely that the Glu binds to the $-NH_2$ of the C_6 of the adenine base in the hydrated Ade–Ura base pair, as shown in Fig. 4a, because of the evidence of the net charge [10]. According to eqn. (1), ΔE was estimated to be about -8.8 kJ mol^{-1}.

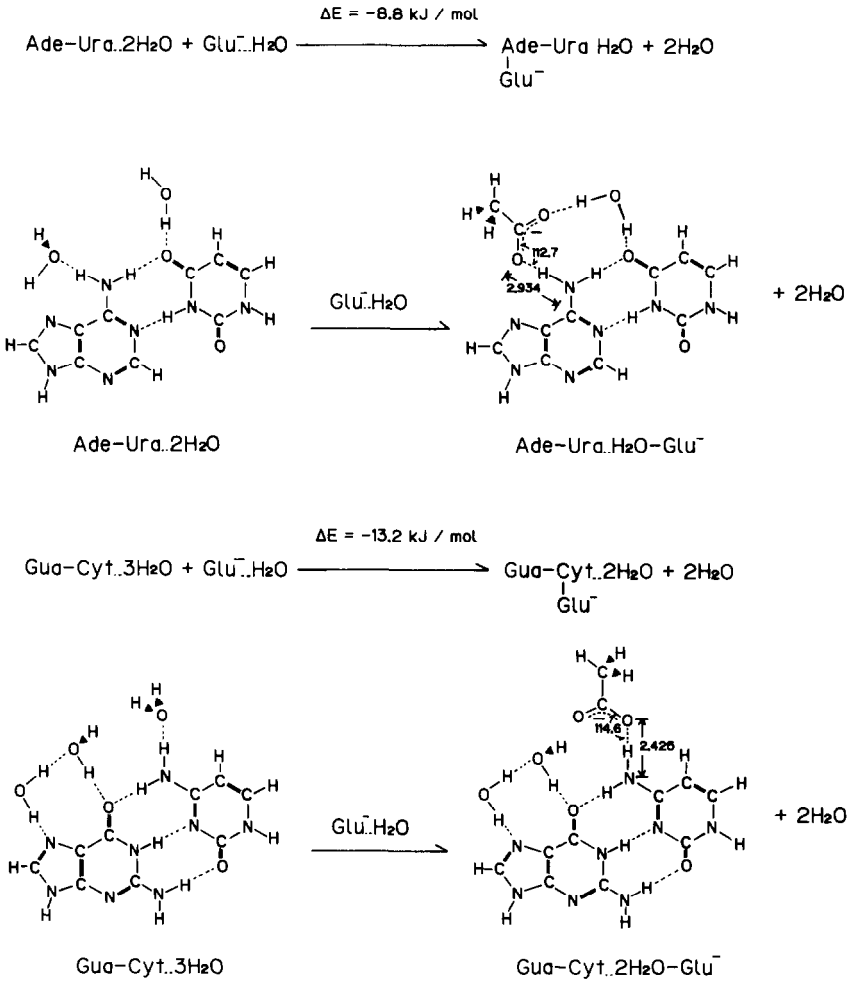

Fig. 4. The reaction processes and geometrical structures between: a, Ade–Ura; and/or b, Gua–Cyt duplexes and Glu. Units are ångströms and degrees.

TABLE 4

Enthalpy change accompanying interaction between duplex and amino acid estimated from *ab initio* MO calculation and calorimetric measurement

System	E_{react} (a.u.) [a]	E_{prod} (a.u.) [a]	ΔE (kJ mol^{-1}) [b]	ΔH (kJ mol^{-1}) [b]	ΔH_{elect} (kJ mol^{-1}) [b]
Duplex I–Lys$^+$	−1185.156273	−1185.162267	−15.7	−58	−42
Duplex II–Lys$^+$	−1314.451648	−1314.460657	−23.7	−56	−32
Duplex I–Glu$^-$	−1314.725912	−1314.729255	−8.8	−42	–
Duplex II–Glu$^-$	−1444.021287	−1444.026319	−13.2	−29	–

[a] a.u. here means atomic unit. 1 a.u. = 2625.5 kJ.

[b] mol here means mole of amino acid.

However, for the hydrated Gua–Cyt base pair interacting with the Glu system, it is believed (from the net charge [11]) that the Glu binds to the $-NH_2$ of the C_6 of the cytosine base in the hydrated Gua–Cyt base pair, as shown in Fig. 4b. In this reaction, ΔE was estimated to be -13.2 kJ mol^{-1}; the results obtained are listed in Table 4.

All ΔE values obtained from *ab initio* MO calculation for the four reaction processes (4)–(7) are summarised in Table 4, together with the ΔH values determined by flow microcalorimetry for the systems of duplexes I and II. As seen in Table 4, the signs of ΔH are in good agreement with those of ΔE. The absolute values of ΔH, however, do not agree with those of ΔE. One possible explanation could be as follows; considering the electrostatic interaction for duplex I– and/or II–Lys systems, ΔH can be expressed as the sum of the heat (ΔH_{elect}) based on electrostatic interaction between the $-PO_4^-$ group of the nucleotide and the $-NH_3^+$ group of the lysine residue, and the heat (ΔH_{base}) accompanying binding to the base of the nucleotide as shown in Fig. 3a and b, i.e. $\Delta H = \Delta H_{elect} + \Delta H_{base}$. ΔH_{elect} can be easily estimated by subtracting ΔH_{base} from ΔH and is estimated to be about -42 kJ mol^{-1} for duplex I–Lys and -32 kJ mol^{-1} for duplex II–Lys systems, and the results obtained are listed in the last column of Table 4.

From studies on the model system of these interactions using calorimetric and *ab initio* MO calculation methods, it can be suggested that the interaction between the base of DNA and amino acid, with the exception of the electrostatic interaction of the duplex I– and/or II–Lys systems, plays an important role in complex formation between duplex and amino acid. However, for duplex I– and duplex II–Glu systems, because $\Delta H_{elect} = 0$, $\Delta H = \Delta H_{base}$ must be equal to ΔE. But the absolute values of ΔH in these systems do not agree with those of ΔE. Further study is needed to solve this problem.

ACKNOWLEDGEMENT

We are grateful to the Computer Centre of the Institute for Molecular Science, Okazaki, Japan for the use of the HITAC M-680 computer system.

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