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ORIGINAL PAPER

How does modification of adenine by hydroxyl radical influence the stability and the nature of stacking interactions in adenine-cytosine complex?

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Abstract This study reports on *ab initio* calculations of adenine - cytosine complexes in two different context alignments appearing in B-DNA. The influence of adenine modification by hydroxyl radical on the stability of the complexes is also discussed. The analysis was performed on over 40 crystallographic structures for each of the sequence contexts. In most cases, modification of adenine by hydroxyl radical leads to less negative intermolecular interaction energies. The issue of the influence of alteration of structural base step parameters on the stability of modified and unmodified adenine - cytosine complexes is also addressed. Analysis of the dependence of intermolecular interaction energy on base step parameters reveals that for *twist* and *shift* modification of adenine by hydroxyl radical leads to quite different interaction energy profiles in comparison with unmodified complexes. In order to elucidate the physical origins of this phenomenon, *i.e.* to analyze how the modification of adenine by hydroxyl radical is reflected in the change of intermolecular interaction energy components, a variational-perturbational decomposition scheme was applied at the MP2/aug-cc-pVDZ level of theory.

Keywords Intermolecular interactions · Nucleic acid base complexes · Stacking interactions

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Introduction

The biological consequences of damage to nucleic acids have been the subject of numerous experimental studies [1–3]. DNA may be exposed in vivo to hydroxyl radicals produced during endogenic cellular processes [4–7]. Modification of nucleic acid bases (NABs) is the most frequent scenario. This type of damage can be partially eliminated due to the presence of specific repair glycosylases that remove oxided purines and pyrimidines from DNA [8, 9]. An accumulation of defects may lead to mutations [9]. The transversion can cause the onset of many serious diseases and aging [10]. An elevated concentration of biomarkers of oxidative stress has been measured in tissues of patients with lung, breast and stomach cancer, to name only a few. The presence of modified forms of nucleic acid bases causes changes in local structure and hence influences the stability of DNA. This implies also the alteration of the nature of intermolecular interactions. A relatively large number of crystallographic structures of native B-DNA have been collected till now. However, the structures of modified (with oxidized DNA bases) chains of DNA are scarcely available. Due to the lack of crystallographic data for oxidized DNA strands, the relationship between oxidation of NAB complexes and their structure is not well understood. One might expect that modification can strongly influence structural parameters describing the mutual orientation of nucleic acid bases in DNA chains.

It is the aim of the present study to gain some insight into this subject. For this purpose we shall determine intermolecular interaction energy (IIE) profiles, as a function of base step parameters, for adenine-cytosine and 2-oxo-adenine - cytosine complexes. Both 8-oxo-guanine

and 2-oxo-adenine are biologically important systems - increased concentration of both molecules has been observed in cancer cells. In contrast to 2-oxo-adenine, 8-oxo-guanine have been much more extensively studied theoretically [11–15]. Here, we analyze 2-oxo-adenine - cytosine system in two context alignments. This is the extension of our previous study of complexes composed of 2-oxo-adenine with adenine and guanine [16]. The conformation of stacked nucleic acid bases strongly influences IIE [17, 18]. In particular, the modification of geometrical parameters may lead to a change in IIE components [19–21]. It is well known that the dynamics of nucleic acid complexes are strongly influenced by the stacking interactions. Hence, this type of interactions has been extensively studied theoretically [22–24]. Experimental in vitro investigations have been devoted both to native and oxidized nucleic acid complexes but theoretical studies of oxidized nucleic acid bases are rare [11–15, 25–28]. On the other hand, a plethora of studies of native nucleic acid base complexes is available in the literature (see [29] and references therein). An effort to analyze the nature of intermolecular interactions has been undertaken only recently [16, 19, 21, 30–37]. In particular, it is still not well understood how modification of nucleic acid bases by hydroxyl radical is reflected in the change of the intermolecular interaction energy components for stacked nucleic acid bases. The second aim of the present study is to address this issue by calculations of IIE components both for oxidized and unoxidized complexes in selected conformations.

Results and discussion

Structure of investigated complexes

In this paper we shall analyze the stacked nucleic acid base complexes formed by adenine and cytosine. The structures of the investigated complexes for two different context alignments appearing in B-DNA were chosen from a crystallografic database. For every context alignment we selected over 40 structures. For the two possible context alignments we chose 44 and 49 structures, respectively. The structures of tetramers can be uniquely defined by a set of 18 parameters. For the purpose of an analysis of the stability of adenine - cytosine and 2-oxo-adenine - cytosine complexes it is sufficient to consider six step parameters, namely *rise*, *twist*, *roll*, *tilt*, *shift* and *slide*. Based on the geometries of monomers optimized using the Gaussian 03 package [38] at the MP2/6-31++G(d,p) level of theory and the set of experimentally determined parameters we then generated the structures of adenine - cytosine as well as 2-oxo-adenine - cytosine complexes with the aid of the 3DNA program [39]. The ranges of variability of these parameters were determined based on the crystallographic data.

Intermolecular interaction energies for experimentally determined conformations of adenine - cytosine complex

As mentioned in the previous section, the experimentally determined conformations of adenine - cytosine complex were considered for both context alignments, in this study referred to as A–C and C–A. The complexes modified by hydroxyl radical are investigated as well, and will be denoted further as AA–C and C-AA. An analysis of intermolecular interaction energies for the set of experimentally determined configurations of monomers in the complex is presented in Figs. 1 and 2. The IIE was calculated at the MP2/aug-cc-pVDZ level of theory within the supermolecular approach using the MOLPRO package and was corrected for the basis set superposition error by the counterpoise procedure [40, 41]. Every crystallographic conformation of the studied complex can be described by six base step parameters. For a given context alignment, namely A–C and C–A, the analysis of the dependence of IIE on these parameters may provide some information on the relationship between the mutual orientation of monomers and the stability of whole complex. Nevertheless, many other stabilizing factors are neglected in such approach. It is interesting to note, however, that a larger *average* stability is observed for A–C than for C–A complex. In the case of A–C context alignment we observe that intermolecular interaction energy for most structures is located in the range −5 – −7 kcal/mol, while for the C–A complexes in the range −3 – −5 kcal/mol. It is not possible to assess the direct dependence of the stability of the complex on a given base step parameter based on the Figs. 1 and 2, because every structure is characterized by a

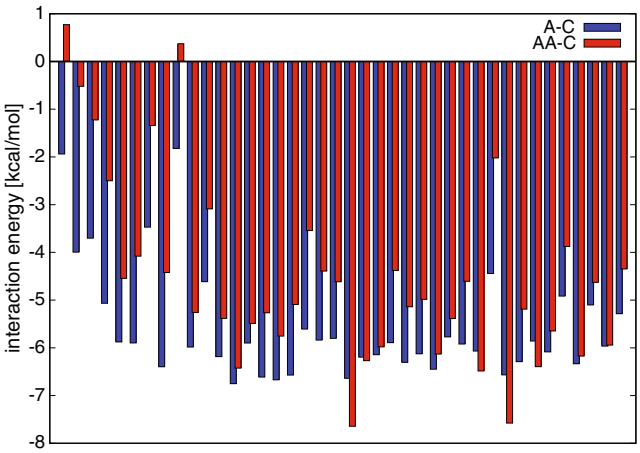

Fig. 1 The influence of modification of A–C complex on intermolecular interaction energy

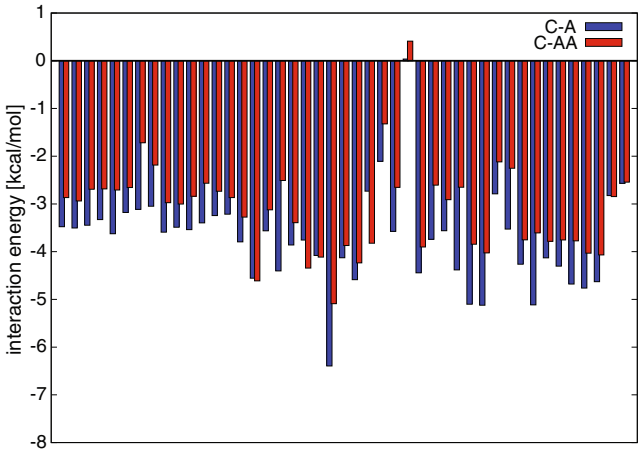

Fig. 2 The influence of modification of C–A complex on intermolecular interaction energy

unique set of all six parameters. It is, however, possible to analyze the influence of modification of adenine by hydroxyl radical on the stability of the whole complex under the assumption that its geometry remains unrelaxed. The intermolecular interaction energies of the 2-oxo-adenine - cytosine complex for two context alignments are presented in Figs. 1 and 2. For the majority of structures considered in both contexts, the modification leads to less negative IIE for the complex in comparison with the unmodified system. In a few cases, the 2-oxo-adenine - cytosine complex is characterized by positive values of IIE. It is worth noticing that the effect of modification is less pronounced for C–A context.

Dependence of the intermolecular interaction energy of the adenine - cytosine complex on base step parameters

In order to analyze the dependence of IIE on parameters describing mutual orientation of monomers, two lowest-energy structures (one for each sequence context) were selected. Then, the scan was performed with respect to a given base step parameter with the remaining five kept fixed at values corresponding to complex with the lowest energy. A schematic representation of base step parameters is given in Fig. 3 and the results are presented in Figs. 4 and 5. As mentioned previously, the ranges of variability were determined based on the crystallographic data. As expected, the comparison of plots for unmodified complexes for two different contexts does not reveal any significant similarities between the two sets of data. It is due to the different mutual alignments of monomers in the complex. As can be seen, in the case of the A–C complex minima are located for all six base step parameters, while for the C–A context the minima are not observed for *shift* and *rise*. The actual differences in absolute values of *shift, slide, rise, tilt, roll* and *slide* between crystallographic and relaxed geometry is 0.54 Å, 0.15 Å, 0.02 Å, 1.31 deg., 2.34 deg. and 4.74 deg. for A–C, and 0.11 Å, 0.36 deg., 2.13 deg. and 5.09 deg. for *slide, tilt, roll* and *twist* in the case of C–A. It is interesting to trace the dependence of IIE of modified complexes on base step parameters. Firstly, we shall discuss the C–A context. As can be seen from Fig. 5a–f, the 2-oxo-adenine complex is less stable in the whole studied range for all six base step parameters. With the exception of *shift* parameter, one observes that the difference of IIE between the C–A and the C–AA complexes is approximately constant in the whole range of variability of *slide*, *rise*, *twist* and *roll*. In the case of the *shift* parameter, the difference increases for increasing *shift* values (for *shift* −1.50 Å the difference is 0.56 kcal/mol while for *shift* 1.07 the difference is 1.84 kcal/mol). In the second context alignment, the picture of influence of modification of adenine is much more complicated in comparison to the C–A context. In the case of *tilt* and *rise* parameters, the location of minima on IIE curve for modified and unmodified complexes is identical.

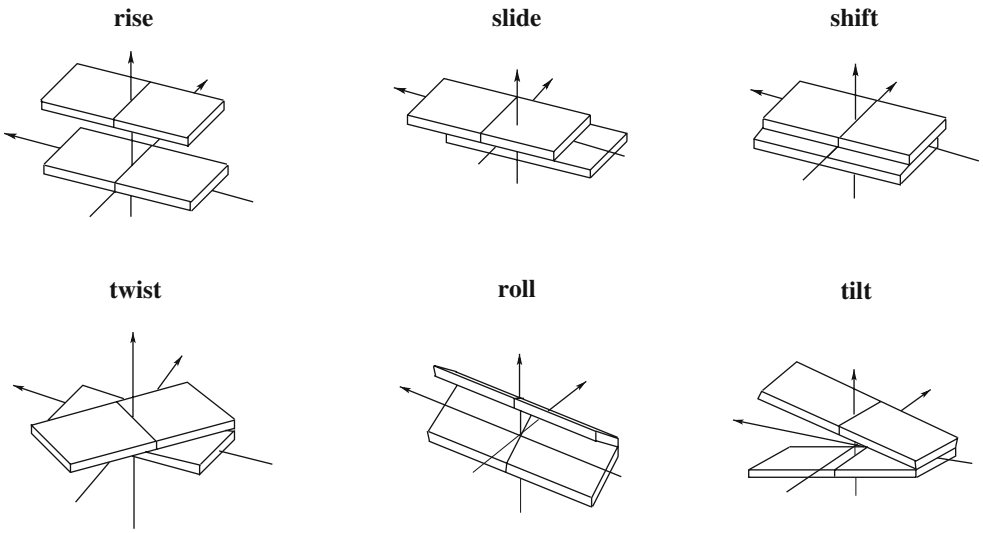

Fig. 3 Schematic representation of base step parameters

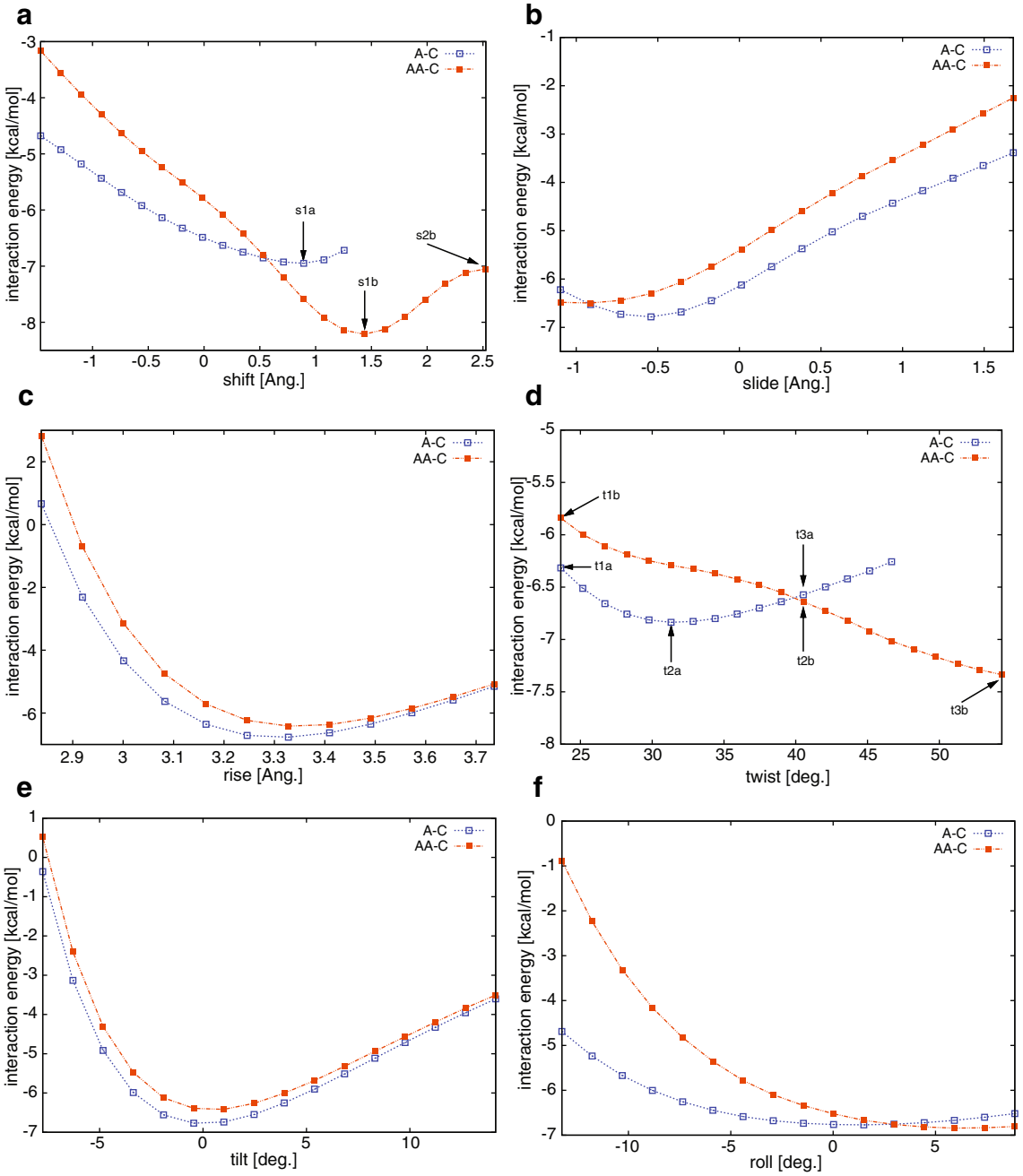

Fig. 4 The dependence of intermolecular interaction energy of A–C and AA–C complexes on structural parameters

For *slide* and *roll* the minima are slightly shifted. However, the stabilization energy corresponding to the minima in both cases is very similar. The two most interesting plots are namely Fig. 4a and d. These plots present the dependence of stabilization energy of modified and unmodified complexes as a function of *shift* and *twist*, respectively. In the case of the *shift* we see that the minimum for the AA–C is shifted by more than 0.5 Å with respect to minima for the A–C context and the IIE difference is 1.5 kcal/mol. Moreover, the minimum for *shift* is located near the border of range determined from crystallographic data. The most interesting observation is that in the case of *twist* we do not find the minima for AA–C complex. In the whole studied range of variability of *twist* the stabilization energy systematically increases. It was observed by Kamiya, that various types of base pairs involving 2-oxo-adenine may be due to the presence of the *syn* and *anti* conformers [42]. A preferred orientation (*syn* or *anti*) depends on many factors, but in this case we clearly see that preferred orientation of the unmodified complex is quite different than that for the oxidized system. Although IIE profiles presented in Figs. 4 and 5 provide very useful

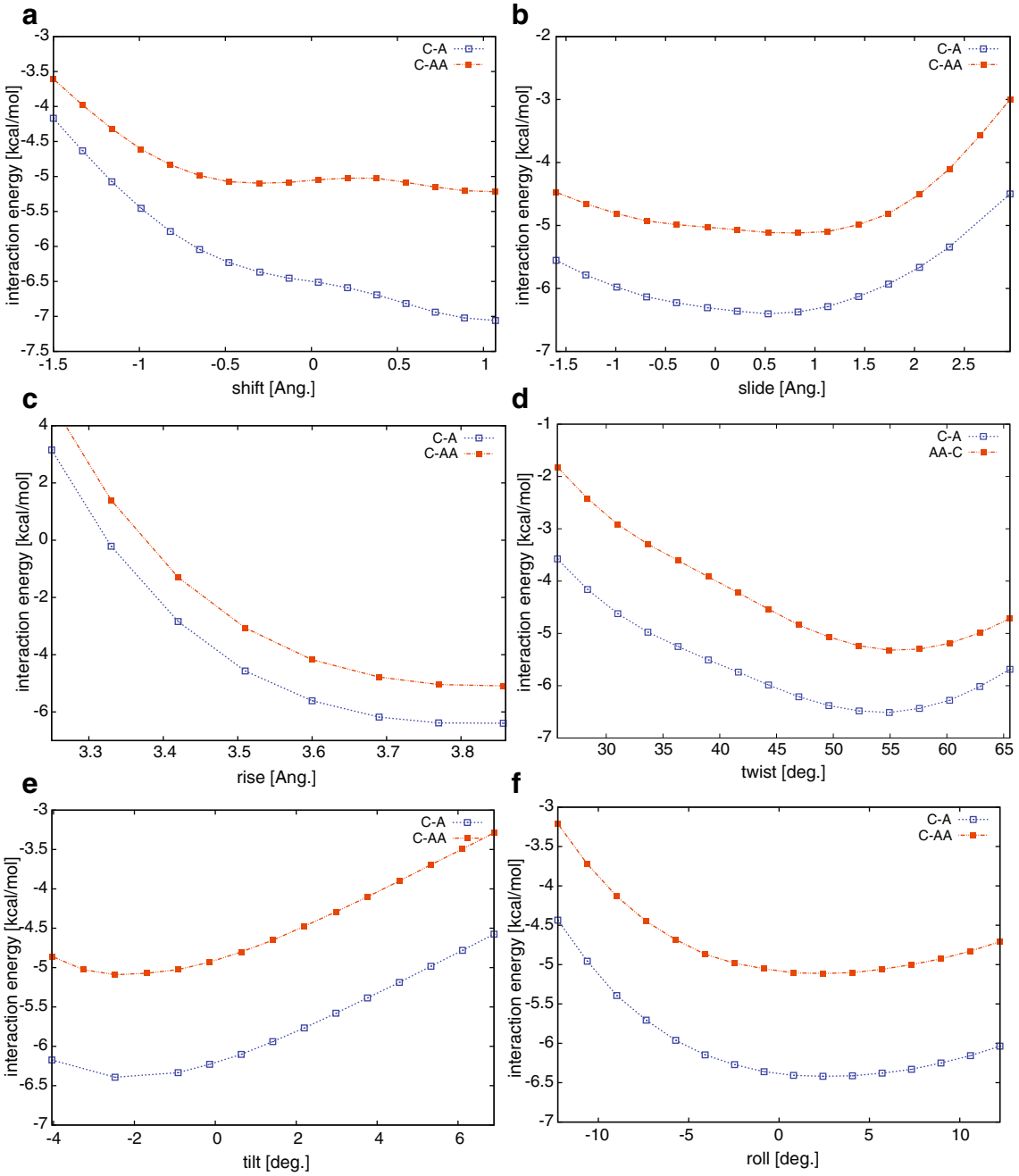

Fig. 5 The dependence of intermolecular interaction energy of C–A and C–AA complexes on structural parameters

information about the dependence on base step parameters, they do not say much about the nature of intermolecular interactions. This type of analysis, presented in the next section, might be a step towards better understanding of processes involving oxidized NABs.

Nature of interactions in the adenine - cytosine complex

As mentioned in the previous section, the dependence of interaction energy on *shift* and *twist* parameters was quite different for modified and unmodified complexes. In order to gain an insight how the IIE profiles are related to intermolecular interaction energy components, we selected a few structures for which the intermolecular interaction energy decomposition at the MP2/aug-cc-pVDZ level of theory was performed [43–45]. Within the variational-perturbational scheme that we employ, the SCF interaction energy is partitioned into electrostatic, Heitler-London exchange and delocalization energy term:

$$\Delta E^{HF} = \varepsilon_{el}^{(10)} + \varepsilon_{ex}^{HL} + \Delta E_{del}^{HF}. \quad (1)$$

Table 1 The intermolecular interaction energy components

complex	label	parameter	$\varepsilon_{el}^{(10)}$	ε_{ex}^{HL}	ΔE_{del}^{HF}	$\varepsilon_{el,r}^{(12)}$	$\varepsilon_{disp}^{(20)}$	$\Delta E_{ex-del}^{(2)}$	ΔE^{HF}	$\varepsilon_{MP}^{(2)}$	ΔE^{MP2}
A–C	s1a	*shift* 0.89	−3.22	12.69	−1.93	−0.78	−17.31	3.64	7.54	−14.45	−6.91
AA–C	s1b	*shift* 1.44	−5.07	15.76	−2.56	−1.41	−19.05	4.25	8.13	−16.21	−8.08
AA–C	s2b	*shift* 2.53	−7.20	18.82	−3.00	−1.23	−19.04	4.57	8.62	−15.70	−7.08
A–C	t1a	*twist* 23.6	−2.82	13.28	−2.02	−0.93	−17.62	3.84	8.44	−14.71	−6.27
AA–C	t1b	*twist* 23.6	−0.71	13.29	−2.28	−2.11	−17.79	3.81	10.30	−16.09	−5.79
A–C	t2a	*twist* 31.3	−2.72	11.33	−1.74	−0.72	−16.27	3.33	6.87	−13.67	−6.80
A–C	t3a	*twist* 40.5	−2.30	9.46	−1.41	−0.59	−14.53	2.83	5.75	−12.29	−6.54
AA–C	t2b	*twist* 40.5	−0.73	9.71	−1.88	−1.72	−14.96	2.97	7.11	−13.71	−6.60
AA–C	t3b	*twist* 54.4	−1.92	7.18	−1.55	−1.03	−12.31	2.29	3.71	−11.05	−7.33

All values are given in kcal/mol

The total intermolecular interaction energy at the MP2 level of theory is given by:

$$\Delta E^{MP2} = \Delta E^{HF} + \varepsilon_{el,r}^{(12)} + \varepsilon_{disp}^{(20)} + \Delta E_{ex-del}^{(2)}, \quad (2)$$

where $\varepsilon_{el,r}^{(12)}$ stands for the component of the intermolecular interaction energy due to the second-order electrostatic interaction including relaxation effects, $\varepsilon_{disp}^{(20)}$ denotes second-order dispersion interaction term and $\Delta E_{ex-del}^{(2)}$ is the exchange-delocalization component.

More details about this scheme can be found elsewhere [46–48].

The values of intermolecular interaction energy components are listed in Table 1. Based on the data presented therein, it is possible to assess the influence of both the change in adenine-cytosine geometry and the modification of the complex by hydroxyl radical on various contributions to IIE. It follows from Fig. 4d (points t1a and t1b) that modification of adenine is reflected mainly in a change of the electrostatic component. The value of the $\varepsilon_{el}^{(10)}$ term for *twist* 23.6° is about 2 kcal/mol smaller for a modified complex than for an unmodified one. On the other hand, modification of adenine in this conformation leads to a larger stabilizing contribution (by 1.18 kcal/mol) of $\varepsilon_{el,r}^{(12)}$ term. Likewise, the first-order electrostatic component for the A–C complex is about 1.5 kcal/mol greater than for the AA–C system for the value of *twist* equal 40.5° (points t3a and t2b on Fig. 4d). For this conformation one also observes that the value of $\varepsilon_{el,r}^{(12)}$ term is smaller for unmodified complex by 1.13 kcal/mol in comparison with the modified system. Based on the data presented in Table 1 it is also possible to arrive at the conclusion that strong interdependence between analyzed base step parameters, namely *shift* and *twist*, and the components of intermolecular interaction energy exists. In the case of the AA–C complex (points denoted as s1b and s2b) we see that first-order electrostatic component is about 2 kcal/mol larger for *shift* equal 2.53 Å than for *shift* value which is 1.44 Å. The exchange component increases by a value of 3 kcal/mol. The remaining components of interaction energy do not reveal significant dependence on changes of the *shift* parameter. In the case of the *twist* parameter, we see that its increase influences mostly the exchange and dispersion components both for modified and unmodified complexes.

Although for all conformations for which intermolecular interaction energy components were evaluated we observe that first-order electrostatic contribution is completely canceled out by ε_{ex}^{HL}, the absolute values of $\varepsilon_{el}^{(10)}$ might be still quite significant (see point s2b in Table 1). Similar to other stacked complexes (*i.e.* guanine-guanine [30, 31], guanine-adenine [16, 30]) the dispersion contribution is the main origin of their stabilization. The data reported in Table 1 fully support this conclusion.

Conclusions

In the present study we have reported on the theoretical calculations of intermolecular interaction energies for the adenine-cytosine complex in two context alignments. The results of computations within supermolecular approach reveal that for selected experimental configurations, the modification of adenine by hydroxyl radical leads to less negative intermolecular interaction energies. In a few cases, we observed that modification makes the complex unstable. An analysis of the dependence of interaction energy on base step parameters shows clearly that for the studied range of variability of these parameters minima are not located in all cases. This might explain why the oxidation introduces local strains to DNA strands. For most base step parameters (in both context alignments) a similar pattern of dependence of IIE is observed both for a modified and an unmodified complex. The decomposition of intermolecular interaction energy for selected configurations allowed us to draw the conclusion that the dispersion component is the most important stabilizing factor being almost an order of magnitude larger than any other stabilizing contribution. The effect of modification of adenine by hydroxyl radical is mainly reflected in the change of the magnitude of electrostatic interactions.

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