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Theoretical insights into the nature of intermolecular interactions in cytosine dimer

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ABSTRACT

In this study we discuss stacking interactions in cytosine dimer in conformations appearing in B-DNA crystals. The variational–perturbational scheme was applied for decomposition of the intermolecular interaction energy at the MP2 level of theory. The significant influence of the mutual orientation of cytosine monomers was observed not only on the total intermolecular interaction energy but also on its components: Different components of intermolecular interaction energy depend in different manner on parameters describing mutual orientation of cytosine monomers.

1. Introduction

Non-covalent interactions contribute substantially to stabilization of biochemically significant complexes. Structure and dynamics of such systems are dependent on various interplaying contributions (electrostatics, London forces, ion-mediated and hydrophobic interactions). Non-covalent interactions are also involved in many important phenomena such as expression of the genetic code, DNA replication process and transcription. Furthermore, they play a key role in the recognition mechanism in protein–DNA complexes and intercalation of drugs into DNA [1–3]. Flexibility and conformational diversity of DNA and RNA can be attributed to hydrogen bonding (HB) and stacking interactions [4–6]. The stability of HB and stacked complexes is due to the different components of intermolecular interaction energies (IIEs). Toczyłowski and collaborators investigated their dependence on geometry of hydrogen bonded nucleic acid base (NAB) pairs [7]. They demonstrated that electrostatic energy constitutes the origin of stabilization of HB NAB complexes. However, the exchange, dispersion and induction contributions also play an important role [7]. So far, the attention has been mainly focused on the calculations of the total stabilization energies of NAB complexes [8–23]. It is well established that dispersion component is the main source of stabilization of stacked nucleic acid bases. The analysis of the nature of interactions in base pairs, however, has been settled on quantitative ground only quite recently [23–31]. Hill and collaborators analyzed the importance of electrostatics for stabilization of DNA bases [24]. Sedlak et al. performed analysis for hydrogen bonded and stacked nucleic acid bases in configurations appearing in crystals using DFT-SAPT approach [32]. Likewise, Hesselman and coworkers employed DFT-SAPT to analyze the interaction energy components in stacked nucleic acid bases [25,26]. Langner et al. used a hybrid variation–perturbation decomposition scheme to investigate the relationships between IIE components and found an interesting correlation between the exchange and dispersion contributions to the interaction energy [27]. Despite the significance of the above mentioned studies, they lack the systematic analysis of the dependence of the intermolecular interaction energy components on the geometry of stacked NAB complexes. Hunter and Lu used empirical potentials to calculate the conformational and energetical properties of nucleic acid base pairs [33]. They analyzed dependence of the structural base step parameters (see Fig. 1) describing mutual orientation of nucleobases in DNA on van der Waals and the electrostatic interactions. It was observed that van der Waals forces occurred to determine *rise*, *tilt* and *roll* parameters. Electrostatic interactions, on the other hand, determine the values of *shift* and *slide*. They also concluded that the stacking energy is essentially independent of the *twist* parameter [33]. The aim of our study is the systematic investigation of the dependence of the components of intermolecular interaction energy on parameters describing the structure of cytosine–cytosine dimer using non-empirical approach. Thus, in this work we shall present the results of *ab initio* calculations for conformations of the complex appearing in B-DNA crystals.

2. Results and discussion

2.1. Structure of investigated complexes

In this letter, sixty three experimentally determined structures of stacked complexes formed by two cytosine molecules were

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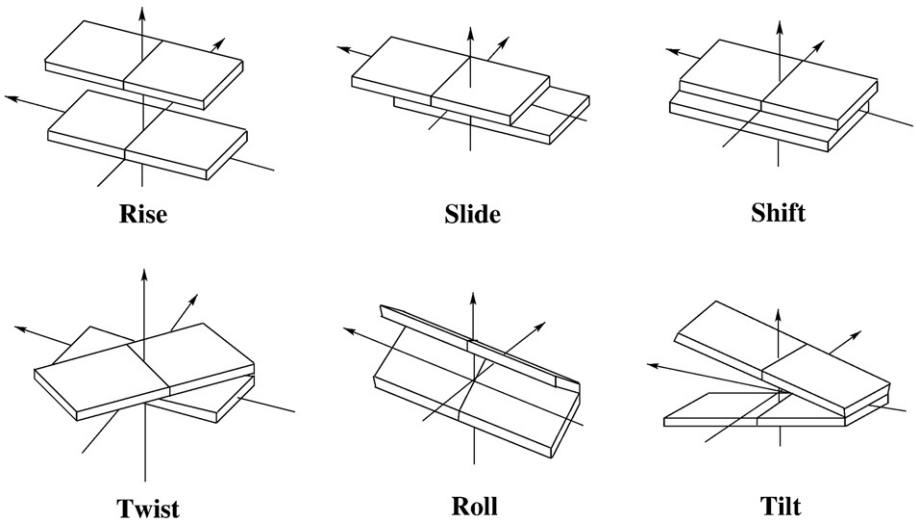

Fig. 1. Definition of base step parameters.

investigated. Thus, the number of complexes selected for this study is large enough to see structural and energetical diversity. Geometry of analyzed complexes appearing in B-DNA crystals can be described by two sets of six parameters. The geometry of two hydrogen bonded cytosine–guanine pairs belonging to opposite strands of B-DNA is defined by *shear*, *stretch*, *stagger*, *buckle*, *propeller* and *opening* parameters. The remaining six parameters, namely *shift*, *slide*, *rise*, *tilt*, *roll* and *twist*, are responsible for mutual orientation of stacked NABs [34]. However, it should be pointed out that these two sets of parameters are mutually dependent. The geometry of the monomer was optimized at the MP2/6-31++G(d,p) level of theory with Gaussian03 package [35] and used for generation of the geometries of the complexes with the aid of the 3DNA program based on the experimentally determined values of the above mentioned parameters [36].

2.2. Intermolecular interaction energy. Nature of stacking interactions

The supermolecular interaction energy, corrected for basis set superposition error [37], was calculated using the MOLPRO package at the DF-MP2/aug-cc-pVDZ level of theory [38]. Fig. 2. shows the intermolecular interaction energies for all investigated complexes. We adopted the notation used in the Nucleic Acid Database for labelling structures [39]. As can be seen, the values of stacking energy of cytosine dimer are rather small and do not exceed −2.56 kcal/mol. Moreover, fifteen unstable complexes were found. The cytosine dimer appearing in numerous conformation was also analyzed by Jurečka et al. [16]. The authors performed extensive *ab initio* calculations including the CCSD(T) level of theory. The data presented by Jurečka et al. show that the average difference between the IIEs calculated at the MP2/aug-cc-pVDZ level of theory and the MP2 complete basis set stacking energy corrected for the so-called *CCSD(T) term* is 0.3 kcal/mol. Hence, one can assume that the

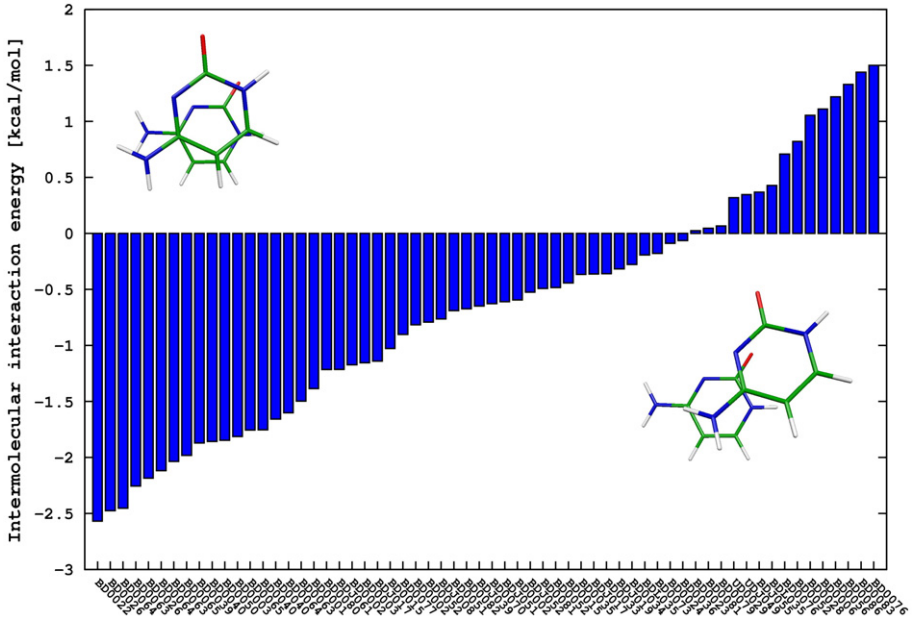

Fig. 2. The intermolecular interaction energy for the cytosine dimer in conformations appearing in B-DNA. The inset figures, presenting the geometries of complexes, correspond to the lowest negative (BD0022, on the left) and the highest positive (BD0076, on the right) intermolecular interaction energy.

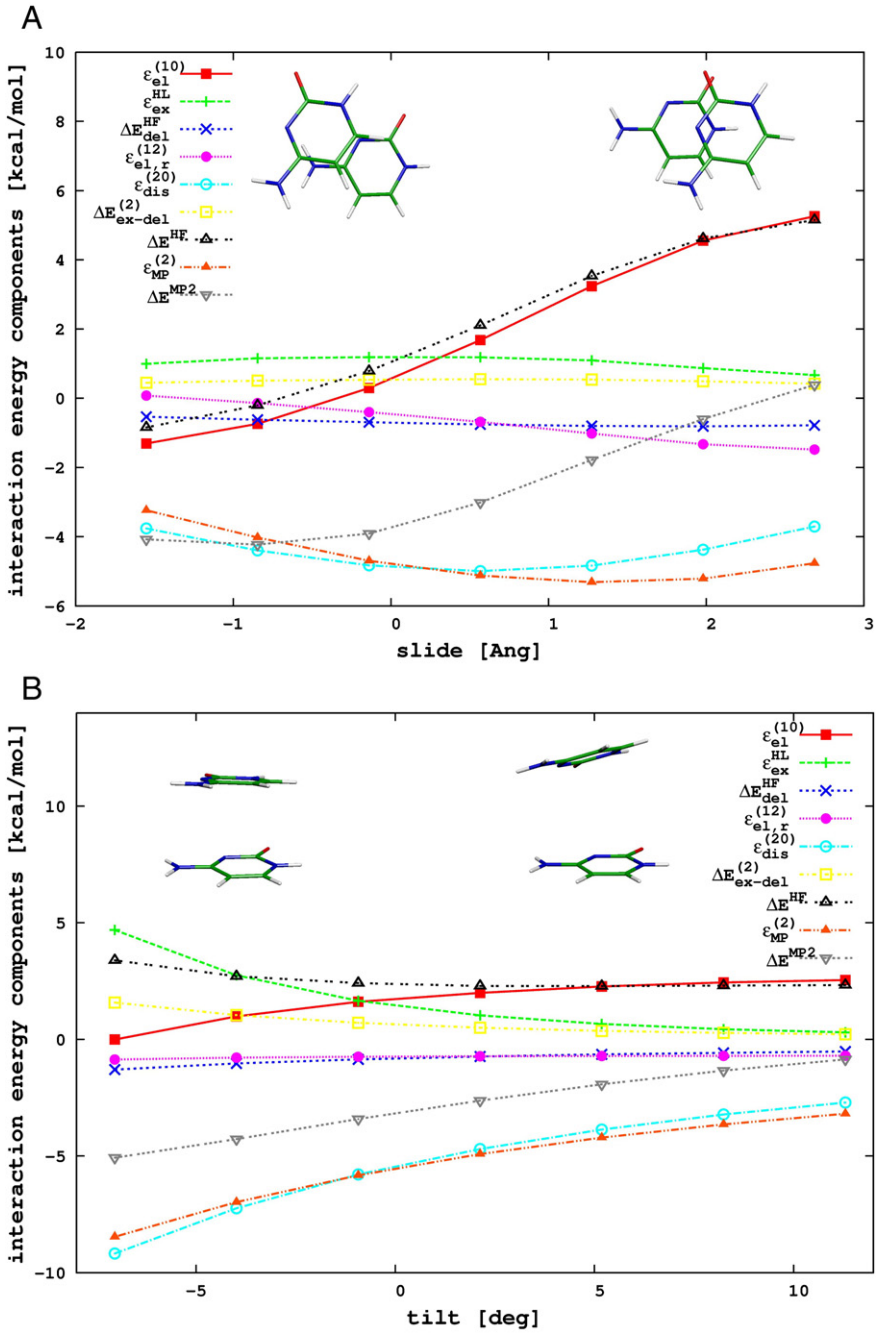

Fig. 3. The influence of variability of *slide* (upper plot) and *tilt* (lower plot) parameters on intermolecular interaction energy components. The geometries of monomers correspond to border values of the base step parameters.

MP2/aug-cc-pVDZ level of theory provides quantitatively correct values of stacking interaction energies for the system under consideration. It is also interesting to note that the values of intermolecular interaction energies reported by Jurečka et al. vary within the very broad range, *i.e.* from +2.45 to −9.93 kcal/mol. The values reported here fall into much narrower range, *i.e.* from +1.50 to −2.56 kcal/mol. However, we report on the results of calculations for experimentally determined configurations which differ from the structures considered by Jurečka et al. [16].

In order to analyze the dependence of intermolecular interaction energy and its components on structural parameters describing mutual orientation of monomers, the lowest energy structure was selected (BD0022). Then, the scan was performed with respect to a given base step parameter with remaining five kept fixed at values corresponding to the complex with the lowest energy (BD0022). The range of variability of the scanned base step parameters was determined on the basis of experimental data. The whole range of parameters was divided into seven intervals for which interaction energy decomposition was performed. The structure of complexes corresponding to minimum (BD0022) and maximum (BD0076) energy values is presented in Fig. 2.

The intermolecular interaction energy of cytosine dimer was decomposed using the variational–perturbational scheme [40–44] as implemented in the modified version of GAMESS package [45–47]. In this approach, the intermolecular interaction energy can be presented as:

$$\Delta E^{\mathrm{MP2}} = \sum_{i=0}^{2} \Delta\varepsilon_{\mathrm{MP}}^{(i)} = \Delta \mathrm{E}^{\mathrm{HF}} + \varepsilon_{\mathrm{MP}}^{(2)}. \tag{1}$$

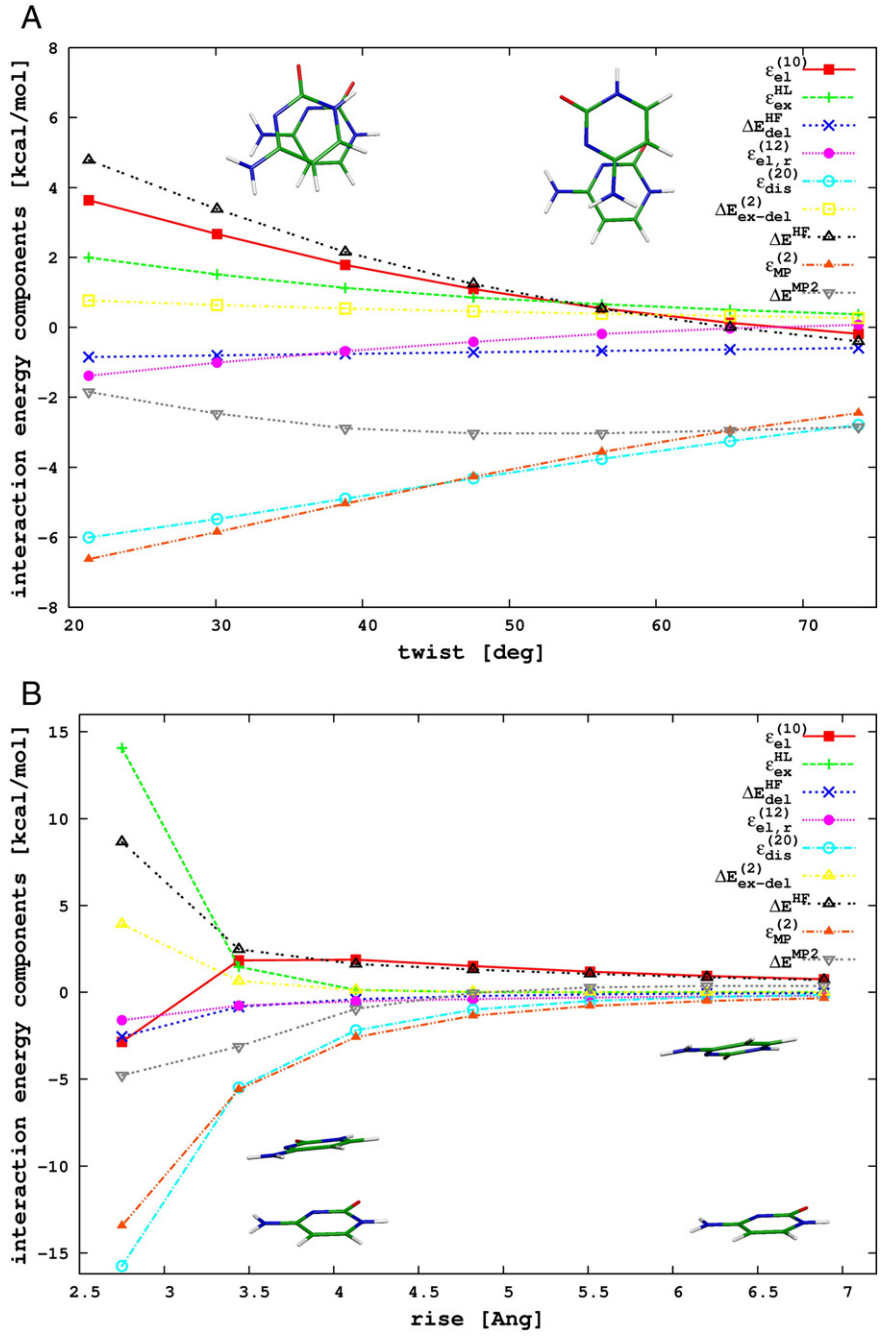

Fig. 4. The influence of variability of *twist* (upper plot) and *rise* (lower plot) parameters on intermolecular interaction energy components. The geometries of monomers correspond to border values of the base step parameters.

ΔE^{HF} is further divided into Heitler–London (ΔE^{HL}) and delocalization term (E^{HF}_{del}):

$$\Delta E^{HF} = \Delta E^{HL} + \Delta E^{HF}_{del}, \tag{2}$$

where ΔE^{HL} is defined as a sum of first-order electrostatic interaction energy and Heitler–London exchange term:

$$\Delta E^{HL} = \varepsilon^{HL}_{ex} + \varepsilon^{(10)}_{el}. \tag{3}$$

The $\varepsilon^{(2)}_{MP}$ term appearing in Eq. (1) comprises electron correlation corrections:

$$\varepsilon^{(2)}_{MP} = \varepsilon^{(12)}_{el,r} + \varepsilon^{(20)}_{disp} + \Delta E^{(2)}_{ex-del}, \tag{4}$$

where $\varepsilon^{(12)}_{el,r}$ denotes the term arising due to the dispersion and correlation corrections to the first-order electrostatic interaction, $\varepsilon^{(20)}_{disp}$ is the dispersion contribution and $\Delta E^{(2)}_{ex\text{-}del}$ is the exchange-delocalization component.

The dependence of the intermolecular interaction energy components on the base step parameters together with the structure of complexes corresponding to the border values of considered range of *slide*, *tilt*, *twist*, *rise*, *roll* and *shift* is presented in Figs. 3–5. The insets on the left side of Figs. 2–4 present the structures of cytosine complexes for the minimum value of a given parameter, while the insets on the right side correspond to the maximum value of considered parameter. In the whole range of variability of *slide* parameter the C/C complex is stabilized only by dispersion and ΔE^{HF}_{del} terms. $\varepsilon^{(12)}_{el,r}$ component is also of stabilizing character for *slide* values

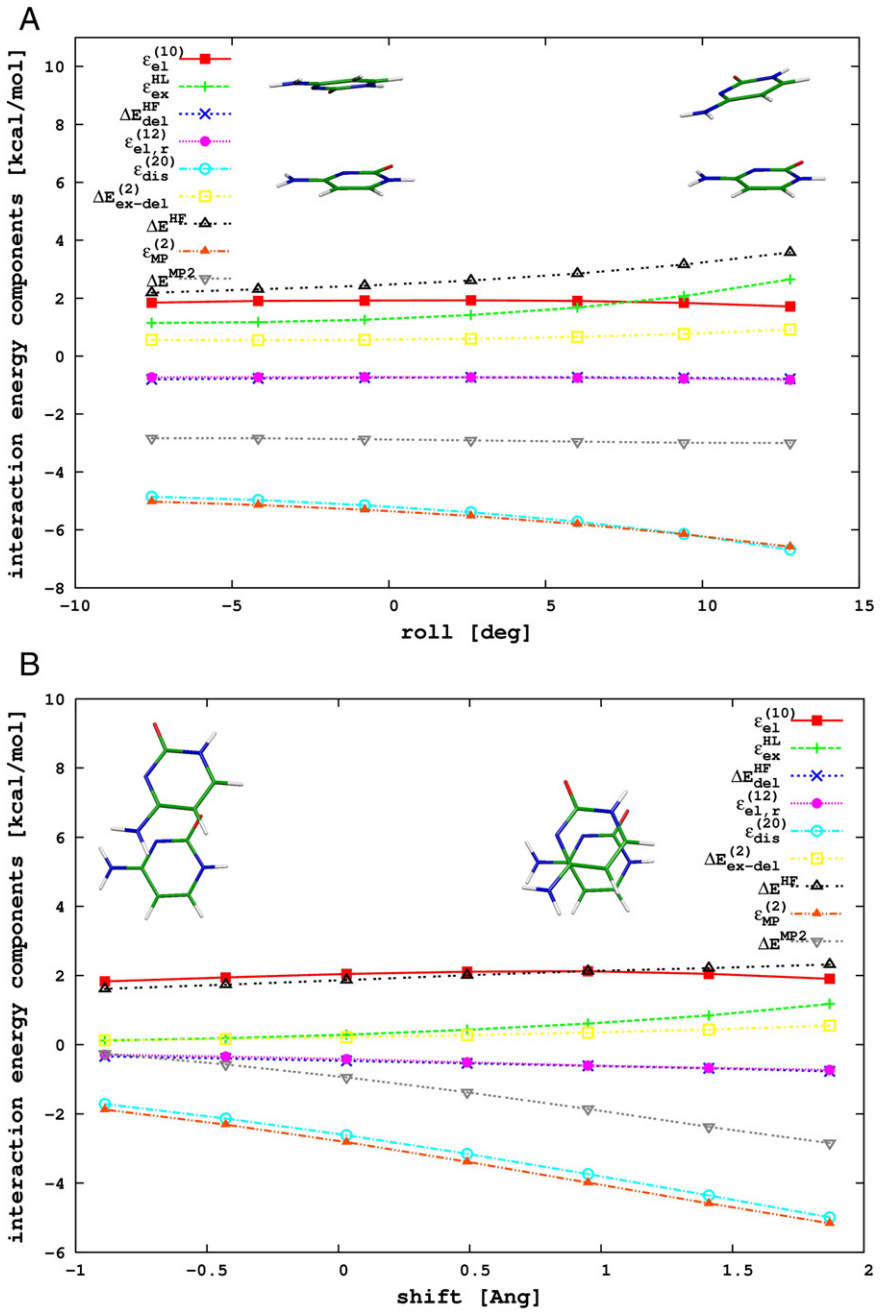

Fig. 5. The influence of variability of *roll* (upper plot) and *shift* (lower plot) parameters on intermolecular interaction energy components. The geometries of monomers correspond to border values of the base step parameters.

greater than −1 Å, while the first-order electrostatic contribution is of negative sign only for *slide* values less than 0.5 Å. Opposite to $\varepsilon_{el}^{(10)}$ and $\varepsilon_{disp}^{(20)}$, $\Delta E_{ex\text{-}del}^{(2)}$ and ε_{ex}^{HL} do not exhibit strong dependence on the *slide* parameter. Interestingly, the values of $\varepsilon_{el}^{(10)}$ fall into very wide range, *i.e.* from −2 to 5 kcal/mol. The impact of variability of the *tilt* parameter on the interaction energy components is presented in Fig. 3b. The increase of *tilt* value leads to smaller stabilization energy of investigated complex. This is mainly due to the weaker interaction of π electrons (see Fig. 1 containing the definition of *tilt* parameter). Among considered components, the largest sensitivity to *tilt* changes is observed for $\varepsilon_{disp}^{(20)}$. The differences of absolute values can be as large as 6 kcal/mol. It can be explained qualitatively based on Fig. 2b, *i.e.* increasing the *tilt* value leads to non-parallel alignment of cytosine monomers. It is also interesting to note, that $\varepsilon_{MP}^{(2)}$ term follows the dispersion contribution dependence on *tilt* very closely.

As it was mentioned in the previous section, it was observed by Hunter et al. that the *twist* parameter did not affect the intermolecular interaction energy for stacked complexes of nucleic acid bases [33]. In the case of investigated C/C complex, one finds indeed that the total IIE does not exhibit significant dependence on the *twist* parameter. Fig. 4a, however, brings an explanation to this observation. Two most important contributions are, namely $\varepsilon_{el}^{(10)}$ and $\varepsilon_{disp}^{(20)}$. In the whole range of variability of *twist*, the former component is positive while the latter contribution is stabilizing the C/C complex. For every *twist* value, for which decomposition of intermolecular interaction energy was performed, the absolute value of $\varepsilon_{el}^{(10)}$ is about 2 kcal/mol smaller than the dispersion contribution. Remaining components do not reveal such significant dependence on *twist*. The influence of *rise* parameter on interaction energy components is presented in Fig. 4b. It should be underlined

Table 1
The values of Pearson product-moment correlation coefficients between the interaction energy components and the base step parameters

	Shift	Twist	Tilt	Roll	Slide	Rise
ΔE^{HL}	0.999	−0.979	−0.871	0.959	0.994	−0.765
$\varepsilon_{el}^{(10)}$	0.359	−0.982	0.939	−0.563	0.993	0.391
ε_{ex}^{HL}	0.970	−0.972	−0.913	0.932	−0.656	−0.666
ΔE_{del}^{HF}	−0.999	1.000	0.962	0.343	−0.910	−0.797
ΔE^{HF}	0.997	−0.978	−0.781	0.973	0.994	−0.754
$\varepsilon_{MP}^{(2)}$	−0.999	0.997	0.980	−0.978	−0.779	0.834
$\varepsilon_{el,r}^{(12)}$	−0.997	0.982	0.883	−0.852	−0.997	0.858
$\varepsilon_{disp}^{(20)}$	−0.998	0.999	0.974	−0.972	0.030	0.802
$\Delta E_{ex\text{-}del}^{(2)}$	0.985	−0.989	−0.936	0.903	−0.163	−0.701
ΔE^{MP2}	−0.997	−0.736	0.996	−0.985	0.958	0.894

that for *rise* values larger than 3.5 Å, the first-order electrostatic contribution is weakly repulsive. The selected lowest-energy structure (BD0022) is characterized by *rise* value 3.53 Å. For this value of *rise* one finds, that besides significant stabilization due to the dispersion, the $\varepsilon_{el,r}^{(12)}$ and ΔE_{HF}^{del} also contribute to the stabilization of the C/C complex. Fig. 5 presents the relation between the interaction energy contributions and the *roll* and *shift* parameters. In both cases, most of the components do not exhibit significant dependence on these base step parameters. The only contribution, for which variations larger than 2 kcal/mol are observed, is $\varepsilon_{disp}^{(20)}$.

The Pearson product-moment correlation coefficients, presented in Table 1., were calculated in order to characterize quantitatively the above discussed trends and provide complementary information. The most important observation is that the smallest covariation is between *slide* and $\varepsilon_{disp}^{(20)}$ term. The value of 0.03 of correlation coefficient means that in the studied range the dependence of the latter quantity on the *slide* parameter is far from being linear. From the definition of *slide* we may infer that its change in both directions, relative to equilibrium value corresponding to the largest overlap of adjacent bases, will result in the paraboloidal dependence of $\varepsilon_{disp}^{(20)}$ term on *slide*. This is confirmed by our calculations presented in Fig. 3a and also explains why the correlation coefficient is close to zero. For the majority of cases, however, the variance in common is larger than 80%. As can be seen from Table 1, the variance in common not exceeding 25% between the first-order electrostatic interaction and *shift*, *roll* and *rise* is observed. Finally, we notice that the smallest correlation between the total MP2 interaction energy and the base step parameters is observed for *twist*.

3. Conclusions

Systematic analysis of the influence of six base step parameters describing mutual orientation of cytosine monomers in B-DNA on the intermolecular interaction energy components was performed using the variational–perturbational scheme at the MP2/aug-cc-pVDZ level of theory. The range of variability of the base step parameters was determined on the basis of crystallographic data. It has been found that different components of IIE behave in different manner upon change of base step parameters: Significant dependence of $\varepsilon_{el}^{(10)}$ term on *slide*, *twist* and *rise* parameters is observed. Moreover, the changes of absolute values of dispersion contribution larger than 3 kcal/mol are noticed for three parameters, namely *tilt*, *rise* and *shift*. The most important source of cytosine–cytosine complex stabilization is the dispersion contribution. However, $\varepsilon_{el,r}^{(12)}$ component is also of stabilizing character for great majority of analyzed conformations of C/C complex. Interestingly, the first-order electrostatic term is repulsive in most of the considered configurations.

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