EFFECTIVE ATOMIC CHARGES OF CANONICAL 2′-DEOXYRIBONUCLEOTIDES AND THEIR CONFORMATIONAL DEPENDENCES

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Effective charges for the atoms of canonical 2′-deoxyribonucleotides (the molecules of 5′-deoxycytidylic, 5′-thymidylic, 5′-deoxyadenylic, and 5′-deoxyguanylic acids) averaged over all of their possible conformers and the corresponding root-mean-square deviations have been obtained. It is shown that the charge deviations for carbon atoms can exceed the average values of the charge itself. A capability of reproducing the conformer dipole moments with the use of averaged charges has been analyzed. It is found that the neglect of the dependence of effective atomic charges on the molecule conformation may result in errors for the dipole moment magnitude exceeding 100%. The results obtained can be used for the improvement of electrostatic components in the existing force fields.

1. Introduction

Various physical properties of DNA fragments with different lengths and/or their structural links have been studied for a long time and continue to be a matter of the close attention for researchers [1–10]. This fact stems from the importance of indicated DNA properties for understanding the basic physical principles of the DNA functioning. Along with plenty of experimental methods such as x-ray and neutron diffraction analyses, vibrational and NMR spectroscopies, light scattering, electron diffraction, and so forth, the researches carried out within molecular dynamics (MD) methods play a more and more important role nowadays (see, e.g., works [11–13] and references therein). Although the MD method is extremely informative and requires much less computation resources in comparison with the methods of quantum chemistry, the proper choice of a specific "force field", i.e. the model potential for the determination of the interaction energy of atoms in a biomolecule, has to be done in order to make the results obtained in MD researches reliable. The potential energy of a molecule is represented, as a rule, in the form of the sum [14, 15]

$$U = U_{\text{chem}} + U_{\text{conf}} + U_{\text{lr}},$$

where

$$U_{\text{chem}} = \sum_b K_b \cdot (l_b - l_{0b})^2 + \sum_q K_q \cdot (\theta_q - \theta_{0q})^2$$

is the elastic deformation energy for rather rigid chemical bonds (here, the summations are carried out over all chemical bond lengths l_b and all valence angles θ_q in the molecule);

$$U_{\text{conf}} = \sum_s K_s \cdot [1 + \cos(n_s \cdot \varphi_s - \delta_s)]$$

is the "conformational" energy needed for relative rotations of neighbor atomic groups around single chemical bonds (here, the summation is carried out over all torsion angles φ_s's; and n_s, δ_s, and K_s are constants); and

$$U_{\text{lr}} = \sum_{i,j} \left(\frac{q_i \cdot q_j}{r_{ij}} + \frac{A_{ij}}{(r_{ij})^m} - \frac{C_{ij}}{(r_{ij})^n} \right)$$

is the energy of long-range interactions (here, the summation is carried out over the pairs of chemically nonbonded atoms; r_{ij} are interatomic distances; A_{ij}, C_{ij}, m, and n are constants; and q_i and q_j are effective atomic charges). The electrostatic energy q_iq_j/r_{ij} is an essential component of the energy of long-range interactions $U_{\rm lr}$; for its evaluation, an effective charge q_i needs to be assigned to every atom [14–16].

At the same time, it is known that the *bio*molecules are characterized by a considerable conformational capacity. For instance, each of four canonical 2′-deoxyribonucleotides (DRNs)–they are elementary (monomer) units of the DNA chain–can acquire 600 to 700 different conformations [17–20]. Atomic charges in the molecule are not observable physical quantities, but they are introduced on the basis of that or another model [21–27]. Therefore, one may expect that the effective charges q_i depend on the specific biomolecule conformation (on the angles φ_s), because, irrespective of the selected model, the magnitudes of those charges are determined by specific electron configurations, which are different for different conformers. Hence, for the solution of molecular simulation problems within MD methods to be correct, it is important to elucidate if the application of atomic charges with definite fixed values is well substantiated for the force field construction.

The purpose of this work is to analyze, using canonical DRNs as examples, to what extent the effective atomic charges can depend on the biomolecule conformation and to determine how precisely the atomic charges averaged over all biomolecular conformers can reproduce dipole moments of individual conformers.

2. Objects and Methods of Research

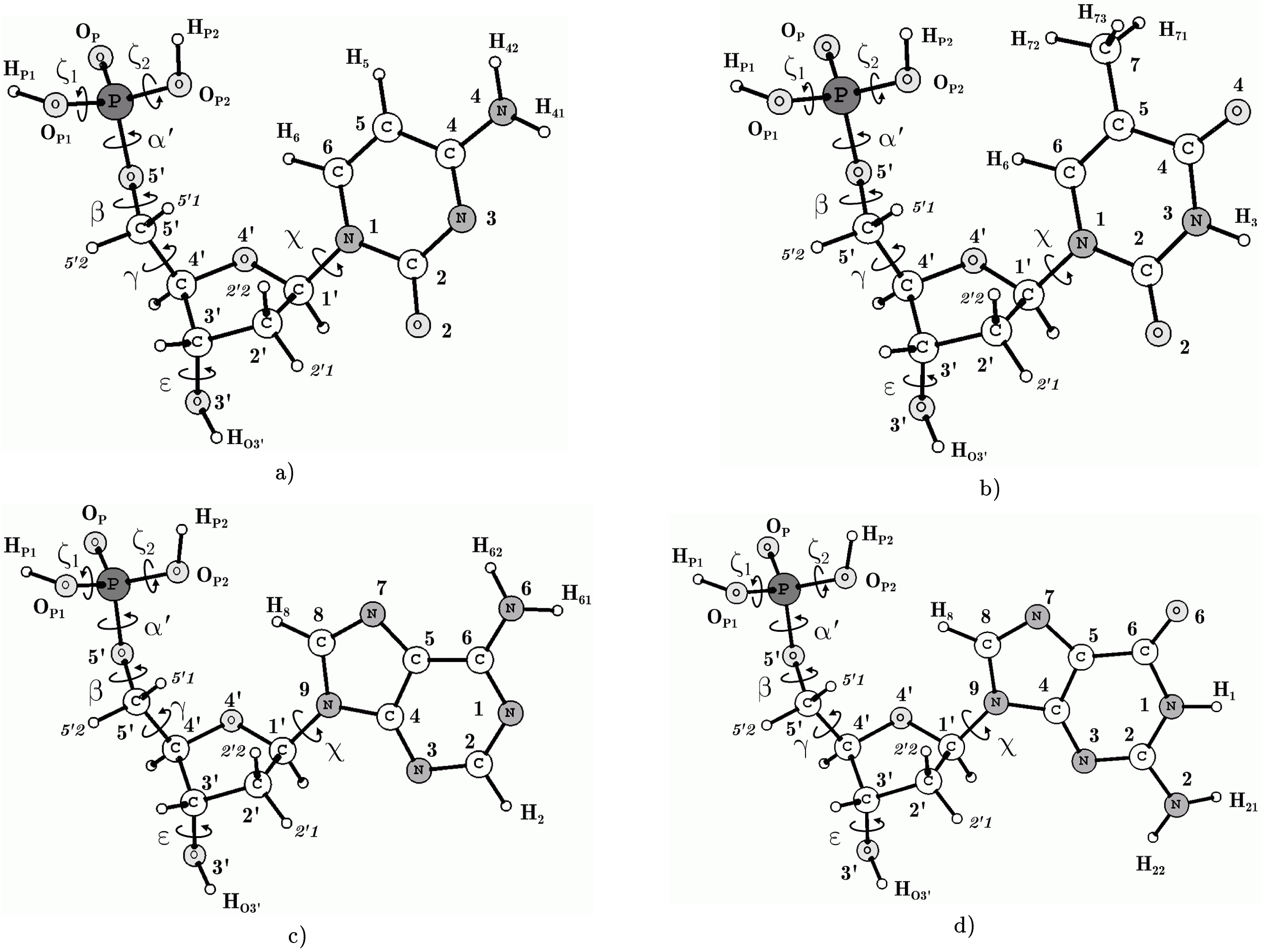
To solve the formulated problem, we used the complete conformer families of canonical isolated DRNs (molecules of 5′-deoxycytidylic (5DCA), 5′-thymidylic (5TA), 5′-deoxyadenylic (5DAA), and 5′-deoxyguanylic (5DGA) acids (see Figure)) obtained by us earlier [17–20] in the framework of the exhausting quantum-mechanical conformational analysis. The analysis was carried out by applying the quantum-mechanical method of density functional theory (DFT) and using the exchange-correlation functional B3LYP [29, 30] and the standard basic set 6-31G(d,p) [21]. The same theoretical level was used to determine the spatial distributions of the charge density in conformers. The effective atomic charges were found separately for each conformation of each studied DRN with the use of the Merz–Kollman method [24, 25] without imposing any additional conditions on multipole moments. The Merz–Kollman method was chosen among others, because it was developed for the most accurate [21, 28] reconstruction of the real electrostatic potential of a molecule by introducing a system of point charges centered at the atomic nuclei in the molecule. The obtained charges were used to find the charge of each atom averaged over all the conformersin of the given DRN, and the corresponding root-mean-square deviations were calculated. The latter served as an indicator for the conformational sensitivity of effective atomic charges. Taking into account that the magnitudes of effective atomic charges find the most practical application in molecular simulations by the MD method, these values must be equally suitable for any conformation of the molecule. Accordingly, all the conformers were regarded to be equiprobable so that the averaged charges were calculated as the arithmetic means for all available conformers (613 conformers for 5DCA [17], 660 ones for 5TK [18], 726 ones for 5DAA [19], and 745 ones for 5DGA [20]).

3. Results and Discussion

3.1. Charges of atoms in the sugar-phosphate backbone

The sugar-phosphate backbone of a DRN is the part of a DRN molecule and consists of the sugar residue (atoms $C_{1'}$, $C_{2'}$, $C_{3'}$, $C_{4'}$, $C_{5'}$, $O_{3'}$, and $O_{4'}$, as well as hydrogen atoms attached to them – and the phosphate group – atoms P, $O_{\rm P}$, $O_{\rm P1}$, $O_{\rm P2}$, $H_{\rm P1}$, $H_{\rm P2}$, and $O_{5'}$ – which are identical for all canonical DRNs (see Figure).

In Table 1, the effective atomic charges calculated for the atoms in the DRN sugar-phosphate backbone by averaging over all corresponding conformers are quoted. The data obtained testify that the most conformation-sensitive are the charges of carbon atoms. The corresponding root-mean-square deviations σ_q divided by the absolute value of electron charge, $|e|$, range from 0.09 to 0.16. Some smaller σ_q-values are observed for $O_{5'}$ and P atoms. Note that the difference $\Delta_q = q_{\rm max} - q_{\rm min}$ between the maximum and minimum charge values for each atom in the sugar-phosphate backbone is, depending on the specific atom, 4.8 to 8.4 times as large as the corresponding root-mean-square deviation σ_q. Atom $C_{5'}$ in the sugar-phosphate backbone of canonical DRNs has the maximal $\Delta_q = (0.79 \div 0.99) \times |e|$, whereas atom $H_{O3'}$ the minimal $\Delta_q = (0.12–0.13) \times |e|$.



Structures of canonical 2′-deoxyribonucleotides (molecules of 5′-deoxycytidylic (*a*), 5′-thymidylic (*b*), 5′-deoxyadenylic (*c*), and 5′-deoxyguanylic (*d*) acids, and notations for their atoms and conformational parameters

3.2. Charges of atoms in nucleotide bases

Nucleotide bases are "bits" of the genetic information, which is contained in a DNA. The canonical DRNs differ from each other namely by the type of nucleotide base. The average effective atomic charges and the corresponding root-mean-square deviations for the atoms of nucleotide bases in molecules 5DCA, 5TA, 5DAA, and 5DGA are listed in Tables 2 to 5, respectively. For the sake of comparison, the tables also include the values q_{base} for the effective atomic charges in nucleotide bases methylated at the glycoside nitrogen atom, which were determined in work [31] at the same level of the DFT B3LYP/6-31G(d,p) theory, as was used in this work.

For purine nucleotide bases (adenine and guanine) and cytosine, it was found that if the sugar-phosphate backbone is substituted by a methyl group, the maximum change (by $(0.14–0.17) \times |e|$) occurs in the charge of the glycoside nitrogen atom. At the same time, in thymine, the maximum change (by $0.26|e|$) is revealed by the charge of C_7 atom, whereas the charge of the glycoside nitrogen atom varies only by $0.12|e|$. For all other atoms in the nucleotide bases, the difference between the charges averaged over all conformers of canonical DRNs and the charges of nucleotide bases methylated at the glycoside nitrogen atom does not exceed $0.1|e|$.

The charge of the glycoside nitrogen atom turned out the most sensitive to the DRN conformation in cytosine, thymine, adenine ($\sigma_q/|e| = 0.08–0.09$). At the same time, in guanine, it is atom N_3 ($\sigma_q/|e| = 0.10$), whereas the charge of the glycoside nitrogen atom is characterized by the same conformational sensitivity, as it has in other

Table 1. Effective charges $\bar{q}$ of atoms in the backbone of canonical 2′-deoxyribonucleotides[a] averaged over all of their possible conformations and the corresponding root-mean-square deviations σ_q

Atom	$q/\lvert e\rvert$				$\sigma_q/\lvert e\rvert$			
	5DCA	5TA	5DAA	5DGA	5DCA	5TA	5DAA	5DGA
$H_{1'}$	0.05	0.06	0.07	0.06	0.03	0.03	0.03	0.03
$H_{2'1}$	0.13	0.13	0.12	0.13	0.03	0.02	0.02	0.02
$H_{2'2}$	0.12	0.13	0.12	0.11	0.03	0.03	0.03	0.04
$H_{3'}$	0.04	0.03	0.03	0.03	0.04	0.04	0.06	0.05
$H_{O3'}$	0.40	0.40	0.40	0.40	0.02	0.02	0.02	0.02
$H_{4'}$	0.08	0.08	0.08	0.08	0.04	0.04	0.04	0.04
$H_{5'1}$	0.10	0.10	0.08	0.09	0.04	0.03	0.04	0.04
$H_{5'2}$	0.09	0.10	0.08	0.09	0.04	0.04	0.05	0.05
H_{P1}	0.43	0.43	0.43	0.43	0.03	0.02	0.03	0.03
H_{P2}	0.43	0.43	0.43	0.43	0.03	0.02	0.03	0.03
$O_{3'}$	−0.63	−0.63	−0.63	−0.63	0.03	0.03	0.03	0.03
$O_{4'}$	−0.41	−0.40	−0.40	−0.40	0.06	0.06	0.06	0.07
$O_{5'}$	−0.36	−0.36	−0.37	−0.36	0.07	0.08	0.08	0.08
O_P	−0.58	−0.58	−0.58	−0.58	0.02	0.02	0.02	0.02
O_{P1}	−0.57	−0.56	−0.57	−0.57	0.04	0.03	0.04	0.04
O_{P2}	−0.56	−0.56	−0.57	−0.57	0.03	0.04	0.03	0.04
$C_{1'}$	0.37	0.36	0.35	0.35	0.11	0.12	0.13	0.16
$C_{2'}$	−0.36	−0.39	−0.35	−0.35	0.09	0.09	0.11	0.11
$C_{3'}$	0.32	0.35	0.33	0.33	0.11	0.11	0.13	0.12
$C_{4'}$	0.13	0.09	0.10	0.11	0.15	0.14	0.14	0.14
$C_{5'}$	0.00	0.00	0.05	0.03	0.13	0.13	0.15	0.15
P	0.96	0.96	0.97	0.97	0.07	0.07	0.07	0.08

[a] Footnote: Notations for 2′-deoxyribonucleotide molecules: 5′-deoxycytidylic (5DCA), 5′-thymidylic (5TA), 5′-deoxyadenylic (5DAA), and 5′-deoxyguanylic (5DGA) acids.

bases ($\sigma_q/|e| = 0.08$). It is worth noting that, despite a substantial difference between the average charge of atom C_7 in thymine as a component of 5TA and the corresponding value for methylated thymine, the charge of this atom is much less sensitive to conformations of 5TA ($\sigma_q/|e| = 0.03$) than the others.

Table 2. Effective charges $\bar{q}$ of cytosine atoms averaged over all possible 5DCA conformations and the corresponding root-mean-square deviations σ_q normalized to the electron charge magnitude[a]

Quantity	Atom					
	N_1	C_2	N_3	C_4	C_5	C_6
q_{base}	−0.19	0.80	−0.76	0.81	−0.54	0.12
$\bar{q}$	−0.33	0.87	−0.78	0.86	−0.62	0.17
σ_q	0.08	0.06	0.03	0.04	0.03	0.05
Quantity	Atom					
	O_2	N_4	H_{41}	H_{42}	H_5	H_6
q_{base}	−0.56	−0.86	0.39	0.37	0.18	0.12
$\bar{q}$	−0.58	−0.89	0.41	0.39	0.22	0.13
σ_q	0.02	0.03	0.02	0.01	0.01	0.02

[a] Footnote: q_{base}-values correspond to effective atomic charges in 1-methylcytosine [31].

Table 3. Effective charges $\bar{q}$ of thymine atoms averaged over all possible 5TA conformations and the corresponding root-mean-square deviations σ_q normalized to the electron charge magnitude[a]

Quantity	Atom						
	N_1	C_2	N_3	C_4	C_5	C_6	O_2
q_{base}	−0.10	0.66	−0.64	0.65	−0.11	−0.10	−0.53
$\bar{q}$	−0.22	0.70	−0.65	0.63	−0.02	−0.11	−0.54
σ_q	0.09	0.07	0.03	0.03	0.03	0.06	0.02
Quantity	Atom						
	H_3	O_4	H_6	C_7	H_{71}	H_{72}	H_{73}
q_{base}	0.37	−0.52	0.16	−0.15	0.05	0.07	0.07
$\bar{q}$	0.38	−0.50	0.18	−0.42	0.13	0.14	0.14
σ_q	0.01	0.01	0.04	0.03	0.01	0.01	0.01

[a] Footnote: q_{base}-values correspond to effective atomic charges in 1-methylthymine [31].

3.3. Reconstruction of conformer dipole moments

By using the effective atomic charges $\bar{q}_i$ obtained by averaging over all conformations of canonical DRNs, which are quoted in Tables 2 to 5, we analyzed how accurately they correspond to the magnitude and the direction of the dipole moment for each of their individual conformers. For this purpose, the dipole moment vector $\mathbf{d}_q = \sum_i \bar{q}_i \mathbf{R}_i$ calculated for each conformer using the averaged effective atomic charges $\bar{q}_i$ was compared with the dipole moment vector $\mathbf{d}_\rho = \int \mathbf{r}\rho_{\text{mol}}(\mathbf{r})\, d^3r$ determined from the charge density distribution in the molecule, $\rho_{\text{mol}}(\mathbf{r})$, obtained from quantum-mechanical calculations. The difference between the vectors $\mathbf{d}_q$ and $\mathbf{d}_\rho$ was characterized by the relative difference between vector magnitudes, $E_d = ||\mathbf{d}_q| - |\mathbf{d}_\rho|| \,/\, |\mathbf{d}_\rho|$, and the angle Θ between them (the case of equality of the indicated vectors corresponds to the values $E_d = 0$ and $\Theta = 0°$). The calculated values for E_d and Θ are shown in Table 6. From the presented data, it follows that the system of constant effective atomic charges reproduces the dipole moment most accurately in the case of 5TA molecule ($E_d < 0.6$) and least accurately in the case of 5DAA molecule. In the latter case, E_d exceeds 100% in 11 of 726 possible conformers (the maximum of E_d is attained in conformer **382** [19], for which $|\mathbf{d}_q| = 2.27$ D, whereas the exact value is $|\mathbf{d}_q| = 0.46$ D). At the same time, in

Table 4. Effective charges $\bar{q}$ of adenine atoms averaged over all possible 5DAA conformations and the corresponding root-mean-square deviations σ_q normalized to the electron charge magnitude[a]

Quantity	Atom						
	N_1	C_2	N_3	C_4	C_5	C_6	N_7
q_{base}	−0.70	0.53	−0.67	0.46	−0.04	0.65	−0.51
$\bar{q}$	−0.69	0.48	−0.65	0.48	0.00	0.64	−0.54
σ_q	0.03	0.05	0.07	0.06	0.05	0.04	0.02

Quantity	Atom						
	C_8	N_9	H_2	N_6	H_{61}	H_{62}	H_8
q_{base}	0.18	−0.10	0.02	−0.79	0.37	0.36	0.11
$\bar{q}$	0.25	−0.26	0.05	−0.82	0.39	0.38	0.11
σ_q	0.05	0.08	0.01	0.02	0.01	0.01	0.02

[a] Footnote: q_{base}-values correspond to effective atomic charges in 9-methyladenine [31].

Table 5. Effective charges $\bar{q}$ of guanine atoms averaged over all possible 5DGA conformations and the corresponding root-mean-square deviations σ_q normalized to the electron charge magnitude[a]

Quantity	Atom							
	N_1	C_2	N_3	C_4	C_5	C_6	N_7	C_8
q_{base}	−0.73	0.79	−0.66	0.35	−0.01	0.64	−0.48	0.14
$\bar{q}$	−0.68	0.73	−0.61	0.32	0.07	0.57	−0.51	0.20
σ_q	0.06	0.08	0.10	0.08	0.05	0.04	0.02	0.05

Quantity	Atom						
	N_9	H_1	N_2	H_{21}	H_{22}	O_6	H_8
q_{base}	−0.05	0.40	−0.82	0.36	0.36	−0.52	0.11
$\bar{q}$	−0.20	0.39	−0.82	0.37	0.38	−0.49	0.11
σ_q	0.08	0.01	0.04	0.01	0.02	0.01	0.02

[a] Footnote: q_{base}-values correspond to effective atomic charges in 9-methylguanine [31].

the majority of 5DAA conformers (81%), E_d does not exceed 25%.

The direction of the dipole moment vector is reproduced better. Even in the case of 5DAA molecule, which is characterized by the largest angle Θ, this parameter does not exceed 45° in 98% of conformers. However, in two conformers, this angle amounts to 123.5° (conformer **544** [19]) and 120.8° (conformer **344** [19]).

4. Conclusions

To summarize, it was found that, among all atoms in the sugar-phosphate backbone of canonical 2′-deoxyribonucleotides, the effective charges of carbon atoms are the most sensitive to the conformational change. The presence of a sugar-phosphate backbone in DRNs considerably affects the effective charges of glycoside nitrogen atoms in nucleotide bases and C_7 atom in thymine. The effective averaged atomic charges in the overwhelming majority of conformers can serve as a reliable tool for the qualitative determination of the molecular electrostatic potential. However, for some conformers, their values are unsuitable for quantitative calculations. The values of effective atomic charges obtained for canonical 2′-deoxyribonucleotides can be used to improve the available force fields, which are used to study biomolecules in the framework of molecular dynamics methods and to calculate the electrostatic contribution to the interaction energy between various structural DNA units (for example, a nucleotide base and a sugar-phosphate backbone).

Table 6. Statistical characteristics describing the accuracy of the dipole moment reproduction for canonical 2′-deoxyribonucleotides using a system of effective atomic point charges[a]

Molecule	$\langle E_d \rangle$	$\max(E_d)$	$\langle \Theta \rangle$	$\max(\Theta)$
5DCA	0.09	0.98	9.5	54.4
5TA	0.13	0.59	9.0	72.8
5DAA	0.21	3.95	14.8	123.5
5DGA	0.09	0.74	7.5	35.5

[a] Footnote: $E_d = \left| |\mathbf{d}_q| - |\mathbf{d}_\rho| \right| / |\mathbf{d}_\rho|$ is the relative difference between the magnitudes of dipole moment vectors $\mathbf{d}_q$ and $\mathbf{d}_\rho$ (the former was calculated with the use of averaged atomic charges $\bar{q}_i$, and the latter was determined from quantum-mechanical calculations), and Θ is the angle between the vectors $\mathbf{d}_q$ and $\mathbf{d}_\rho$.

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ЕФЕКТИВНІ АТОМНІ ЗАРЯДИ КАНОНІЧНИХ 2′-ДЕЗОКСИРИБОНУКЛЕОТИДІВ ТА ЇХНЯ ЗАЛЕЖНІСТЬ ВІД КОНФОРМАЦІЇ

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Резюме

Одержано середні за усіма можливими конформерами канонічних 2′-дезоксирибонуклеотидів (молекул 5′-дезоксицитидилової, 5′-тимідилової, 5′-дезоксиаденілової та 5′-дезоксигуанілової кислот) значення ефективних зарядів їхніх атомів та знайдено відповідні середньоквадратичні відхилення. Показано, що зазначені відхилення для атомів вуглецю можуть перевищувати середнє значення їхнього заряду. Проаналізовано можливість відтворення дипольного моменту конформерів за допомогою усереднених атомних зарядів і виявлено, що нехтування залежністю ефективних атомних зарядів від конформації молекули може приводити до похибок модуля дипольного моменту, більших за 100%. Одержані результати можуть бути використані для вдосконалення електростатичних складових існуючих силових полів.