

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

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S u m m a r y

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 was 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 using averaged charges has been analyzed. It was found that the neglect of the dependence of effective atomic charges on the molecule conformation may result in the errors for the dipole moment magnitude exceeding 100%. The results obtained can be used for the improvement of electrostatic components in existing force fields.