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Quantum-Chemical Study of the Interactions between DNA Phosphate Groups and Monovalent Ions

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The complexes of monovalent ions (Li^+, Na^+, K^+) with DNA phosphate groups are considered in the present work. The complexes are studied from the simplest to the more complicated ones. In addition, chloride ions (Cl^-) and water molecules are introduced to make the complexes more realistic. Optimized geometries, interaction energies, and vibrational spectra are calculated using density functional theory method (DFT) within the framework of the Gaussian 03 software package.
It is shown that the lithium ion has a tetrahedral hydration shell. The calculated interaction energies show that complexes containing Li^+ and two phosphate groups are energetically more stable than the corresponding complexes containing sodium or potassium ions. IR and Raman spectra are obtained, and all the main vibrational modes are identified. Some of the calculated vibrational modes are in good agreement with experimental data.
The results of the present work may play a crucial role in understanding the possible condensation of DNA molecules in solution in the presence of Li^+ ions, as suggested by some recent molecular dynamics calculations.

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