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Electronic structure and stability of complexes Ag+ with nucleotide base pairs

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Metallized DNA is of considerable interest due to its potential application in molecular electronics. Therefore, the fundamental properties of this system are of paramount interest, in particular those related to electronic structure and dynamics of metallized base pairs. In this work, two different structural motifs of Ag-DNA known from the experiment [1,2] were investigated: one that preserves Watson-Crick base pairing with Ag^+ ions included in the base pairs (based on experiment [1]), and the other that breaks the base pairing (based on experiment [2]). The fundamental questions concerning their relative energetic stability and thermodynamics of formation were considered. To answer these questions the detailed quantum-chemical calculations were performed at the DFT level using the B3LYP functional in the Gaussian 03 software package. Ag+ ions were described by the Def2-TZVP basis set with effective core potential (ECP). Nucleotide base atoms were described by the all-electron basis set 6-311++G(d, p). Solvation effects of the aqueous environment were taken into account using the SMD model. Dispersion corrections were taken into account using method Grimme's of D3. This calculation method for the studied systems was chosen based on the results of our previous work [3]. Several sets of systems were investigated, both with and without Ag+, including purine-Ag-purine, pyrimidine-Ag-pyrimidine, 7-deazapurine-Ag-pyrimidine, and canonical Watson-Crick base pairs. The highest thermodynamic stability was demonstrated by the neutral complex [7-deazaguanine(N1)-Ag+-cytosine(N3)]0, which outperforms its canonical counterpart [guanine(N1)-Ag+-cytosine(N3)]0. Analysis of the calculated IR and Raman vibrational spectra revealed pronounced spectral changes that can be used to characterize the presence of Ag^+ ions in the DNA double helix. In particular, vibrations associated with the motion of Ag^+ ions were detected in the low-frequency region (<250 cm^{-1}).

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Primary authors: OSOKIN, Yevhen (Bogolyubov Institute for Theoretical Physics); PEREPELYTSYA, Sergiy (Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine)

Presenter: OSOKIN, Yevhen (Bogolyubov Institute for Theoretical Physics)

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