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Metallized Ag-DNA: Computational insights into a novel biomolecular material

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Metallized DNA, in which Ag^+ ions form complexes with the nucleotide bases and arrange inside the double helix as a chain of atoms, is of great practical importance due to the potential use of such systems as nanowires in various technological applications. In the present work, the quantum-chemical DFT study of Ag^+ complexes with DNA nucleotide bases has been carried out[a]. The B3LYP and M06-2X functionals in combination with the PCM and SMD solvation models have been used. The results have shown that electrically neutral complexes of silver ions with thymine (Ag^+ at N3) and guanine (Ag^+ at N1) possess the highest thermodynamic stability, whereas the positively charged adenine complexes (Ag^+ at N1) are the least stable (Figure 1). The obtained results are in agreement with experimental X-ray data indicating that silver ions in metallized Ag-DNA displace adenine bases from the double helix[b]. Comparison of computational methods indicates that the B3LYP functional combined with the SMD solvation model provides the most reliable description. These findings contribute to understanding the structural characteristics of metallized Ag-DNA and its potential applications as a nanomaterial.

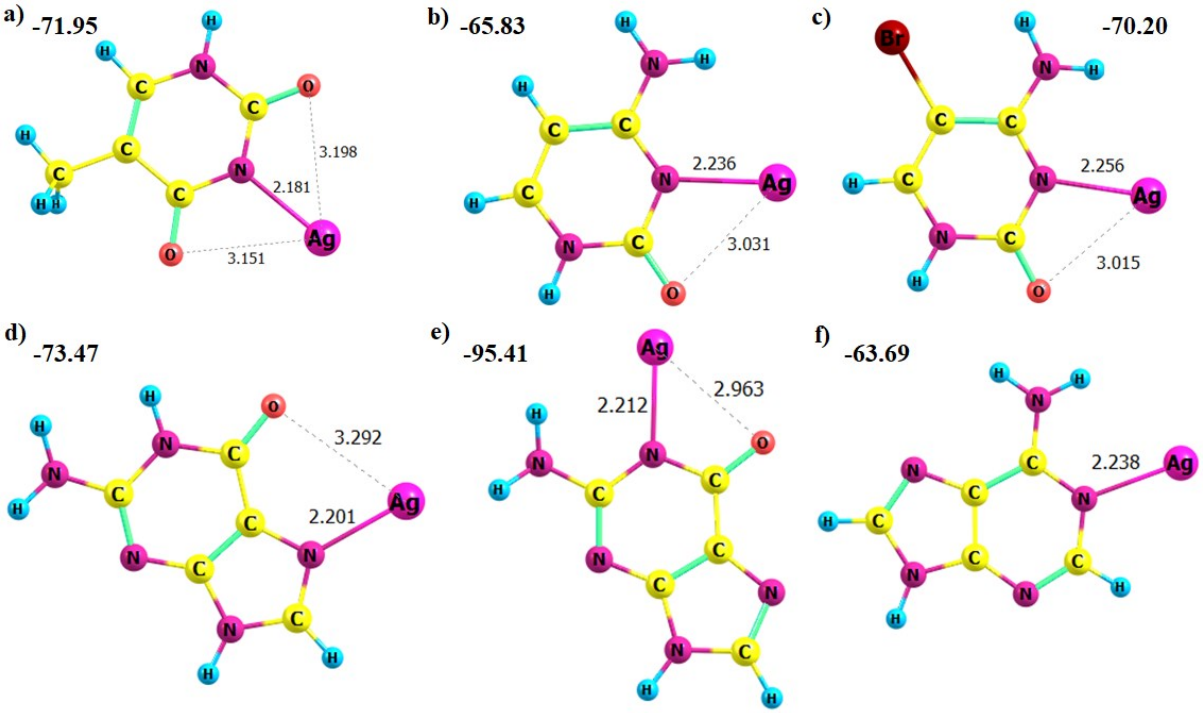

Figure 1. Ag^+-nucleobase complexes: thymine (a), cytosine (b), 5-bromocytosine (c), guanine (d,e), adenine (f). Distances in Å; energies in kJ/mol.

References:
[a]Osokin, Ye.; Perepelytsya, S. Low Temperature Physics, 2026, Volume 52 (accepted)
[b]Kondo, J., et al., Nature Chemistry, 2017, Volume 9, 956–960. https://doi.org/10.1038/nchem.2808