

Supplementary Materials

How the long G·G* Watson-Crick DNA base mispair comprising keto and enol tautomers of the guanine tautomerises? The results of the QM/QTAIM investigation

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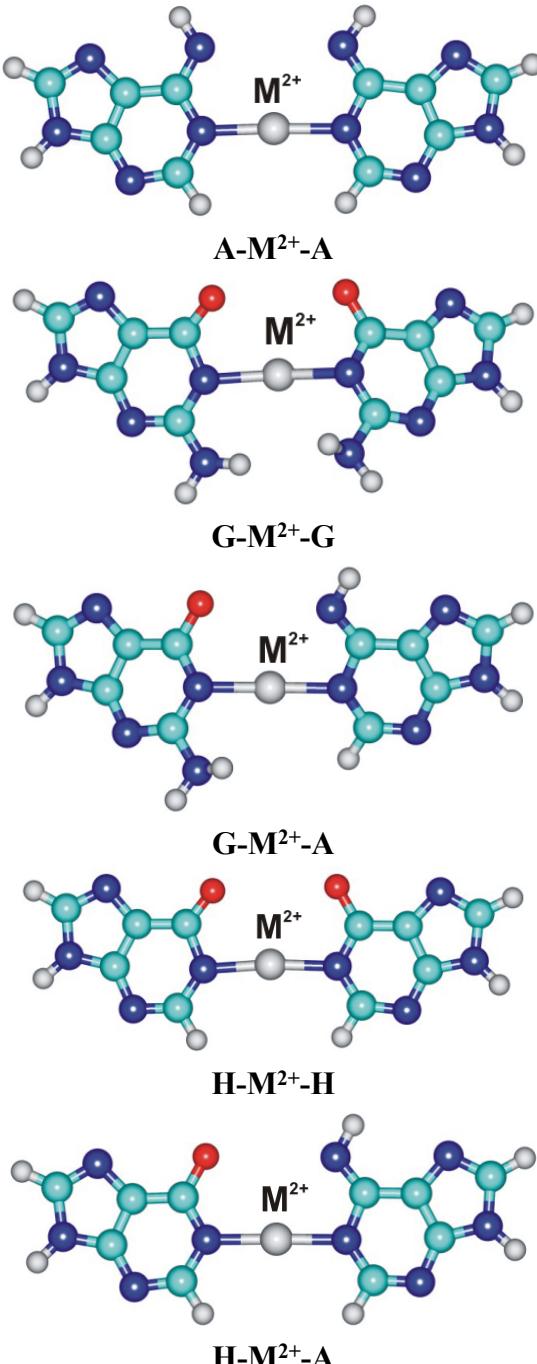


Figure S1. Hypothetical metallized purine-purine pairs of nucleotide bases that can be integrated into the DNA double helix. Designation: M^{2+} – the doubly charged metal cation, for example Hg^{2+} or Ag^{2+} [1-3], H – hypoxanthine, G – guanine, A – adenine.

References:

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3. Torigoe H., Ono A., Kozasa T. Hg^{II} ion specifically binds with T:T mismatched base pair in duplex DNA, *Chem. Eur. J.*, 2010, **16**, 13218–13225.