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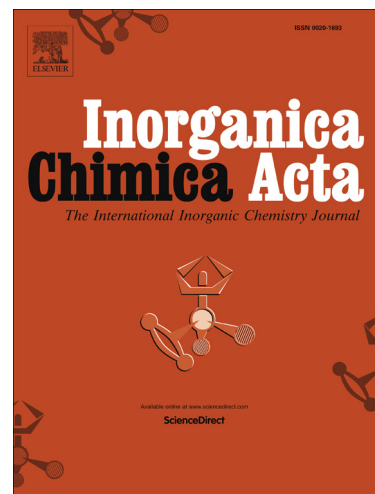
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Structure and properties of a copper-mediated nucleobase pair from density functional theory investigation

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Abstract

The structure and electronic properties of the 6-carboxypurine (Pur^{C}) self pair with Cu^{2+} , $\text{Pur}^{\text{C}}\text{-Cu-Pur}^{\text{C}}$, a new copper-mediated base pair having a core purine and close to Watson-Crick natural adenine-thymine base pair in a DNA double helix, were determined by using density functional theory and employing the M06-L exchange-correlation functional. With the aim to better evaluate the influence of the ligand nature on binding energy of $\text{Pur}^{\text{C}}\text{-Cu-Pur}^{\text{C}}$, comparisons with the A-Cu- Pur^{C} , $\text{Pur}^{\text{C}}\text{-Cu-T}$ systems have been performed. The computations on the corresponding zinc-mediated DNA dimer allow to explore also the role of the metal. The two employed models have different molecular size due to the presence of the sugar-phosphate group in the larger one. Results evidence as the copper ion complexes prefer to assume a square-planar complex that hence preserves the geometrical features of hydrogen-bonded natural base pairs. The computed binding energies well agree with the experimental melting point temperatures.

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