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DFT Study of Hoogsteen-Type Base Pairs

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Abstract : We have performed a theoretical study using dispersion-corrected Density Functional Methods to evaluate a variety of artificial nucleobases as candidates for metal-mediated Hoogsteen-type base pairs. We focus on A-M-T Hoogsteen-type base pair with M=Co(II), Ru(I), Ni(I). All calculations are performed using (ADF 09) program. Metal-mediated Hoogsteen-type base pairs are studied as drug candidates, their geometry optimizations are performed at ZORA/TZ2P/BLYP-D level. The molecular geometries and different energies as total energies, coordination energies, Pauli interactions, orbital interactions and electrostatic energies are determined.

Keywords : chemistry, biology, density functional method, orbital interactions
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