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# Computational modeling of the dinuclear metal complexes with di-*o*-quinones comprising paramagnetic acene linker groups

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The magnetically-active dinuclear metal complexes with previously unstudied di-*o*-quinone ligands comprising paramagnetic acene linkers have been investigated with the use of density functional theory quantum-chemical calculations (UTPSSh/UB3LYP/6-311++G(d,p)). Two types of linker groups are considered: linear acenes comprising various number of six-membered cycles and polycyclic hydrocarbons containing terminal five-membered rings. In sodium complexes replacement of terminal six-atomic hydrocarbon rings of the acene chain by five-membered cycles results in changing the type of the exchange interactions involving *o*-semiquinone radical-anions from antiferromagnetic to ferromagnetic. All paramagnetic centers in copper complexes with dicatecholate forms of the redox-active ligands are antiferromagnetically coupled. The performed computational modeling has shown that the nature and strength of the exchange interactions between paramagnetic centers of the compounds under study depend on the structure of the polycyclic hydrocarbon determined by the type of terminal rings and oxidation state of the redox-active moieties.

**Keywords:** DFT calculations, Di-*o*-quinones, Acenes, Metal complexes, Magnetic properties

## 1. Introduction

The search for paramagnetic molecules, electron spins of which are capable of performing the functions of molecular switches and spin quantum bits, represents one of the priority research directions in the industry of nanosystems. Examples of such type compounds are acenes – a large class of polycyclic aromatic hydrocarbons [1, 2]. These intriguing molecules with unique electronic properties are regarded as the basis for organic field-effect transistors [3, 4] and semiconductors [5, 6]. A distinctive feature of acenes is significant variation of their characteristics with changing the number of condensed rings [7–10]. It was shown by means of quantum-chemical calculations that increasing the number of condensed rings of the linear acenes results in considerable reducing the HOMO-LUMO energy gap, giving rise starting from hexacene to the compounds stabilized in the open-shell singlet biradical state [11], which may find an application in molecular electronics and spintronics [12, 13].

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