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Valence-Tautomeric Adducts of Co(II) Diketonates Based on Annelated Di-*o*-Quinones: Computer Simulation

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Abstract—The computer simulation (DFT B3LYP*/6-311++G(d,p)) is performed for the adducts of divalent cobalt diketonates with di-*o*-quinones in which the quinone rings are separated by the cycloalkane spacers. The isomers containing dianion–diradical forms of the redox-active ligand, the character of exchange between unpaired electrons of which depends on the spacer structure, correspond to the ground states of the considered compounds. Strong antiferromagnetic interactions ($J > 400$ cm^{-1}) are predicted for the most stable electromers of the adducts of Co(II) bis(chelates) with 9,10-dimethyl-9,10-ethanoanthracene-2,3,6,7(9H,10H)-tetraone, whereas a weak exchange favoring paramagnetism in a wide temperature range is expected for the ground states of the binuclear complexes with the isomeric 5,10-dimethyl-4b,5,9b,10-tetrahydroindeno[2,1-a]indene-2,3,7,8-tetraone spacer. The electromers of the complex with the hexafluoroacetylacetone ligands are characterized by close values of the total energies, due to which the complex becomes a promising object for the development of spin qubits.

Keywords: quantum-chemical calculations, cobalt complexes, *o*-quinones, valence tautomerism, exchange interactions

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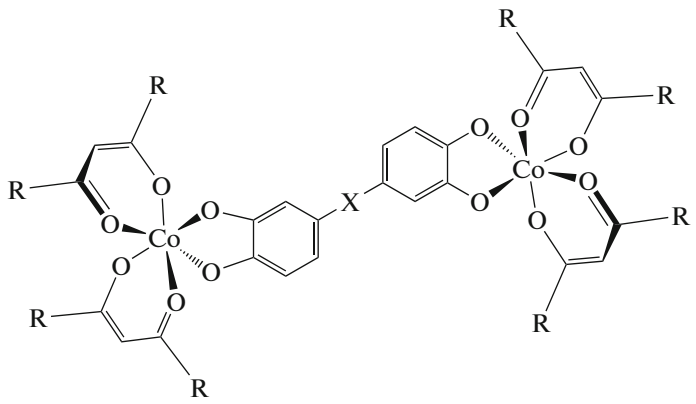
INTRODUCTION

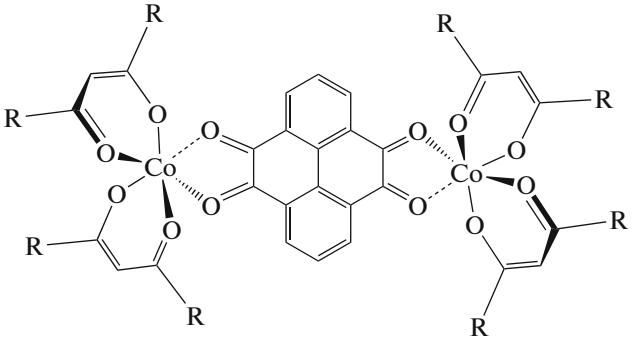
Coordination metal compounds containing weakly coupled paramagnetic centers are considered as promising systems for logical elements of quantum computers [1–3]. Electron spins of these complexes can act as qubits [4] under the condition of their correspondence to the DiVincenzo criteria [5]. The imposed requirements can be fulfilled by using molecular magnets based on transition metal clusters, whose fragments are coupled by appropriate organic or organometallic linkers [2, 4, 6–8].

We have previously studied the tetranuclear copper and nickel complexes based on the 1,3,5-triketone ligands containing two exchange fragments bridged by the methylene linker groups in order to search for coordination compounds with properties appropriate for spin qubits [9]. The weak antiferromagnetic exchange in the Ni(II) complexes predicted by the calculations makes it possible to consider these compounds as candidates for spin qubits. This approach is based on a change in the magnetic characteristics of the paramagnetic centers due to exchange interactions.

Another method for the design of logical elements of quantum computers is the use of magnetic bistability of transition metal complexes. Redox isomerism or valence tautomerism caused by the reversible electron transfer between the metal and ligand system is a well studied effect accompanied by switching of magnetic properties of coordination compounds [10–12]. A group of stable 2 : 1 adducts of Co(II) bis(chelates) with tetradentate di-*o*-quinones (**I**) capable of exhibiting two-step valence tautomerism was revealed by the quantum-chemical calculations (DFT B3LYP*/6-311++G(d,p)) [13]. Exchange interactions between the paramagnetic centers of these complexes can be controlled by linker groups X connecting the quinone fragments and by the functionalization of the auxiliary ligands.



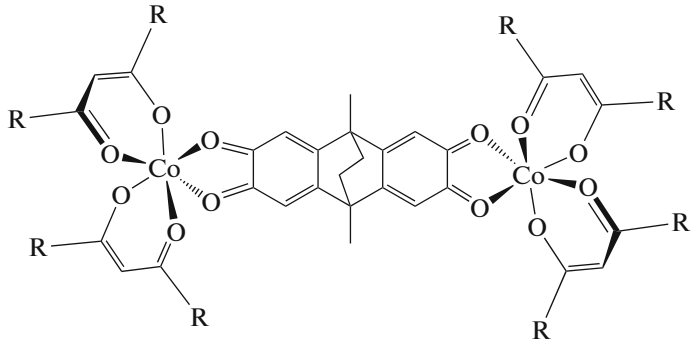
I: R = H, CF_3; X = none, –CH=CH–, $–CH_2–CH_2–$



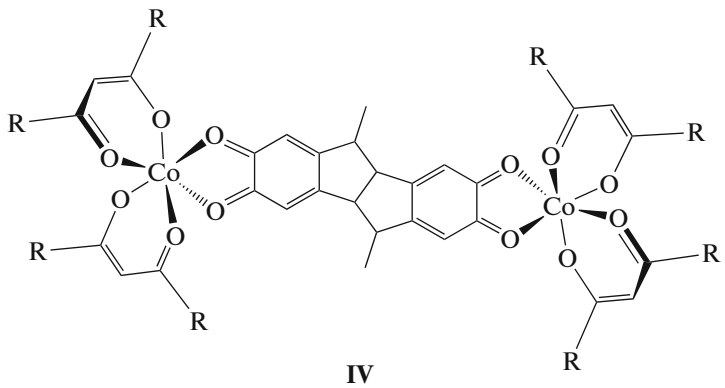
II: R = H, CH_3, CF_3

To develop this trend, we studied the binuclear complexes with di-*o*-quinones based on the polyaromatic systems (**II**) [14]. The weak ferromagnetic exchange interactions predicted for the ground states of these adducts indicate their paramagnetism in a wide temperature range. The obtained results show that the use of valence-tautomeric complexes as molecular magnetics and two-qubit molecular systems is promising.

In order to reveal new coordination compounds with the properties of spin qubits, we performed the theoretical simulation (DFT B3LYP*/6-311++G(d,p)) of the adducts of divalent cobalt diketonates with structurally isomeric di-*o*-quinone ligands (**III**, **IV**) differed by the type of the cycloalkane spacer to which the *o*-quinone rings are annelated and, as expected, by the character of exchange interactions.



III



IV

CALCULATION PROCEDURE

All calculations were performed using the Gaussian 09 program [15] in terms of the density functional theory (DFT) in the B3LYP*/6-311++G(d,p) approximation [16] that correctly reproduced the stabilization energies of the adducts formed by the cobalt bis(chelate) complexes with the redox-active ligands [17, 18] and the mechanisms of intramolecular rearrangements of the open-shell transition metal complexes [19, 20]. The stationary points on the potential energy surface were localized by the full geometry optimization of the molecular structures with the checking of the stability of the DFT wave function. The exchange interactions between unpaired electrons of the paramagnetic centers were estimated using the "broken symmetry" (BS) technique [21]. The exchange interaction constant (J) was calculated using the Yamaguchi equation [22].

RESULTS AND DISCUSSION

The structure $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ (SQ is the semiquinone form), representing a minimum on the triplet potential energy surface, corresponds to the most stable form of the adduct of cobalt(II) bis(malonate) with 9,10-dimethyl-9,10-ethanoanthracene-2,3,6,7(9H,10H)-tetraone **III** (R = H). The geometric characteristics of the isomer $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ presented in Fig. 1 and the absence of the spin density on the cobalt atoms of this isomer (Table 1) indicate the transfer of electrons from the metals to the ligand due to complex formation. This process is accompanied by the formation of an electromer containing the $_{LS}$Co(III) atoms and two semiquinone fragments. The calculated parameter J (–466 cm^{-1}) indicates a strong antiferromagnetic exchange between the unpaired electrons localized on the tetradentate ligand, which allows one to predict diamagnetism of the complex in the ground state.

The calculation on the quintet potential energy surface resulted in the structure $_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ (Q is the quinone form) with different geometric parameters of the quinone fragments (Fig. 1). The spin density is presented at one of the metal atoms (Table 1) and on the quinone fragment, which is not adjacent to this atom. The exchange interactions between the paramagnetic centers in the structure $_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ are ferromagnetic (J = 84 cm^{-1}). The difference in energies between the low-spin structure $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ and the isomer with the intermediate spin $_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ is 9.1 kcal/mol taking into account the zero-point vibration energy (ZPE), which lies in the range of values of valence-tautomeric rearrangements [23–25]. This result allows one to expect the corresponding redox processes in adduct **III** (R = H).

The least favorable form of adduct **III** (R = H) is the structure $_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$, being a molecular complex of di-*o*-benzoquinone and two cobalt bis(malonates). In this isomer, the unpaired electrons are localized on the $_{HS}$Co(II) atoms between which, according to the calculation results, exchange interactions are absent. The energetic preference of the structure $_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$ over the isolated ligand and diketonate molecules taking into account ZPE is 14.2 kcal/mol, indicating the stability of the adduct. At the same time, the destabilization of the structure $_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$ over the structure $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ by 21.6 kcal/mol does not allow one to expect the transfer of the second electron under thermal conditions. Thus, the interaction of di-*o*-benzoquinone with $_{HS}Co^{II}$ bis(malonate) results in the formation of a stable adduct capable of changing the spin state due to the intramolecular redox process.

The earlier theoretical study of the cobalt diketonate complexes with benzoquinones and their imino derivatives showed [26] that the inclusion of trifluoromethyl groups into the bis(chelate) favored a decrease in the energy gap between the electromeric forms. The compounds containing cobalt bis(hexafluoroacetylacetonates) were considered for the search for adducts in

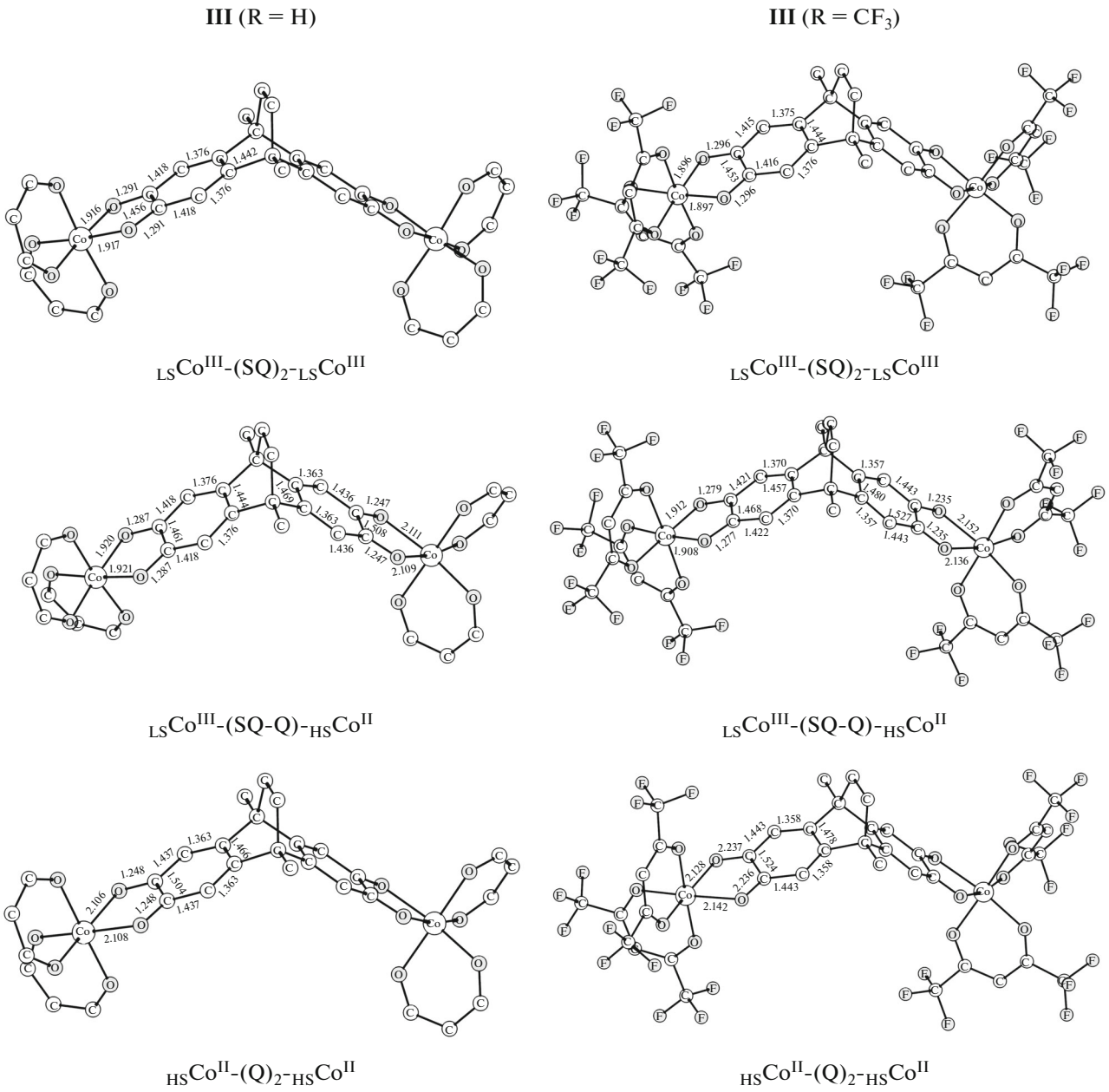


Fig. 1. Geometric characteristics of the isomeric forms of adducts **III** (R = H, CF_3) calculated by the DFT B3LYP*/6-311++G(d,p) method. Hereinafter the bond lengths are given in Å, and hydrogen atoms are omitted for clarity.

which both valence-tautomeric transitions would thermally be achievable.

The structure $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ on the triplet potential energy surface (Fig. 1) containing unpaired electrons on the semiquinone fragments between which strong antiferromagnetic interactions with the constant $J = -439$ cm^{-1} were predicted (Table 1) corresponds to the ground state of the fluorinated cobalt diketonate complex with the 9,10-dimethyl-9,10-ethanoanthracene-2,3,6,7(9H,10H)-tetraone spacer **III** (R = CF_3). The structure $_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ on the quintet potential energy surface includes two nonequivalent paramagnetic centers, one of which contains three unpaired electrons localized on the high-spin ion of divalent cobalt, and another contains one unpaired electron on semiquinone. The geometry optimization on the septet potential energy surface resulted in the structure $_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$ containing two $_{HS}Co^{II}$ ions between unpaired electrons of which no exchange interactions are predicted. As follows from Table 1, the inclusion of trifluoromethyl groups into the diketone favors a sharp decrease in the difference in energies between the isomers

Table 1. Spin (S), stabilization energies without (E_{stab}) and with taking into account ($E_{stabZPE}$) the zero-point vibration energy, relative energies without (ΔE) and with taking into account (ΔE_{ZPE}) the zero-point harmonic vibration energy, exchange interaction parameter (J), and spin densities on the metal atoms (q_s^{M1} and q_s^{M2}) in the isomeric forms of adducts **III** (R = H, CF_3) calculated by the DFT B3LYP*/6-311++G(d,p) method

Structure	S	E_{stab}*	$E_{stabZPE}$	ΔE	ΔE_{ZPE}	J, cm^{-1}	q_s^{M1}	q_s^{M2}
		kcal/mol						
R = H								
$_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ BS	2/2	42.2 43.7	35.9	0.0 −1.5	0.0	−466	0.01	0.01
$_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ BS	4/2	30.3 29.6	26.7	11.9 12.6	9.1	84	0.01	2.83
$_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$	6/2	15.0	14.2	27.2	21.6		2.85	2.85
R = CF_3								
$_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ BS	2/2	43.5 44.9	37.7	0.0 −1.4	0.0	−437	0.03	0.03
$_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ BS	4/2	39.9 39.6	36.4	3.6 3.9	1.4	33	0.03	2.76
$_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$	6/2	32.0	30.7	11.5	7.0		2.77	2.77

* The stabilization energies were calculated relative to isolated molecules of cobalt bis(chelates) and the redox-active ligand.

$_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ and $_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$. The energy gap between the ground state $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ and asymmetric structure $_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ does not exceed 2 kcal/mol. The calculated energy differences between the structures $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ and $_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$, being 7 kcal/mol, allow one to expect the reversible stepwise transfer of two electrons, under thermal conditions, for complex **III** (R = CF_3).

The strong antiferromagnetic exchange predicted for the ground states of the adducts considered above, the structures $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ (**III**), where R = H and CF_3, and the significant ferromagnetic exchange in the structures $_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ (**III**), where R = H and CF_3, would favor a decrease in the residence time of the complex in the excited state. One of the approaches to controlling the strength of interactions between the paramagnetic centers is based on a change in the conditions of magnetic orbital overlapping. Therefore, we considered the adducts with 5,10-dimethyl-4b,5,9b,10-tetrahydroindeno[2,1-a]indene-2,3,7,8-tetraone in which the quinone fragments are parallel to each other.

According to the calculation results, complexes **IV** (R = H) is characterized by weak exchange interactions between the paramagnetic centers. For example, a weak antiferromagnetic exchange between unpaired electrons of the semiquinone fragments ($J = -14$ cm^{-1}) was predicted for the structure $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ corresponding to the ground state of the complex (Table 2, Fig. 2), which makes it possible to expect paramagnetism of adduct **IV** (R = H) in a wide temperature range. Less significant exchange interactions ($J = 1$ cm^{-1}) were predicted for the structure $_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ on the quintet potential energy surface. The difference in energies between the structures $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ and $_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ is 10.2 kcal/mol, which allows one to expect the intramolecular redox process to occur. The destabilization of the high-spin electromer $_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$ (**IV**), where R = H, over the isomer $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ by 24.1 kcal/mol does not allow the thermal occupation of the state in which unpaired electrons are localized on the $_{HS}Co^{II}$ ions.

The study of the cobalt bis(hexafluoroacetylacetonate) complex with di-*o*-quinone, whose fragments are annelated to the C–C bond, showed weak antiferromagnetic exchange interactions between the semiquinone fragments ($J = -9$ cm^{-1}) expected in the low-spin structure $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$, whereas there is no magnetic ordering in the structures $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ and $_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$ (Table 2, Fig. 2). A small difference in energies between the ground form of the $_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$ complex and the structures $_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$ and $_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$ indicates the possibility of

Table 2. Spin (S), stabilization energies without (E_{stab}) and with taking into account ($E_{stabZPE}$) the zero-point harmonic vibration energy, relative energies without (ΔE) and with taking into account (ΔE_{ZPE}) the zero-point vibration energy, exchange interaction parameter (J), and spin densities on the metal atoms (q_s^{M1} and q_s^{M2}) in the isomeric forms of adducts **IV** (R = H, CF_3) calculated by the DFT B3LYP*/6-311++G(d,p) method

Structure	S	E_{stab}*	$E_{stabZPE}$	ΔE	ΔE_{ZPE}	J, cm^{-1}	q_s^{M1}	q_s^{M2}
		kcal/mol						
R = H								
$_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$	2/2	38.3	31.6	0.0	0.0	−14	0.01	0.01
BS		38.4		0.0				
$_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$	4/2	28.2	24.5	10.2	7.1	2	0.01	2.82
BS		28.1		10.2				
$_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$	6/2	14.2	13.5	24.1	18.2		2.84	2.84
R = CF_3								
$_{LS}Co^{III}$-$(SQ)_2$-$_{LS}Co^{III}$	2/2	39.7	33.6	0.0	0.0	−9	0.03	0.03
BS		39.8		0.0				
$_{LS}Co^{III}$-(SQ-Q)-$_{HS}Co^{II}$	4/2	38.4	34.8	1.4	−1.1	1	0.03	2.75
BS		38.4		1.4				
$_{HS}Co^{II}$-$(Q)_2$-$_{HS}Co^{II}$	6/2	32.5	31.2	7.3	2.4		2.76	2.76

* The stabilization energies were calculated relative to isolated molecules of cobalt bis(chelates) and the redox-active ligand.

manifesting two-step valence tautomerism in adduct **IV** (R = CF_3) [23–25]. The predicted energy and magnetic characteristics of the Co(II) bis(hexafluoroacetylacetonate) complex with the 5,10-dimethyl-4b,5,9b,10-tetrahydroindeno[2,1-a]indene-2,3,7,8-tetraone spacer make it possible to consider this compound as a promising candidate for the development of spin qubits.

The orbital analysis of the model compounds in which metal diketonates were replaced by sodium cations (**V**–**VII**) was performed to reveal factors determining the differences in the strength of the exchange interactions in the ground states of the adducts considered. According to the calculations performed, the magnetic orbitals of complexes **V**–**VII** are superposition of the α-SOMO and β-SOMO localized on different semiquinone fragments. These orbitals are significantly overlapped in complex **V** leading to a strong antiferromagnetic exchange (J = −430 cm^{-1}, Fig. 3). There is no this overlap in complex **VII**, which favors a very weak or even the complete absence of the interaction of unpaired electrons (J = −18 cm^{-1}). Therefore, the main factor responsible for the strength of exchange interactions is the degree of overlapping of the orbitals of the semiquinone fragments. The index of biradicaloid character was proposed for the description of the ability of complexes with two unpaired electrons to exist in the paramagnetic state [27]. According to the calculations, this index in complex **V** is 62%, indicating a high probability of diamagnetism of this compound. The index of biradical character for complex **VII** (100%) allows one to expect the stable triplet state.

An analog of compound **V**, complex **VI** containing no dimethylene bridge, was studied to check the correctness of the conclusions made. A decrease in the steric strain favors increasing the angle between the quinone fragments (from 122° to 149°) and the weakening of the overlap of the magnetic orbitals. The calculated magnetic exchange parameter for complex **VI** is −60 cm^{-1}, and its index of biradical character is 92%. These values are intermediate between those predicted for complexes **V** and **VII**, which is well consistent with the conclusion formulated above.

Thus, the performed quantum-chemical study made it possible to extend the range of coordination compounds constructed as 2 : 1 mixed-ligand adducts of cobalt diketonates with the redox-active di-*o*-quinone ligands [13, 14] capable of manifesting two-step valence tautomerism. The complex formation is shown to be accompanied by the intramolecular transfer from the metal to ligand and results in the formation of stable adducts (E_{stab} = 14–32 kcal/mol). The small differences in the energies of the electromeric forms and the weak exchange interactions between the paramagnetic centers in adduct **IV** based on Co(II)

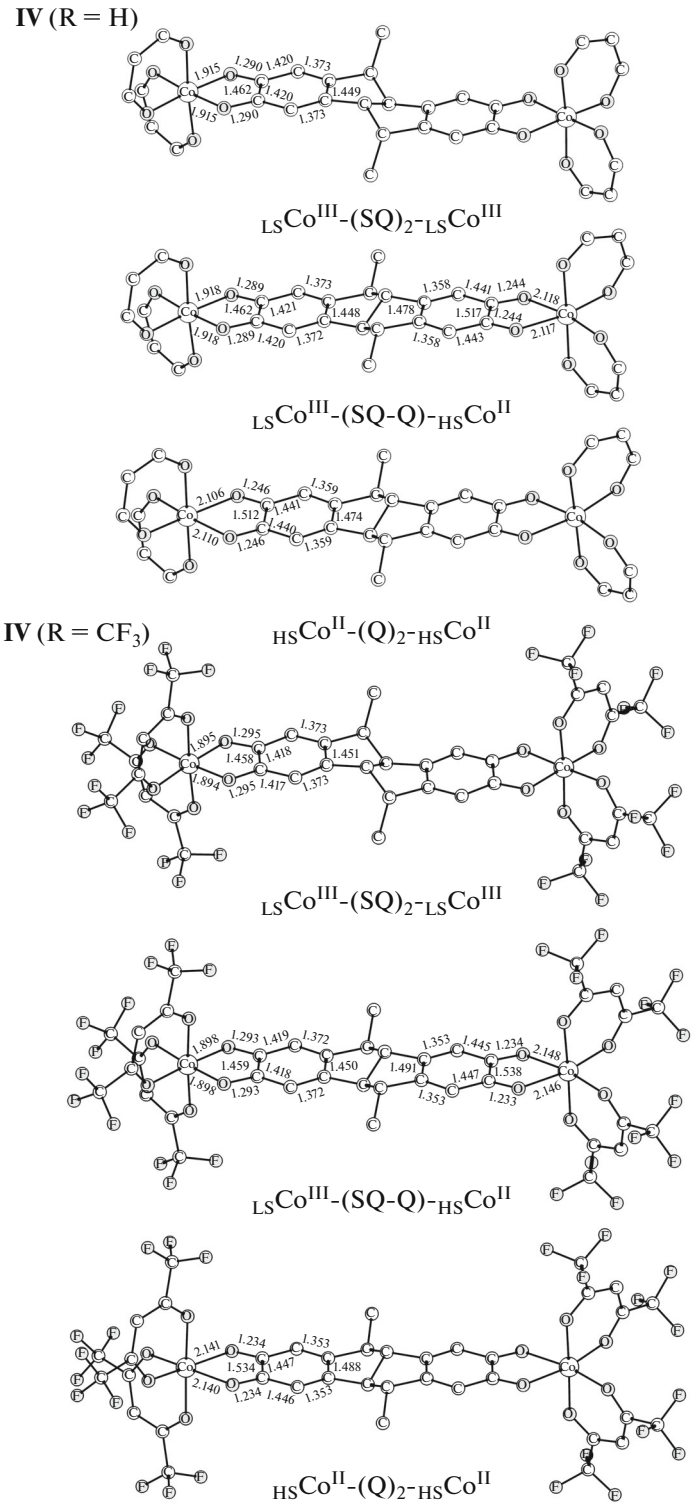


Fig. 2. Geometric characteristics of the isomeric forms of adducts **IV** (R = H, CF_3) calculated by the DFT B3LYP*/6-311++G(d,p) method.

bis(hexafluoroacetylacetonate) with the 5,10-dimethyl-4b,5,9b,10-tetrahydroindeno[2,1-a]indene-2,3,7,8-tetraone spacer make this compound to be an appropriate candidate for using as a spin qubit.

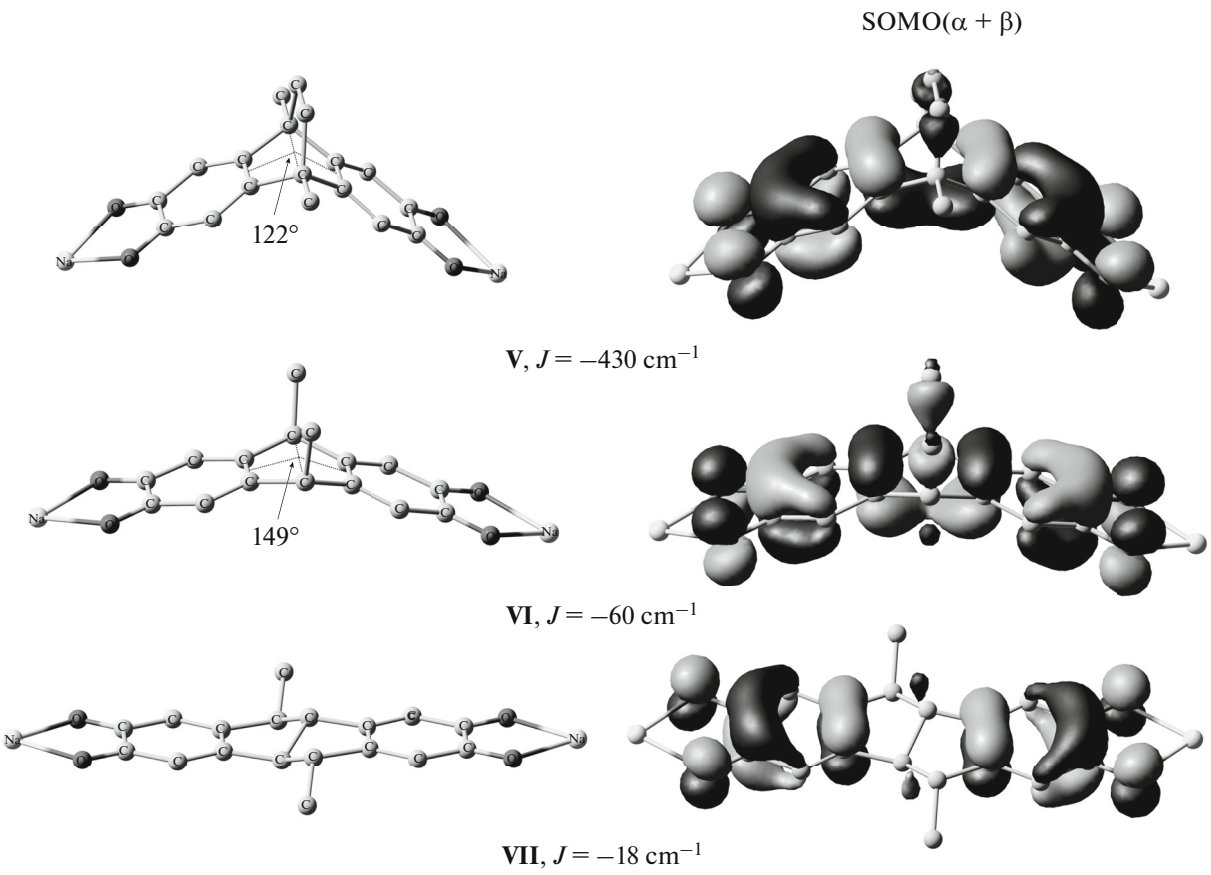


Fig. 3. Forms of magnetic orbitals and the magnetic exchange parameters of complexes **V–VII**.

ACKNOWLEDGMENTS

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