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Computational Modeling of Spin-Crossover in Mixed-Ligand Binuclear Iron and Cobalt Complexes with 5,6-Bis(salicylideneimino)-1,10-Phenanthroline

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Abstract—The quantum chemical modeling (DFT UTPSSh/6-311++G(d,p)) of the binuclear homo- and heterometallic Fe and Co complexes based on the 5,6-bis(salicylideneimino)-1,10-phenanthroline ligand and two bipyridyl molecules is performed. The magnetic properties of these compounds can be switched due to the thermally induced spin-crossover occurring at the cobalt ions. The predicted energetic and magnetic characteristics of isomers of the studied systems allow one to consider them as promising molecular switches.

Keywords: iron complexes, cobalt complexes, spin-crossover, magnetic properties, quantum chemical modeling

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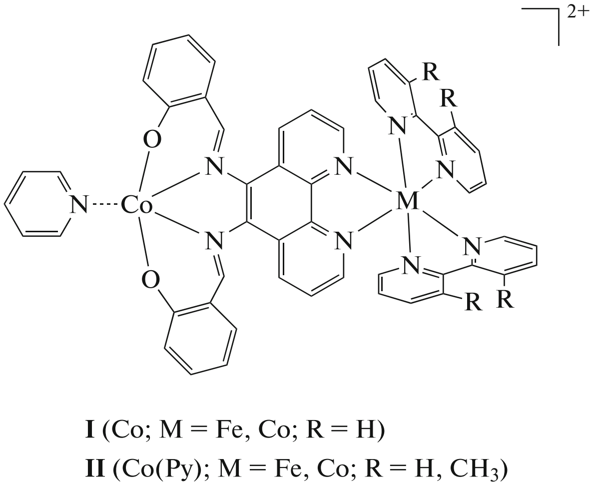
INTRODUCTION

Spin-crossover (SCO) is the studied in detail effect resulting in the manifestation of magnetically active properties by coordination compounds of transition metals [1]. At the molecular level, the SCO is a change in the spin state of the metallocenter induced by the temperature, pressure, irradiation, or magnetic field. The use of the SCO mechanism as a driving force leading to switching spin states of transition metal complexes is one of the actively developed trends in coordination chemistry [2–5]. The complexes demonstrating this behavior can find use in the development of molecular switches and memory with the magnetic function of the response, sensors and information display devices, and quantum bits [6–8].

The broadest class of compounds susceptible to SCO rearrangements is presented by the pseudo-octahedral complexes of divalent iron with the N-donor ligands [9–11]. The cobalt systems in which the field strength of the ligands suitable for the SCO to occur is achieved in the molecules with the pentacoordinated central atom are less studied, and their typical examples are the monoadducts of Co(II) bis(salicylideneiminates) with the nitrogen-containing bases [12–15] and the complexes with six donor nitrogen atoms [16–20].

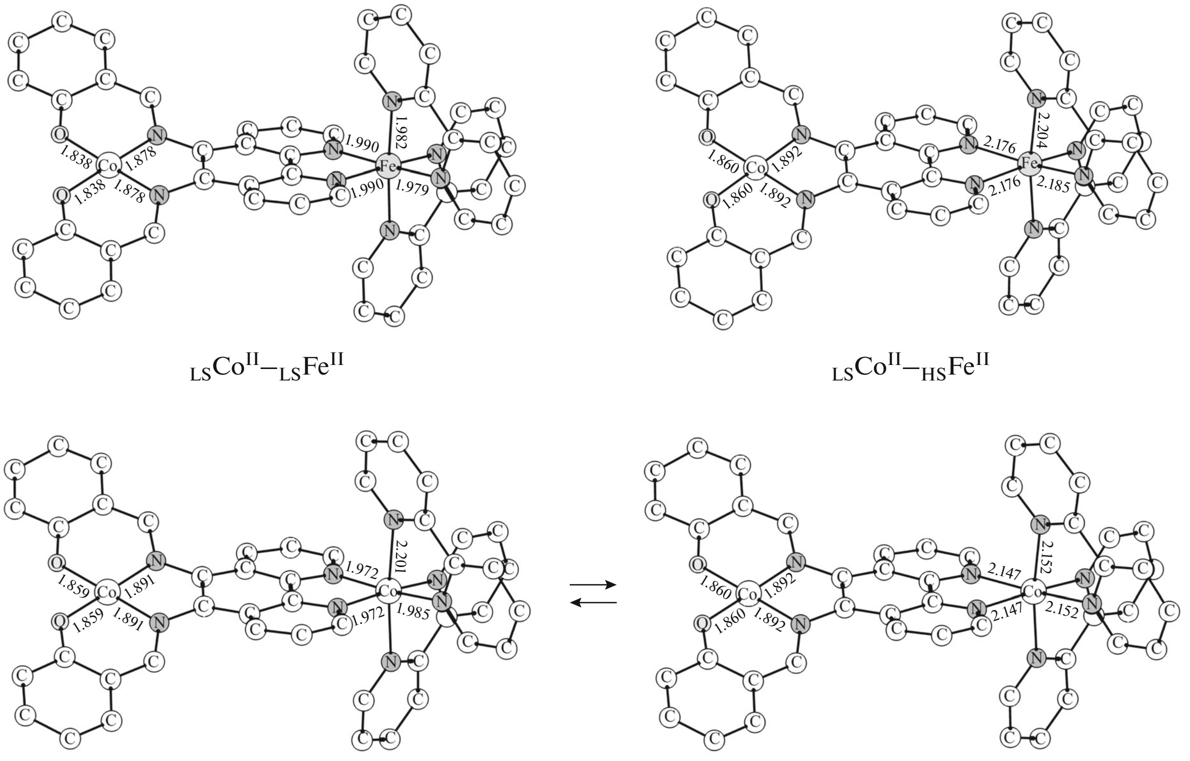
The earlier theoretical studies of the binuclear coordination compounds that undergo SCO transitions show that such systems are promising for the development of the elemental base of molecular electronics and spintronics devices [21, 22]. In this work, we used quantum chemical modeling to study mixed-ligand binuclear complexes **I** (Co; M = Fe, Co; R = H) and **II** (Co(Py); M = Fe, Co; R = H, CH_3) with 5,6-bis(salicylideneimino)-1,10-phenanthroline [23] in which the coordination sites of metals M are completed by bipyridyl molecules.



I (Co; M = Fe, Co; R = H)
II (Co(Py); M = Fe, Co; R = H, CH_3)

CALCULATION PROCEDURE

The density functional theory (DFT) calculations were performed using the Gaussian 09 program [24] with the UTPSSh functional [25, 26] in the 6-311++G(d,p) extended basis set correctly reproducing the energetic characteristics of the SCO in the cationic complexes [27–31]. According to the results



${}_{LS}Co^{II}–{}_{LS}Fe^{II}$ ${}_{LS}Co^{II}–{}_{HS}Fe^{II}$

${}_{LS}Co^{II}–{}_{LS}Co^{II}$ $\rightleftarrows$ ${}_{LS}Co^{II}–{}_{HS}Co^{II}$

Fig. 1. Optimized geometries of the isomers of complexes **I** (Co; M = Fe, Co; R = H) calculated by the DFT UTPSSh/6-311++G(d,p) method. Hereinafter hydrogen atoms are omitted for clarity, bond lengths are given in Å, arrows show a possible SCO transition, and all structures have the charge +2.

obtained in this approximation, spin transitions are expected to occur at the Fe^{2+} ion at $\Delta E_{HS-LS} < 11$ kcal/mol [27, 28] and at Co^{2+} at $\Delta E_{HS-LS} < 5$ kcal/mol [29, 30]. Stationary points were localized on the potential energy surface by the full geometry optimization of molecular structures checking the DFT stability of the wave function. The exchange interaction parameters (J, cm^{-1}) were determined in the framework of the broken symmetry (BS) formalism [32] using the Yamaguchi equation [33] by the calculation of all possible spin states. The graphical images of the molecular structures were obtained using the ChemCraft program [34].

RESULTS AND DISCUSSION

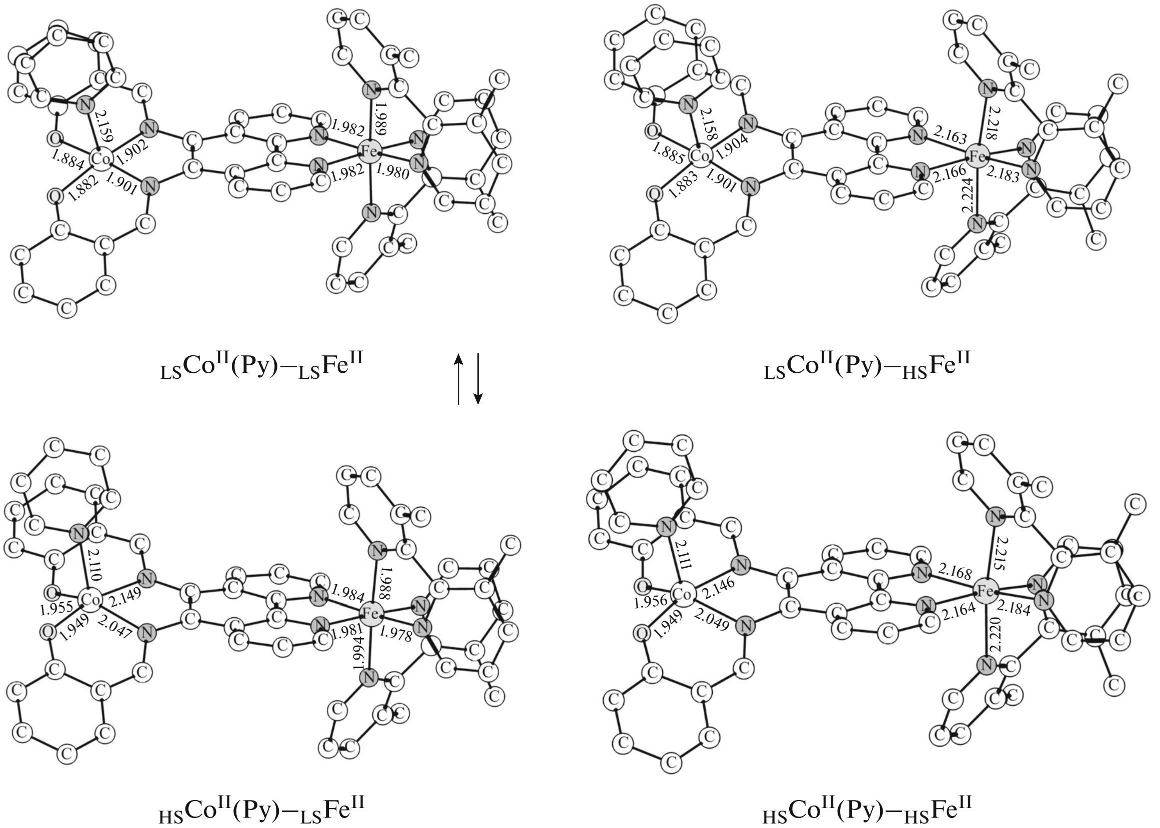
Model systems **I** (Co; M = Fe, Co; R = H) containing no coordinated pyridine molecule were studied to evaluate the character and strength of exchange interactions between the paramagnetic centers and a principal possibility of the SCO to occur at the iron and cobalt ions linked by the bipyridyl ligands (Fig. 1). As follows from the calculation results, the difference in energies between the isomers ${}_{LS}Co^{II}–{}_{LS}Fe^{II}$ and ${}_{LS}Co^{II}–{}_{HS}Fe^{II}$ distinct by the spin states of the iron ion exceeds 11 kcal/mol (Table 1), which does not allow one to expect the SCO rearrangement. In homometallic complex **I** (Co; M = Co; R = H), the electron-excited structure ${}_{LS}Co^{II}–{}_{HS}Co^{II}$ and the ground state ${}_{LS}Co^{II}–{}_{LS}Co^{II}$ are nearly isoenergetic (ΔE_{HS-LS} = 0.5 kcal/mol). Therefore, both isomers of the discussed compound can coexist at equilibrium. The predicted weak antiferromagnetic coupling in the high-spin (HS) electromer and the absence of exchange interactions between the metallocenters in the ${}_{LS}Co^{II}–{}_{LS}Co^{II}$ structure indicate that the complex is paramagnetic in a wide temperature range. Thus, compound **I** (Co; M = Co; R = H) can be interesting as a basis for a molecular switch with the magnetic function of the response.

A substantial destabilization of the ${}_{LS}Co^{II}–{}_{HS}Fe^{II}$ structure with the high-spin iron ion relative to the low-spin (LS) isomer ${}_{LS}Co^{II}–{}_{LS}Fe^{II}$ stimulated us to study the complexes bearing the bipyridyl derivatives with methyl substituents in positions 3 and 3' as auxiliary ligands. It was expected that steric hindrances created by the CH_3 groups upon complex formation would decrease the strength of the ligand field and the possibility of the SCO to occur at the Fe^{2+} ion.

Table 1. Spin (S), total energy (E_{tot}), relative energy (ΔE), spin-squared operator (S^2), spin density on the cobalt ion in the bis(salicylidene) fragment (q_s^{Co}) and metal ion M in the octahedral environment $\left(q_s^{\text{M}}\right)$, and exchange interaction parameter (J) in the isomers of complexes **I** (Co; M = Fe, Co; R = H) and **II** (Co(Py); M = Fe, Co; R = H, CH_3) calculated by the DFT UTPSSh/6-311++G(d,p) method

Structure	S	E_{tot}, au	ΔE*, kcal/mol	S^2	q_s^{Co}	q_s^{M}	J, cm^{-1}
I (Co; M = Fe; R = H)							
$_{\text{LS}}\text{Co}^{\text{II}}$–$_{\text{LS}}\text{Fe}^{\text{II}}$	1/2	−5007.64903	0.0	0.773	1.07	0.00	
$_{\text{LS}}\text{Co}^{\text{II}}$–$_{\text{HS}}\text{Fe}^{\text{II}}$	5/2	−5007.62467	17.8	8.800	1.07	3.75	−6
$_{\text{LS}}\text{Co}^{\text{II}}$–$_{\text{HS}}\text{Fe}^{\text{II}}$ BS	3/2	−5007.62478		4.789			
I (Co; M = Co; R = H)							
$_{\text{LS}}\text{Co}^{\text{II}}$–$_{\text{LS}}\text{Co}^{\text{II}}$	2/2	−5126.67374	0.0	2.020	1.00	0.89	0
$_{\text{LS}}\text{Co}^{\text{II}}$–$_{\text{LS}}\text{Co}^{\text{II}}$ BS	0	−5126.67374		1.021			
$_{\text{LS}}\text{Co}^{\text{II}}$–$_{\text{HS}}\text{Co}^{\text{II}}$	4/2	−5126.67293	0.5	6.021	1.00	2.25	1
$_{\text{LS}}\text{Co}^{\text{II}}$–$_{\text{HS}}\text{Co}^{\text{II}}$ BS	2/2	−5126.67293		3.021			
II (Co(Py); M = Fe; R = CH_3)							
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{LS}}\text{Fe}^{\text{II}}$	1/2	−5413.34042	0.0	0.764	0.84	0.00	
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Fe}^{\text{II}}$	5/2	−5413.32035	12.6	8.789	0.83	3.41	2
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Fe}^{\text{II}}$ BS	3/2	−5413.32032		4.787			
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{LS}}\text{Fe}^{\text{II}}$	3/2	−5413.33253	3.3	3.768	2.55	0.00	
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Fe}^{\text{II}}$	7/2	−5413.31252	17.5	15.793	2.55	3.43	0
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Fe}^{\text{II}}$ BS	1/2	−5413.31251		3.791			
II (Co(Py); M = Co; R = H)							
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{LS}}\text{Co}^{\text{II}}$	2/2	−5375.06589	0.0	2.025	0.85	0.89	1
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{LS}}\text{Co}^{\text{II}}$ BS	0	−5375.06589		1.024			
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Co}^{\text{II}}$	4/2	−5375.06469	0.8	6.025	0.83	2.41	2
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Co}^{\text{II}}$ BS	2/2	−5375.06466		3.028			
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{LS}}\text{Co}^{\text{II}}$	4/2	−5375.05819	4.8	6.029	2.55	0.90	3
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{LS}}\text{Co}^{\text{II}}$ BS	2/2	−5375.05815		3.028			
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Co}^{\text{II}}$	6/2	−5375.05687	5.7	12.029	2.55	2.45	3
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Co}^{\text{II}}$ BS	0	−5375.05676		3.028			
II (Co(Py); M = Co; R = CH_3)							
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{LS}}\text{Co}^{\text{II}}$	2/2	−5532.36833	0.0	2.024	0.86	0.88	15
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{LS}}\text{Co}^{\text{II}}$ BS	0	−5532.36827		1.024			
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Co}^{\text{II}}$	4/2	−5532.36564	1.7	6.025	0.85	2.33	2
$_{\text{LS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Co}^{\text{II}}$ BS	2/2	−5532.36562		3.023			
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{LS}}\text{Co}^{\text{II}}$	4/2	−5532.36058	4.9	6.029	2.55	0.89	8
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{LS}}\text{Co}^{\text{II}}$ BS	2/2	−5532.36048		3.028			
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Co}^{\text{II}}$	6/2	−5532.35590	7.8	12.026	2.55	2.39	15
$_{\text{HS}}\text{Co}^{\text{II}}$(Py)–$_{\text{HS}}\text{Co}^{\text{II}}$ BS	0	−5532.35530		3.028			

*ΔE were calculated relative to the most stable isomer of the complex.



$_{LS}Co^{II}(Py)-{}_{LS}Fe^{II}$ $_{LS}Co^{II}(Py)-{}_{HS}Fe^{II}$

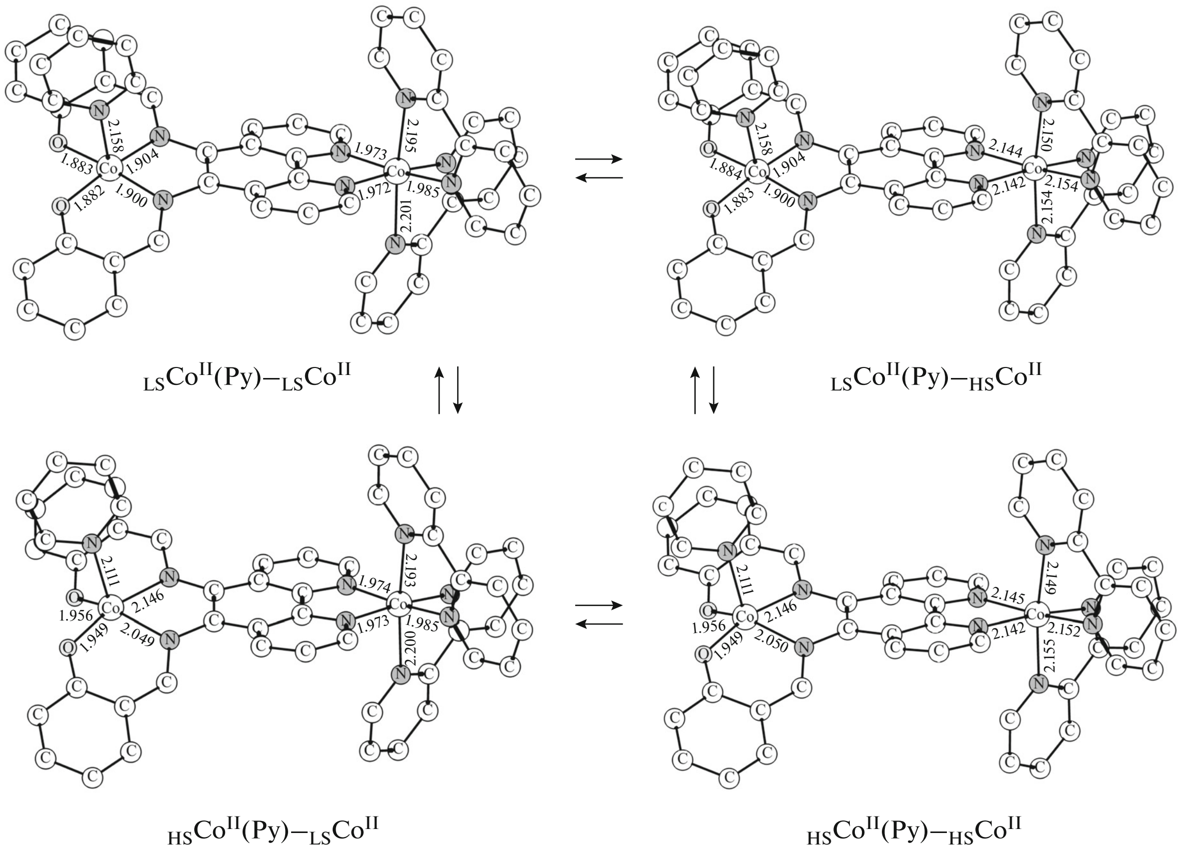
$_{HS}Co^{II}(Py)-{}_{LS}Fe^{II}$ $_{HS}Co^{II}(Py)-{}_{HS}Fe^{II}$

Fig. 2. Optimized geometries of the isomers of complexes **II** (Co(Py); M = Fe; R = CH_3) calculated by the DFT UTPSSh/6-311++G(d,p) method.

Another way to modify model compounds **I** is the coordination of the pyridine molecules capable of providing the SCO in the bis(salicylidene) fragment [12–15, 35].

An analysis of the calculated bond lengths in adduct **II** (Co(Py); M = Fe; R = CH_3) showed the elongation of the Fe–N distances in the $_{LS}Co^{II}(Py)-{}_{LS}Fe^{II}$ and $_{HS}Co^{II}(Py)-{}_{LS}Fe^{II}$ structures decreasing the relative stability of the isomers (Fig. 2, Table 1). These changes favor a decrease (compared to complex **I** (Co; M = Fe; R = H)) in the differences in energies between the electromers containing iron ions in different spin states, but the obtained values (12.6 and 17.5 kcal/mol) still do not reach the values characteristic of the thermally initiated spin transitions on Fe^{2+} ions. At the same time, the difference in energies between the structures $_{LS}Co^{II}(Py)-{}_{LS}Fe^{II}$ and $_{HS}Co^{II}(Py)-{}_{LS}Fe^{II}$ (3.3 kcal/mol) allows one to expect that the SCO would occur at the cobalt ion (Fig. 2). The high-spin form of the complex $_{HS}Co^{II}(Py)-{}_{HS}Fe^{II}$ lies by 4.9 kcal/mol higher in energy than the $_{LS}Co^{II}(Py)-{}_{HS}Fe^{II}$ isomer indicating the possibility of the second spin transition in the bis(salicylidene) fragment of adduct **II** (Co(Py); M = Fe; R = CH_3). However, the destabilization of the discussed electromers relative to the ground state prejudices their formation.

Complex **II** (Co(Py); M = Co; R = H) was studied to search for a compound capable of demonstrating the SCO at two metallocenters. According to the quantum chemical calculation results, the differences in energies of the isomers containing metal ions in different spin states range from 0.8 to 5.7 kcal/mol (Table 1). This allows one to expect that the SCO rearrangements would occur on all cobalt centers (Fig. 3). The calculations of the BS states and the subsequent analysis of the exchange interactions indicate the weak ferromagnetic exchange (J = 1–3 cm^{-1}) between unpaired electrons of the metals (Table 1). The expected synchronized spin transitions in the bis(salicylidene) fragment ($_{LS}Co^{II}(Py)-{}_{LS}Co^{II} \rightleftarrows {}_{HS}Co^{II}(Py)-{}_{LS}Co^{II}$ and $_{LS}Co^{II}(Py)-{}_{HS}Co^{II} \rightleftarrows {}_{HS}Co^{II}(Py)-{}_{HS}Co^{II}$) and in the opposite moiety of the molecule ($_{LS}Co^{II}(Py)-{}_{LS}Co^{II} \rightleftarrows {}_{LS}Co^{II}(Py)-{}_{HS}Co^{II}$ and $_{HS}Co^{II}(Py)-{}_{LS}Co^{II} \rightleftarrows {}_{HS}Co^{II}(Py)-{}_{HS}Co^{II}$) accompanied by a change in the spin of the system from $S = 2/2$ to $S = 6/2$, as well as paramagnetism of all electromeric forms in a wide temperature range, make it possible to consider adduct **II** (Co(Py); M = Co; R = H) as a promising molecular switch.



${}_{LS}Co^{II}(Py)—{}_{LS}Co^{II}$

${}_{LS}Co^{II}(Py)—{}_{HS}Co^{II}$

${}_{HS}Co^{II}(Py)—{}_{LS}Co^{II}$

${}_{HS}Co^{II}(Py)—{}_{HS}Co^{II}$

Fig. 3. Optimized geometries of the isomers of complexes **II** (Co(Py); M = Co; R = H) calculated by the DFT UTPSSh/6-311++G(d,p) method.

The theoretical consideration of binuclear cobalt complex **II** (Co(Py); M = Co; R = CH_3) bearing 3,3'-dimethyl-2,2'-bipyridyl molecules showed that both metallocenters can undergo spin transitions due to the SCO as in compound **II** (Co(Py); M = Co; R = H) (Fig. 4). According to the calculated geometric characteristics, alkyl substituents in the pyridine rings favor the elongation of bonds Co—donor atom of the auxiliary ligands, whereas the distances between the metallocenter and nitrogen atom of the phenanthroline shorten. The predicted increase in the differences in energies between the electromers and an insignificant enhancement of the ferromagnetic interactions (Table 1) compared to the above described adduct containing no methyl groups will not prevent the involvement of all forms of the complex in the synchronized spin transitions and their manifestation of the molecular switch properties.

To conclude, the data of the quantum chemical calculations (DFT UTPSSh/6-311++G(d,p)) of the binuclear homo- and heterometallic iron and cobalt complexes with 5,6-bis(salicylideneimino)-1,10-phenanthroline showed a possibility of controlling the energetic and magnetic characteristics of the electromers of the studied coordination compounds by the modification of the metal nature and coordination of the additional nitrogen-containing base. In compounds **I** (Co; M = Fe, Co; R = H), switching of the spin states is expected only at the cobalt ions in the octahedral environment formed by the nitrogen atoms of the phenanthroline fragments and bipyridyls. The coordination of pyridine to the cobalt ion in the bis(salicylidene) moiety of the complex favors the SCO. Regardless of the presence of methyl groups in the bidentate ligands (adduct **II** (Co(Py); M = Fe; R = CH_3), the difference in energies of the isomers with the high- and low-spin Fe^{2+} ions exceeds the values that allow one to expect spin transitions to occur at this metal ion. Paramagnetism of all isomers of homometallic cobalt complexes **II** (Co(Py); M = Co; R = H) and **II** (Co(Py); M = Co; R = CH_3), possible synchronized spin transitions, and spin states of the system varied in a wide range allow one to consider these compounds as efficient molecular switches with the magnetic function of the response.

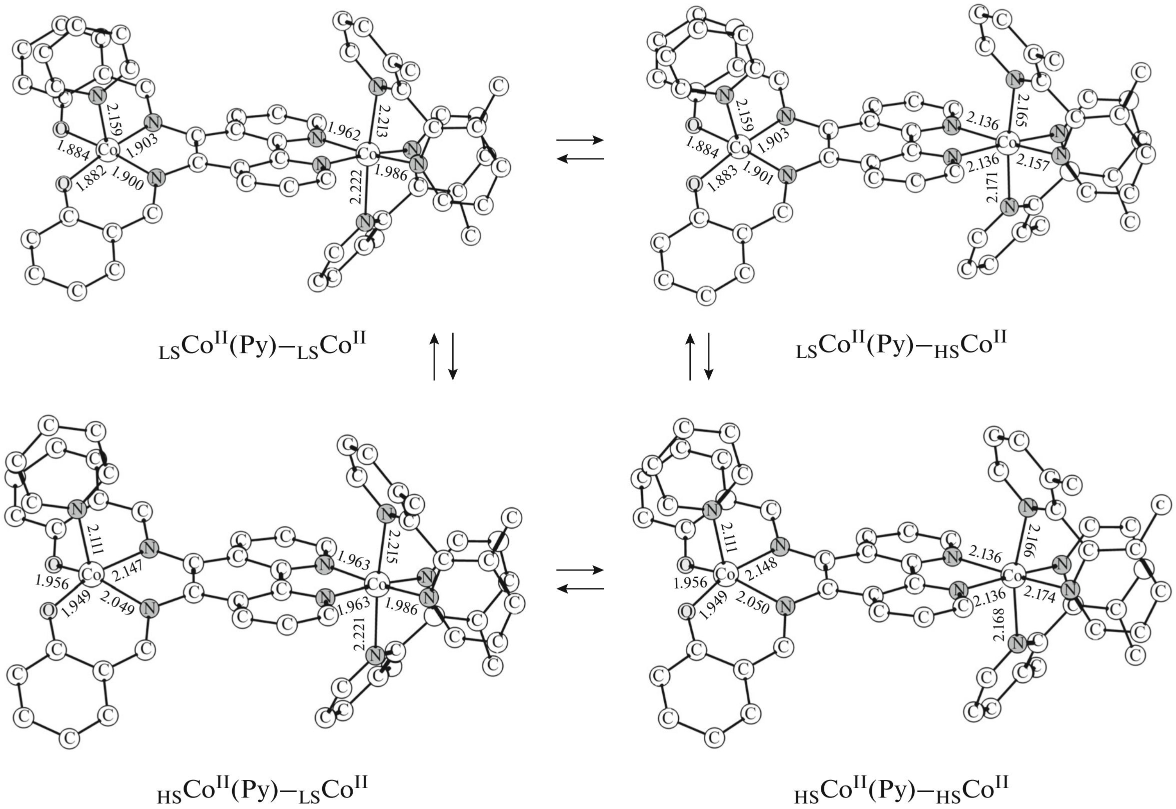


Fig. 4. Optimized geometries of the isomers of complexes **II** (Co(Py); M = Co; R = CH_3) calculated by the DFT UTPSSh/6-311++G(d,p) method.

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