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Combining Open-Shell Verdazyl Environment and Co(II) Spin-Crossover: Spinmerism in Cobalt Oxoverdazyl Compound

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Abstract: The spin states of a Co(II) oxoverdazyl compound are investigated by means of wavefunction-based calculations. Within a ca. 189 K energy window, the ground state and excited states display a structure-sensitive admixture of low-spin $S_M = 1/2$ in a dominant high-spin $S_M = 3/2$ Co(II) ion as read from localized molecular orbitals. This puzzling spins zoology that results from the coupling between open-shell radical ligands and a spin-crossover metal ion gives rise to this unusual scenario which extends the views in molecular magnetism. In agreement with experimental observation, the low-energy spectroscopy is very sensitive to deformations of the coordination sphere, and a growing admixture of Co(II) low-spin is evidenced from the calculations. In analogy with mesomerism that accounts for charge delocalization, entanglement combines different local spin states to generate a given total spin multiplicity, a *spinmerism* phenomenon.

Introduction

The synthesis and characterization of molecule-based magnetic systems remains an active field of research due to potential applications as molecular switches^[1], thermal sensors^[2] and photomechanical properties^[3]. Spin crossover phenomenon and valence tautomerism are manifestations of the electronic lability in such coordination chemistry compounds. Even though mostly based on metal ions, organic radicals have significantly extended the panel of building blocks of molecular magnetism to design purely organic materials or metal-radical architectures. Redox-active ligands are known to stabilize high oxidation states of metal ions^[4,5]. Besides, the resulting transition-metal complexes can be very sensitive to oxidation, and interestingly the oxidative process may involve all partners. As suggested in a *metal field*^[6], the metal and the ligands should thus be treated on the same footing. As evidenced by means of wavefunction calculations, the spin nature of diradical non-innocent ligands can be controlled by the electrostatic field generated by the metal ion. Such observation had led to the *excited state coordination chemistry* concept developed for various coordination compounds^[7]. Importantly, the redox activity of radical-ligands such as verdazyls^[8] is preserved when coordinated to metal centers, introducing exchange interactions between the cation and its coordination sphere. A well-accepted and robust picture to describe magnetic properties is the Heisenberg-Dirac-Van Vleck (HDVV) spin Hamiltonian. Depending on the metal ion, different regimes were reported in

verdazyl coordination complexes, ranging from strong ferromagnetic^[9] to weak antiferromagnetic^[10] interactions between local spin states. However, deviations from the HDVV picture can be observed. The importance of excited non-Hund forms were identified as contributions to the non-Heisenberg behaviour^[11].

In self-assemblies and materials, a spin transition picture may be favoured over exchange-interaction models, reflecting the flexibility of the contacts in purely organic verdazyl radicals-based materials^[12,13]. In this context, cobalt compounds are known to be interesting targets since valence tautomerization as well as temperature-dependent spin crossover can be triggered by varying the coordination sphere of the Co ion. In coordination chemistry materials, the Co ion has attracted much attention with the growing interest for photomagnetic properties in FeCo Prussian analogue^[14]. The cyanide bimetallic network is very sensitive to the alkali environment and a low-spin Co(III) to high-spin Co(II) is observed^[15].

As a prime example, valence tautomerization has been recently reported^[16] in the $[\text{Co}(\text{dipyvd})_2]^{2+}$ (dipyvd = 1-isopropyl-3,5-dipyridil-6-oxoverdazyl) coordination compound **1** (see Figure 1). A combination of magnetic susceptibility, temperature-dependent UV and EPR experiments concluded on a valence tautomeric equilibrium between a high-spin $S_M = 3/2$ Co(II) and a low-spin $S_M = 0$ Co(III). Nevertheless, the occurrence of a high-spin Co(II) in tetragonal environment, not to mention the strong ferromagnetic coupling traditionally observed in cobalt-verdazyl compounds^[17], question the intimate nature of the interactions that characterize this complex. The possibility to manipulate spin state and to trigger valence tautomerism in solution makes this cobalt-verdazyl coordination compound particularly fascinating. The authors concluded that there is still to be learned and that a coherent explanation remains *elusive*. Part of the answer may be found in moving away from *overly simplistic* models as mentioned by Hicks and coworkers^[18]. How much robust is the traditional view of a metal ion, either high-spin or low-spin, in a crystal field? Singlet and triplet spin values can emerge from the environment generated by two open-shell dipyvd radical ligands. Besides, Co(II) being a spin-crossover (SCO) ion, a high-spin $S_M = 3/2$ and a low-spin $S_M = 1/2$ Co(II) ion (non-Hund form following Bastardis *et al.*^[19]) are likely to compete depending on the crystal field strength. As a consequence, the observed spin states of the complex may result from several intricated local spin states on the ligands and the metal ion.

Herein, wavefunction-based calculations (Difference Dedicated Configuration Interaction (DDCI)) were conducted to examine the electronic structures of low-lying states of **1**. Not only can

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wavefunction-based calculations reach spectroscopic accuracy (a few tens of wave-numbers), but the nature of the spin states can be analyzed based on localized orbitals, *i.e.* site orbitals. The energy splittings cannot be reproduced by a mere Heisenberg-Dirac-Van Vleck (HDVV) Hamiltonian picture whilst the structures of the correlated wavefunctions deviate from the picture given by the spin-coupling between a local Co(II) high-spin and dipyv radicals.

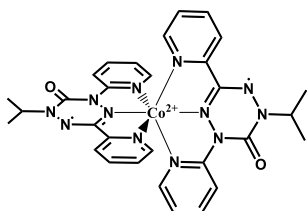


Figure 1. Compound 1.

The presence of open-shells on both the metal ion suggests the use of a wavefunction-based method. Using such methodology, the microscopic origin of exchange couplings can be investigated and spin Hamiltonians rationalized or invalidated. In the complete active space self-consistent field method (CASSCF), the complete active space includes the three unpaired electrons on the Co and two on the oxoverdazyl ligands in 1. The CAS[5,5]SCF hexuplet MOs are then transformed into localized MOs and shown in Figure 3. The localization procedure^[20] affords a reading of the multireference wavefunction following a Lewis valence-like picture. All CASSCF calculations were performed on the available Xray structure without any geometry optimization, and used the MOLCAS 8.0 package. The Co and first coordination sphere atoms were described with 4s3p2d and 3s2p1d basis sets, respectively. Smaller basis sets were used for all other atoms, 3s2p whilst hydrogen atoms were depicted with a 1s basis set. The dynamical and polarization effects were included following the Difference Dedicated Configuration Interaction (DDCI) method as implemented in the CASDI code^[21]. Depending on the classes of configurations involved in the CI expansion, different levels (CAS+S, CAS+DDC2 and CAS+DDCI) can be reached beyond the CAS picture. This variational method that follows a step-by-step construction of the wavefunction has produced a wealth of interpretations^[22–24] and rationalizations^[25,26] by concentrating the numerical effort on the hierarchising contributions in molecular magnetism compounds. The CI calculations eigenfunctions were projected onto the local spin states of the oxoverdazyl ligands ($S_{L1} = S_{L2} = 1/2$) and the cobalt ion ($S_M = 1/2$ or $3/2$). This allows for a decomposition into the different intricate metal-ligand contributions. A fictitious $[\text{Zn}(\text{dipyvd})_2]^{2+}$ coordination compound 2 was constructed with a closed-shell diamagnetic divalent cation to mimic the electrostatic presence of the Co(II). For this analogue 2, a similar procedure was used starting from a CAS[2,2]SCF calculation to generate a set of MOs, followed by the DDCI evaluation of the singlet-triplet energy difference.

Results and Discussion

From a traditional crystal field picture, one would naturally start by considering the two radical ligands as the so-called environment of the metal center. Following this view, the Co(II) ion undergoes a field that is characterized by singlet or triplet spin multiplicities. Thus, our first intention was to evaluate the energy difference between those spin states. From a CAS[2,2]SCF calculation performed on 2, the magnetic orbitals of the triplet state are essentially the singly occupied MOs localized on each dipyv radical (see Figure 2). As expected, the singlet and triplet states are quasi-degenerated with a triplet-singlet DDCI energy difference $E_S - E_T = 3$ K. This result suggests that the spin states

in 1 may involve a local $S_L = 1$ as well as a $S_L = 0$ environment. From this point of view, one can anticipate modulations of the crystal field acting on the SCO Co(II) metal center.

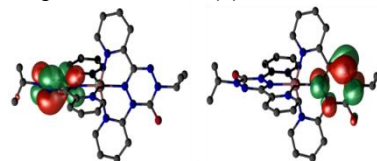


Figure 2. CAS[2,2] triplet molecular orbitals of the fictitious compound 2, Zn analog of 1.

In order to explore deeper the magnetic behaviour and to provide a spin description of 1, calculations were then conducted starting from a picture that involves five unpaired electrons in five MOs (CAS[5,5]SCF). The resulting MOs were then localized either on the metal center (see Figure 3) or on the dipyv ligands. This procedure allows for a valence-bond like reading of the wavefunctions constructed on orthogonal site-orbitals.

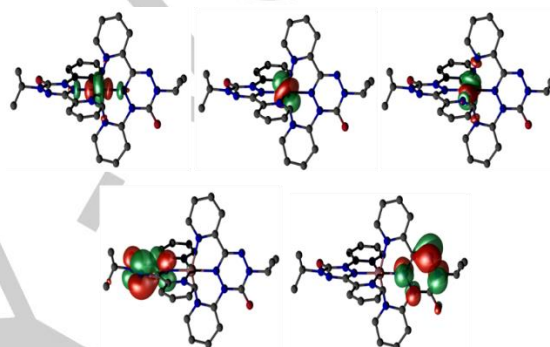


Figure 3. CAS[5,5] hexuplet localized molecular orbitals of 1.

Assuming a $S_M = 3/2$ high-spin value on the cobalt ion, four low-lying spin states S_T can be anticipated, namely a doublet, two quartets and a hexuplet. A very different scenario holds for a Co(II) low-spin $S_M = 1/2$, resulting in two doublet and a quartet states. Clarifications are readily accessible from *ab initio* DDCI calculations which give access to the low-energy spectrum. Due to the system size and the number of open-shells, a CAS+DDCI level of calculation cannot be reached and our conclusions are based on CAS+DDC2 spectrum. Even though part of the screening effects is not included, the structures of the wavefunctions are well-defined at this level of approximation. First, the ground state is a doublet (see Figure 4) which can be analyzed using the expansion over determinants built on localized MOs. It is dominated by a $S_M = 3/2$ cobalt ion and a $S_L = 1$ environment. A similar analysis holds for the first quartet state, and naturally for the hexuplet state.

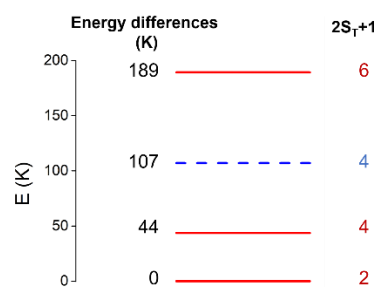


Figure 4. Low-energy spectrum of 1 calculated at the DDC2 level. The ground state energy is used as reference energy. Spin multiplicities $2S_T+1$ are given.

Therefore, it is rather tempting to fit the low-energy spectrum using a single-parameter Heisenberg Hamiltonian $\hat{H} = -2J\hat{S}_M\hat{S}_L$, where J is the exchange coupling between $S_M = 3/2$ and $S_L = 1$ local spins. Within this description, the ratio between the quartet-doublet and hexuplet-doublet energy differences is readily

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evaluated 0.375. However, the DDC2 ratio (ca. 0.23) strongly deviates from this value, not to mention the presence of a competing quartet state dominated by a $S_L = 0$ environment which cannot be described (see blue state in Figure 4). Thus, the spin Hamiltonian was extended by the introduction of two exchange coupling constants j_1 and j_2 between the metal center and the two individual ligands $\hat{H} = -2j_1\hat{S}_M\hat{S}_{L1} - 2j_2\hat{S}_M\hat{S}_{L2}$ (two-parameter Hamiltonian). Lifting the $S_L = 1$ constraint allows for the description of four spin states resulting from $S_M = 3/2$, and $S_{L1} = S_{L2} = 1/2$ local spin states. Four DDC2 energy values give access to three energy differences which can be compared to the analytical expressions of such Heisenberg Hamiltonian. A measure of the robustness of this picture is the identification of a set (j_1, j_2) that reproduces the *ab initio* excitation energies. Besides, the geometry of **1** suggests that j_1 and j_2 should be very similar and any strong deviation might not be acceptable from a physical point of view. From the fitting procedure using the $S_T = 1/2$, first excited 3/2 and 5/2 states, we find $j_1 = -12$ K and $j_2 = -35$ K. Our calculations support that both ligands are antiferromagnetically coupled to the Co ion. This conclusion is to be contrasted with some model that suggested with great care the simultaneous presence of ferromagnetic and antiferromagnetic interactions in some Co analogue^[18]. Nevertheless, not only do the antiferromagnetic couplings j_1 and j_2 values strongly differ, but the second excited quadruplet is then positioned 141 K above the ground state, in disagreement with the calculated value (see Figure 4). Finally, the interaction between the ligand spins was introduced in a three-parameter spin Hamiltonian $\hat{H} = -2j_1\hat{S}_M\hat{S}_{L1} - 2j_2\hat{S}_M\hat{S}_{L2} - 2j_{12}\hat{S}_{L1}\hat{S}_{L2}$ constructed on three coupling constants. Evidently, the three DDC2 energy differences can be reproduced and $j_1 = -16$ K, $j_2 = -32$ K and $j_{12} = -19$ K are found. This picture is consistent with spin frustration consideration. However, the exchange couplings ratio j_1/j_2 still deviates from unity without any particular justification. Besides, the antiferromagnetic coupling between the dipyvd radicals j_{12} is significantly larger than the singlet-triplet energy difference previously calculated in **2**. Whatever the extension of the Heisenberg Hamiltonian, the fitting to the *ab initio* spectrum leads to some inconsistencies that deserve further investigations.

At this stage, one may wonder whether a given total spin state S_T may be produced through different spin coupling schemes, involving the contacts between a versatile environment generated by two radical ligands ($S_L = 0$ or 1) and a spin crossover ion ($S_M = 1/2$ or 3/2). As a matter of fact, ingredients for entanglement manifestation are gathered in this particular compound. While the flexibility of the environment is rather natural and immediately invalidates the single-parameter Hamiltonian $\hat{H} = -2J\hat{S}_M\hat{S}_L$ ($S_M = 3/2$ and $S_L = 1$), the local spin S_M on the metal center might not be uniquely defined.

To push further the analysis of the interactions in **1**, the *ab initio* wavefunctions were projected onto the local metal and ligands spin states S_M and S_L . For the $S_T = 3/2$ (first excited state, or ground state under distortion), the configurations amplitudes are given in Table 1 and compared to the ones resulting from a $S_M = 3/2$ and $S_L = 1$ coupling scheme (so-called Clebsch-Gordan coefficients). Let us mention that the first two configurations necessarily involve a $S_M = 3/2$ spin state on the metal whereas the ligands spin state can be either $S_L = 0$ or 1. The last three configurations are characteristic of $S_L = 1$ and a metal spin state $S_M = 3/2$ or 1/2. Though small, the observed deviations are indicative of a contribution of $S_M = 1/2$ and $S_L = 0$. Quantitatively, a proportion of 0.06% for $S_M = 1/2$ and 0.001% for $S_L = 0$ were estimated. Remembering the valence tautomeric behaviour of **1** in solution, these contributions might be influenced by structural changes. In particular, it is known that spin crossover phenomenon is accompanied by modulations of the coordination sphere (ca. 0.2Å variations)^[27]. Besides, a significant charge redistribution is calculated in this kind of compounds^[28]. For all those reasons, the structures of the wavefunctions were examined as the geometry of the complex is varied. First, a

breathing deformation that symmetrically modifies the Co-N' axial bonds (slippage in Figure 5) was applied to modulate the crystal field generated by the ligands. Upon contraction $\delta = -0.2\text{\AA}$, the spin state ordering is modified with a $S_T = 3/2$ ground state dominated by $S_M = 3/2$ and $S_L = 1$. As expected from Tanabe Sugano view, the growth of the $S_M = 1/2$ spin contribution on the Co ion is observed (Table 1), while the so-called high-field regime is reached. The $S_M = 1/2$ weight significantly increases to reach 0.14% for $\delta = -0.2\text{\AA}$. On the contrary, this contribution is reduced to 0.04% when the coordination sphere is expanded with $\delta = +0.1\text{\AA}$. This sensitivity to environment was reported for this particular compound by comparing the solid and solution phases, but also in other organic-based materials^[13,29]. Then, a torsion of the two ligands was applied (see Figure 5) and similar conclusions can be drawn. Upon weak distortions, the spin multiplicity of the ground state is changed and the mixing of different spin states on the metal varies, entangled to the spin environment.

Table 1. Wavefunction structure (DDC2 level) of the $S_T = 3/2$ state for the Xray structure and distorted geometries $\delta = -0.2\text{\AA}$ and $\theta = 5^\circ$ (see Figure 5).

L_1 .MMM.L ₂	Clebsch-Gordan	X-ray	Slippage	Torsion
$\downarrow\uparrow\uparrow\uparrow$	0.548	0.545	0.441	0.544
$\uparrow\uparrow\uparrow\downarrow$	0.548	0.550	0.642	0.551
$\uparrow\downarrow\uparrow\uparrow$	-0.365	-0.350	-0.339	-0.346
$\uparrow\uparrow\downarrow\uparrow$	-0.365	-0.362	-0.355	-0.358
$\uparrow\uparrow\uparrow\downarrow$	-0.365	-0.384	-0.390	-0.390

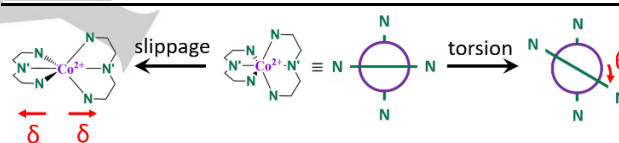


Figure 5. Deformations of the coordination sphere of **1**. Left: symmetric slippage of the ligands along the (N'-N') axis. Right: torsion of the two ligands around the (N'-N') axis.

Despite small deviations observed in Table 1, our suggestion is supported by the observed modification of the $S_M = 3/2$ and $S_M = 1/2$ contributions to the $S_T = 3/2$ state of **1**. Evidently, the electrostatic changes that accompany the $S_L = 1$ to 0 spin change are rather small ($E_S - E_T = 3$ K from our calculations). Should the field generated by the ligands be stronger, the metal ion might consist of a more pronounced weight on the $S_M = 1/2$ state. Such compound that gathers a spin crossover ion and organic radical ligands offers a variety of spin-coupling schemes that may not be reproduced by a given spin state on the Co center. This is to be considered as a limiting case where Hund and non-Hund forms are close in energy in an intermediate crystal field produced by radical ligands.

Conclusion

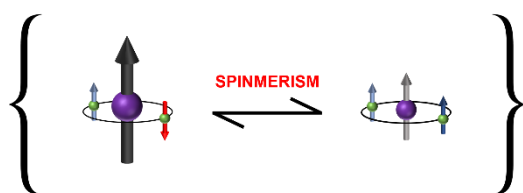
While trapped as high-spin in the solid state, the electronic structure of bis(oxoverdazyl) Co compound **1** is deeply modified in solution. This compound is particularly intriguing for magnetic interactions that were inspected using the correlated quantum chemistry DDC2 method. The controversy regarding the magnetic exchange interactions is reflected by a structure sensitive low-energy spectrum. The ground state spin multiplicity is modulated and is highly sensitive. From our *ab initio* calculations, we observed that the spin states emerge from an unusual scenario that combines various local spin states. The manifestation of

entanglement results from the simultaneous presence of a spin-crossover Co(II) ion and a crystal field produced by a set of open-shell radicals. The mixing of high-spin and low-spin in the construction of the total spin state has strong similarity with hybrids of resonance built from limiting forms accounting for charge delocalization. In analogy with mesomerism effect, our observations led to the recognition of a *spinmerism* phenomenon involving spin degree of freedom. These views somewhat extend the traditional picture in transition metal complexes where the spin multiplicity is fixed and governed by the metal ion.

Keywords: *ab initio* calculations • molecular magnetism • radicals • valence tautomerism • verdazyl

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Combination of Spin Crossover metal ion and open-shell environment results in the mixing of high- and low- spin metal, named as *spinmerism*.