Supporting information for the manuscript:

Magnetic behavior and ground spin states for coordination $\{L\cdot[M^{II}(Hal)_2]_3\}^{3-}$ assemblies (Hal = Cl or I) of radical trianion hexacyanohexaazatriphenylenes (L) with three coordinated high-spin Fe^{II} (S = 2) or Co^{II} (S = 3/2) centers

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Table S1. IR-spectra (cm^{-1} in KBr pellets) of starting compounds and salts **1-3**.

	CVCl	Cryptand	HATNA $(CN)_6$	HAT $(CN)_6$	$C_6H_4Cl_2$	$\{Cryptand(K^+)\}_3$ $\{HATNA(CN)_6\cdot(FeI_2)_3\}^{3-}$ $\cdot 2C_6H_4Cl_2$ (**1**)	$\{\{Cryptand(K^+)\}_3$ $\{HATNA(CN)_6\cdot(CoI_2)_3\}^{3-}$ $\cdot 2C_6H_4Cl_2$ (**2**)	$(CV^+)_3$ $\{HAT(CN)_6\cdot(CoCl_2)_3\}^{3-}$ $0.5(CVCl)\cdot$ $2.5C_6H_4Cl_2$ (**3**)
Cat^+	CV^+	Cryptand				Cryptand	Cryptand	CV^+
	420w	476w				-	-	422w*
	522w	528w				520w	520w	524w
	561w	735m				-	-	560w
	722m	922m				930w*	930w*	723w
	744m	948w				949m*	949m*	744w
	760m	982m				-	-	760w*
	825w	1038w				-	-	826w
	847w	1071m				1078m*	1078m*	-
	913m	1100s				1105s	1105s	912w
	940m	1127s				1134m	1134m	942w
	1172s	1213w				-	-	1172s
	1190m	1295m				1296w*	1292w*	1186m sh
	1226w	1329m				1334m*	1335m*	1227w*
	1296m	1360s				1352m*	1353m*	1296w
	1360s	1446m				1445w	1445w	1360s*
	1450w	1462m				1477w*	1477w*	1456w*
	1477w	1490w				-	-	1481w
	1523w	2790w				2813w	2813w	1523w
	1586s	2877w				2883w	2881w	1583vs
	2856w	2943w				2955w	2955w	2860w
	2915w							2910w
HAT						$HATNA(CN)_6$	$HATNA(CN)_6$	$HAT(CN)_6$
			409m	418s		-	-	422w*
			483w	462w		493w	-	-
			538s	534w		536w	538w	-
			615m	621w		-	-	620w
			718w	709w		-	-	-
			744w	808w		753w*	754w*	-
			903w	923w		930w*	930w*	920w
			936s	1146m		949m*	949m*	-
			1084vs	1230s		1078m*	1078m*	1227w*
			1202m	1341s		-	-	1335m
			1248w	1364m		1257w	1258w	1360s*
			1293m	1464m		1296w*	1292w*	1456w*
			1321w	1560m		1334m*	1334m*	-
			1368s	1706m		1352m*	1352m*	-
			1469s	2241m		1421m 1477w*	1423m 1477w*	2198m 2213m
			1514m			1526w	1528w	
			1561m			-	-	
			1619m			1584w	1584w	
			2239vs			2226w	2228w	
			3050w			-	-	
$C_6H_4Cl_2$					657w	649w	645w	650w
					748s	753w*	754w*	760w*
					1030m	1028w	1026w	1031w
					1122m	-	-	-
					1453m	1454w	1453w*	1456w*

*****bands coincide, w - weak, m - middle, s – strong intensity, sh- shoulder, sp.- split band

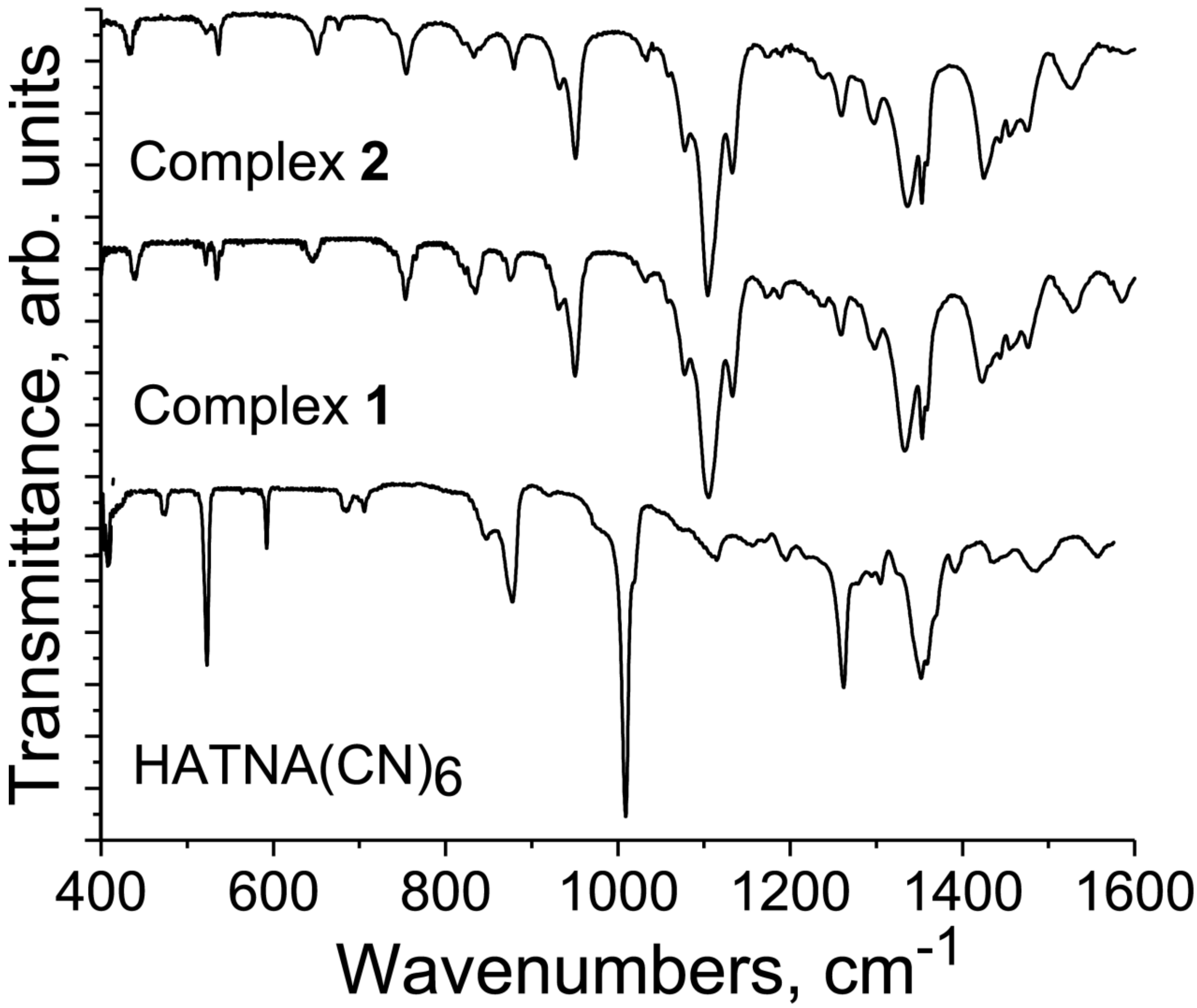


Figure S1. IR-spectra of starting HATNA(CN)$_6$, and salts {Cryptand(K^+)}$_3${HATNA(CN)$_6$$\cdot$(FeI$_2$)$_3$}$^{3-}$$\cdot$2$C_6H_4Cl_2$ (**1**) and {Cryptand(K^+)}$_3${HATNA(CN)$_6$$\cdot$(CoI$_2$)$_3$}$^{3-}$$\cdot$2$C_6H_4Cl_2$ (**2**) measured in KBr pellets. Pellets for **1** and **2** were prepared in anaerobic conditions.

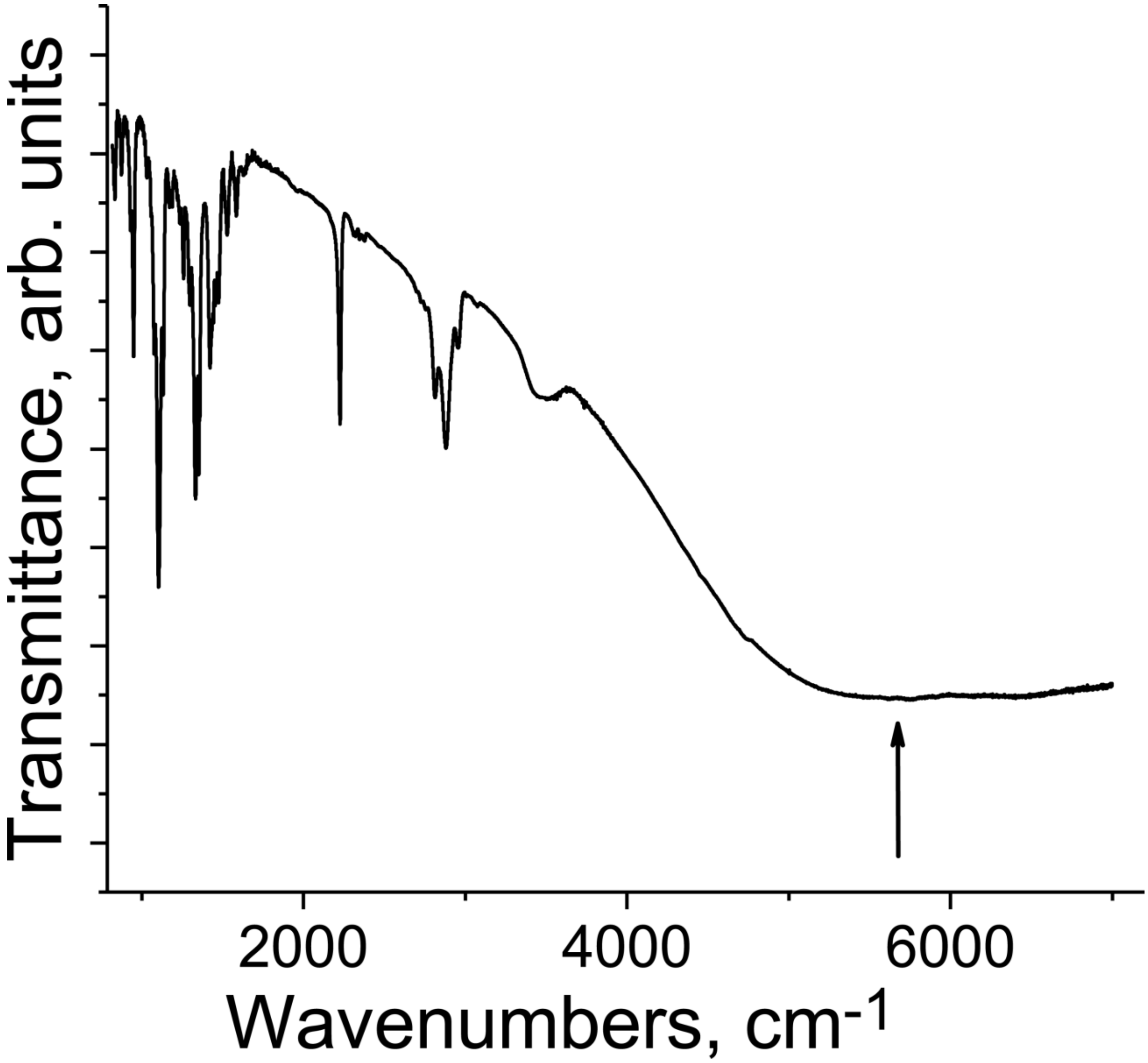


Figure S2. IR spectrum of {Cryptand(K^+)}$_3${HATNA$(CN)_6\cdot(FeI_2)_3$}$^{3-}\cdot 2C_6H_4Cl_2$ (**1**) in a KBr pellet in the 400-7000 cm^{-1} range.

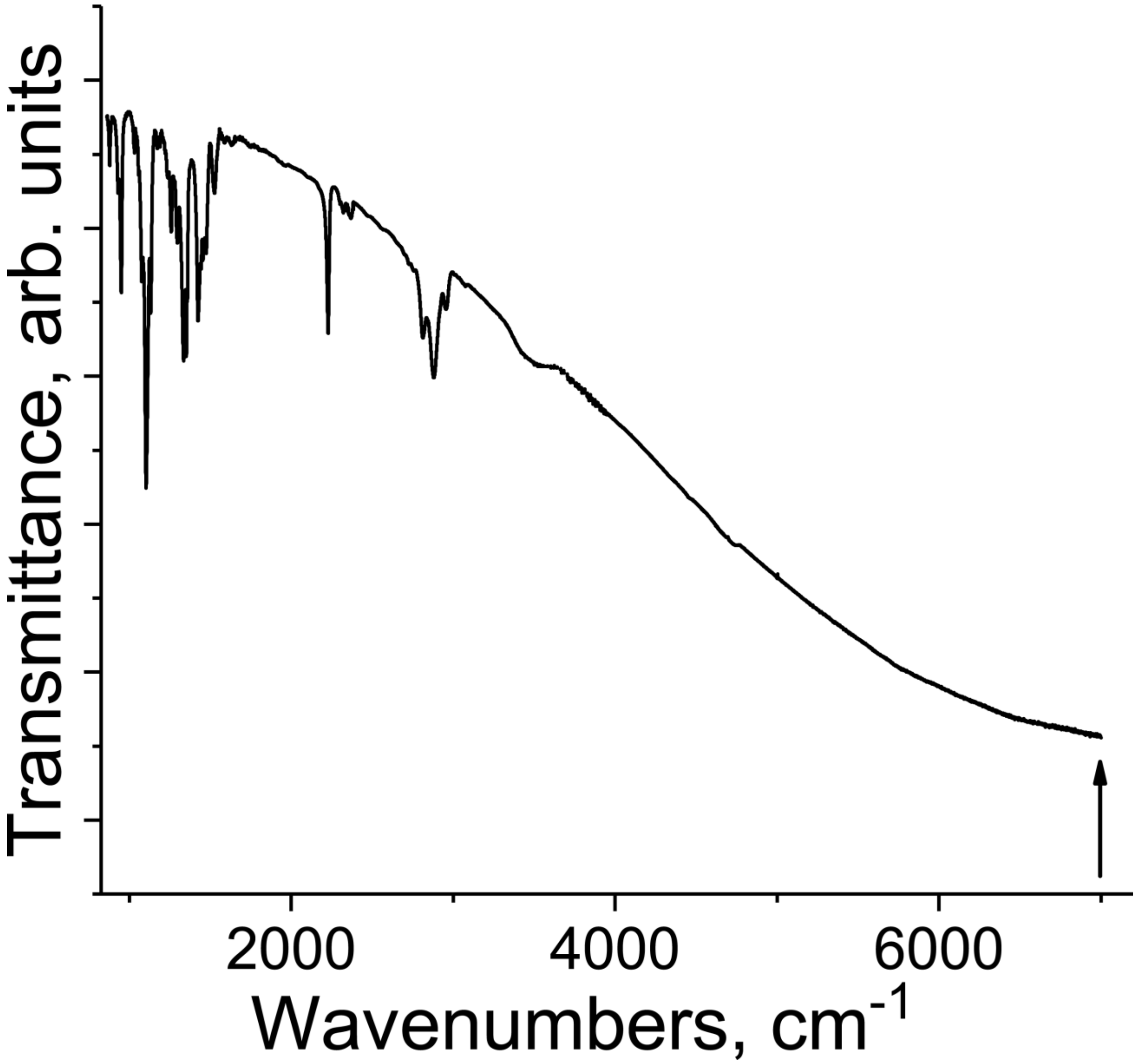


Figure S3. IR spectrum of {Cryptand(K^+)}$_3${HATNA$(CN)_6$·$(CoI_2)_3$}$^{3-}$·$2C_6H_4Cl_2$ (**2**) in a KBr pellet in the 400-7000 cm^{-1} range.

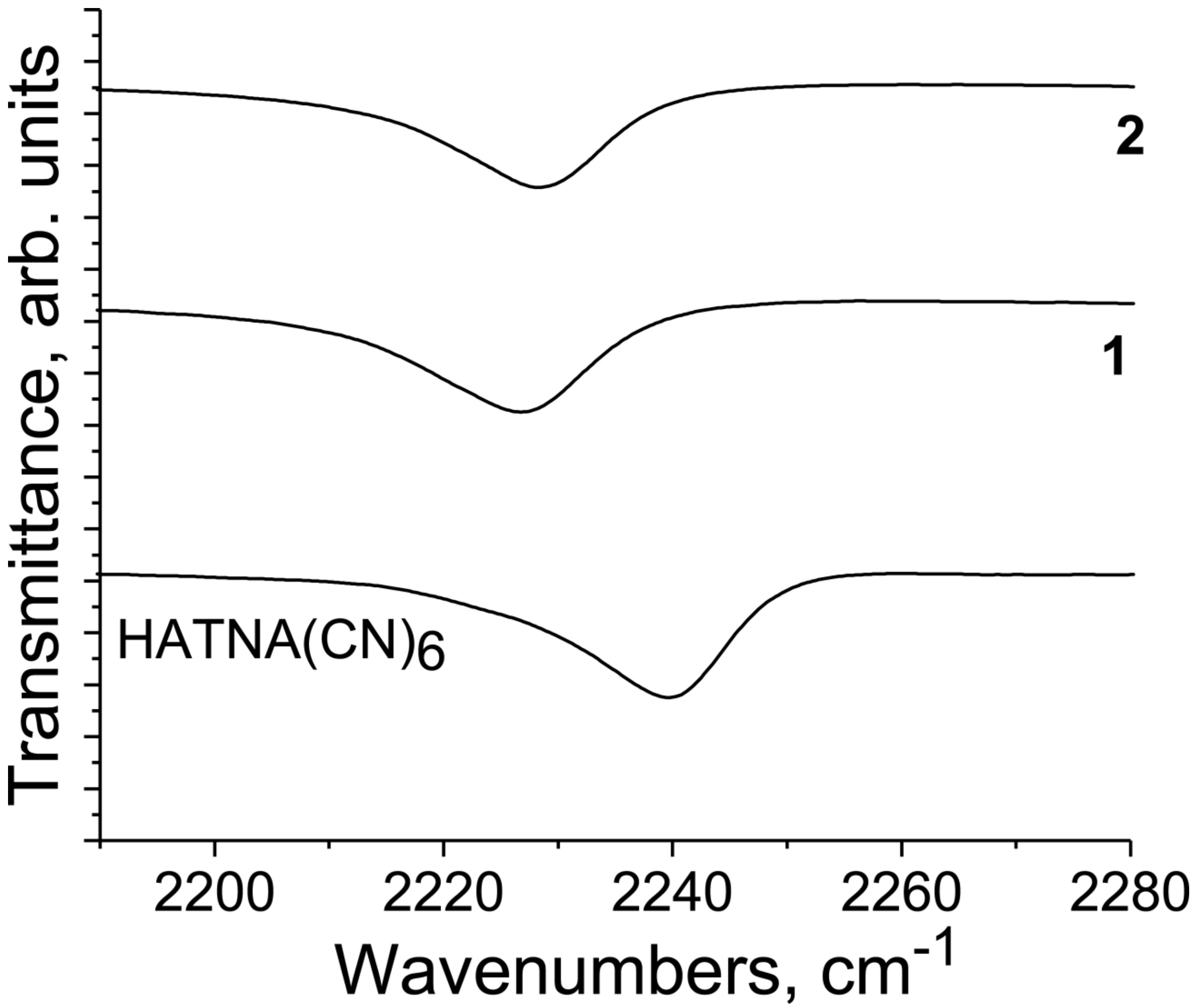


Figure S4. IR-spectra in the range of C≡N vibrations for starting HATNA$(CN)_6$ and salts **1** and **2** in KBr pellets. Pellets for **1** and **2** were prepared in anaerobic conditions.

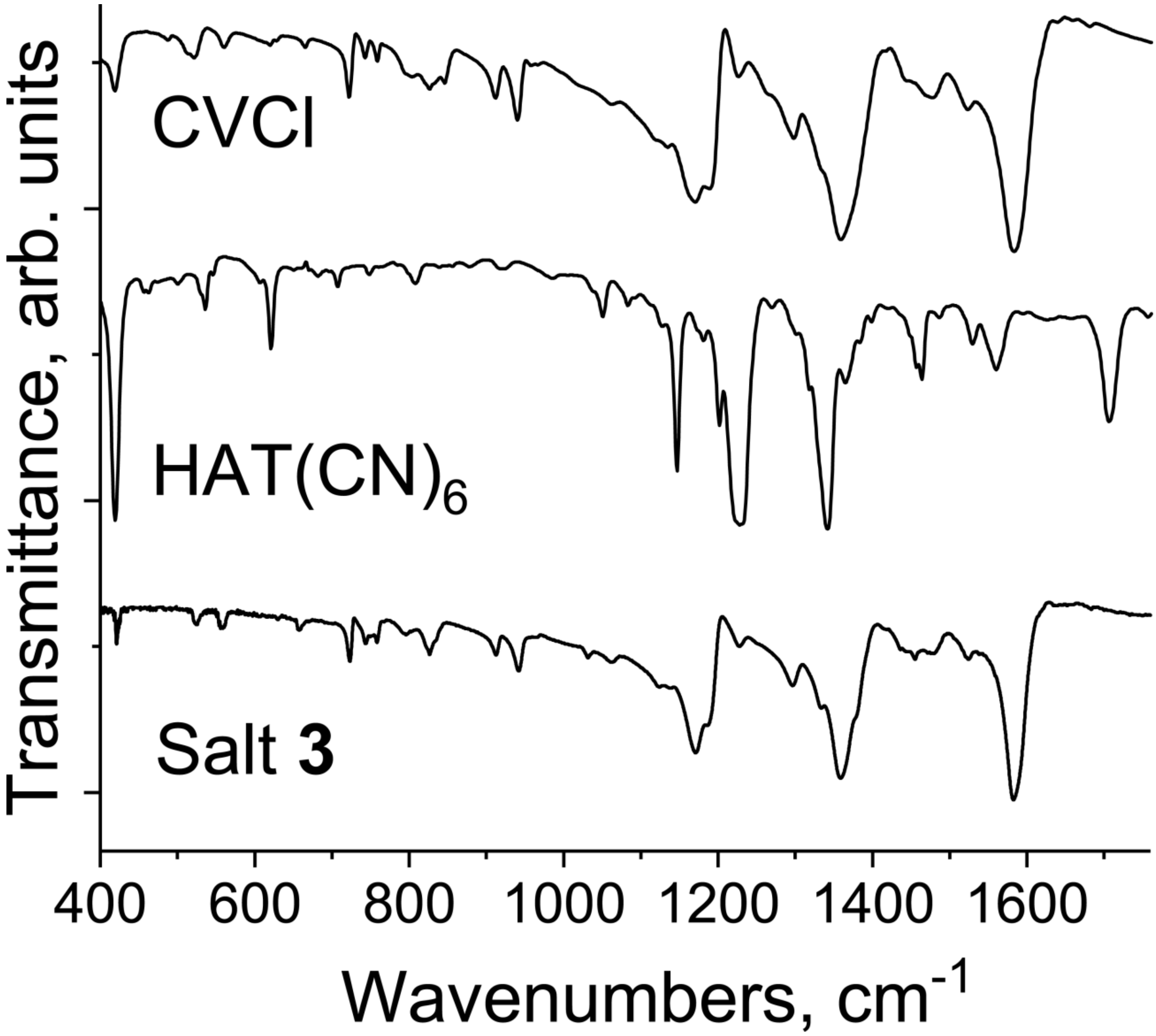


Figure S5. IR-spectra of pristine salt of crystal violet (CVCl), starting $HAT(CN)_6$, and salt $(CV^+)_3$ $\{HAT(CN)_6{\cdot}(CoCl_2)_3\}^{3-}{\cdot}0.5(CVCl){\cdot}2.5C_6H_4Cl_2$ (**3**) in KBr pellets. Pellet for **3** was prepared in anaerobic conditions.

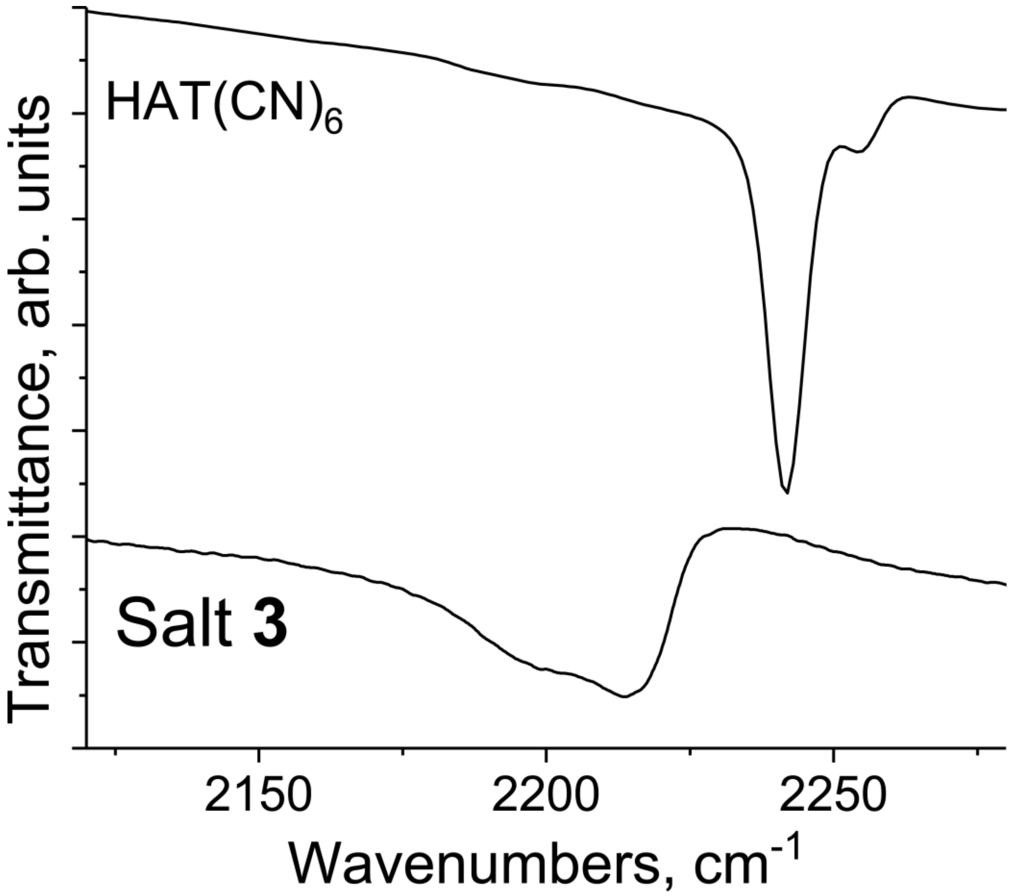


Figure S6. IR-spectra in the range of C≡N vibrations for starting $HAT(CN)_6$ and **3** in KBr pellets. Pellet for **3** was prepared in anaerobic conditions.

Spectra in the UV-visible-NIR range.

Table S2. Optical spectra of starting compounds and obtained salts **1-3**.

N	Units	Bands in the UV range	Bands in the visible range	Bands in the NIR range
	$HATNA(CN)_6$	304, 335	400sh, 615(weak)	-
	$\{HATNA(CN)_6\}^{2-}$ Ref. [1]	286, 345,	374, 620	1160, 1400, 1800
1	$\{Cryptand(K^+)\}_3\{HATNA(CN)_6\cdot(FeI_2)_3\}^{3-}\cdot 2C_6H_4Cl_2$	286, 386 (new)	510 (shoulder)	1000, 1820
2	$\{Cryptand(K^+)\}_3\{HATNA(CN)_6\cdot(CoI_2)_3\}^{3-}\cdot 2C_6H_4Cl_2$	284, 387 (new)	544 (shoulder)	928, 1455
	$HAT(CN)_6$	290 (shoulder)		
3	$(CV^+)_3\{HAT(CN)_6\cdot(CoCl_2)_3\}^{3-}\cdot 0.5(CVCl)\cdot 2.5C_6H_4Cl_2$	305 (CV^+)	600 (CV^+) 770 (shoulder)	

Crystal structure of 3.

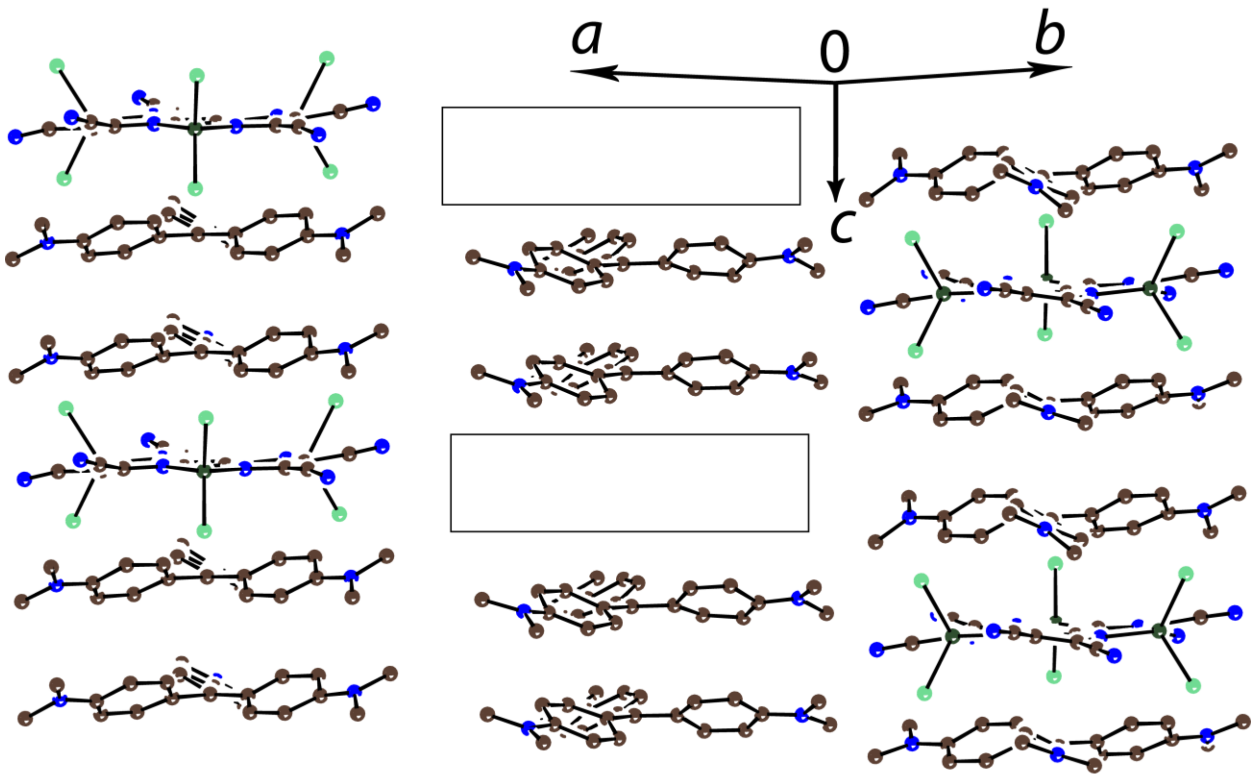


Fig. S7. View on the crystal structure of **3**. There are two types of columns containing alternating ions. Two columns contain only the $\{HAT(CN)_6 \cdot (CoCl_2)_3\}^{3-}$ trianions alternatig with two CV^+ cations (left and right columns). Central column contains two ordered CV^+ cations and one position (shown by black rectangle) contains an electroneutral CVCl unit. Disordered solvent $C_6H_4Cl_2$ molecules positioned between the columns are not shown.

Magnetic data for 1.

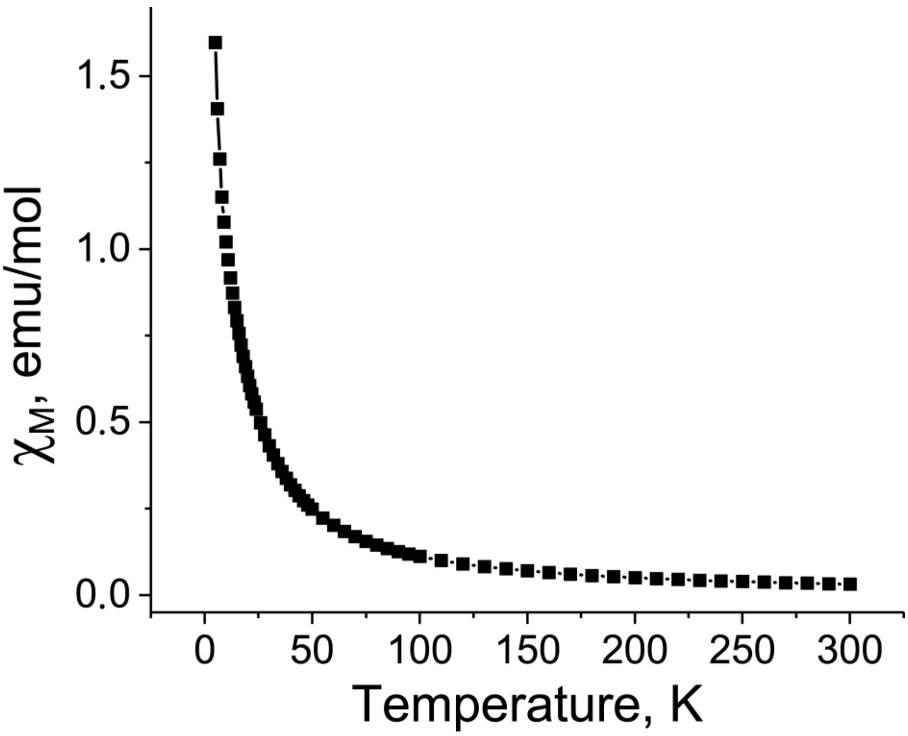


Figure S8. Temperature dependence of molar magnetic susceptibility for salt **1** in the 1.9-300 K range after the subtraction of a temperature independent part.

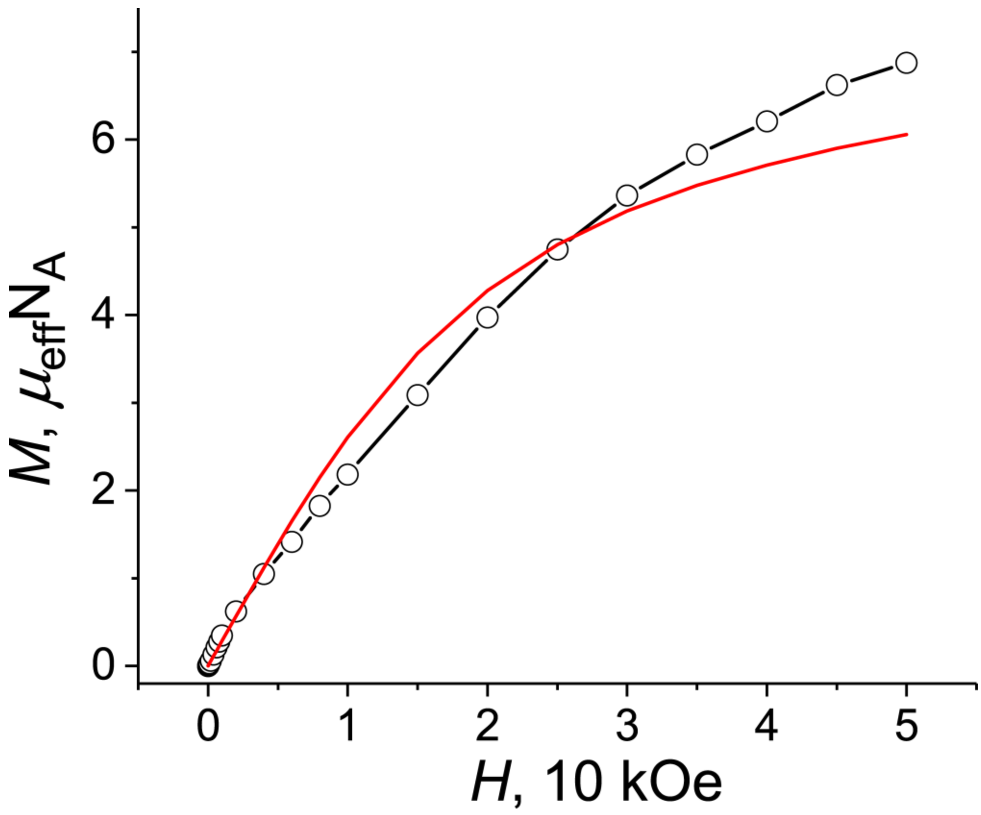


Figure S9. Dependence of magnetization vs magnetic field up to 50 kOe magnetic field for **1** at 6 K (black line is a guide to the eye): experimental data (black circles) and calculated data obtained from simultaneous fitting of susceptibility and magnetization by PHI (red curve).

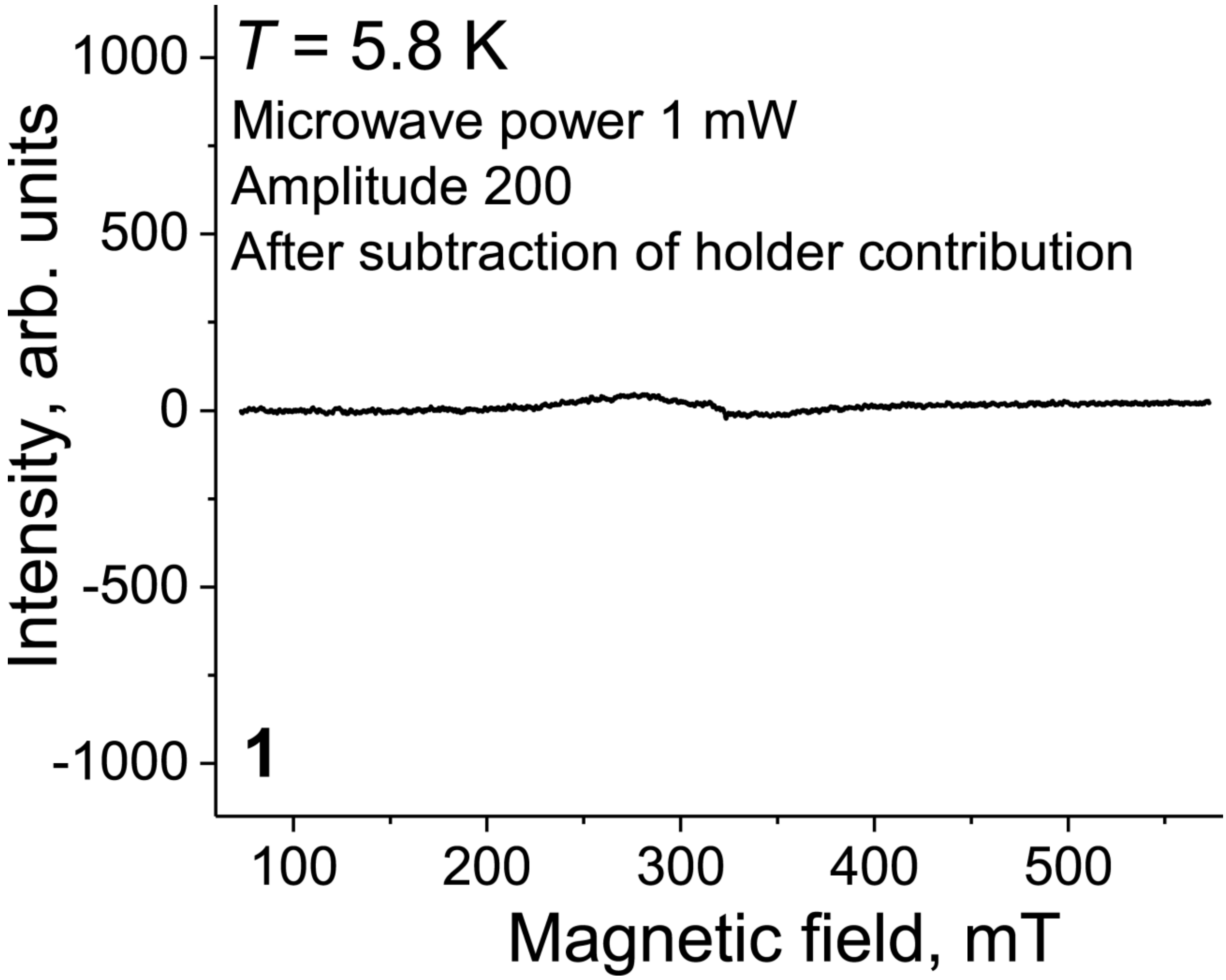


Figure S10. EPR spectrum of polycrystalline **1** at 5.8 K at high amplitude (200) and large magnetic field range (70-580 mT) after subtraction of sample holder contribution. Weak broad signal at g = 2.11 (ΔH = 60 mT) most probably can be attributed to impurities.

Magnetic data for 2

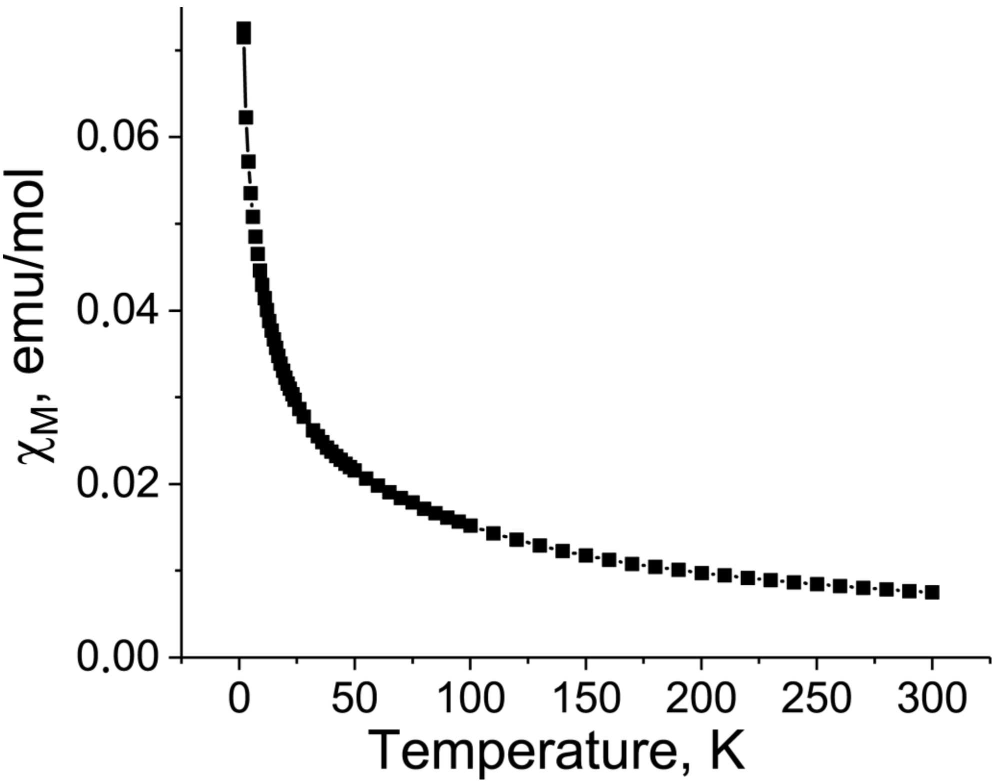


Figure S11. Temperature dependence of molar magnetic susceptibility for salt **2** in the 1.9-300 K range after the subtraction of a temperature independent part.

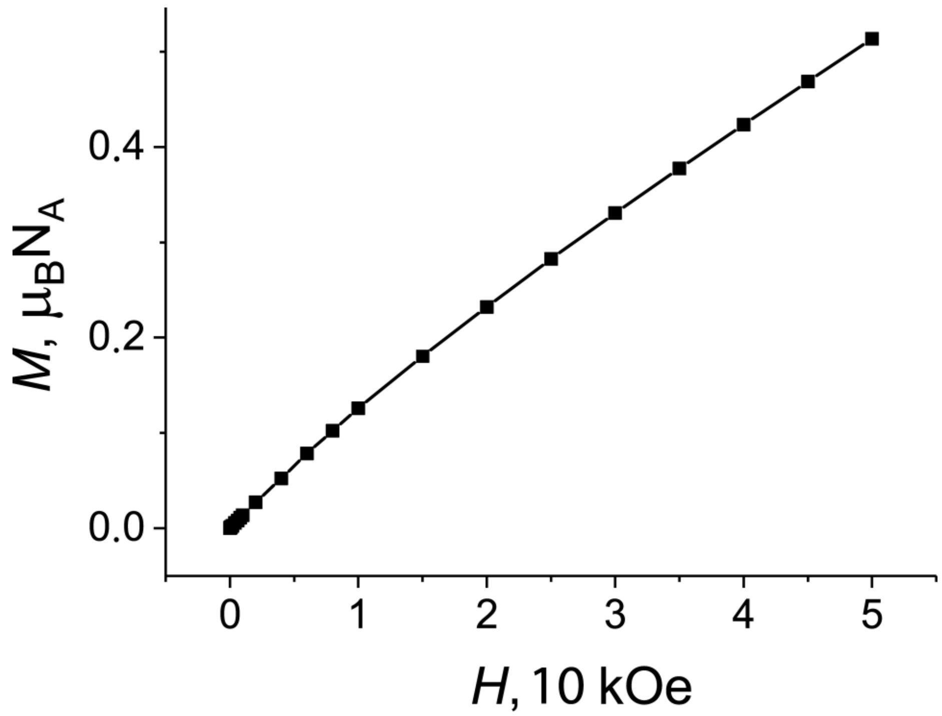


Figure S12. Dependence of magnetization *vs* magnetic field up to 50 kOe magnetic field for **2** at 2 K (black line is a guide to the eye).

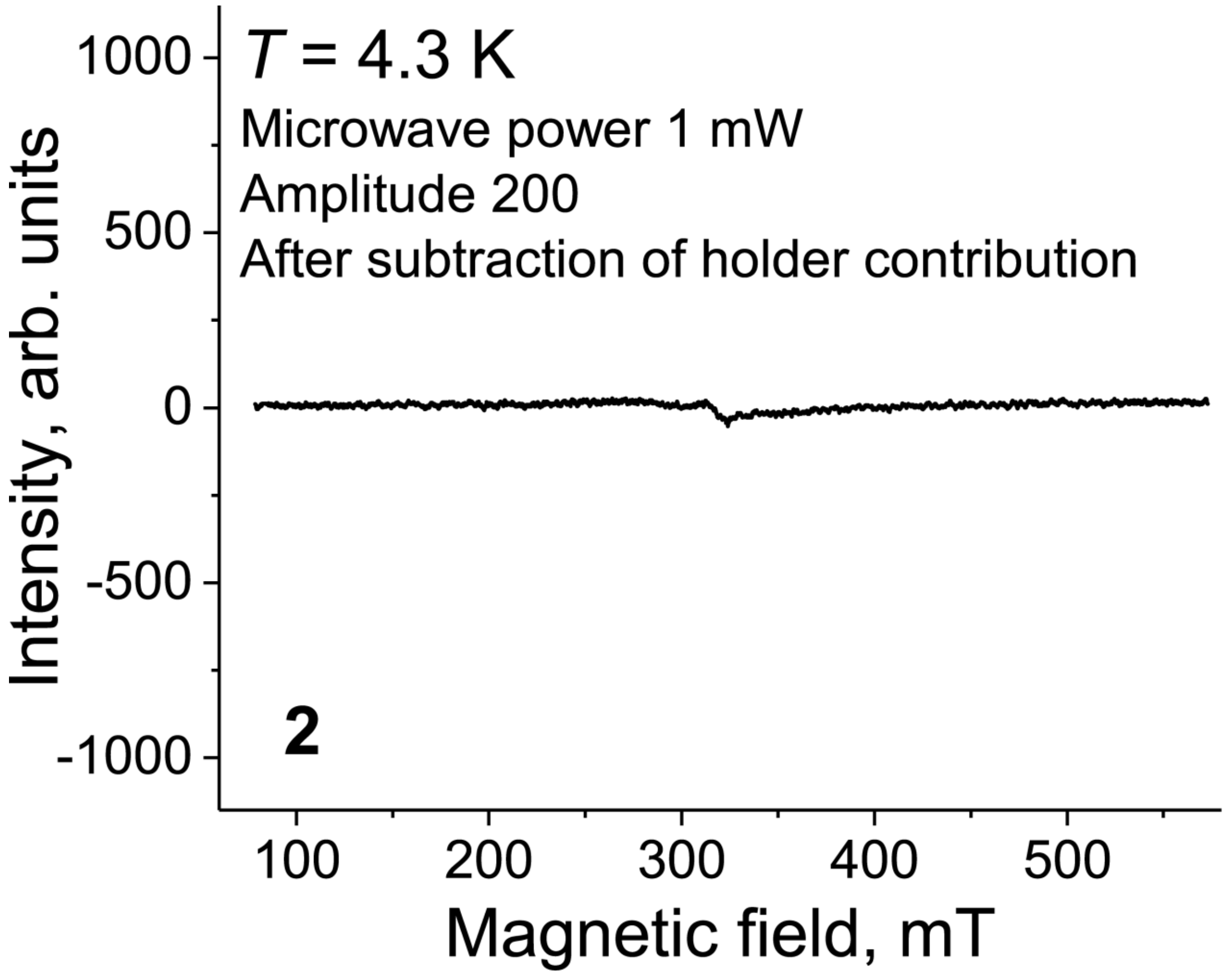


Figure S13. EPR spectrum of polycrystalline **2** at 4.3 K at high amplitude (200) and large magnetic field range (70-580 mT) after subtraction of sample holder contribution. Very weak broad signal at g = 2.11 (ΔH = 60 mT) most probably can be attributed to impurities.

Magnetic data for 3

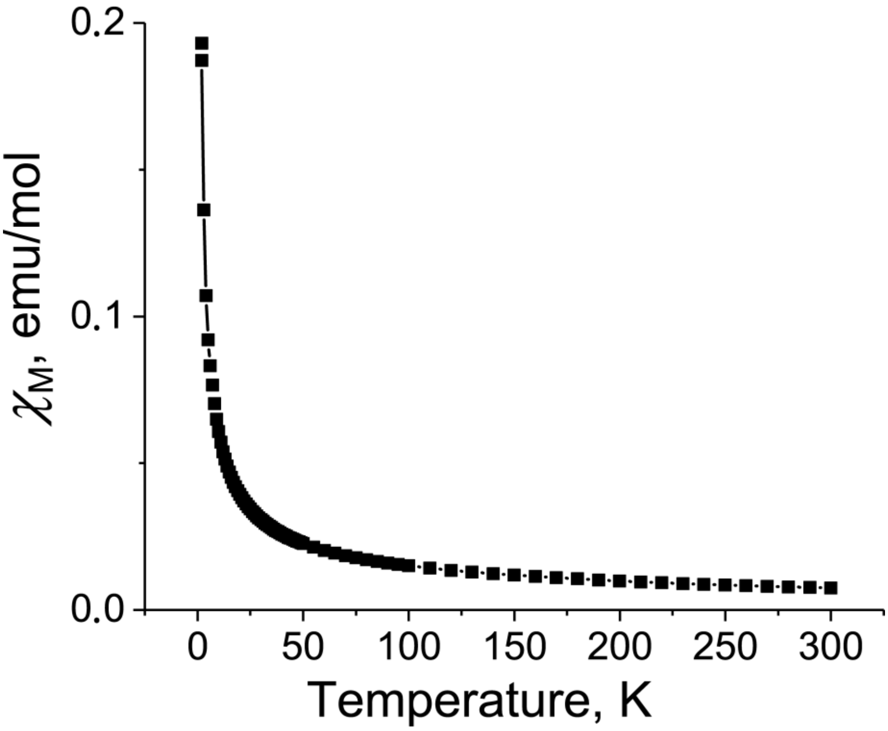


Figure S14. Temperature dependence of molar magnetic susceptibility for salt **3** in the 1.9-300 K range after the subtraction of a temperature independent part.

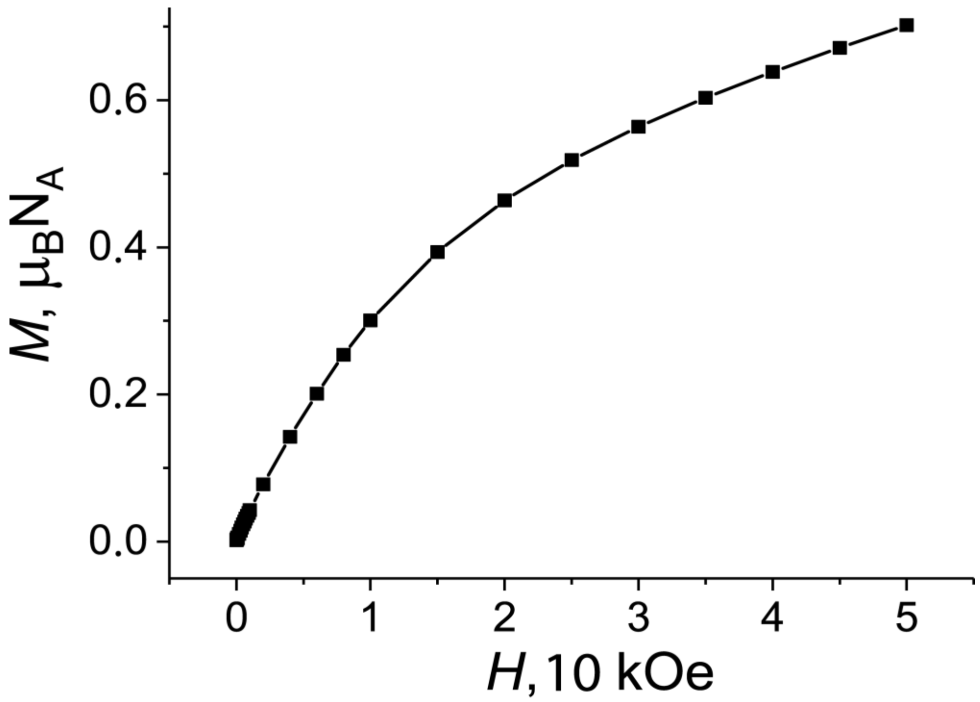


Figure S15. Dependence of magnetization *vs* magnetic field up to 50 kOe magnetic field for **3** at 2 K (black line is a guide to the eye).

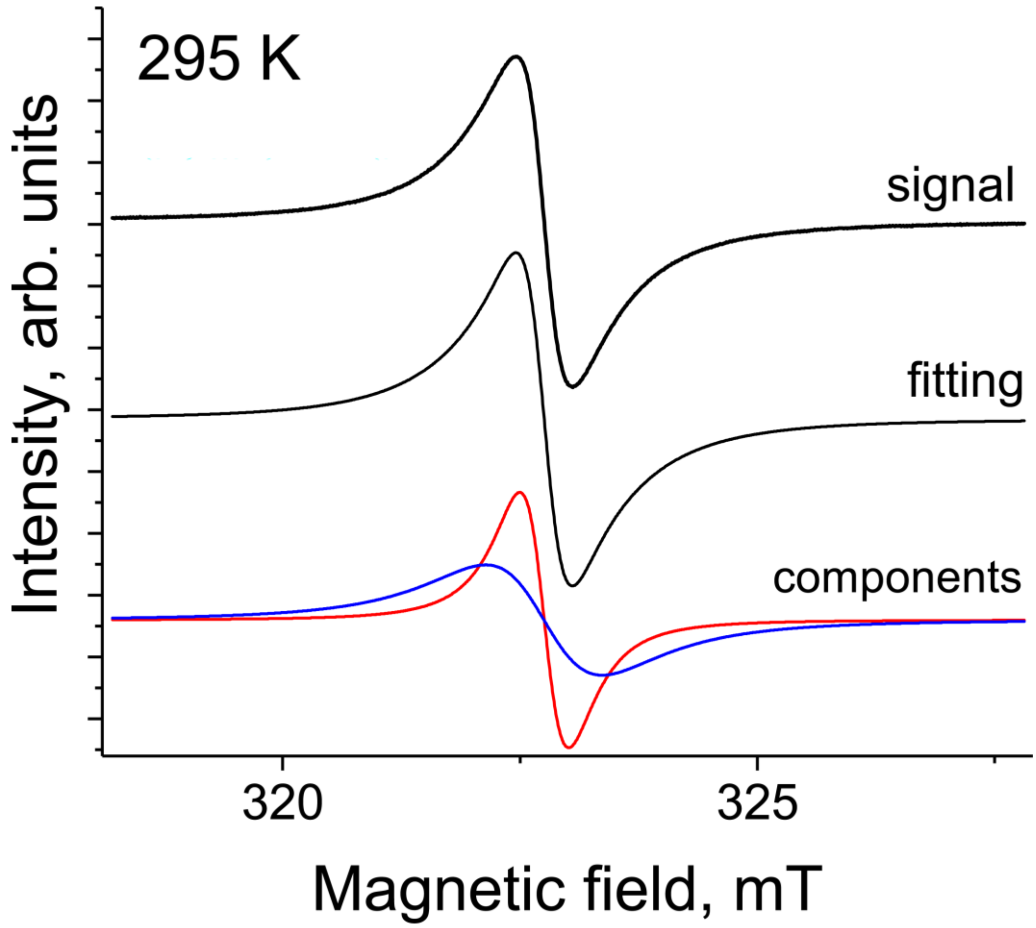


Figure S16. Weak EPR signal from polycrystalline **3** at room temperature (295K) and fitting of the signal by two Lorentzian lines (red and blue curves)..

Theoretical calculations

The molecular structures of $\{HAT(CN)_6(CoCl_2)_3\}^{3-}$ and $\{HAT(CN)_6(CoCl_2)_3\}^{3-}$ complexes were optimized using the PBE exchange-correlation functional [2] and with the Λ2 basis set Fe:Co [23s18p13d8f4g/8s7p5d3f1g], Cl [18s13p5d2f/5s4p2d1f], N,C : [12s8p4d2f/4s3p2d1f], H :[8s4p2d/3s2p1d] [3] of triple zeta quality implemented in the **PRIRODA** package [4].

Relativistic effect must be taken into account for the iodide atom. In this case when describing iodine-containing complexes, the calculations were carried out in the scalar relativistic approximation, which is based on the complete four-component one-electron Dirac equation with excluded spin-orbit effects [5]. An energy-optimized extended Gaussian basis was used for large components: I [29s26p18d2f/7s6p4d1f], Fe:Co [25s20p13d8f4g/8s7p5d3f1g], Cl [19s13p5d2f/5s4p2d1f], N,C : [12s8p4d2f/4s3p2d1f], H :[8s4p2d/3s2p1d] and corresponding kinetically balanced basis for small components. The Hirschfeld method [6] was used to calculate atomic charges. All calculations were performed at Joint Supercomputer Center of the Russian Academy of Sciences.

In the DFT approach wave functions are described in one-determinant approximation, and that imposes certain restrictions when studying trinuclear complexes with open shells. As a result, the energies of spin-correct states can be directly obtained only when the value of the total spin coincides with its projection $S = S_z$. In the system of three metal centers with spin s, there is a lot of spin states in the system: $S_M = 3s$, $3s$-1, $3s$-2 and so on. In the particular case of three high-spin Co^{II} ions with spin $s = 3/2$, there are 1, 2, 3, 4 and 2 states with a total spin equal to 9/2, 7/2, 5/2, 3/2, and 1/2, correspondingly. For each Co-center, the d_{xz}, d_{yz} and d_{z^2} orbitals are singly occupied (the x-axis is in the ligand plane, and the y-axis is in the CoX_2 plane). Group-theoretical analysis shows that these states give the following set of terms: ${}^{10}A''$, ${}^{8}E''$, ${}^{6}A_2''$, ${}^{6}E''$, ${}^{4}A_1''$, ${}^{4}A_2''$, ${}^{4}E''$ and ${}^{2}E''$.

At a parallel orientation of all spins localized at metal centers, a state arises with a total spin $S_M = 3s$, which is well described by one determinant. In the presence of the spin 1/2 on the ligand, two states appear, and only the state with total spin $S_M + 1/2$ is described by one determinant. Another one-determinant state with spin projection $S_z = S_M - 1/2$ (β electron is localized on the ligand) is the following combination of states with the correct spin:

$$\left|S_z = S_M - 1/2\right\rangle = \frac{\left|S_M - 1/2, S_M - 1/2\right\rangle - \sqrt{2S_M}\left|S_M + 1/2, S_M - 1/2\right\rangle}{\sqrt{2S_M + 1}}$$

Therefore, its energy, $E(S_z = S_M - 1/2)$, differs from the energy of the state with spin $S_M - 1/2$, $E(S_M - 1/2)$. Nevertheless, it is possible to find the energy of the state with the total spin $S_M - 1/2$ from the calculated energies of one-determinant states:

$$E(S_M - 1/2) = E(S_z = S_M - 1/2) + \frac{1}{2S_M}\left[E(S_z = S_M - 1/2) - E(S_M + 1/2)\right] \qquad \text{(Equation 1)}$$

In this case, the same geometry is used to calculate the energies (the optimized geometry of true $S_M + 1/2$ state should be used for that purpose). The difference between the energies of the states with spin $S_M + 1/2$ and $S_M - 1/2$ is equal to $2J_1^*(S_M + 1/2)$, where J_1^* is the exchange parameter of high-spin state of metal center with the radical trianion ligand.

The optimized geometry of $\{HAT(CN)_6{\cdot}(MCl_2)_3\}^{3-}$ trianions (M = Co^{II} and Fe^{II}) for the $S = 3s + 1/2$ and $S_z = 3s - 1/2$ spin states is different. According to Equation 1, the energies of $S = 3s - 1/2$ spin state can be found for both geometries of Co and Fe complexes from the calculated

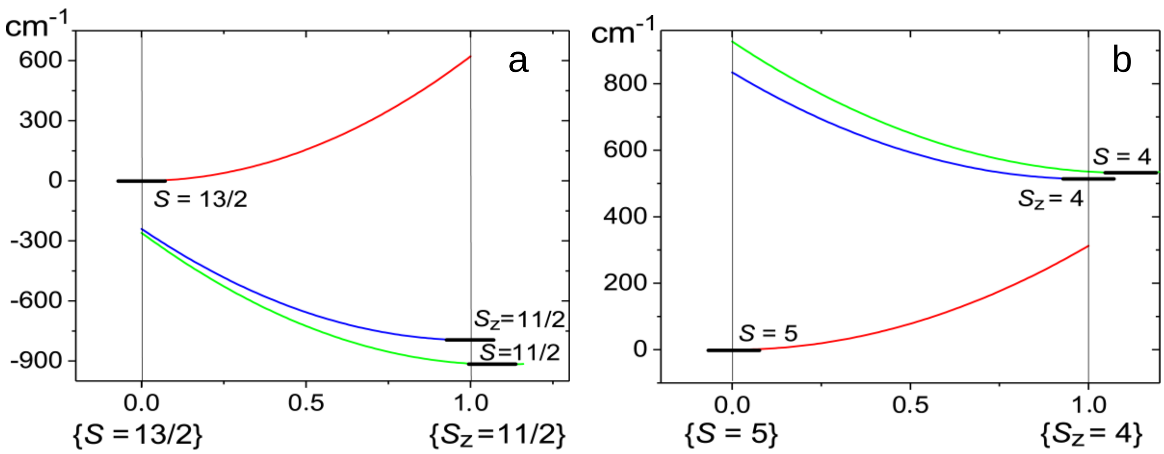


Fig. S17. Theoretically found energy terms $S = 11/2$ and $S = 4$ for the $\{HAT(CN)_6 3M^{II}Cl_2\}^{3-}$ trianion complex, M = Fe^{II} (a) and M = Co^{II} (b) which are based on calculated energies with $S = 3s + 1/2$ and $S_z = 3s - 1/2$ for two geometries $\{S = 3s + 1/2\}$ and $\{S_z = 3s - 1/2\}$.

energies of the $S = 3s + 1/2$ and $S_z = 3s - 1/2$ spin states. Then one can recover the values of the energy of the optimized state with a total spin $S = 3s - 1/2$ in some approximation. We will characterize the geometry change by dimensionless parameter Q, which varies from 0 for the $S = 3s + 1/2$ state geometry to Q = 1 for the $S_z = 3s - 1/2$ state geometry. Then, assuming that for intermediate geometries the difference in energy of $S = 3s + 1/2$ and $S_z = 3s - 1/2$ terms depends linearly on Q, it is possible to find the energy minimum for $S = 3s - 1/2$ term. The corresponding illustration for the chloride complexes of Co and Fe is shown in Figure S17.

At a minimum point of the $S = 3s - 1/2$ term, parameter Q is close to 1. Thus, geometric characteristics of this state are close to those of the optimized state with $S_z = 3s - 1/2$ state, and we accept the equality of the zero-point vibration energy contributions for the $S = 3s -1/2$ and $S_z= 3s - 1/2$ states.

Changes in the Co-Cl and the Co-N bond lengths in the $S = 3s + 1/2$ and $S_z=3s - 1/2$ states are only 0.005 and 0.017 Å, respectively. However, there are distortions of bond angles of the complex in the $S_z = 3s - 1/2$ state since the values of the root-mean-square displacements of Cl atoms are much higher, 0.037 Å, under the change in spin state. In the case of the Fe complex, changes in the Fe-Cl and the Fe-N bond lengths are smaller, 0.002 and 0.005 Å, respectively. However pronounced rotation of the two $FeCl_2$ fragments relative to the macrocycle plane appears which lead to much higher root-mean-square displacements of Cl atoms, 0.253 Å. These rather small structural distortions are accompanied by energy changes of the order of 1000 cm^{-1}, which are very significant in the scale of magnetic interactions.

One-determinant states with projection of total spin of metal centers less than the maximal value $S_{Mz} < 3s$ have in general an admixture of high lying excited electronic states. For example, one-determinant states $|d_{xz}\alpha\ d_{yz}\alpha\ d_{z^2}\beta|$ state of Co-center is superposition of true state with projection 1/2 of local spin 3/2 $|d_{xz}\alpha\ d_{yz}\alpha\ d_{z^2}\beta| + |d_{xz}\alpha\ d_{yz}\beta\ d_{z^2}\alpha| + |d_{xz}\beta\ d_{yz}\alpha\ d_{z^2}\alpha|$ and higher electronic states with local spin 1/2 $|d_{xz}\alpha\ d_{yz}\alpha\ d_{z^2}\beta| - |d_{xz}\alpha\ d_{yz}\beta\ d_{z^2}\alpha|$ and $|d_{xz}\alpha\ d_{yz}\beta\ d_{z^2}\alpha| - |d_{xz}\beta\ d_{yz}\alpha\ d_{z^2}\alpha|$ for open shells with 3 unpaired electrons. The only exception occurs when spin is flipped at one of metal centers, and those states the spin density on each center corresponds to 3 unpaired electrons for Co and 4 unpaired electrons for Fe center.

In this case the one-determinant state $|S_{Mz}=s>$ is the superposition of true spin states $|S_M,s>$ with total spin $s \le S_M \le 3s$ with the same spin projection $S_{Mz}=s$

$$\left|S_{Mz}=s\right\rangle = \sum_{S_M=s,i}^{S_M=3s} x_{S_M}^i \left|S_M, s\right\rangle$$

The index *i* takes into account the presence of several states with spin S_M. To find the expansion coefficients directly, it is necessary to know the explicit form of spin functions. This can easily be done for the state with maximum spin $S_M = 3s$ using the lowering spin operator $\mathbf{S}^-$

$|S_M,s> = (\mathbf{S}^-)^{2s} |S_M, S_M>$

, which gives the coefficient for the state with maximum spin

$$x_{3s} = \frac{1}{\sqrt{C_{6s}^{2s}}}$$

Other coefficients can easily be found by solving the system of equations:

$$\sum_{S_M=s}^{S_M=3s} (x_{S_M}^i)^2 = 1$$
$$\sum_{S_M=s}^{S_M=3s} (x_{S_M}^i)^2 [S_M(S_M+1) - s(s+1)]^n = \left\langle S_{Mz} = s \middle| P_s^n \middle| S_{Mz} = s \right\rangle$$
$$n = 1,2,..,2s-1$$

, where P_s is the projection operator onto a state with spin $S_M = s$. It can be represented in terms of the product of the lowering and raising spin operator $\mathbf{S}^+$

$P_s = \mathbf{S}^- \mathbf{S}^+$

For local spin $s = 3/2$, after simple algebraic transformations, one can find the values of two matrix elements $<P_s>$ and $<P_s^2>$ equal to 3 and 27, respectively. Taking into account the numerical values $x_{9/2}$, it follows from the above system of linear equations that the total contribution of the states with spin $S = 3/2$, 5/2 , 7/2 and 9/2 (the sum of the squares of the corresponding coefficients) is equal to 48/84, 27/84, 8/84 and 1/84, respectively.

The next step is to take into account that in presence of spin 1/2 on the ligand there are two one-determinant states of the complex with the projection of the total spin $S_z = s + 1/2$ and $S_z = s - 1/2$. Both states are a superposition of multi-determinant states with true spin, whose contribution can be found theoretically.

It is important that expansion in true spin functions opens us the possibility to find all energy levels on the base of the calculated energies of $S = 3s + 1/2$, $S_z = 3s - 1/2$, $S_z = s + 1/2$ and $S_z = s - 1/2$ states only. If we adopt the spin Hamiltonian approximation then the energy explicitly depends on square of the total spin. For the state with the maximum spin of metal centers, the energies of two possible levels with total spin $3s + 1/2$ and $3s - 1/2$ are directly known from the calculations. Thus, the modified model of the spin Hamiltonian was used:

$$E(S \pm 1/2) = E_0 + J_2 S(S+1) \pm J_1 (S+1/2), S < 3s$$
$$E(S \pm 1/2) = E_0 + J_2 S(S+1) \pm J_1^* (S+1/2), S = 3s$$

Here E_0 is determined by the energy reference point. Taking into account general Equation 1 it is easy found the formula :

$$E\big|_{SMz=s+1/2} - E\big|_{SMz=s-1/2} = J_1 \sum_{S_M=s}^{S_M=3s-1} (x_{S_M}^i)^2 2S_M + (x_{3s})^2 J_1^* 6s$$

which is directly connect the value of parameter J_1 with the energy difference of one-determinant states. Then it is possible to calculate the value of exchange interaction parameter J_2 between the metal centers, taking into account the value of the matrix element of projector P_s

$$E\big|_{SMz=s+1/2} = E_0 + \sum_{S_M=s}^{S_M=3s} (x_S^i)^2 J_2 S_M (S_M+1) + \sum_{S_M=s}^{S_M=3s-1} (x_{S_M}^i)^2 J_1 (S_M + 1/2) + (x_{3s})^2 J_1^* (3s+1/2)) =$$
$$= E_0 + J_2[s(s+1) + \langle P_s \rangle] + \sum_{S_M=s}^{S_M=3s-1} (x_{S_M}^i)^2 J_1 (S_M + 1/2) + (x_{3s})^2 J_1^* (3s+1/2)$$

and the energy of the state with maximum spin S_M=3s of metal centers

$E(S_M + 1/2) = E_0 + J_2(S_M)(S_M + 1) + J_1^*(S_M + 1/2)$

The trinuclear complex with the maximum spin $3s + 1/2$ has most symmetric geometry. In this case, there is only a Jahn-Teller distortion of ligand geometry with spin 1/2. It is logical that the optimized geometry of this complex can be used to calculate the energies of other one-determinant states with the projection of the total spin 3*s*-1/2, *s*+1/2 and *s*-1/2 to restore the parameters of the spin Hamiltonian.

The values of these energies, as well as the theoretical values of the energies of all spin states for the for $\{HAT(CN)_6{\cdot}(Co^{II}Cl_2)_3\}^{3-}$ complex, calculated for the theoretically calculated parameters J_1 = -211.4 cm^{-1} and J_2 = -79.7 cm^{-1}, are shown in Fig. S18. The scheme also shows the positions of the energy levels S = 5, S_z = 4, S_z = 2 and S_z = 1 for the geometries of the

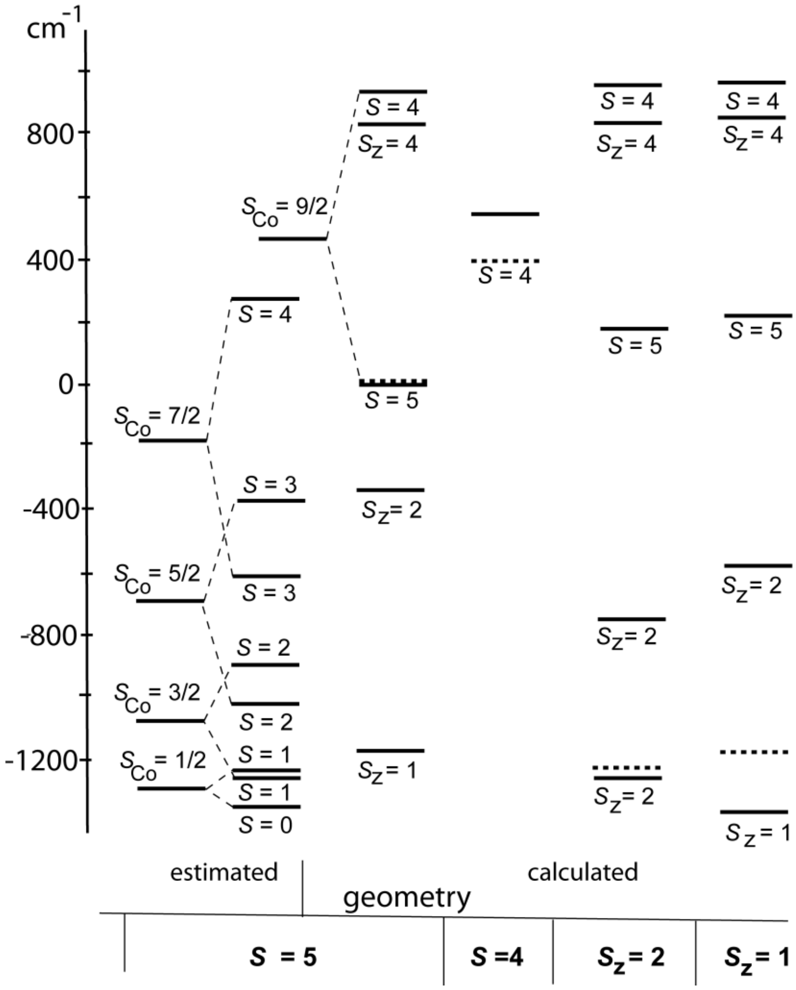


Fig. S18. Schematic energy levels in cm^{-1} for the $HAT(CN)_6{\cdot}(Co^{II}Cl_2)_3\}^{3-}$ complex. Estimated levels for the Co_3 system with total spin S_{Co} interacting with S = 1/2 spin of radical trianion for the equilibrium geometry of S = 5 state are given on the left. The geometry used for calculation of different spin states is specified in the bottom. Dashed lines show the position of levels corrected for a zero-point vibrational energy contribution.

complex found when optimizing the $S_z = 2$ and $S_z = 1$ states, as well as the optimized level $S = 4$ relative to the level $S = 5$. The dashed line shows the energy levels, taking into account the zero-point vibration energy contributions also calculated relative to level S=5. A comparison of these data shows that states with maximum spin are little sensitive to geometry variations in contrast to states with $S_z = 2$ and $S_z = 1$. This leads to a stronger perturbation of the position of the true optimized energy levels with small spin values. Therefore, the error of the calculated magnetic moment according to the Van Vleck equation will increase with decreasing temperature.

In case of 3 Fe atoms with spin 2, there are 1, 2, 3, 4, 5, 3 and 1 states with spin 6, 5, 4, 3, 2, 1 and 0 correspondingly. Each metal center has 4 unpaired electrons, $s = 2$, and $x_6 = \frac{1}{\sqrt{C_{12}^4}}$. In order to restore the contribution of other spin states to the state with $S_z = s$, the matrix element $< P_s^3>$ should be found as well. After algebraic transformations, one can find the values of the matrix elements $<P_s>$, $<P_s^2>$ and $< P_s^3>$, 4, 48 and 768, respectively, and then the total contribution of other states with the spin of the metal centers S_M = 2, 3, 4, 5 and 6 are 275 /495, 154/495, 54/495, 11/495 and 1/495, respectively. This allows one to find the parameters of the spin Hamiltonian $J_1 = -110.3$ cm^{-1} and $J_2 = -7.2$ cm^{-1} to describe all levels with spin from 1/2 to 13/2. Estimated and calculated energy levels for different geometries of $\{HAT(CN)_6{\cdot}(Fe^{II}Cl_2)_3\}^{3-}$ complex are shown in Fig. S19.

In contrast to the $\{HAT(CN)_6{\cdot}(Co^{II}Cl_2)_3\}^{3-}$ complex, the energy levels with high-spin projection $S_z = 11/2$ for the $\{HAT(CN)_6{\cdot}(Fe^{II}Cl_2)_3\}^{3-}$ complex are also sensitive to variations in its geometry. This will lead to perturbation of low-lying energy levels and to large errors in the theoretical magnetic moment at low temperatures.

For the $\{HATNA(CN)_6{\cdot}(Co^{II}I_2)_3\}^{3-}$ $\{HATNA(CN)_6{\cdot}(Fe^{II}I_2)_3\}^{3-}$ and complexes the same approach gives the parameters are $J_1 = -44.9$ and $J_2 = -37.3$ cm^{-1} and $J_1 = -47.9$ and $J_2 = -1.86$ cm^{-1} respectively. The energies of all found states and calculated spin states for these complexes are given in Tables S3 and S4.

Distributions of electronic and spin density in the ligands and complexes in the highest spin states are given in Table S5. Cartesian coordinates of calculated structures are given in the end of theoretical section.

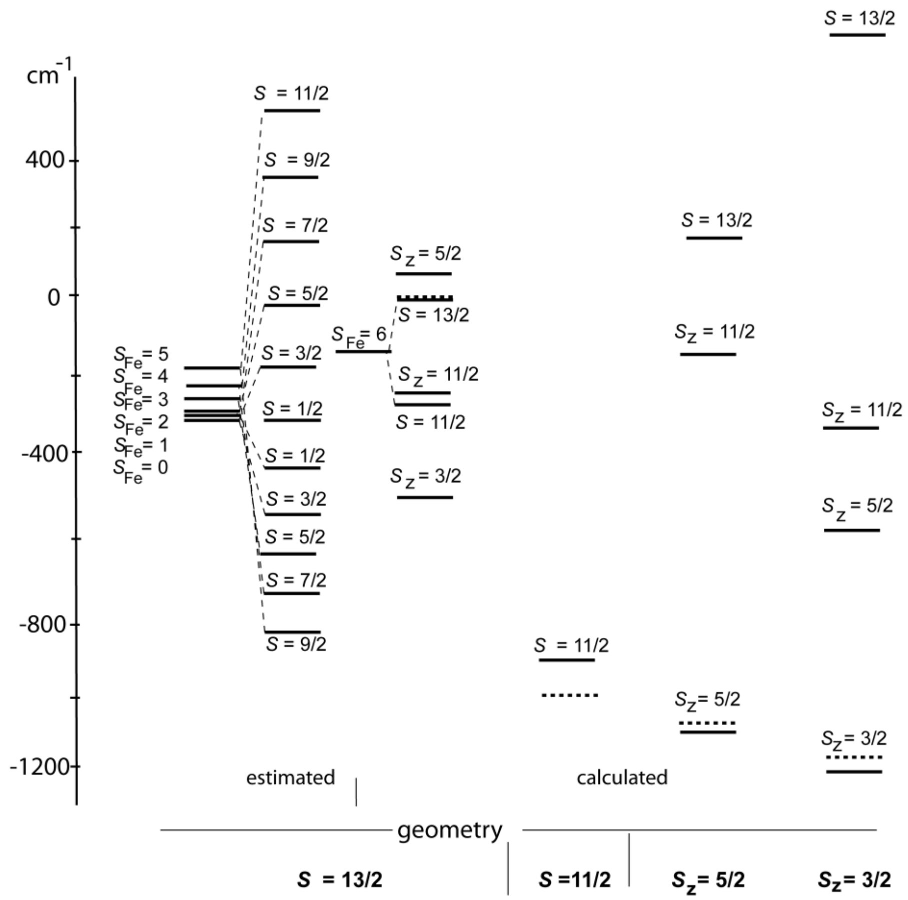


Fig. S19. Schematic energy levels in cm^{-1} for the $\{HAT(CN)_6 \cdot (Fe^{II}Cl_2)_3\}^{3-}$ complex. Estimated levels for the Fe_3 system with total spin S_{Fe} interacting with S = 1/2 spin of radical trianion for the equilibrium geometry of S = 13/2 state are given on the left. The geometry used for calculation of different spin states is specified in the bottom. Dashed lines show the position of levels corrected for zero-point vibrational energy contribution.

Table S3. The calculated and estimated positions of energy levels in the $\{HATNA(CN)_6 \cdot (Co^{II}I_2)_3\}^{3-}$ complex in cm^{-1}.[#]

Spin state	Geometry's type					
	{S=5}		{S_z=4}	{S=4}	{S_z=2}	{S_z=1}
S=6	4385* (4590)					
S_z=3	693** (923)					
S=5	0 (0)		209			
S_z=4	-398		-564 (-321)			
S=4	-442		-650	-653 (-410)		
S_z=2	-755				-914 (-903)	-368
S_z=1	-936				-940	-1472 (-1262)
	Estimated					
	$S=S_M+1/2$	$S=S_M-1/2$				
S_M=7/2	-478	-635				
S_M=5/2	-762	-874				
S_M=3/2	-971	-1038				
S_M=1/2	-1105	-1127				

[#]The values in parenthesis include zero point vibration energy contribution
* Calculate at optimized geometry of S=6 state
** Calculate at optimized geometry of S_z=3 state

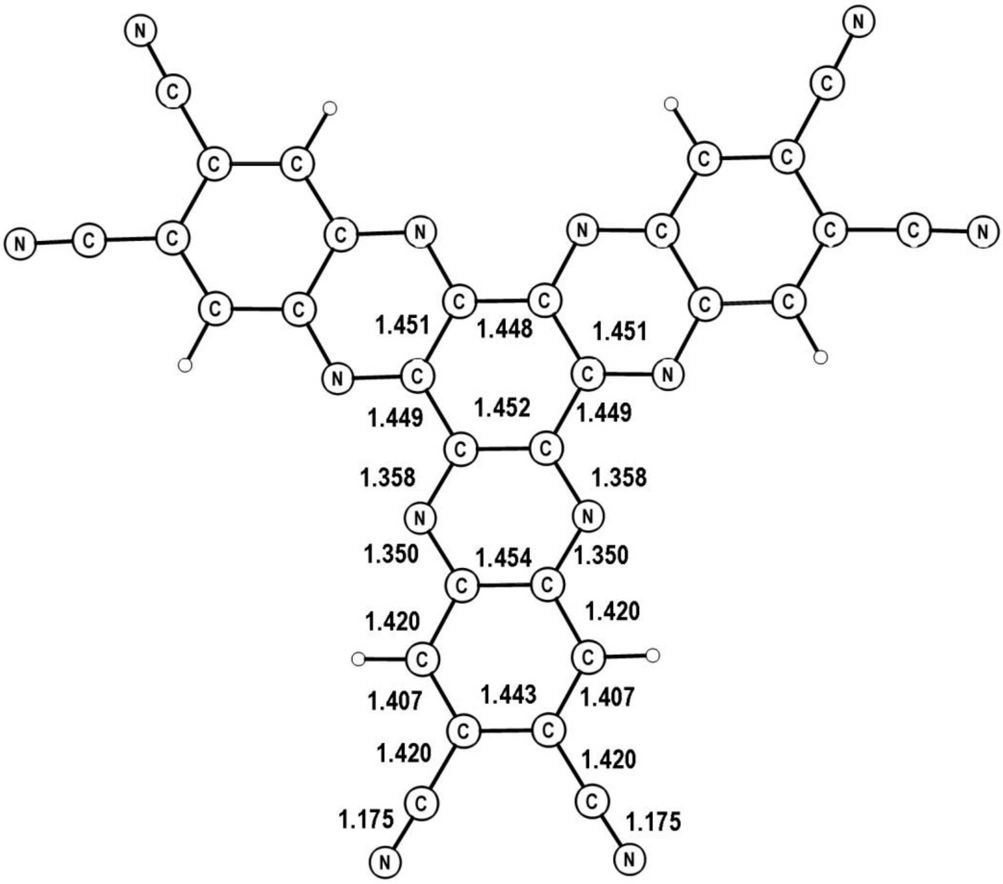
Table S4. The calculated and estimated positions of energy levels in the $\{HATNA(CN)_6 \cdot (Fe^{II}I_2)_3\}^{3-}$ complex in $cm^{-1\#}$

Spin state	Geometry's type					
	{S=13/2}		$\{S_z=11/2\}$	{S=11/2}	$\{S_z=5/2\}$	$\{S_z=3/2\}$
S=15/2	1686* (1906)					
$S_z=9/2$	1584** (1828)					
S=13/2	0 (0)		292		369	122
$S_z=11/2$	-737		-1048 (-740)		-586	-848
S=11/2	-799		-1159	-1161 (-853)		
$S_z=5/2$	-271				-769 (-724)	-324
$S_z=3/2$	-520				-229	-674 (-554)
	Estimated					
	$S=S_M+1/2$	$S=S_M-1/2$				
$S_M=5$	-182	-661				
$S_M=4$	-249	-632				
$S_M=3$	-312	-599				
$S_M=2$	-371	-563				
$S_M=1$	-426	-522				
$S_M=0$	-478					

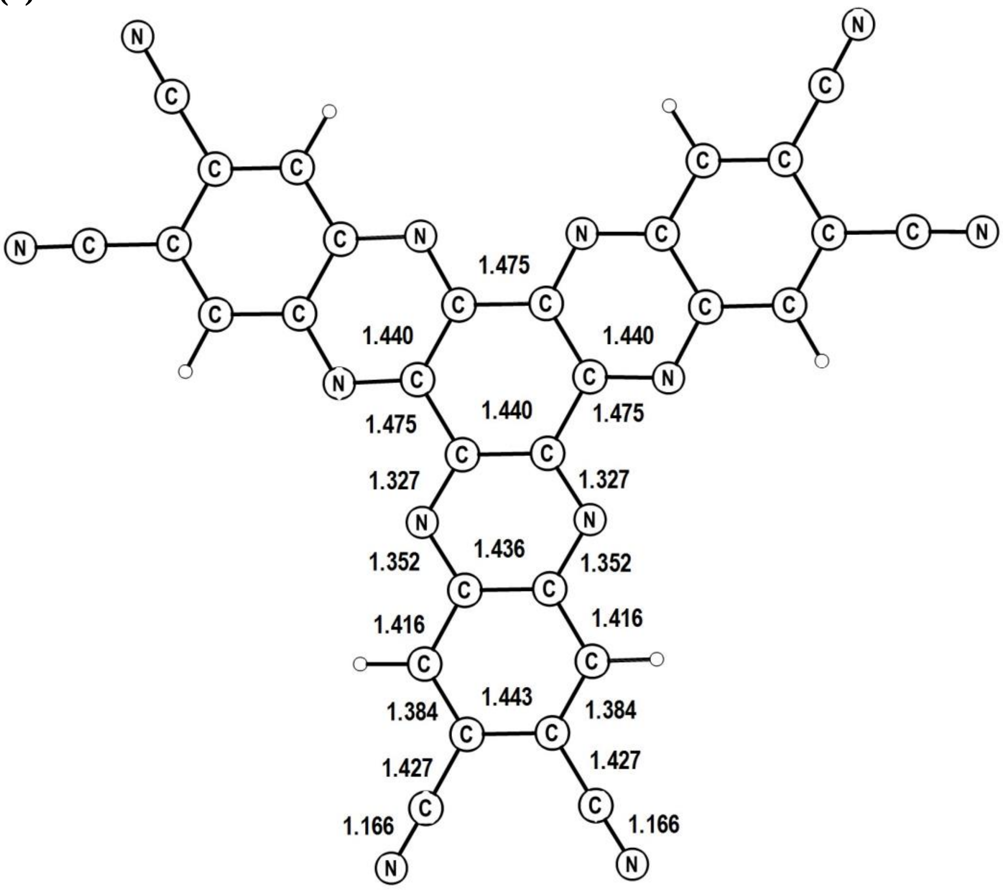
#The values in parenthesis include zero point vibration energy contribution
* Calculated at optimized geometry of S=15/2 state
** Calculated at optimized geometry of $S_z=9/2$ state

Table S5. The calculated charges and spin densities by Hirshfeld method [6] on selected atoms and atomic groups. The value of spin is maximal for the $3MX_2$ systems with open shells.

	6CN		6N		Macrocycle without 6CN		$3MX_2$	
	q	s	q	s	q	s	q	s
$HAT(CN)_6$	-0.35	0	-0.54	0	+0.35	0		
$\{HAT(CN)_6\}^{\bullet 3-}$	-1.83	0.67	-1.12	0.97	-1.17	2.33		
$\{HAT(CN)_6 \cdot (FeCl_2)_3\}^0$	-0.25	-0.13	-0.25	-0.13	+0.47	-0. 73	-0.22	12.86
$\{HAT(CN)_6 \cdot (FeCl_2)_3\}^{3-}$	-1.16	0.43	-0.63	1.20	-0.30	2.42	-1.54	12.15
$\{HAT(CN)_6 \cdot (CoCl_2)_3\}^0$	-0.21	-0.12	-0.29	-0.14	+0.60	-0.57	-0.39	9.69
$\{HAT(CN)_6 \cdot (CoCl_2)_3\}^{3-}$	-1.11	0.44	-0.54	1.31	-0.17	2.59	-1.72	8.97
$HATNA(CN)_6$	-0.57	0	-0.65	0	+0.57	0		
$\{HATNA(CN)_6\}^{\bullet 3-}$	-1.64	0.36	-1.08	0.80	-1.36	2.64		
$\{HATNA(CN)_6 \cdot (FeI_2)_3\}^0$	-0.52	-0.07	-0.23	-0.18	+0.63	-0.76	-0.11	12.83
$\{HATNA(CN)_6 \cdot (FeI_2)_3\}^{3-}$	-1.22	0.16	-0.66	1.12	-0.37	2.49	-1.41	12.35
$\{HATNA(CN)_6 \cdot (CoI_2)_3\}^0$	-0.50	-0.05	-0.35	0.02	+0.80	-0.38	-0.30	9.43
$\{HATNA(CN)_6 \cdot (CoI_2)_3\}^{3-}$	-1.21	0.18	-0.56	1.22	-0.19	2.78	-1.60	9.08



(a)



(b)

Fig. S20. Geometry of HATNA(CN)$_6$ (a) and HATNA(CN)$_6$$^{\bullet 3-}$ in quartet *S* = 3/2 spin state (b).

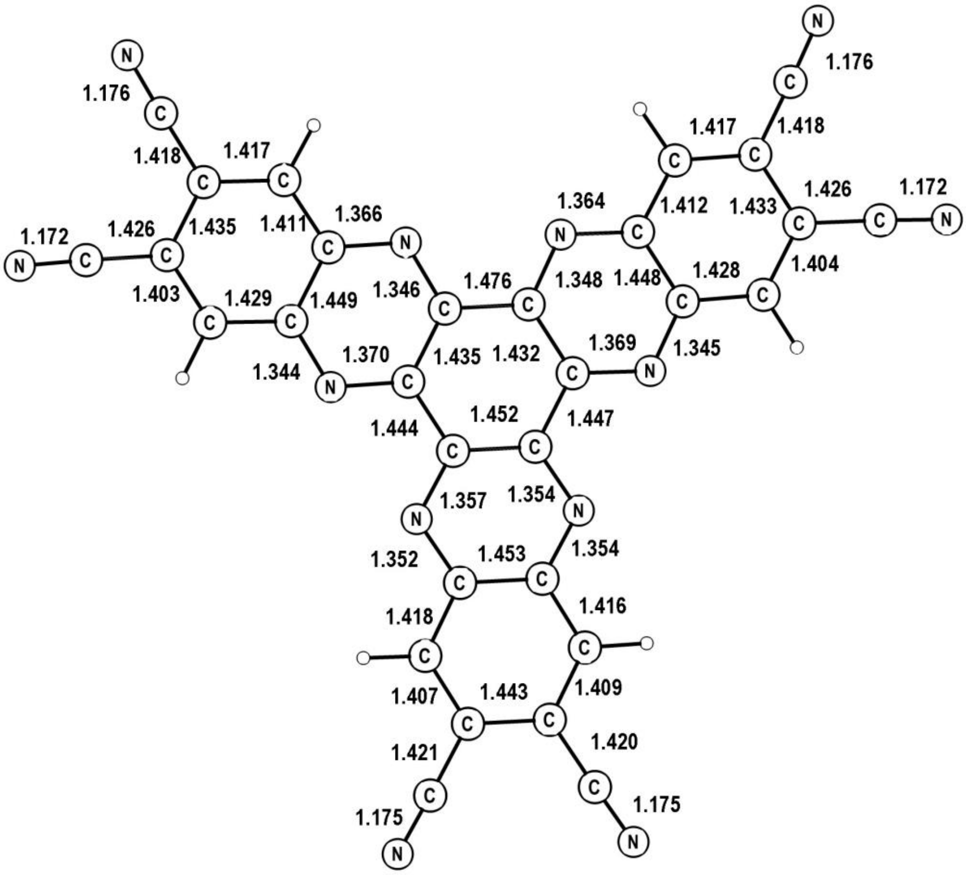


Fig. S21. Geometry of HATNA(CN)$_6^{\bullet 3-}$ in doublet S = 1/2 spin state.

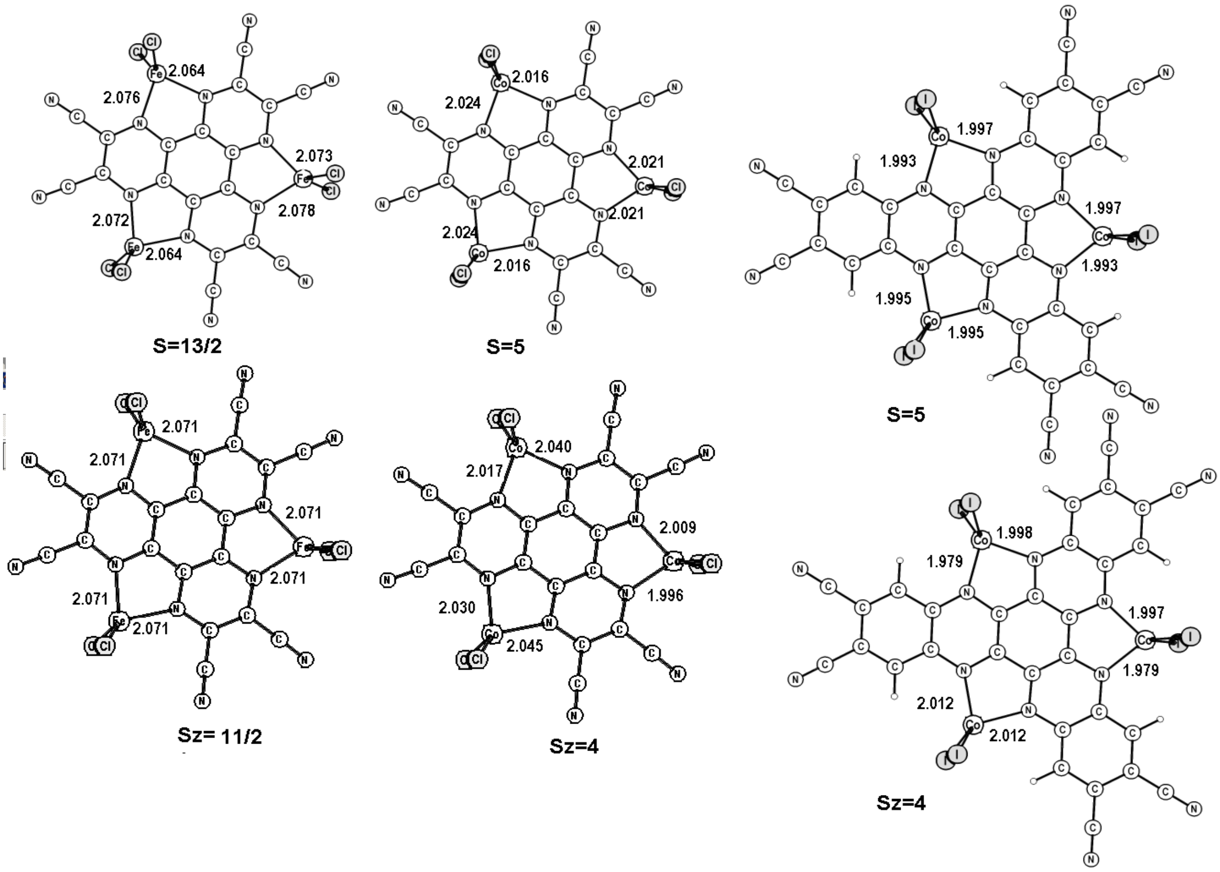


Fig. S22. Calculated lengths of M-N bonds in the $\{HAT(CN)_6 \cdot 3M^{II}(Hal)_2\}^{3-}$ trianions, where M = Co, Fe, Hal is Cl or I.

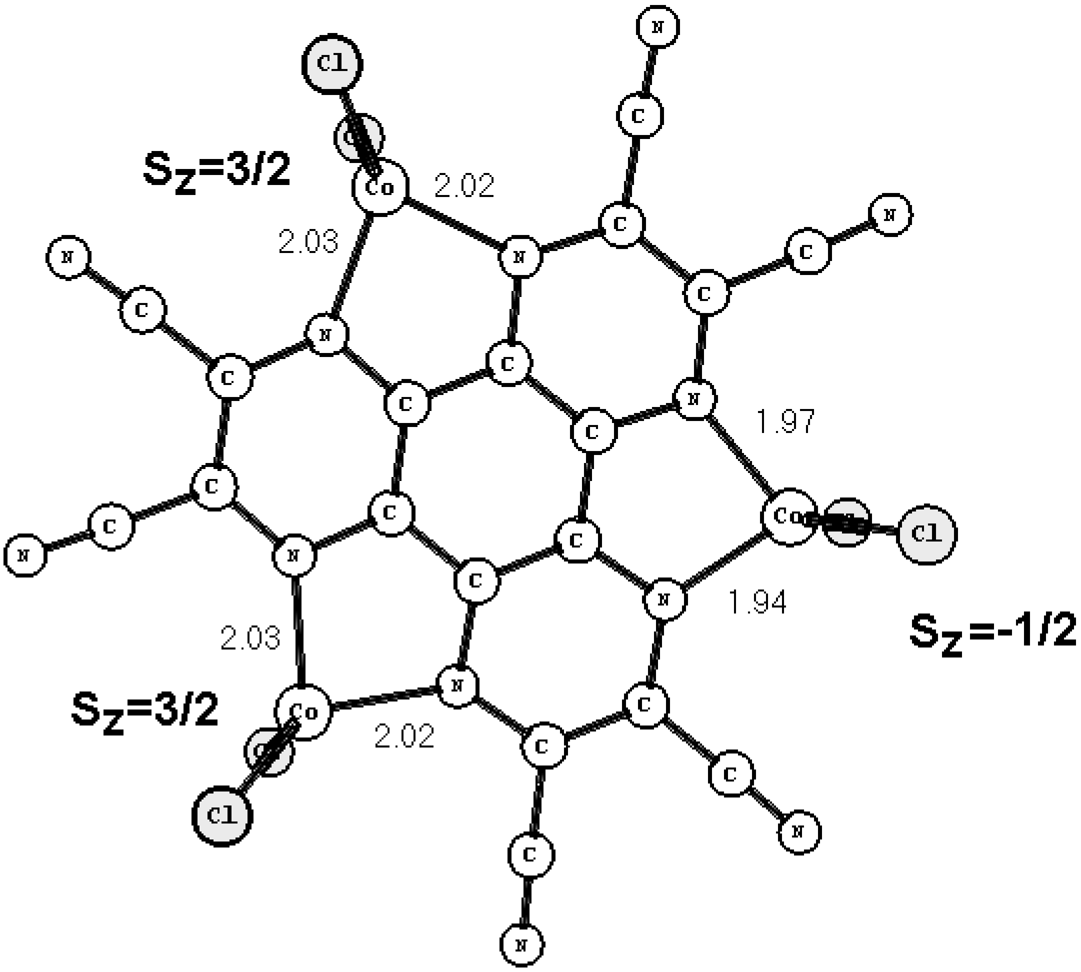


Fig. S23. Calculated geometry of the $\{HAT(CN)_6{\cdot}(Co^{II}Cl_2)_3\}^{3-}$ trianion having state with the +3/2, -1/2, +3/2 and -1/2 projections and described the system with one low (S = 1/2) spin and two high-spin (S = 3/2) Co^{II} centers.

Cartesian coordinates of calculated structures

$HAT(CN)_6$, S = 0

7	3.80612687	4.19465269	2.33406174
6	3.02004348	3.37129282	2.08570913
6	1.30238039	0.71321197	-3.28893150
7	1.50619803	1.14030916	-2.04614218
7	1.88689021	1.97359157	0.54798339
7	0.36679085	0.83594712	2.63105246
6	0.34103282	-0.30774036	-3.57922992
7	-1.87270876	-1.97647230	-0.58480861
6	2.04621251	2.35667144	1.81144764
6	1.27383534	1.77867368	2.86983078
7	-0.38910542	-0.86590679	-2.61807173
7	-1.49750783	-1.10794514	2.07018472
6	-2.38743209	-2.04872260	1.76776241
6	-2.57641731	-2.49166916	0.41910226
6	-0.18663206	-0.43349894	-1.36202012
6	-0.97495510	-1.02375737	-0.28149709
6	0.20479166	0.44721700	1.35501063
6	-0.78397892	-0.58772478	1.05731946
6	0.97114014	1.02073837	0.30485912
6	0.77079985	0.57596034	-1.07333707
7	2.69527836	1.77696064	-5.20646122
6	2.07715331	1.30844420	-4.33701150
7	1.62667135	2.56306343	5.32112365
6	1.45821115	2.20219025	4.22617188
7	-0.00999186	-1.11218094	-6.02428394
6	0.13758229	-0.76080739	-4.92324484
7	-3.79628460	-3.08238019	3.69008696
6	-3.15787627	-2.61023286	2.83742004
7	-4.32242551	-4.33964144	-0.11483207
6	-3.53582290	-3.51024444	0.11074549

$HAT(CN)_6^{\bullet-}$, S = 1/2

7	3.79944612	4.19790014	2.33259860
6	3.01175361	3.37145067	2.09328233
6	1.30121484	0.70354874	-3.28899989
7	1.51996737	1.14565612	-2.03872692
7	1.89221938	1.97811953	0.53458728
7	0.35650309	0.82854304	2.63925302
6	0.34394399	-0.30025156	-3.57731930
7	-1.87653658	-1.97413277	-0.60053847
6	2.03985482	2.35496225	1.81626100
6	1.27585125	1.78305253	2.86331735
7	-0.40419856	-0.87208753	-2.61826719
7	-1.48806968	-1.10598347	2.08367111
6	-2.38375068	-2.05475963	1.76106691
6	-2.57703418	-2.48663351	0.42568790
6	-0.18809092	-0.43093386	-1.35841563
6	-0.97392551	-1.01911835	-0.28149965
6	0.20397002	0.44560576	1.35137201

6	-0.78055443	-0.58687862	1.05483797
6	0.96852864	1.01792944	0.30355630
6	0.76981390	0.57365451	-1.06989811
7	2.70954122	1.76055584	-5.20173081
6	2.08137686	1.29083994	-4.33829218
7	1.62110588	2.56739993	5.31786096
6	1.46066625	2.21042708	4.21896147
7	-0.01980309	-1.10133789	-6.02377282
6	0.13785110	-0.74691283	-4.92364636
7	-3.77954314	-3.09666233	3.69119362
6	-3.14952506	-2.62461871	2.83037903
7	-4.33058670	-4.32801467	-0.11611916
6	-3.54198983	-3.50131980	0.11933965

$HAT(CN)_6^{2-}$, $S = 0$

7	3.79916877	4.19826300	2.34325019
6	3.00848118	3.36961845	2.10598123
6	1.29913542	0.70176477	-3.29181396
7	1.52917943	1.15625144	-2.03576301
7	1.89978652	1.98393322	0.52388829
7	0.34858533	0.82280722	2.64973873
6	0.34681287	-0.29801217	-3.57871132
7	-1.87781798	-1.97900429	-0.61398506
6	2.03929935	2.35472357	1.82011099
6	1.27877818	1.78544430	2.86237381
7	-0.41334997	-0.88281907	-2.62095562
7	-1.48647606	-1.10107379	2.09706067
6	-2.38607787	-2.05674520	1.75860664
6	-2.57788660	-2.48723591	0.42944546
6	-0.18762175	-0.43017764	-1.35438120
6	-0.97083526	-1.01641290	-0.28104609
6	0.20303182	0.44415519	1.34763070
6	-0.77827155	-0.58484089	1.05207331
6	0.96579931	1.01511378	0.30229127
6	0.76768951	0.57237292	-1.06660481
7	2.70436961	1.75689394	-5.21053028
6	2.07369109	1.28374939	-4.34652015
7	1.62928557	2.57415822	5.31686514
6	1.47018999	2.21822188	4.21408088
7	-0.01193761	-1.09623902	-6.02893276
6	0.14780164	-0.73872822	-4.92675112
7	-3.78713869	-3.10211721	3.68569744
6	-3.15621500	-2.63095844	2.82078163
7	-4.33361439	-4.33109613	-0.10632726
6	-3.54384287	-3.50201041	0.13244625

$HAT(CN)_6^{2-}$, $S = 1$

7	3.81864346	4.21262867	2.32455153
6	3.02714143	3.38309467	2.08504879
6	1.31310141	0.71485772	-3.30728075
7	1.51715234	1.14334013	-2.05485515
7	1.89589479	1.98373961	0.54949760

7	0.36748460	0.83961470	2.64417659
6	0.34123268	-0.30848173	-3.60026493
7	-1.88474132	-1.98287931	-0.58923224
6	2.05703918	2.37170332	1.82123437
6	1.27973514	1.78983753	2.88656479
7	-0.39473356	-0.86781763	-2.63105004
7	-1.50103931	-1.11602075	2.08154521
6	-2.39825498	-2.06328316	1.77901208
6	-2.59296861	-2.50460696	0.42073217
6	-0.20080802	-0.44594550	-1.36619050
6	-0.97890723	-1.02832704	-0.29985159
6	0.19450689	0.43939549	1.36926230
6	-0.78072697	-0.58253302	1.07554960
6	0.98149970	1.02850637	0.29065970
6	0.78433040	0.58900581	-1.06933707
7	2.72252074	1.78182752	-5.21010479
6	2.09295672	1.30818319	-4.34334349
7	1.61646127	2.56414856	5.34269641
6	1.45555956	2.20665737	4.23893712
7	-0.02842900	-1.11974829	-6.03968330
6	0.12921016	-0.76215868	-4.93548525
7	-3.78972991	-3.09328758	3.71511241
6	-3.15608684	-2.62119602	2.85047566
7	-4.33933747	-4.34566418	-0.13271054
6	-3.54870724	-3.51459079	0.10433330

$HAT(CN)_6^{3-}$, S = 3/2

7	3.82055777	4.21906353	2.33021012
6	3.02451122	3.38515035	2.09602317
6	1.31454988	0.71151864	-3.31480615
7	1.52842895	1.15083996	-2.05262025
7	1.90306966	1.99006089	0.54014766
7	0.36030884	0.83515267	2.65451948
6	0.34412419	-0.30516252	-3.60703384
7	-1.88881215	-1.98591673	-0.60191261
6	2.05819831	2.37564453	1.82821621
6	1.28407738	1.79611379	2.88918024
7	-0.40527152	-0.87553365	-2.63495186
7	-1.49782969	-1.11449543	2.09479924
6	-2.40220935	-2.07059521	1.77883838
6	-2.59855186	-2.50770771	0.42563995
6	-0.20006267	-0.44344229	-1.36344112
6	-0.97752732	-1.02530274	-0.29804782
6	0.19497231	0.43910934	1.36557950
6	-0.77899462	-0.58236262	1.07222189
6	0.97890802	1.02595539	0.29119252
6	0.78234578	0.58640410	-1.06756911
7	2.72970178	1.77641013	-5.21729118
6	2.09270303	1.29846131	-4.35141477
7	1.61879836	2.57107124	5.34753438
6	1.46221695	2.21574941	4.23705093
7	-0.03005373	-1.11511626	-6.04835838

6	0.13414960	-0.75300265	-4.94117468
7	-3.79040894	-3.10404434	3.71816373
6	-3.15856370	-2.63224447	2.84516832
7	-4.34846830	-4.34751527	-0.13023795
6	-3.55486818	-3.51426340	0.11437403

$HAT(CN)_6^{3-}$, S = 1/2

7	3.82953756	4.22091819	2.33041999
6	3.03202159	3.38748302	2.09799426
6	1.31770090	0.72071767	-3.32009149
7	1.51450973	1.14510454	-2.05251168
7	1.90426388	1.99056438	0.54784703
7	0.36664667	0.83964689	2.65504554
6	0.34067486	-0.31291181	-3.61274223
7	-1.89177604	-1.99467132	-0.59501678
6	2.06435786	2.37954626	1.83461324
6	1.28999538	1.79993912	2.89581610
7	-0.39721178	-0.87602092	-2.64317696
7	-1.50111146	-1.11219362	2.08026405
6	-2.40909204	-2.06893722	1.78733108
6	-2.60110605	-2.51490138	0.41880624
6	-0.20892322	-0.45586950	-1.36886152
6	-0.98007732	-1.03312367	-0.31201270
6	0.19634991	0.44151194	1.37266561
6	-0.78131625	-0.58229237	1.07533031
6	0.98412303	1.03116709	0.29307558
6	0.78385736	0.58928122	-1.06965877
7	2.72571447	1.79675891	-5.21648882
6	2.09282311	1.31609955	-4.34655221
7	1.62198684	2.56846458	5.35579261
6	1.46593306	2.21520970	4.24425050
7	-0.03084240	-1.13233543	-6.05084164
6	0.12853746	-0.76940330	-4.94304314
7	-3.80018027	-3.08822980	3.72707488
6	-3.16224477	-2.61757784	2.85535268
7	-4.34348929	-4.36005228	-0.14095073
6	-3.55166278	-3.52389259	0.10026896

$HATNA(CN)_6$, S = 0

6	2.24765230	-1.68655298	4.12182213
6	1.68830662	-0.91869288	3.07162954
7	1.08467152	-1.55229681	2.04102383
7	-0.14591871	-2.77966997	-0.06437074
7	-1.26092510	-1.22374388	-2.15970740
6	-1.32495308	-2.57414688	-2.17881184
6	-0.76083237	-3.36135687	-1.11869154
6	1.77137798	0.51403281	3.11887554
7	0.17631005	2.77613937	0.11868857
6	-1.96126490	-3.21982888	-3.26672780
6	-0.84775232	-4.77370658	-1.17414130

7	1.24885434	1.27938328	2.13440352
6	2.41161938	1.14155088	4.21509451
7	-1.10301762	1.50027547	-2.06985428
6	-1.01063448	2.84734245	-2.00008434
6	-1.56402435	3.63215230	-3.04085391
6	-0.36332086	3.49287683	-0.89278667
6	-0.28626131	4.90638764	-0.85517420
1	2.17626557	-2.77229759	4.07095116
1	2.46622189	2.22925957	4.23592415
1	0.20807880	5.38067361	-0.00828342
1	-0.41479025	-5.35641455	-0.36202208
1	-2.38410133	-2.60831878	-4.06284848
1	-2.05166876	3.12712108	-3.87373309
6	0.65892652	0.64640230	1.12820227
6	0.07948454	1.45498198	0.03928277
6	-0.65510536	-0.66417103	-1.11999844
6	-0.56976037	0.80745208	-1.07147934
6	-0.08919827	-1.45382107	-0.05660414
6	0.57559124	-0.79075220	1.08081618
7	-2.50694833	6.41470077	-4.91614846
6	-2.04297945	5.79325309	-4.04609910
6	-1.48186658	5.01287441	-2.99184649
6	-0.83123028	5.66170176	-1.87892178
6	-0.74760668	7.08505204	-1.83027865
7	-0.66996086	8.24661791	-1.77383191
7	4.11803874	1.56494545	7.22462916
6	3.59680478	1.02248685	6.33440283
6	2.95415872	0.37933021	5.23500872
6	2.87067899	-1.06069330	5.18750902
6	3.43058879	-1.84454506	6.23983657
7	3.88231088	-2.50085816	7.09051247
7	-3.21213728	-5.74574642	-5.31694588
6	-2.68282223	-5.24049930	-4.40975170
6	-2.03936379	-4.60101958	-3.30870231
6	-1.47236923	-5.39224871	-2.24316454
6	-1.55392115	-6.81583517	-2.28829019
7	-1.61120636	-7.97977750	-2.30845894

HATNA(CN)$_6^{-}$, S = 1/2

6	-2.11866138	4.36030738	1.16880427
6	-1.25511590	3.26339891	0.94786701
7	-1.75673324	2.12400750	0.40901560
7	-2.69854422	-0.18931532	-0.66853031
7	-0.93006792	-2.38531623	-1.10001065
6	-2.24596908	-2.46199977	-1.42042261
6	-3.13608873	-1.35666740	-1.20330428
6	0.13229129	3.37942059	1.29831279
7	2.68672009	0.26118135	0.69153798
6	-2.75102639	-3.65747742	-1.98032315
6	-4.49902952	-1.48654840	-1.55439224
7	0.99974651	2.35451747	1.10524250
6	0.60609618	4.58817560	1.85700241

7	1.69864949	-2.16542496	-0.43617547
6	3.00370264	-2.02285488	-0.09471561
6	3.89293394	-3.10163231	-0.30267201
6	3.50100256	-0.80142662	0.47276772
6	4.86968861	-0.70283436	0.81158237
1	-3.16853209	4.25518418	0.89717895
1	1.66170864	4.65914163	2.11721719
1	5.23037104	0.23121977	1.24113367
1	-5.16061123	-0.63803112	-1.38295924
1	-2.06180806	-4.48637945	-2.13832210
1	3.49887834	-4.02113657	-0.73428851
6	0.49377466	1.23844029	0.57439639
6	1.40428597	0.10826376	0.35125776
6	-0.51168545	-1.23103555	-0.57457252
6	0.90738420	-1.11232328	-0.21618597
6	-1.40136605	-0.12642985	-0.35727733
6	-0.89290562	1.12246897	0.22414484
7	6.81175684	-5.01131979	-0.37473956
6	6.11312038	-4.09606680	-0.18576396
6	5.23846127	-2.99248644	0.03496551
6	5.73547662	-1.77184904	0.60192282
6	7.11113227	-1.64499619	0.95283215
7	8.23327471	-1.51992725	1.24715656
7	0.68426679	7.84762173	3.09858780
6	0.25066321	6.86859367	2.63494340
6	-0.25390925	5.66123385	2.06984641
6	-1.64038062	5.54529806	1.71963704
6	-2.53346583	6.63572766	1.93179638
7	-3.28152747	7.51582877	2.09702173
7	-4.95156664	-5.99569512	-3.34468634
6	-4.57752422	-4.99056120	-2.88504418
6	-4.09500969	-3.77332749	-2.32186048
6	-4.98447274	-2.66867317	-2.10510486
6	-6.36361386	-2.77231304	-2.44989683
7	-7.49577104	-2.83598213	-2.72492300

HATNA$(CN)_6^{2-}$, $S = 0$

6	-2.11498223	4.36540294	1.17152847
6	-1.25708890	3.26453968	0.94784814
7	-1.76073952	2.12562674	0.40870922
7	-2.70243857	-0.18748989	-0.66874116
7	-0.92930216	-2.38937004	-1.10128830
6	-2.24594192	-2.46412578	-1.42117502
6	-3.13823522	-1.35603823	-1.20356235
6	0.13375406	3.38085186	1.29917138
7	2.68991357	0.26354219	0.69311946
6	-2.75780377	-3.65661321	-1.98143038
6	-4.49995186	-1.49282328	-1.55701716
7	1.00306493	2.35676616	1.10681004
6	0.60073228	4.59252783	1.85746113
7	1.69924034	-2.16949035	-0.43750405

6	3.00440691	-2.02492901	-0.09530591
6	3.89923091	-3.09968282	-0.30050916
6	3.50297487	-0.80049569	0.47354639
6	4.87276455	-0.70881566	0.80997712
1	-3.16528704	4.26012229	0.89974422
1	1.65681853	4.66339347	2.11775166
1	5.23348526	0.22570375	1.23968038
1	-5.16169720	-0.64384478	-1.38549476
1	-2.06820687	-4.48582241	-2.13941442
1	3.50488380	-4.01954275	-0.73229540
6	0.49194795	1.23369587	0.57221584
6	1.39903895	0.10792646	0.34998027
6	-0.50967242	-1.22641570	-0.57235934
6	0.90388266	-1.10817958	-0.21536899
6	-1.39605155	-0.12587481	-0.35589396
6	-0.88957155	1.11815833	0.22326130
7	6.81633548	-5.02232699	-0.37783889
6	6.12237117	-4.10112364	-0.18561183
6	5.25384626	-2.99660477	0.03681990
6	5.74912380	-1.78027667	0.60173346
6	7.12114121	-1.64824156	0.95374100
7	8.24415208	-1.51558225	1.25106401
7	0.69164065	7.85614390	3.10347054
6	0.24999003	6.87842993	2.63852627
6	-0.25890367	5.67578059	2.07422556
6	-1.64047655	5.56024437	1.72524196
6	-2.53619222	6.64538631	1.93484792
7	-3.29158961	7.52292467	2.09749560
7	-4.95241021	-6.00712425	-3.34907795
6	-4.58484501	-4.99697814	-2.88902003
6	-4.10857961	-3.77984824	-2.32728893
6	-4.99487529	-2.67906230	-2.11135293
6	-6.37219057	-2.77702868	-2.45366633
7	-7.50770674	-2.83341585	-2.72675396

HATNA$(CN)_6^{2-}$, S = 1

6	-2.11670015	4.38211505	1.17732203
6	-1.26753982	3.26347260	0.94509183
7	-1.77916814	2.14242493	0.41090262
7	-2.71272922	-0.19523847	-0.67382504
7	-0.93988459	-2.39592852	-1.10635192
6	-2.24926318	-2.47055318	-1.42442948
6	-3.14592919	-1.35721892	-1.20564943
6	0.12657895	3.37930009	1.29703018
7	2.67143557	0.25410540	0.68554831
6	-2.76209738	-3.66351069	-1.98516947
6	-4.50852972	-1.49527420	-1.55960081
7	0.98807386	2.34261497	1.09824920
6	0.60785007	4.57872752	1.85392905
7	1.71124125	-2.19018685	-0.44284998
6	3.00031990	-2.03380087	-0.09963651
6	3.91555225	-3.10557666	-0.29924624

6	3.49934823	-0.80636153	0.47057396
6	4.86059503	-0.69867326	0.81122982
1	-3.16931609	4.29022927	0.90997402
1	1.66575810	4.63732815	2.11005763
1	5.20940822	0.24072073	1.24024719
1	-5.16977971	-0.64553844	-1.38754625
1	-2.07124521	-4.49223142	-2.14281998
1	3.53417729	-4.03110402	-0.73035947
6	0.47371187	1.23052671	0.56694866
6	1.39072895	0.09255350	0.34232290
6	-0.50538611	-1.23961290	-0.57654449
6	0.89220597	-1.12692974	-0.22516424
6	-1.40884757	-0.11801094	-0.35582824
6	-0.91251568	1.11281249	0.21611305
7	6.83825521	-5.00143035	-0.36514747
6	6.13810978	-4.08546694	-0.17626538
6	5.26031684	-2.98389298	0.04299862
6	5.75388865	-1.76355618	0.60917212
6	7.12072588	-1.62336704	0.96320935
7	8.24346692	-1.48307398	1.26342922
7	0.72578886	7.84639410	3.10742141
6	0.27602058	6.87114767	2.64158951
6	-0.24023201	5.67561897	2.07831245
6	-1.62563736	5.56278373	1.72940538
6	-2.51569099	6.65561998	1.94305613
7	-3.26370811	7.53755347	2.10890413
7	-4.95560216	-6.01209493	-3.35179578
6	-4.58264303	-5.00351890	-2.89107850
6	-4.10711263	-3.78772594	-2.32995206
6	-5.00232363	-2.67611451	-2.11172242
6	-6.37814497	-2.77410689	-2.45354531
7	-7.51353156	-2.83595011	-2.72851031

HATNA(CN)$_6^{3-}$, S = 1/2

6	-2.11499733	4.38926908	1.18038269
6	-1.26825327	3.26573290	0.94576848
7	-1.77783604	2.14537714	0.41227023
7	-2.71642129	-0.19406747	-0.67422528
7	-0.93942257	-2.39904430	-1.10739782
6	-2.25018203	-2.47442171	-1.42606968
6	-3.15002937	-1.35679238	-1.20641118
6	0.12959840	3.38554534	1.30003520
7	2.67931561	0.25602970	0.68799654
6	-2.76939751	-3.66391689	-1.98690452
6	-4.51118511	-1.50202823	-1.56275355
7	0.99208697	2.34898644	1.10150493
6	0.60256800	4.58907639	1.85665678
7	1.71448369	-2.18946231	-0.44184055
6	3.00267434	-2.03483255	-0.09949110
6	3.92325158	-3.10585563	-0.29761793
6	3.50651027	-0.80514320	0.47260164
6	4.87010674	-0.70617822	0.81048473

1	-3.16827213	4.29646351	0.91253948
1	1.66101770	4.64942254	2.11356743
1	5.22105793	0.23314136	1.23992496
1	-5.17363453	-0.65207671	-1.39090358
1	-2.07840966	-4.49358128	-2.14486121
1	3.54058633	-4.03165110	-0.72909442
6	0.47578254	1.22890287	0.56678047
6	1.38953226	0.09501038	0.34296570
6	-0.50472576	-1.23422407	-0.57437998
6	0.89069961	-1.12021158	-0.22297866
6	-1.40333028	-0.11838476	-0.35476791
6	-0.90650241	1.10955655	0.21619871
7	6.83817446	-5.02047139	-0.37225690
6	6.14549225	-4.09600056	-0.17855798
6	5.27627026	-2.99213860	0.04344047
6	5.77419302	-1.77543621	0.60917462
6	7.13714591	-1.63711145	0.96162896
7	8.26349848	-1.49515318	1.26324305
7	0.71998073	7.86726770	3.11403343
6	0.26672231	6.88954452	2.64648476
6	-0.24676839	5.69730330	2.08503433
6	-1.62979818	5.57934005	1.73471947
6	-2.52478996	6.66494161	1.94457541
7	-3.28371857	7.54231410	2.10630542
7	-4.95362837	-6.02903216	-3.35765174
6	-4.59025432	-5.01271334	-2.89617562
6	-4.12318381	-3.79778401	-2.33726805
6	-5.01656440	-2.68807248	-2.11938011
6	-6.38939697	-2.77834940	-2.45767042
7	-7.53004713	-2.82909031	-2.72965969

HATNA(CN)$_6^{3-}$, S = 3/2

6	-2.11796496	4.37852749	1.17580970
6	-1.26430045	3.27078379	0.94860583
7	-1.76381411	2.13966247	0.41334545
7	-2.71434319	-0.19502988	-0.67410919
7	-0.94024518	-2.39798390	-1.10721386
6	-2.24751122	-2.47283255	-1.42489469
6	-3.14766716	-1.35503585	-1.20522026
6	0.13878113	3.38814966	1.30299849
7	2.70403046	0.25812304	0.69424469
6	-2.76803931	-3.66474400	-1.98692300
6	-4.51122789	-1.49980463	-1.56191992
7	1.00145873	2.37095160	1.11176490
6	0.59930851	4.60585779	1.86211270
7	1.71287436	-2.17607129	-0.43726603
6	3.00888843	-2.03320207	-0.09755862
6	3.91195085	-3.10599949	-0.30024602
6	3.51181544	-0.79805316	0.47644749
6	4.88598259	-0.71386358	0.81118435
1	-3.16922185	4.27280376	0.90365282
1	1.65647142	4.67649940	2.12251302

1	5.24671158	0.22164364	1.24140501
1	-5.17335223	-0.64985212	-1.38998176
1	-2.07751821	-4.49454315	-2.14504366
1	3.51692664	-4.02657069	-0.73255956
6	0.50225037	1.23090972	0.57337846
6	1.39900415	0.11794010	0.35365493
6	-0.50051912	-1.23196032	-0.57262168
6	0.89695794	-1.11507658	-0.21971507
6	-1.39927450	-0.11611124	-0.35299423
6	-0.89854135	1.11374958	0.21958268
7	6.82537934	-5.04076837	-0.38275735
6	6.13242947	-4.11362125	-0.18808968
6	5.27201632	-3.01050148	0.03560196
6	5.77138625	-1.78408616	0.60537995
6	7.13670907	-1.64698053	0.95796840
7	8.26304148	-1.50918283	1.25807277
7	0.70328491	7.87166232	3.11177180
6	0.25565658	6.89221307	2.64488226
6	-0.25662364	5.69694461	2.08263905
6	-1.64971557	5.58037803	1.73075088
6	-2.54637009	6.65770052	1.93718927
7	-3.30844747	7.53570370	2.09850899
7	-4.95479199	-6.02650650	-3.35698666
6	-4.59042808	-5.01067426	-2.89546762
6	-4.12166005	-3.79622862	-2.33635679
6	-5.01536726	-2.68631591	-2.11845532
6	-6.38793998	-2.77824476	-2.45730723
7	-7.52843116	-2.83035911	-2.7297776

Complex $\{HAT(CN)_6 \cdot (FeCl_2)_3\}^{3-}$, S = 13/2

7	4.11042644	3.84865570	2.46314944
6	3.28705768	3.07247620	2.17411171
6	1.23471767	0.77921191	-3.30952406
7	1.54358230	1.13951277	-2.02494306
7	2.04158372	1.85498307	0.53910919
7	0.47788269	0.66357158	2.65267799
6	0.19374283	-0.14035787	-3.60955685
7	-2.06614635	-1.79119594	-0.64827083
6	2.25887125	2.13285888	1.85403404
6	1.50936075	1.56359032	2.90329291
7	-0.56761539	-0.72594146	-2.63295078
7	-1.43440510	-1.12913970	2.08958385
6	-2.44292882	-2.02640300	1.75168125
6	-2.73882795	-2.32749611	0.40721195
6	-0.27372412	-0.35537605	-1.34170864
6	-1.04164638	-0.90773197	-0.30573278
6	0.27182276	0.36374352	1.34351582
6	-0.76063505	-0.58850652	1.04147622
6	1.02335224	0.93485930	0.29148498
6	0.77297797	0.56897216	-1.04060775
7	2.63468192	1.75639465	-5.25873286
6	2.00761669	1.32947834	-4.36753576

7	2.01838474	2.25481196	5.34491746
6	1.78062215	1.92685809	4.24573172
7	-0.23263871	-0.77649068	-6.08488783
6	-0.05759064	-0.49452804	-4.96253670
7	-3.77958384	-3.19028071	3.63770306
6	-3.17120979	-2.65074592	2.79449090
7	-4.70141857	-3.95616423	-0.08063830
6	-3.81000302	-3.22996317	0.12417022
26	2.93873031	2.45001811	-1.22213261
17	5.08042446	1.77748710	-1.21017895
17	2.48523721	4.53680486	-1.91518702
26	-2.16158757	-2.04849161	-2.69435967
17	-1.69838843	-4.19376907	-3.16923597
17	-3.88993326	-1.08205147	-3.75295173
26	-0.79274855	-0.37759417	3.91727646
17	-2.45973276	0.79567484	4.84802004
17	0.40968857	-1.75773564	5.20803293

Complex $\{HAT(CN)_6{\cdot}(FeCl_2)_3\}^{3-}$, $S_z = 11/2$

7	4.12770329	3.82037364	2.45957406
6	3.28643119	3.06098515	2.17137943
6	1.23137971	0.77566831	-3.30961373
7	1.53525013	1.15656395	-2.02344716
7	2.04110050	1.82766780	0.53141757
7	0.48218874	0.66083117	2.66826783
6	0.20652578	-0.14473722	-3.60667472
7	-2.01770782	-1.81712103	-0.64487447
6	2.25402714	2.13249196	1.85564184
6	1.49419255	1.56374418	2.89717061
7	-0.56736181	-0.73163338	-2.63281213
7	-1.47401494	-1.09572141	2.10134792
6	-2.46063473	-1.98762674	1.75101746
6	-2.72565311	-2.33932278	0.41244812
6	-0.26651640	-0.35312625	-1.34407476
6	-1.02925757	-0.92399186	-0.29861207
6	0.26577391	0.35298814	1.34421098
6	-0.76298262	-0.57074910	1.04605367
6	1.02911476	0.92431071	0.29792053
6	0.76305199	0.57139640	-1.04565918
7	2.59823247	1.79137757	-5.26522948
6	1.99072352	1.34202350	-4.37277772
7	2.02496213	2.24636648	5.34189346
6	1.77375939	1.92868956	4.24487895
7	-0.23790585	-0.75586417	-6.08726187
6	-0.04951084	-0.49035005	-4.96410698
7	-3.88969772	-3.06455900	3.62782648
6	-3.23691308	-2.57063150	2.79274507
7	-4.62298368	-4.03793248	-0.07660804
6	-3.76442040	-3.27079559	0.12794074
26	2.93956349	2.45300975	-1.22636545
17	5.03749746	1.68569444	-1.44015552
17	2.49525970	4.60048176	-1.70261365

26	-2.12436054	-2.09555718	-2.69409267
17	-1.45018729	-4.14236657	-3.32004407
17	-3.99306181	-1.22818224	-3.58369442
26	-0.81504207	-0.35764635	3.92045234
17	-2.31527689	0.99912583	4.89221552
17	0.22675131	-1.91587538	5.15431550

Complex $\{HAT(CN)_6{\cdot}(FeCl_2)_6\}^{3-}$, $S_z = 5/2$

7	4.11106421	3.83654666	2.47978951
6	3.26447054	3.08739565	2.18319603
6	1.16415359	0.86357691	-3.30929261
7	1.46202122	1.23871666	-2.02427647
7	2.04230828	1.83996218	0.54796087
7	0.49515471	0.64006367	2.67145734
6	0.18387609	-0.11399465	-3.60549861
7	-1.97694626	-1.87405125	-0.63494122
6	2.23739208	2.15199513	1.86172397
6	1.48857190	1.56965303	2.91127333
7	-0.55318854	-0.73314799	-2.62837458
7	-1.37900506	-1.19914198	2.10896085
6	-2.31495557	-2.15665008	1.76720814
6	-2.60733150	-2.46932201	0.41919507
6	-0.26425326	-0.35612080	-1.33676665
6	-0.99528341	-0.95896694	-0.29404763
6	0.29722553	0.32254570	1.35531253
6	-0.71026015	-0.63521277	1.05597768
6	1.02983587	0.92710841	0.30268172
6	0.73676119	0.60938609	-1.03786738
7	2.42145121	2.00898737	-5.26492212
6	1.86839139	1.49412965	-4.37171030
7	1.99672076	2.27116709	5.35191598
6	1.75264339	1.94425666	4.25463809
7	-0.21058229	-0.78146702	-6.07847418
6	-0.04905694	-0.48516240	-4.95822133
7	-3.59280549	-3.39704771	3.64754078
6	-3.00993327	-2.82333469	2.80993545
7	-4.47539099	-4.20466075	-0.05966081
6	-3.62533088	-3.42722622	0.13774832
26	3.00076509	2.34646370	-1.22254873
17	4.90238453	1.20284013	-1.59535381
17	3.02805243	4.56804255	-1.48947234
26	-2.18319581	-1.98951424	-2.69822561
17	-1.90426864	-4.11029367	-3.36160378
17	-3.90676436	-0.82406109	-3.55132882
26	-0.96979756	-0.19080714	3.84687010
17	-2.58306064	1.29416905	4.31402391
17	-0.17183337	-1.48682291	5.49517730

Complex $\{HAT(CN)_6{\cdot}(FeCl_2)_3\}^{3-}$, $S_z = 3/2$

7	4.17289130	3.77104948	2.46867323
6	3.32208565	3.02203004	2.17771206
6	1.32438854	0.67187750	-3.29432187

7	1.59449635	1.08057315	-2.01823551
7	2.05288964	1.81792416	0.53146143
7	0.45941438	0.69204704	2.66721567
6	0.28539344	-0.24606823	-3.59431336
7	-2.03167668	-1.80194396	-0.64760947
6	2.27725774	2.11334715	1.85867851
6	1.49131171	1.56636027	2.89769611
7	-0.51631727	-0.78458881	-2.62538165
7	-1.45668941	-1.12150592	2.10480313
6	-2.44752548	-2.00141239	1.75370755
6	-2.73636025	-2.33500670	0.41185577
6	-0.23788277	-0.38881874	-1.34012538
6	-1.03045538	-0.93322894	-0.30030986
6	0.25405588	0.36306453	1.33792547
6	-0.75389289	-0.57440385	1.04323107
6	1.04351135	0.91863702	0.29869730
6	0.80141848	0.52871853	-1.03955806
7	2.77252194	1.58673603	-5.24044313
6	2.12654752	1.19022659	-4.35018622
7	1.97707262	2.29626528	5.33768634
6	1.75315603	1.95142865	4.24285451
7	-0.08721714	-0.93654253	-6.06491684
6	0.06087908	-0.63281604	-4.94543471
7	-3.81305940	-3.14936031	3.63566915
6	-3.19585465	-2.61703298	2.79727536
7	-4.66833405	-3.99030835	-0.07786212
6	-3.79092219	-3.24365232	0.12805419
26	2.82542182	2.55438554	-1.23986160
17	5.02397462	2.16769732	-1.42251778
17	2.01030521	4.56587401	-1.80320611
26	-2.24092500	-1.93470449	-2.69973587
17	-1.94881167	-4.03104594	-3.43456225
17	-3.92770835	-0.70287182	-3.51203873
26	-0.77980193	-0.38226456	3.89307969
17	-2.43944597	0.73105194	4.92720449
17	0.47388718	-1.78171734	5.13713948

Complex $\{HAT(CN)_6{\cdot}(FeCl_2)_3\}^{3-}$, S = 15/2

7	4.21862471	3.73917620	2.44943555
6	3.35886881	2.99503747	2.17055405
6	1.05457544	0.97818026	-3.32560989
7	1.44098640	1.24768988	-2.03631193
7	2.06586582	1.79688856	0.54535678
7	0.53841290	0.61813526	2.67229350
6	0.02422927	0.05276846	-3.62294910
7	-1.99534321	-1.84940636	-0.62606290
6	2.31055901	2.08736145	1.86408312
6	1.55699577	1.50570003	2.91312231
7	-0.64829524	-0.62851017	-2.63908612
7	-1.43466800	-1.15414301	2.10310343
6	-2.41119201	-2.05838997	1.76837477
6	-2.68804115	-2.40136426	0.42210334

6	-0.30285009	-0.32471513	-1.34623894
6	-1.01545484	-0.94723051	-0.29919370
6	0.30256977	0.30716544	1.35670039
6	-0.72379250	-0.61464011	1.06062035
6	1.05108217	0.90827495	0.29693844
6	0.73741362	0.60931280	-1.04613522
7	2.26978833	2.17663291	-5.27494431
6	1.73085973	1.64137227	-4.38401648
7	2.10125865	2.15150377	5.36239163
6	1.84417425	1.85118311	4.26038548
7	-0.58977475	-0.39237962	-6.10038659
6	-0.32211231	-0.20267575	-4.97651783
7	-3.80368134	-3.15382471	3.65865282
6	-3.16715207	-2.65080982	2.81454603
7	-4.54814570	-4.13333107	-0.08007385
6	-3.70546858	-3.34883830	0.13243676
26	3.06931932	2.26920679	-1.22623476
17	4.90584104	0.99243453	-1.39853379
17	3.17030273	4.43946404	-1.70738329
26	-1.96269811	-2.24734997	-2.67809393
17	-0.80979802	-4.13694850	-3.04223728
17	-3.88158486	-1.88695603	-3.74564386
26	-0.96561274	-0.17378752	3.88815401
17	-2.50286506	1.41794485	4.26605382
17	-0.27319719	-1.48013217	5.55034718

Complex $\{HAT(CN)_6{\cdot}(FeCl_2)_3\}^{3-}$, $S_z = 9/2$

7	4.12276843	3.81739379	2.47123072
6	3.28690759	3.06083285	2.16269496
6	1.23371468	0.77821349	-3.30266131
7	1.53331897	1.15470201	-2.02414143
7	2.03966816	1.82663896	0.53358667
7	0.48377562	0.66200576	2.66634117
6	0.20187092	-0.14860989	-3.60172806
7	-2.01741235	-1.81641699	-0.64220211
6	2.25338768	2.13131781	1.84797444
6	1.48831922	1.55862717	2.89670541
7	-0.56517887	-0.73002806	-2.63235155
7	-1.47450482	-1.09667807	2.09878146
6	-2.45519564	-1.98286584	1.75378546
6	-2.72221042	-2.33672406	0.40596056
6	-0.26921285	-0.35595253	-1.34711550
6	-1.03165229	-0.92647425	-0.30214393
6	0.26456564	0.35230010	1.34900092
6	-0.76370274	-0.57108385	1.05098986
6	1.03267626	0.92722517	0.29612895
6	0.76679781	0.57442308	-1.04685668
7	2.58981563	1.78347736	-5.27149857
6	1.99441224	1.34577769	-4.36587417
7	2.03346131	2.25350613	5.33511916
6	1.76709661	1.92317324	4.24600425
7	-0.22775114	-0.74775595	-6.08815940

6	-0.05528203	-0.49544360	-4.95995994
7	-3.89431691	-3.07054341	3.61705729
6	-3.23125863	-2.56590460	2.79734071
7	-4.62385410	-4.03645450	-0.06367126
6	-3.76184420	-3.26866528	0.11985139
26	2.96329510	2.47275054	-1.23624531
17	5.04725678	1.67676761	-1.43960343
17	2.48812352	4.61125628	-1.70407516
26	-2.14174469	-2.11214515	-2.71581041
17	-1.44343496	-4.15298243	-3.32004788
17	-4.00229267	-1.21789695	-3.58557710
26	-0.82155803	-0.36063747	3.95209769
17	-2.32603776	1.00713135	4.89206748
17	0.23721294	-1.92425752	5.15700465

Complex $\{HAT(CN)_6{\cdot}(FeCl_2)_3\}^{3-}$, $S_z = 7/2$

7	4.17892277	3.76711943	2.44287402
6	3.31814685	3.02551110	2.16508365
6	1.36540540	0.62697522	-3.30230107
7	1.57994716	1.09592552	-2.02926531
7	2.02568416	1.83762729	0.54400276
7	0.45975161	0.68483345	2.66303183
6	0.33666896	-0.29619952	-3.60019294
7	-2.03123588	-1.80328805	-0.63069071
6	2.26382118	2.12050295	1.85705948
6	1.49328509	1.55340662	2.90635827
7	-0.51164809	-0.78114360	-2.63490653
7	-1.49446886	-1.06767424	2.09732494
6	-2.45519587	-1.98811575	1.76328720
6	-2.71689658	-2.34856463	0.41493327
6	-0.27621714	-0.34926218	-1.35266890
6	-1.05982638	-0.88929661	-0.30848864
6	0.22261682	0.39887262	1.34642778
6	-0.80477248	-0.52294917	1.04895801
6	1.00166415	0.96068342	0.28842948
6	0.76268206	0.58318401	-1.05181914
7	2.87477741	1.49144110	-5.22299884
6	2.20043845	1.10912834	-4.34600138
7	2.08252004	2.20738797	5.34323829
6	1.79287781	1.89304634	4.25389890
7	0.01619538	-1.07384897	-6.05113229
6	0.14966691	-0.73125053	-4.93990027
7	-3.85916609	-3.12097449	3.62305190
6	-3.20906433	-2.59283612	2.80586080
7	-4.57360989	-4.08593390	-0.09133793
6	-3.73320470	-3.30125995	0.12335542
26	2.78839827	2.60279089	-1.26840461
17	4.97029561	2.31407002	-1.58143075
17	1.83565995	4.59732801	-1.64108713
26	-2.24516811	-1.91977047	-2.72684165
17	-1.99394612	-3.94956385	-3.59807523
17	-3.97302412	-0.62418929	-3.32728746

26	-0.80281786	-0.37933042	3.94874404
17	-2.28599675	0.93434486	5.00295670
17	0.30683323	-1.97872741	5.06595402

Complex {HAT(CN)$_6$·(FeCl$_2$)$_3$}$^{3-}$, S_z = 1/2

7	4.27797051	3.64608380	2.48805966
6	3.40425361	2.93506980	2.17231313
6	1.16915012	0.84922951	-3.30050073
7	1.48286536	1.20839666	-2.02053574
7	2.05682633	1.80540985	0.53714119
7	0.52191686	0.64048708	2.67468854
6	0.13691838	-0.07871306	-3.59948188
7	-1.99722504	-1.83926027	-0.63718088
6	2.32813222	2.06010452	1.85705065
6	1.56896330	1.48489573	2.90765212
7	-0.61426775	-0.67666033	-2.62795902
7	-1.45726925	-1.13874224	2.10136363
6	-2.39059231	-2.07492568	1.76067769
6	-2.65874096	-2.42339333	0.41249275
6	-0.31298854	-0.30977619	-1.34219080
6	-1.04913832	-0.91270365	-0.29731209
6	0.25828412	0.35647783	1.35750324
6	-0.76892824	-0.56713617	1.05992934
6	1.01826229	0.94588279	0.30154577
6	0.72322537	0.62184382	-1.04202853
7	2.49377298	1.88883257	-5.27271831
6	1.91401746	1.43452964	-4.36488142
7	2.16182545	2.07345584	5.36228318
6	1.88449578	1.79962876	4.25969771
7	-0.32304485	-0.64272104	-6.08853208
6	-0.13608120	-0.40803993	-4.95864847
7	-3.73609696	-3.22871830	3.65314947
6	-3.12178676	-2.70114088	2.80941378
7	-4.46964645	-4.21907392	-0.04756721
6	-3.64775396	-3.40552934	0.12920409
26	2.96900904	2.46104296	-1.22893413
17	5.01808257	1.59034209	-1.48995563
17	2.57756612	4.62891850	-1.64620380
26	-2.13372692	-2.12220356	-2.70658482
17	-1.34915891	-4.12541782	-3.33616316
17	-4.04250695	-1.31329117	-3.56060686
26	-0.97685395	-0.17275724	3.90864396
17	-2.51224625	1.42018657	4.26743864
17	-0.26748430	-1.49061417	5.54773703

Complex {HAT(CN)$_6$·(FeCl$_2$)$_3$}^{0}, S = 6

7	3.69227115	4.29497492	2.31228579
6	2.92451856	3.44677626	2.08588449
6	1.28050380	0.72191072	-3.30559853
7	1.52084939	1.13542491	-2.03019513
7	1.87000788	1.98414223	0.52201691
7	0.33488663	0.83447080	2.62641701

6	0.29261938	-0.24641164	-3.59943520
7	-1.93634571	-1.90444922	-0.61677437
6	1.98728133	2.41138314	1.81050439
6	1.22487532	1.84037800	2.85566179
7	-0.47205539	-0.80937079	-2.62278054
7	-1.47617643	-1.10845341	2.07753337
6	-2.41356613	-2.04331566	1.75713187
6	-2.64001801	-2.44072456	0.41894193
6	-0.22054336	-0.40502159	-1.34605652
6	-0.98902460	-0.98004571	-0.29303036
6	0.18302077	0.44293589	1.33001719
6	-0.77722605	-0.56886782	1.04039110
6	0.94375472	1.01259015	0.28723249
6	0.75183036	0.57569071	-1.05515882
7	2.71067048	1.75123677	-5.20324868
6	2.06541129	1.28904245	-4.34876277
7	1.51802837	2.66645363	5.29253257
6	1.38584265	2.29431090	4.19518142
7	-0.13410042	-0.98230440	-6.04536954
6	0.05909443	-0.65167384	-4.94378697
7	-3.77558908	-3.10518682	3.68671618
6	-3.16335965	-2.62554678	2.81766781
7	-4.44872629	-4.20964467	-0.13397618
6	-3.63334296	-3.41393676	0.11526663
26	3.08810154	2.18090836	-1.14947036
17	4.66231828	0.72461259	-0.87434881
17	3.47600106	4.16043438	-1.87222783
26	-2.27970276	-1.83450389	-2.66554908
17	-2.35664386	-3.69009987	-3.73265205
17	-3.77497594	-0.29046881	-2.91542312
26	-0.57232726	-0.56169013	3.86893373
17	-1.84849821	0.16876902	5.42750195
17	0.94033471	-2.06472947	4.22602626

Complex $\{HAT(CN)_6 \cdot (FeCl_2)_3\}^0$, $S_z = 2$

7	3.66842515	4.31136984	2.30794756
6	2.90845869	3.45604460	2.08226169
6	1.28494904	0.71459978	-3.30204212
7	1.52458247	1.12934501	-2.02695628
7	1.88147055	1.96670108	0.52348979
7	0.34474394	0.81860288	2.62504639
6	0.30237395	-0.25963667	-3.59501735
7	-1.94734432	-1.89169569	-0.61855350
6	1.98169030	2.41068961	1.80900946
6	1.21840362	1.84304440	2.85231824
7	-0.46035169	-0.82486775	-2.61805462
7	-1.45454401	-1.13098138	2.07850959
6	-2.40605258	-2.05590605	1.75649999
6	-2.65159309	-2.43033064	0.41802001
6	-0.20632421	-0.42102081	-1.34322088
6	-0.98173294	-0.99230121	-0.29068061
6	0.20648071	0.41866044	1.33488932

6	-0.75720179	-0.59595122	1.04407804
6	0.96358677	0.99088451	0.29182954
6	0.76518274	0.55821366	-1.05252912
7	2.70602693	1.75805898	-5.19886358
6	2.06500112	1.28836118	-4.34525820
7	1.47910683	2.68821338	5.28577635
6	1.36242455	2.30889032	4.18902173
7	-0.11997315	-1.00401481	-6.03915082
6	0.07103872	-0.66870961	-4.93857305
7	-3.74744116	-3.12313249	3.69706771
6	-3.14709589	-2.64280140	2.81999330
7	-4.50266292	-4.15377405	-0.13853813
6	-3.66713836	-3.37948150	0.11136558
26	3.09767994	2.19789004	-1.16761792
17	4.67258263	0.73375245	-0.93191531
17	3.43168708	4.20951262	-1.82438106
26	-2.29036073	-1.82618679	-2.68238955
17	-2.41632359	-3.71197581	-3.68952543
17	-3.71877922	-0.22156628	-2.95512718
26	-0.57220659	-0.57280223	3.89210015
17	-1.85538637	0.16864528	5.43642665
17	0.96661687	-2.06434365	4.20274363

Complex $\{HAT(CN)_6{\cdot}(FeCl_2)_3\}^0$, S = 2

7	3.50213969	3.96224056	2.40266695
6	2.70178211	3.14762917	2.16730731
6	0.97247228	0.52565616	-3.16035177
7	1.23142015	0.86701441	-1.88050408
7	1.60457445	1.67634710	0.64754454
7	-0.01057998	0.66719826	2.74061016
6	-0.05083336	-0.41288029	-3.46208042
7	-2.21023944	-2.21508113	-0.45906733
6	1.71992792	2.14844065	1.90668056
6	0.89380462	1.63951134	2.94472336
7	-0.78500290	-1.01540775	-2.51185705
7	-1.81646217	-1.36524899	2.19967723
6	-2.70287697	-2.31015223	1.89786307
6	-2.90336610	-2.74149058	0.54698302
6	-0.53669182	-0.66686183	-1.24561570
6	-1.31000484	-1.26622374	-0.15589592
6	-0.13292727	0.20939621	1.49082079
6	-1.11158700	-0.83671163	1.18653721
6	0.65080792	0.72272139	0.42936804
6	0.45211435	0.29165791	-0.91701271
7	2.40226907	1.57754957	-5.04750979
6	1.76347527	1.11221175	-4.19021009
7	1.11951880	2.59220802	5.34912468
6	1.01570070	2.15965479	4.27199851
7	-0.54355807	-1.02413127	-5.93661214
6	-0.32503310	-0.75470683	-4.82407466
7	-4.08397880	-3.37238279	3.82430835
6	-3.45739807	-2.88710421	2.97023219

7	-4.65170052	-4.58694638	0.01350753
6	-3.86381646	-3.75849367	0.23811615
26	2.85259717	1.84714592	-1.01248659
17	4.28996048	0.24953849	-0.71370837
17	3.32349189	3.81770163	-1.71108308

Complex $\{HAT(CN)_6{\cdot}(FeCl_2)_6\}^0$, $S = 1$

7	3.68391060	3.80379609	2.34348991
6	2.86036115	3.00853328	2.11636062
6	1.08124570	0.40431420	-3.14707939
7	1.26117253	0.80449249	-1.87749971
7	1.65252633	1.61926851	0.58325449
7	0.09041575	0.58985947	2.73124604
6	0.08448752	-0.56578653	-3.46290352
7	-2.27862951	-2.17234926	-0.47520507
6	1.85199377	2.04088109	1.87122909
6	1.05589449	1.50685850	2.91491594
7	-0.70765859	-1.11709159	-2.53017342
7	-1.86370049	-1.30034770	2.17320893
6	-2.79307897	-2.20509547	1.87779910
6	-3.00455188	-2.64881910	0.53296562
6	-0.52691567	-0.71740163	-1.26778693
6	-1.34020950	-1.25922849	-0.18044164
6	-0.09926709	0.18181826	1.46856037
6	-1.12817246	-0.81640600	1.15910497
6	0.66359958	0.68003059	0.39531970
6	0.45750352	0.24424623	-0.93676682
7	2.58548785	1.43822137	-4.98741969
6	1.91175019	0.97656107	-4.15560120
7	1.45760553	2.32605618	5.34727830
6	1.27754717	1.95876957	4.25640227
7	-0.23421825	-1.31484627	-5.92793717
6	-0.09807603	-0.98444293	-4.81866046
7	-4.23911440	-3.16769019	3.80921231
6	-3.58309429	-2.72727995	2.95292431
7	-4.83335943	-4.41853529	0.01322210
6	-4.00960301	-3.62418033	0.23228418
26	2.57021293	2.18195261	-0.90700456
17	4.44104727	1.16780463	-0.77922202
17	1.75288771	4.10603658	-1.32507662

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