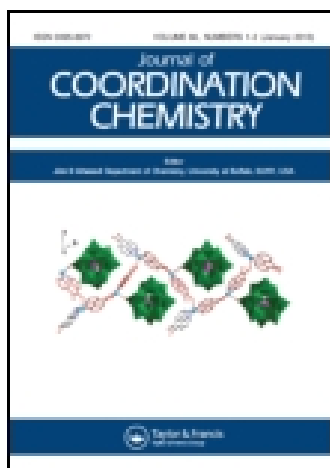


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Journal of Coordination Chemistry

Publication details, including instructions for authors and subscription information:

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Synthesis, crystal structures, and magnetic properties of three iron(II) complexes with 3-(p-bromophenyl)-4-phenyl-5-(2-pyridyl)-1,2,4-triazole

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Accepted author version posted online: 23 Dec 2013. Published online: 20 Jan 2014.



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To cite this article: Xin He, Dong-Yong Cao, Jing-Jing Jiang, Xuan Shen & Dun-Ru Zhu (2014) Synthesis, crystal structures, and magnetic properties of three iron(II) complexes with 3-(p-bromophenyl)-4-phenyl-5-(2-pyridyl)-1,2,4-triazole, *Journal of Coordination Chemistry*, 67:2, 227-235, DOI: [10.1080/00958972.2013.877585](https://doi.org/10.1080/00958972.2013.877585)

To link to this article: <http://dx.doi.org/10.1080/00958972.2013.877585>

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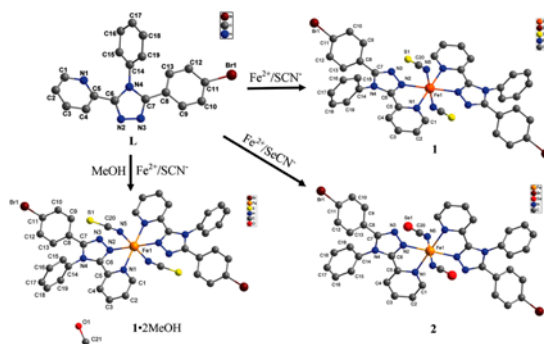
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Synthesis, crystal structures, and magnetic properties of three iron(II) complexes with 3-(*p*-bromophenyl)-4-phenyl-5-(2-pyridyl)-1,2,4-triazole

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(Received 8 October 2013; accepted 5 December 2013)



Three iron(II) complexes with an asymmetrically 3,4,5-triarylsubstituted 1,2,4-triazole, $[\text{FeL}_2(\text{NCS})_2]$ (1), $[\text{FeL}_2(\text{NCS})_2] \cdot 2\text{MeOH}$ ($1 \cdot 2\text{MeOH}$) and $[\text{FeL}_2(\text{NCSe})_2]$ (2), have been synthesized and characterized by single-crystal X-ray crystallography.

Three iron(II) complexes with 3-(*p*-bromophenyl)-4-phenyl-5-(2-pyridyl)-1,2,4-triazole (**L**), *trans*- $[\text{FeL}_2(\text{NCS})_2]$ (**1**), *trans*- $[\text{FeL}_2(\text{NCS})_2] \cdot 2\text{MeOH}$ ($1 \cdot 2\text{MeOH}$), and *trans*- $[\text{FeL}_2(\text{NCSe})_2]$ (**2**), have been synthesized and characterized by elemental analysis, FT-IR, ESI-MS, and single-crystal X-ray crystallography. Crystallographic studies reveal that all the complexes contain a distorted octahedral $[\text{FeN}_6]$ core with two *trans* $\text{NCS}(\text{Se})^-$ ions. Each **L** adopts a chelating bidentate coordination via one N of pyridyl and one N of triazole. Magnetic susceptibility measurement indicated that both **1** and $1 \cdot 2\text{MeOH}$ are in a high-spin state from 2 to 300 K.

Keywords: Synthesis; Triazole; Crystal structure; Iron(II) complex

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1. Introduction

Over the past decade, coordination of triaryltriazoles and related ligands has attracted attention due to versatile structures and the intriguing magnetic properties of their resulting transition metal complexes [1–3]. Some iron(II) complexes with triaryltriazole ligands show interesting spin crossover (SCO) properties which can be applied in molecular electronics, memory devices, information storage, and switching materials [4, 5].

Recently, some 4-arylsubstituted 3,5-di(2-pyridyl)-1,2,4-triazoles and their metal complexes have been prepared [6–12]. However, complexes with asymmetrically 3,4,5-triarylsubstituted 1,2,4-triazole have been little studied [13]. As a continuation of our investigation of asymmetrically substituted triaryltriazole [14–19], we present here the synthesis of three iron(II) complexes, $[\text{FeL}_2(\text{NCS})_2]$ (**1**), $[\text{FeL}_2(\text{NCS})_2] \cdot 2\text{MeOH}$ (**1**·2MeOH), and $[\text{FeL}_2(\text{NCSe})_2]$ (**2**) with 3-(*p*-bromophenyl)-4-phenyl-5-(2-pyridyl)-1,2,4-triazole (**L**) [20]. Their molecular structures were investigated by single-crystal X-ray diffraction and their magnetic properties were explored by variable-temperature magnetic susceptibility. The influence of the solvent, the different co-ligands, and intermolecular interactions on the crystal packing and magnetic behavior are also discussed. All the complexes contain a similar $[\text{FeN}_6]$ octahedral geometry with two *trans* $\text{NCS}(\text{Se})^-$ groups. Compared to **1**, complex **1**·2MeOH contains two MeOH molecules, whereas complex **2** has two different co-ligands.

2. Experimental

2.1. Materials and measurements

All chemicals used were of analytical grade. Solvents were purified by conventional methods. **L** was synthesized using a modified method [20]. Elemental analyses were carried out with a Thermo Finnigan Flash 1112A elemental analyzer. IR spectra were recorded on a Nicolet Avatar 380 FT-IR instrument with KBr pellets from 4000 to 400 cm^{-1} . Electrospray ionization mass spectra (ESI-MS) were recorded with a LCQ ADVANTAGE MAX mass spectrometer, with MeOH on the mobile phase; the flow rate of the mobile phase was 0.2 $\text{cm}^3 \text{min}^{-1}$. The spray voltage was 4 kV and the capillary voltage was 40 V. The temperature dependence of the magnetic susceptibility for **1** and **1**·2MeOH were measured on a Quantum Design MPMS-7 SQUID magnetometer from 2 to 300 K under 2000 Oe of external field. Diamagnetic correction was made with Pascal's constants.

2.2. Syntheses and characterization of **1** and **2**

To a solution of KSCN (0.8 mmol) in anhydrous MeOH (4 mL) was added a solution of $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ (0.4 mmol) in MeOH (3 mL). The mixture was stirred for 30 min, the K_2SO_4 precipitate was filtered off and then washed with 3 mL of anhydrous MeOH. The methanolic fractions containing $\text{Fe}(\text{SCN})_2$ were collected and then were poured into a methanol solution of **L** (0.8 mmol). The resulting solution was stirred for 1.5 h during which an orange precipitate formed, which was isolated by filtration, washed with H_2O , and dried thoroughly in vacuo to give $[\text{FeL}_2(\text{NCS})_2]$ (318.7 mg, 86%) as an orange powder.

Complex 1. Red single crystals suitable for X-ray diffraction were obtained by evaporation from an acetone and *n*-butyl alcohol (1 : 1) solution of $[\text{FeL}_2(\text{NCS})_2]$ under argon.

Anal. Calcd for $C_{40}H_{26}Br_2FeN_{10}S_2$ (%): C, 51.85; H, 2.83; N, 15.12; S, 6.92. Found (%): C, 51.73; H, 2.67; N, 15.01; S, 7.11. FT-IR (cm^{-1}): 2061(s), 1600(m), 1570(m), 1497(m), 1476(m), 1460(m), 1396(m), 1076(m), 837(m), 795(m), 737(w). ESI-MS: $m/z = 868.2, 777.4, 379.2$.

Complex 1·2MeOH. Orange single crystals suitable for X-ray diffraction were obtained by evaporation from a methanol solution of $[FeL_2(NCS)_2]$ under argon. Anal. Calcd for $C_{42}H_{34}Br_2FeN_{10}O_2S_2$ (%): C, 50.93; H, 3.46; N, 14.14; S, 6.47. Found (%): C, 50.74; H, 3.27; N, 14.32; S, 6.64. FT-IR (cm^{-1}): 3426(m,b), 2920(w), 2848(w), 2060(s), 1598(m), 1572(m), 1496(m), 1477(m), 1463(m), 1395(m), 1076(m), 838(m), 794(m), 741(w). ESI-MS: $m/z = 868.2, 777.4, 379.2$.

Complex 2. The complex was obtained following the same method as for **1** except replacing KSCN with KSeCN. An orange powder of **2** was obtained in a yield of 88.2%. Single crystals suitable for X-ray diffraction were obtained by evaporation from a methanol solution under argon. Anal. Calcd for $C_{40}H_{26}Br_2FeN_{10}Se_2$ (%): C, 47.09; H, 2.57; N, 13.73. Found (%): C, 47.28; H, 2.37; N, 13.42. FT-IR (cm^{-1}): 2065(s), 1598(m), 1496(m), 1476(m), 1395(m), 1075(m), 838(m), 795(m), 742(m). ESI-MS: $m/z = 915.2, 777.2, 401.3, 379.4$.

2.3. Crystal structure determination

Crystals of **1**, **1**·2MeOH and **2** were selected for lattice parameter determination and collection of intensity data at 296 K on a Bruker Smart APEX II CCD diffractometer with monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$) using a ϕ - ω scan mode. The structures were solved by direct methods and refined on F^2 by full matrix least-squares using SHELXTL [21]. All non-hydrogen atoms were refined anisotropically. Hydrogens for C–H were placed in calculated positions and allowed to ride on the parent to which they are attached. The contribution of these hydrogens was included in the structure factor

Table 1. Crystal data and structure refinements for **1**–**2**.

Complex	1	1 ·2MeOH	2
Empirical formula	$C_{40}H_{26}Br_2FeN_{10}S_2$	$C_{42}H_{34}Br_2FeN_{10}O_2S_2$	$C_{40}H_{26}Br_2FeN_{10}Se_2$
Formula weight	926.50	990.58	1020.30
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	9.917(5)	9.311(18)	11.0863(13)
b (Å)	8.546(4)	16.18(3)	8.1863(10)
c (Å)	23.555(11)	14.44(3)	22.494(3)
β (°)	90.551(7)	102.54(3)	95.302(2)
V (Å ³)	1996.1(17)	2122(7)	2032.7(4)
Z	2	2	2
D_{Calcd} ($g\ cm^{-3}$)	1.541	1.550	1.667
μ (mm^{-1})	2.527	2.386	4.170
$F(000)$	928	1000	1000
Crystal size (mm)	0.16×0.13×0.10	0.18×0.14×0.12	0.13×0.10×0.08
θ Range	1.73–25.00	1.9–25.00	1.82–25.00
Reflections collected	13,764	14,439	14,027
Independent reflections	3518 [$R_{\text{int}} = 0.057$]	3737 [$R_{\text{int}} = 0.0897$]	3580 [$R_{\text{int}} = 0.0619$]
Reflections observed [$I > 2\sigma(I)$]	2346	2332	2191
Data/restraints/parameters	3518/12/250	3737/6/271	3580/0/250
Goodness-of-fit on F^2	0.975	1.000	1.009
R/wR [$I > 2\sigma(I)$]	0.0377/0.0715	0.0577/0.1456	0.0451/0.1014
R/wR (all data)	0.0735/0.0788	0.1013/0.1664	0.0920/0.1154
Max., Min. $\Delta\rho$ ($e\cdot\text{\AA}^{-3}$)	0.293, -0.387	0.635, -0.593	0.654, -0.786

Table 2. Selected bond distances (Å) and angles (°) for **1**–**2**.

Complex	1	1·2MeOH	2
Fe1–N1	2.214(3)	2.163(5)	2.208(4)
Fe1–N2	2.134(3)	2.137(5)	2.131(4)
Fe1–N5	2.137(3)	2.118(6)	2.144(5)
N5–C20	1.156(4)	1.143(6)	1.132(6)
C20–S1(Se1)	1.621(4)	1.617(6)	1.799(7)
Br1–C11	1.896(3)	1.865(6)	1.898(5)
N1–Fe1–N2	74.80(10)	74.9(2)	75.21(15)
N1–Fe1–N5	86.21(11)	90.80(19)	87.41(16)
N2–Fe1–N5	84.27(11)	95.09(19)	87.33(16)
N5–C20–S1(Se1)	179.2(4)	177.8(5)	177.3(5)
Fe1–N5–C20	148.5(3)	154.3(5)	150.6(5)

calculations. Crystallographic data are summarized in table 1. Selected bond lengths and angles for **1**, **1·2MeOH** and **2** are listed in table 2.

3. Results and discussion

3.1. Synthesis

L reacts with iron(II) and KNCS(Se) in molar ratio 2 : 1 : 2 to form three mononuclear iron (II) complexes, *trans*-[FeL₂(NCX)₂], **1** (X = S), **1·2MeOH** (X = S), and **2** (X = Se), which are stable in air. The elemental analyses were satisfactory and indicate that all the complexes contain one iron(II), two triazole ligands and two NCS(Se)[−] except **1·2MeOH** has two MeOH molecules.

3.2. Crystal structures of **1**, **1·2MeOH**, and **2**

The crystal structures of **1**, **1·2MeOH**, and **2** were determined by X-ray crystallography, and all the complexes crystallize in the monoclinic space group *P2₁/c* and have similar mononuclear structure (figure 1). There is an inversion center at iron(II). Each Fe(II) is coordinated by four nitrogens from two **L** in the equatorial plane and two nitrogens from two NCS(Se)[−] in the axial positions to form a distorted octahedron. Each **L** coordinates to Fe(II) via N1 of pyridyl and N2 of the triazole, similar to those observed in related triazole-based iron(II) complexes [5, 22, 23]. In **1**, **1·2MeOH**, and **2**, the average Fe–N bond length is 2.162, 2.139, and 2.161 Å, respectively, within the typical range for high-spin Fe(II)–N (2.051–2.248 Å) [23]. The spin-state assignment based on the Fe(II)–N bond distance is associated with octahedral distortion parameter (Σ), which is commonly used for quantification of the angular deviation of an octahedron from ideal [24]. A smaller Σ value is generally related with a stronger ligand field and, therefore, a low spin state of the metal ion, while the opposite suggests a high-spin state [24, 25]. In the present case, Σ of **1** and **1·2MeOH** are 85.2° and 87.5°, respectively, suggesting that the Fe(II) center is in a high-spin state at 296 K (vide infra). The Fe–N_{py} distance in all the complexes is always larger than Fe–N_{trz}, consistent with those found in the analogous triazole-based Fe(II)

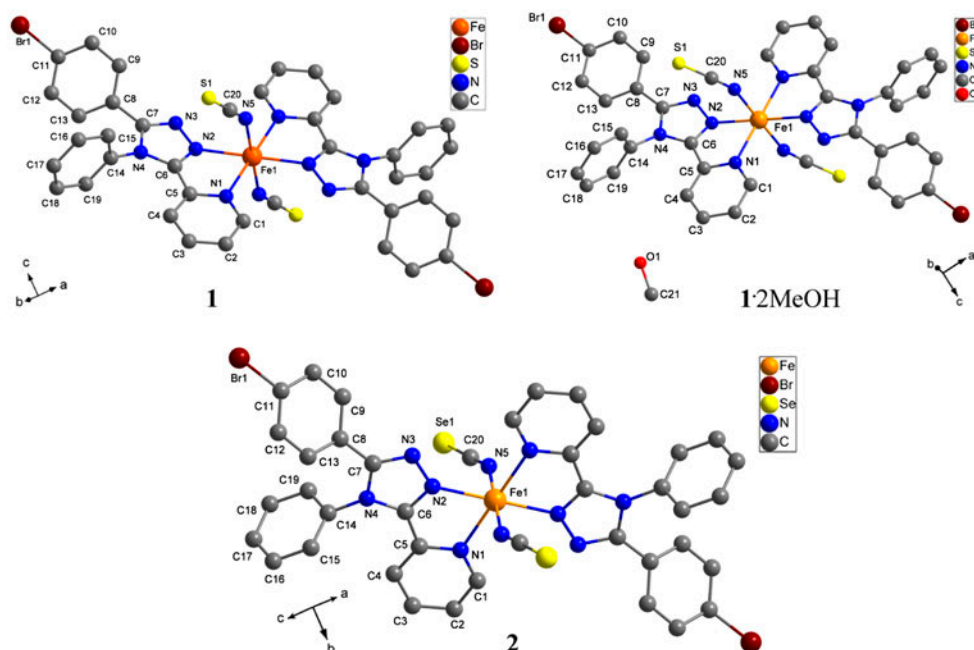


Figure 1. Projection of the structures of **1–2** with the atomic labeling system. Hydrogens are omitted for clarity.

complexes [4, 5, 22, 26–29]. The dihedral angle between pyridyl and triazole ring in **1**, **1·2MeOH**, and **2** are 7.0°, 16.2°, and 4.2°, respectively, smaller than (35.3°) in free **L** [20]. Compared to free **L** (25.2°), the *p*-bromophenyl-triazole twist angle in **1** and **2** is larger (44.5° and 45.4°), while that (22.7°) in **1·2MeOH** becomes smaller due to the influence of CH₃OH. In addition, the Fe1–N6–C14 angle in **1·2MeOH** is slightly larger than those in **1** and **2** (table 2).

Table 3. Hydrogen-bond geometry, C–H··· π and π ··· π interactions (Å, °) for **1–2**.

Complex	D–H···A	d(D–H)	d(H···A)	d(D···A)	\angle D–H···A
1	C1–H1A···N3 ⁱⁱ	0.93	2.77	3.564	144
	C10–H10A···N5 ⁱ	0.93	2.74	3.392	127
	C19 ⁱ –H19A ⁱ ···Br1	0.93	2.97	3.869	162
	C5–H5A··· π (C14–C19)	0.93	3.03	3.832	145
	π ··· π interaction	cent··cent (Å)		π ··· π (Å)	dihedral angle (°)
	π (Ph–Br)··· π (Ph–Br) ⁱⁱⁱ	3.899		3.750	0
1·2MeOH	O1–H1B···S1 ^{vi}	0.82	2.42	3.188	157
	C1–H1A···N3 ^{iv}	0.93	2.69	3.492	145
	C2–H2A···S1 ^v	0.93	2.86	3.741	159
	C3–H3A···O1	0.93	2.46	3.154	131
	π ··· π interaction	cent··cent (Å)		π ··· π (Å)	dihedral angle (°)
	π (Ph–Br)··· π (py) ^{vii}	3.921		–	10.5
2	C10 ^{ix} –H10A ^{ix} ···Br1 ^{viii}	0.93	2.996	3.732	137
	C15–H15A···Br1 ^{ix}	0.93	2.972	3.827	153
	π ··· π interaction	cent··cent (Å)		π ··· π (Å)	dihedral angle (°)
	π (Ph–Br)··· π (Ph–Br) ^{viii}	3.774		3.554	0

Symmetry codes: (i) 2–x, –y, –z; (ii) 2–x, –1–y, –z; (iii) 1–x, –y, –z; (iv) 2–x, 1–y, 1–z; (v) 3–x, 1–y, 1–z; (vi) x, 1/2–y, 1/2+z; (vii) x–1, y, z; (viii) 2–x, 2–y, 1–z; (ix) –x, y–1, z.

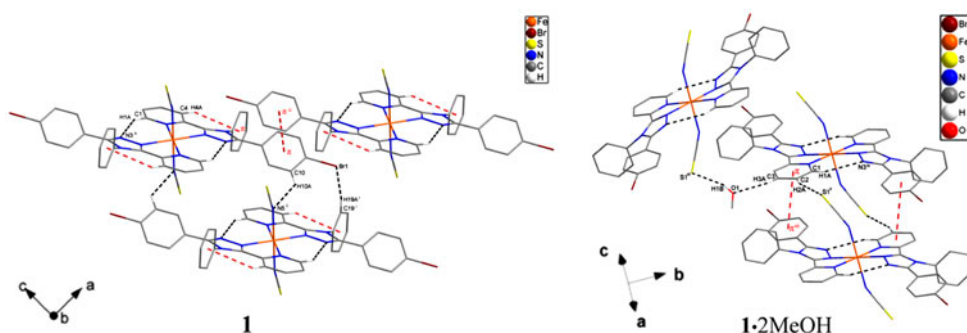


Figure 2. Hydrogen bonding and C–H $\cdots\pi$ interactions in **1** and **1·2MeOH**.

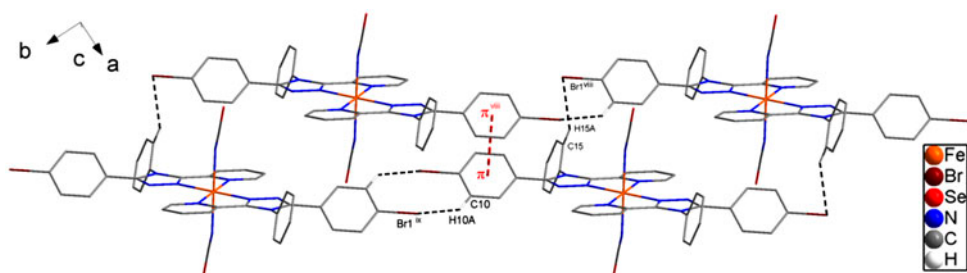


Figure 3. Hydrogen bonding and C–H $\cdots\pi$ interaction in **2**.

There are three kinds of hydrogen bonds [C1–H1A \cdots N3ⁱⁱ, C10–H10A \cdots N5ⁱ, and C19ⁱ–H19Aⁱ \cdots Br1], a kind of C–H $\cdots\pi$ [C5–H5A $\cdots\pi$ (C14–C19)] and one face-to-face $\pi\cdots\pi$ interaction [π (Ph–Br) $\cdots\pi$ (Ph–Br)ⁱⁱⁱ] in the structure of **1** (table 3). Due to the presence of CH₃OH in **1·2MeOH**, there are four kinds of hydrogen bonds [O1–H1B \cdots S1^{vi}, C1–H1A \cdots N3^{iv}, C2–H2A \cdots S1^v, C3–H3A \cdots O1], and one weak face-to-face $\pi\cdots\pi$ interaction [π (Ph–Br) $\cdots\pi$ (py)^{vii}], linking the molecules of **1·2MeOH** to form a 1-D chain along the *c* axis (figure 2). In **2**, there are only two kinds of hydrogen bonds [C10^{ix}–H10A^{ix} \cdots Br1^{vii}, C15–H15A \cdots Br1^{ix}], and one strong face-to-face $\pi\cdots\pi$ interaction [π (Ph–Br) $\cdots\pi$ (Ph–Br)^{ix}], connecting the molecules of **2** to form a 2-D framework (figure 3).

3.3. IR spectra

In **1**, **1·2MeOH**, and **2**, strong bands at 2061, 2060, and 2065 cm⁻¹ are assigned to C \equiv N stretches of two *trans*-coordinated NCS(Se)⁻ groups, respectively [4, 22]. Bands at 1076, 1076, and 1075 cm⁻¹ are attributed to stretch of C(Ph)–Br bond in **1**, **1·2MeOH**, and **2**, respectively [30]. In addition, a broad band at 3426 cm⁻¹ in **1·2MeOH** is due to the O–H stretch of MeOH. These features are in agreement with the results of X-ray crystallography analyses.

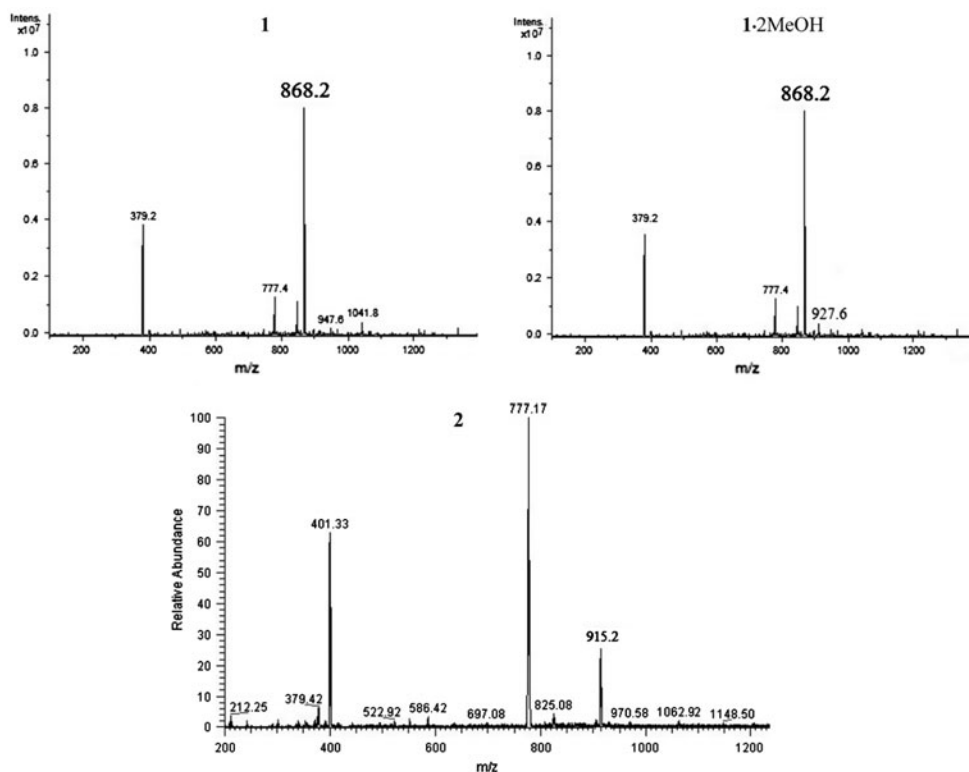


Figure 4. ESI-MS spectra of 1–2 in methanol solution.

3.4. Electrospray ionization mass spectra

The structures of 1, 1·2MeOH, and 2 in solution were also studied by ESI-MS [31, 32]. Figure 4 displays the positive ESI mass spectra of the three complexes in methanol. The ESI-MS of 1 and 1·2MeOH are similar, the base peak at m/z 868.2 is $[\text{FeL}_2(\text{NCS})]^+$ and the

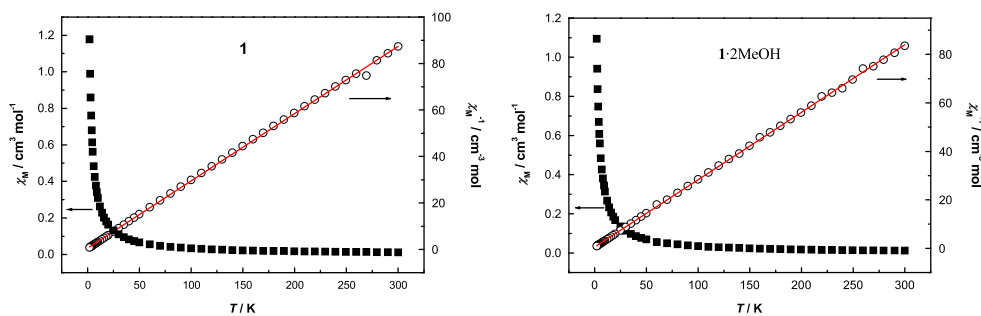


Figure 5. Plots of χ_M (■) vs. T and χ_M^{-1} (○) vs. T for 1 and 1·2MeOH. Solid red line represents the best linear fit (see <http://dx.doi.org/10.1080/00958972.2013.877585> for color version).

peaks at 777.4 and 379.2 are $[\text{NaL}_2]^+$ and $[\text{L} + \text{H}]^+$, respectively. In **2**, four main peaks were observed; the base peak at 777.2 is $[\text{NaL}_2]^+$, and the peaks at m/z 915.2, 401.3, and 379.4 are $[\text{FeL}_2(\text{NCSe})]^+$, $[\text{L} + \text{Na}]^+$, and $[\text{L} + \text{H}]^+$ ion, respectively.

3.5. Magnetic properties of **1** and **1**·2MeOH

The temperature dependences of the magnetic susceptibilities of **1** and **1**·2MeOH were measured on the crystalline sample at an applied field of 2000 Oe. The χ_M and χ_M^{-1} versus T plots are shown in figure 5. The results show that both **1** and **1**·2MeOH remained in a high-spin state from 2 to 300 K, which indicates that the crystal-field splitting energy ($\Delta = 10 \text{ Dq}$) is lower than the electron pairing energy (P). The results are also consistent with the octahedral distortion parameter (Σ). In accord with the Curie–Weiss law, $\chi_M = C/(T - \theta)$, the data for **1** and **1**·2MeOH exhibit a good linear relationship between χ_M^{-1} and T with a Curie value of $3.45(1) \text{ cm}^3 \text{ mol}^{-1} \text{ K}$ for **1** and $3.59(1) \text{ cm}^3 \text{ mol}^{-1} \text{ K}$ for **1**·2MeOH, and Weiss constant of $-1.9(5) \text{ K}$ for **1** and $-1.8(3) \text{ K}$ for **1**·2MeOH. The results are in agreement with those found in *trans*- $[\text{FeL}'_2(\text{NCS})_2]$ ($\text{L}' = 4\text{-amino-3-(}p\text{-bromophenyl)-5-(2-pyridyl)-1,2,4\text{-triazole}$) [23]. Recently, we reported that the transition modes and temperature of a family of mononuclear iron(II) SCO complexes, *trans*- $[\text{Fe}(\text{L1-L4})_2(\text{NCS})_2]$ ($\text{L1-L4} = \text{triaryltriazole}$), can be tuned by remote substituent effects [5]. Compared to *trans*- $[\text{Fe}(\text{L4})_2(\text{NCS})_2]$ ($\text{L4} = 3\text{-}(p\text{-fluorophenyl})\text{-4-(}p\text{-methylphenyl)-5-(2-pyridyl)-1,2,4\text{-triazole}$) displaying an incomplete (70%) spin transition with $T_{1/2} = 97 \text{ K}$, **1** and **1**·2MeOH are still high-spin species, revealing that after both p -fluorophenyl at the 3-position and p -methylphenyl at the 4-position of L4 are replaced simultaneously by p -bromophenyl and phenyl group, the ligand field strength resulting from **L** cannot be shifted to the region of SCO for Fe(II) complexes with NCS^- as co-ligands.

4. Conclusion

Three mononuclear iron(II) complexes, *trans*- $[\text{FeL}_2(\text{NCS})_2]$ (**1**), *trans*- $[\text{FeL}_2(\text{NCS})_2] \cdot 2\text{-MeOH}$ (**1**·2MeOH), and *trans*- $[\text{FeL}_2(\text{NCSe})_2]$ (**2**), with 3-(p -bromophenyl)-4-phenyl-5-(2-pyridyl)-1,2,4-triazole (**L**), have been synthesized and characterized by elemental analysis, FT-IR, ESI-MS, and single crystal X-ray diffraction. Crystallographic studies reveal that **1**, **1**·2MeOH, and **2** possess a similar distorted octahedral $[\text{FeN}_6]$ core with two *trans* NCS (Se^-) anions. Each **L** coordinates to iron(II) via N1 of the pyridyl ring and N2 of the triazole. Both **1** and **1**·2MeOH are high-spin species from 2 to 300 K. Their paramagnetism is similar to that observed in a related triazole-based iron(II) complex, $[\text{Cd}_{2.98}\text{Fe}_{2.02}(\text{atrz})_6(\text{SCN})_{10}] \cdot 2\text{H}_2\text{O}$ ($\text{atrz} = 4\text{-amino-1,2,4-triazole}$) [33].

Supplementary material

Crystallographic data for the structures reported in this article have been deposited with the Cambridge Crystallographic Data Center as supplementary publication Nos. CCDC 961234 (**1**), 961235 (**1**·2MeOH), and 961236 (**2**). Copies of the data can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Center, 12 Union Road, Cambridge CB21EZ, UK; Fax: +44 1223 336033; E-mail: deposit@ccdc.cam.ac.uk).

Funding

This work was funded by the National Nature Science Foundation of China [grant numbers 20771059 and 21171093].

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