Electronic Supplementary Information (ESI)

Electroneutral Mononuclear Iron(III) Schiff Base Complexes involving Terminal Pseudohalido Ligands

P. Masárová, P. Zoufalý, J. Moncoľ, I. Nemec, J. Pavlik, M. Gembický, Z. Trávníček, R. Boča, and I. Šalitroš

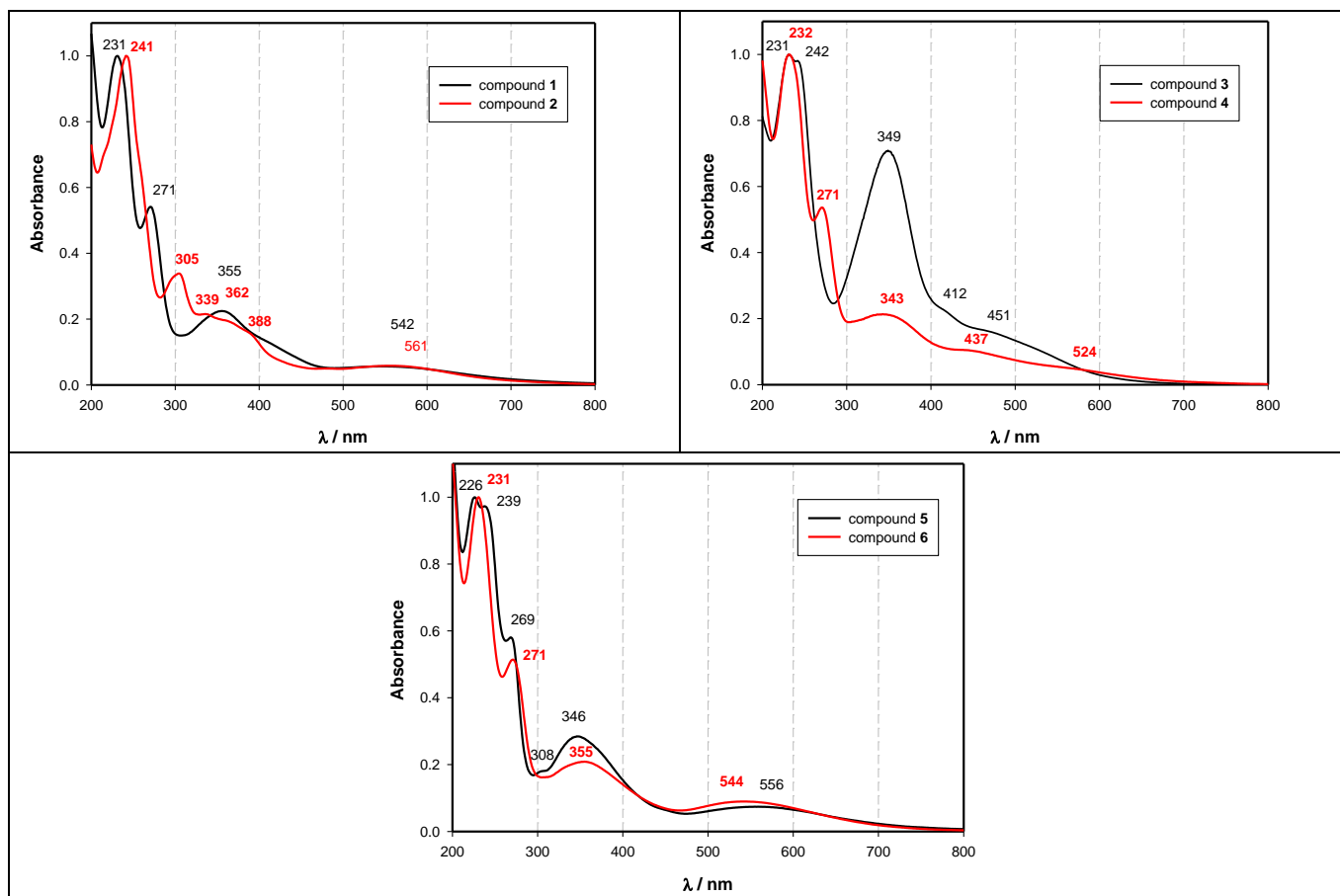## S1. UV-VIS spectra of the reported complexes

Figure S1 UV-VIS spectra of compound **1**-**6** in acetonitrile solution

S2. **Selected non-covalent interactions in the reported complexes**
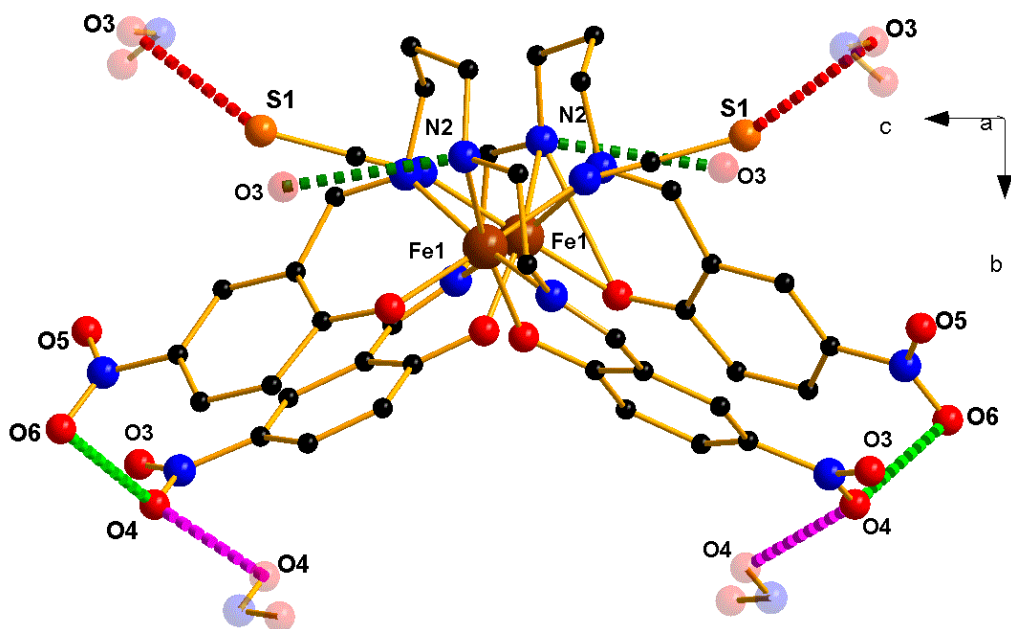
Compound 3 [Fe(L3)(NCS)]

Figure S2 A perspective view of non-covalent interactions in the crystal lattice of **3**. At 150 K corresponding bond distances are d(O3···N2) = 3.071(3) Å; d(O3···S1) = 3.265(2) Å; d(O4···O6) = 2.922(3) Å; d(O4···O4) = 3.443(3) Å at 150 K.

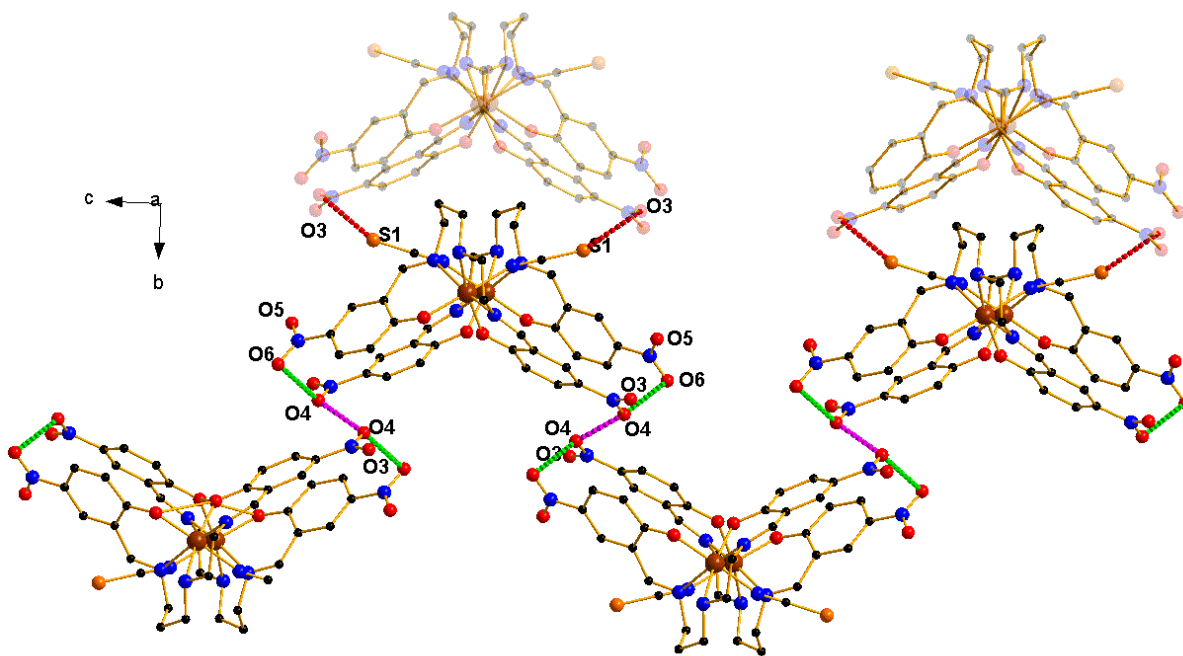**Figure S3** A perspective view of non-covalent interactions in the crystal lattice of **3** along *bc* plane. d(O3···N2) = 3.071(3) Å; d(O3···S1) = 3.265(2) Å; d(O4···O6) = 2.922(3) Å; d(O4···O4) = 3.443(3) Å at 150 K.
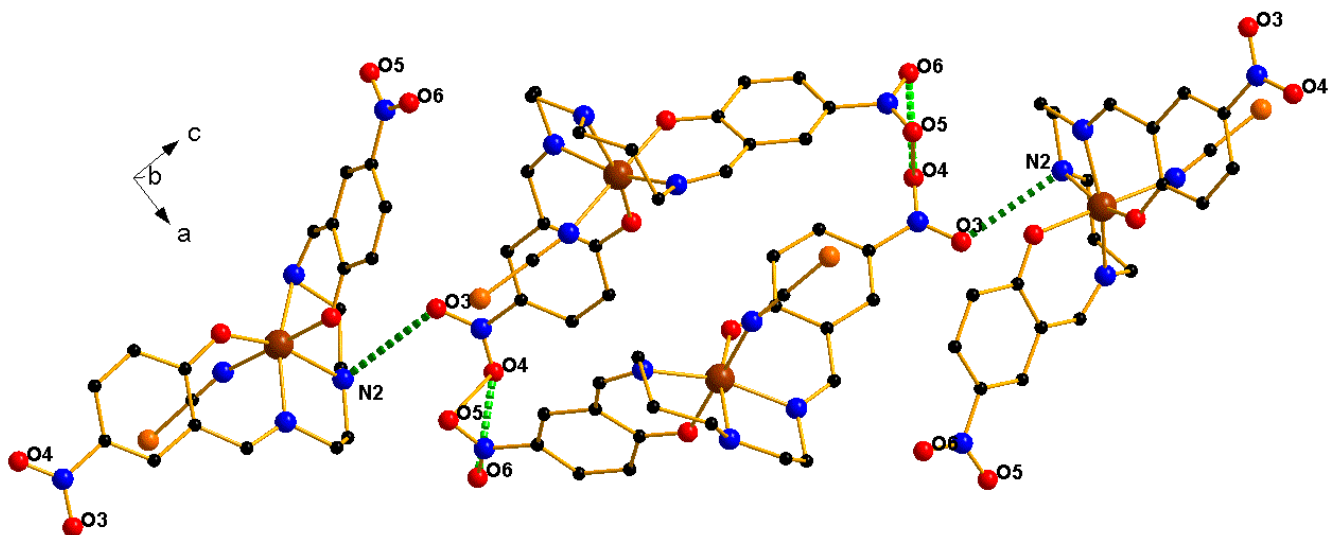
Figure S4 A perspective view of non-covalent interactions in the crystal lattice of **3** along *ac* plane
d(O3⋯N2) = 3.071(3) Å; d(O3⋯S1) = 3.265(2) Å; d(O4⋯O6) = 2.922(3) Å; d(O4⋯O4) = 3.443(3) Å
at 150 K.

*Compound **5** [Fe(L5)(NCS)]*

Figure S7 A perspective view on N$_{(am)}$⋯S1 hydrogen bonding in [Fe(L5)NCS]. The corresponding
donor⋯acceptor distances: d(N2⋯S1) = 3.529(2) Å (150 K).
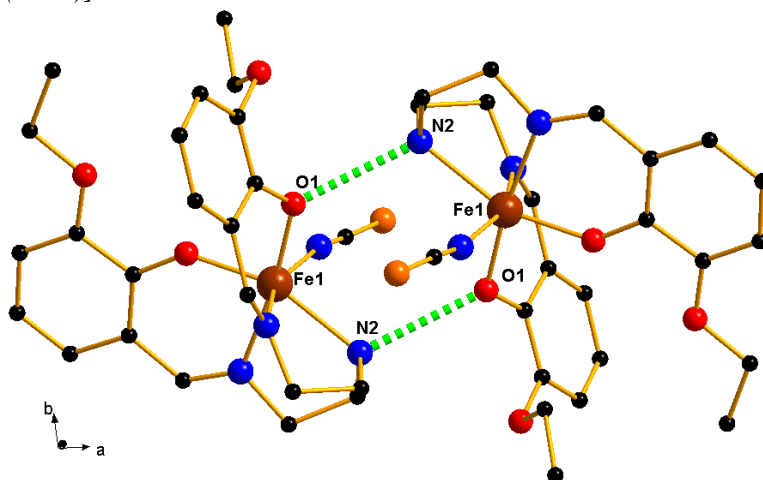
*Compound **6** [Fe(L5)(NCS)]*

Figure S8 A perspective view on $N_{(am)} \cdots O_1$ hydrogen bonding in [Fe(L6)NCS]. Corresponding bond distances: $d(N2 \cdots O1) = 2.878(2)$ Å (100 K).

S3 Collection of alternative fits of magnetic functions with sign reversal of the *D* parameter

In following cases the sign of the parameter *D* was fixed opposite as found in the article (the absolute value was not limited), other parameters were unrestricted.
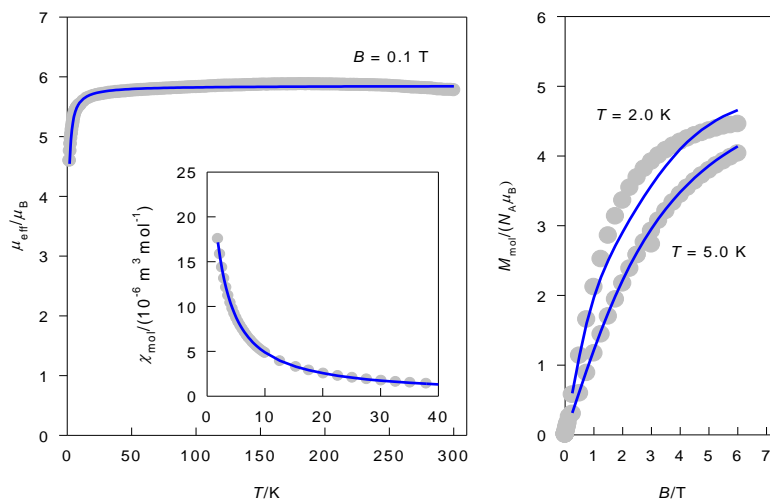

Figure S9 Magnetic functions for **3**: effective magnetic moment *vs* temperature (left), magnetization *vs* magnetic field (right), magnetic susceptibility *vs* temperature (inset); grey circles: experimental data, solid line: fitted.

Figure S10 Magnetic functions for **4**: effective magnetic moment *vs* temperature (left), magnetization *vs* magnetic field (right), magnetic susceptibility *vs* temperature (inset); grey circles: experimental data, solid line: fitted.

Figure S11 Magnetic functions for **5**: effective magnetic moment *vs* temperature (left), magnetization *vs* magnetic field (right), magnetic susceptibility *vs* temperature (inset); grey circles: experimental data, solid line: fitted.
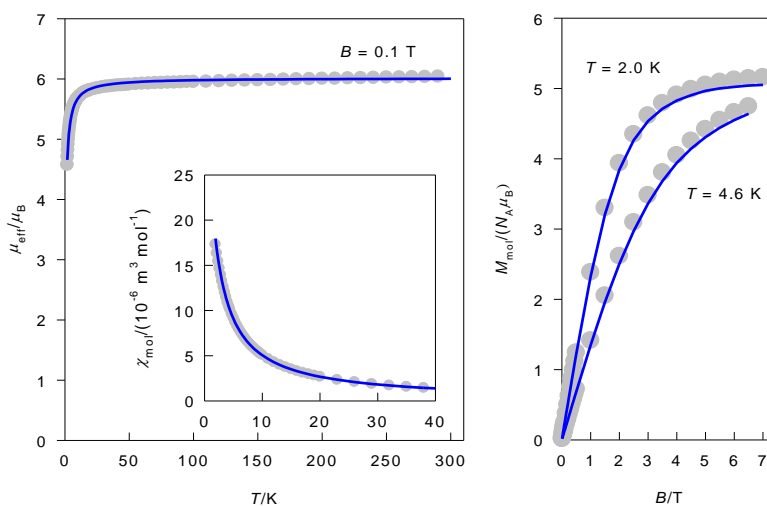
Figure S12. Magnetic functions for **6** per monomeric unit: effective magnetic moment *vs* temperature (left), magnetization *vs* magnetic field (right), magnetic susceptibility *vs* temperature (inset); grey circles: experimental data, solid line: fitted.
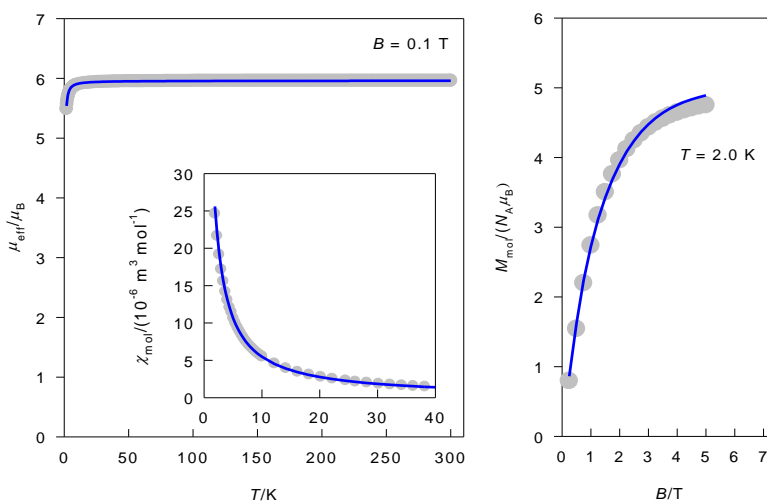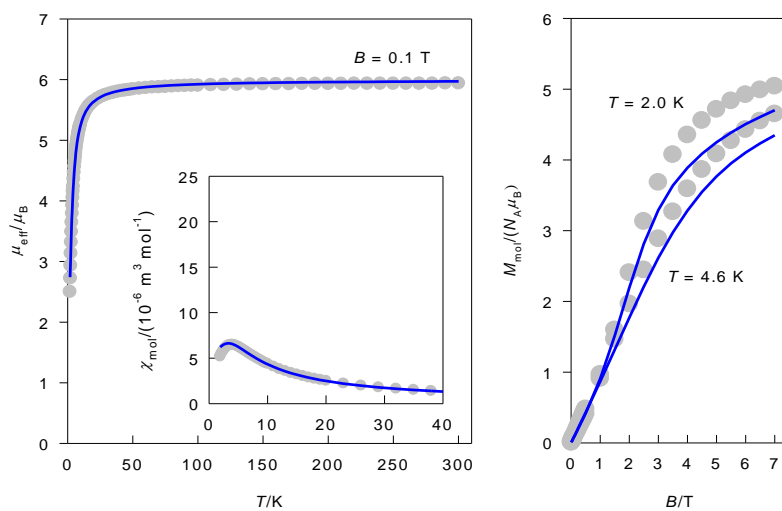
Table S1. Summary of alternative magnetic parameters for the high spin complexes **3**-**6** with opposite sign of the parameter D

Complex	J/cm^{-1}	g	D/cm^{-1}	$(zj)/\text{cm}^{-1}$	$R(\chi)/R(M)$
3, [Fe(L3)(NCS)]	−	1.98	-1.00	-0.23	0.012/0.055
4, [Fe(L1)(N$_3$)]	−	2.03	-0.11	-0.28	0.016/0.023
5, [Fe(L5)(NCS)]	−	2.01	-0.52	-0.04	0.020/0.021
6, [Fe(L6)(NCS)]	-0.56	2.03	+1.00	-0.05	0.054/0.086