Supplementary material for

High spin iron(II) complexes based on imidazolyl- and 1,2,3-triazolyl-thione ligands and NCE (E = S, Se or BH_3) co-ligands: effect of the S-functional group on the structural and magnetic properties

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1. Spectroscopic characterisation.

1.1. Pyiridotetrazole (A^1).

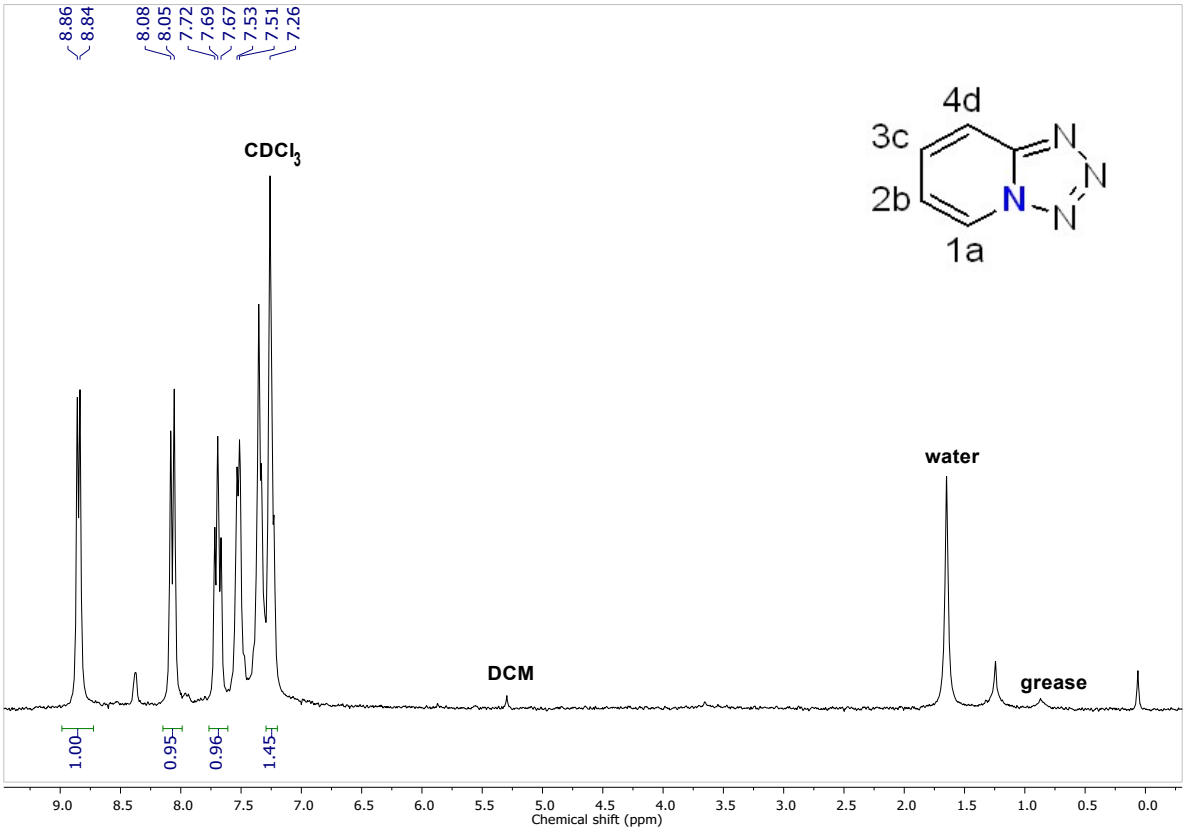

Figure **S1**. ^{1}H-NMR spectrum for (**A^1**) in chloroform-*d*.

1.2. 2-(4-Phenyl-1-(*1H*-1,2,3-triazolyl))pyridine (A^2).

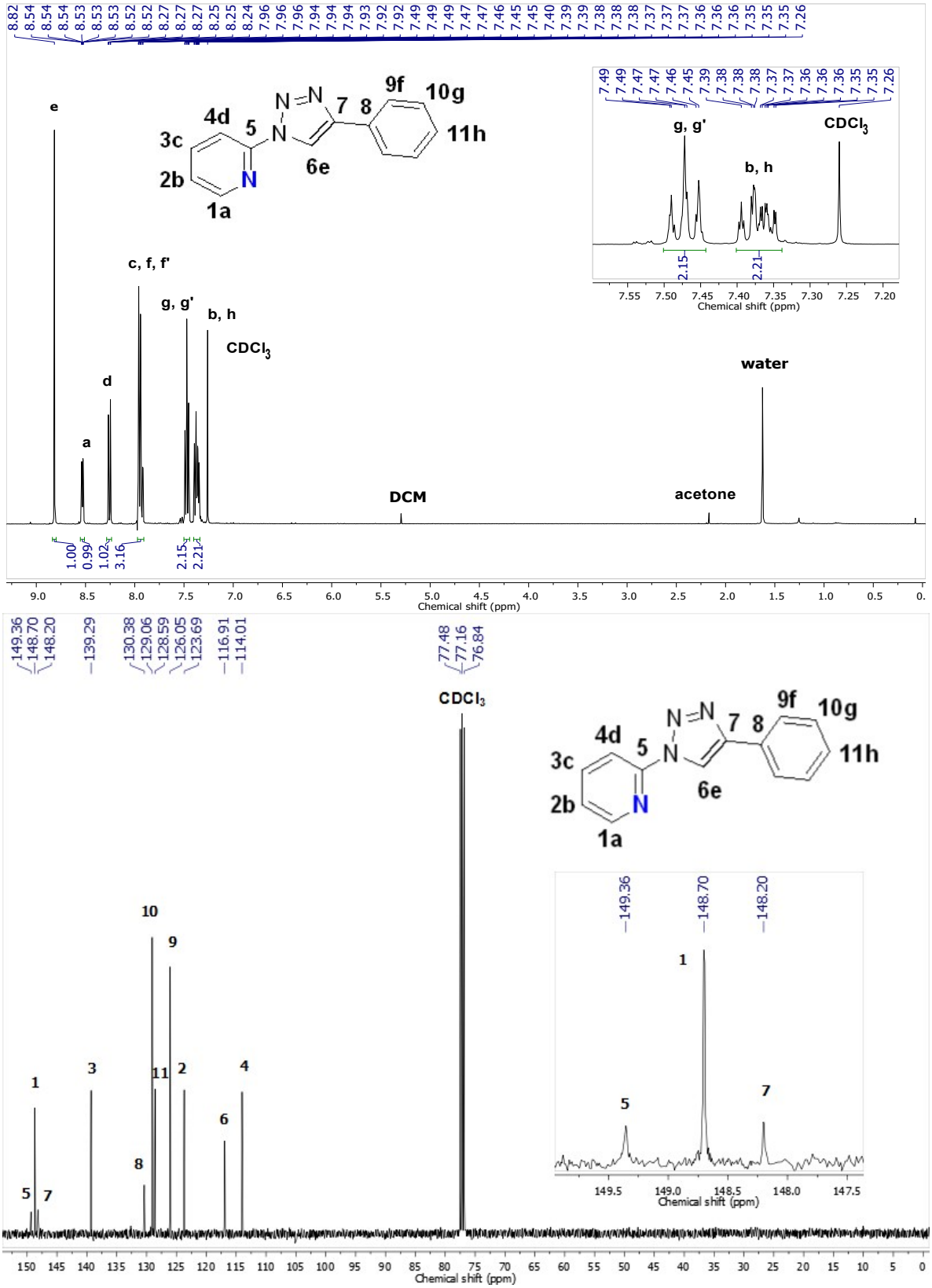

Figure **S2**. ^{1}H- (top) and ^{13}C{^{1}H}-NMR (bottom) spectra for (**A^2**) in chloroform-*d*.

1.3. 3-Methyl-4-phenyl-1-(2-pyridyl)-*1H*-1,2,3-triazole trifluoromethanesulfonate (A³).

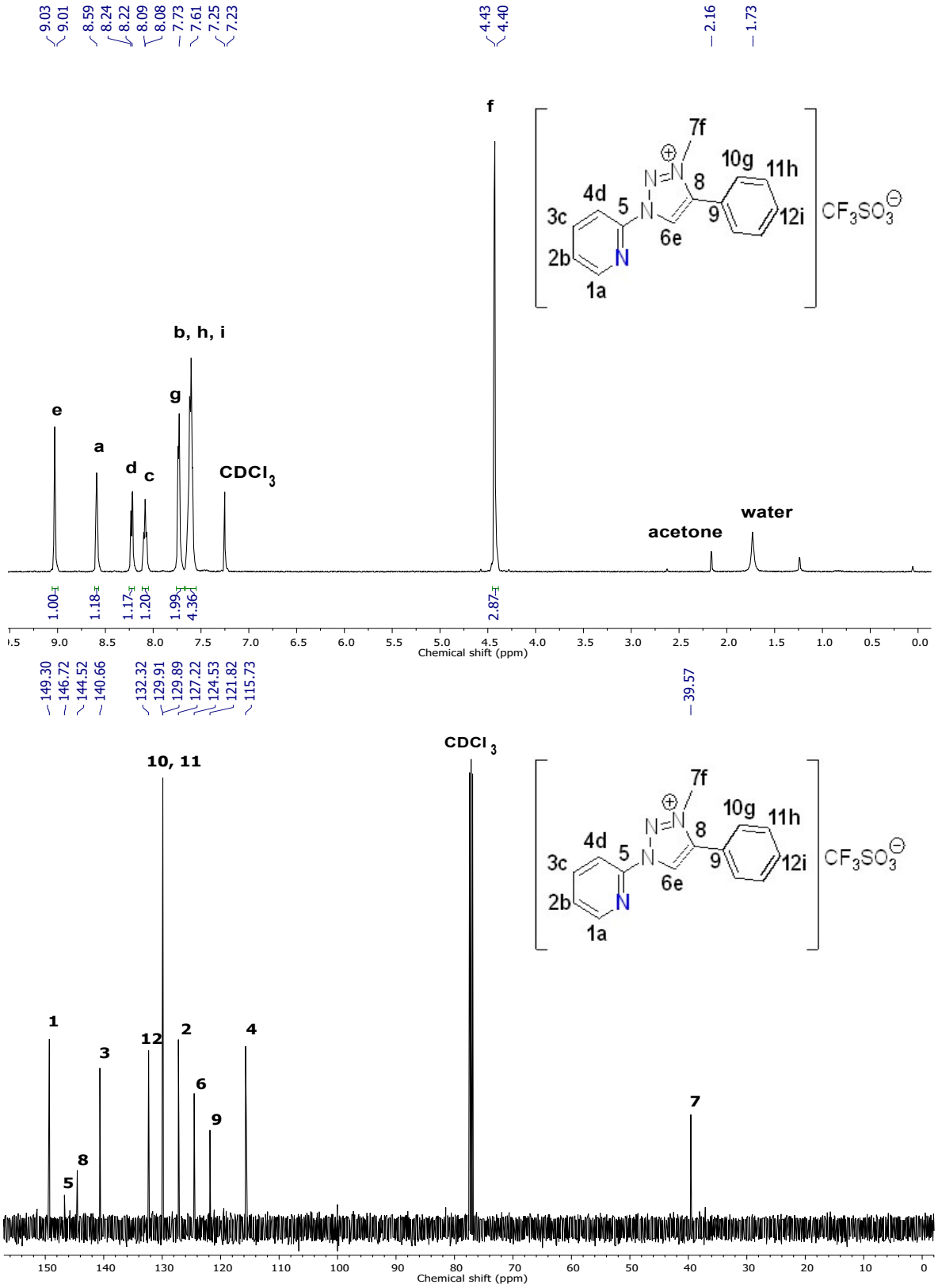

Figure **S3**. ^{1}H- (top) and ^{13}C{^{1}H}-NMR (bottom) spectra for (**A³**) in chloroform-*d*.

1.4. 3-Methyl-4-phenyl-1-(2-pyridyl)-1,2,3-triazolyl-5-thione (TrzPyS).

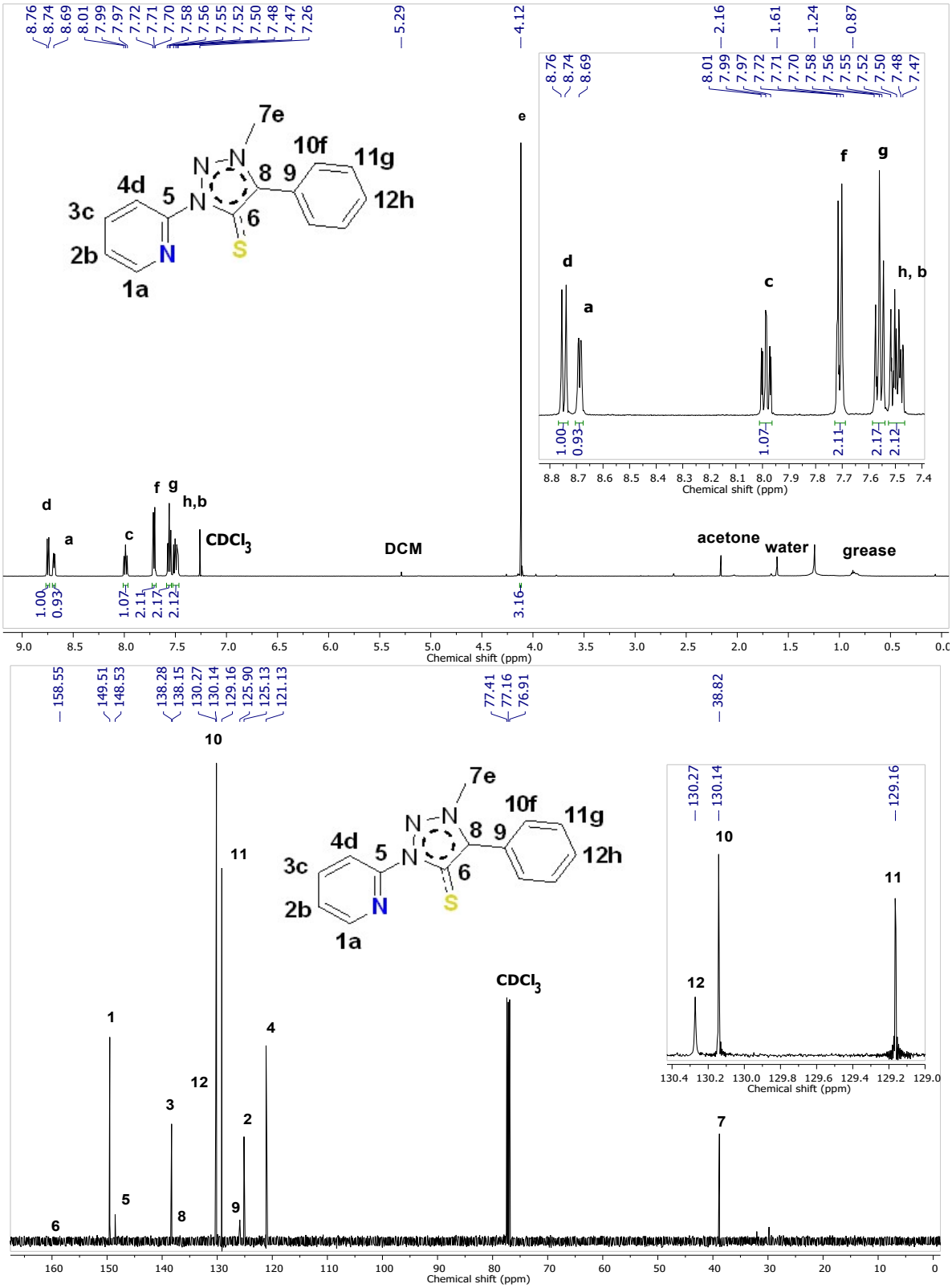

Figure **S4**. ^{1}H- (top) and ^{13}C{^{1}H}-NMR (bottom) spectra (**TrzPyS**) in chloroform-*d*.

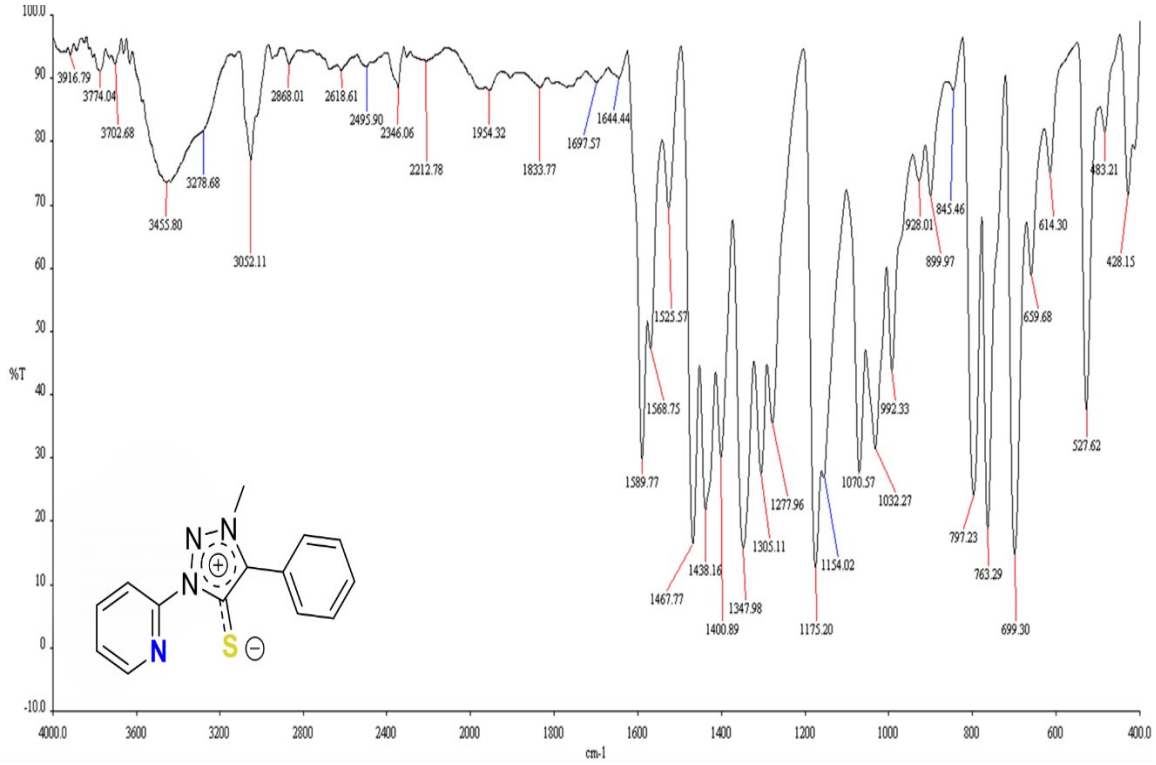

Figure **S5**. Infrared spectrum for (**TrzPyS**).

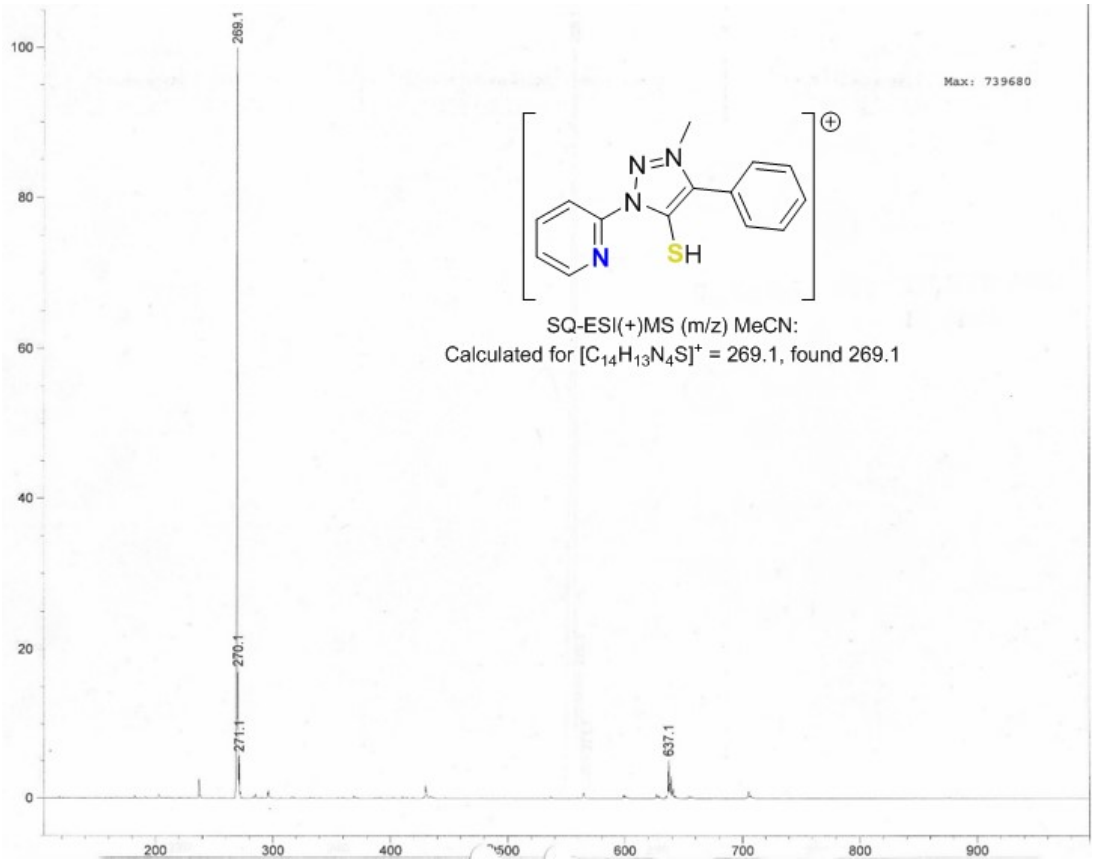

Figure **S6**. Mass spectrum for (**TrzPyS**).

1.5. Complex *trans*-$[Fe^{II}(Py)_4(NCS)_2]$ (P^1).

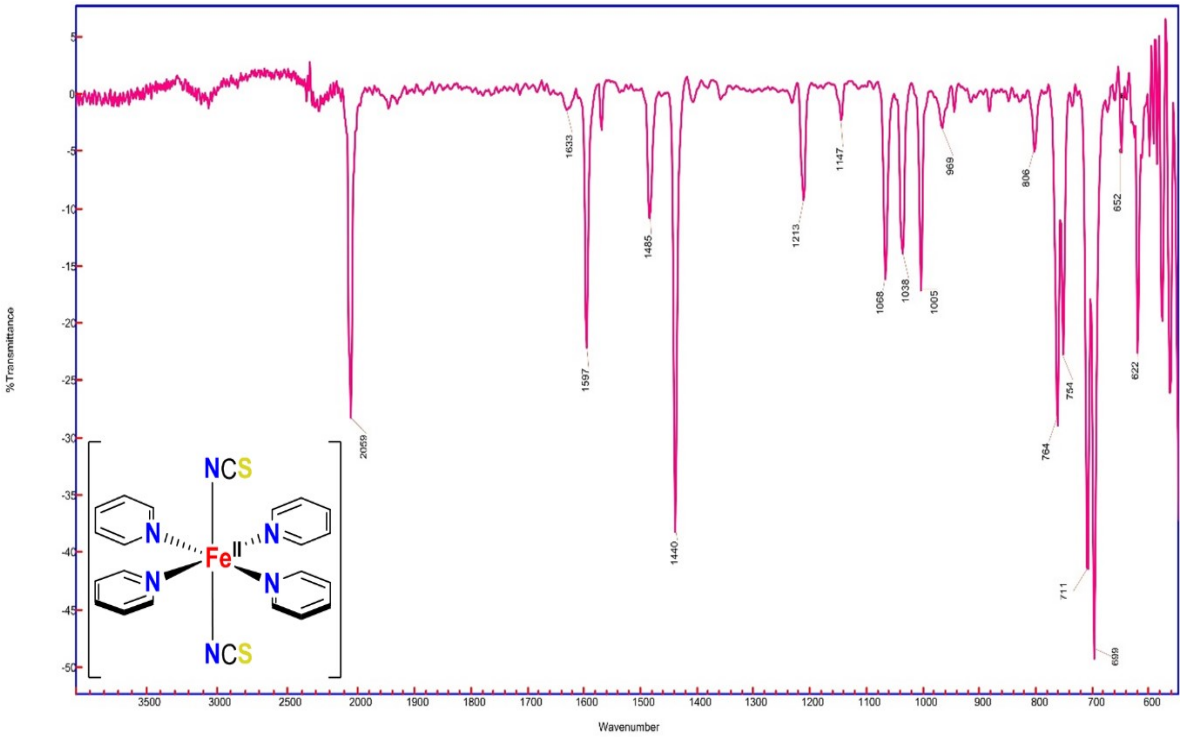

Figure **S7**. Infrared spectrum for (P^1).

1.6. Complex *trans*-$[Fe^{II}(Py)_4(NCSe)_2]$ (P^2).

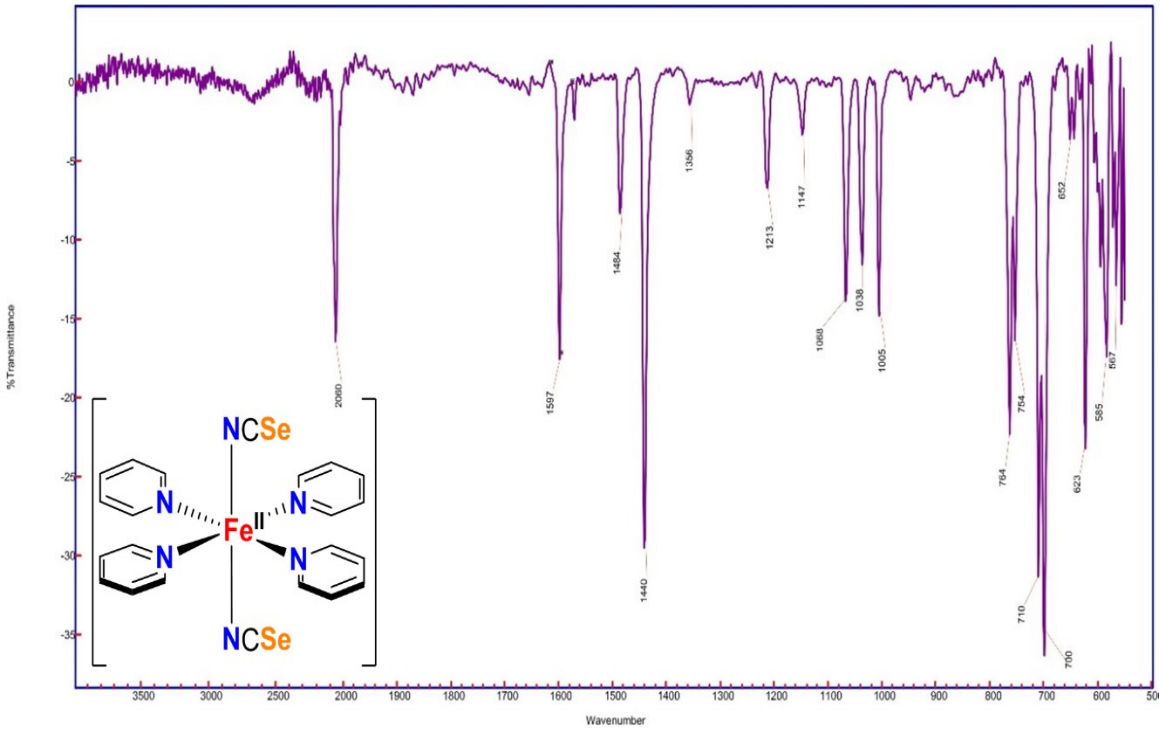

Figure **S8**. Infrared spectrum for (P^2).

1.7. Complex *trans*-$[Fe^{II}(Py)_4(NCBH_3)_2]$ (P^3).

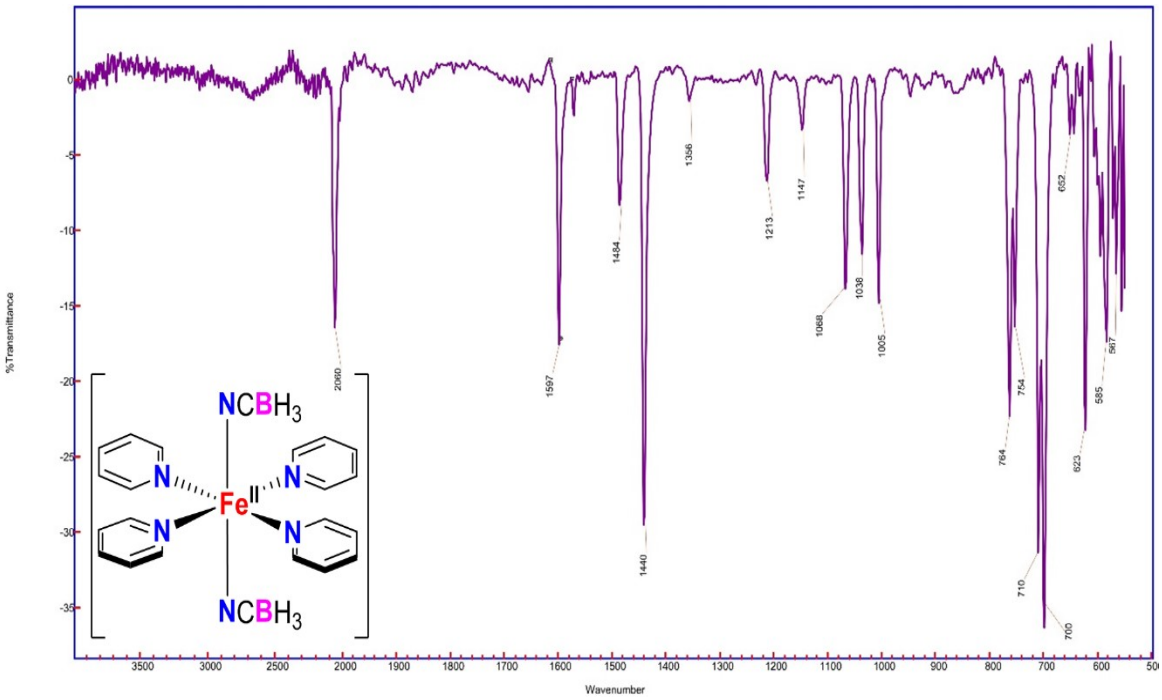

Figure **S9**. Infrared spectrum for (P^3).

1.8. Complex *trans*-$[Fe^{II}(ImPyS)_2(NCS)_2]$ (1a).

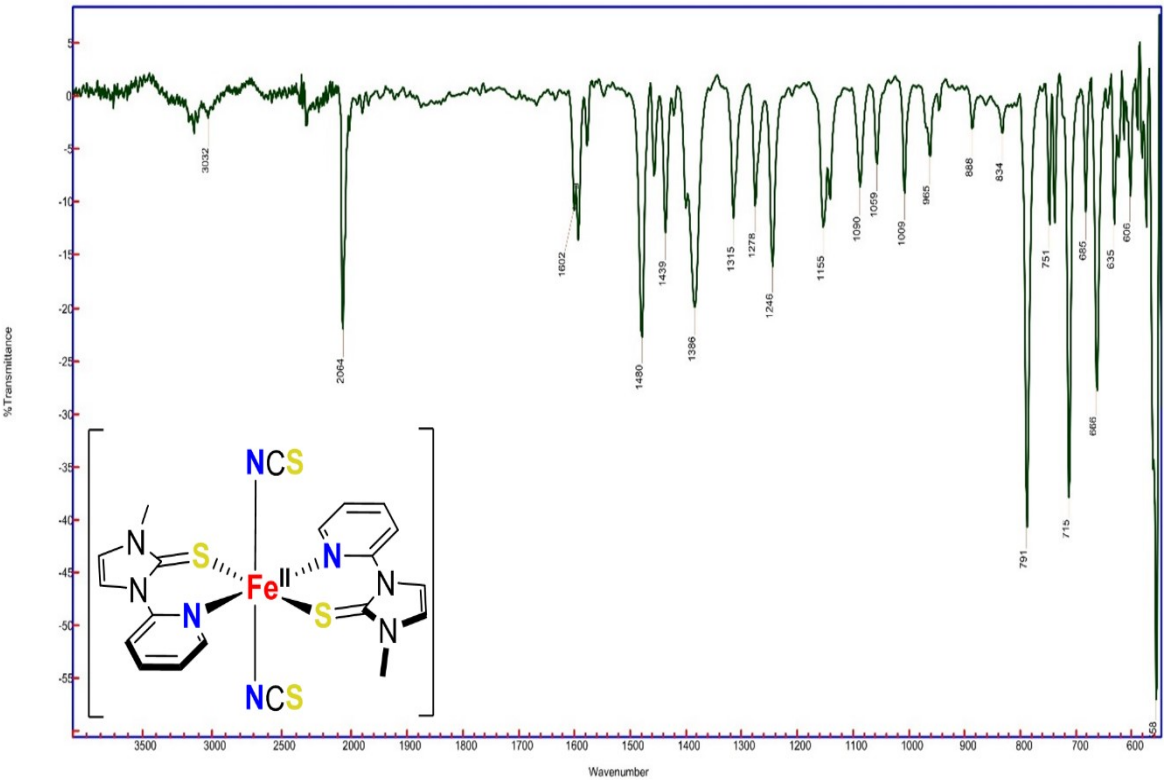

Figure **S10**. Infrared spectrum for (**1a**).

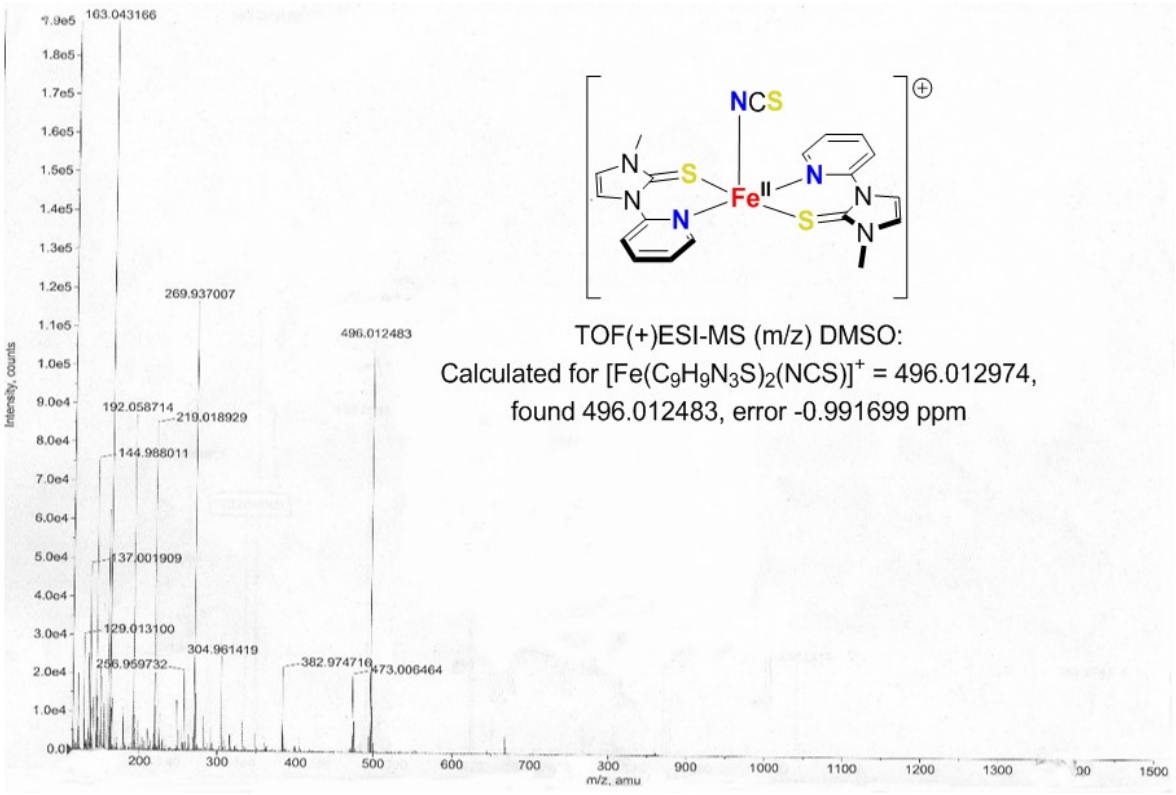

Figure **S11**. Mass spectrum for (**1a**).

1.9. Complex *trans*-[$Fe^{II}(ImPyS)_2(NCSe)_2$] (1b).

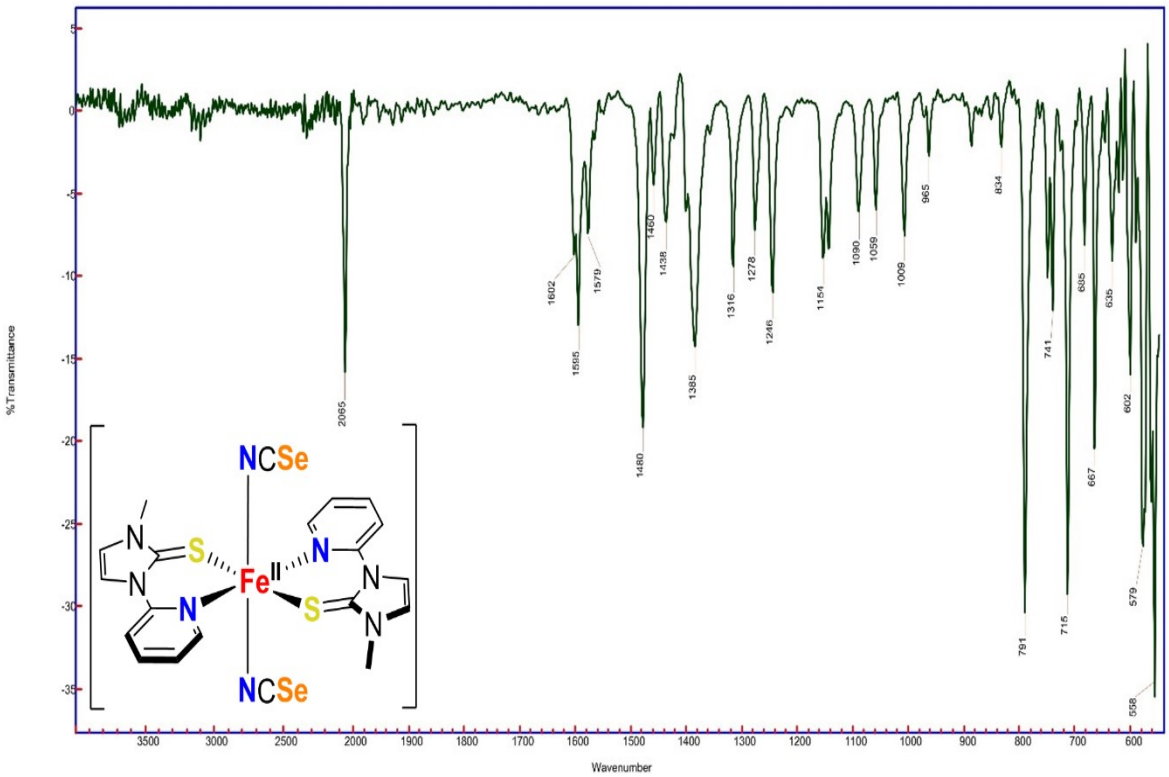

Figure **S12**. Infrared spectrum for (**1b**).

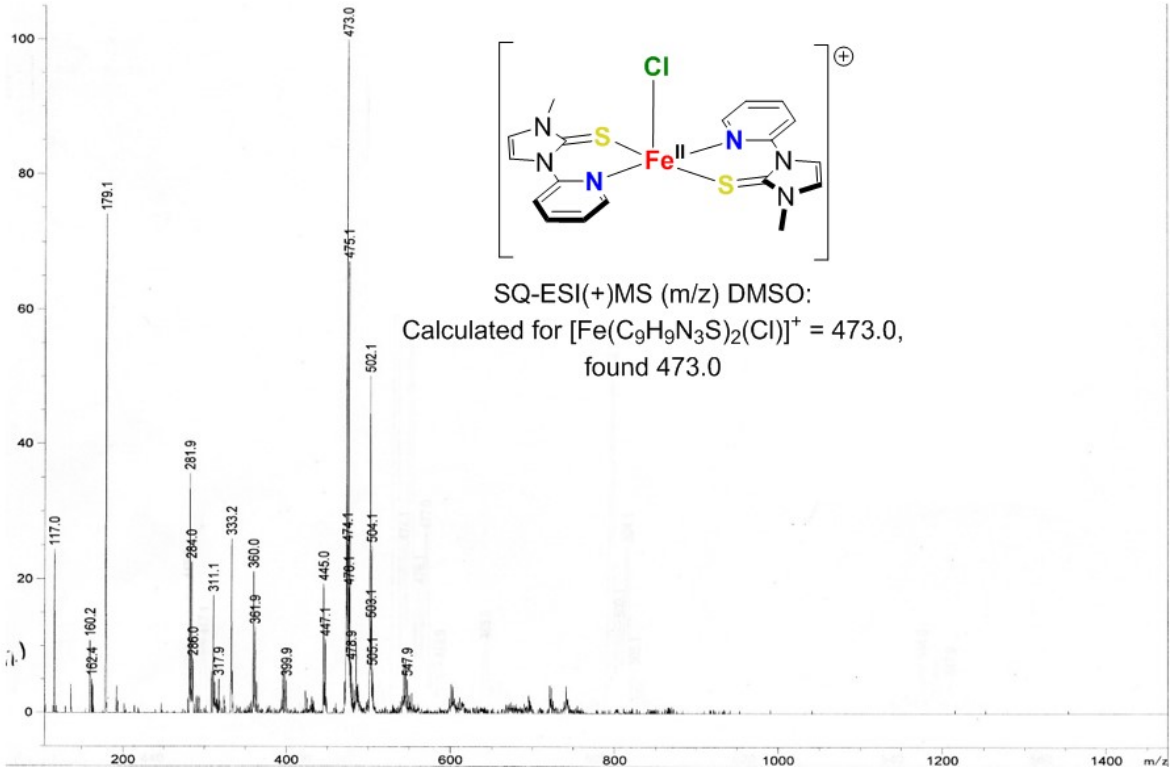

Figure **S13**. Mass spectrum for (**1b**).

1.10. Complex *trans*-[Fe^{II}(ImPyS)$_2$(NCBH$_3$)$_2$] (1c).

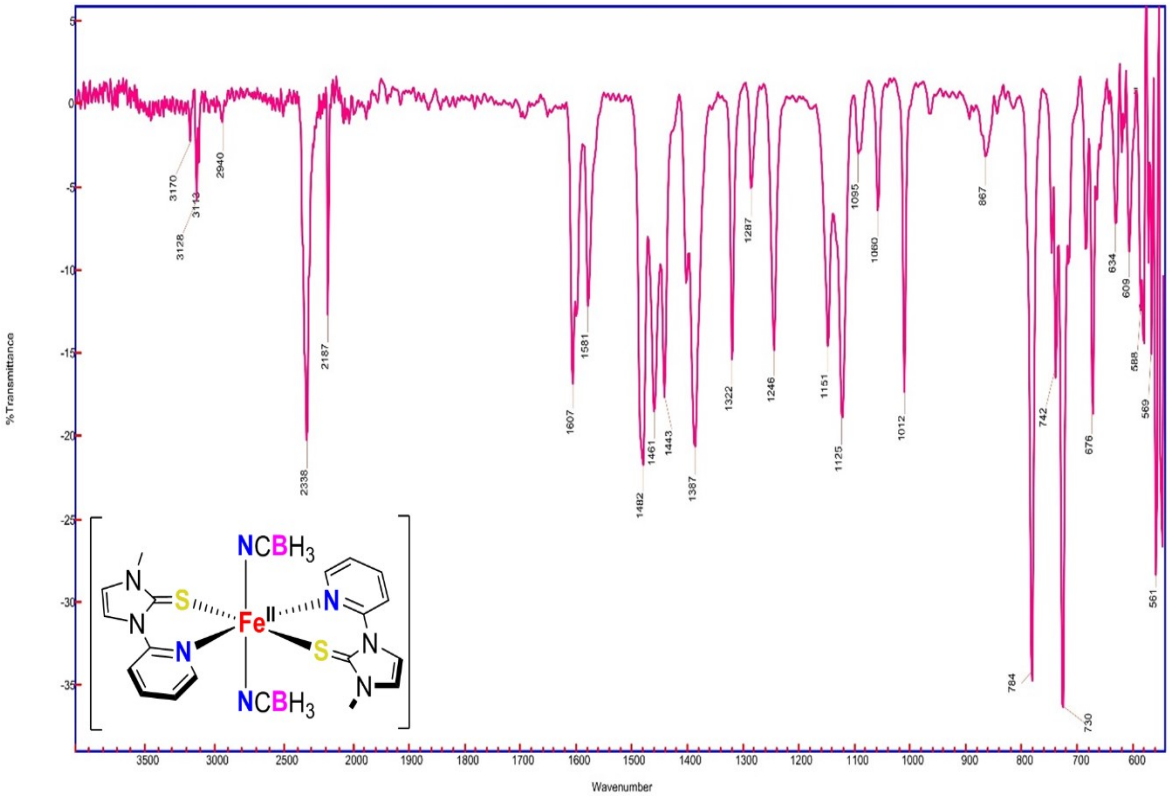

Figure **S14**. Infrared spectrum for (**1c**).

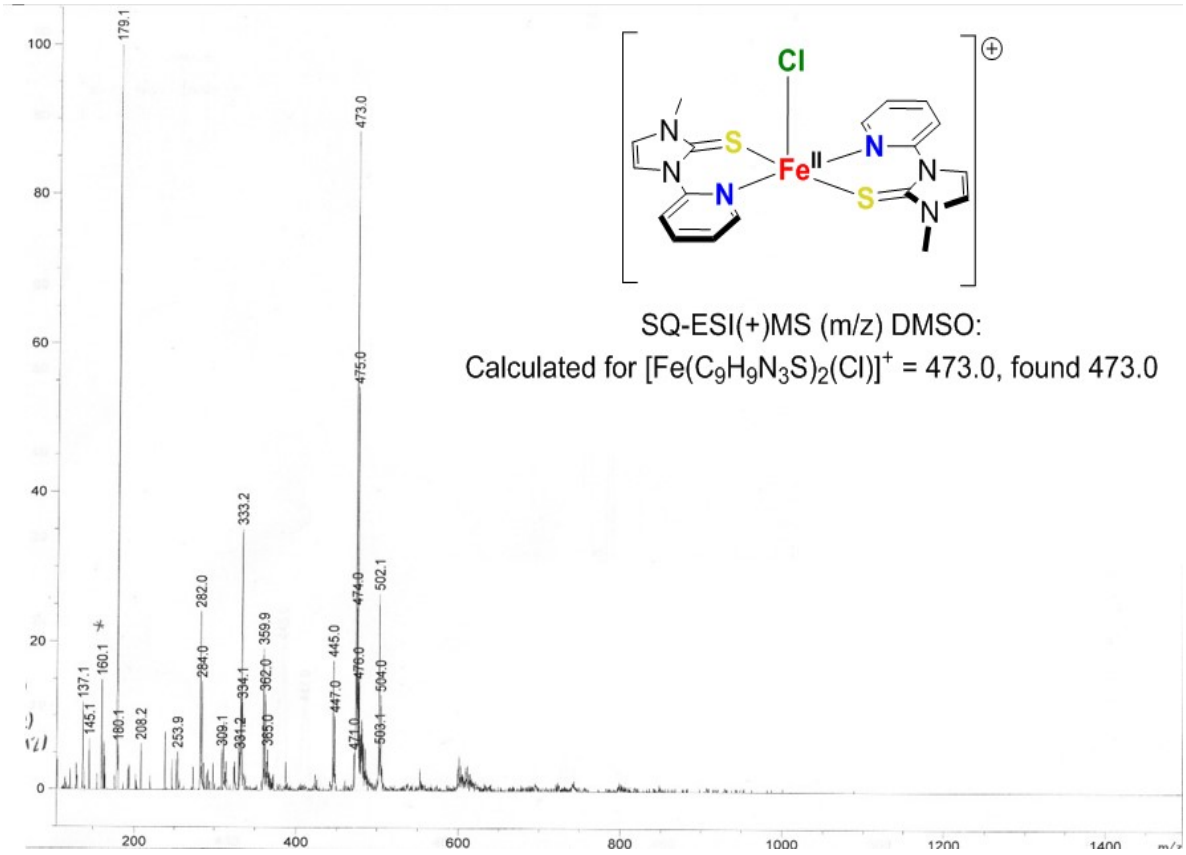

Figure **S15**. Mass spectrum for (**1c**).

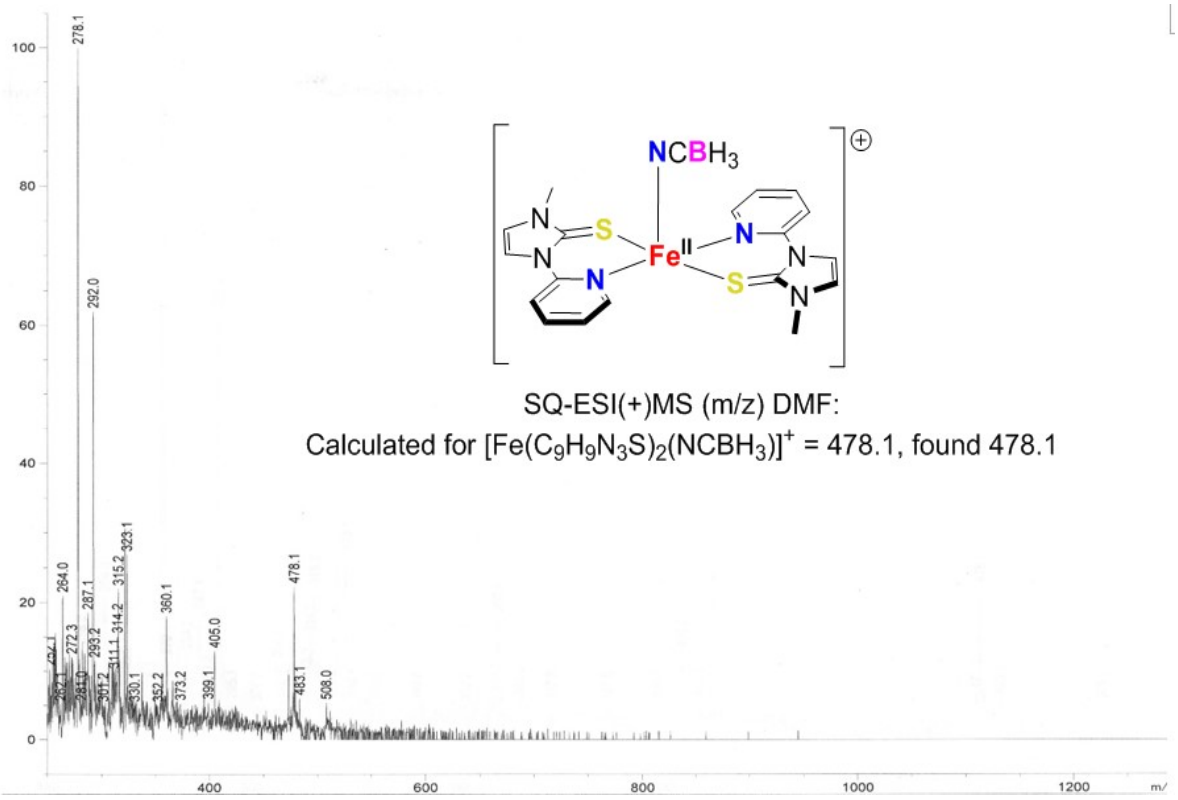

Figure **S16**. Mass spectrum for (**1c**).

1.11. Complex *trans*-[$Fe^{II}(TrzPyS)_2(NCS)_2$] (2a).

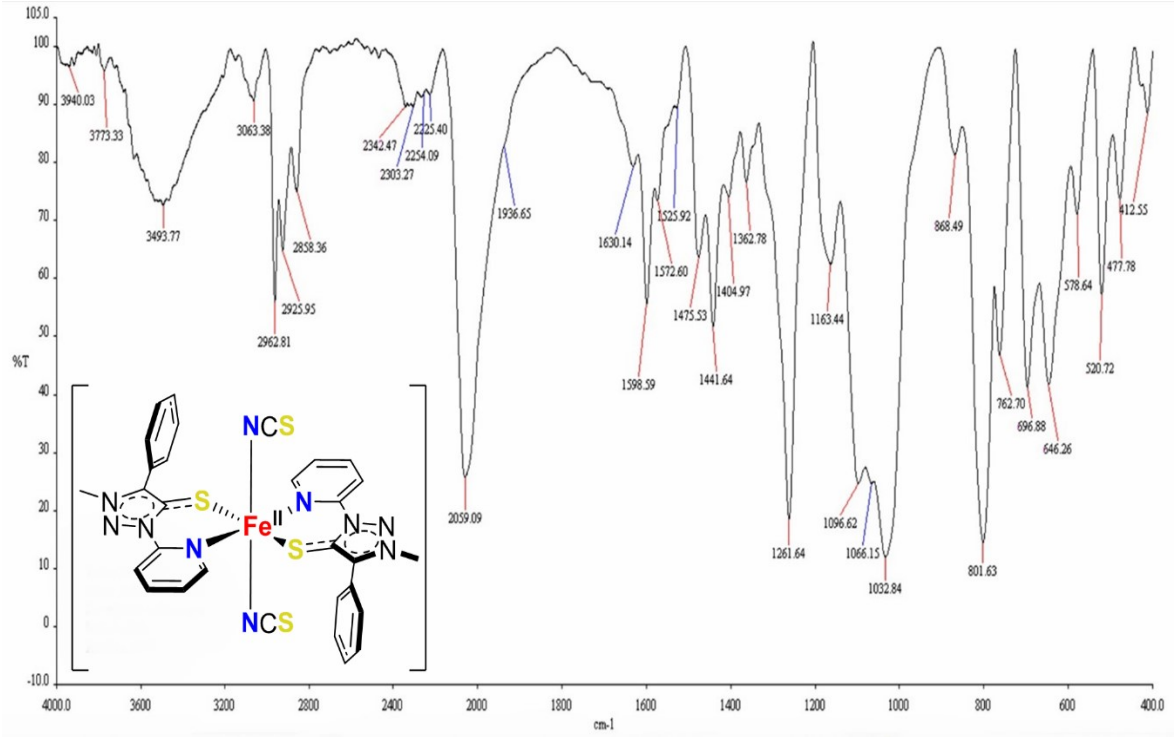

Figure **S17**. Infrared spectrum for (**2a**).

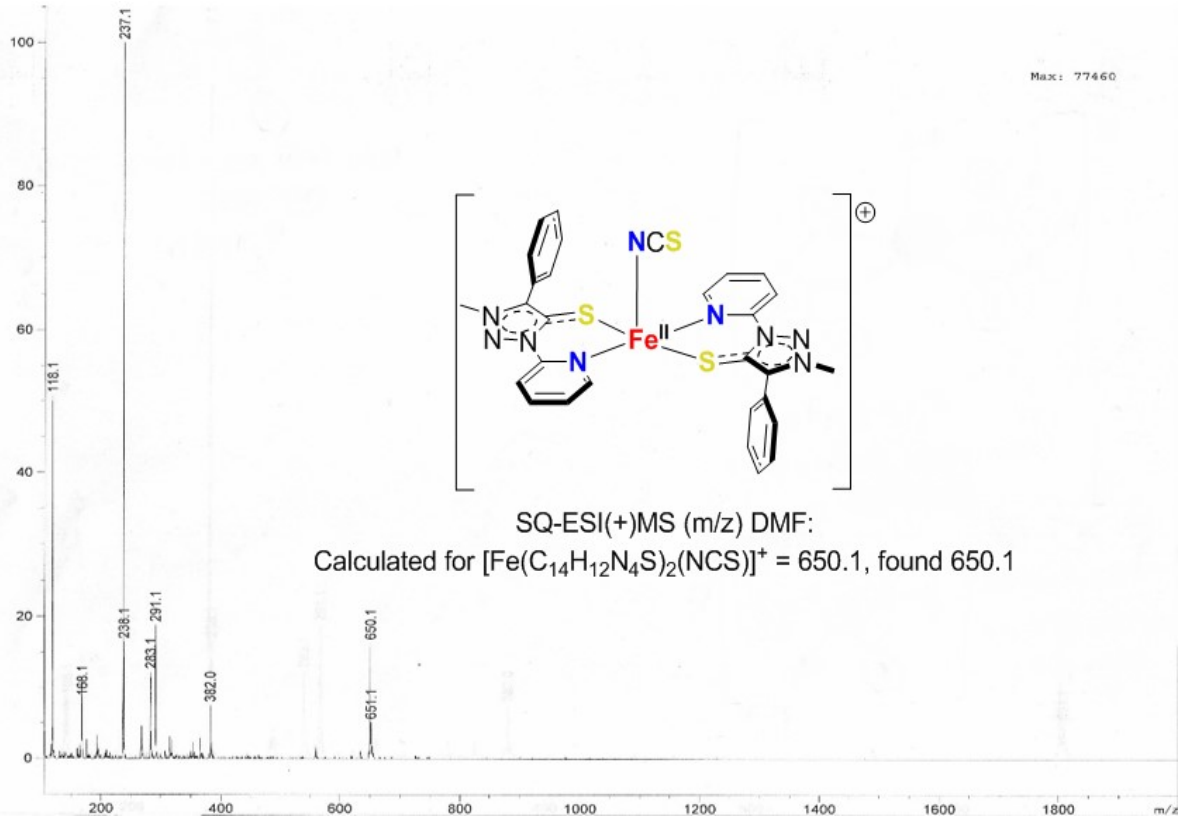

Figure **S18**. Mass spectrum for (**2a**).

1.12. Complex *trans*-$[Fe^{II}(TrzPyS)_2(NCSe)_2]$ (2b).

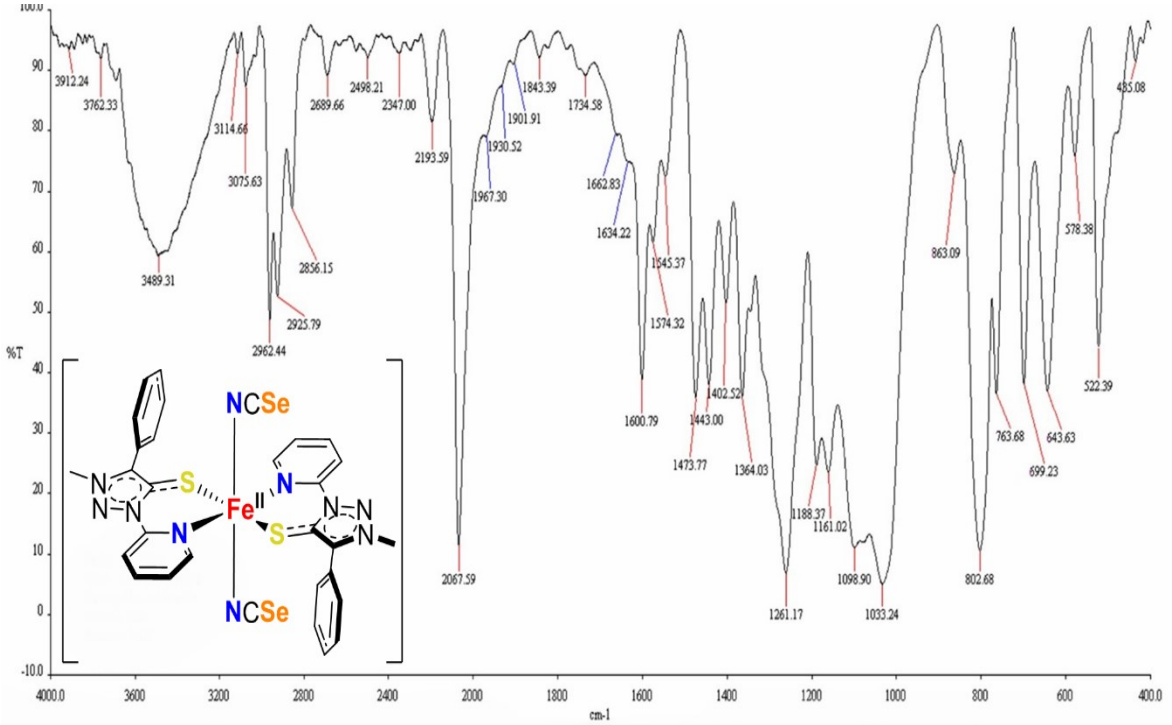

Figure **S19**. Infrared spectrum for (**2b**).

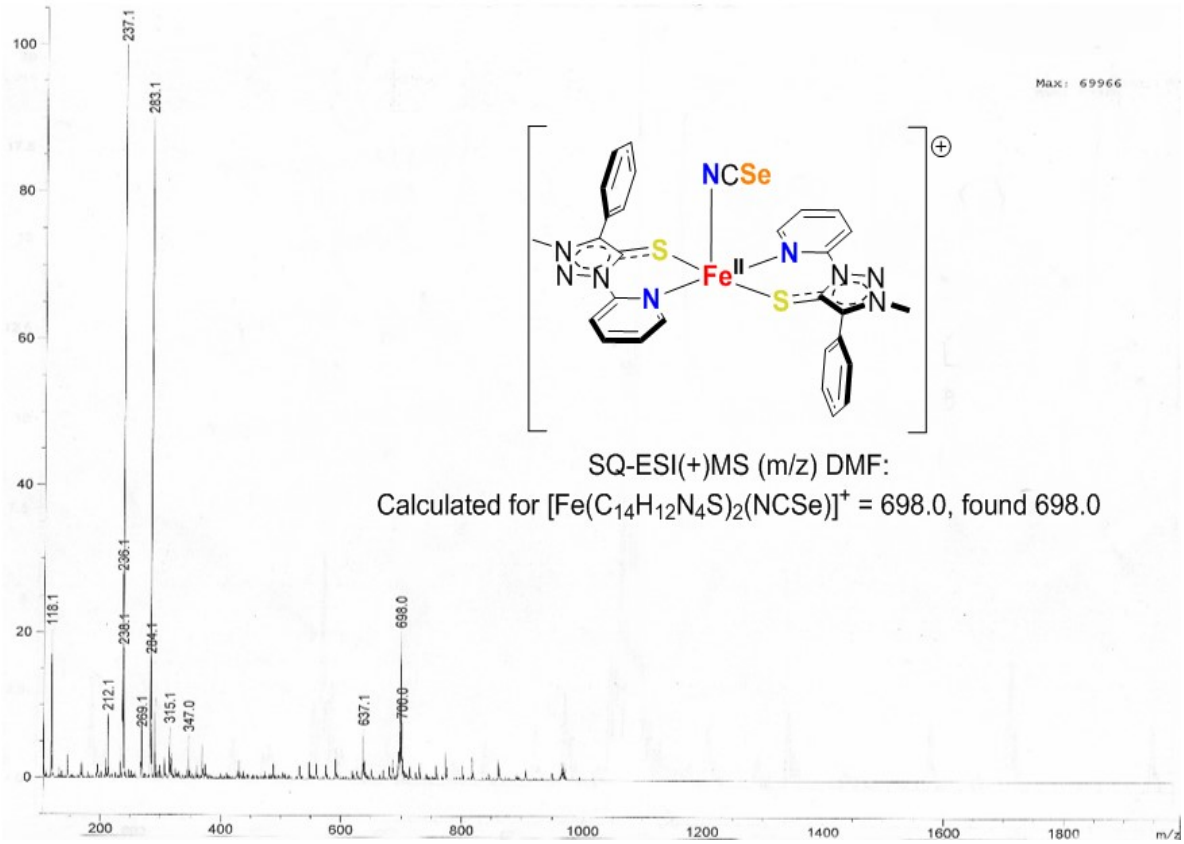

Figure **S20**. Mass spectrum for (**2b**).

1.13. Complex *trans*-$[Fe^{II}(TrzPyS)_2(NCBH_3)_2]$ (2c).

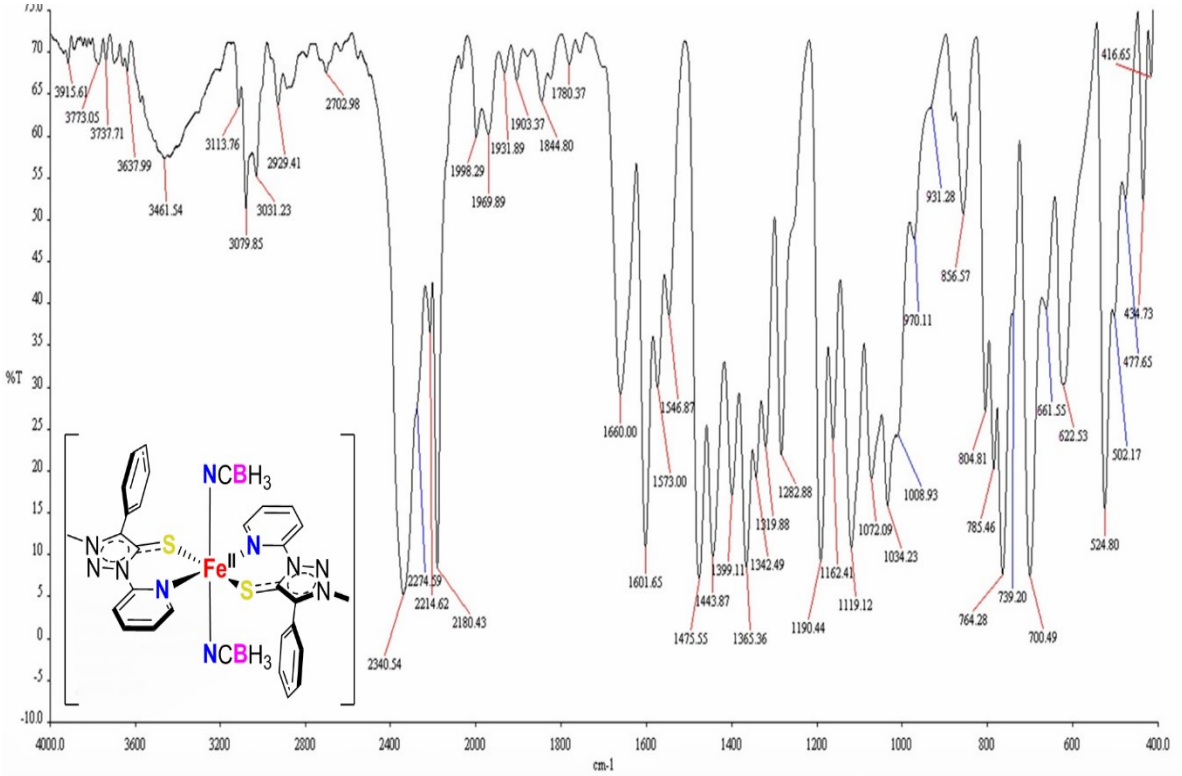

Figure **S21**. Spectrum for (**2c**).

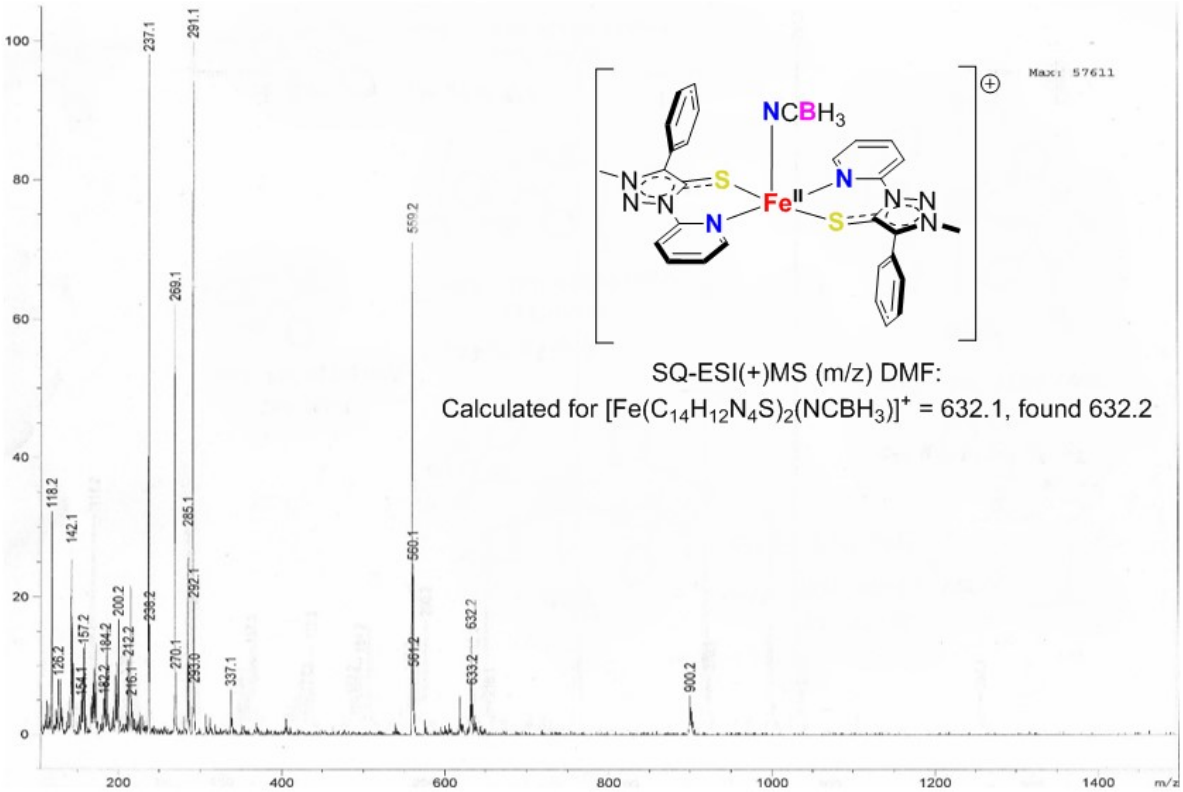

Figure **S22**. Mass spectrum for (**2c**).

2. X-ray analysis.

2.1. Single crystal data, structure refinement and selected bond parameters.

Single crystal data, structures refinement and selected bond lengths (Å) and bond angles (˚), average bond lengths (Å), average bond angles (˚) and Hendrickson octahedral distortion parameter are summarised in the next Tables **S1**-**S5**.

Table **S1**. Single crystal data and structure refinement for complex family *trans*-$[Fe^{II}(ImPyS)_2(NCE)_2]$ E = S and Se; complexes **1a** and **1b** respectively.

Complex	**1a**	**1b**
Empirical formula	$C_{20}H_{18}Fe_1N_8S_4$	$C_{20}H_{18}Fe_1N_8S_2Se_2$
Formula weight	554.51	648.31
Temperature (K)	150(2)	296(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
a (Å)	9.8211(7)	10.0926(7)
b (Å)	15.7029(11)	15.8607(10)
c (Å)	7.7911(6)	7.8392(5)
α (°)	90	90
β (°)	99.618(2)	99.955(2)
γ (°)	90	90
Volume ($Å^3$)	1184.65(15)	1235.97(14)
Z	2	2
Density (calculated) (g/cm^3)	1.555	1.742
Absorption coefficient (mm^{-1})	1.016	3.750
F(000)	568	640
Crystal size (mm) / colour / shape	0.303 x 0.277 x 0.254 / amber / prism	0.121 x 0.115 x 0.077 / amber / plate
Theta range for data collection (°)	2.471 to 32.575	2.418 to 26.371
Index ranges	-14 ≤ h ≤ 14 -23 ≤ k ≤ 23 -11 ≤ l ≤ 11	-12 ≤ h ≤ 12 -19 ≤ k ≤ 19 -9 ≤ l ≤ 9
Reflections collected	36368	33828
Independent reflections	4290 [R(int) = 0.0355]	2527 [R(int) = 0.0744]
Completeness to theta = 25.242°	98.9 %	100.0 %
Max. and min. transmission	0.7465 and 0.7019	0.7454 and 0.6393
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	4290 / 0 / 152	2527 / 0 / 152
Goodness-of-fit on F^2	1.091	1.027
Final R indices [I>2sigma(I)]	R_1 = 0.0244, wR_2 = 0.0630	R_1 = 0.0440, wR_2 = 0.1011
R indices (all data)	R_1 = 0.0275, wR_2 = 0.0646	R_1 = 0.0713, wR_2 = 0.1156
Largest diff. peak and hole ($e.Å^{-3}$)	0.417 and -0.473	0.742 and -0.749

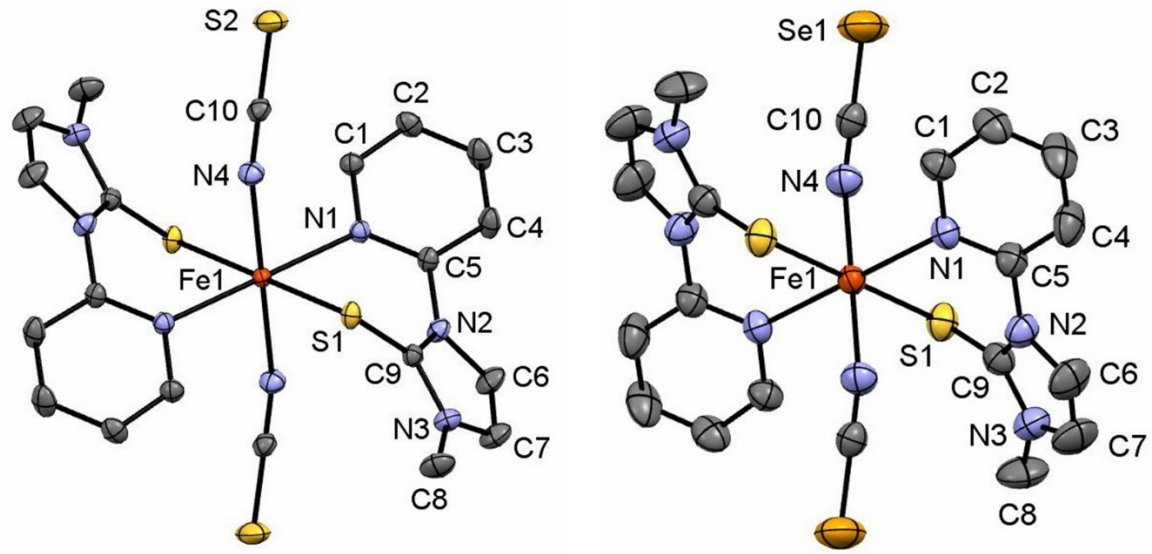

Figure **S23**. Perspective view of complex *trans*-[$Fe^{II}(ImPyS)_2(NCS)_2$] (**1a**) acquired at 150(2) K (left), and complex *trans*-[$Fe^{II}(ImPyS)_2(NCSe)_2$] (**1b**) acquired at 296(2) K (right). Ellipsoids are drawn at the 50 % probability level. Hydrogen atoms are omitted for the sake of clarity.

Table **S2**. Selected bond lengths (Å) and bond angles (˚) of complexes *trans*-[$Fe^{II}(ImPyS)_2(NCE)_2$] E = S and Se; complexes **1a** and **1b** respectively.

Complex	**1a**	**1b**
Temperature (K)	150(2)	296(2)
Fe(1)-N(1) (Å)	2.2474(8)	2.249(3)
Fe(1)-N(4) (Å)	2.1177(9)	2.128(4)
Fe(1)-S(1) (Å)	2.4800(3)	2.4741(10)
C(9)-S(1) (Å)	1.6942(10)	1.687(4)
N(1)-Fe(1)-N(1)#1 (°)	180.0	180.00(15)
N(4)-Fe(1)-N(4)#1 (°)	180.00(4)	180.0
S(1)-Fe(1)-S(1)#1 (°)	180.0	180.0
N(1)-Fe(1)-N(4) (°)	87.52(3)	87.79(13)
N(1)-Fe(1)-N(4)#1 (°)	92.48(3)	92.21(13)
N(4)-Fe(1)-S(1) (°)	89.59(3)	89.16(10)
N(4)-Fe(1)-S(1)#1 (°)	90.41(3)	90.84(10)
N(1)-Fe(1)-S(1) (°)	85.70(2)	85.38(8)
N(1)-Fe(1)-S(1)#1 (°)	94.30(2)	94.62(8)
C(9)-S(1)-Fe(1) (°)	96.73(3)	96.48(14)

Table **S3**. Single crystal data and structure refinement for complexes *trans*-[$Fe^{II}(TrzPyS)_2(NCE)_2$] E = S, Se and BH_3; **2a**, **2b** and **2c** respectively.

Complex	**2a**	**2b**	**2c**	
Empirical formula	$C_{30}H_{24}Fe_1N_{10}S_4$	$C_{30}H_{24}Fe_1N_{10}S_2Se_2$	$C_{30}H_{30}Fe_1N_{10}S_2B_2$	$C_{30}H_{30}Fe_1N_{10}S_2B_2$
Formula weight	708.68	802.48	672.23	672.23
Temperature (K)	170(2)	171(2)	302(2)	166(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1	*P*-1
a (Å)	8.2200(8)	8.1749(10)	8.2630(4)	8.2367(7)
b (Å)	8.4119(8)	8.4576(10)	8.4919(4)	8.4429(9)
c (Å	13.0015(13)	12.8781(16)	13.1039(7)	12.9792(13)
α (°)	106.039(3)	104.556(4)	104.846(2)	104.946(4)
β (°)	102.841(4)	101.501(4)	103.820(2)	103.136(3)
γ (°)	99.914(3)	100.261(4)	99.454(2)	99.831(3)
Volume ($Å^3$)	815.80(14)	819.69(17)	837.79(7)	823.62(14)
Z	1	1	1	1
Density (calculated) (g/cm^3)	1.442	1.626	1.332	1.355
Absorption coefficient (mm^{-1})	0.757	2.846	0.612	0.622
F(000)	364	400	348	348
Crystal size (mm) / colour / shape	0.263 x 0.177 x 0.098 / red / prism	0.196 x 0.181 x 0.054 / red / prism	0.088 x 0.058 x 0.022 / yellow / square	0.088 x 0.058 x 0.022 / yellow / square
Theta range for data collection (°)	2.624 to 27.481	2.563 to 26.372	2.556 to 26.732	2.575 to 25.124
Index ranges	$-10 \le h \le 10$ $-10 \le k \le 10$ $-16 \le l \le 16$	$-10 \le h \le 10$ $-9 \le k \le 10$ $-16 \le l \le 16$	$-10 \le h \le 10$ $-10 \le k \le 10$ $-16 \le l \le 16$	$-9 \le h \le 9$ $-10 \le k \le 10$ $-15 \le l \le 15$
Reflections collected	84766	59596	87200	64134
Independent reflections	3732 [R(int) = 0.0678]	3347 [R(int) = 0.0458]	3564 [R(int) = 0.1879]	2923 [R(int) = 0.0804]
Completeness to theta = 25.242°	99.8 %	99.8 %	99.8 %	99.6 %
Max. and min. transmission	0.7273 and 0.6653	0.7458 and 0.6205	0.7457 and 0.7265	0.7452 and 0.6934
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	3732 / 0 / 242	3347 / 0 / 253	3569 / 0 / 246	2923 / 0 / 265
Goodness-of-fit on F^2	1.052	0.998	1.112	1.090
Final R indices [I>2sigma(I)]	$R_1 = 0.0269$, $wR_2 = 0.0695$	$R_1 = 0.0265$, $wR_2 = 0.0616$	$R_1 = 0.0445$, wR2 = 0.1053	$R_1 = 0.0281$, $wR_2 = 0.0606$
R indices (all data)	$R_1 = 0.0305$, $wR_2 = 0.0720$	$R_1 = 0.0328$, $wR_2 = 0.0652$	R1 = 0.0530, wR2 = 0.1096	$R_1 = 0.0369$, $wR_2 = 0.0637$
Largest diff. peak and hole ($e.Å^{-3}$)	0.314 and -0.526	0.543 and -0.591	0.381 and -0.502	0.213 and -0.238

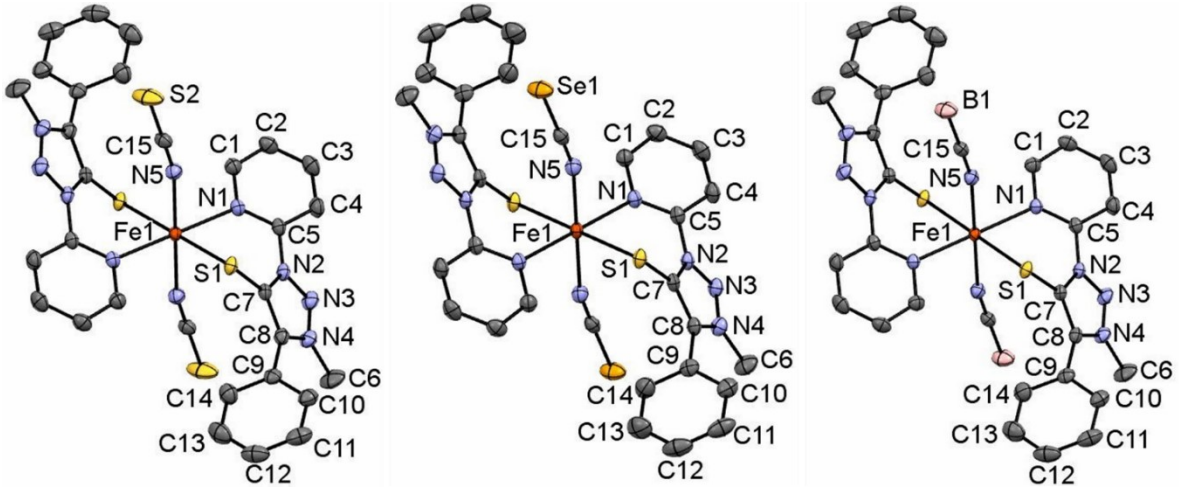

Figure **S24**. Perspective view of the family complex *trans*-[$Fe^{II}(TrzPyS)_2(NCE)_2$] E = S, Se and BH_3 **2a**, **2b** and **2c** acquired at 170(2) K, 171(2) K and 166(2) K; from left to right respectively. Ellipsoids are drawn at the 50 % probability level. Hydrogen atoms are omitted for the sake of clarity.

Table **S4**. Selected bond lengths (Å) and bond angles (˚) of complex family *trans*-[$Fe^{II}(TrzPyS)_2(NCE)_2$] E = S, Se and BH_3; complexes **2a**, **2b** and **2c** respectively.

Complex	**2a**	**2b**	**2c**	
Temperature (K)	170(2)	171(2)	302(2)	166(2)
Fe(1)-N(1) (Å)	2.2680(11)	2.2657(17)	2.2663(18)	2.2611(14)
Fe(1)-N(5) (Å)	2.1201(12)	2.1418(19)	2.1453(19)	2.1443(16)
Fe(1)-S(1) (Å)	2.4860(4)	2.4695(6)	2.4818(5)	2.4780(5)
C(7)-S(1) (Å)	1.7074(13)	1.708(2)	1.709(2)	1.7094(17)
N(1)-Fe(1)-N(1)#1 (°)	180.0	180.0	180.0	180.00(7)
N(5)-Fe(1)-N(5)#1 (°)	180.0	180.00(10)	180.0	180.0
S(1)-Fe(1)-S(1)#1 (°)	180.0	180.0	180.0	180.0
N(1)-Fe(1)-N(5) (°)	90.99(4)	90.55(7)	89.71(7)	90.14(5)
N(1)-Fe(1)-N(5)#1 (°)	89.01(4)	89.45(7)	90.29(7)	89.86(5)
N(5)-Fe(1)-S(1) (°)	90.29(3)	90.48(5)	90.96(5)	89.32(4)
N(5)-Fe(1)-S(1)#1 (°)	89.71(3)	89.52(5)	89.04(5)	90.68(4)
N(1)-Fe(1)-S(1) (°)	85.93(3)	86.05(5)	85.47(5)	85.76(4)
N(1)-Fe(1)-S(1)#1 (°)	94.07(3)	93.95(5)	94.53(5)	94.24(4)
C(7)-S(1)-Fe(1) (°)	95.91(4)	96.38(7)	96.00(7)	96.26(6)

Table **S5**. Average bond lengths (Å) and angles (°) and Σ_{Oh} parameter for the family complex *trans*-[$Fe^{II}(ImPyS)_2(NCE)_2$] E = S and Se; complexes **1a** and **1b** respectively, *trans*-[$Fe^{II}(TrzPyS)_2(NCE)_2$] E = S, Se and BH_3; complexes **2a**, **2b** and **2c** respectively. Σ_{Oh} = Hendrickson octahedral distortion parameter.

Complex	**1a**[a]	**1b**[b]	**2a**[a]	**2b**[b]	**2c**[c]	
Temperature (K)	150(2)	296(2)	170(2)	171(2)	302(2)	166(2)
Space group	$P2_1/c$	$P2_1/c$	P-1	P-1	P-1	P-1
Fe-N_{Py} (Å)	2.2474(8)	2.249(3)	2.2680(11)	2.2657(17)	2.2663(18)	2.2611(14)
Fe-N_{NCE} (Å)	2.1177(9)	2.128(4)	2.1201(12)	2.1418(19)	2.1453(19)	2.1443(16)
Fe-S (Å)	2.4800(3)	2.4741(10)	2.4860(4)	2.4695(6)	2.4818(5)	2.4780(5)
C=S (Å)	1.6942(10)	1.687(4)	1.7074(13)	1.708(2)	1.709(2)	1.7094(17)
trans-N_{Py}-Fe-N_{Py} (°)	180.00	180.00(15)	180.00	180.00	180.00	180.00(7)
trans-N_{NCE}-Fe-N_{NCE} (°)	180.00(4)	180.00	180.00	180.00(10)	180.00	180.00
trans-S-Fe-S (°)	180.00	180.00	180.00	180.00	180.00	180.00
Fe-S-C (°)	96.73(3)	96.48(14)	95.91(4)	96.38(7)	96.00(7)	96.26(6)
Av. cis-N-Fe-N (°)	90.00(4)	90.00(18)	90.00(6)	90.00	90.00(10)	90.00(7)
Av. cis-N-Fe-S (°)	90.00(5)	90.00(18)	90.00(6)	90.00	90.00(10)	90.00(8)
Av. Fe-N-C(E) (°)	157.21	157.26	165.11	163.97	168.18	166.69
Σ_{Oh}[d]	28.76(9)	30.68(36)	21.40(12)	19.92(20)	23.12(20)	20.24(15)

[a] E = S for complexes **1a** and **2a**. [b] E = Se for complexes **1b** and **2b**. [c] E = BH_3 for complex **2c**.
[d] The octahedral distortion parameter, Σ_{Oh}, is defined as the sum of the absolute values of the difference of each of the twelve cis angles from 90°. Σ_{Oh} = 0 indicates a perfect octahedral geometry.[S1,2]

2.2. Chemical structure of the literature complexes.[S3]

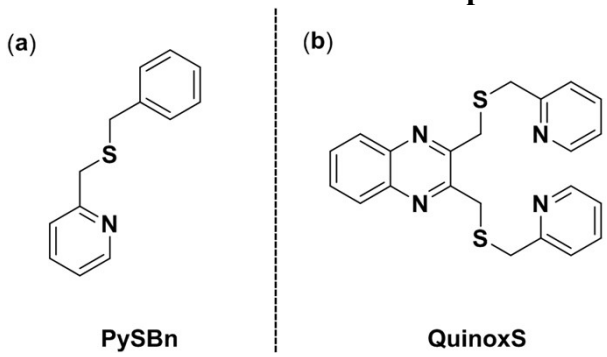

Figure **S25**. Chemical structure of ligands (**a**) benzylpicolylthioether (**PySBn**) and (**b**) 2,3-bis(((2-pyridylmethyl)thio)methyl)quinoxaline (**QuinoxS**).[S3]

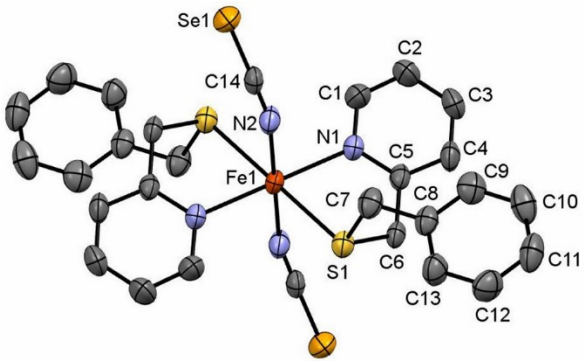

Figure **S26**. Crystal structure view of complex *trans*-[$Fe^{II}(PySBn)_2(NCSe)_2$] **3b** acquired at 199(2) K. Ellipsoids are drawn at the 50 % probability level. Hydrogen atoms are omitted for the sake of clarity.[S3]

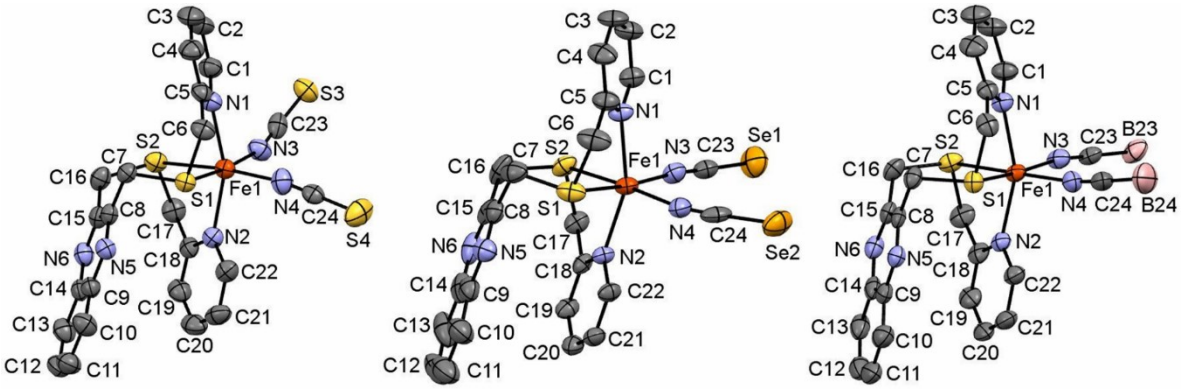

Figure **S27**. Crystal structure of the family complex *cis*-[$Fe^{II}(QuinoxS)(NCE)_2$] E = S, Se and BH_3; complexes **4a**, **4b** and **4c** acquired at 177(2) K, 177(2) K and 175(2) K; left, centre and right respectively. Ellipsoids are drawn at the 50 % probability level. Hydrogen atoms and acetonitrile solvent molecules are omitted for the sake of clarity.[S3]

2.3. Comparison of structural parameters with literature complexes of iron(II) in $\{N_4S_2\}$ coordination sphere.[S3-5]

In order to compare the structural characteristics of the complexes for this work with $Fe^{II}(N_4S_2)$ SCO-active complexes published in the literature, which contain cyanide co-ligands NCE E = S, Se and BH_3, Table **S6** shows the most relevant structural parameters for complex *trans*-$[Fe^{II}(PySBn)_2(NCSe)_2]$ and complex family *cis*-$[Fe^{II}(QuinoxS)(NCE)_2]$ E = S, Se and BH_3, PySBn = benzylpicolylthioether and QuinoxS = 2,3-bis(((2-pyridylmethyl)thio)methyl)quinoxaline.

Table **S6**. Average bond lengths (Å) and angles (°) and Σ_{Oh} parameter for complexes *trans*-$[Fe^{II}(ImPyS)_2(NCE)_2]$ E = S and Se, **1a** and **1b** respectively; complexes *trans*-$[Fe^{II}(TrzPyS)_2(NCE)_2]$ E = S, Se and BH_3, **2a**, **2b** and **2c** respectively; complex[S3] *trans*-$[Fe^{II}(PySBn)_2(NCSe)_2]$ **3b** and complexes[S3] *cis*-$[Fe^{II}(QuinoxS)(NCE)_2]$ E = S, Se and BH_3, **4a**, **4b** and **4c** respectively. Σ_{Oh} = Hendrickson octahedral distortion parameter.

Complex	**1a**[b]	**1b**[c]	**2a**[b]	**2b**[c]	**2c**[d]		**3b**[a, c]	**4a**[a, b]		**4b**[a, c]		**4c**[d]	
SCO activity	No	No	No	No	No		Yes	No		No		No	
Temperature (K)	150(2)	296(2)	170(2)	171(2)	302(2)	166(2)	199(2)	297(2)	177(2)	298(2)	177(2)	298(2)	175(2)
Spin state	High	High	High	High	High	High	High	High	High	High	High	High	High
Space group	$P2_1/c$	$P2_1/c$	P-1	P-1	P-1	P-1	$C2/c$	$P2_1/c$	$P2_1/c$	P-1	P-1	P-1	P-1
Fe-N_{Py} (Å)	2.2474(8)	2.249(3)	2.2680(11)	2.2657(17)	2.2663(18)	2.2611(14)	2.182(4)	2.181(4)	2.177(4)	2.167(7)	2.094(8)	2.163(6)	2.127(6)
Fe-N_{NCE} (Å)	2.1177(9)	2.128(4)	2.1201(12)	2.1418(19)	2.1453(19)	2.1443(16)	2.105(4)	2.090(4)	2.094(4)	2.089(19)	2.091(10)	2.106(8)	2.107(7)
Fe-S(Å)	2.4800(3)	2.4741(10)	2.4860(4)	2.4695(6)	2.4818(5)	2.4780(5)	2.6004(13)	2.6069(13)	2.5964(13)	2.6142(28)	2.6044(32)	2.5978(26)	2.5899(23)
C=S (Å)	1.6942(10)	1.687(4)	1.7074(13)	1.708(2)	1.709(2)	1.7094(17)	-	-	-	-	-	-	-
trans-N_{Py}-Fe-N_{Py} (°)	180.00	180.00(15)	180.00	180.00	180.00	180.00(7)	180.00	158.02(10)	158.70(10)	155.74(21)	156.59(23)	157.66(18)	158.87(17)
trans-N_{NCE}-Fe-N_{NCE} (°)	180.00(4)	180.00	180.00	180.00(10)	180.00	180.00	180.00	-	-	-	-	-	-
trans-S-Fe-N_{NCE} (°)	-	-	-	-	-	-	-	172.88(13)	172.505(13)	173.52(26)	173.20(29)	172.13(22)	172.00(20)
trans-S-Fe-S (°)	180.00	180.00	180.00	180.00	180.00	180.00	180.00	-	-	-	-	-	-
Fe-S-C (°)	96.73(3)	96.48(14)	95.91(4)	96.38(7)	96.00(7)	96.26(6)	-	-	-	-	-	-	-
Av. *cis*-N-Fe-N (°)	90.00(4)	90.00(18)	90.00(6)	90.00(10)	90.00(10)	90.00(7)	90.00(21)	96.82(25)	96.56(26)	97.24(50)	96.96(54)	96.44(42)	95.99(38)
Av. *cis*-S-Fe-S (°)	-	-	-	-	-	-	-	98.95(3)	99.28(3)	101.00(7)	101.37(7)	101.78(6)	101.81(6)
Av. *cis*-N-Fe-S (°)	90.00(5)	90.00(18)	90.00(6)	90.00(10)	90.00(10)	90.00(8)	90.00(23)	83.15(19)	83.35(20)	82.60(39)	82.81(43)	83.35(33)	83.62(30)
Av. Fe-N-C(E) (°)	157.21	157.26	165.11	163.97	168.18	166.69	155.30	160.8(4)	161.1(4)	163.3(6)	163.4(1.2)	167.0(8)	166.5(8)
Σ_{Oh}[e] (°)	28.76(9)	30.68(36)	21.4(12)	19.92(20)	23.12(20)	20.24(15)	81.02(44)	84.17(32)	82.00(33)	91.58(64)	89.32(69)	83.87(54)	80.06(67)

[a] Crystal data taken from the published reference.[S3] [b] E = S for complexes **1a**, **2a** and **4a**. [c] E = Se for complexes **1b**, **2b**, **3b** and **4b**. [d] E = BH_3 for complex **2c** and **4c**. [e] The octahedral distortion parameter, Σ_{Oh}, is defined as the sum of the absolute values of the difference of each of the twelve cis angles from 90°. Σ_{Oh} = 0 indicates a perfect octahedral geometry.[S1,2]

In order to compare the structural characteristics of the complexes for this work with $Fe^{II}(N_4S_2)$ SCO-active complexes published in the literature,[S4,5] which contain cyanide co-ligands NCE E = S, Se and BH_3, Table **S7** shows the most relevant structural parameters for complex family *cis*-$[Fe^{II}(bpte)_2(NCE)_2]$ E = S, Se and BH_3, bpte = *S,S'*-bis(2-pyridylmethyl)-1,2-thioethane.

Table **S7**. Average bond distances (Å) and angles (°) and Σ_{Oh} parameter for complex family *cis*-$[Fe^{II}(bpte)_2(NCE)_2]$ E = S, Se and BH_3, bpte = *S,S'*-bis(2-pyridylmethyl)-1,2-thioethane.[S4,5]

Complex	$[Fe^{II}(bpte)_2(NCS)_2]$ [a]		α-$Fe^{II}(bpte)_2(NCSe)_2$ [b,c]		β-$[Fe^{II}(bpte)_2(NCSe)_2]$ [b]		γ-$[Fe^{II}(bpte)_2(NCSe)_2]$ [b,c]		$[Fe^{II}(bpte)_2(NCBH_3)_2]$ [a]	
SCO activity	No		Yes		No		Yes		Yes	
Temperature (K)	90(2)	230(2)	90(2)	300(2)	120(2)	300(2)	100(2)	300(2)	150(2)	295(2)
Spin state	High	High	Low	High	High	High	Low	High	Low	High
Space group	*Pbcn*	*Pbcn*	$P2_1/n$	$P2_1/c$	$C2/c$	$C2/c$	$P2_1/c$	$P2_1/c$	$C2/c$	$C2/c$
Av. Fe-N_{Py} (Å)	2.198(2)	2.206(2)	2.001(3)	2.199(3)	2.1758(11)	2.1799(15)	2.007(3)	2.192(3)	2.008(2)	2.161(1)
Av. Fe-N_{NCE} (Å)	2.076(2)	2.075(2)	1.947(3)	2.080(3)	2.0925(13)	2.0870(18)	1.952(3)	2.071(3)	1.960(2)	2.093(2)
Av. Fe-S (Å)	2.5416(6)	2.556(1)	2.2383(9)	2.547(1)	2.6034(4)	2.6117(6)	2.239(1)	2.551(1)	2.2503(5)	2.5233(9)
trans-N_{Py}-Fe-N_{Py} (°)	158.76(9)	160.07(9)	174.3(1)	162.8(1)	170.95(6)	170.21(8)	172.5(1)	161.7(1)	177.91(8)	170.64(7)
Av. *trans*-S-Fe-N_{NCE} (°)	174.91(8)	173.74(8)	170.44(13)	173.2(1)	166.48(6)	166.37(8)	178.93(12)	171.89(13)	176.12(6)	169.23(6)
Av. *cis*-N-Fe-N (°)	95.37(18)	95.24(20)	92.29(24)	95.00(30)	95.41(8)	95.52(17)	91.66(24)	95.03(24)	91.09(15)	93.56(15)
Av. *cis*-S-Fe-S (°)	86.37(3)	84.99(5)	90.26(4)	84.48(5)	81.227(17)	80.68(2)	90.87(3)	83.29(3)	89.75(3)	84.17(4)
Av. *cis*-N-Fe-S (°)	84.10(12)	84.44(12)	88.14(18)	85.12(19)	86.55(12)	99.04(12)	87.84(18)	84.83(18)	88.70(9)	86.51(10)
Av. Fe-N-C(E) (°)	167.53	165.92	166.8(60)	163.5(50)	149.97(17)	150.13(25)	173.68(60)	171.4(60)	165.65	161.88
Σ_{Oh} [d]	68.2(2)	67.4(3)	35.24(3)	60.75(8)	73.11(15)	73.33(21)	24.64	67.75	41.7(2)	62.8(2)

[a] Crystal data taken from the published reference.[S4] [b] Crystal data taken from the published reference.[S5] [c] There are two symmetry independent complex molecule in the structure of polymorphs α at 90(2) K and γ at 150(2) K and 295(2) K. [d] The octahedral distortion parameter of Hendrickson, Σ_{Oh}, is defined as the sum of the absolute values of the difference of each of the twelve cis angles from 90°. Σ_{Oh} = 0 indicates a perfect octahedral geometry.[S1,2]

2.4. Supramolecular analysis.

2.4.1. Supramolecular interactions of complexes *trans*-[$Fe^{II}(ImPyS)_2(NCE)_2$] E = S, Se; complexes 1a and 1b respectively.

The supramolecular interactions present in the crystal structure of complexes **1a** and **1b** comprise CH···π and CH···E (E = S or Se) hydrogen bonds, Figure **S28**. The former arises from the interaction between C-H of a pyridine ring at the 3-position with the centroid of a pyridine ring of a neighbouring complex molecule. Whilst, the CH···E (E = S or Se) interactions are formed between the 4-position C-H of the pyridine ring with the coordinated Se-CN co-ligand of a neighbouring complex molecule, in addition the 4-position C-H of the imidazolyl ring interacts with the coordinated Se-CN co-ligand of a different neighbouring molecule. Finally, there is an interaction between the CH_3 group of the imidazolyl ligand with the Se-CN co-ligand of a neighbouring complex. Both types of interactions can be considered weak to medium strength with range values from 3.492—4.018 Å, Figure **S28**. All this type of interactions form 2D sheets within the crystal structure.

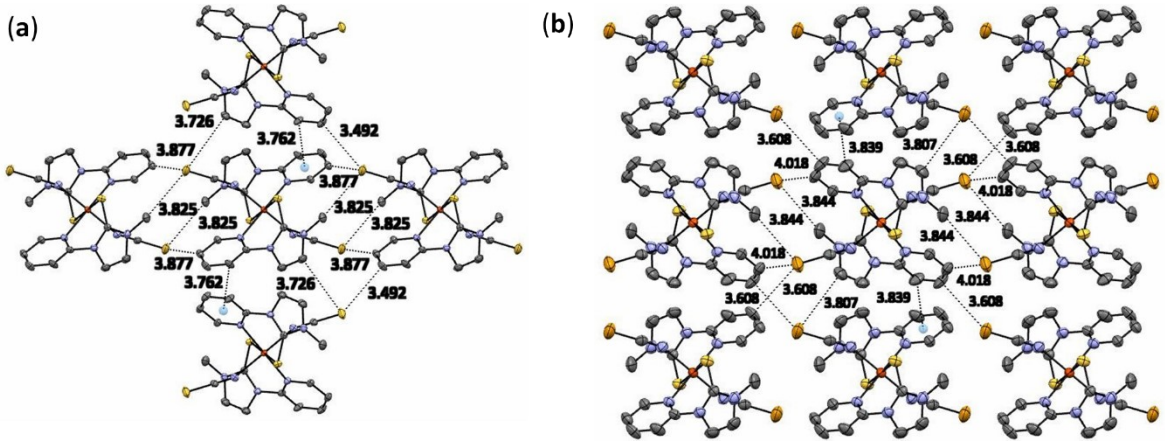

Figure **S28**. Supramolecular C-H···π y C-H···E (E = S or Se) interactions present in the crystal structure of complexes **1a** at 150(2) K (**a**) and **1b** at 296(2) K (**b**). Ellipsoids are drawn at 50 % probability level. Hydrogen atoms are omitted for the sake of clarity.

2.4.2. Supramolecular interactions of family complex *trans*-[$Fe^{II}(TrzPyS)_2(NCE)_2$] E = S, Se and BH_3; complexes 2a, 2b and 2c respectively.

In the case of complexes **2a-c** it is possible to observe two types of π-π interactions within the crystal structure. One of them comprises a moderate interaction between two off-set pyridine rings of neighbouring complex molecules, blue centroids Figure **S29**, with a distance between centroids ranging 3.527—2.557 Å. The second type of off-set π-π interaction occurs between a pyridine ring and the phenyl ring of a neighbouring complex molecule, (grey centroid for phenyl ring in Figure **S29**) with a centroid-centroid distance varying 4.041—4.097 Å, indicating a weak interaction and forming a supramolecular polymer. In addition, it is possible to observe H-bond interactions between the methyl group and a C-H group of a pyridine ring with the E (E = S, Se and BH_3) atom of the co-ligand, both of them being weak interactions with a value ranging 3.763—2.557 Å, Figure **S29**.

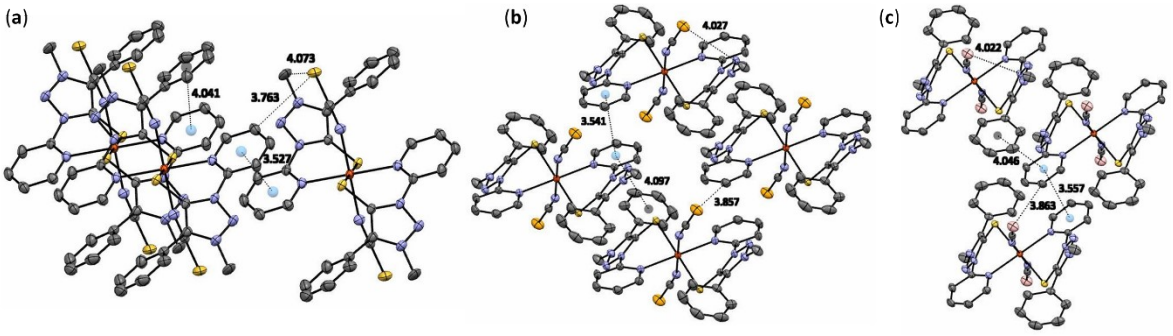

Figure **S29**. Supramolecular π-π and C-H···E (E = S, Se and BH_3) interactions observed for complexes **2a** at 170(2) K (a), **2b** at 171(2) K and **2c** at 166(2) K. Ellipsoids are drawn at 50 % probability level. Hydrogen atoms are omitted for the sake of clarity.

3. DFT Calculations

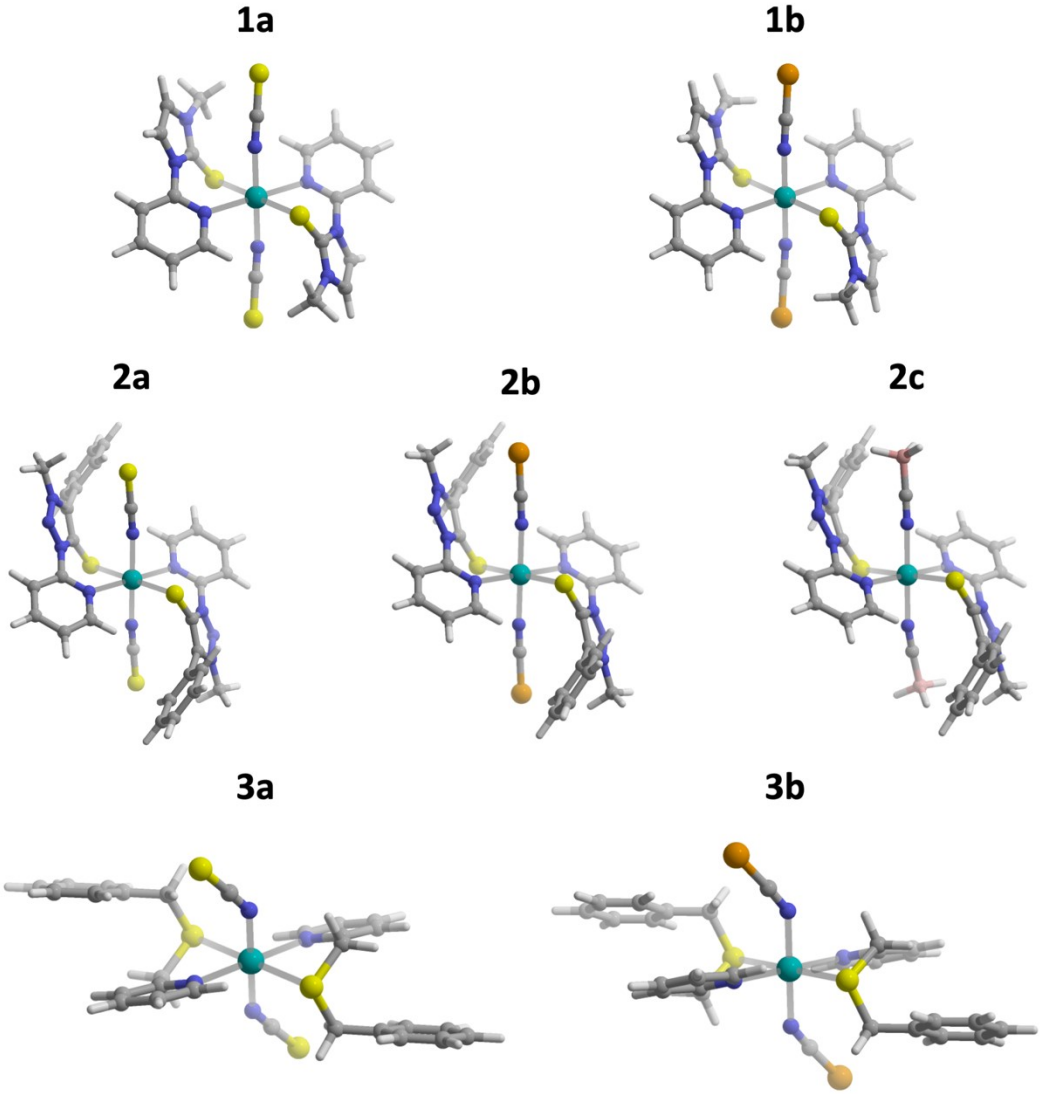

Figure **S30**. Optimised geometries for the iron(II) complexes in the HS-state.

Table **S8**. Experimental and calculated Fe-L bond length distances, showing the percentage deviations compared to the experimental HS-structures; as expected the LS-states show larger deviations.

		Fe-L bond length (Å)			Deviations (%)	
Complex	Ligand	X-ray	Calculated LS	Calculated HS	LS	HS
1a	N_ax	2.1176	1.9818	2.0640	-6.4162	-2.5319
	N_ax	2.1176	1.9817	2.0640	-6.4176	-2.5327
	N_eq	2.2474	2.0782	2.3111	-7.5309	2.8330
	N_eq	2.2474	2.0783	2.3110	-7.5254	2.8300
	S_eq	2.4800	2.4080	2.6170	-2.9043	5.5231
	S_eq	2.4800	2.4079	2.6169	-2.9052	5.5200
1b	N_ax	2.1279	1.9787	2.0770	-7.0116	-2.3920
	N_ax	2.1279	1.9787	2.0770	-7.0092	-2.3933
	N_eq	2.2481	2.0782	2.3027	-7.5576	2.4280
	N_eq	2.2481	2.0788	2.3026	-7.5312	2.4234
	S_eq	2.4741	2.4033	2.6067	-2.8614	5.3596
	S_eq	2.4741	2.4041	2.6066	-2.8284	5.3566
2a	N_ax	2.1201	1.9753	2.0849	-6.8281	-1.6569
	N_ax	2.1201	1.9754	2.0851	-6.8245	-1.6470
	N_eq	2.2680	2.0669	2.2891	-8.8650	0.9317
	N_eq	2.2680	2.0669	2.2890	-8.8672	0.9282
	S_eq	2.4860	2.3899	2.5795	-3.8652	3.7629
	S_eq	2.4860	2.3897	2.5792	-3.8734	3.7506
2b	N_ax	2.1417	1.9708	2.0990	-7.9797	-1.9954
	N_ax	2.1417	1.9706	2.0989	-7.9890	-1.9987
	N_eq	2.2658	2.0658	2.2868	-8.8278	0.9262
	N_eq	2.2658	2.0657	2.2869	-8.8310	0.9288
	S_eq	2.4696	2.3866	2.5598	-3.3611	3.6545
	S_eq	2.4696	2.3881	2.5599	-3.3002	3.6565
2c	N_ax	2.1443	1.9714	2.1257	-8.0633	-0.8687
	N_ax	2.1443	1.9715	2.1191	-8.0592	-1.1752
	N_eq	2.2611	2.0673	2.2856	-8.5737	1.0822
	N_eq	2.2611	2.0672	2.2770	-8.5786	0.7027
	S_eq	2.4780	2.3848	2.5384	-3.7619	2.4385
	S_eq	2.4780	2.3844	2.5376	-3.7763	2.4058
3b	N_ax	2.1050	1.9528	2.0690	-7.2292	-1.7123
	N_ax	2.1050	1.9528	2.0690	-7.2330	-1.7108
	N_eq	2.1816	2.0452	2.2385	-6.2565	2.6069
	N_eq	2.1816	2.0472	2.2385	-6.1615	2.6060
	S_eq	2.6004	2.3296	2.6351	-10.4112	1.3363
	S_eq	2.6004	2.3131	2.6352	-11.0475	1.3379

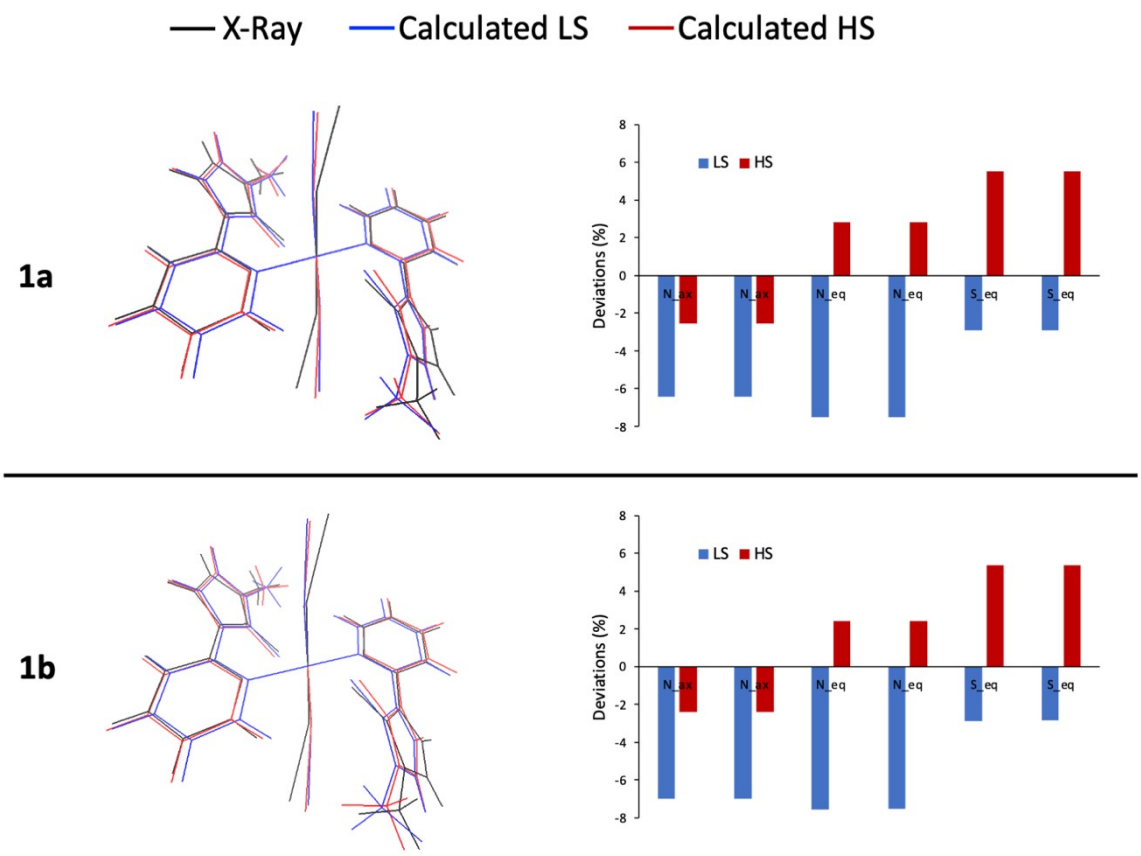

Figure **S31**. Left: Overlayed structures for the calculated HS-state (red), calculated LS-state (blue) and the experimental X-ray structure (black) for complexes **1a** and **1b**. Right: Percentage deviations bar plot for the six Fe-L bond lengths for complexes **1a** and **1b.**

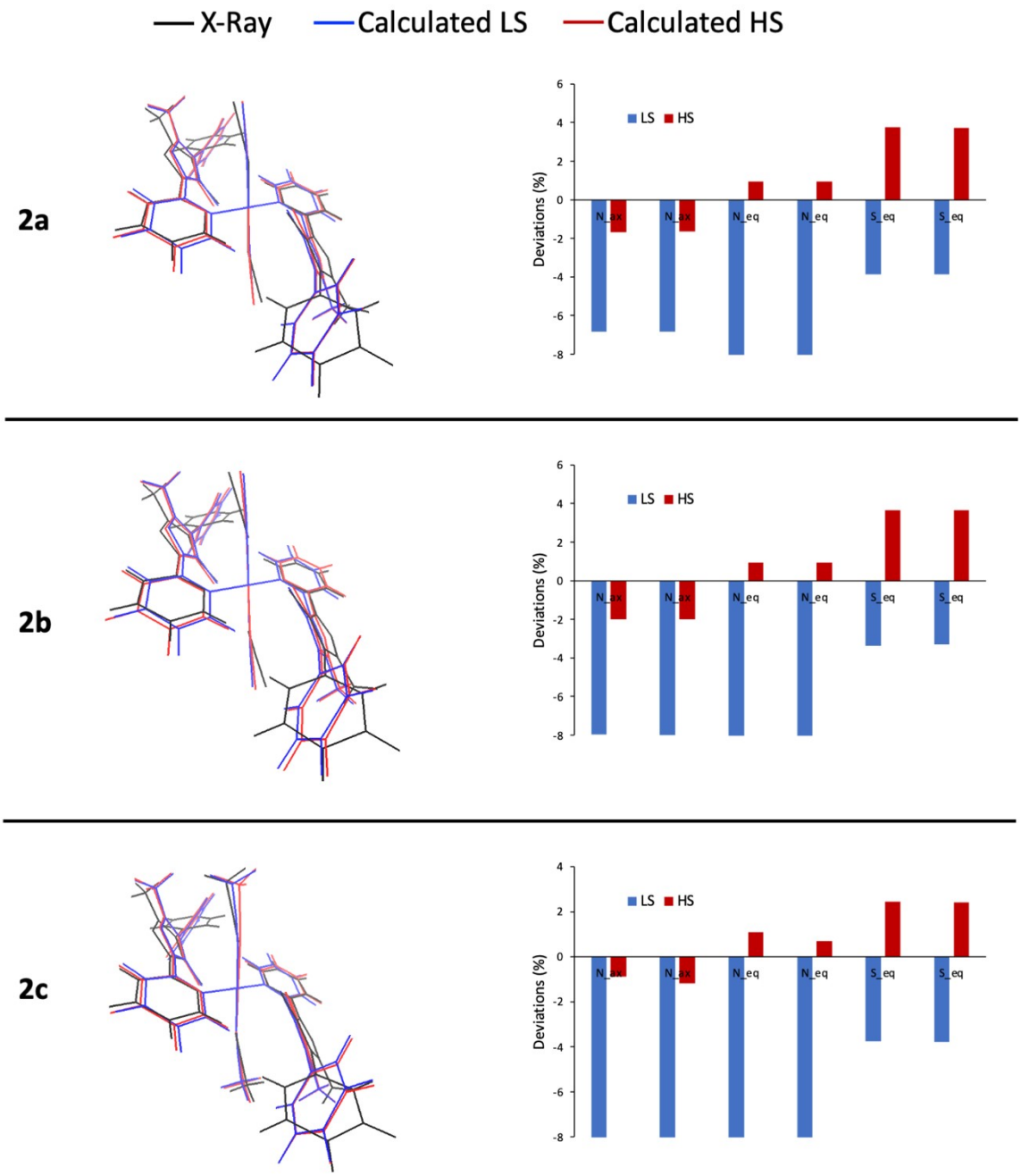

Figure **S32**. Left: Overlayed structures for the calculated HS-state (red), calculated LS-state (blue) and the experimental X-ray structure (black) for complexes **2a-c**. Right: Percentage deviations bar plot for the six Fe-L bond lengths for complexes **2a-c.**

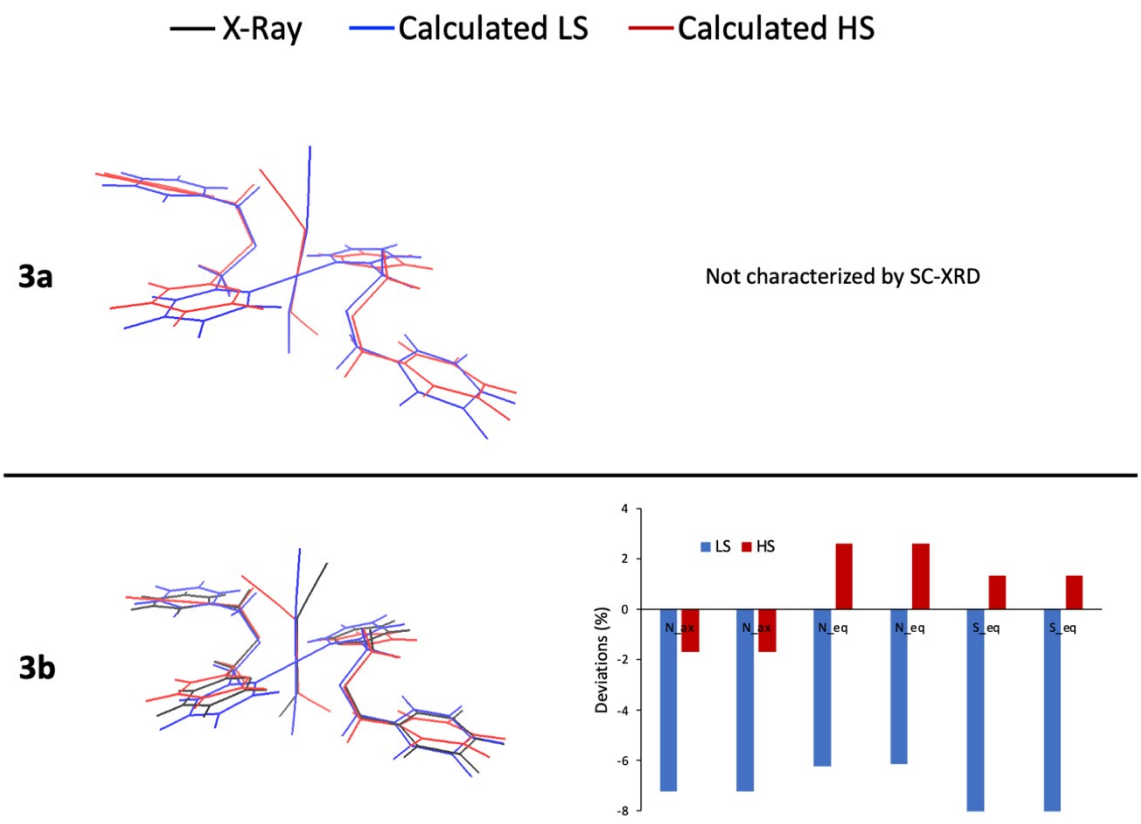

Figure **S33**. Left: Overlayed structures for the calculated HS-state (red), calculated LS-state (blue) and the experimental X-ray structure (black) for complexes **3a-b**. Right: Percentage deviations bar plot for the six Fe-L bond lengths for complexes **3a-b.**

Table **S9**. Calculated total energies, and their corresponding adiabatic energy gaps for the HS- and LS-states of the iron(II) complexes shown in Figure **S30**.

Complex	E_{LS} (kcal/mol)	E_{HS} (kcal/mol)	ΔE_{HL} (kcal/mol)
1a	-2552557.8459	-2552577.0343	-19.1885
1b	-5066880.8734	-5066898.0968	-17.2234
2a	-2862634.5534	-2862650.0663	-15.5129
2b	-5376957.4727	-5376971.0956	-13.6229
2c	-2396319.6215	-2396332.2004	-12.5789
3a	-2609458.9017	-2609472.1131	-13.2114
3b	-5123780.2019	-5123791.9262	-11.7243

Table **S10**. Cartesian coordinates of the optimized structures of iron(II) complexes with their total energies and smallest vibrational frequencies.

1a (HS)

E (Eh) =	-4067.7910	ν (cm^{-1}) =	6.30
Atom	x	y	z
Fe	4.2595	7.8515	3.8408
C	6.7135	6.1212	4.7631
H	7.0481	6.6211	3.8626
N	5.4234	6.2706	5.0604
S	3.3799	8.5191	6.2134
N	3.5830	5.7981	6.4468
C	7.5840	5.3794	5.5400
H	8.6223	5.2928	5.2512
S	8.5544	9.9350	4.2227
C	2.7673	4.7006	6.6852
H	3.1438	3.6945	6.6459
C	1.5283	5.1725	6.8812
H	0.5995	4.6564	7.0461
N	1.5880	6.5472	6.7755
C	7.0974	4.7792	6.6870
H	7.7486	4.2022	7.3315
C	4.9672	5.6867	6.1587
C	5.7618	4.9377	7.0100
H	5.3391	4.5112	7.9095
N	5.9056	9.0711	4.0921
C	0.4331	7.4208	6.8332
H	-0.1387	7.3229	5.9087
H	0.7839	8.4427	6.9493
H	-0.1850	7.1434	7.6858

C	7.0117	9.4469	4.1636
C	2.8440	6.9437	6.4864
C	1.8058	9.5819	2.9184
H	1.4709	9.0820	3.8188
N	3.0959	9.4325	2.6213
S	5.1392	7.1839	1.4684
N	4.9365	9.9048	1.2353
C	0.9354	10.3239	2.1414
H	-0.1029	10.4106	2.4300
S	-0.0354	5.7677	3.4588
C	5.7525	11.0022	0.9972
H	5.3762	12.0085	1.0368
C	6.9914	10.5301	0.8010
H	7.9203	11.0461	0.6361
N	6.9314	9.1554	0.9061
C	1.4223	10.9241	0.9945
H	0.7712	11.5013	0.3499
C	3.5523	10.0165	1.5231
C	2.7579	10.7655	0.6718
H	3.1808	11.1921	-0.2277
N	2.6133	6.6320	3.5894
C	8.0860	8.2815	0.8476
H	8.6573	8.3775	1.7726
H	7.7349	7.2599	0.7292
H	8.7047	8.5604	-0.0040
C	1.5073	6.2560	3.5179
C	5.6753	8.7592	1.1956

1b (HS)

E (Eh) =	-8074.6172	ν (cm^{-1}) =	8.78
Atom	x	y	z
Se	-0.0787	10.0343	3.4252
N	3.2202	6.3653	2.6218
Fe	4.3686	7.9302	3.8606
S	5.3091	8.5995	1.5236
C	1.9228	6.2243	2.8925
H	1.5704	6.7345	3.7799
N	5.0851	5.8742	1.2757
C	1.0654	5.4779	2.1064
H	0.0206	5.4021	2.3736

C	1.5741	4.8604	0.9785
H	0.9342	4.2784	0.3271
N	7.0810	6.6268	0.9582
C	2.9170	5.0086	0.6827
H	3.3562	4.5689	-0.2024
N	2.7301	9.1735	3.5720
C	3.6972	5.7655	1.5403
C	8.2142	7.5269	0.8890
H	8.4025	7.9564	1.8721
H	8.0135	8.3206	0.1719
H	9.0859	6.9538	0.5838
C	7.1429	5.2536	0.8429
H	8.0732	4.7390	0.6824
C	5.9033	4.7790	1.0321
H	5.5291	3.7719	1.0686
C	5.8246	7.0192	1.2450
C	1.6252	9.5395	3.5009
Se	8.8157	5.8265	4.2987
N	5.5171	9.4950	5.0992
S	3.4278	7.2612	6.1978
C	6.8144	9.6359	4.8282
H	7.1667	9.1255	3.9409
N	3.6524	9.9864	6.4456
C	7.6720	10.3825	5.6141
H	8.7168	10.4582	5.3466
C	7.1635	11.0001	6.7420
H	7.8036	11.5822	7.3931
N	1.6564	9.2342	6.7632
C	5.8207	10.8520	7.0380
H	5.3817	11.2919	7.9231
N	6.0069	6.6867	4.1493
C	5.0404	10.0950	6.1807
C	0.5230	8.3344	6.8322
H	0.3355	7.9041	5.8493
H	0.7228	7.5412	7.5501
H	-0.3489	8.9080	7.1360
C	1.5948	10.6075	6.8785
H	0.6647	11.1223	7.0392
C	2.8345	11.0818	6.6892
H	3.2089	12.0888	6.6529

C	2.9127	8.8416	6.4762
C	7.1118	6.3209	4.2213

2a (HS)

E (Eh) =	-4561.9239	ν (cm^{-1}) =	6.64
Atom	x	y	z
Fe	6.0515	2.0669	5.9883
S	3.6127	1.2296	5.9253
N	5.0718	4.0550	6.5608
C	5.6440	4.7190	7.5631
H	6.5873	4.3177	7.9150
N	3.3467	3.7996	4.9944
S	5.7881	3.4840	1.3353
C	5.0827	5.8537	8.1198
H	5.5867	6.3594	8.9319
N	2.9637	4.5145	3.9503
C	3.8777	6.3128	7.6195
H	3.4063	7.1951	8.0338
C	3.2727	5.6251	6.5819
H	2.3310	5.9392	6.1555
N	2.5525	3.6340	3.0949
C	3.9201	4.5061	6.0950
N	5.9923	2.5650	3.9646
C	2.1212	4.0930	1.7853
H	2.9889	4.1075	1.1255
H	1.7154	5.0938	1.9006
H	1.3649	3.4094	1.4087
C	2.6545	2.3602	3.5399
C	3.1850	2.4455	4.8243
C	2.3347	1.1647	2.7511
C	1.4388	0.2246	3.2527
H	0.9746	0.3897	4.2171
C	1.1595	-0.9210	2.5270
H	0.4597	-1.6485	2.9196
C	1.7770	-1.1382	1.3037
H	1.5568	-2.0356	0.7378
C	2.6830	-0.2116	0.8102
H	3.1823	-0.3843	-0.1353
C	2.9674	0.9368	1.5317
H	3.7080	1.6433	1.1696

C	5.9192	2.9524	2.8653
S	8.4905	2.9044	6.0512
N	7.0316	0.0790	5.4160
C	6.4595	-0.5851	4.4137
H	5.5164	-0.1837	4.0614
N	8.7562	0.3346	6.9828
S	6.3123	0.6534	10.6431
C	7.0209	-1.7200	3.8574
H	6.5170	-2.2259	3.0453
N	9.1383	-0.3800	8.0274
C	8.2257	-2.1792	4.3582
H	8.6970	-3.0617	3.9443
C	8.8304	-1.4913	5.3958
H	9.7719	-1.8054	5.8226
N	9.5488	0.5007	8.8829
C	8.1830	-0.3721	5.8822
N	6.1108	1.5684	8.0121
C	9.9792	0.0420	10.1929
H	9.1118	0.0312	10.8533
H	10.3811	-0.9604	10.0786
H	10.7382	0.7233	10.5683
C	9.4473	1.7744	8.4375
C	8.9177	1.6888	7.1528
C	9.7670	2.9701	9.2259
C	10.6629	3.9101	8.7238
H	11.1270	3.7446	7.7595
C	10.9424	5.0559	9.4492
H	11.6422	5.7832	9.0563
C	10.3250	5.2736	10.6725
H	10.5453	6.1711	11.2381
C	9.4190	4.3472	11.1664
H	8.9198	4.5203	12.1120
C	9.1345	3.1985	10.4454
H	8.3937	2.4924	10.8078
C	6.1826	1.1830	9.1122

2b (HS)

E (Eh) =	-8568.7500	ν (cm^{-1}) =	9.97
Atom	x	y	z
Se	2.3387	0.8209	1.2070

S	4.4154	3.2550	5.8962
Fe	2.0500	2.2846	6.0235
C	2.6382	-0.2914	7.6780
H	1.6880	0.0730	8.0502
N	3.1476	0.3769	6.6441
N	4.8221	0.6798	5.0283
C	3.2676	-1.3870	8.2402
H	2.8116	-1.8970	9.0776
N	5.2557	-0.0379	4.0066
C	4.4771	-1.8018	7.7115
H	5.0017	-2.6526	8.1278
C	5.0180	-1.1085	6.6430
H	5.9607	-1.3860	6.1940
N	5.6379	0.8419	3.1374
C	6.1133	0.3753	1.8458
H	5.2660	0.3453	1.1596
H	6.8755	1.0614	1.4854
H	6.5221	-0.6212	1.9847
C	4.3053	-0.0307	6.1534
N	2.1114	1.7363	3.9984
C	4.9193	2.0363	4.8284
C	5.4685	2.1194	3.5517
C	6.6259	4.2844	3.2786
H	7.0494	4.1471	4.2658
C	6.9087	5.4251	2.5470
H	7.5677	6.1785	2.9605
C	6.3449	5.6041	1.2917
H	6.5669	6.4981	0.7210
C	5.4887	4.6444	0.7731
H	5.0311	4.7882	-0.1980
C	5.1994	3.5012	1.5015
H	4.4938	2.7708	1.1172
C	2.1896	1.3712	2.8963
C	5.7794	3.3113	2.7533
Se	1.7628	3.7430	10.8420
S	-0.3153	1.3141	6.1506
C	1.4611	4.8612	4.3698
H	2.4111	4.4968	3.9970
N	0.9521	4.1924	5.4036
N	-0.7217	3.8888	7.0200

C	0.8316	5.9573	3.8085
H	1.2873	6.4677	2.9712
N	-1.1548	4.6060	8.0423
C	-0.3776	6.3719	4.3380
H	-0.9022	7.2230	3.9225
C	-0.9181	5.6782	5.4064
H	-1.8605	5.9555	5.8560
N	-1.5368	3.7257	8.9111
C	-2.0116	4.1916	10.2032
H	-1.1640	4.2207	10.8891
H	-2.7740	3.5055	10.5634
H	-2.4199	5.1884	10.0652
C	-0.2053	4.6000	5.8951
N	1.9887	2.8338	8.0485
C	-0.8190	2.5323	7.2191
C	-1.3677	2.4484	8.4960
C	-2.5256	0.2835	8.7678
H	-2.9492	0.4216	7.7808
C	-2.8085	-0.8577	9.4986
H	-3.4677	-1.6107	9.0846
C	-2.2445	-1.0377	10.7537
H	-2.4666	-1.9320	11.3237
C	-1.3880	-0.0786	11.2728
H	-0.9303	-0.2232	12.2438
C	-1.0986	1.0652	10.5452
H	-0.3928	1.7951	10.9300
C	1.9107	3.1958	9.1515
C	-1.6787	1.2560	9.2936

2c (HS)

E (Eh) =	-3818.7989	ν (cm^{-1}) =	12.26
Atom	x	y	z
Fe	6.0626	2.1085	6.0042
S	3.6785	1.2506	5.8502
N	5.0642	4.0811	6.5491
C	5.6174	4.7498	7.5603
H	6.5474	4.3434	7.9401
N	3.3659	3.8298	4.9468
C	5.0577	5.8974	8.0898
H	5.5475	6.4047	8.9094

N	2.9313	4.5467	3.9241
C	3.8735	6.3674	7.5514
H	3.4036	7.2610	7.9423
C	3.2871	5.6757	6.5063
H	2.3614	5.9977	6.0521
N	2.4989	3.6673	3.0783
C	3.9303	4.5414	6.0481
N	6.0582	2.6040	3.9438
C	1.9737	4.1275	1.8032
H	2.7555	4.0429	1.0498
H	1.6815	5.1660	1.9262
H	1.1184	3.5120	1.5352
C	2.6363	2.3917	3.5076
C	3.2140	2.4747	4.7707
C	2.2871	1.2039	2.7191
C	1.3910	0.2697	3.2314
H	0.9495	0.4299	4.2073
C	1.0815	-0.8640	2.4992
H	0.3818	-1.5876	2.8990
C	1.6689	-1.0742	1.2598
H	1.4253	-1.9625	0.6893
C	2.5748	-0.1532	0.7560
H	3.0523	-0.3205	-0.2017
C	2.8883	0.9843	1.4826
H	3.6286	1.6825	1.1073
C	5.9934	2.8465	2.8174
S	8.4428	2.9757	6.1522
N	7.0739	0.1356	5.4483
C	6.5256	-0.5325	4.4343
H	5.5876	-0.1376	4.0624
N	8.7728	0.3971	7.0463
C	7.1023	-1.6642	3.8889
H	6.6165	-2.1702	3.0661
N	9.1830	-0.3211	8.0764
C	8.2985	-2.1184	4.4138
H	8.7818	-2.9989	4.0096
C	8.8794	-1.4278	5.4630
H	9.8131	-1.7383	5.9090
N	9.5809	0.5553	8.9409
C	8.2189	-0.3108	5.9366

N	6.0627	1.5574	8.0571
C	10.0374	0.0887	10.2408
H	9.1805	0.0473	10.9125
H	10.4575	-0.9039	10.1079
H	10.7883	0.7806	10.6133
C	9.4471	1.8335	8.5127
C	8.9061	1.7516	7.2346
C	9.7661	3.0261	9.3064
C	10.6412	3.9809	8.7958
H	11.0884	3.8300	7.8211
C	10.9244	5.1217	9.5276
H	11.6091	5.8597	9.1285
C	10.3318	5.3193	10.7665
H	10.5558	6.2123	11.3377
C	9.4470	4.3777	11.2698
H	8.9686	4.5337	12.2290
C	9.1594	3.2341	10.5421
H	8.4401	2.5135	10.9159
C	6.1682	1.0583	9.0928
B	5.8602	3.1589	1.2773
H	6.7849	3.8668	0.9454
H	5.8695	2.0912	0.6920
B	6.3746	0.3388	10.4824
H	7.0165	-0.6725	10.2534
H	6.9937	1.0981	11.2112
H	4.7939	3.7345	1.1212
H	5.2884	0.0785	10.9502

3a (HS)

E (Eh) =	-4158.4591	ν (cm^{-1}) =	18.12
Atom	x	y	z
S	6.1538	6.0501	8.0918
Fe	10.1511	3.8540	8.6731
N	9.1214	4.4005	10.5961
C	8.8839	5.6732	10.9056
H	9.3043	6.4126	10.2339
N	8.6254	4.8301	7.6980
C	8.1261	6.0505	11.9976
H	7.9487	7.0982	12.1972
S	8.7289	1.6832	9.2090

C	8.8781	2.0102	10.9749
H	9.9167	1.7619	11.2024
H	8.2266	1.3336	11.5267
C	8.5999	3.4380	11.3593
C	7.5890	5.0572	12.7968
H	6.9779	5.3083	13.6551
C	7.8260	3.7336	12.4717
H	7.3990	2.9288	13.0561
C	6.9978	2.1253	8.8925
H	6.8939	3.2077	8.9351
H	6.8353	1.8290	7.8547
C	7.5845	5.3584	7.8449
C	5.9078	0.0852	9.9192
H	6.5487	-0.5454	9.3125
C	6.0154	1.4697	9.8216
C	5.1926	2.2664	10.6090
H	5.2674	3.3458	10.5284
C	4.9961	-0.4888	10.7890
H	4.9202	-1.5676	10.8544
C	4.2774	1.6927	11.4803
H	3.6392	2.3268	12.0841
C	4.1791	0.3139	11.5743
H	3.4657	-0.1366	12.2537
S	14.1502	1.6613	9.2529
N	11.1824	3.3084	6.7505
C	11.4208	2.0360	6.4406
H	10.9984	1.2960	7.1104
N	11.6766	2.8769	9.6484
C	12.1818	1.6595	5.3506
H	12.3598	0.6120	5.1506
S	11.5728	6.0242	8.1407
C	11.4264	5.6990	6.3742
H	10.3879	5.9467	6.1454
H	12.0783	6.3764	5.8241
C	11.7061	4.2715	5.9895
C	12.7214	2.6535	4.5538
H	13.3351	2.4031	3.6972
C	12.4833	3.9769	4.8793
H	12.9120	4.7821	4.2968
C	13.3037	5.5832	8.4586

H	13.4095	4.5011	8.4111
H	13.4637	5.8750	9.4980
C	12.7187	2.3510	9.5010
C	14.3919	7.6297	7.4423
H	13.7478	8.2568	8.0493
C	14.2872	6.2445	7.5345
C	15.1142	5.4527	6.7467
H	15.0415	4.3728	6.8231
C	15.3053	8.2090	6.5779
H	15.3790	9.2882	6.5169
C	16.0311	6.0317	5.8807
H	16.6725	5.4011	5.2766
C	16.1267	7.4110	5.7923
H	16.8414	7.8658	5.1171

3b (HS)

E (Eh) =	-8165.2833	ν (cm^{-1}) =	17.71
Atom	x	y	z
Fe	10.1525	3.8563	8.6765
N	9.1398	4.4111	10.5943
C	8.9241	5.6854	10.9135
H	9.3661	6.4235	10.2543
N	8.6224	4.8524	7.7032
C	8.1630	6.0683	12.0011
H	8.0059	7.1177	12.2081
S	8.7306	1.6989	9.1938
C	8.8621	2.0225	10.9620
H	9.8951	1.7634	11.2025
H	8.1982	1.3493	11.5029
C	8.5935	3.4523	11.3462
C	7.5948	5.0792	12.7833
H	6.9780	5.3350	13.6361
C	7.8095	3.7534	12.4492
H	7.3619	2.9523	13.0232
C	6.9963	2.1237	8.8646
H	6.8798	3.2054	8.8964
H	6.8408	1.8126	7.8302
C	7.6002	5.3962	7.8826
C	5.9445	0.0804	9.9226
H	6.6025	-0.5470	9.3309

C	6.0214	1.4651	9.7998
C	5.1783	2.2587	10.5687
H	5.2287	3.3380	10.4673
C	5.0446	-0.4981	10.8016
H	4.9939	-1.5769	10.8878
C	4.2745	1.6797	11.4489
H	3.6198	2.3103	12.0385
C	4.2079	0.3011	11.5698
H	3.5039	-0.1524	12.2570
N	11.1651	3.3016	6.7588
C	11.3808	2.0273	6.4395
H	10.9389	1.2892	7.0987
N	11.6825	2.8601	9.6498
C	12.1418	1.6444	5.3518
H	12.2989	0.5950	5.1448
S	11.5744	6.0138	8.1593
C	11.4428	5.6902	6.3910
H	10.4097	5.9493	6.1506
H	12.1066	6.3634	5.8501
C	11.7114	4.2604	6.0068
C	12.7099	2.6336	4.5696
H	13.3266	2.3778	3.7167
C	12.4952	3.9593	4.9037
H	12.9427	4.7604	4.3297
C	13.3087	5.5891	8.4884
H	13.4252	4.5075	8.4561
H	13.4639	5.8997	9.5231
C	12.7048	2.3165	9.4705
C	14.3603	7.6330	7.4316
H	13.7021	8.2600	8.0234
C	14.2836	6.2482	7.5538
C	15.1270	5.4552	6.7846
H	15.0768	4.3758	6.8855
C	15.2603	8.2121	6.5530
H	15.3107	9.2910	6.4673
C	16.0308	6.0347	5.9049
H	16.6858	5.4045	5.3151
C	16.0972	7.4133	5.7846
H	16.8013	7.8673	5.0978
Se	6.0557	6.1726	8.2330

Se	14.2490	1.5398	9.1199

1a (LS)

E (Eh) =	-4067.7604	ν (cm^{-1}) =	26.21
Atom	x	y	z
Fe	4.2596	7.8513	3.8406
C	6.6511	6.3246	4.6261
H	6.9890	6.8897	3.7713
N	5.3551	6.4597	4.9277
S	3.3670	8.5735	5.9572
N	3.5406	5.8858	6.3245
C	7.5211	5.5233	5.3378
H	8.5575	5.4661	5.0359
S	8.3571	10.1707	4.2399
C	2.7369	4.8004	6.6431
H	3.1042	3.7907	6.6174
C	1.5101	5.2846	6.8788
H	0.5880	4.7780	7.1004
N	1.5659	6.6548	6.7132
C	7.0426	4.8331	6.4351
H	7.6942	4.2098	7.0343
C	4.9085	5.7860	5.9851
C	5.7104	4.9733	6.7699
H	5.2899	4.4882	7.6399
N	5.7840	9.0894	4.1063
C	0.4052	7.5227	6.7396
H	-0.2367	7.2767	5.8918
H	0.7479	8.5512	6.6638
H	-0.1335	7.3844	7.6759
C	6.8467	9.5637	4.1769
C	2.8056	7.0285	6.3499
C	1.8679	9.3781	3.0548
H	1.5299	8.8128	3.9094
N	3.1640	9.2431	2.7534
S	5.1523	7.1295	1.7239
N	4.9788	9.8172	1.3570
C	0.9981	10.1795	2.3430
H	-0.0384	10.2366	2.6446
S	0.1622	5.5316	3.4421
C	5.7825	10.9026	1.0387

H	5.4153	11.9124	1.0646
C	7.0095	10.4185	0.8034
H	7.9316	10.9252	0.5822
N	6.9536	9.0483	0.9689
C	1.4768	10.8699	1.2459
H	0.8253	11.4933	0.6467
C	3.6109	9.9170	1.6962
C	2.8091	10.7298	0.9114
H	3.2298	11.2151	0.0415
N	2.7352	6.6131	3.5749
C	8.1144	8.1804	0.9429
H	8.7562	8.4268	1.7906
H	7.7716	7.1519	1.0192
H	8.6530	8.3181	0.0065
C	1.6725	6.1387	3.5047
C	5.7137	8.6745	1.3315

1b (LS)

E (Eh) =	-8074.5897	ν (cm^{-1}) =	19.48
Atom	x	y	z
Se	0.1272	10.2703	3.3362
N	3.2941	6.5289	2.7650
Fe	4.3687	7.9299	3.8611
S	5.3020	8.6373	1.7615
C	1.9914	6.3972	3.0396
H	1.6359	6.9626	3.8870
N	5.1365	5.9476	1.4073
C	1.1340	5.5992	2.3091
H	0.0908	5.5478	2.5876
C	1.6340	4.9064	1.2235
H	0.9930	4.2854	0.6106
N	7.1114	6.7190	1.0238
C	2.9741	5.0403	0.9185
H	3.4116	4.5516	0.0590
N	2.8491	9.1595	3.5541
C	3.7617	5.8514	1.7187
C	8.2694	7.5909	0.9877
H	8.9201	7.3457	1.8292
H	7.9240	8.6182	1.0674
H	8.7993	7.4551	0.0461

C	7.1708	5.3480	0.8655
H	8.0956	4.8420	0.6537
C	5.9436	4.8623	1.0972
H	5.5785	3.8519	1.1276
C	5.8694	7.0913	1.3789
C	1.7921	9.6300	3.4487
Se	8.6114	5.5910	4.3831
N	5.4434	9.3317	4.9570
S	3.4357	7.2232	5.9602
C	6.7460	9.4638	4.6823
H	7.1015	8.8984	3.8348
N	3.6010	9.9127	6.3149
C	7.6033	10.2619	5.4126
H	8.6464	10.3137	5.1340
C	7.1034	10.9545	6.4985
H	7.7443	11.5756	7.1113
N	1.6256	9.1416	6.6965
C	5.7633	10.8203	6.8036
H	5.3258	11.3088	7.6632
N	5.8889	6.7011	4.1686
C	4.9758	10.0091	6.0034
C	0.4677	8.2697	6.7320
H	-0.1841	8.5169	5.8920
H	0.8128	7.2427	6.6493
H	-0.0611	8.4033	7.6746
C	1.5662	10.5126	6.8545
H	0.6413	11.0186	7.0656
C	2.7937	10.9982	6.6239
H	3.1588	12.0086	6.5935
C	2.8680	8.7692	6.3427
C	6.9462	6.2309	4.2728

2a (LS)

E (Eh) =	-4561.8991	ν (cm^{-1}) =	18.32
Atom	x	y	z
Fe	6.0521	2.0677	5.9886
S	3.8379	1.1758	5.8765
N	5.1817	3.8404	6.5986
C	5.7373	4.4721	7.6373
H	6.6209	4.0059	8.0473

N	3.4743	3.7182	4.9789
S	5.8039	3.4614	1.4322
C	5.2411	5.6520	8.1560
H	5.7418	6.1152	8.9950
N	3.0476	4.4466	3.9651
C	4.1124	6.2106	7.5878
H	3.6932	7.1332	7.9689
C	3.5131	5.5585	6.5275
H	2.6207	5.9359	6.0503
N	2.5881	3.5793	3.1213
C	4.0876	4.3851	6.0772
N	6.0161	2.6524	4.1022
C	2.1266	4.0523	1.8276
H	2.9827	4.0757	1.1522
H	1.7221	5.0513	1.9614
H	1.3639	3.3715	1.4593
C	2.7046	2.2977	3.5472
C	3.3008	2.3712	4.7987
C	2.3649	1.1107	2.7534
C	1.4711	0.1701	3.2564
H	1.0128	0.3309	4.2245
C	1.1833	-0.9704	2.5254
H	0.4854	-1.6993	2.9186
C	1.7896	-1.1798	1.2953
H	1.5625	-2.0726	0.7250
C	2.6942	-0.2522	0.8005
H	3.1855	-0.4202	-0.1502
C	2.9881	0.8902	1.5273
H	3.7303	1.5975	1.1688
C	5.9453	2.9915	2.9910
S	8.2666	2.9593	6.1005
N	6.9220	0.2950	5.3781
C	6.3658	-0.3366	4.3399
H	5.4822	0.1299	3.9302
N	8.6302	0.4165	6.9971
S	6.2965	0.6764	10.5460
C	6.8613	-1.5168	3.8210
H	6.3599	-1.9798	2.9824
N	9.0571	-0.3123	8.0105
C	7.9901	-2.0756	4.3886

H	8.4087	-2.9984	4.0073
C	8.5901	-1.4236	5.4484
H	9.4826	-1.8013	5.9252
N	9.5165	0.5546	8.8548
C	8.0163	-0.2500	5.8989
N	6.0879	1.4834	7.8752
C	9.9782	0.0808	10.1480
H	9.1214	0.0532	10.8226
H	10.3870	-0.9163	10.0129
H	10.7379	0.7640	10.5186
C	9.3995	1.8364	8.4295
C	8.8040	1.7634	7.1776
C	9.7372	3.0232	9.2244
C	10.6293	3.9658	8.7221
H	11.0880	3.8066	7.7538
C	10.9147	5.1064	9.4540
H	11.6110	5.8369	9.0615
C	10.3075	5.3141	10.6838
H	10.5324	6.2072	11.2545
C	9.4048	4.3843	11.1781
H	8.9128	4.5508	12.1286
C	9.1133	3.2416	10.4506
H	8.3724	2.5328	10.8084
C	6.1573	1.1454	8.9868

2b (LS)

E (Eh) =	-8568.7283	ν (cm^{-1}) =	14.89
Atom	x	y	z
Se	2.1957	0.8592	1.3144
S	4.2323	3.2341	5.8662
Fe	2.0484	2.2845	6.0226
C	2.4546	-0.1033	7.6707
H	1.5620	0.3370	8.0899
N	2.9751	0.5372	6.6193
N	4.6542	0.6988	4.9735
C	2.9952	-1.2619	8.1925
H	2.5213	-1.7317	9.0432
N	5.0982	-0.0214	3.9615
C	4.1326	-1.7898	7.6124
H	4.5863	-2.6947	7.9960

C	4.6944	-1.1297	6.5363
H	5.5907	-1.4835	6.0485
N	5.5328	0.8548	3.1133
C	6.0123	0.3894	1.8232
H	5.1608	0.3444	1.1424
H	6.7614	1.0869	1.4578
H	6.4383	-0.5998	1.9619
C	4.0770	0.0212	6.0849
N	2.0573	1.6966	4.1417
C	4.7916	2.0491	4.7877
C	5.3814	2.1347	3.5341
C	6.5550	4.2959	3.2597
H	7.0027	4.1487	4.2349
C	6.8211	5.4447	2.5337
H	7.4911	6.1932	2.9380
C	6.2286	5.6369	1.2940
H	6.4375	6.5366	0.7276
C	5.3601	4.6832	0.7847
H	4.8793	4.8368	-0.1737
C	5.0883	3.5321	1.5063
H	4.3720	2.8050	1.1350
C	2.0917	1.3621	3.0313
C	5.6973	3.3295	2.7425
Se	1.9151	3.7065	10.7323
S	-0.1373	1.3354	6.1794
C	1.6398	4.6712	4.3733
H	2.5313	4.2303	3.9524
N	1.1214	4.0315	5.4261
N	-0.5545	3.8705	7.0749
C	1.0983	5.8296	3.8520
H	1.5703	6.2987	2.9999
N	-0.9944	4.5904	8.0890
C	-0.0377	6.3581	4.4342
H	-0.4922	7.2629	4.0509
C	-0.5974	5.6988	5.5118
H	-1.4928	6.0528	6.0013
N	-1.4275	3.7137	8.9376
C	-1.9017	4.1773	10.2303
H	-1.0492	4.2124	10.9106
H	-2.6560	3.4841	10.5934

H	-2.3195	5.1706	10.0960
C	0.0206	4.5480	5.9625
N	2.0403	2.8723	7.9038
C	-0.6931	2.5203	7.2598
C	-1.2796	2.4343	8.5148
C	-2.4713	0.2838	8.7994
H	-2.9329	0.4394	7.8320
C	-2.7379	-0.8647	9.5257
H	-3.4228	-1.6045	9.1300
C	-2.1272	-1.0681	10.7546
H	-2.3366	-1.9678	11.3206
C	-1.2406	-0.1254	11.2535
H	-0.7458	-0.2877	12.2032
C	-0.9690	1.0260	10.5323
H	-0.2413	1.7459	10.8961
C	2.0099	3.2034	9.0153
C	-1.5955	1.2393	9.3066

2c (LS)

E (Eh) =	-3818.7789	ν (cm^{-1}) =	18.04
Atom	x	y	z
Fe	6.0407	2.2056	6.0103
C	5.6824	4.6262	7.6223
N	5.1382	3.9724	6.5912
S	3.8449	1.2837	5.8853
B	6.3176	0.5847	10.4094
H	5.2277	0.3759	10.8949
H	6.9447	1.3899	11.0817
H	6.9486	-0.4507	10.2688
N	3.4399	3.8116	4.9629
C	5.1773	5.8130	8.1153
C	3.4626	5.6815	6.4752
N	2.5552	3.6388	3.1068
N	3.0017	4.5212	3.9412
C	4.0513	6.3565	7.5272
N	6.0594	1.6146	7.8910
C	4.0442	4.5015	6.0523
H	2.5734	6.0468	5.9828
C	1.4961	0.2034	3.3308
C	1.7719	-1.1653	1.3758

C	1.2090	-0.9537	2.6260
H	3.6294	1.6570	1.1336
C	2.6321	-0.2220	0.8340
H	3.0898	-0.3900	-0.1332
H	1.5458	-2.0714	0.8265
C	2.9238	0.9372	1.5343
H	0.5452	-1.6936	3.0558
C	6.1318	1.1976	8.9632
H	1.0706	0.3657	4.3136
H	2.9285	4.1395	1.1305
H	1.3302	3.3922	1.4501
H	1.6490	5.0829	1.9413
H	3.6265	7.2852	7.8863
C	2.3460	1.1596	2.7817
H	5.6702	6.2940	8.9487
C	2.6859	2.3631	3.5499
H	6.5667	4.1741	8.0466
C	3.2845	2.4606	4.7978
C	2.0779	4.0938	1.8105
C	6.3986	-0.2151	4.3984
N	6.9431	0.4388	5.4293
S	8.2360	3.1278	6.1357
B	5.7675	3.8223	1.6093
H	6.8583	4.0352	1.1275
H	5.1460	3.0142	0.9354
H	5.1319	4.8552	1.7470
N	8.6422	0.5996	7.0569
C	6.9039	-1.4016	3.9049
C	8.6195	-1.2698	5.5440
N	9.5278	0.7720	8.9126
N	9.0814	-0.1102	8.0779
C	8.0304	-1.9447	4.4922
N	6.0221	2.7966	4.1297
C	8.0376	-0.0900	5.9675
H	9.5090	-1.6349	6.0358
C	10.5847	4.2082	8.6901
C	10.3086	5.5757	10.6460
C	10.8713	5.3651	9.3955
H	8.4531	2.7519	10.8872
C	9.4493	4.6314	11.1875

H	8.9918	4.7985	12.1550
H	10.5343	6.4816	11.1957
C	9.1581	3.4724	10.4867
H	11.5343	6.1058	8.9659
C	5.9510	3.2115	3.0567
H	11.0099	4.0469	7.7071
H	9.1552	0.2698	10.8886
H	10.7528	1.0187	10.5692
H	10.4354	-0.6720	10.0771
H	8.4554	-2.8731	4.1326
C	9.7356	3.2512	9.2389
H	6.4107	-1.8825	3.0716
C	9.3963	2.0478	8.4702
H	5.5138	0.2367	3.9747
C	8.7972	1.9507	7.2224
C	10.0057	0.3167	10.2085

3a (LS)

E (Eh) =	-4158.4380	ν (cm^{-1}) =	5.42
Atom	x	y	z
S	6.4358	5.8381	6.5139
Fe	10.1529	3.8564	8.6763
N	9.2927	4.6097	10.3729
C	9.1400	5.9180	10.5834
H	9.5162	6.5720	9.8085
N	8.7211	4.7160	7.6459
C	8.5229	6.4315	11.7065
H	8.4233	7.5020	11.8216
S	8.8431	2.0020	9.2019
C	8.9333	2.2912	10.9739
H	9.9201	1.9327	11.2680
H	8.1740	1.7054	11.4905
C	8.7978	3.7539	11.2765
C	8.0297	5.5502	12.6523
H	7.5353	5.9144	13.5444
C	8.1623	4.1928	12.4274
H	7.7689	3.4671	13.1274
C	7.1036	2.4065	8.8653
H	6.9516	3.4681	9.0497
H	6.9939	2.2539	7.7912

C	7.7680	5.1947	7.1663
C	5.9963	0.2056	9.4126
H	6.5652	-0.2596	8.6149
C	6.1489	1.5664	9.6621
C	5.4113	2.1479	10.6870
H	5.5143	3.2106	10.8790
C	5.1284	-0.5570	10.1757
H	5.0161	-1.6144	9.9690
C	4.5419	1.3858	11.4538
H	3.9715	1.8550	12.2465
C	4.4009	0.0311	11.2016
H	3.7239	-0.5672	11.7989
S	13.8648	1.8711	10.8447
N	11.0132	3.1030	6.9798
C	11.1660	1.7947	6.7693
H	10.7897	1.1407	7.5441
N	11.5842	2.9967	9.7069
C	11.7834	1.2813	5.6464
H	11.8831	0.2109	5.5313
S	11.4631	5.7107	8.1509
C	11.3726	5.4215	6.3790
H	10.3855	5.7799	6.0855
H	12.1315	6.0076	5.8621
C	11.5082	3.9589	6.0764
C	12.2769	2.1626	4.7007
H	12.7715	1.7985	3.8088
C	12.1440	3.5201	4.9256
H	12.5376	4.2459	4.2257
C	13.2022	5.3048	8.4879
H	13.3532	4.2430	8.3040
H	13.3117	5.4578	9.5620
C	12.5354	2.5168	10.1889
C	14.3138	7.5039	7.9419
H	13.7467	7.9695	8.7406
C	14.1579	6.1437	7.6911
C	14.8935	5.5617	6.6649
H	14.7879	4.4994	6.4719
C	15.1828	8.2654	7.1789
H	15.2976	9.3223	7.3866
C	15.7639	6.3226	5.8982

H	16.3325	5.8531	5.1045
C	15.9080	7.6768	6.1518
H	16.5859	8.2742	5.5545

3b (LS)

E (Eh) =	-8165.2646	ν (cm^{-1}) =	8.20
Atom	x	y	z
Se	6.6809	6.1442	6.1655
Fe	10.1644	3.9292	8.7844
N	9.4075	4.6843	10.5278
C	9.3370	5.9940	10.7733
H	9.6964	6.6457	9.9884
N	8.7299	4.8188	7.8023
C	8.8238	6.5127	11.9448
H	8.7902	7.5840	12.0874
S	8.8433	2.1137	9.3402
C	8.9636	2.3693	11.1148
H	9.9191	1.9341	11.4114
H	8.1655	1.8277	11.6225
C	8.9274	3.8337	11.4451
C	8.3500	5.6363	12.9050
H	7.9383	6.0045	13.8365
C	8.3949	4.2796	12.6446
H	8.0165	3.5596	13.3586
C	7.1105	2.5547	9.0371
H	6.9424	3.5706	9.3921
H	7.0277	2.5855	7.9503
C	7.9110	5.3461	7.1638
C	6.0221	0.2918	9.1165
H	6.6158	0.0077	8.2544
C	6.1534	1.5726	9.6459
C	5.3884	1.9236	10.7520
H	5.4736	2.9231	11.1658
C	5.1430	-0.6169	9.6780
H	5.0486	-1.6077	9.2505
C	4.5054	1.0137	11.3174
H	3.9092	1.3026	12.1746
C	4.3810	-0.2575	10.7818
H	3.6886	-0.9669	11.2182
Se	13.6074	1.6827	11.4290

N	10.9103	3.1698	7.0357
C	10.9941	1.8598	6.7951
H	10.6645	1.2069	7.5919
N	11.5918	3.0376	9.7748
C	11.4856	1.3431	5.6134
H	11.5313	0.2716	5.4750
S	11.5048	5.7436	8.2027
C	11.3150	5.4859	6.4337
H	10.3424	5.9089	6.1796
H	12.0847	6.0350	5.8929
C	11.3572	4.0224	6.1039
C	11.9232	2.2216	4.6379
H	12.3174	1.8548	3.6983
C	11.8667	3.5786	4.8936
H	12.2216	4.3010	4.1700
C	13.2395	5.2583	8.4445
H	13.3324	4.1934	8.2395
H	13.4100	5.3924	9.5132
C	12.3980	2.4984	10.4198
C	14.4200	7.4146	7.8824
H	13.9249	7.8841	8.7254
C	14.1853	6.0701	7.6093
C	14.8261	5.4829	6.5244
H	14.6543	4.4333	6.3094
C	15.2747	8.1559	7.0846
H	15.4513	9.2008	7.3096
C	15.6830	6.2236	5.7232
H	16.1786	5.7508	4.8840
C	15.9073	7.5621	6.0008
H	16.5747	8.1439	5.3771

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