Supplementary Information

Synthesis, spectral characterization, DFT calculations and investigation of anticancer properties of carbothioamide and metal (Fe^{II} and Cr^{III}) complexes

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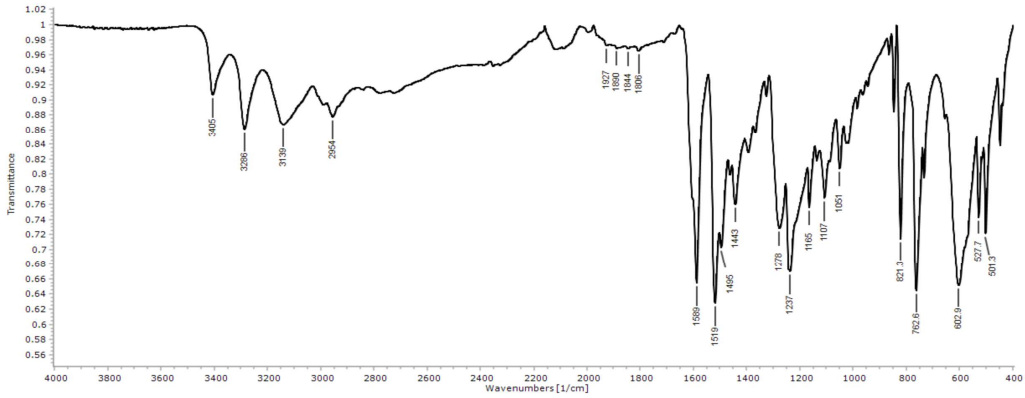
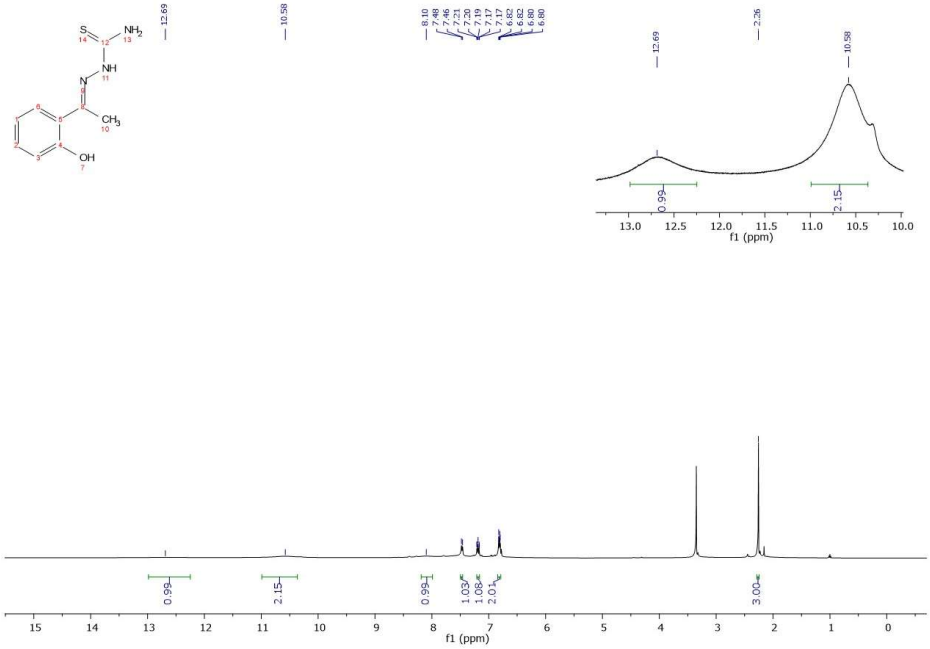
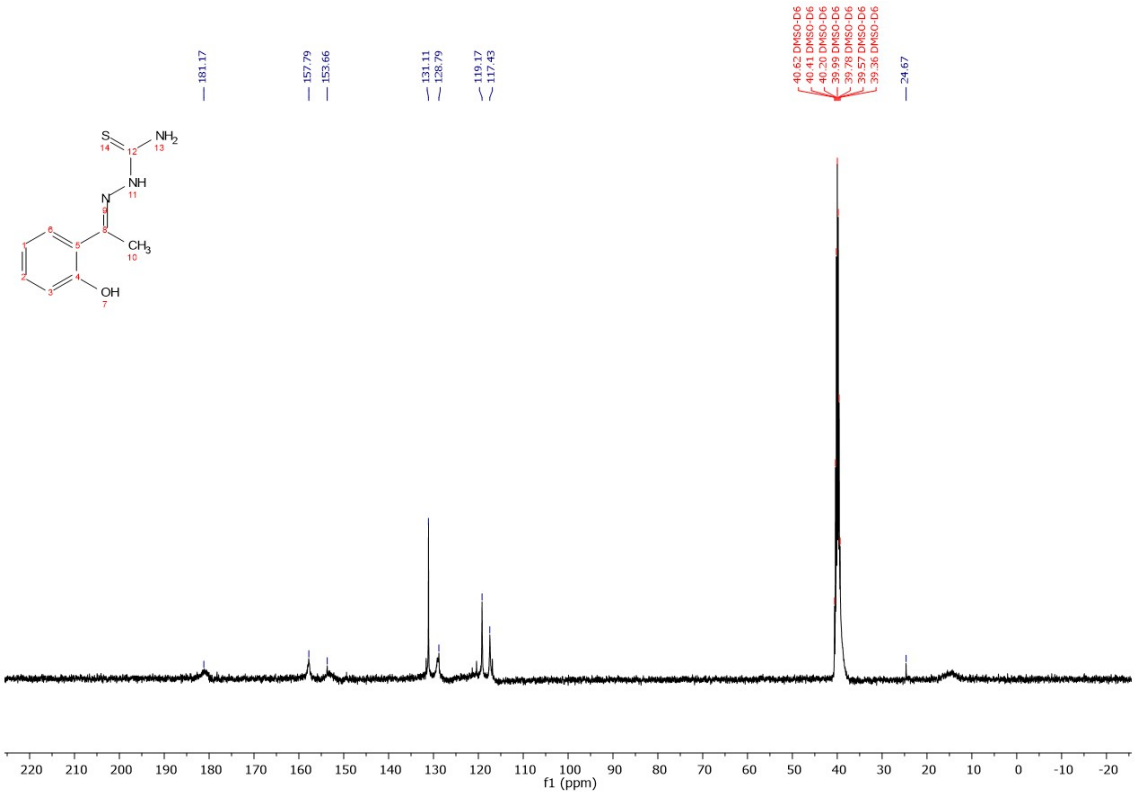


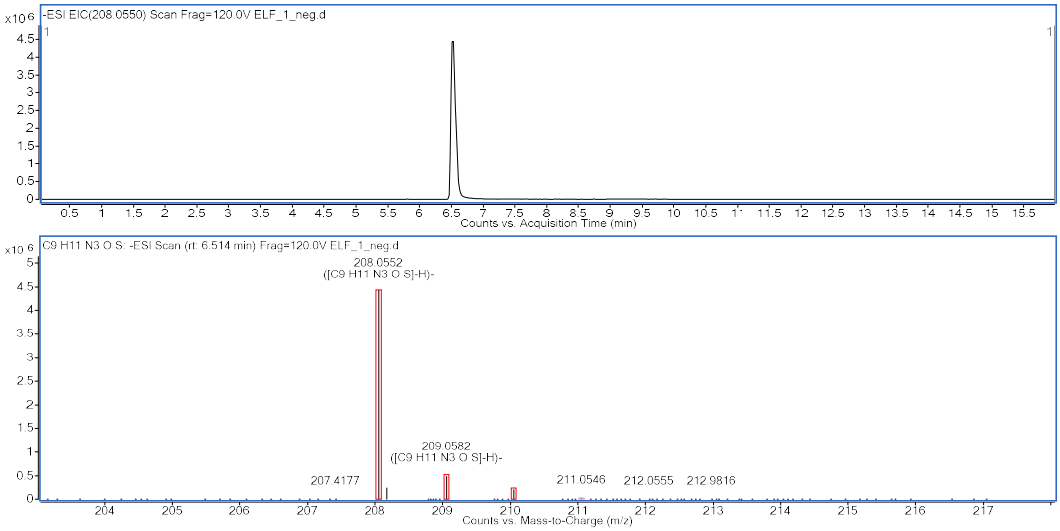
Supp. Fig. S1. IR spectrum of HL.



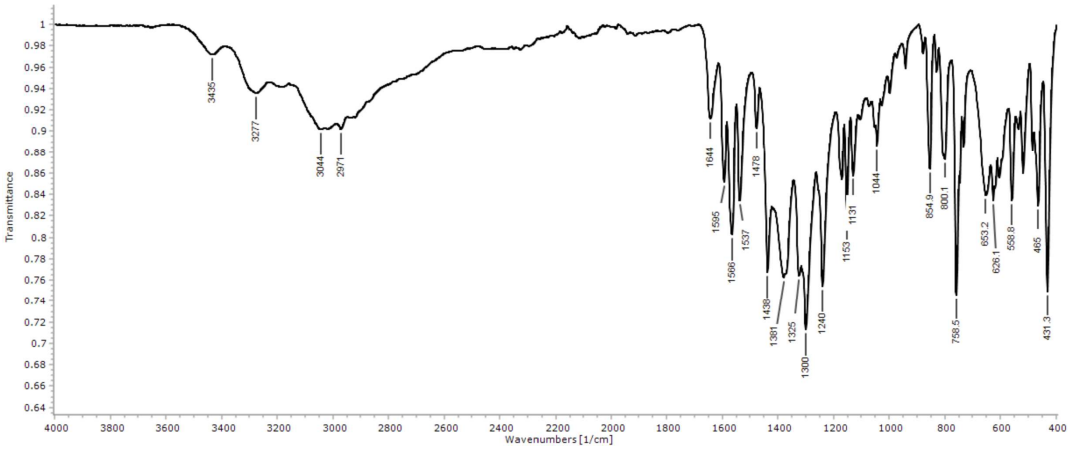
Supp. Fig. S2. ^{1}H-NMR spectrum of HL.



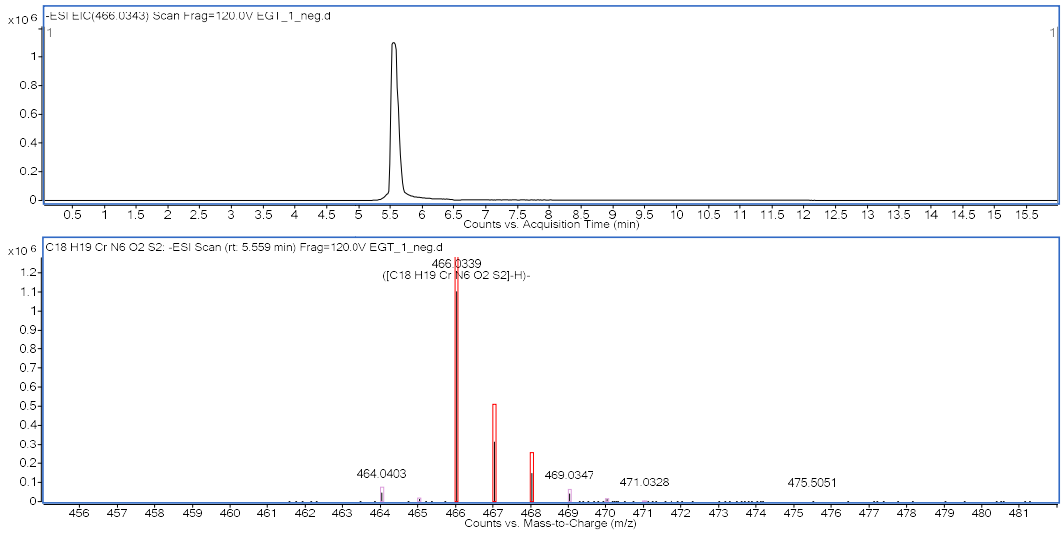
Supp. Fig. S3. ^{13}C-NMR spectrum of HL.



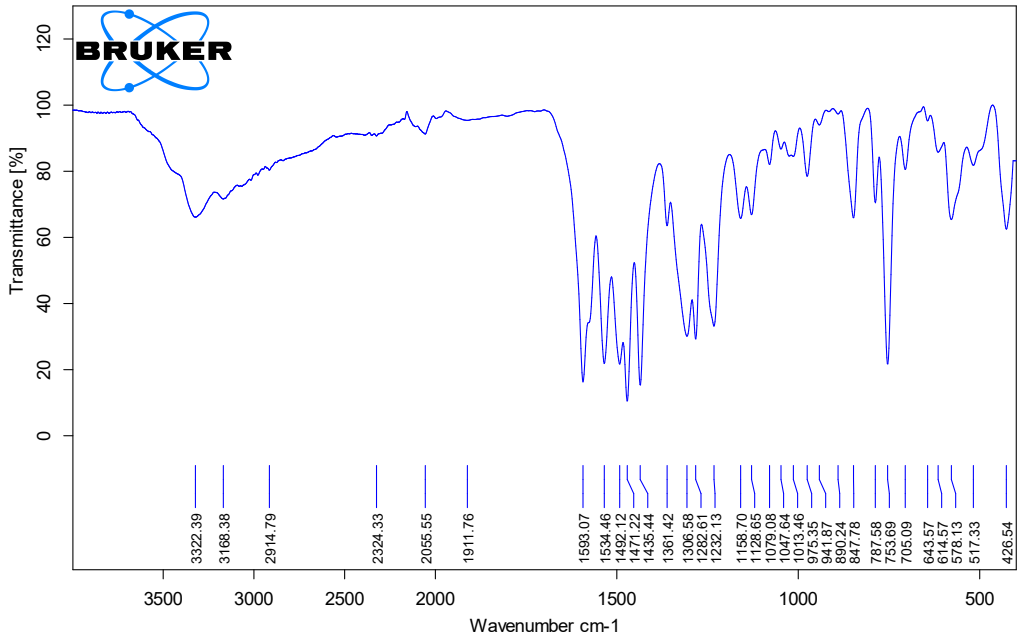
Supp. Fig. S4. LC-QTOF/MS spectrum of HL.



Supp. Fig. S5. IR spectrum of $[CrL_2]^+$.



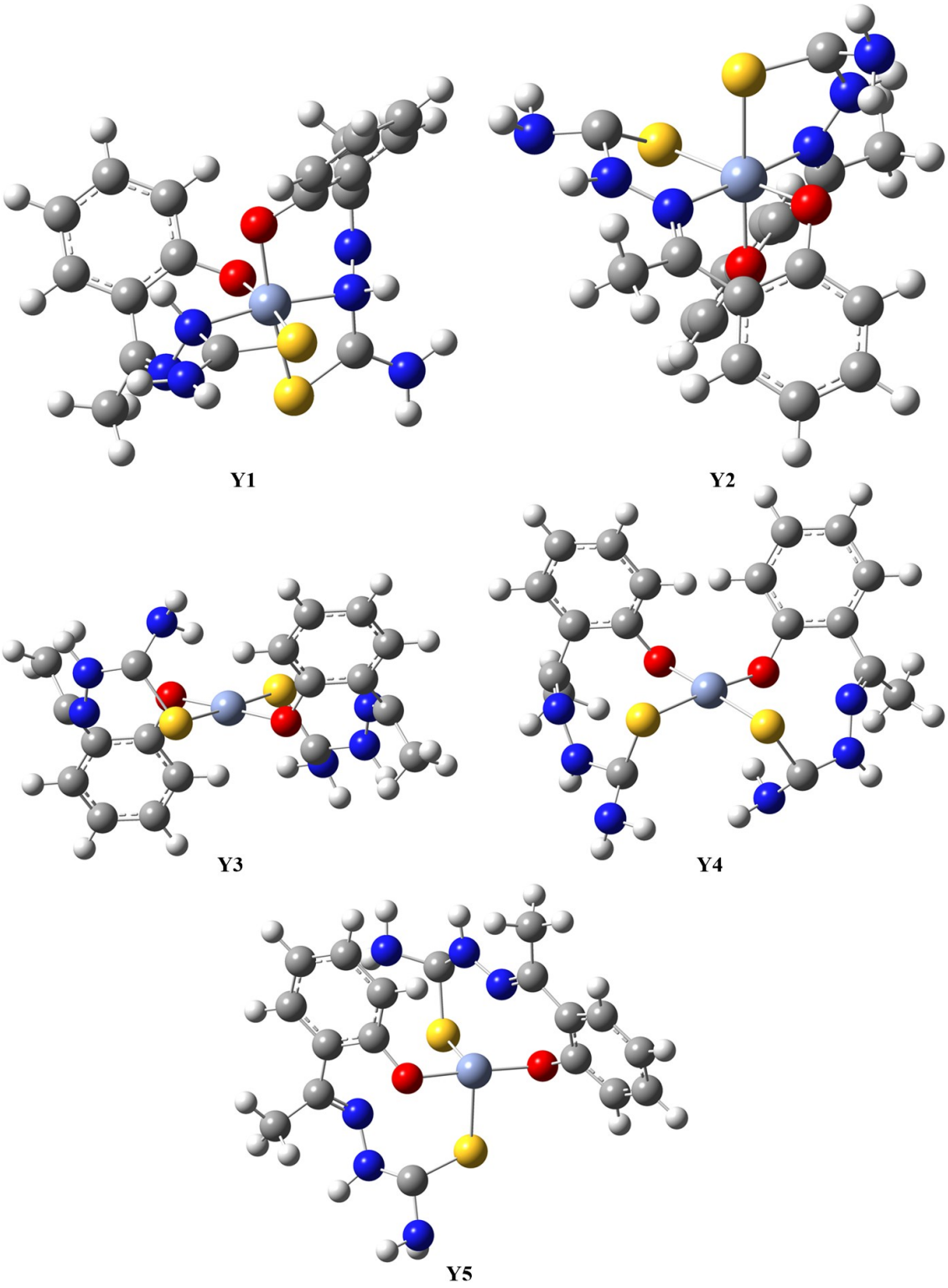
Supp. Fig. S6. LC-QTOF/MS spectrum of $[CrL_2]^+$.



Supp. Fig. S7. ^{13}C-NMR spectrum of IR spectrum of [FeL_2].

Supp. Table S1. Crystal data of the HL labeled molecule.

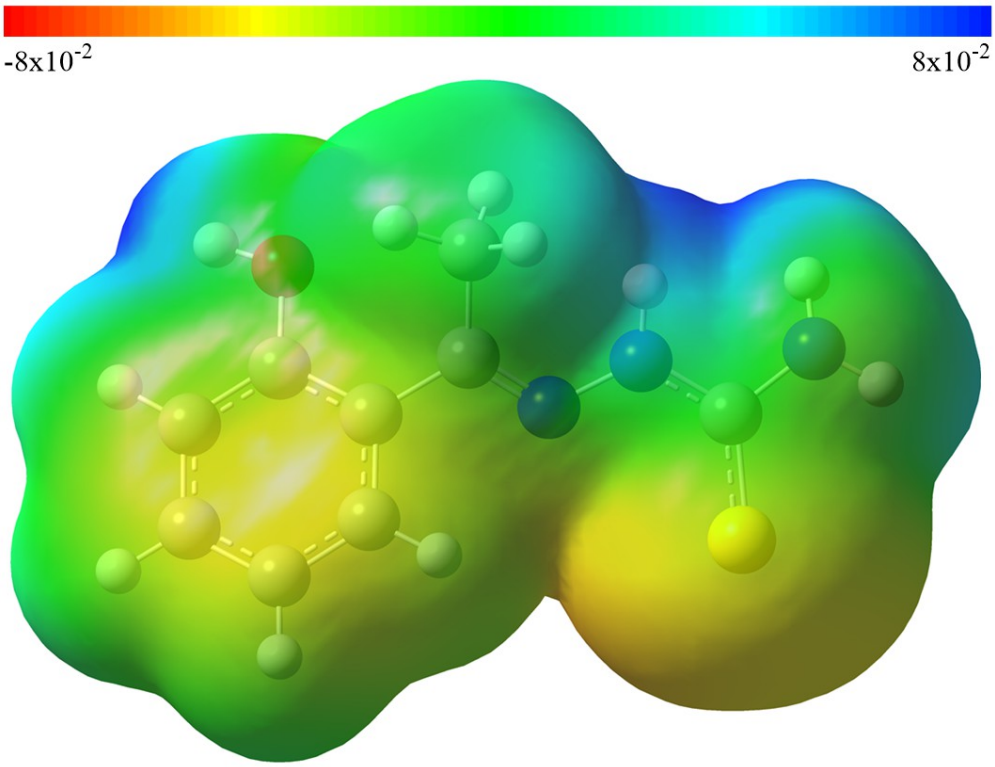
Empirical formula	$C_9H_{12}N_3O_{1.5}S$
Formula weight	218.28
Temperature	273.15 K
Wavelength	0.71073 Å
Crystal system	*Monoclinic*
Space group	*C2/c*
Unit cell dimensions	a = 14.383(3) Å α= 90° b = 14.725(3) Å β= 114.893(3)° c = 10.864(2) Å γ= 90°
Volume (Å^3)	2087.2(2)
Z	8
Density (calculated) (mg/m^3)	1.389
Absorption coefficient (mm^{-1})	0.288
Crystal size (mm^3)	0.218 x 0.161 x 0.092
Reflections collected	8201
Independent reflections	2390 [R_{int} = 0.0475]
Final R indixes [I>2σ (I)]	R_1 = 0.0482, wR_2 = 0.1152
R indixes (all data)	R_1 = 0.0723, wR_2 = 0.1289
CCDC	2296872



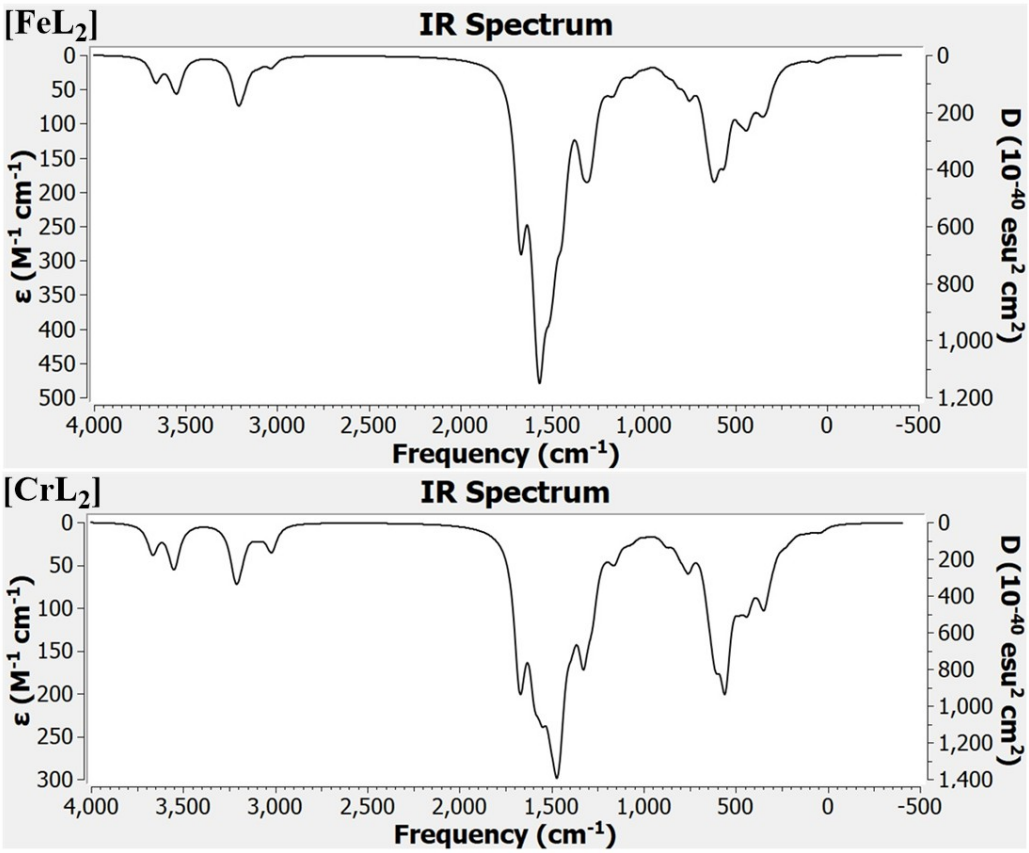
Supp. Fig. S8. Possible geometric structures of the synthesized complexes and their bonding patterns according to donor atoms.

Supp. Table S2. Calculated structural parameters of the complexes

Assignment	$[CrL_2]^+$	$[FeL_2]$
Bond Lenght (Å)		
M-S001	2.510	2.409
M-O003	1.906	1.913
M-N004	2.048	1.974
M-S001'	2.541	2.403
M-O003'	1.893	1.914
M-N004'	2.026	1.966
Bond Angle (º)		
S001-M-O003	167.96	178.18
S001-M-N004	82.43	86.13
S001-M-S001'	84.30	92.22
S001-M-O003'	89.87	88.51
S001-M-N004'	102.23	93.76
O003-M-N004	89.32	92.62
O003-M-S001'	88.48	89.19
O003-M-O003'	98.75	90.10
O003-M-N004'	86.24	87.46
N004-M-S001'	99.67	94.97
N004-M-N004'	175.22	178.79



Supp. Fig. S9. MEP map of HL compound.



Supp. Fig. S10. Calculated IR spectrum of studied complexes.

Supp. Table S3. Stretching frequencies (cm^{-1}) of $[FeL_2]$ ve $[CrL_2]^+$ complexes

	$[FeL_2]$		$[CrL_2]^+$	
Etiketleme	Hesapsal	Deneysel	Hesapsal	Deneysel
ν_{NH}	3667, 3546	3453, 3326	3667, 3549	3435, 3277
$\nu_{CH\_Aromatik}$	3217	3074	3215	3044
$\nu_{CH\_Alifatik}$	3027	2916	3023	2944
$\nu_{C=N}$	1618	1590	1601	1595
ν_{C-O}	1566	1534	1475	1539
ν_{C-N}	1329	1363	1325	1381
ν_{N-N}	1103	1127	1170	1171
$\nu_{C=S}$	810	844	808	800
ν_{M-O}	645	702	662	653
ν_{M-N}	629	616	648	626
ν_{M-S} [a]	322	-	319	-

[a] This frequency was appropriate with the result of Schelvis et al. in 2002 (Schelvis et al., 2002).