Supporting Information

"Photosensitizing activity of ferrocenyl bearing Ni(II) and Cu(II) dithiocarbamates in dye sensitized TiO_2 solar cells"

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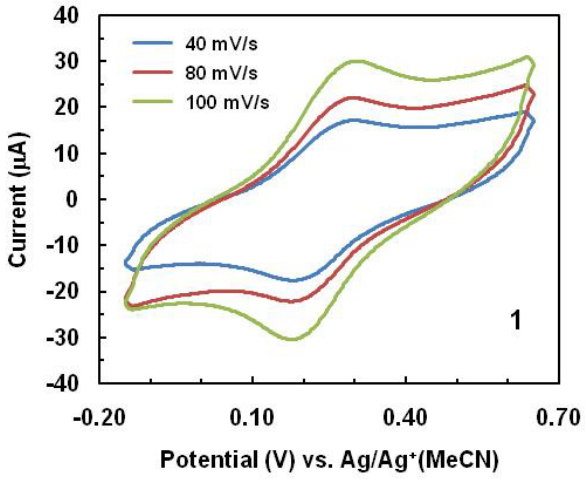
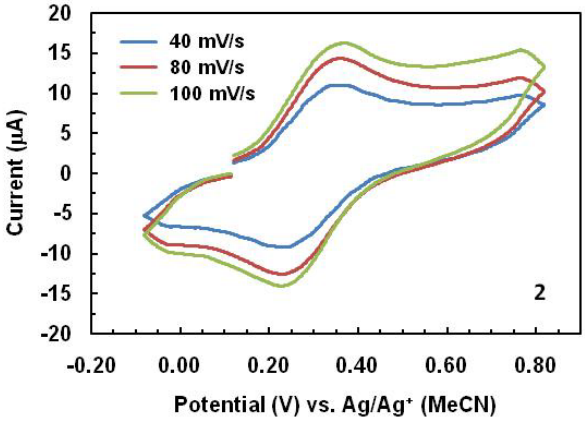
Contents

Table S1. Crystallographic Data and Structure Refinement Details for 1, **2**, and **4.**

	1	2	4
Formula	$C_{34}H_{32}CuFe_2N_2O_2S_4$	$C_{40}H_{36}CuFe_2N_2O_4S_4$	$C_{34}H_{32}NiFe_2N_2O_2S_4$
Crystal System	Tetragonal	Triclinic	Tetragonal
Space Group	$P4_2/n$	P-1	$P4_2/n$
Formula weight	804.10	912.19	799.27
Temperature(K)	293(2)	298(2)	293(2)
Z	4	1	4
a/(Å)	23.6577(12)	7.5963(13)	23.414(4)
b/(Å)	23.6577(12)	11. 2271(8)	23.414(4)
c/ (Å)	5.8825(4)	11.6787(19)	5.832(1)
α /deg	(90)	84.763(9)	(90)
β/ deg	(90)	77.404 (15)	(90)
γ/deg	(90)	85.766(9)	(90)
V(Å^3)	3292.4(4)	966.5 (2)	3197(1)
D_α (g/cm^3)	1.622	1.567	1.660
Crystal size (mm^3)	0.45 x 0.38x 0.30	0.45x 0.40 x 0.38	0.45 x 0.38 x 0.35
F(000)	1644	467	1640
Reflections collected	8002	7101	19350
Unique reflections	3646 R(int) = 0.1000]	4220 [R(int) = 0.026]	3676 [R_{int}= 0.1219]
μ (Mo Kα),	1.798	1.546	1.776
Final R indices R [I > 2σ(I)]	R1 = 0.0787, wR2 = 0.0830	R1 = 0.0445, wR2 = 0.0819	R1 = 0.0706, wR2 = 0.1589
R indices [all data]	R1 = 0.2152, wR2 = 0.1097	R1 = 0.074, wR2 = 0.0927	R1 = 0.1403, wR2 = 0.1885
Goodness-of-fit on F^2	0.907	1.007	0.994
largest peak difference and hole /e Å^{-3}	0.423 and -0.403	0.283 and -0.366	0.860 and -0.498

$R_1 = \Sigma \| F0| - |Fc \| / \Sigma |F0|$. $R_2 = \{[\Sigma w (F_0^2 - Fc^2)/ \Sigma w (F_0^2)^2] \}^{1/2}$, $w = 1/ [\sigma^2 (F_0^2) + (xP)^2]$, where $P = (F_0^2 + 2Fc^2)/3$





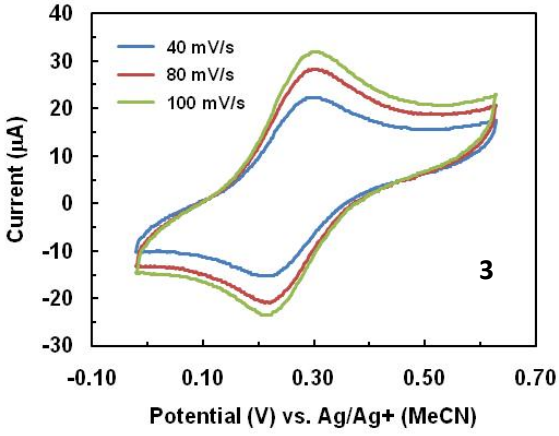


Fig. S1. Cyclic voltammograms of the compounds **1**, **2** and **3** recorded at different scan rates (40-100mV/s) in 10^{-3} M dichloromethane solution (0.1 M Bu_4NClO_4 was used as supporting electrolyte).

Table S2. Electrochemical Parameters Derived From the Voltammograms for (1-6).

Scan rate (mVs^{-1})	$E_{p,a}$ (V)	$E_{p,c}$ (V)	$\Delta E = E_{p,a} - E_{p,c}$ (V)	$E^0 = (E_{p,a} + E_{p,c})/2$ (V)
1				
40	0.29	0.18	0.10	0.23
80	0.29	0.18	0.11	0.23
100	0.30	0.18	0.12	0.24
2				
40	0.36	0.23	0.13	0.29
80	0.36	0.22	0.13	0.29
100	0.36	0.22	0.14	0.29
3				
40	0.30	0.21	0.09	0.26
80	0.30	0.21	0.09	0.26
100	0.31	0.21	0.09	0.26
4				
40	0.40	0.30	0.10	0.35
80	0.39	0.29	0.10	0.34
100	0.38	0.28	0.10	0.33
5				
40	0.38	0.27	0.11	0.32
80	0.39	0.27	0.12	0.33
100	0.39	0.27	0.12	0.33
6				
40	0.33	0.24	0.09	0.28
80	0.34	0.24	0.09	0.28
100	0.34	0.24	0.10	0.29

^{1}H NMR Spectra of the Ligands (L1-L3) and Complexes(1-6).

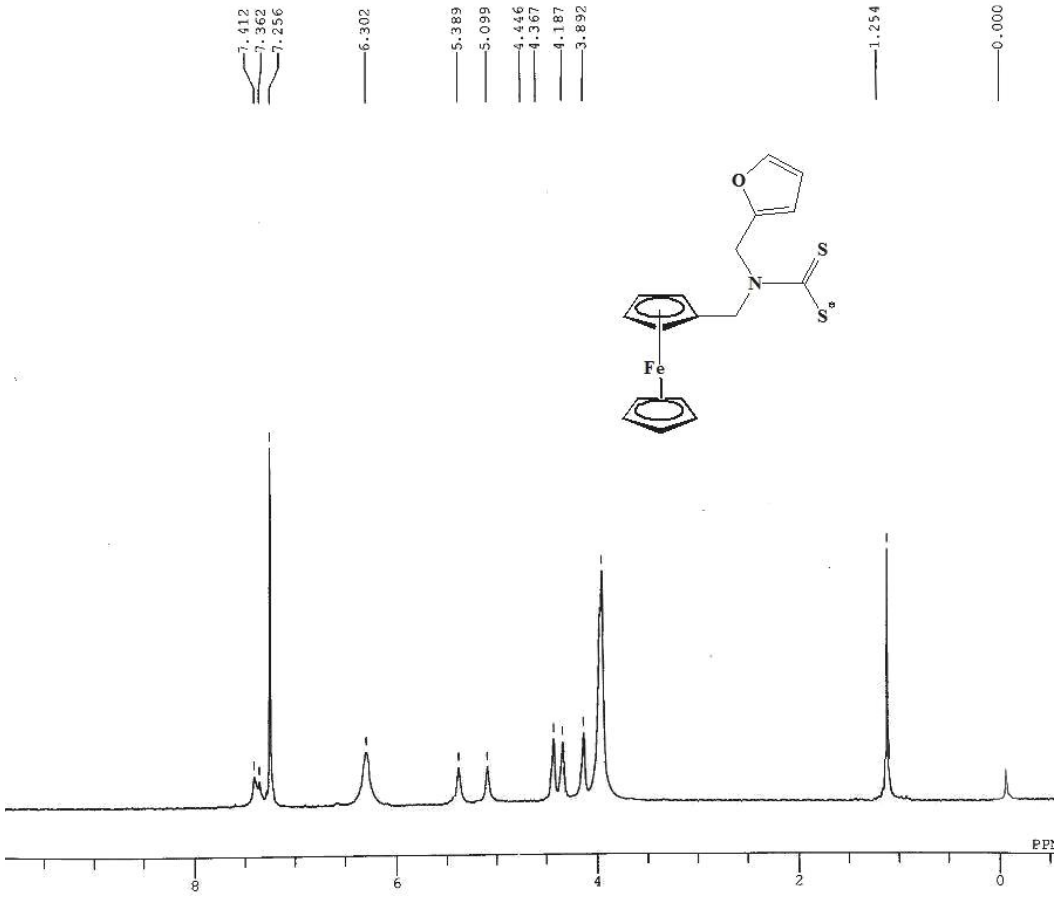


Fig.S2 (a) ^{1}H NMR of L1, potassium-N-methyl furfuryl-N-methyl ferrocenyl dithiocarabamate.

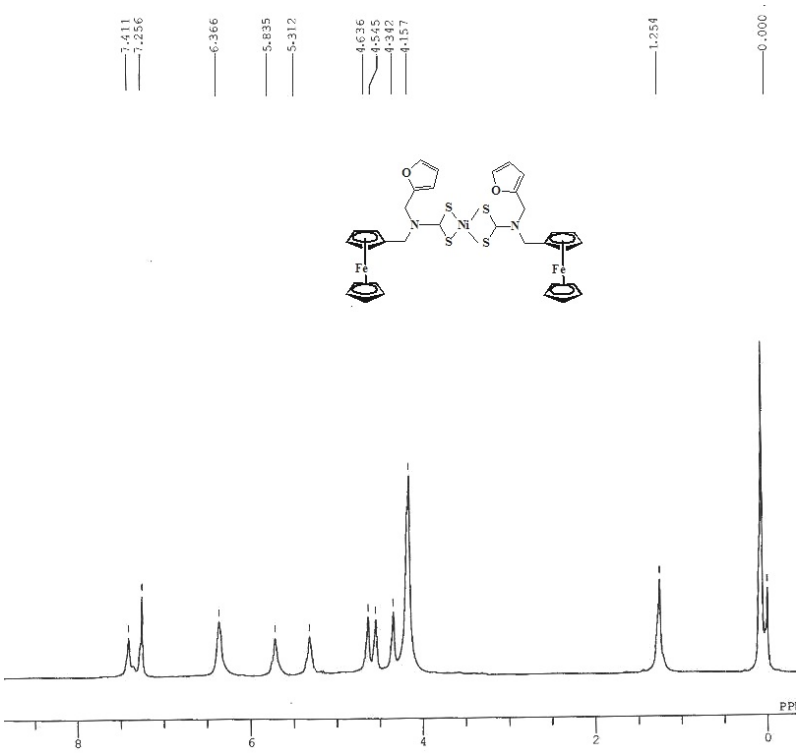


Fig. S2 (b) ^{1}H NMR of **4**, [Ni($FcCH_2NCS_2CH_2C_4H_3O)_2$].

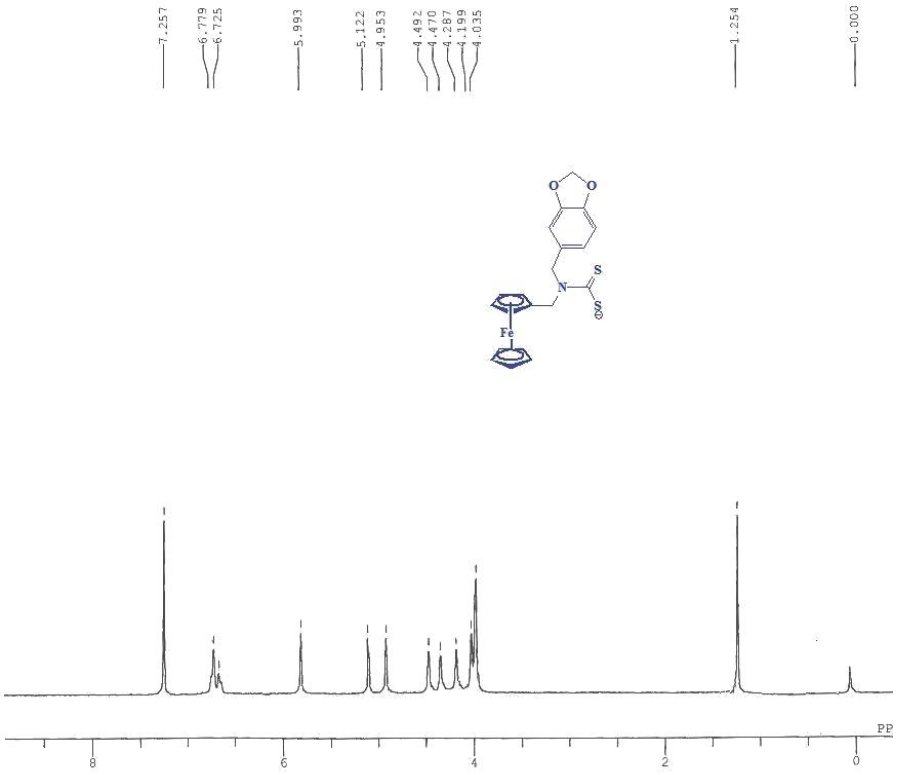


Fig. S2(c) ^{1}H NMR of L2, potassium-N-methylpiperonyl-N-methyl ferrocenyl dithiocarbamate.

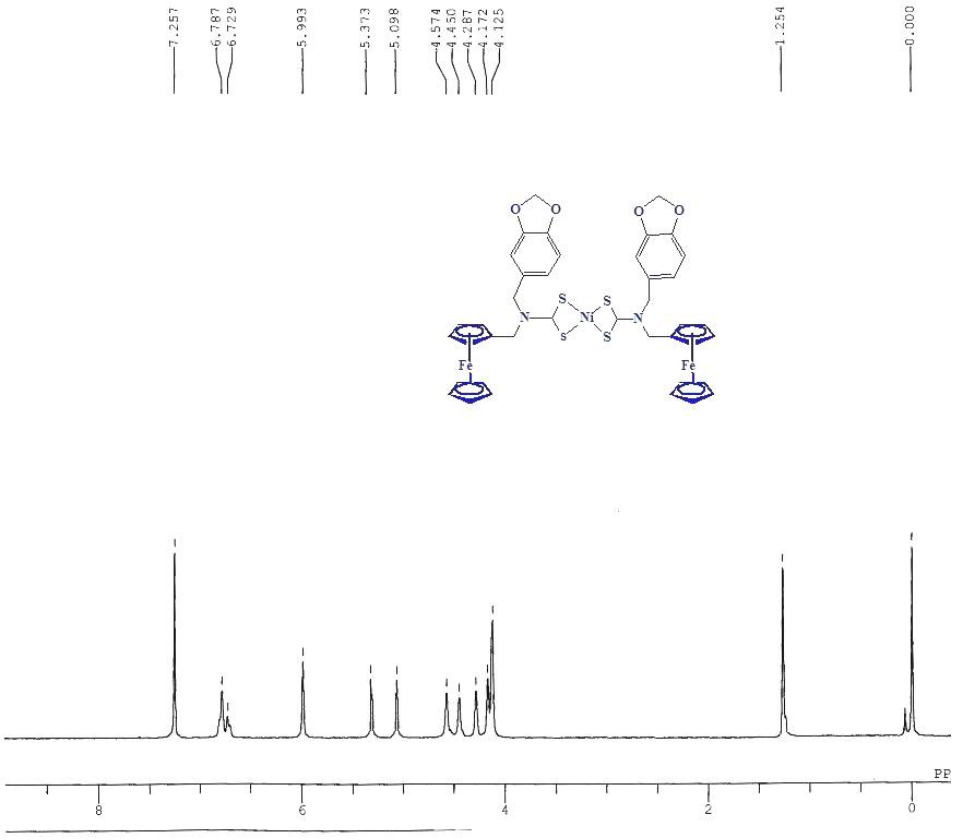


Fig. S2(d) ^{1}H NMR of **5**, [Ni(FcCH$_2$NCS$_2$CH$_2$C$_7$H$_5$O$_2$)$_2$].

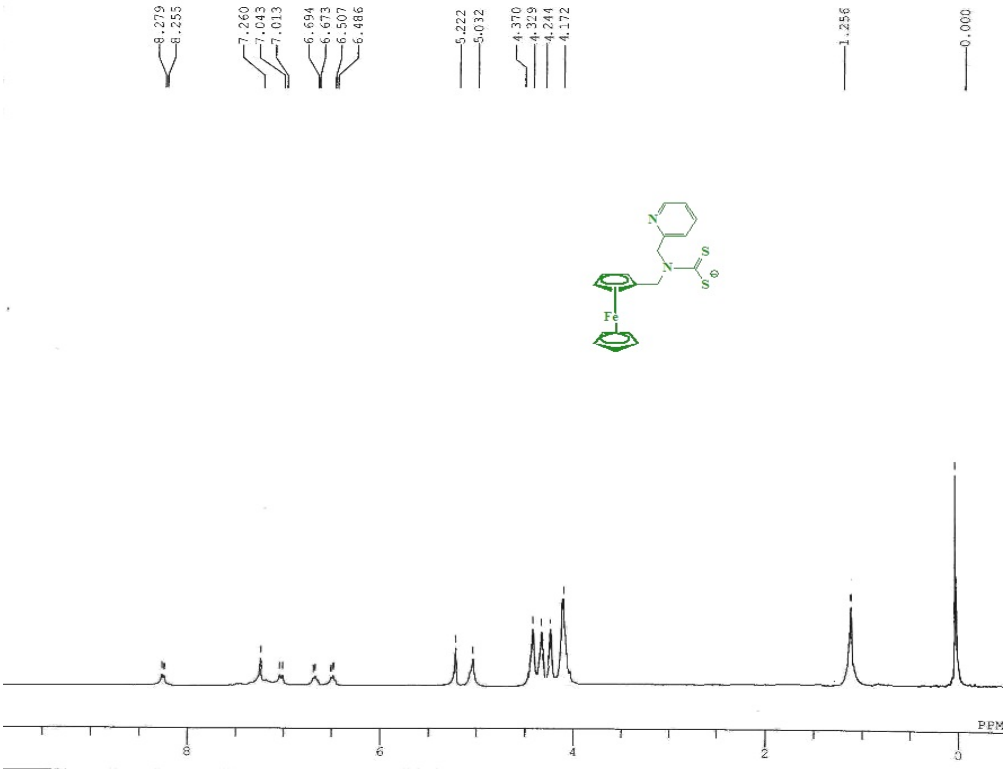


Fig. S2 (e) ^{1}H NMR of L3, potassium-N-methylpyridyl-N-methylferrocenyl dithiocarbamate.

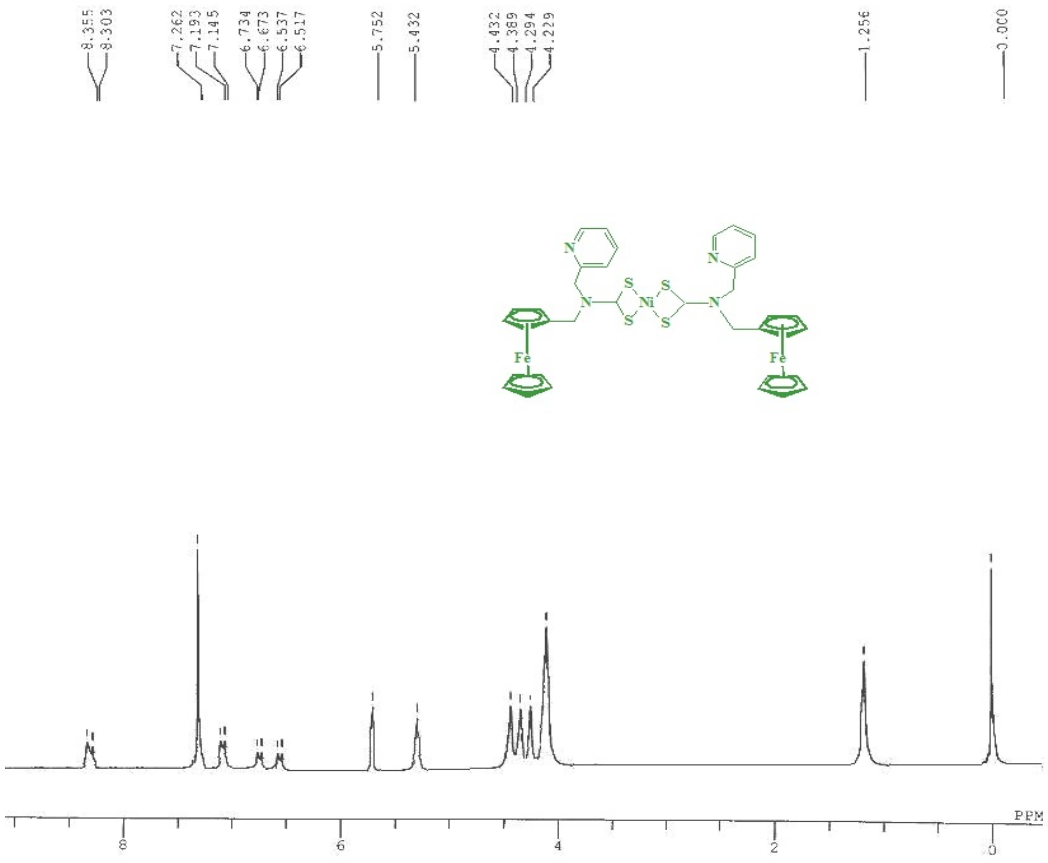


Fig. S2(f) ^{1}H NMR of **6**, [Ni(FcCH$_2$NCS$_2$CH$_2$C$_5$H$_4$N)$_2$].

IR Spectra of the Complexes, 1, 2 and 3

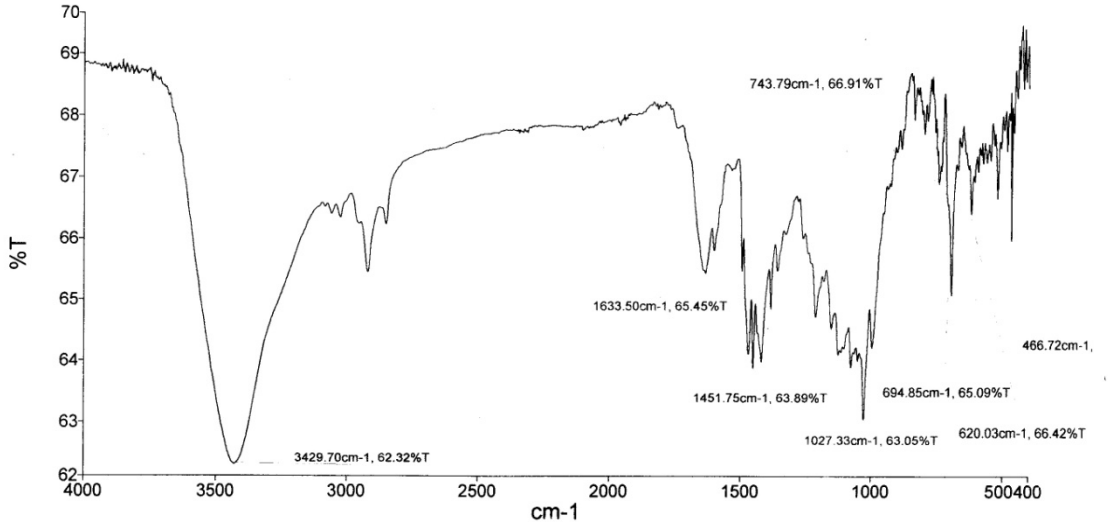


Fig.S2 (g) IR specrum of **1**, $[Cu(FcCH_2NCS_2CH_2C_4H_3O)_2]$.

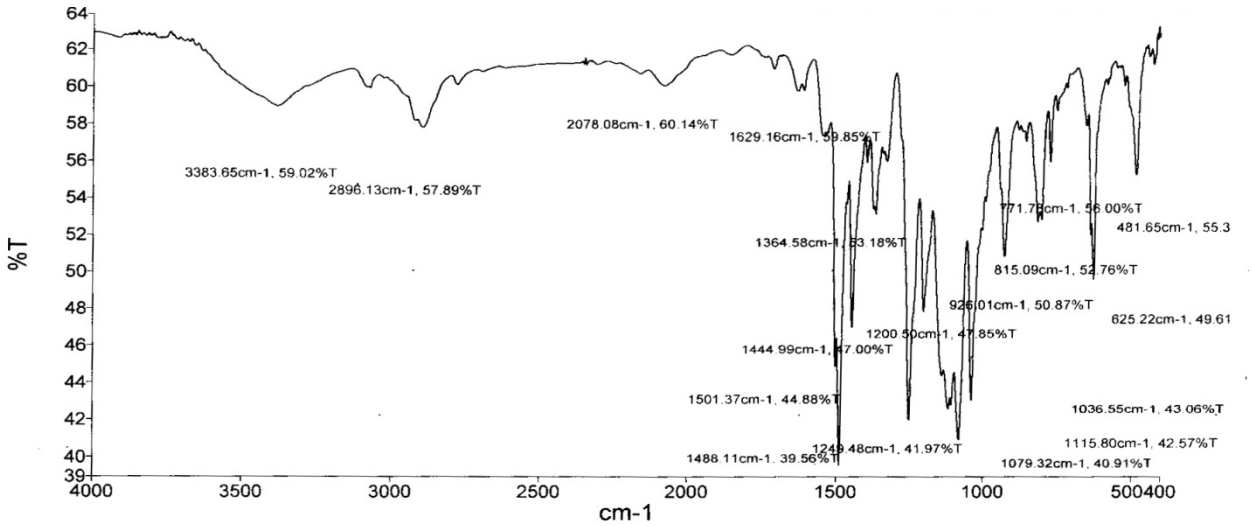


Fig.S2 (h) IR spectrum of **2**, $[Cu(FcCH_2NCS_2CH_2C_7H_6O)_2]$.

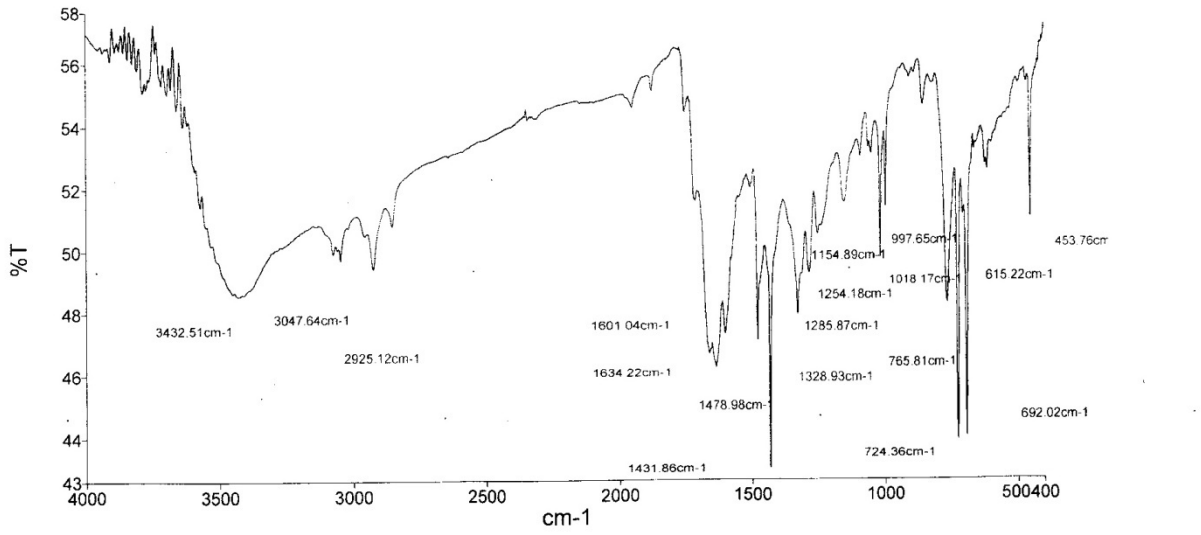


Fig.S2(i). IR spectrum of **3**, $[Cu(FcCH_2NCS_2CH_2C_5H_4N)_2]$.