Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Nickel(II) dithiocarbamate complexes containing pyrrole moiety for sensing of anions and synthesis of nickel sulfide and nickel oxide nanoparticles

*Ethiraj Sathiyaraj, Govindasamy Gurumoorthy and SubbiahThirumaran**

New Journal of Chemistry

Table:S1 Correlations in the HSQC spectrum of complex

^{13}C Chemical shifts (δ, ppm)	Correlation in the **HSQC** spectrum
43.6 (CH_2- pyrrole)	4.67 (furyl)
44.7 (CH_2-furyl)	4.71(pyrrole)
123.9 (C-2) pyrrole	-
110.3(C-3) pyrrole	6.21
108.1(C-4) pyrrole	6.13
119.8 (C-5) pyrrole	6.83
147.4(C-2) furyl	-
143.1(C-5) furyl	7.43
110.8 (C-3), 110.9 (C-4) furyl	6.38

Table: S2 Correlations in the HMBC spectrum of complex 2

^{13}C Chemical shifts (δ, ppm)	Correlation in the **HMBC** spectrum
43.6 (CH_2-pyrrole)	4.71 (H-1)
44.7 (CH_2-furyl)	4.67 (H-1)
123.9 (C-2) pyrrole	6.83(H-5), 6.21(H-4), 4.71(furyl)
119.8 (C-5) pyrrole	-
110.3(C-3) pyrrole	-
108.1(C-4) pyrrole	-
147.4(C-2) furyl	7.43 (H-5), 6.38 (H-4), 4.66 (pyrrole)
143.1(C-5) furyl	-
110.8, 110.9 (C-3) (C-4) furyl	-

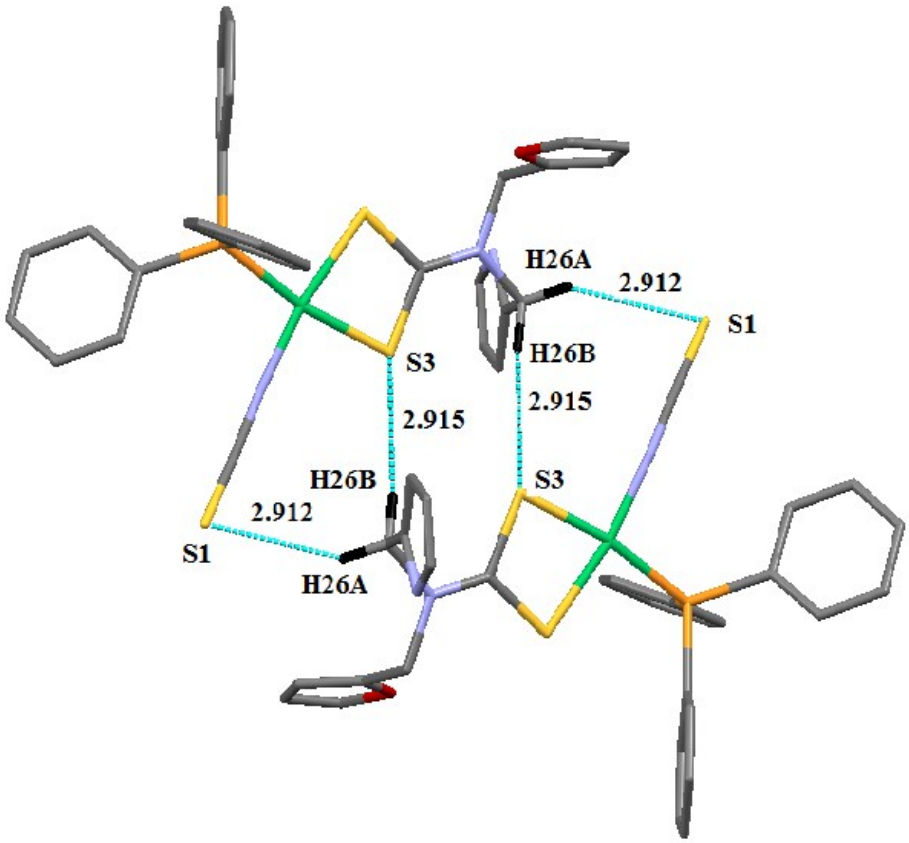

Fig. S1 Intermolecular S···H–C interactions (2.91 and 2.92 Å) in complex **5**.

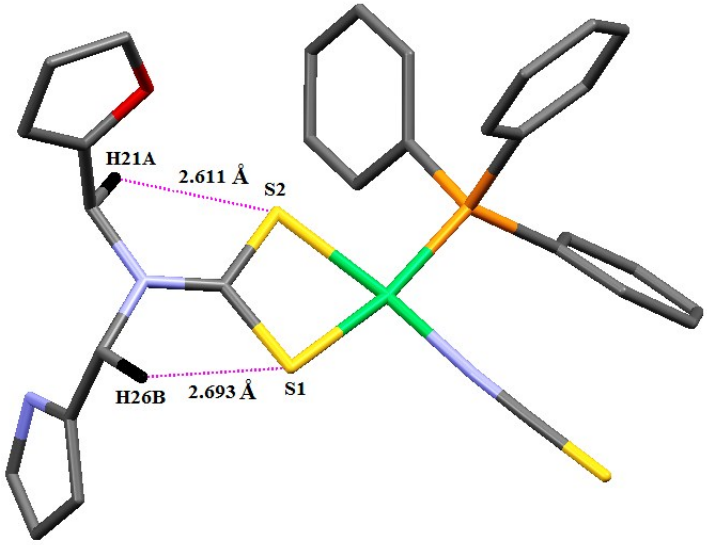

Fig. S2 Intramolecular S···H–C interactions (2.61 and 2.69 Å) in complex **5**.

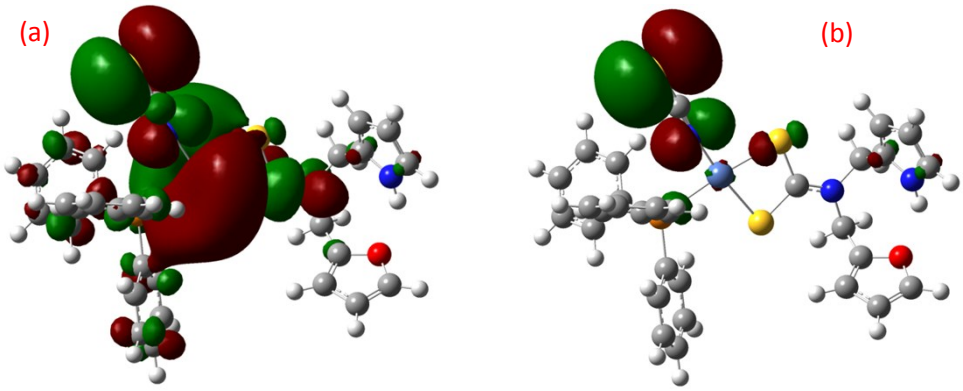

Fig. S3 HOMO and **LUMO** plots of complex **5**

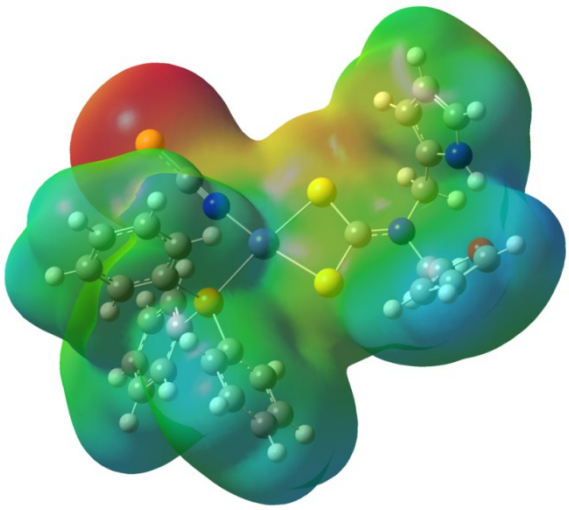

Fig. S4 MEP plot of complex **5**

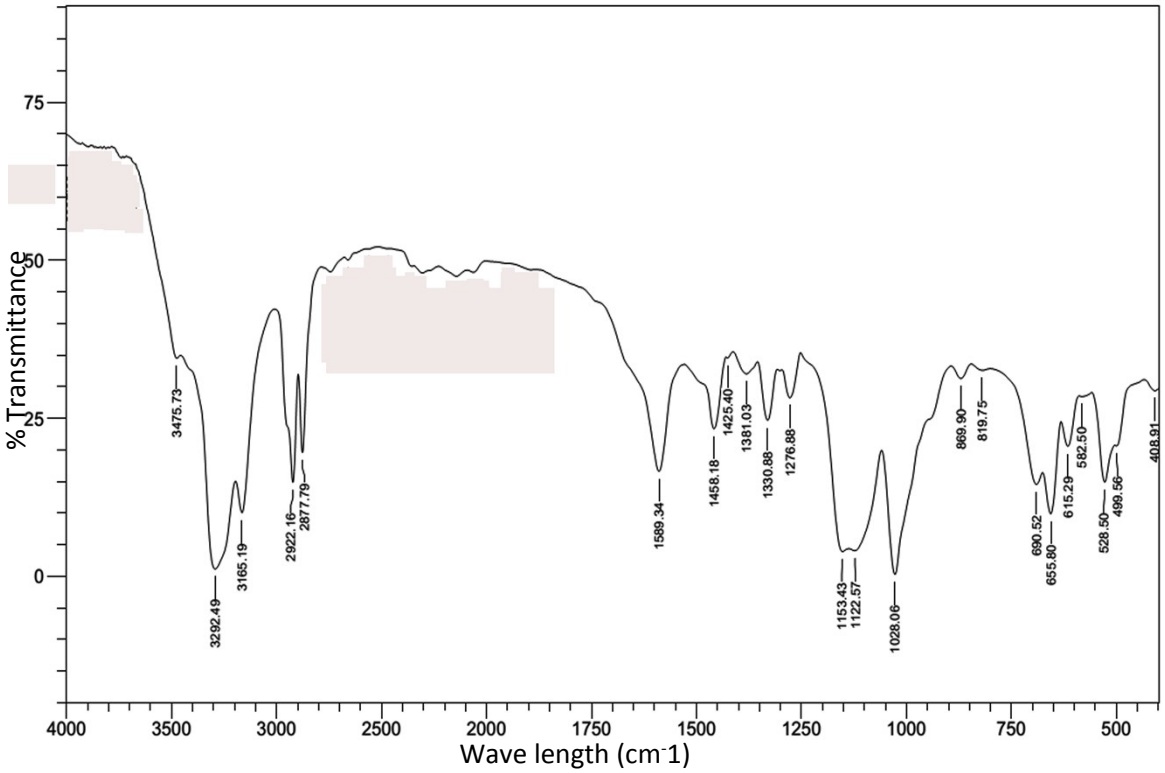

Fig. S5 FT-IR spectrum of the as-synthesized Nickel sulfide NPs