Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2020

New main group ferrocenyldithiocarbamates and conversion to ferrocene oxazolidine-2-thione and -2-one

Reena Yadav,^a Suryabhan Singh,^b Manoj Trivedi,^c Gabriele Kociok-Köhn,^d Nigam P. Rath,^e Randolf D. Köhn,^{f*} Mohd. Muddassir,^g and Abhinav Kumar^{a*}

^{a.} Department of Chemistry, University of Lucknow, Lucknow 226 007, India. Email: <u>abhinavmarshal@gmail.com</u>

- b. Department of Chemistry, Guru GhasidasVishwadiyalaya, Bilaspur India
 - c. Department of Chemistry, University of Delhi, Delhi 110 007, India.
- d. Material and Chemical Characterisation Facility (MC²), University of Bath, Bath BA2 7AY, UK
- e. Department of Chemistry & Biochemistry and Centre for Nanoscience, University of Missouri-St. Louis, One University Boulevard, St. Louis, MO 63121-4499, USA
 - ^{f.} Department of Chemistry, University of Bath, Bath BA2 7AY, UK Email:

chsrdk@bath.ac.uk

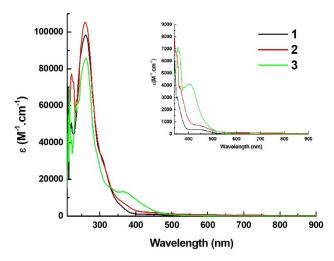


Fig. S1 Electronic absorption spectra for the complexes recorded in 10-5 M dichloromethane solution (inset: spectra recorded in 10⁻³ M solution).

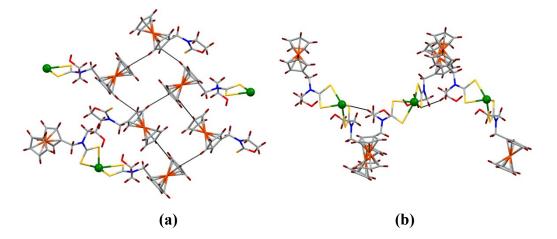


Fig. S2 (a) 2D sheet along b-axis due to CH... π and (b) 1D chain due to CH₂...S interactions in 1.

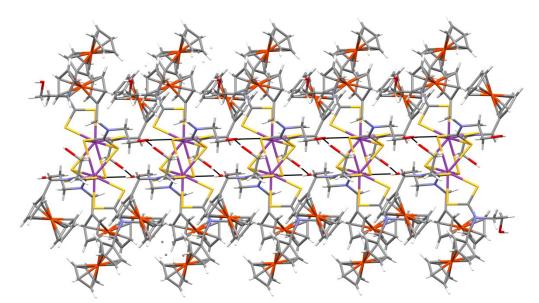


Figure S3. One dimensional chain formed due to intermolecular O-H…S interactions in 3.

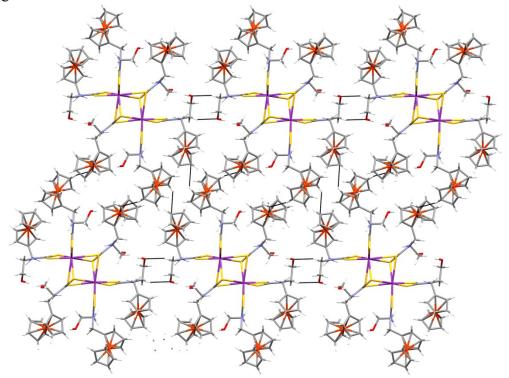


Figure S4 A 2D sheet formed due to $CH \cdots \pi$ and $CH_2 \cdots O$ (OH group, 2.496 Å) interactions in **3**.

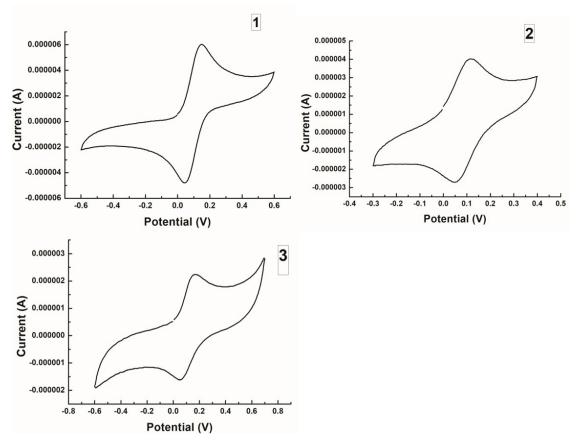


Fig. S5 The cyclic voltammograms for the complexes 1-3.

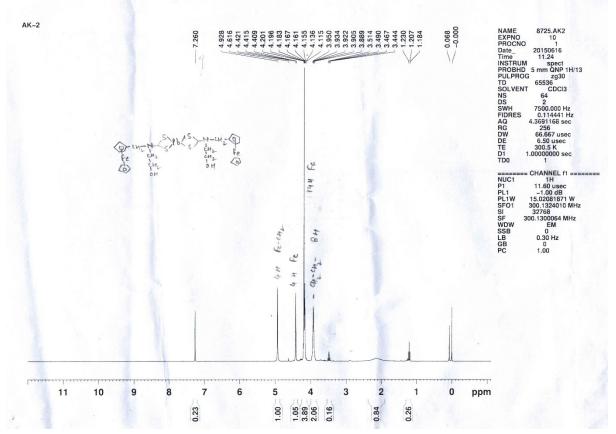


Fig. S6 ¹H NMR spectra for 1.

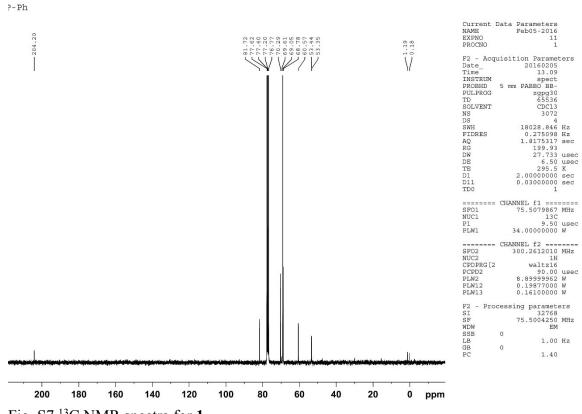


Fig. S7 ¹³C NMR spectra for **1**.

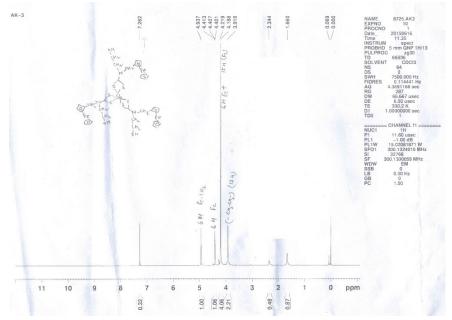


Fig. S8 ¹H NMR spectra for **2**.

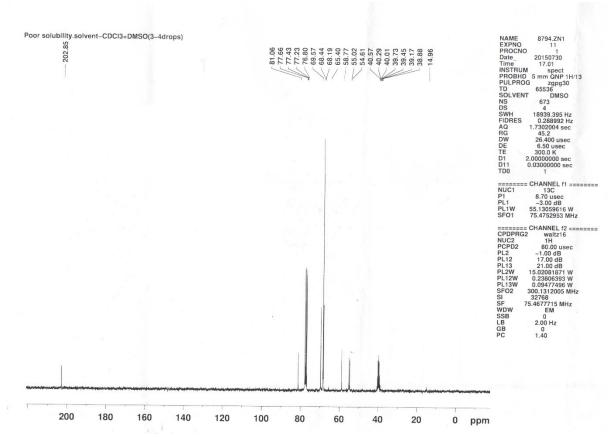


Fig. S9 ¹³C NMR spectra for 2.

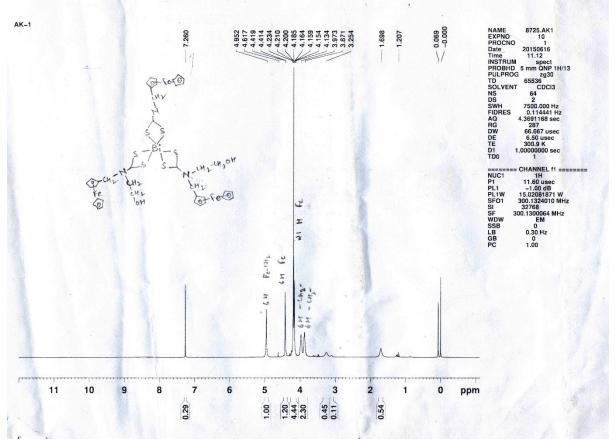


Fig. S10 ¹H NMR spectra for **3**.

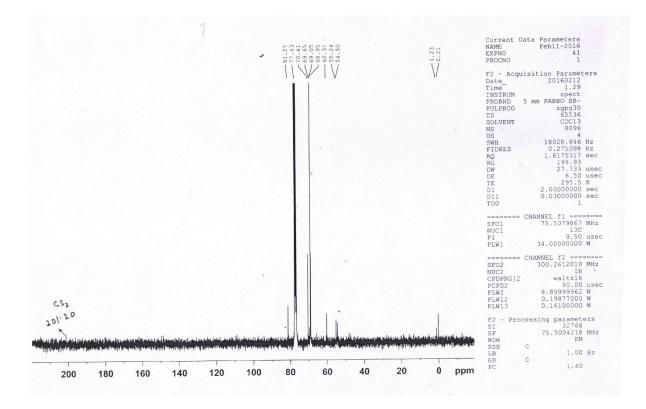


Fig. S11 ¹³C NMR spectra for **3**.

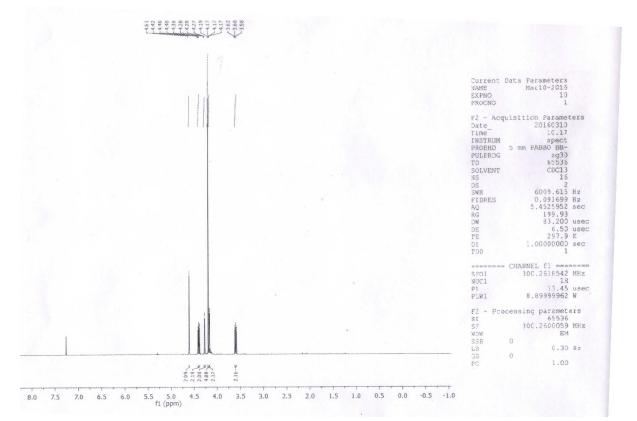


Fig. S12 ¹H NMR spectra for 4.

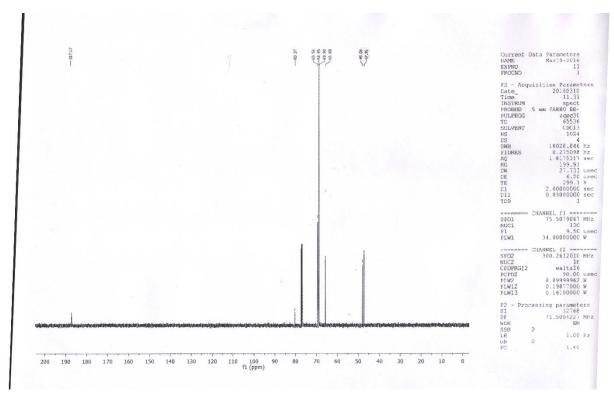


Fig. S13 ¹³C NMR spectra for 4.

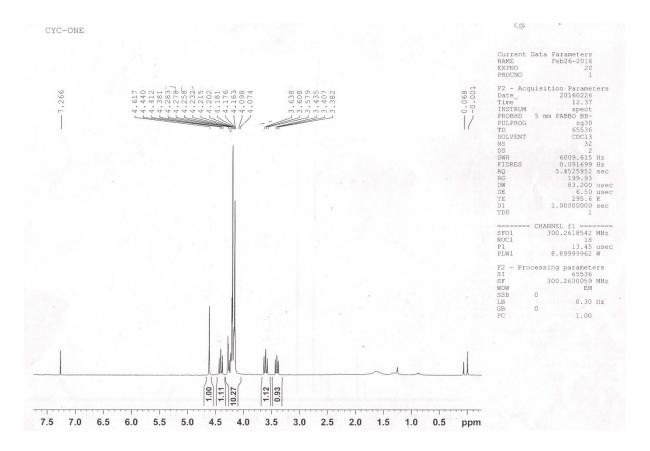


Fig. S14 ¹H NMR spectra for **5**.

