Supporting Information

Synthesis of Pyrite Thin Films and Transition Metal Doped Pyrite Thin Films by Aerosol-Assisted Chemical Vapour Depositionfrom Single-Source Precursors

Sadia Khalid,[a,b,c]EjazAhmed,[a] M. Azad Malik,[c]David J. Lewis,[c,d]Shahzad Abu Bakar,[b]YaqoobKhan,[b] and Paul O'Brien[c,d]*

[a]Department of Physics, BahauddinZakariya University, Multan 60800, Pakistan.
[b] Nanoscience and Catalysis Division, National Centre for Physics, Quaid-i-Azam University Campus, 45320- Islamabad, Pakistan
[c]School of Chemistry, The University of Manchester, Oxford Road, Manchester, M13 9PL, U.K..
[d]School of Chemistry, The University of Manchester, Oxford Road, Manchester, M13 9PL, U.K..

Corresponding Author
Professor Paul O'Brien FRS.
Email: paul.o'brien@manchester.ac.uk.

Tel: +44 161 275 4653.
Fax: +44 161 275 4616.

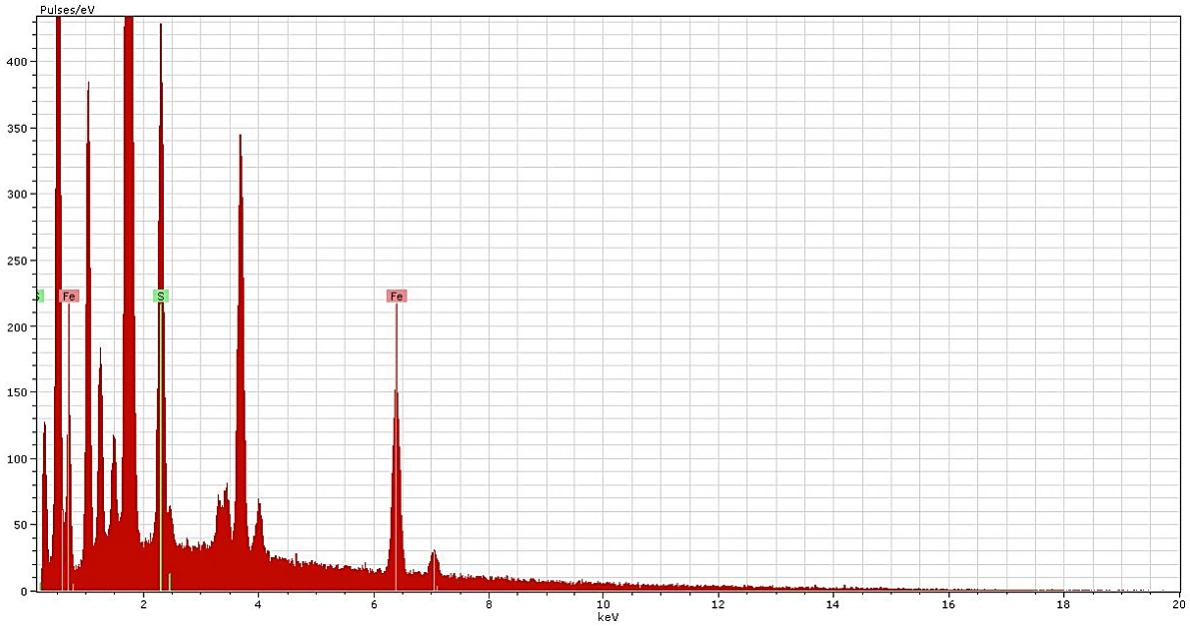

Figure S1. EDX spectra of pyrite (FeS_2) thin films deposited from complex [$Fe(S_2CNEt_2)_3$] (1) on glass substrate by AACVD at 350 °C.

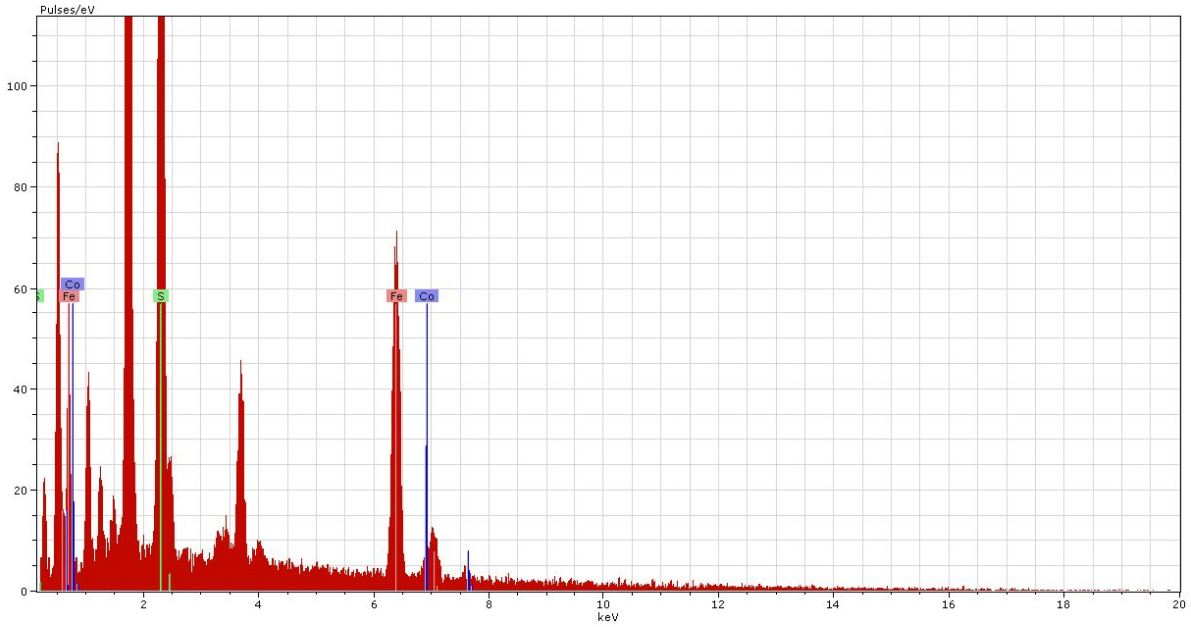

Figure S2. EDX spectra of cobalt doped pyrite ($Co_xFe_{1-x}S_2$) thin films deposited from complexes [$Fe(S_2CNEt_2)_3$] (1) and [$Co(S_2CNEt_2)_3$] (2) on glass substrate by AACVD at 350 °C.

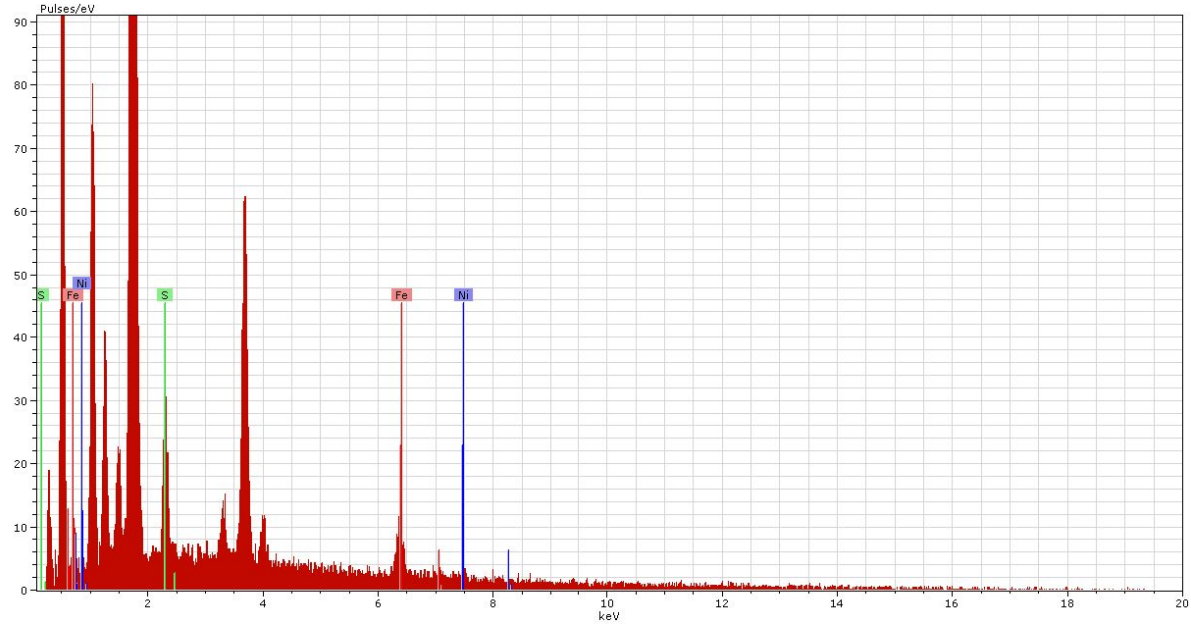

Figure S3.EDX spectrum of nickel doped pyrite ($Ni_xFe_{1-x}S_2$) thin films deposited from complexes [$Fe(S_2CNEt_2)_3$] (1) and [$Ni(S_2CNEt_2)_2$] (3) on glass substrate by AACVD at 350 °C.

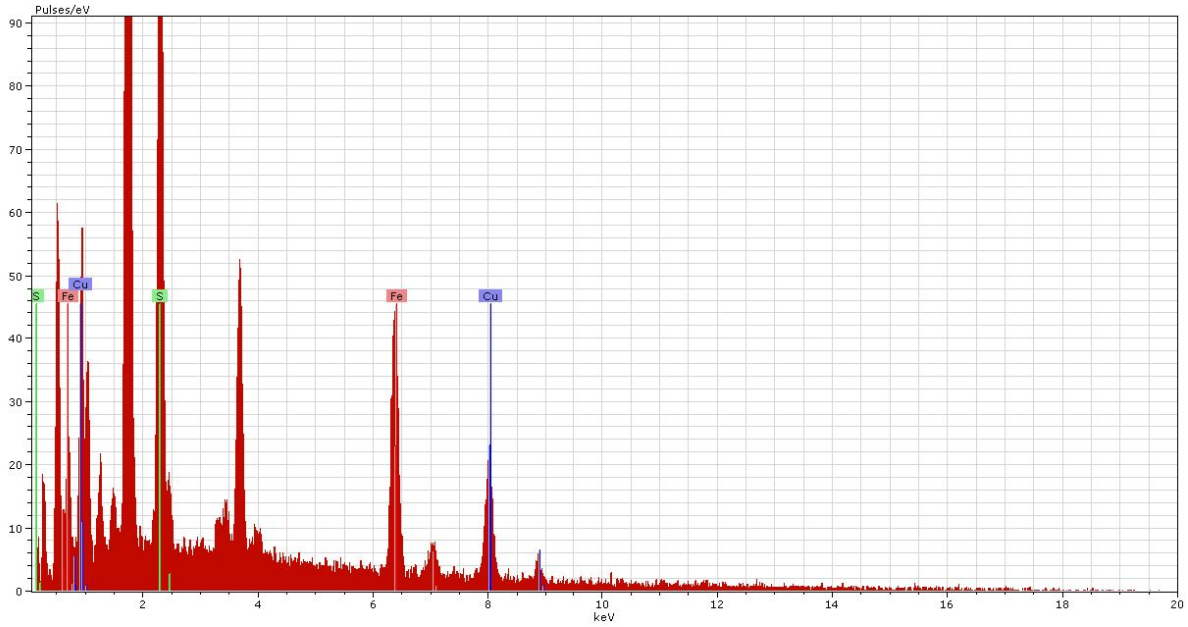

Figure S4.EDX spectra of copper doped pyrite ($Cu_xFe_{1-x}S_2$) thin films deposited from complexes [$Fe(S_2CNEt_2)_3$] (1) and [$Cu(S_2CNEt_2)_2$] (4) on glass substrate by AACVD at 350^{o}C.

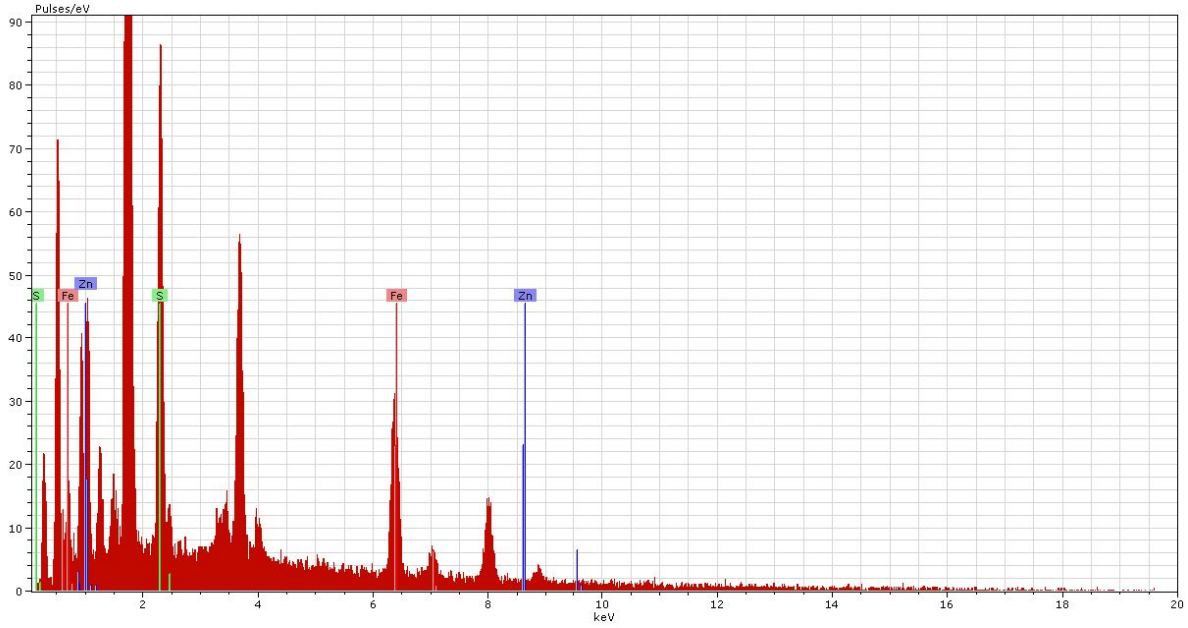

Figure S5.EDX spectra of zinc doped pyrite ($Zn_xFe_{1-x}S_2$) thin films deposited from complex [$Fe(S_2CNEt_2)_3$](1) [$Zn(S_2CNEt_2)_2$] (5) on glass substrate by AACVD at 350 ^{o}C.

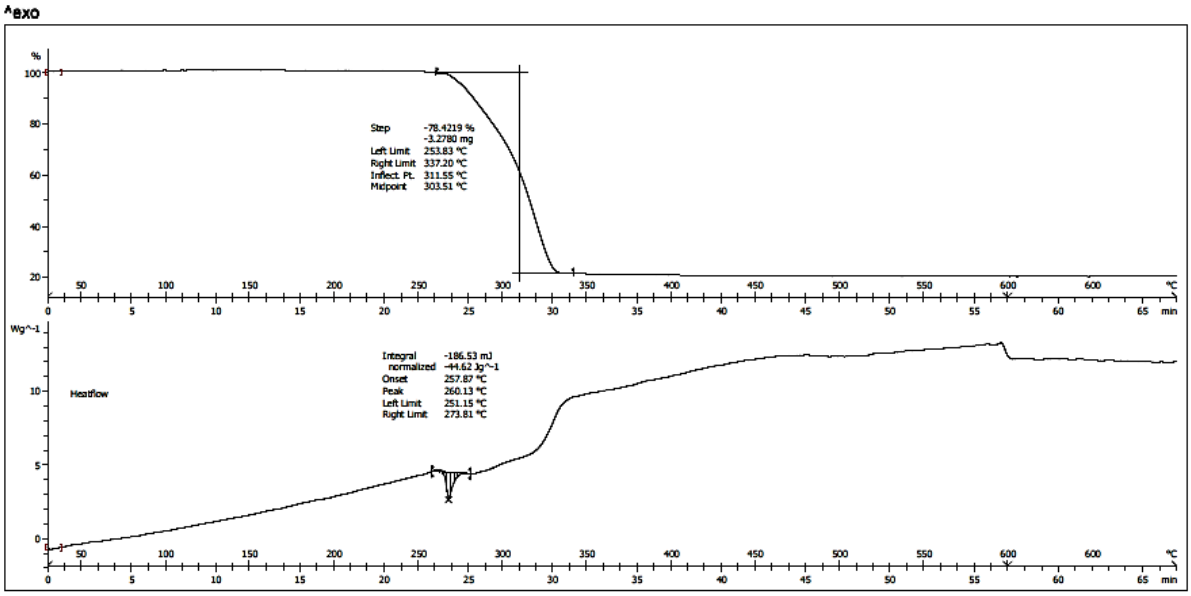

Figure S6. TGA/DSC curve of complex [$Fe(S_2CNEt_2)_3$] (1).

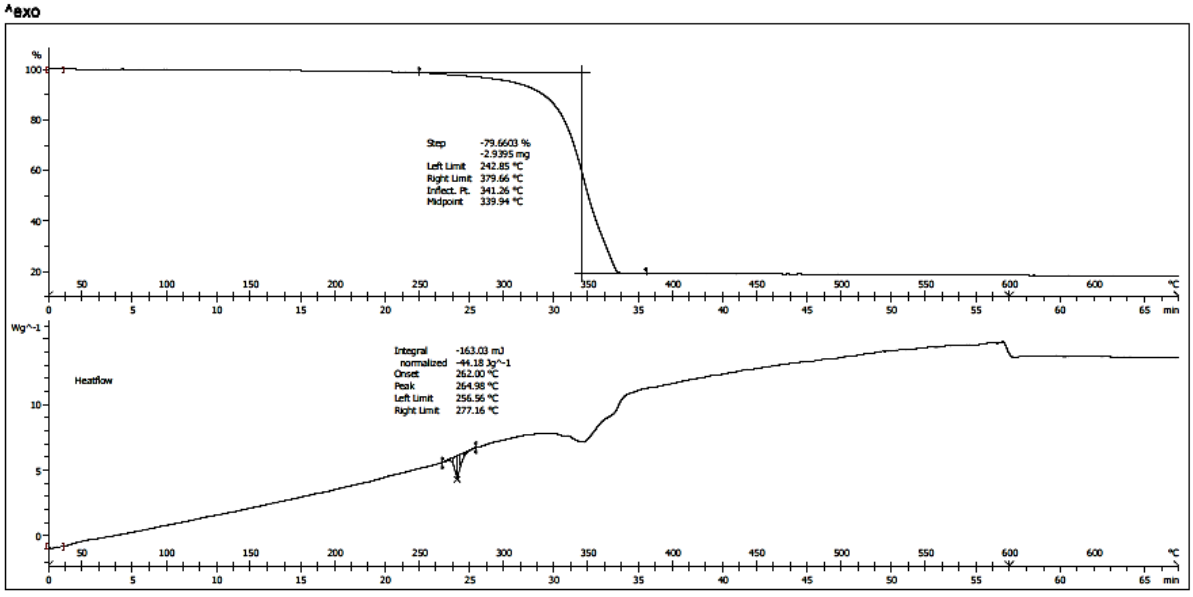

Figure S7. TGA/DSC curve of complex [$Co(S_2CNEt_2)_3$] (2).

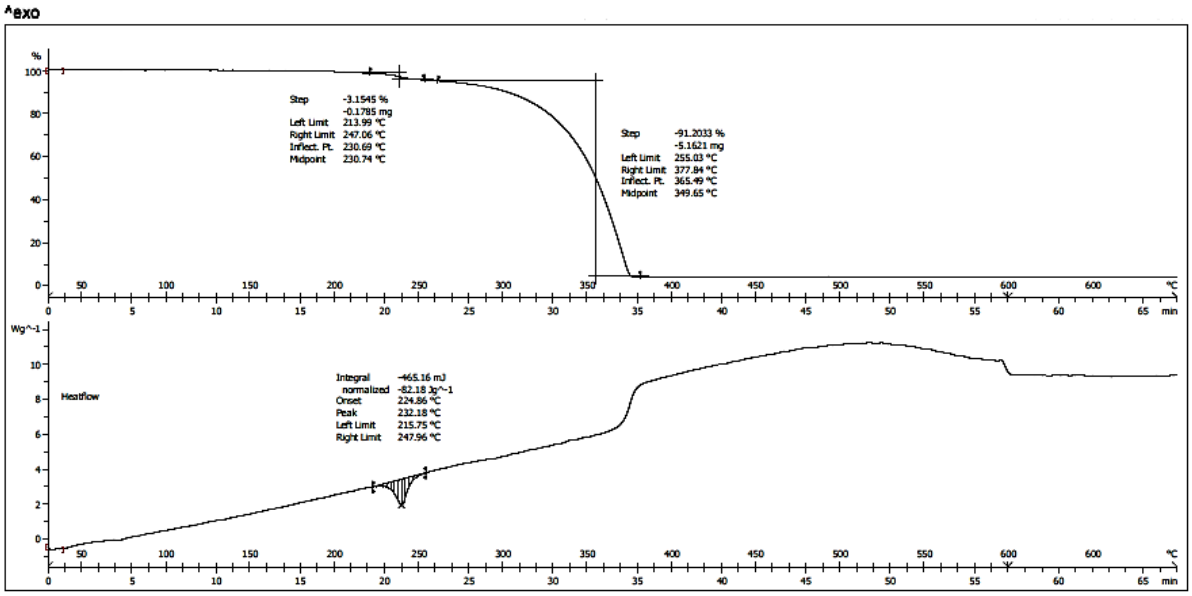

Figure S8. TGA/DSC curve of complex [Ni(S_2CNEt_2)$_2$] (3).

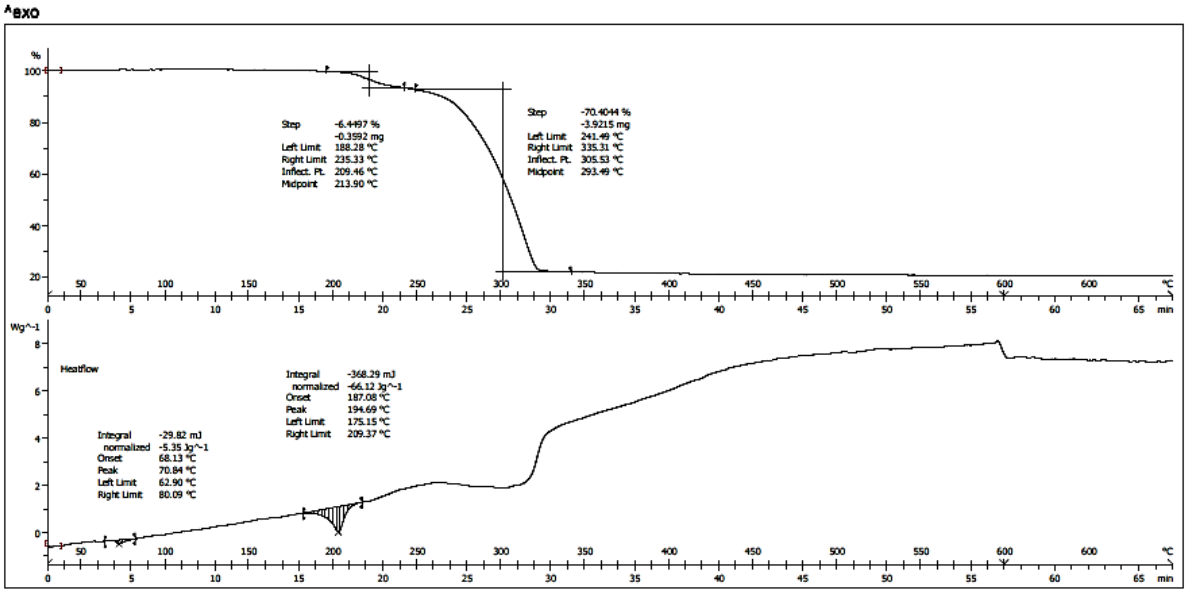

Figure S9. TGA/DSC curve of complex [Cu(S_2CNEt_2)$_2$] (4).

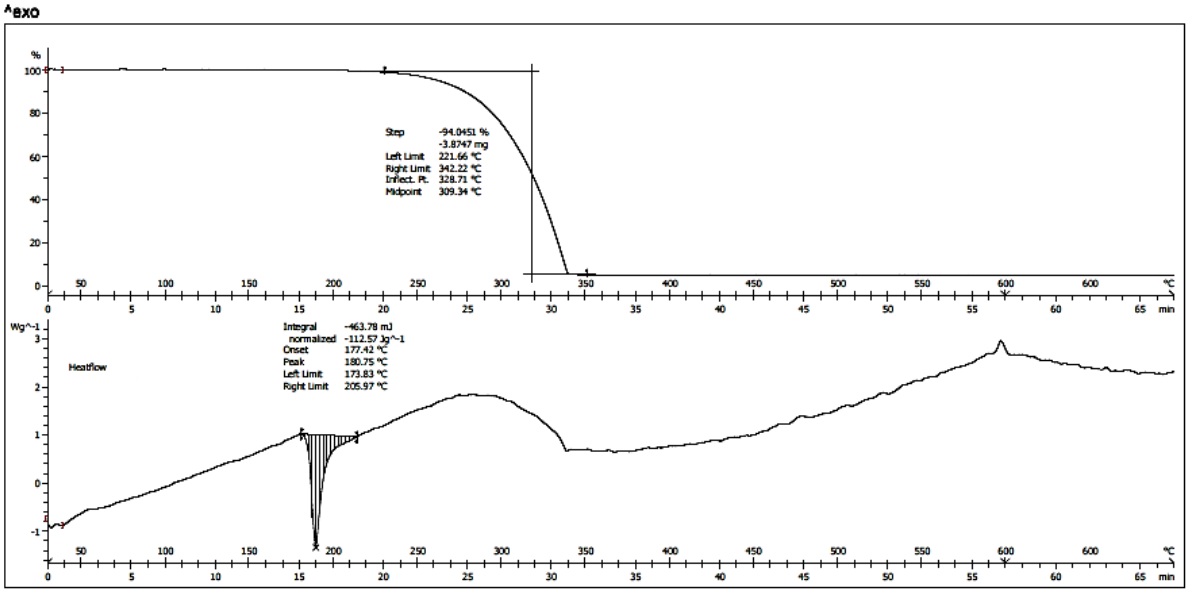

Figure S10. TGA/DSC curve of complex $[Zn(S_2CNEt_2)_2]$ (5).

FTIR

The IR spectra of dithiocarbamato complexes consist of three basic regions; the first region extents from 1450 to 1550 cm^{-1} and account for the thioureide (NCSS) band whose position typically lies in between C-N and C=N band. The position of this sharp and strong band is indicative of an important mark of double bond character shown by a number of resonating states. The absorption band at 1500 cm^{-1} is attributed as arising from polar structure —NCS_2.The second region (1070-930 cm^{-1}) is descriptive of coordination mode of dithiocarbamato moiety (CSS)[i]. The third region around 350-400 cm^{-1} is attributed to M-S bonds.

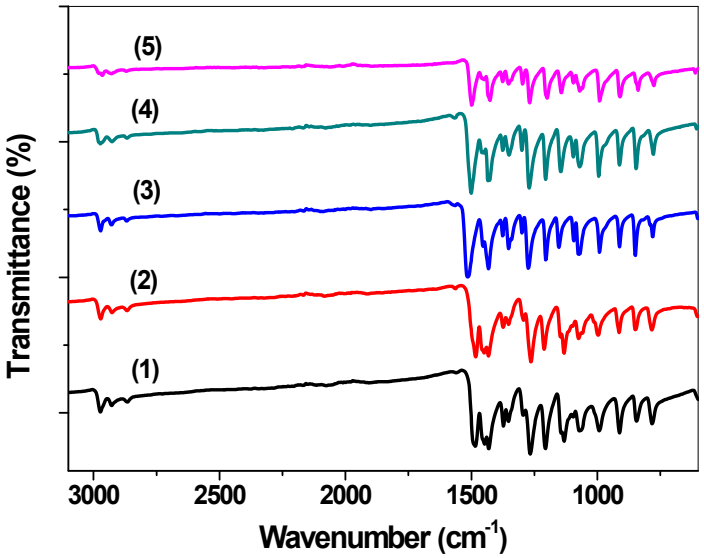

Figure S11. FTIR spectra of transition metals complexes$[Fe(S_2CNEt_2)_3]$ (1), $[Co(S_2CNEt_2)_3]$ (2), $[Ni(S_2CNEt_2)_2]$ (3), $[Cu(S_2CNEt_2)_2]$ (4) and $[Zn(S_2CNEt_2)_2]$ (5).

[i] D.C. Bradley, M.H. Gitlitz, Journal of Chemical Society A (1969) 1152.