Supplementary Material (ESI) for New Journal of Chemistry

Assembling Coordination Networks of Bis-amido Pyridines *via* Hydrogen Bonds: Isostructurality and Large Hydrophobic Cavities for Guest Inclusion

Lalit Rajput and Kumar Biradha*

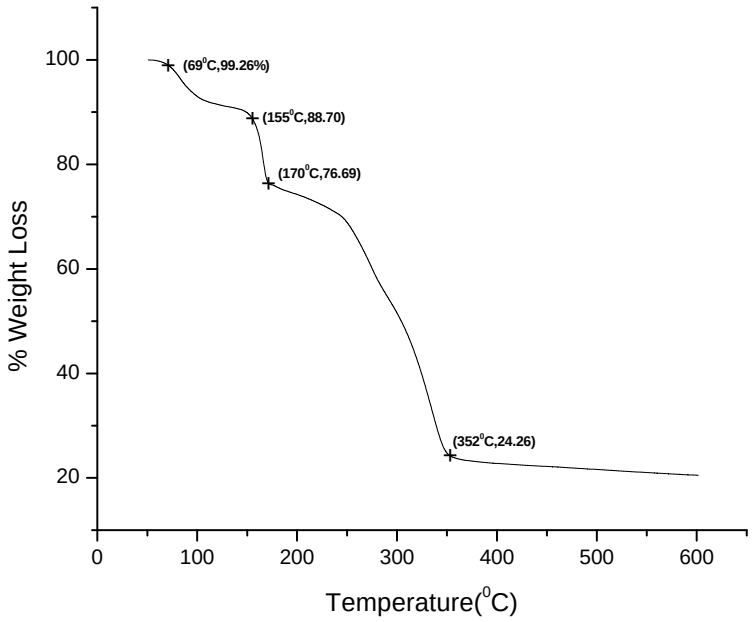
Department of Chemistry, Indian Institute of Technology, Kharagpur-721302, India

Fax:+91-3222-282252; Tel: +91-3222-283346;

E-mail: kbiradha@chem.iitkgp.ernet.in

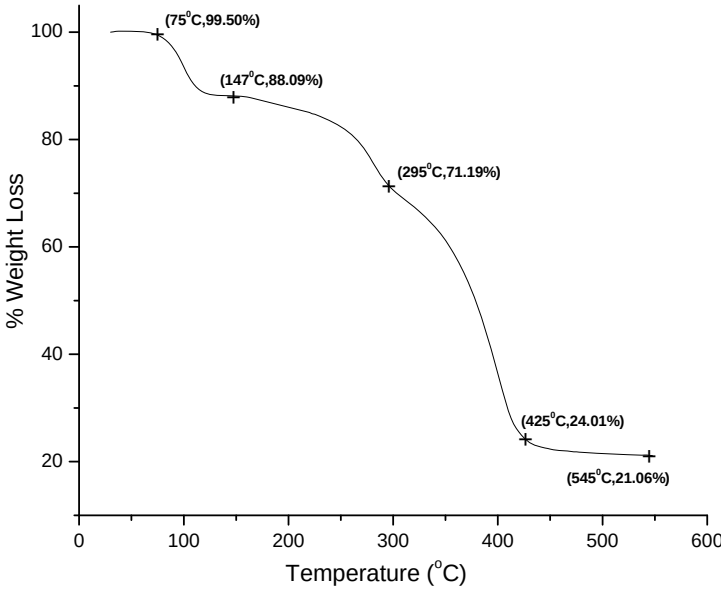
TGA:

{Cu (**2b**)$(SCN)_2(DMF)_2$} (**5**)



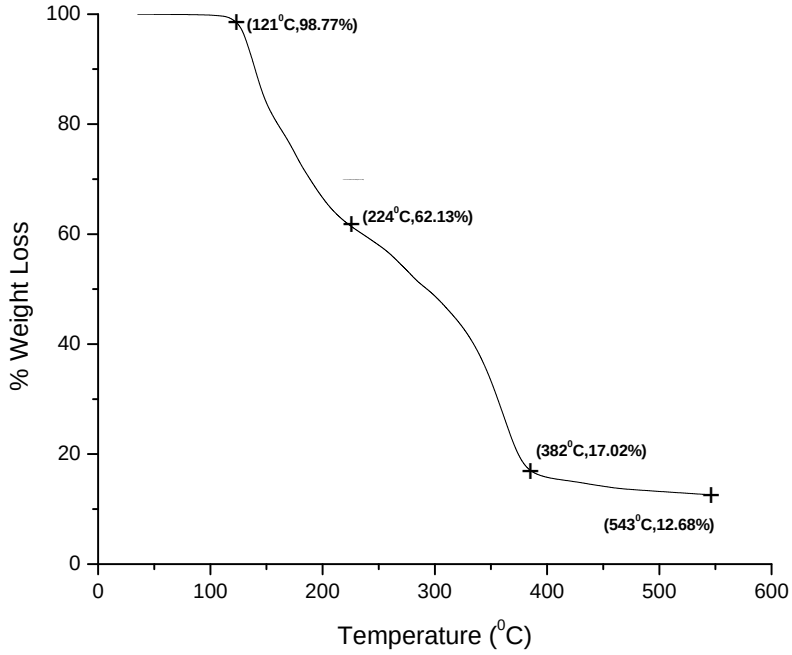
At 155˚C 11.30% weight loss corresponds to the loss of first DMF molecule (Cal: 11.70%), from 155˚C to 170˚C 12.01% weight loss corresponds to the loss of second DMF molecule (Cal: 11.70%) and from 170˚C onwards ligand degradation takes place.

{[Cu (**1c**)$(SCN)_2(H_2O)_2$]·2(H_2O)} (**6**)



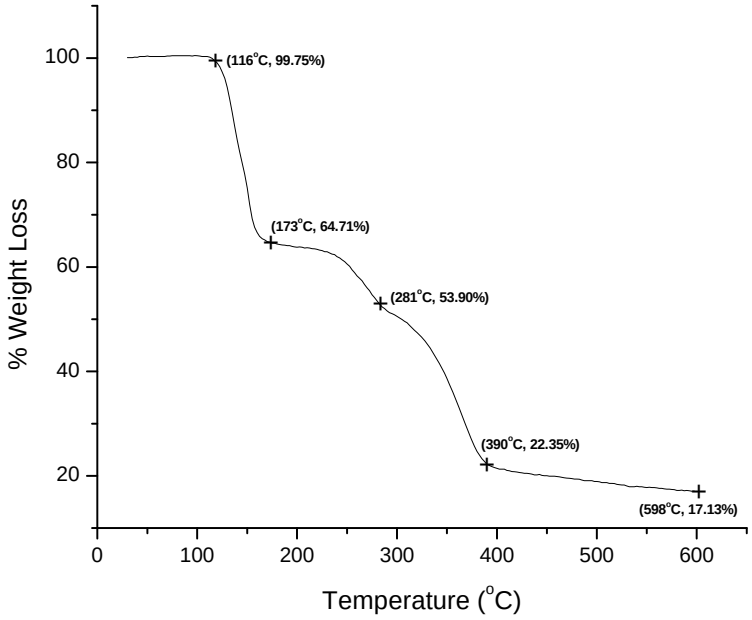
At 147˚C 11.91% weight loss corresponds to the loss of two free & two coordinated water molecules i.e. total four waters molecules (Cal: 12.44%).

{[Cu (**2d**)$(SCN)_2(DMF)_2$] **(**anthracene)} (**9**)



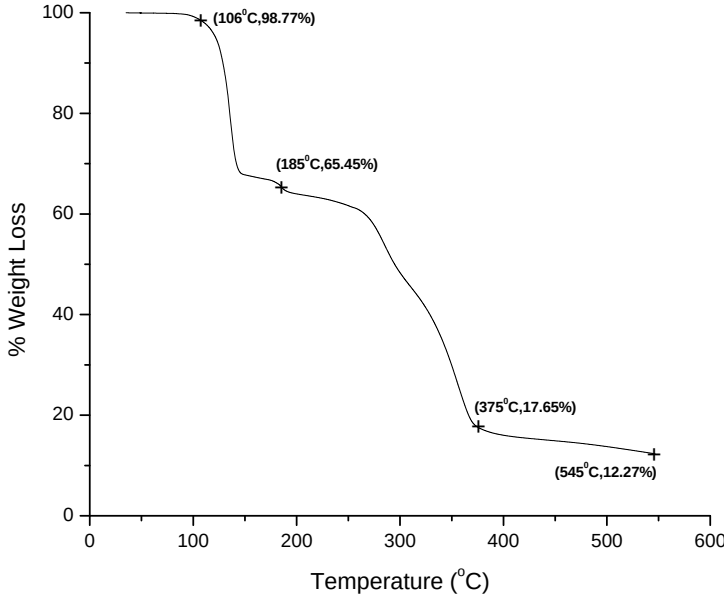
At 224˚C 36.64% weight loss corresponds to the loss of one anthracene molecules and two DMF molecules (Cal: 36.01%) and from 224˚C onwards ligand degradation takes place.

{[Cu(**2d**)$(SCN)_2(DMF)_2$]**·(**biphenyl)} (**10**)



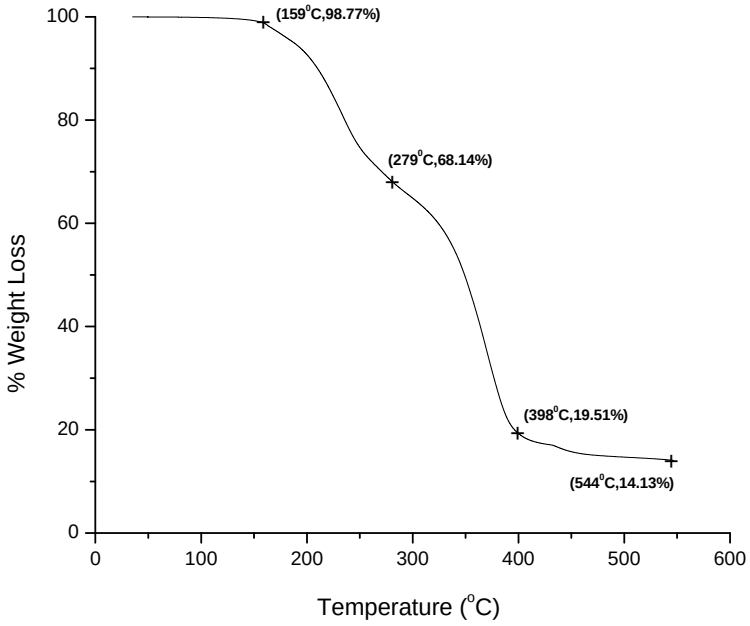
At 173˚C 35.29% weight loss corresponds to the loss of one biphenyl molecules and two DMF molecules (Cal: 36.01%) and from 173˚C onwards ligand degradation takes place.

{[Cu(**1b**)$(SCN)_2$]·2(nitrobenzene)} (**13**)



At 185˚C 34.55% weight loss corresponds to the loss of two nitrobenzene molecules (Cal: 34.00%), and from 185˚C onwards ligand degradation takes place.

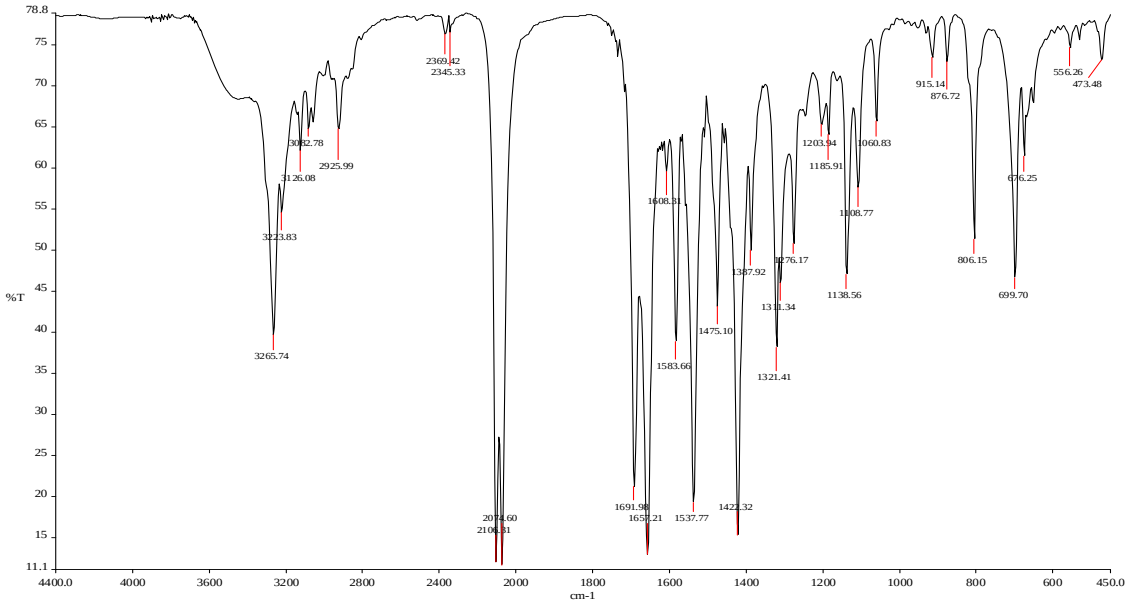
{[Cu (**2d**)$_2(SCN)_2$] 2(9-anthraldehyde)} (**16**)



At 279˚C 31.86% weight loss corresponds to the loss of two 9-anthraldehyde molecules (Cal: 31.70%) and from 279˚C onwards ligand degradation takes place.

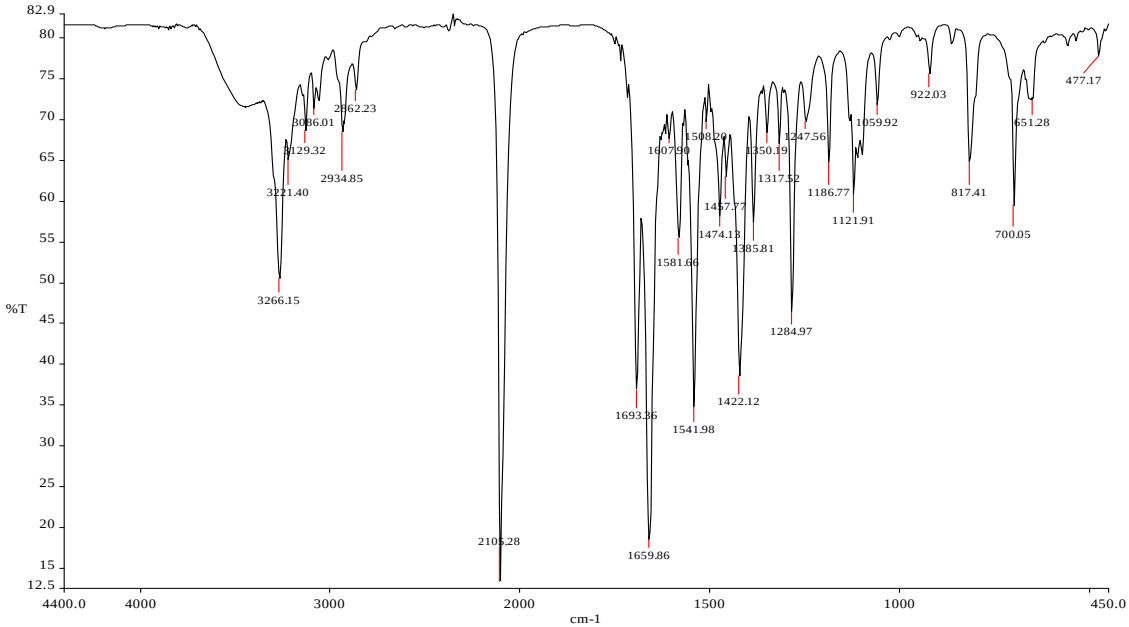
IR:

{Cu(**2a**)$(SCN)_2(DMF)_2$} (**3**) & {[Cu(**2a**)$(SCN)_2(DMF)_2$]·2(DMF)} (**4**)



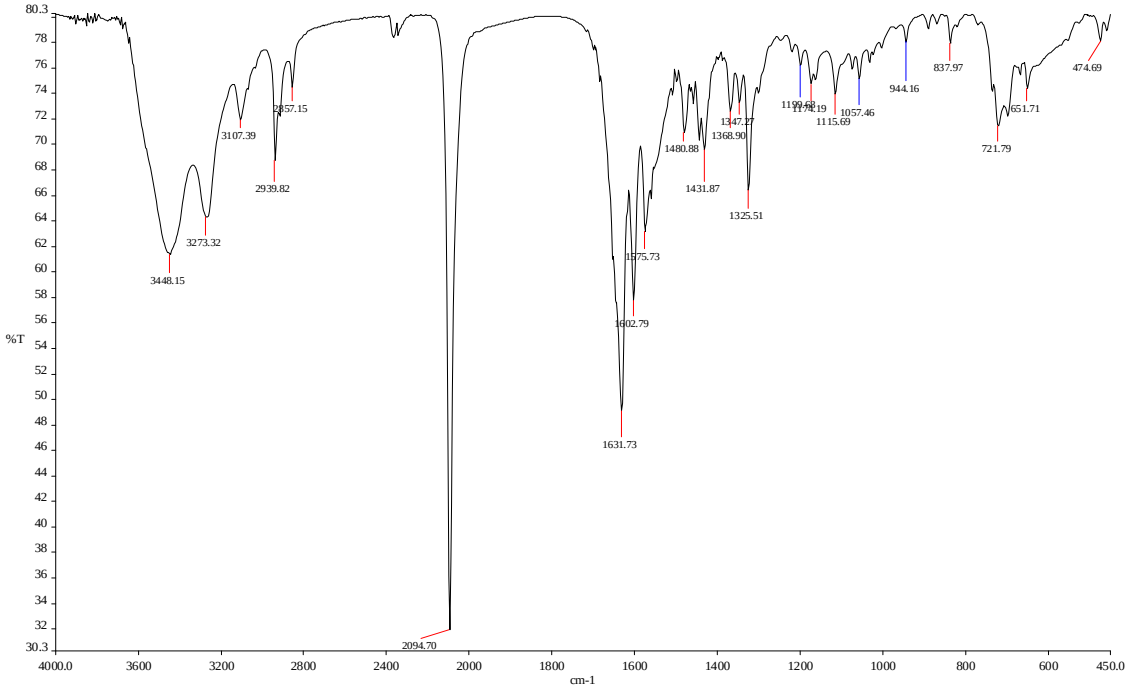
The N-H stretch; 3265 cm^{-1}; CN vibrational stretch of the thiocyanate, 2074 cm^{-1} & 2106 cm^{-1}; amide C=O stretch (amide-I band), 1657 cm^{-1}; N-H bending (amide-II band), 1537 cm^{-1}.

{Cu(**2b**)$(SCN)_2(DMF)_2$} (**5**)



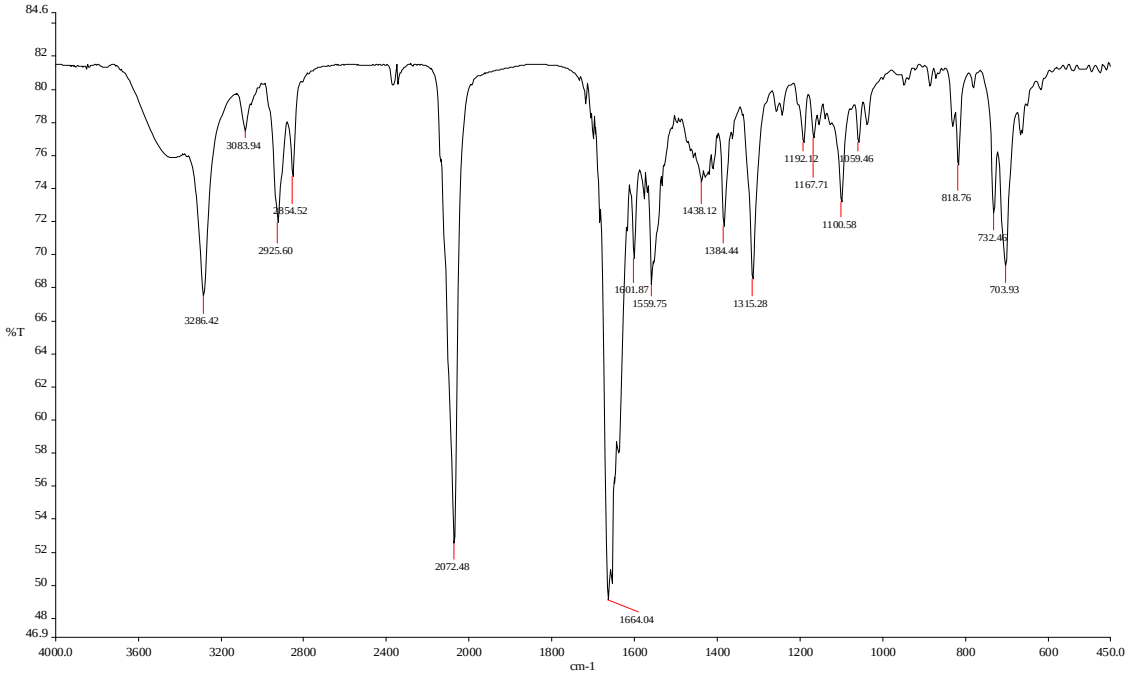
The N-H stretch; 3266 cm^{-1}; CN vibrational stretch of the thiocyanate, 2105 cm^{-1}; amide C=O stretch (amide-I band), 1659 cm^{-1}; N-H bending (amide-II band), 1541 cm^{-1}.

{[Cu(**1c**)$(SCN)_2(H_2O)_2$]·$2(H_2O)$} (**6**)



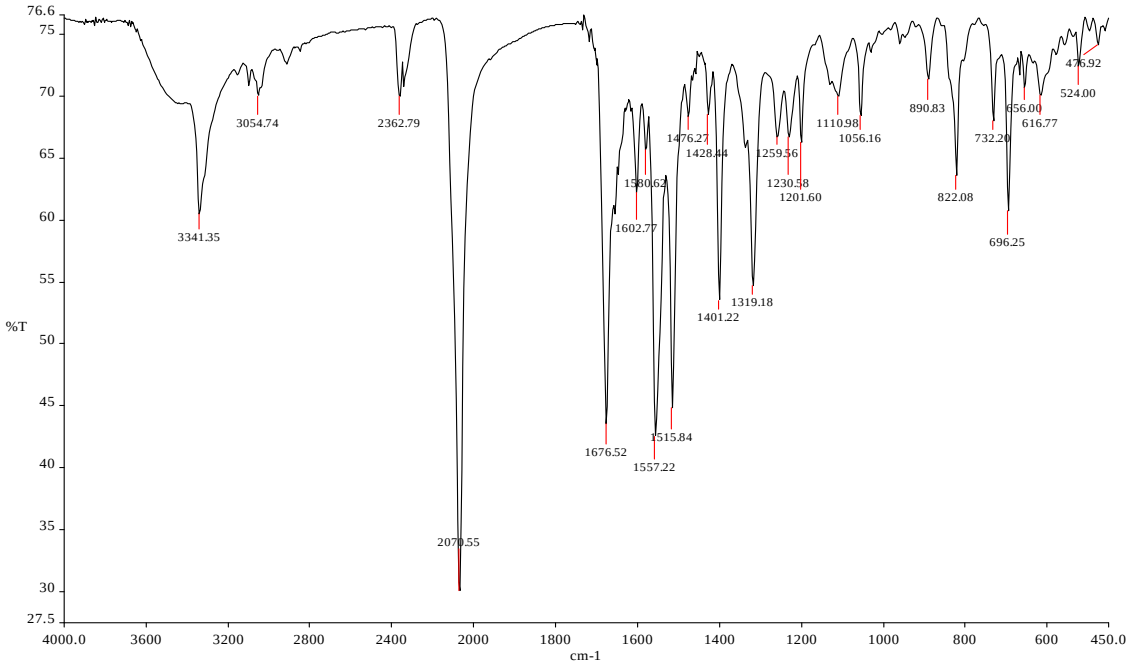
The N-H stretch; 3273 cm^{-1}; CN vibrational stretch of the thiocyanate, 2094 cm^{-1}; amide C=O stretch (amide-I band), 1631 cm^{-1}; N-H bending (amide-II band), 1575 cm^{-1}.

{[Cu(**1d**)$(SCN)_2(DMF)_2$]·$2(H_2O)$} (**7**)



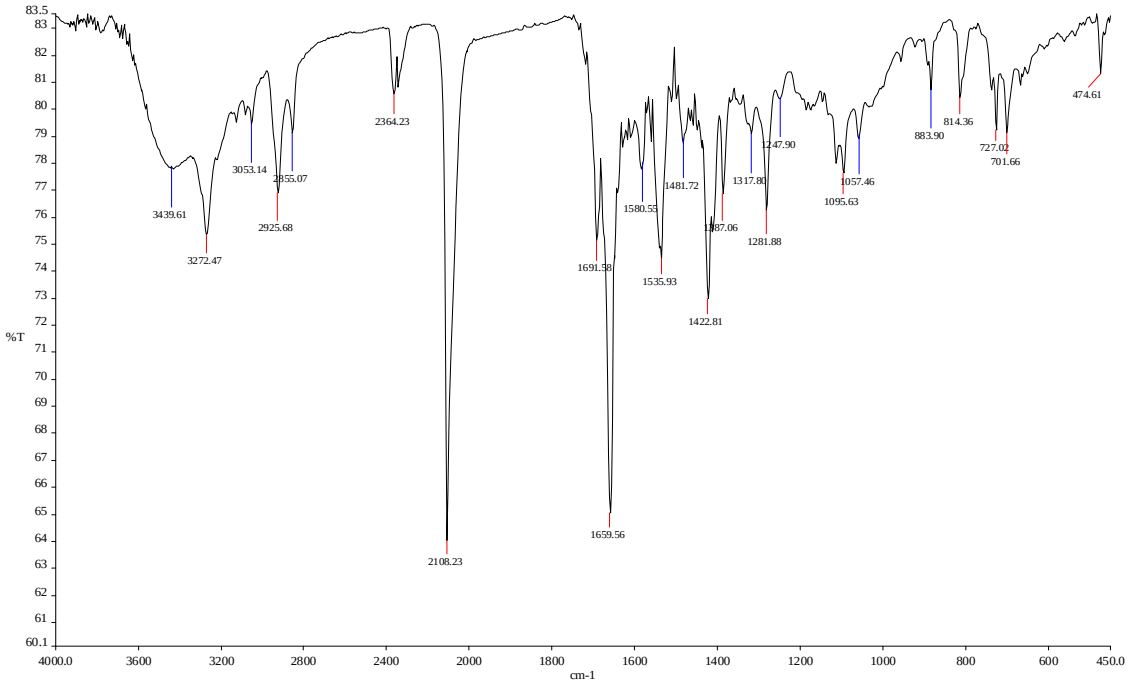
The N-H stretch; 3286 cm^{-1}; CN vibrational stretch of the thiocyanate, 2072 cm^{-1}; amide C=O stretch (amide-I band), 1664 cm^{-1}; N-H bending (amide-II band), 1559 cm^{-1}.

{[Cu(**1e**) $(SCN)_2(DMF)_2$] **2(**DMF)}$_n$ (**8**)



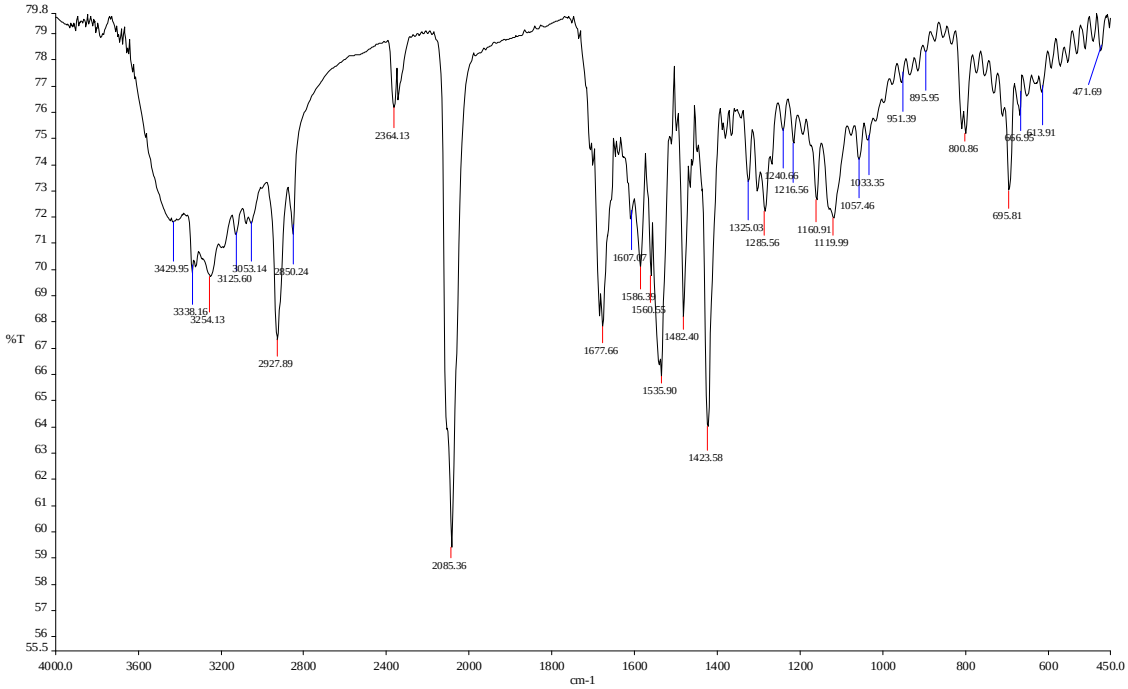
The N-H stretch; 3341 cm^{-1}; CN vibrational stretch of the thiocyanate, 2070 cm^{-1}; amide C=O stretch (amide-I band), 1676 cm^{-1}; N-H bending (amide-II band), 1557 cm^{-1}.

{[Cu(**2d**)$(SCN)_2(DMF)_2$]**·(**anthracene)} (**9**)



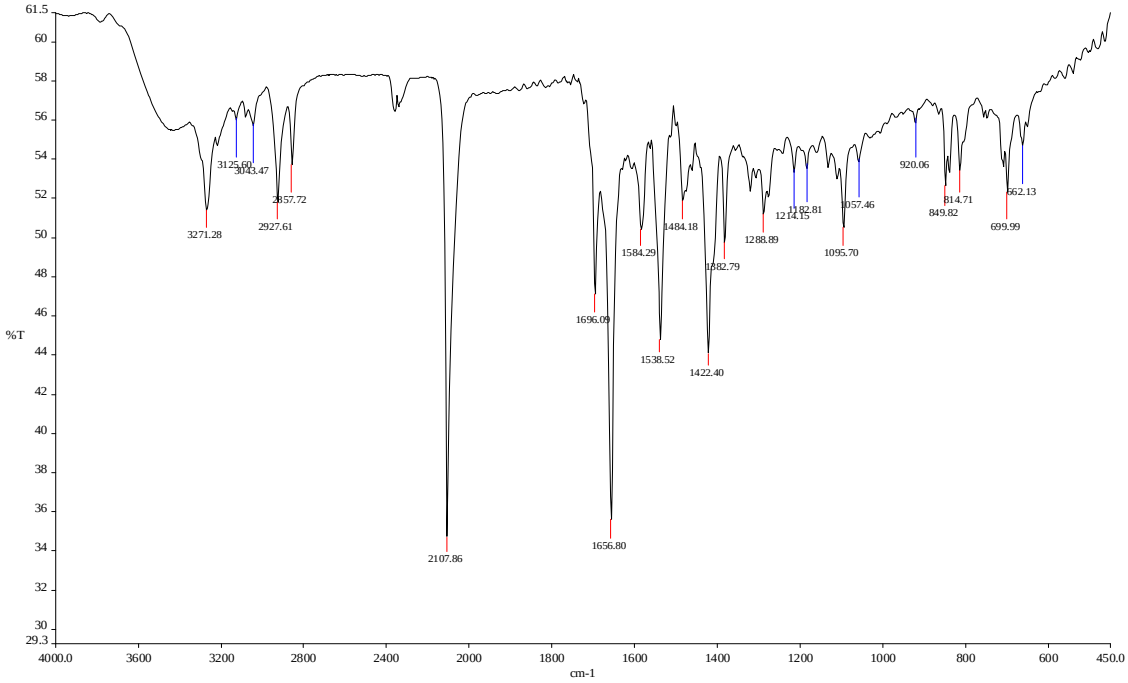
The N-H stretch; 3272 cm^{-1}; CN vibrational stretch of the thiocyanate, 2108 cm^{-1}; amide C=O stretch (amide-I band), 1659 cm^{-1}; N-H bending (amide-II band), 1535 cm^{-1}.

{[Cu(**2d**)$(SCN)_2(DMF)_2$]·**(**biphenyl)} (**10**)



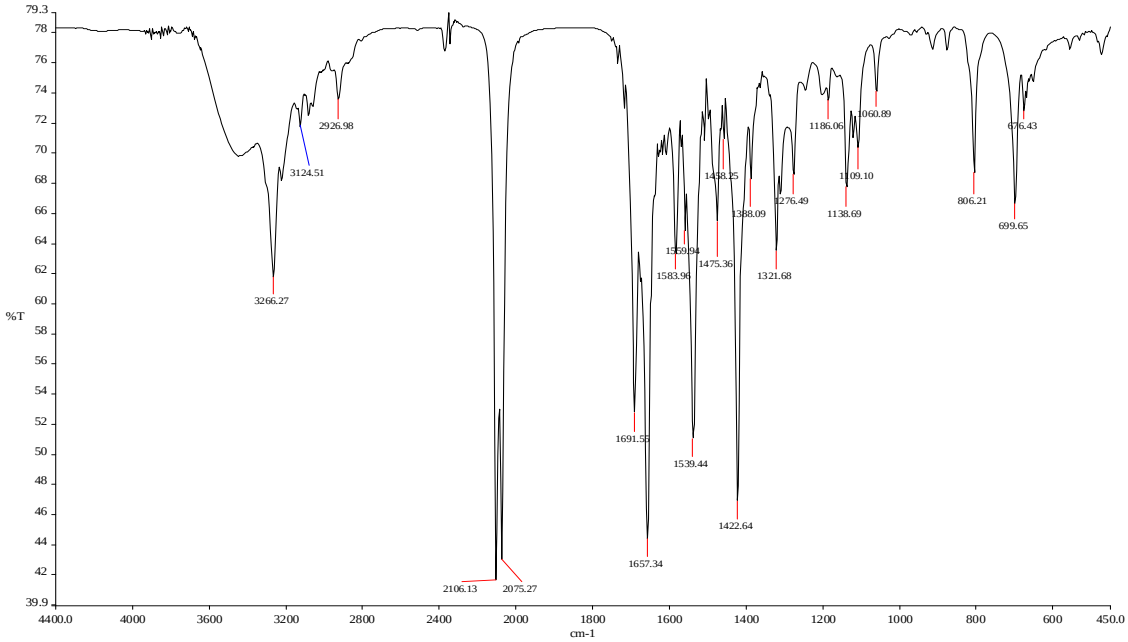
The N-H stretch; 3254 cm^{-1}; CN vibrational stretch of the thiocyanate, 2085 cm^{-1}; amide C=O stretch (amide-I band), 1677 cm^{-1}; N-H bending (amide-II band), 1535 cm^{-1}.

{[Cu(**2d**)$(SCN)_2(DMF)_2$]·**(**pyrene)} (**11**)



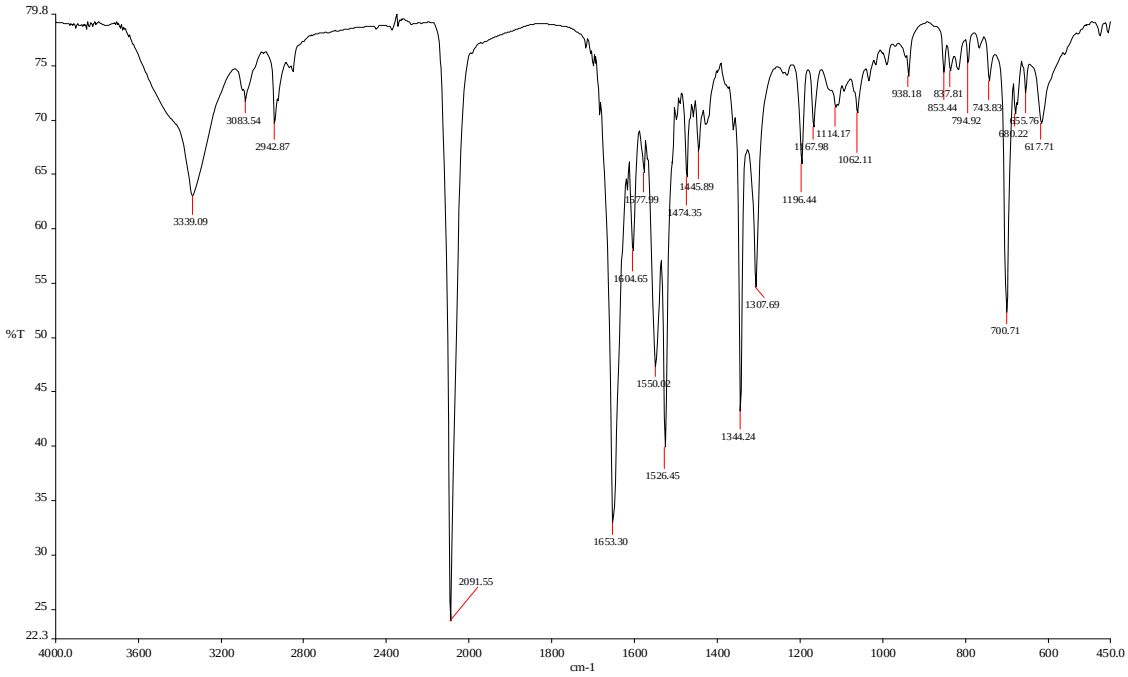
The N-H stretch; 3271 cm^{-1}; CN vibrational stretch of the thiocyanate, 2107 cm^{-1}; amide C=O stretch (amide-I band), 1656 cm^{-1}; N-H bending (amide-II band), 1538 cm^{-1}.

{[Cu(**2a**)$(SCN)_2$]·2(DMF)·(nitrobenzene)}$_n$ (**12**)



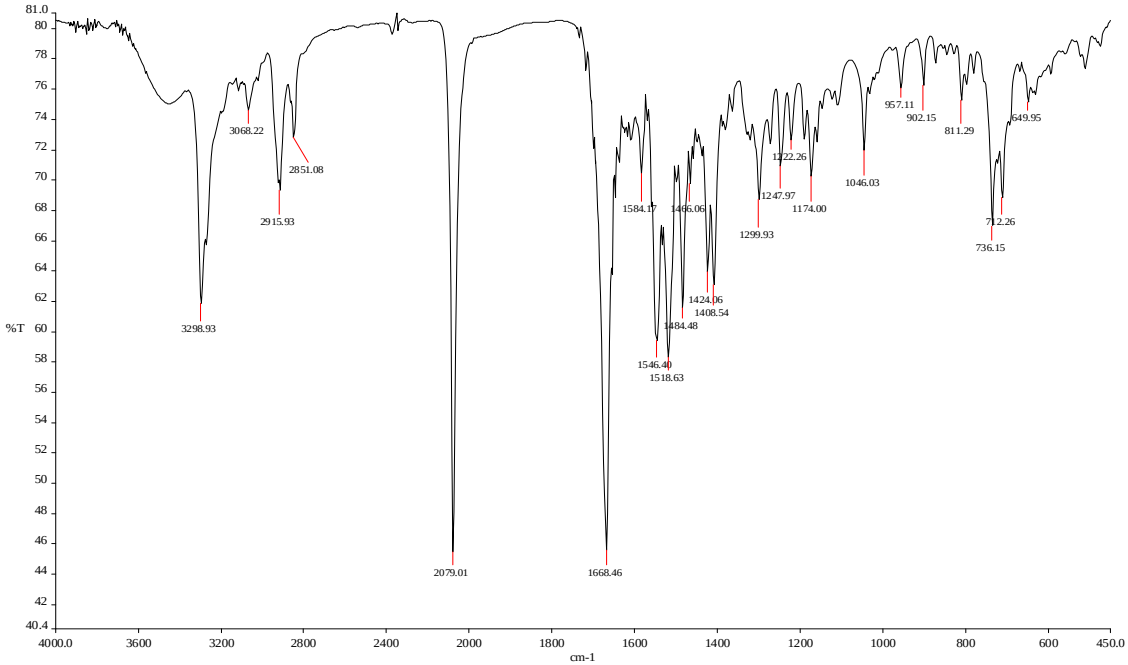
The N-H stretch; 3266 cm^{-1}; CN vibrational stretch of the thiocyanate, 2107 cm^{-1} & 2075 cm^{-1}; amide C=O stretch (amide-I band), 1657 cm^{-1}; N-H bending (amide-II band), 1539 cm^{-1}.

{[Cu(**1b**)$(SCN)_2$]·2(nitrobenzene)} (**13**)



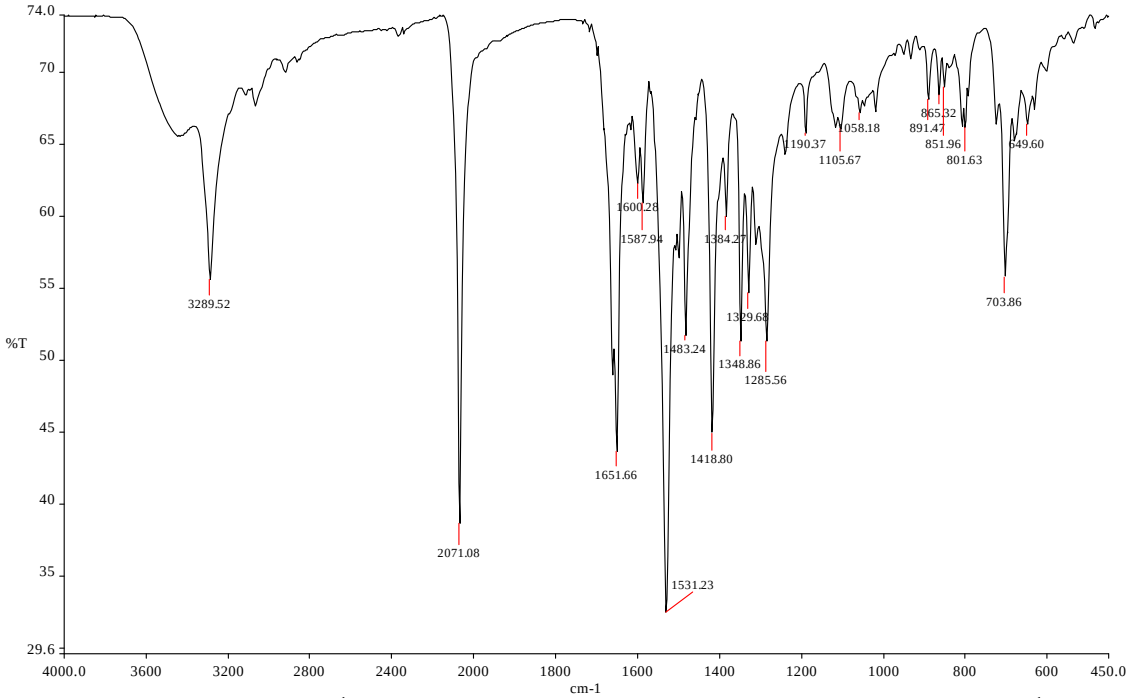
The N-H stretch; 3339 cm^{-1}; CN vibrational stretch of the thiocyanate, 2091 cm^{-1}; amide C=O stretch (amide-I band), 1653 cm^{-1}; N-H bending (amide-II band), 1550 cm^{-1}.

{[Cu(**2d**)$_2$(SCN)$_2$] 2(9-anthraldehyde)} (**16**)



The N-H stretch; 3298 cm^{-1}; CN vibrational stretch of the thiocyanate, 2079 cm^{-1}; amide C=O stretch (amide-I band), 1668 cm^{-1}; N-H bending (amide-II band), 1546 cm^{-1}.

{[Cu(**2e**)$_2$(SCN)$_2$]·2(nitrobenzene)}n, (**18b**)



The N-H stretch; 3289 cm^{-1}; CN vibrational stretch of the thiocyanate, 2071 cm^{-1}; amide C=O stretch (amide-I band), 1651 cm^{-1}; N-H bending (amide-II band), 1531 cm^{-1}.

Discussion on IR spectra

The -NH stretching vibration in all the CPs observed near 3340-3250 cm^{-1} because of the involvement of amide moiety in the hydrogen bond formation. The C=O stretching vibration (amide-I band) of the CPs involving amide to amide recognition shows differences in the stretching frequencies for amide, **1** and reverse amide, **2** CPs. In case of amide CPs where C=O is in conjugation with pyridyl group the stretching frequency is observed in the range of 1645-1630 cm^{-1}. However in reverse amides CPs where C=O is not in conjugation with pyridyl group, the stretching frequency observed in between 1670-1650 cm^{-1}. In the reverse amide CPs where C=O is involved in C-H···O hydrogen bond with pyridyl -CH, the stretching frequency of C=O is observed at 1680-1655 cm^{-1}. The -NH bending (amide-II band) in complexes involving N-H···O or N-H···S hydrogen bond shifted to lower wave number and appears in between 1545-1535 cm^{-1}.