Electronic Supplementary Material (ESI) for CrystEngComm.

Investigation of structure-directing interactions within copper(I) thiocyanate complexes through X-ray analyses and Non-Covalent Interaction (NCI) theoretical approach

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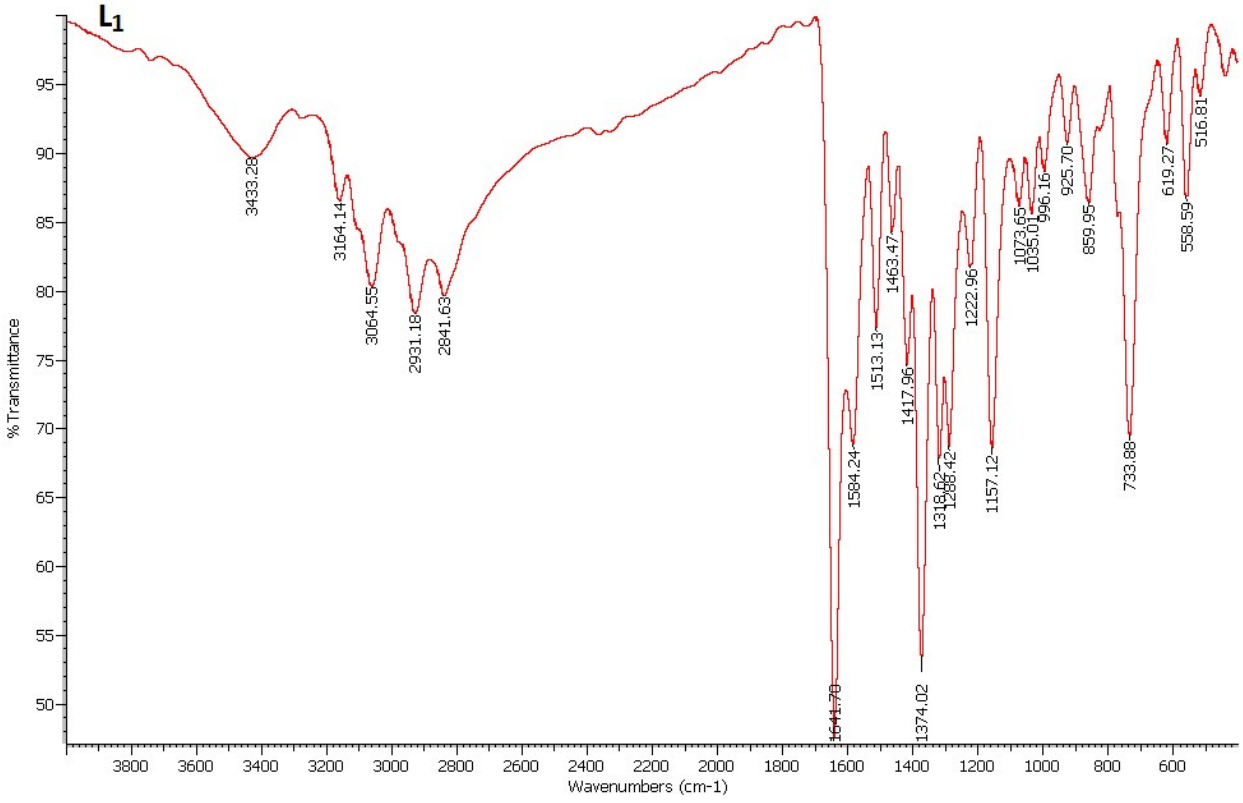
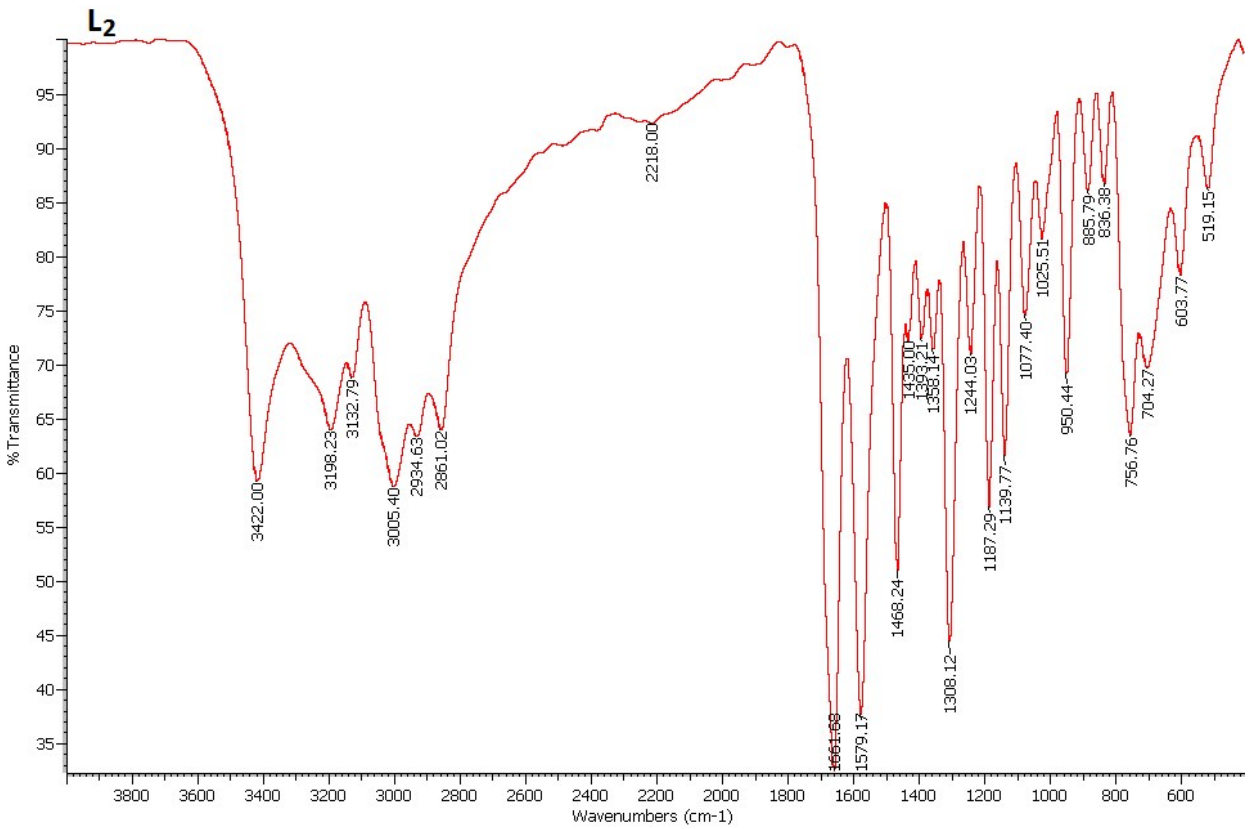
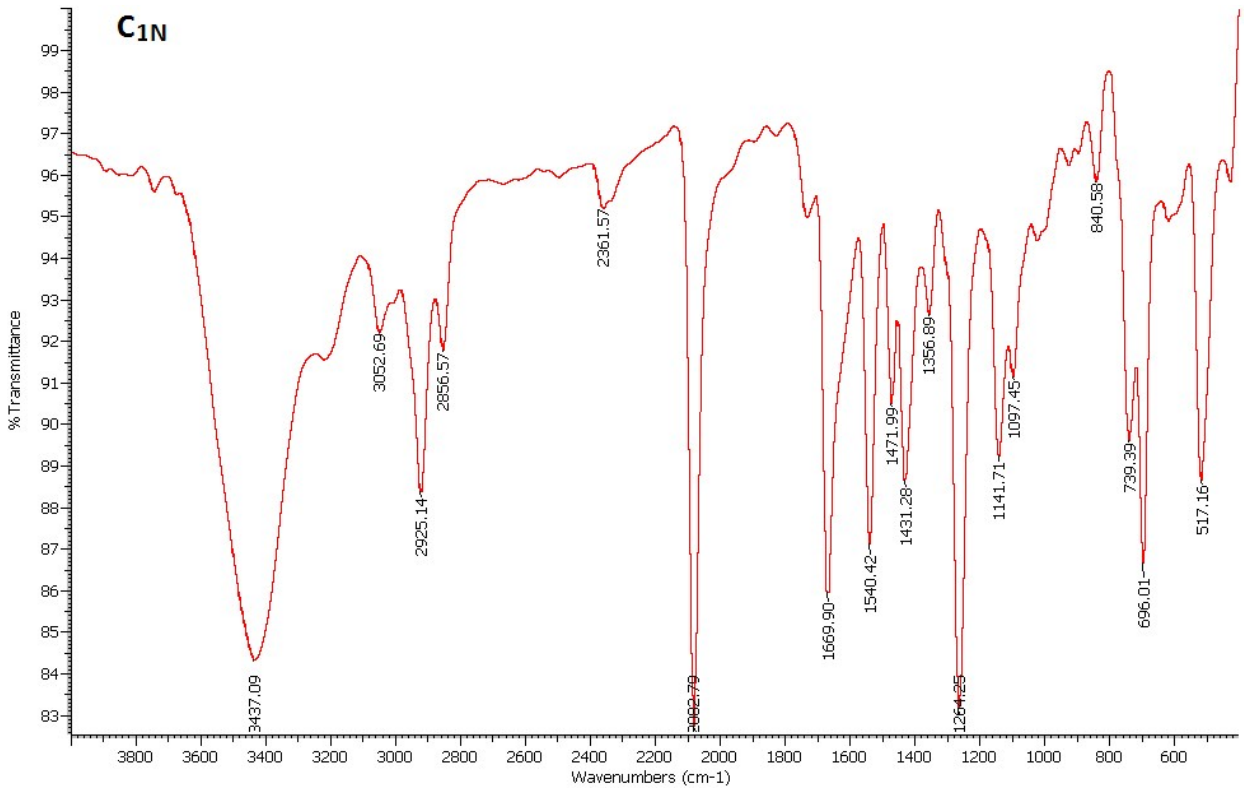
IR spectra of all compounds as well as NMR spectra of ligands are presented below. Complexes are only soluble in DMSO which decomposes them. ^{13}C NMR spectrum of $\mathbf{L_1}$ has not been also reported as the signals was not distinguishable due to the low solubility.



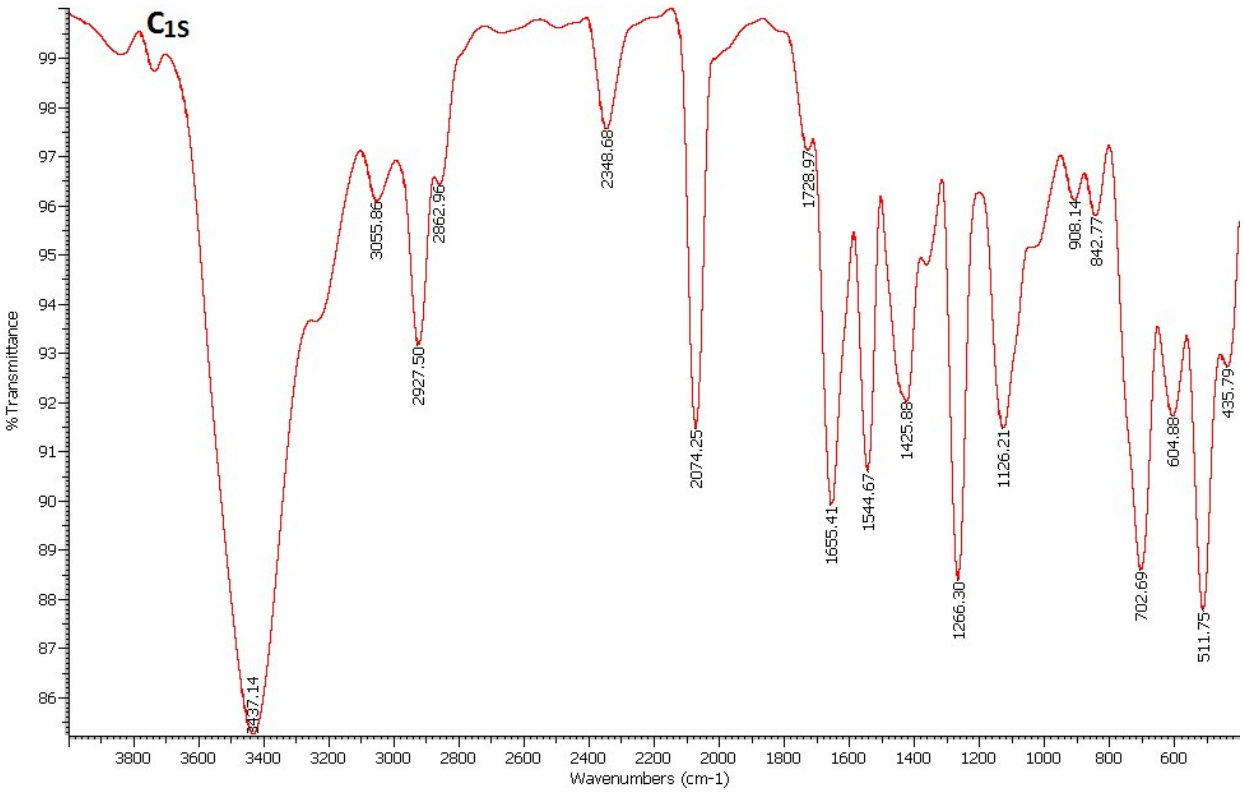
IR spectrum of $\mathbf{L_1}$



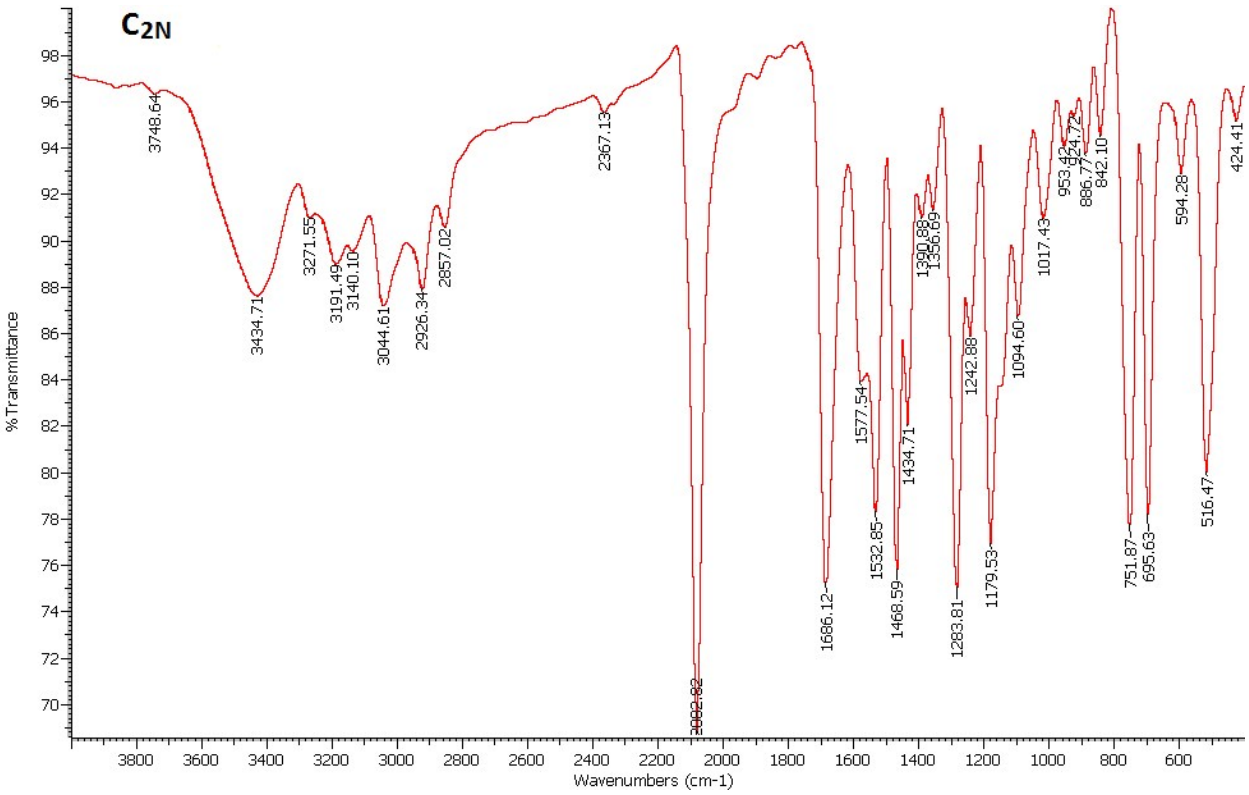
IR spectrum of $\mathbf{L_2}$



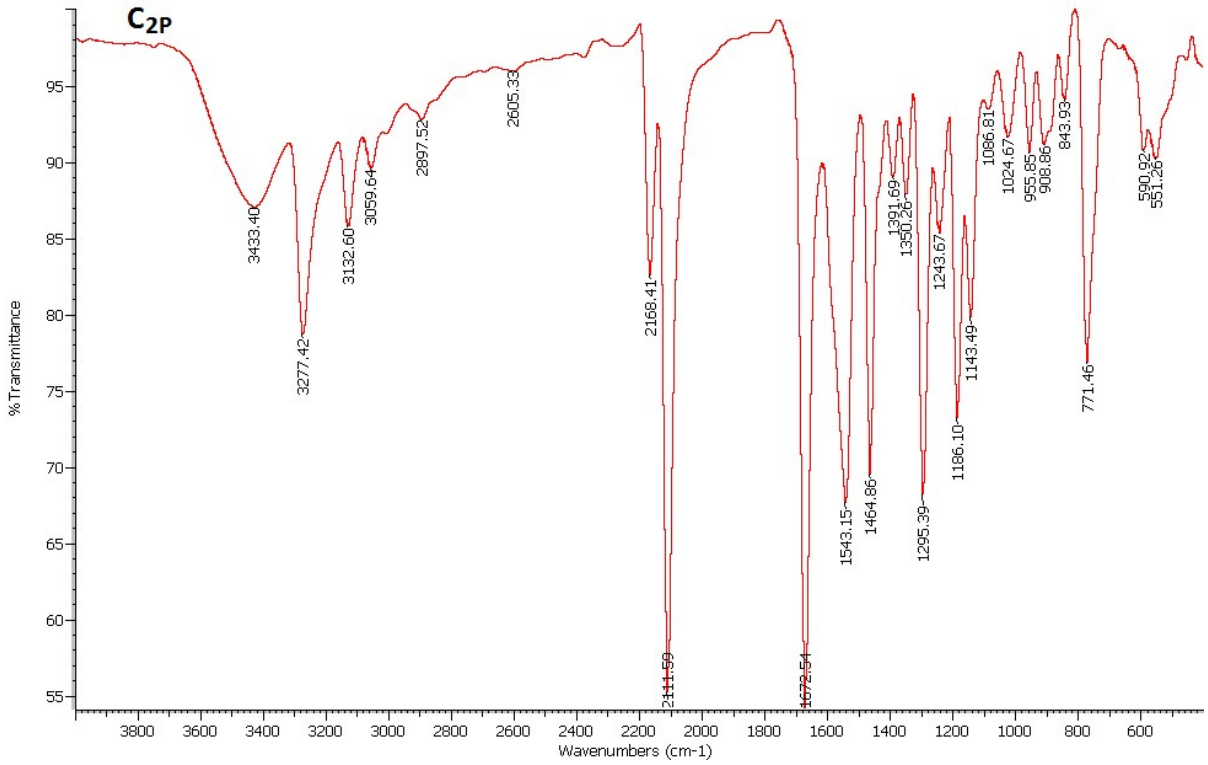
IR spectrum of **C_{1N}**



IR spectrum of **C_{1S}**

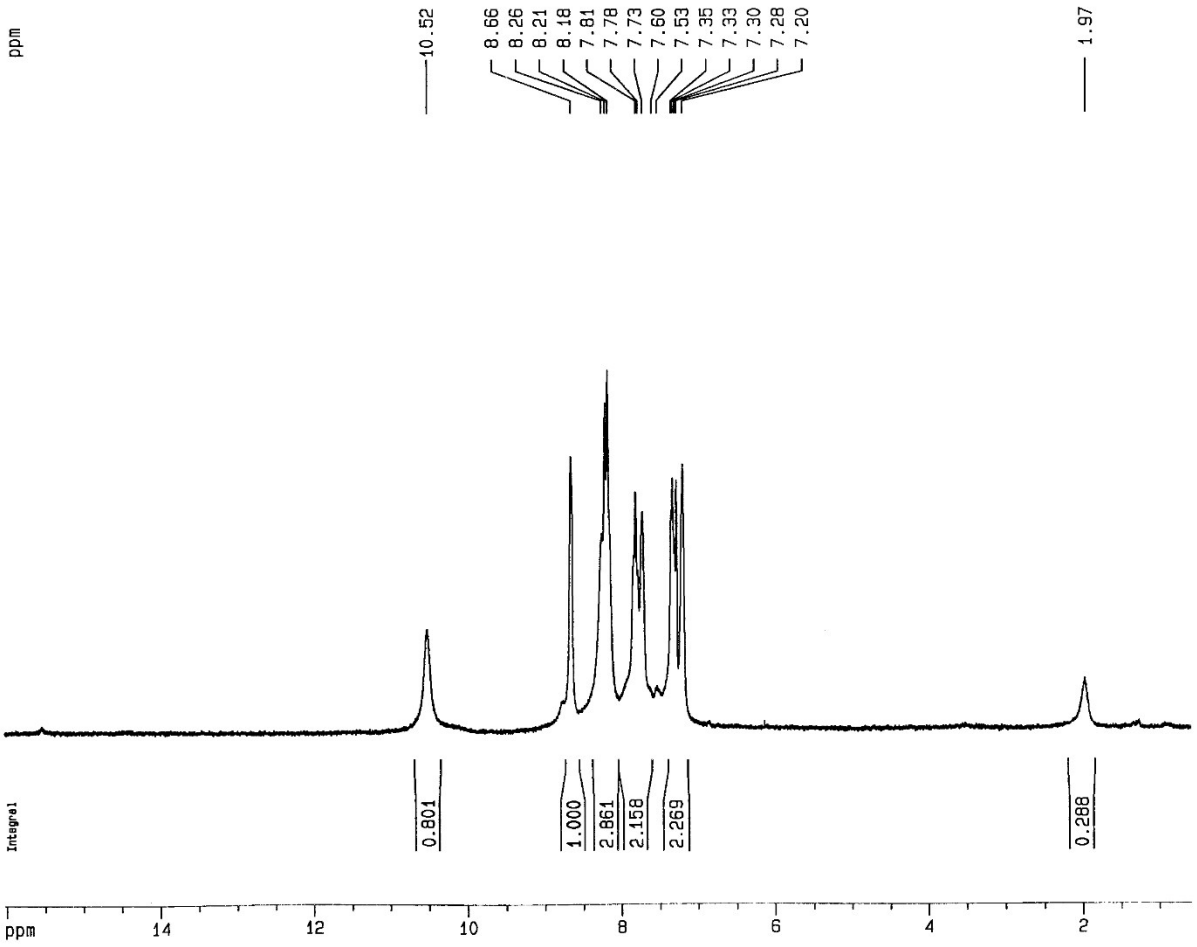


IR spectrum of **C_{2N}**



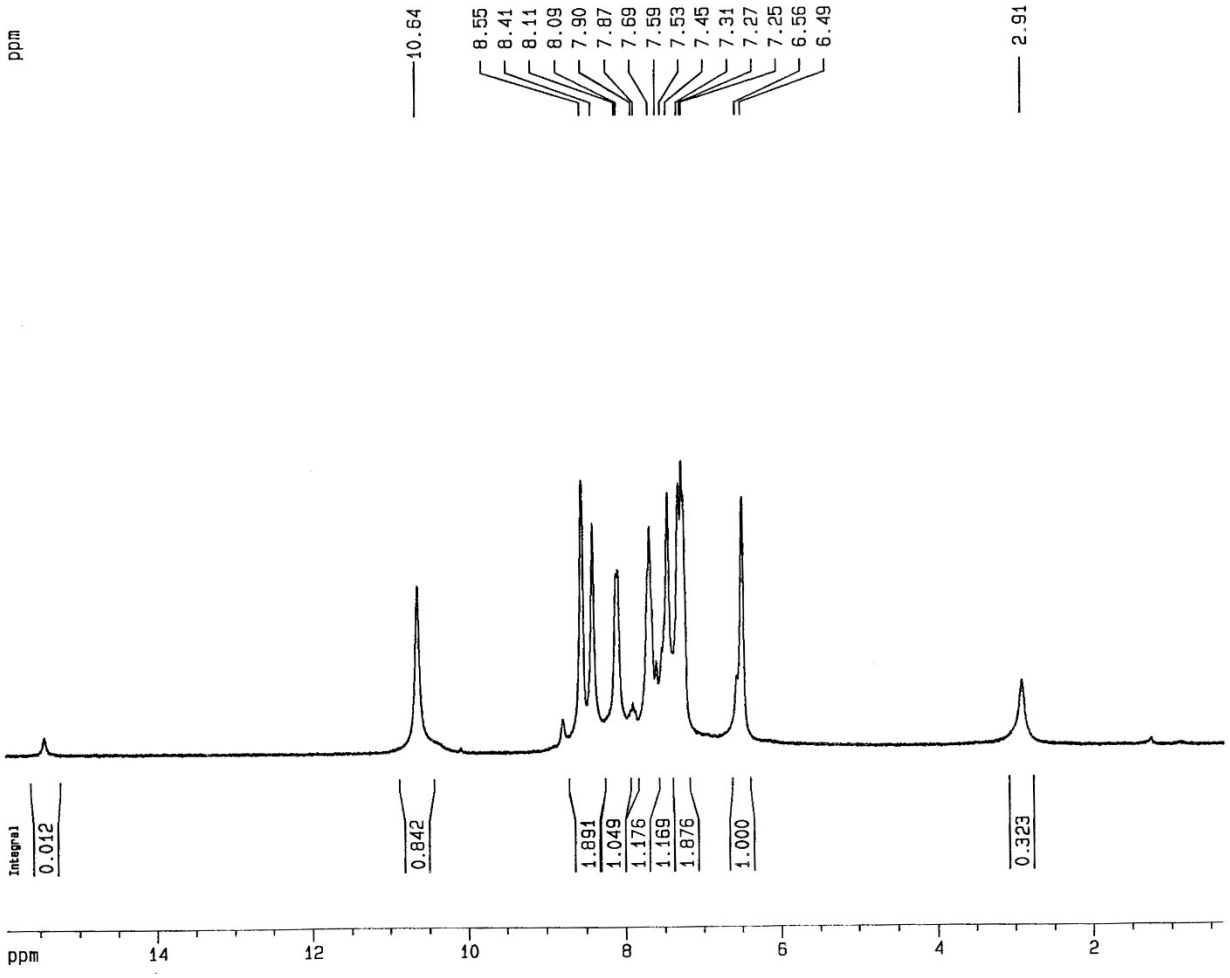
IR spectrum of **C_{2P}**

L_1



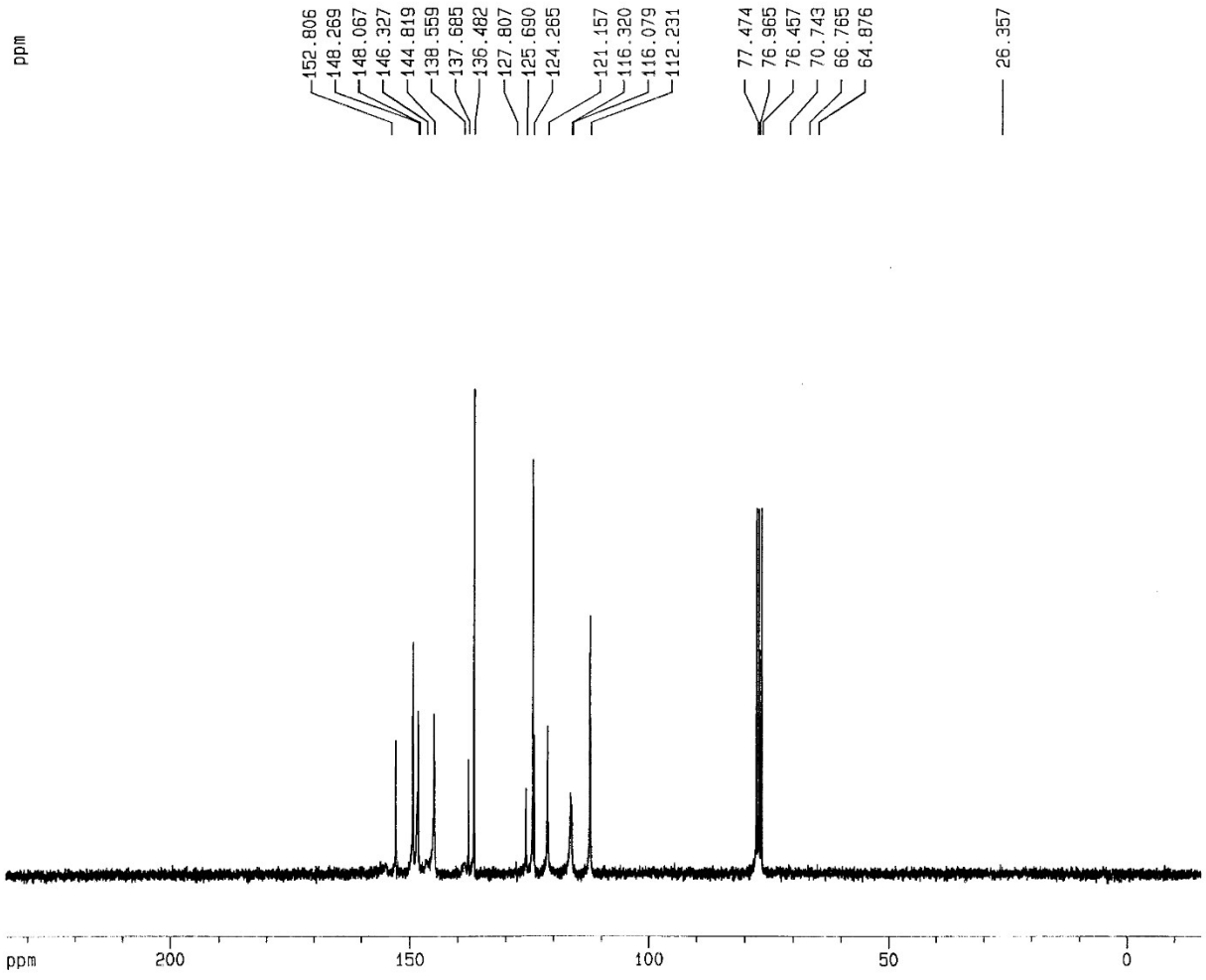
^{1}H NMR spectrum of **L_1** in $CDCl_3$

L_2



^{1}H NMR spectrum of **L_2** in $CDCl_3$

L_2



^{13}C NMR spectrum of **L_2** in $CDCl_3$