

**SUPPLEMENTARY MATERIALS TO: STRUCTURAL
FEATURES OF COPPER(II) COMPLEXES BASED
ON 3-(5-PHENYL-2H-TETRAZOL-2-YL)PYRIDINE
AND 2,2'-BIPYRIDINE/1,10-PHENANTHROLINE**

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TABLE S1. Crystallographic data and structure refinement results for the copper(II) complex

Compound	1a
Chemical formula	C ₁₈ H ₂₆ ClCuFeNO ₃
M, g/mol	459,25
Crystal system, space group	Monoclinic, <i>P2₁/c</i>
Temperature, K	150
<i>a</i> /Å	15,30(2)
<i>b</i> /Å	6,069(8)
<i>c</i> /Å	21,61(2)
<i>α</i> /°	90
<i>β</i> /°	110,67(9)
<i>γ</i> /°	90
Volume / Å ³	1878(4)
<i>Z</i>	4
ρ_{cal} g/cm ³	1,624
μ /mm ⁻¹	9,038
Crystal dimensions / mm	0,2 × 0,02 × 0,02
2 θ scanning range/ °	6,17 – 101,81
hkl index range	-11 ≤ <i>h</i> ≤ 15, -6 ≤ <i>k</i> ≤ 4, -21 ≤ <i>l</i> ≤ 18
Number of reflections measured / independent	3802 / 1567
<i>R</i> _{int} , <i>R</i> _σ	<i>R</i> _{int} = 0,0716, <i>R</i> _σ = 0,0949
Number of restraints / parameters	3 / 232
Goodness on F ²	1,022
R-factors [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0,0645, w <i>R</i> ₂ = 0,1552
R-factors (for all reflections)	<i>R</i> ₁ = 0,0939, w <i>R</i> ₂ = 0,1689
Residual electron density (max/min), e Å ⁻³	0,81 / -0,58
CCDC	2406334

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TABLE S2. Bond lengths in the [Cu(MeOH)LCI]_n complex

Complex	1a
Cu–O(L), Å	1.968(7) 1.959(7)
Cu–N(L), Å	1.996(9)
Cu–O(MeOH), Å	2.233(8)
Cu–Cl	2.257(3)

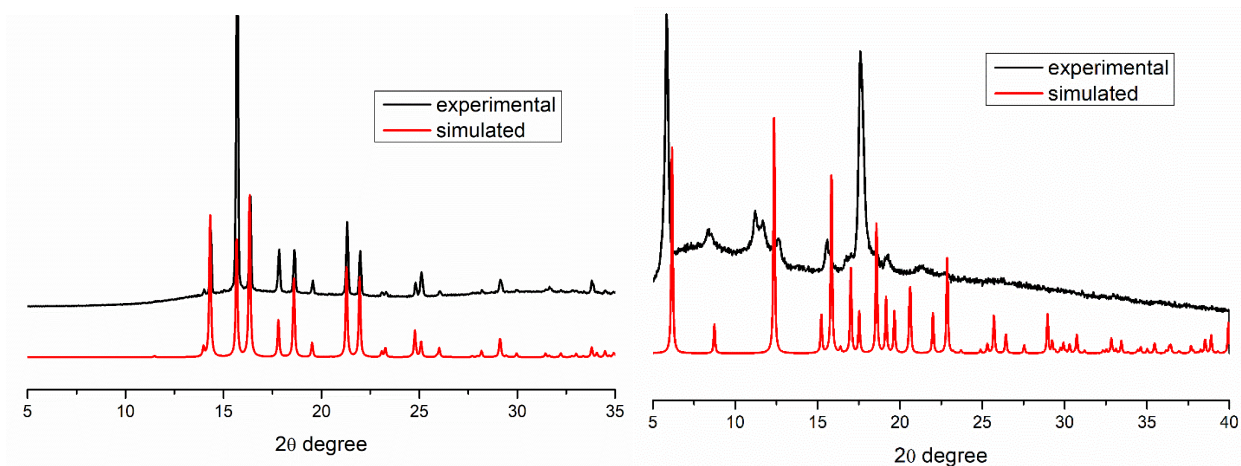


Fig. S1. Experimental and simulated (CCDC refcode: DEJZAT01) XRD pattern of formylferrocene (left) and complex **1**, **1a** (right).

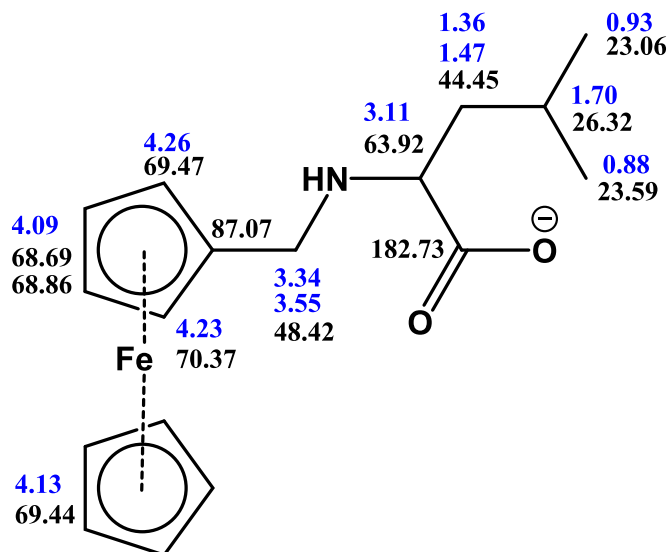


Fig. S2. Structure of HL with the signal assignment in the NMR spectrum.

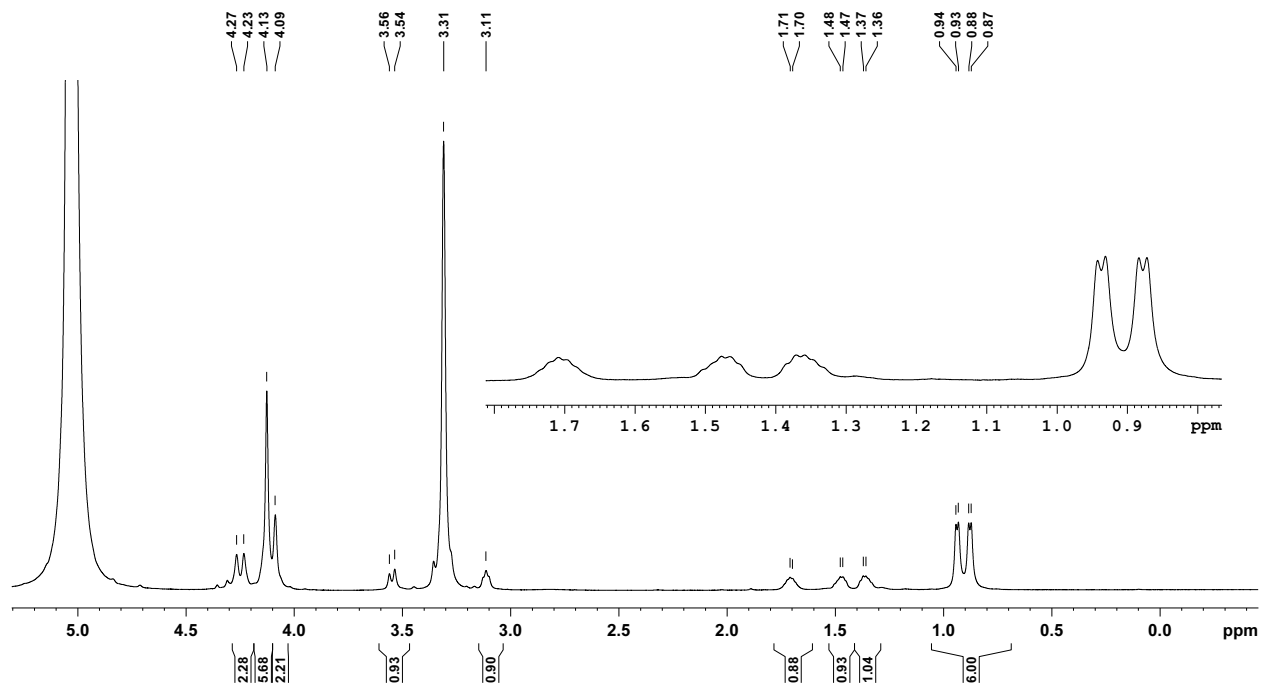


Fig. S3. ^1H NMR spectrum of the HL ligand.

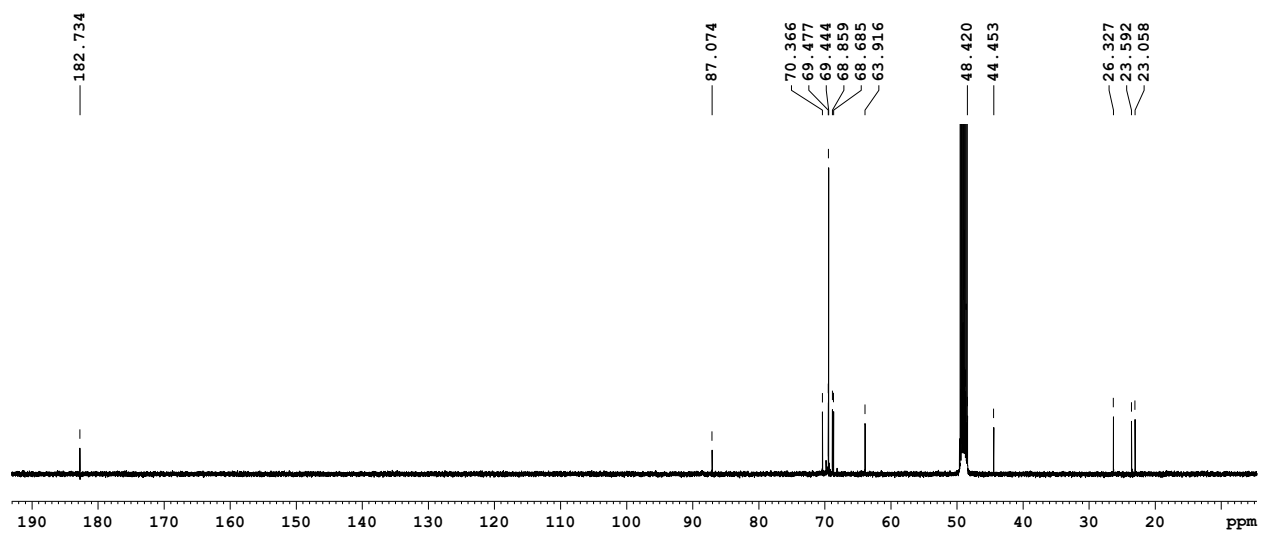


Fig. S4. $^{13}\text{C}\{^1\text{H}\}$ PMR spectrum of the HL ligand.

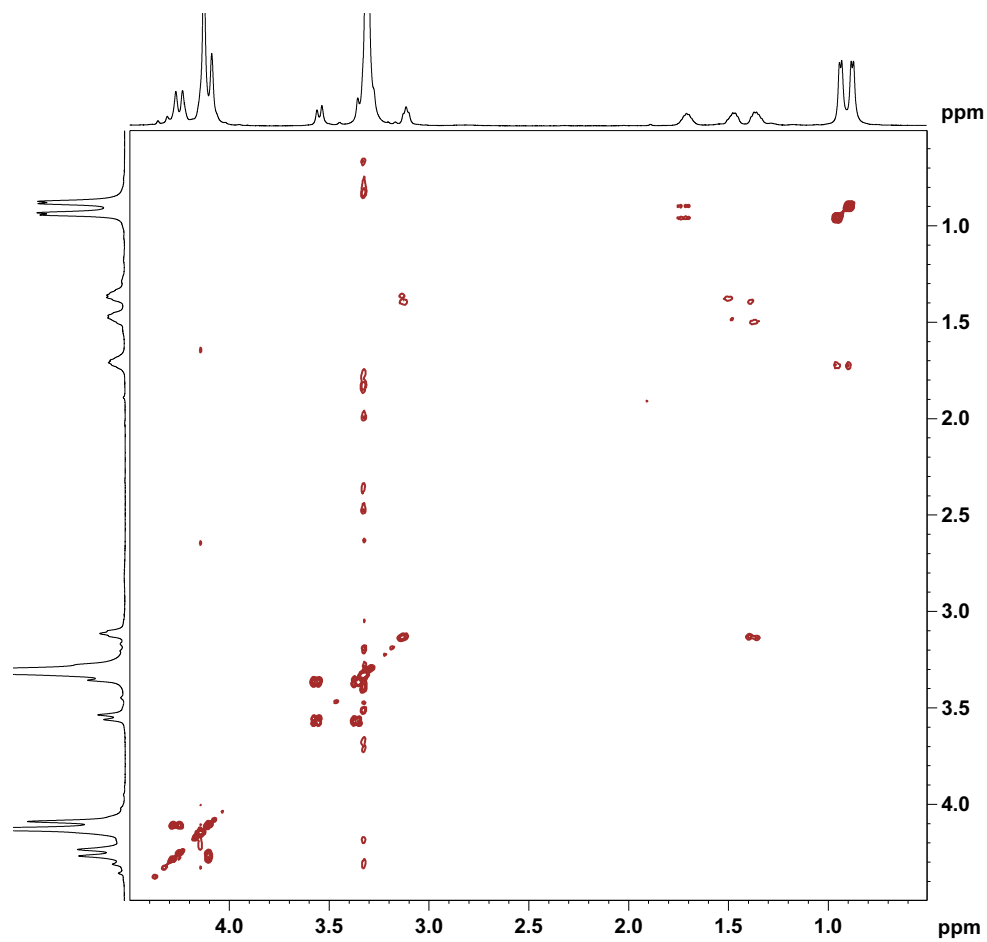


Fig. S5. 2D ^1H , ^1H COSY spectrum of the HL ligand.

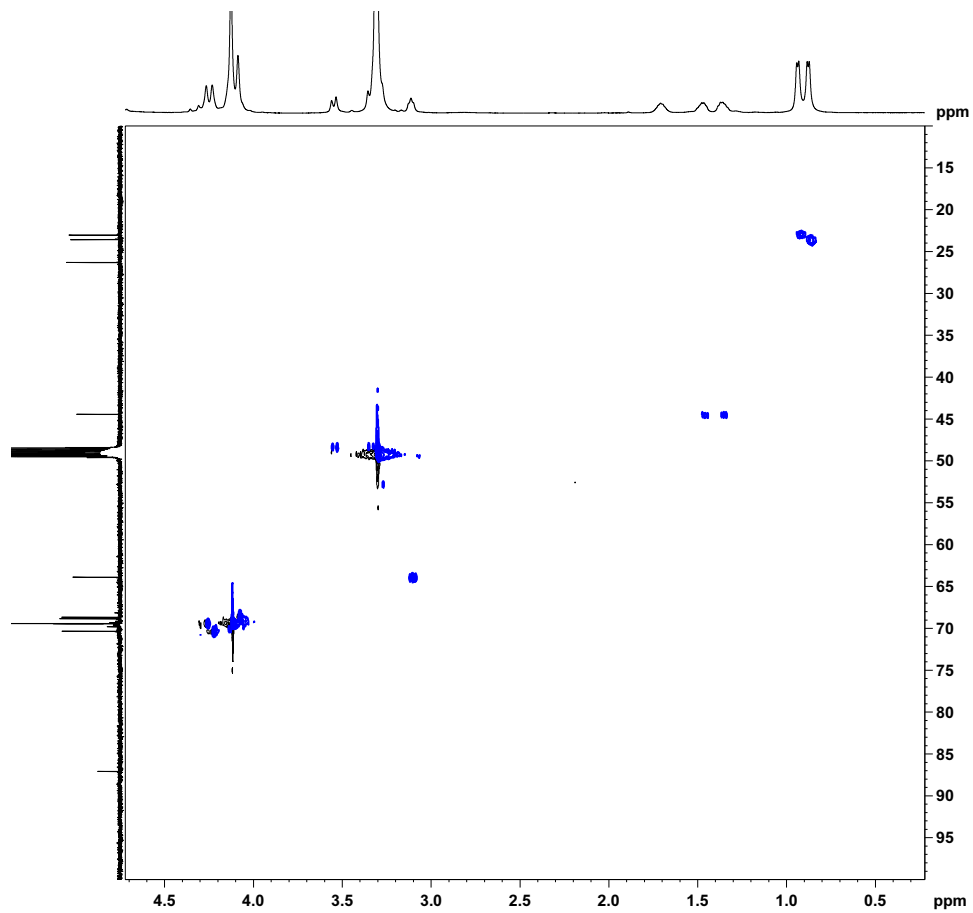


Fig. S6. 2D ^1H , ^{13}C HSQC spectrum of the HL ligand.

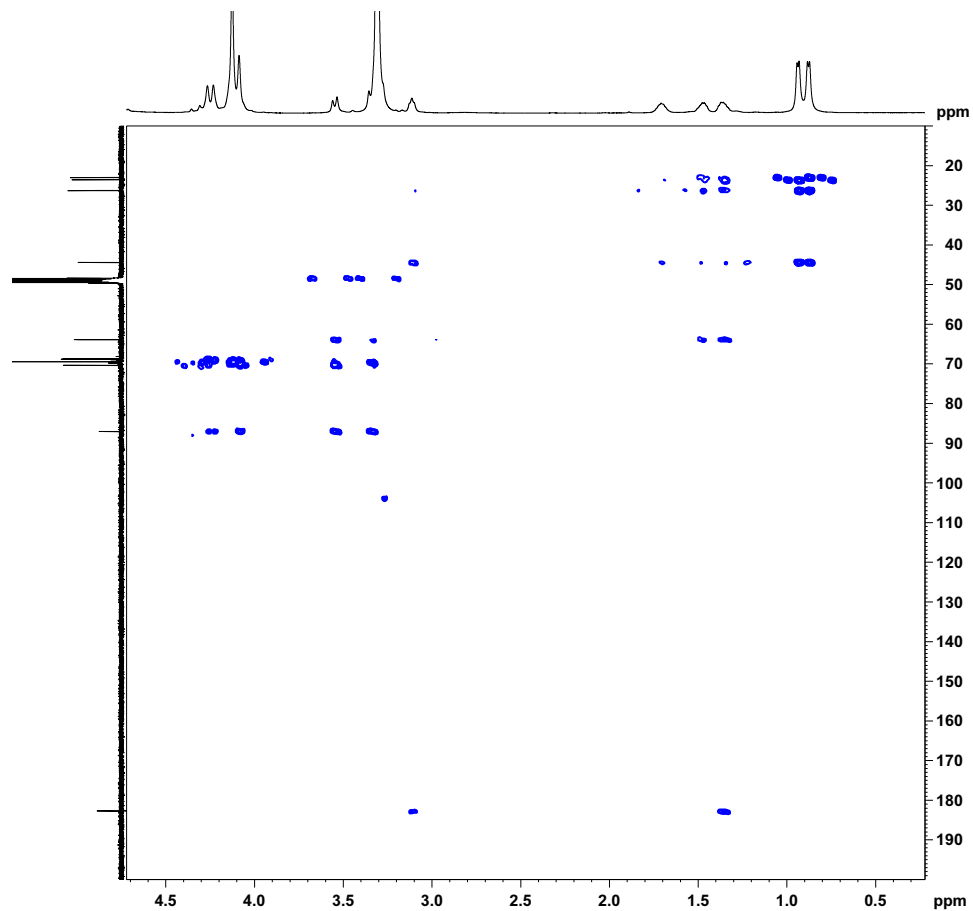


Fig. S7. 2D ^1H , ^{13}C HMBC spectrum of the HL ligand.

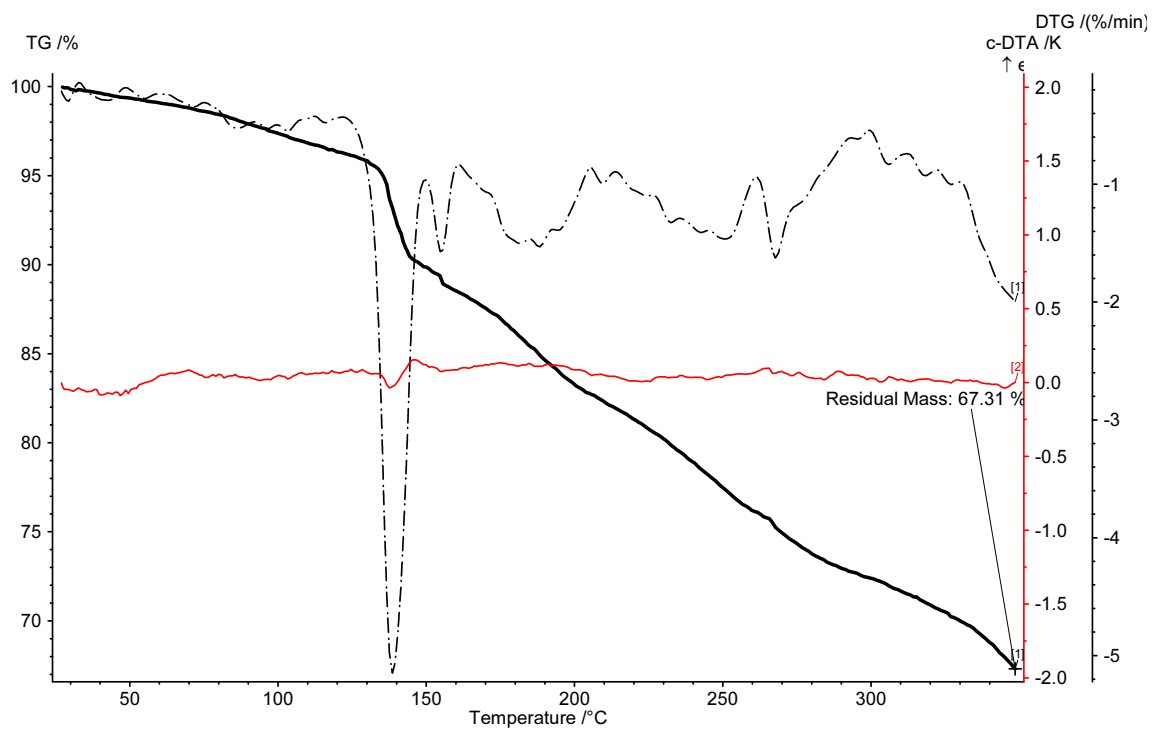
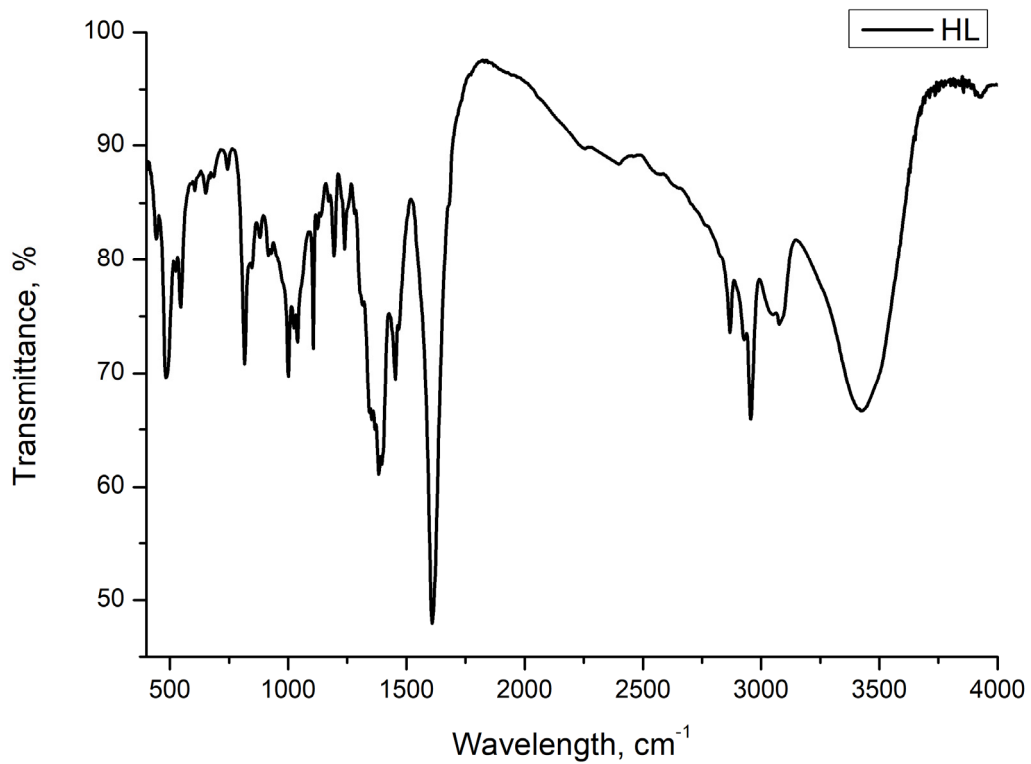
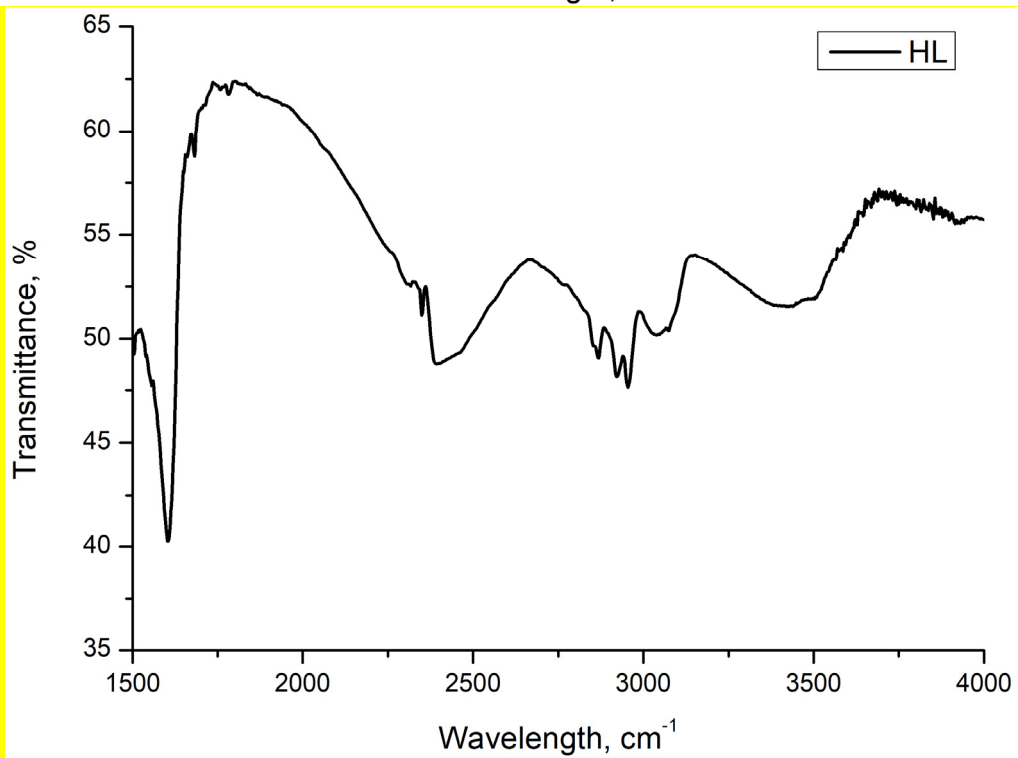


Fig. S8. TGA data for complex 1.

a



b



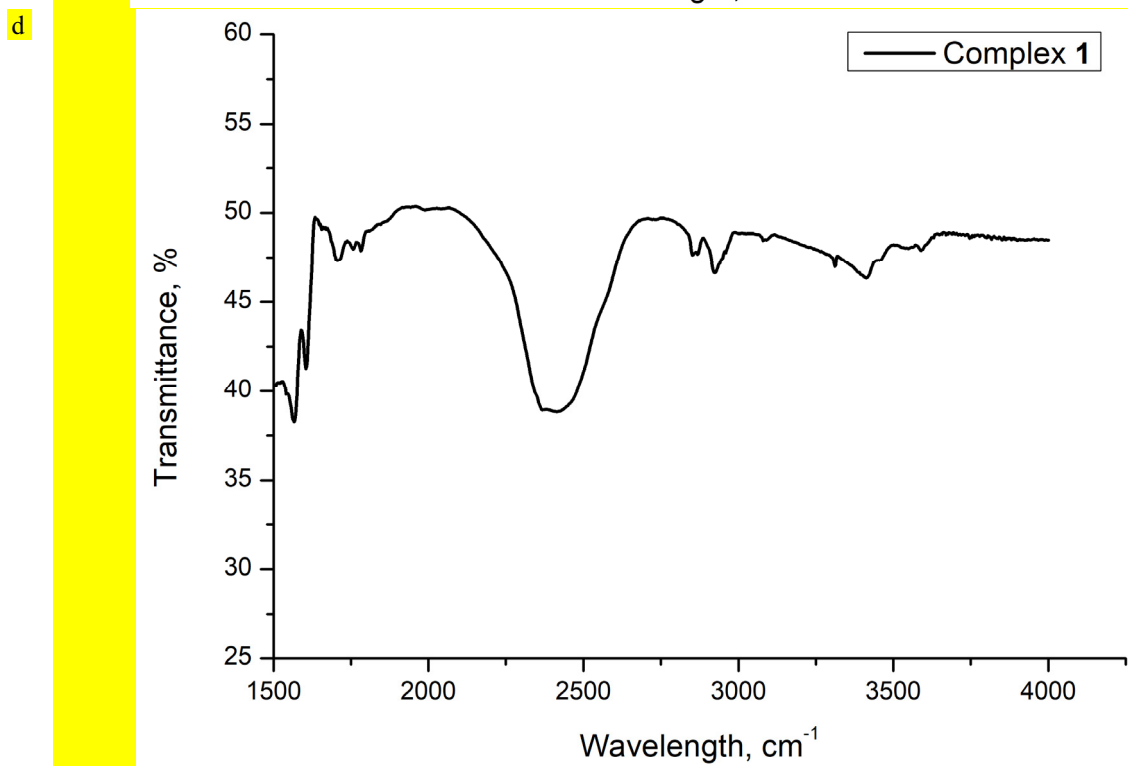
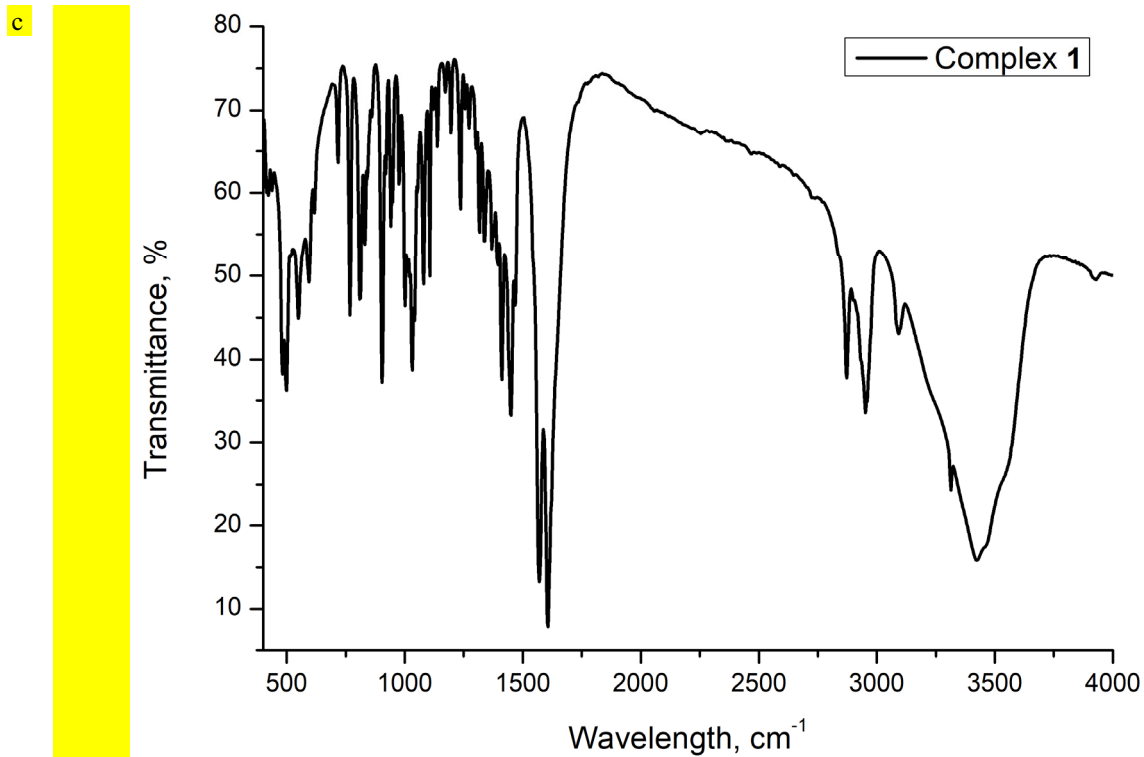


Fig. S9. IR spectra of the HL ligand and complex **1** in KBr (a, c) and in fluorinated oil (b, d).

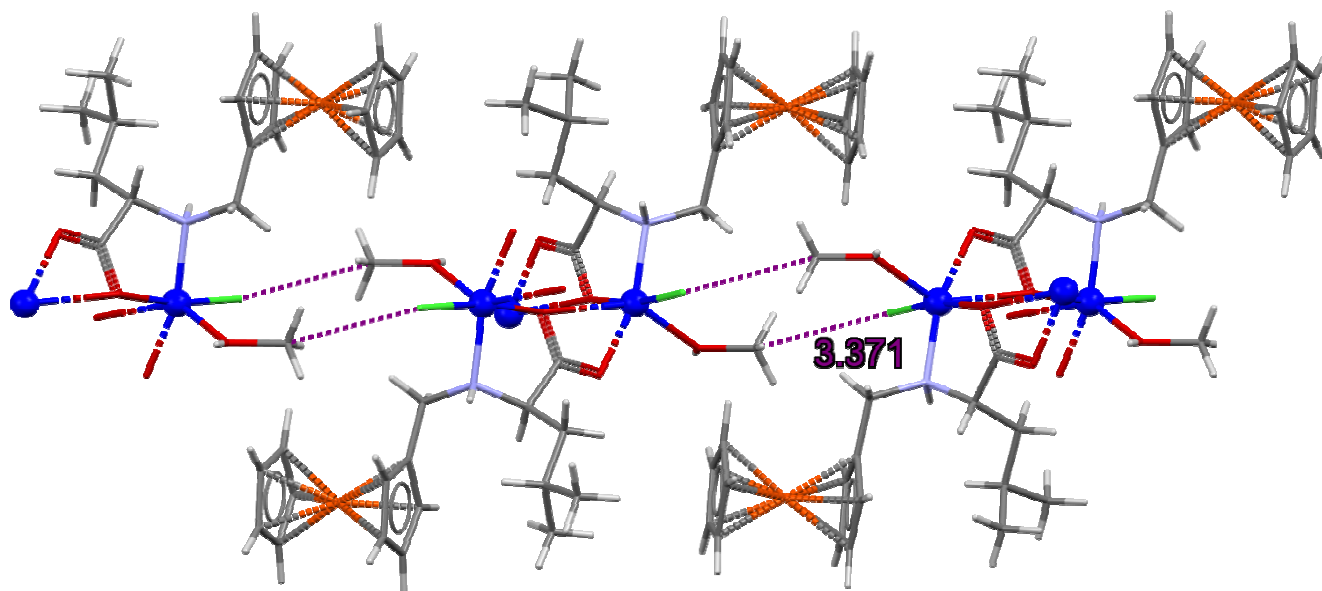


Fig. S10. Halogen bonds (purple dotted lines) between the neighboring $[\text{Cu}(\text{MeOH})\text{LCI}]_n$ polymer chains.