Thioether-Triphenolate Bimetallic Iron(III) Complexes as Robust and Highly Efficient Catalysts for Cycloaddition of Carbon Dioxide to Epoxides

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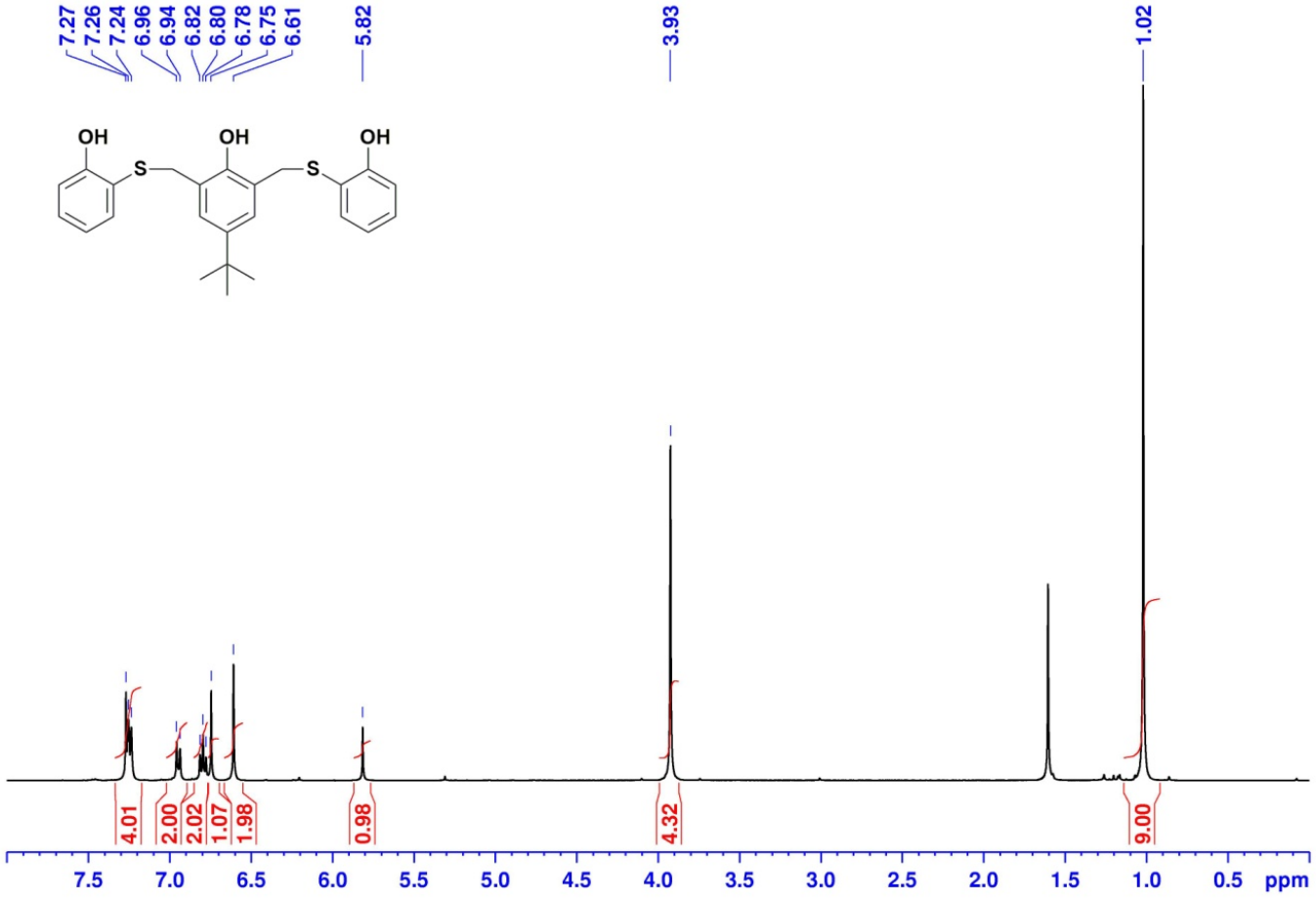


Figure S1. ^{1}H NMR spectrum of the pro-ligand $\mathbf{L}_{\boldsymbol{H}}$ (CD_2Cl_2, 400 MHz).

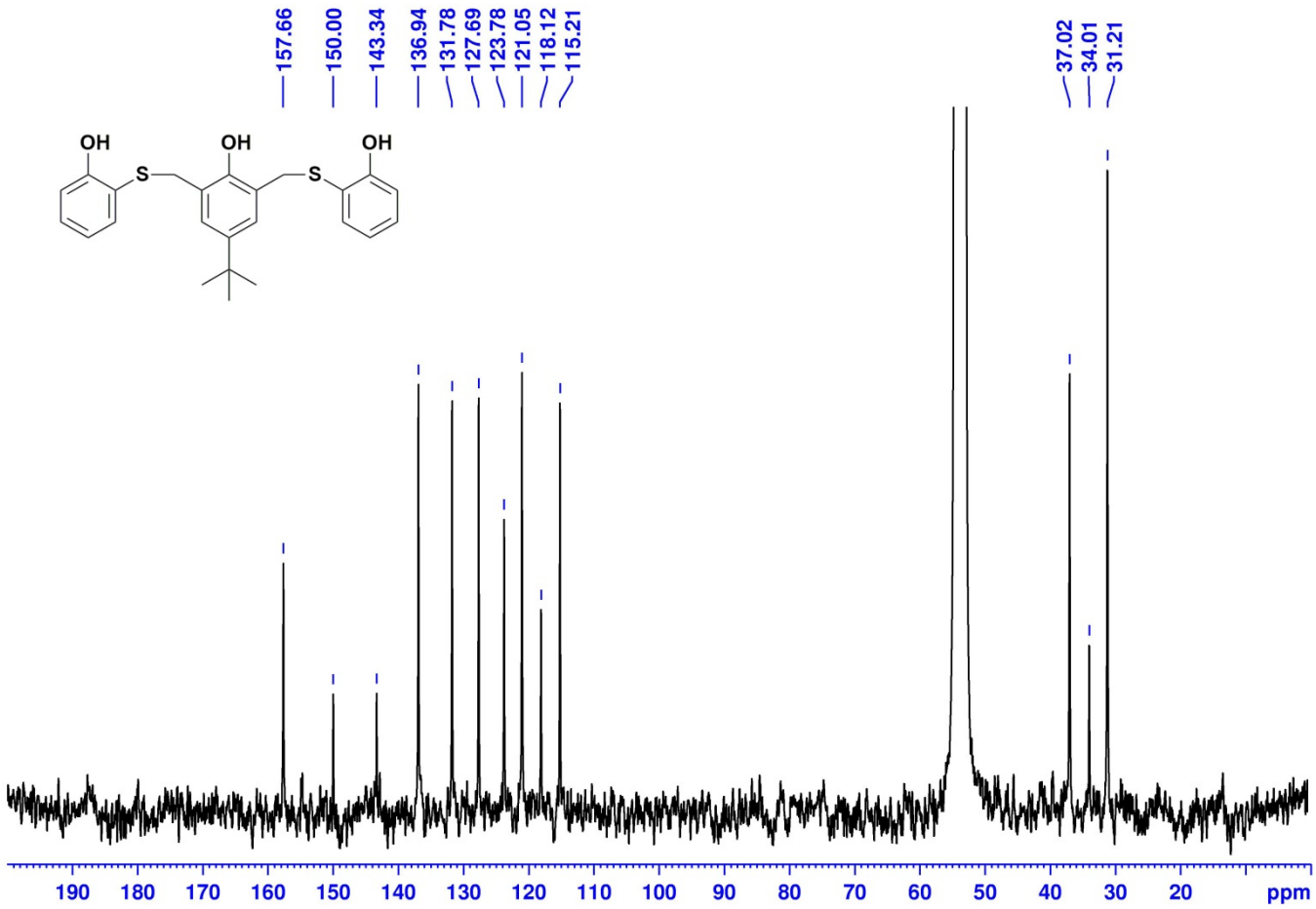


Figure S2. ^{13}C NMR spectrum of the pro-ligand $\mathbf{L}_{\boldsymbol{H}}$ (CD_2Cl_2, 250 MHz).

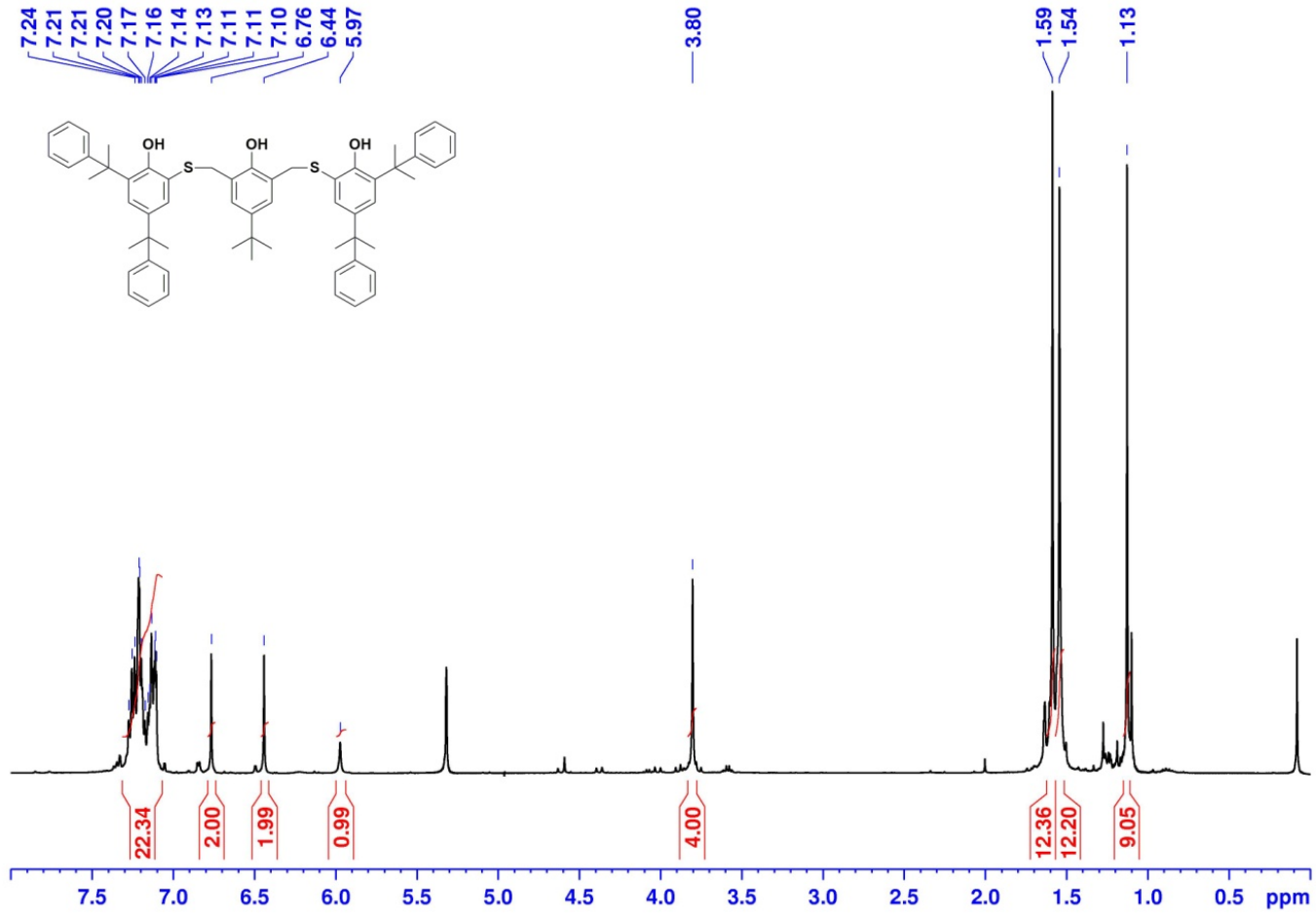


Figure S3. ^{1}H NMR spectrum of the pro-ligand $\mathbf{L}_{Cum}$(CD_2Cl_2, 400 MHz).

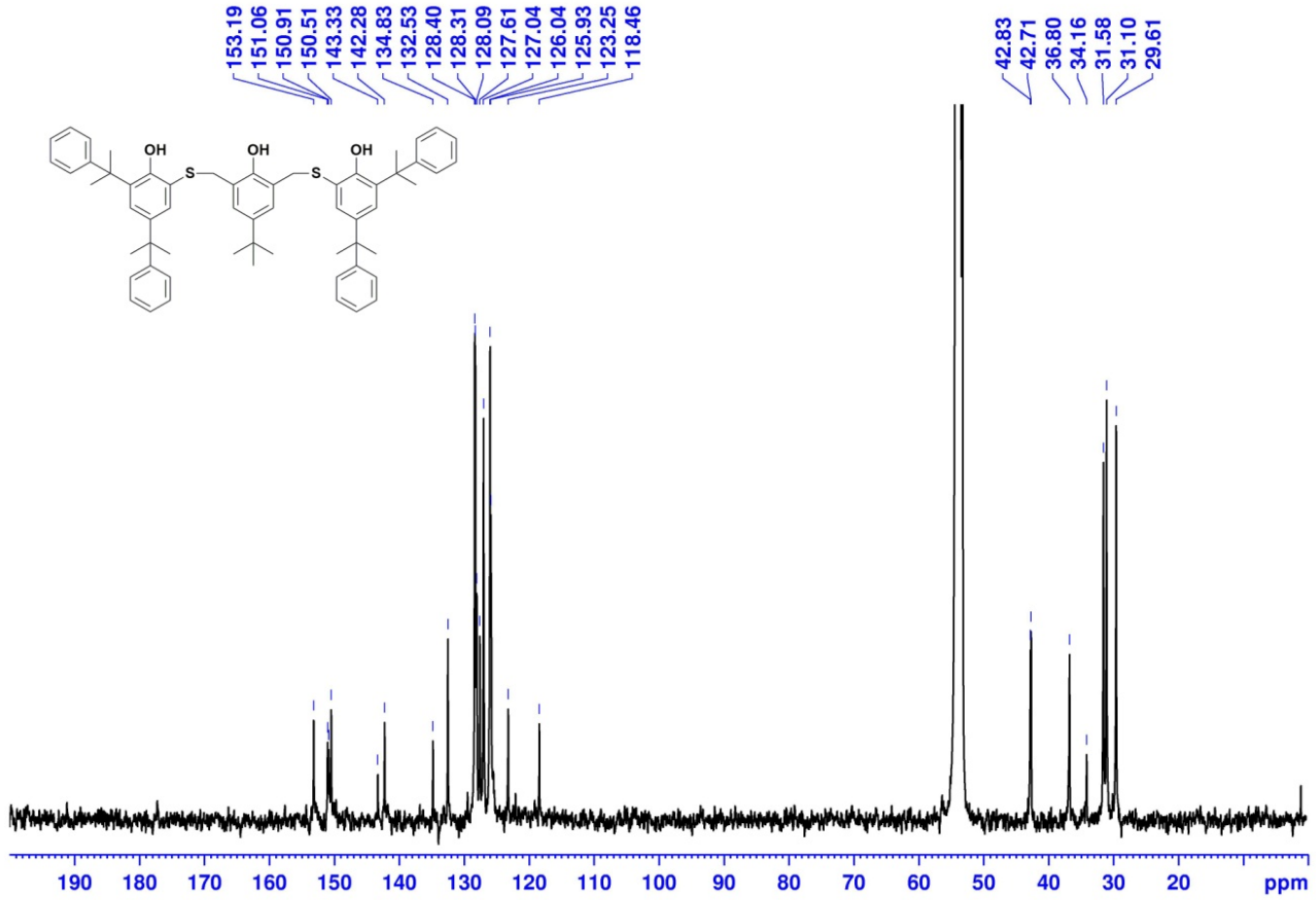


Figure S4. ^{13}C NMR spectrum of the pro-ligand $\mathbf{L}_{\boldsymbol{Cum}}$ (CD_2Cl_2, 400 MHz).

ESI-MS Characterization.

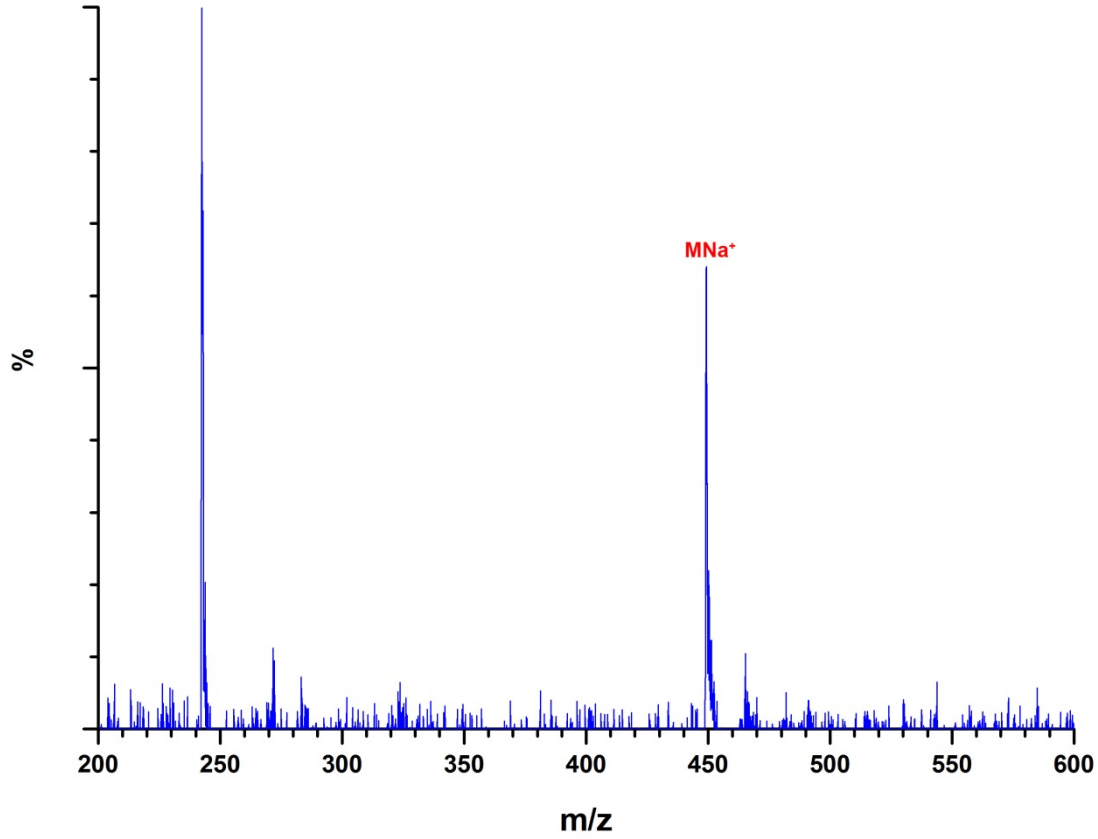


Figure S5. Mass spectrum of the pro-ligand $\mathbf{L}_{H}$ (acetonitrile as solvent).

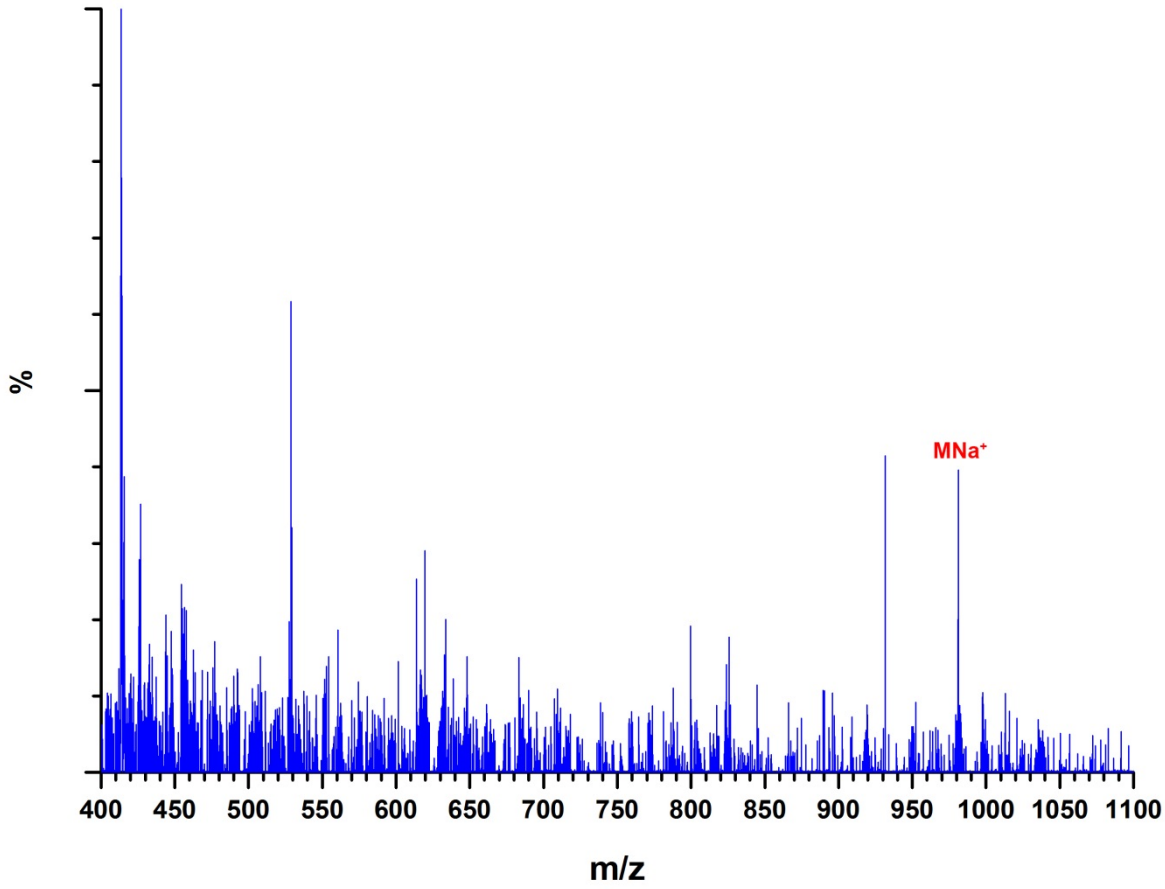


Figure S6. Mass spectrum of the complex $\mathbf{C}_{\boldsymbol{H}}$ (acetonitrile as solvent).

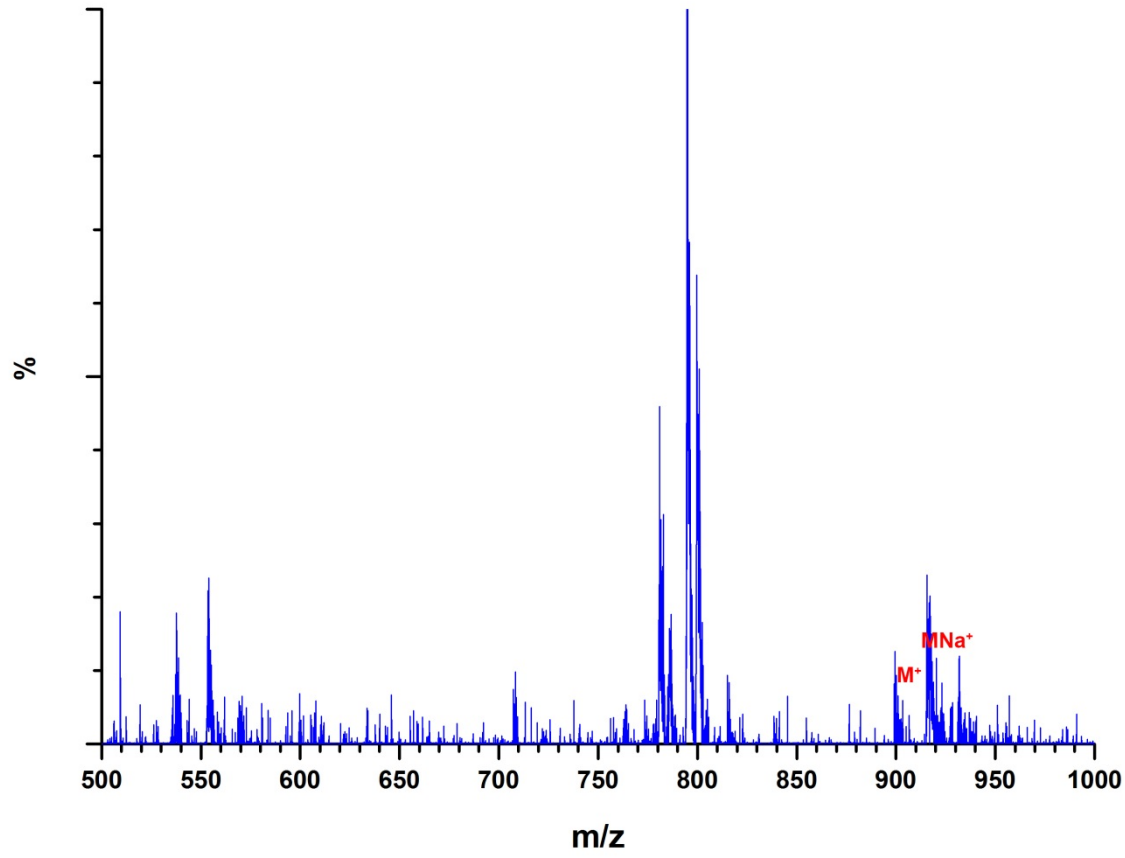


Figure S7. Mass spectrum of the pro-ligand $\mathbf{L}_{Cum}$ (acetonitrile as solvent).

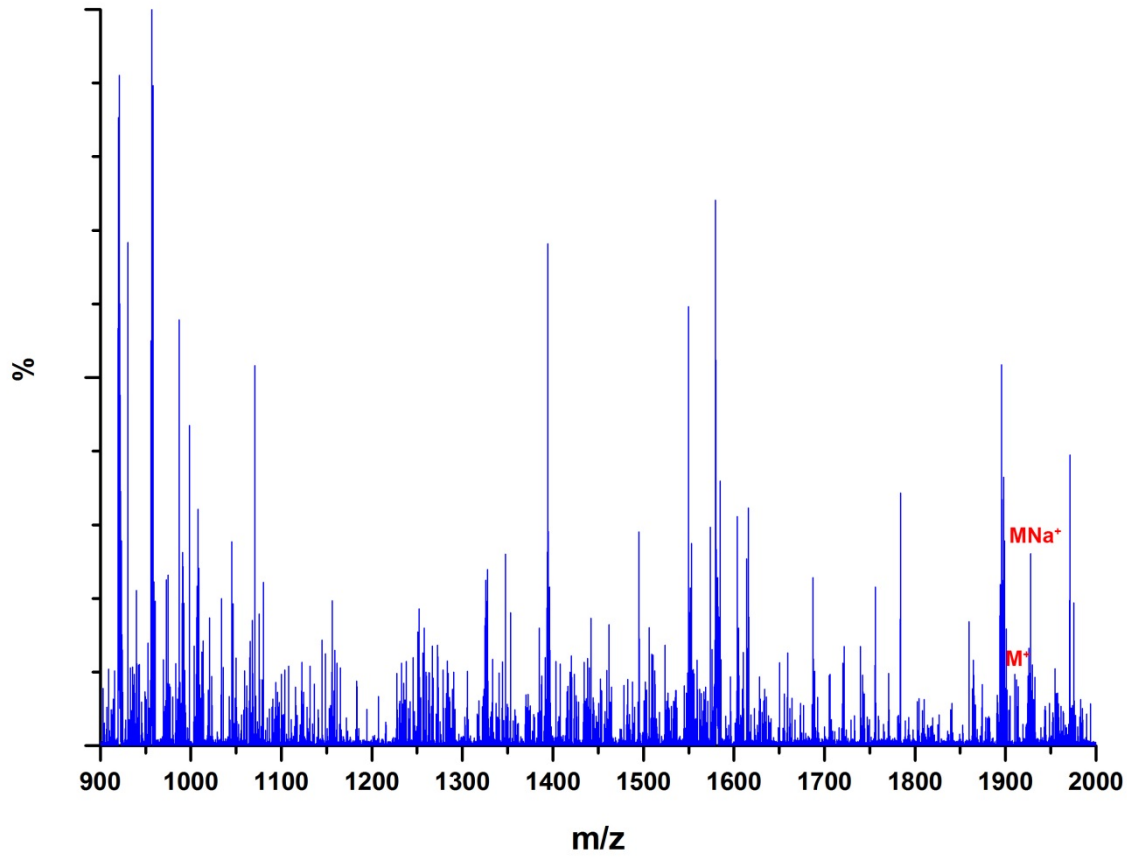


Figure S8. Mass spectrum of the complex $\mathbf{C}_{Cum}$ (acetonitrile as solvent).

FT-IR Characterization.

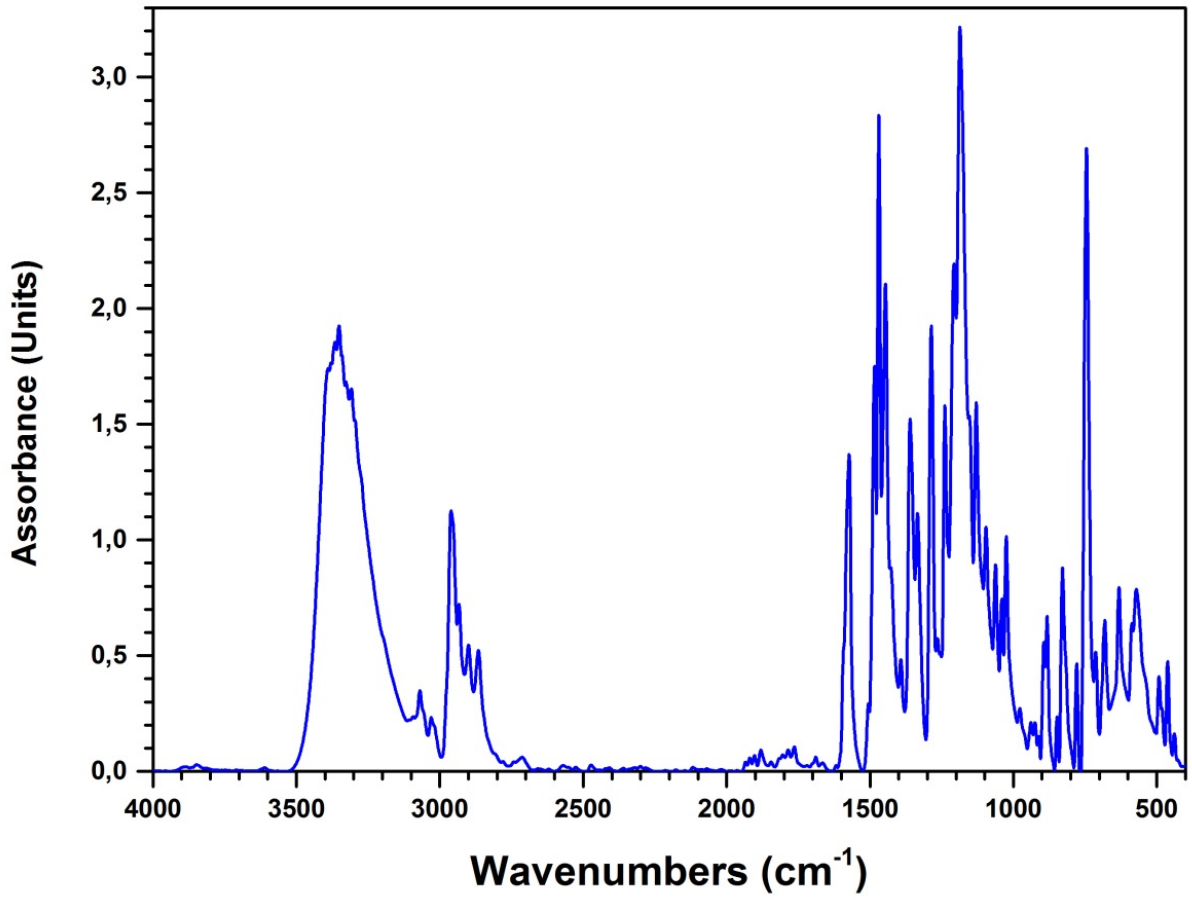


Figure S9. FT-IR spectrum of the pro-ligand $\mathbf{L}_{H}$ (KBr disk).

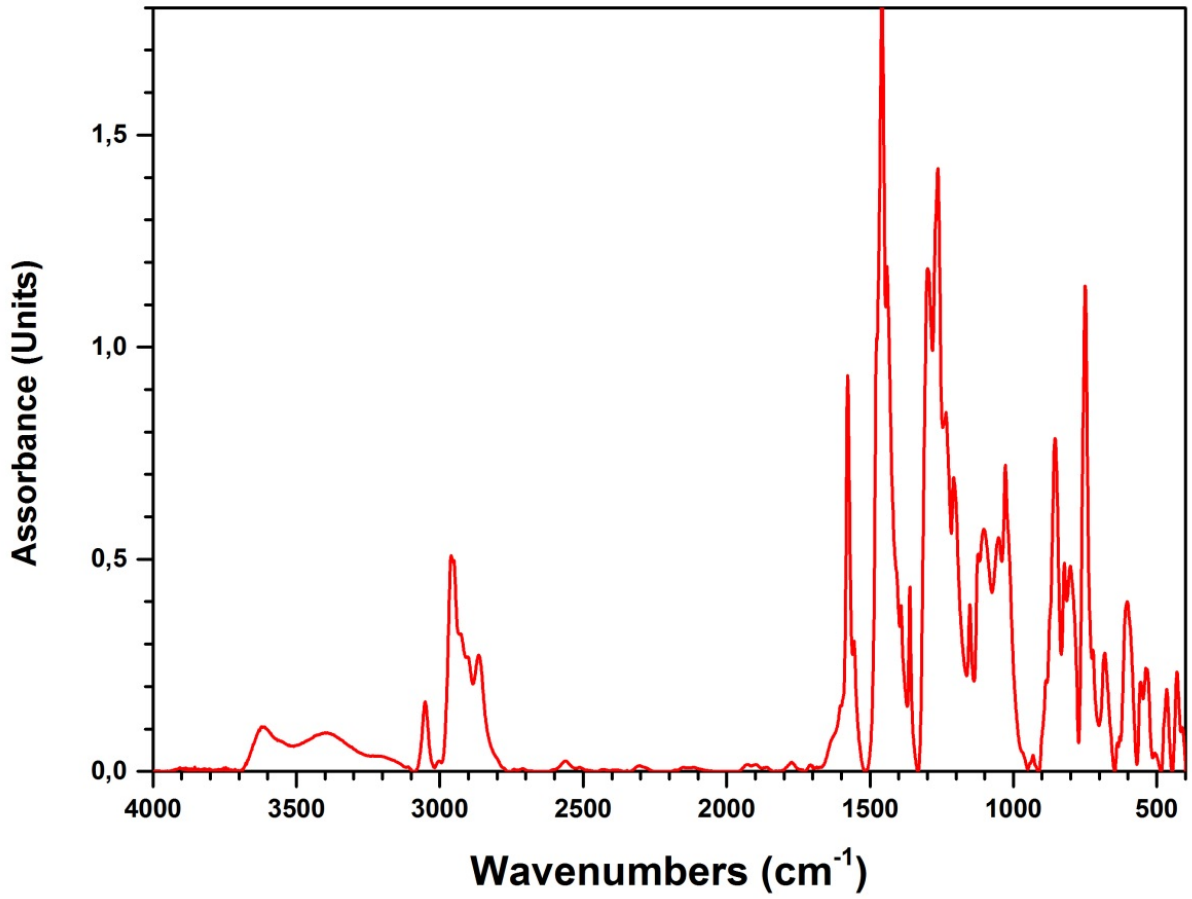


Figure S10. FT-IR spectrum of the complex $\mathbf{C}_{\boldsymbol{H}}$ (KBr disk).

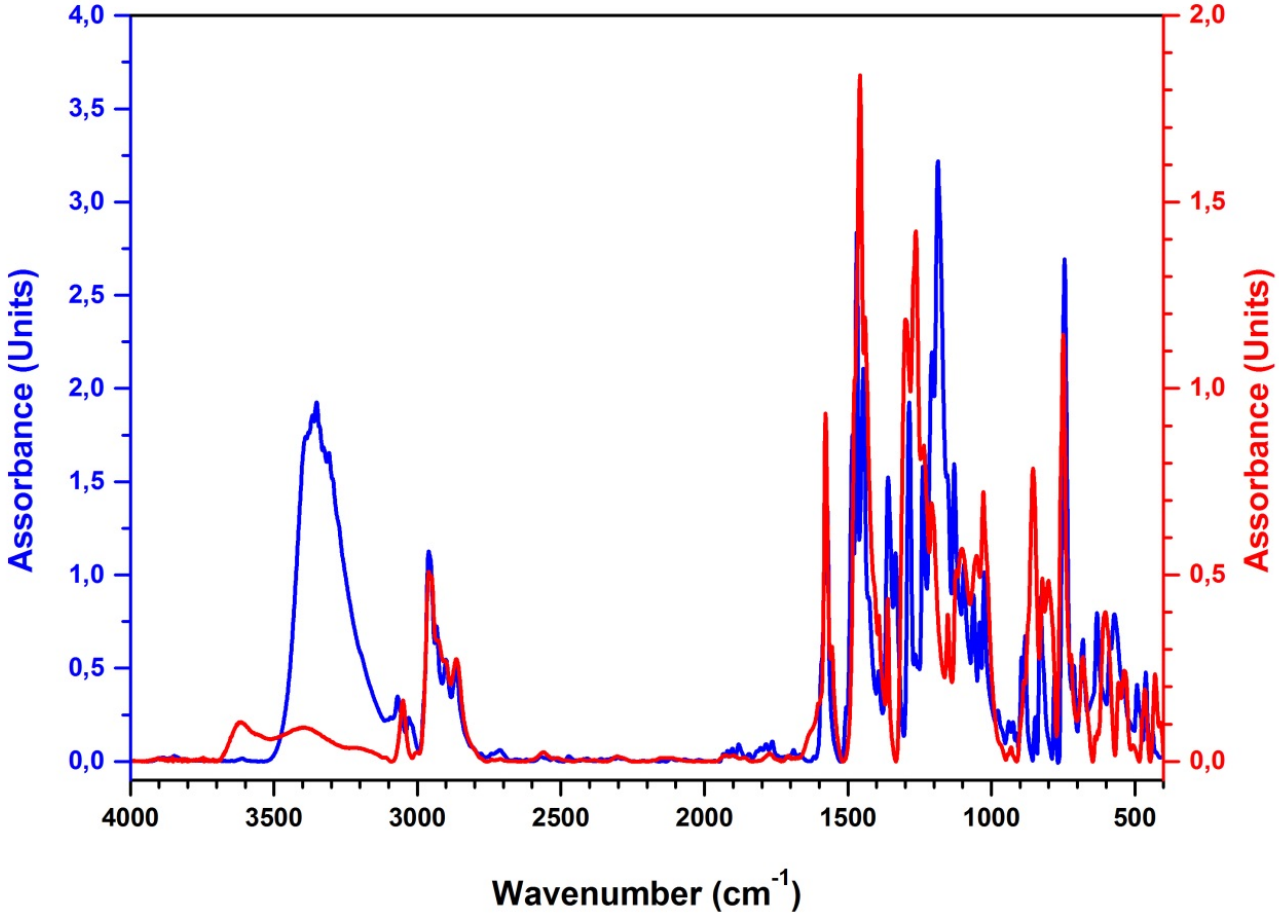
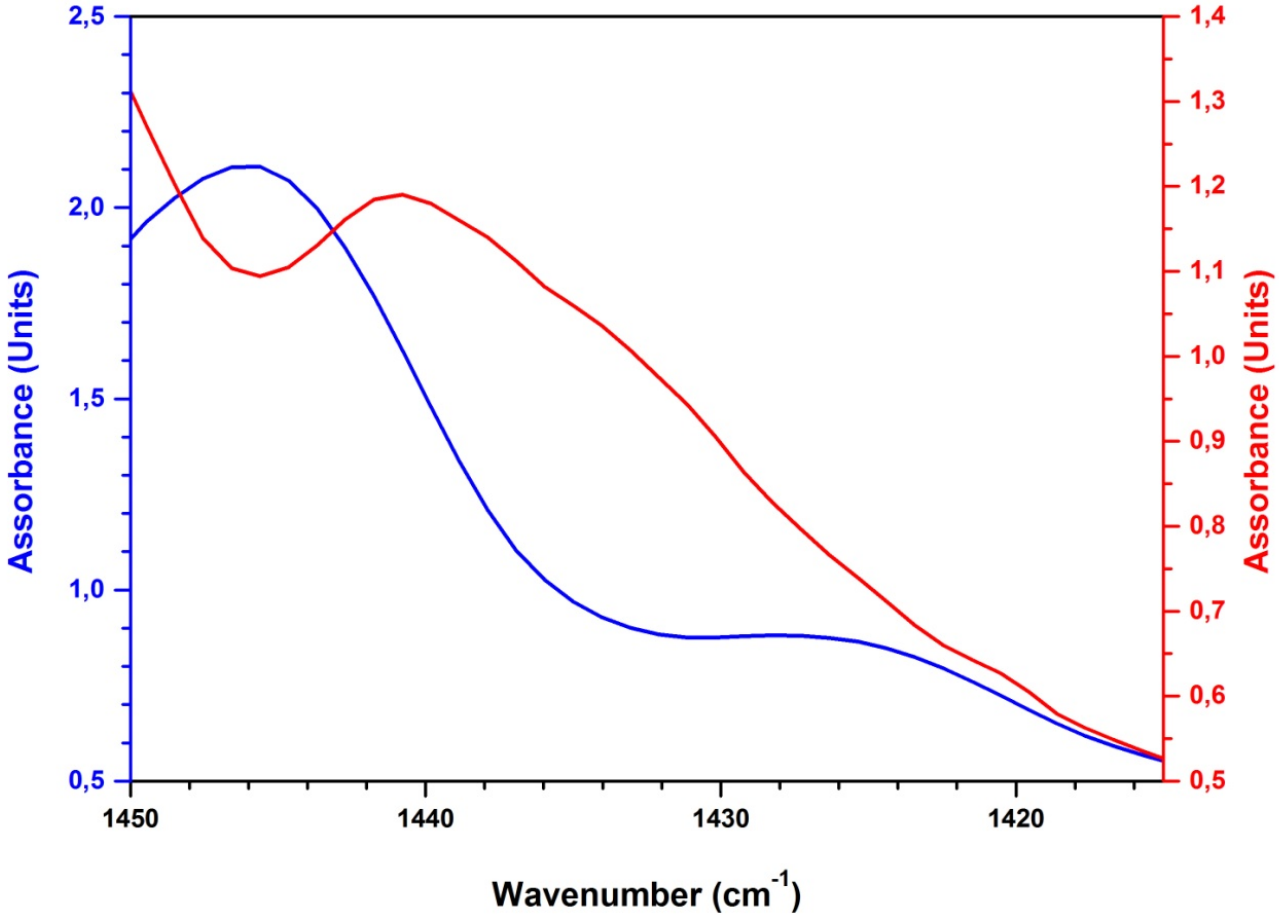


Figure S11. Comparison of the FT-IR spectra of the pro-ligand $\mathbf{L}_{H}$ (blue curve) and of the iron(III) complex $\mathbf{C}_{H}$ (red curve).



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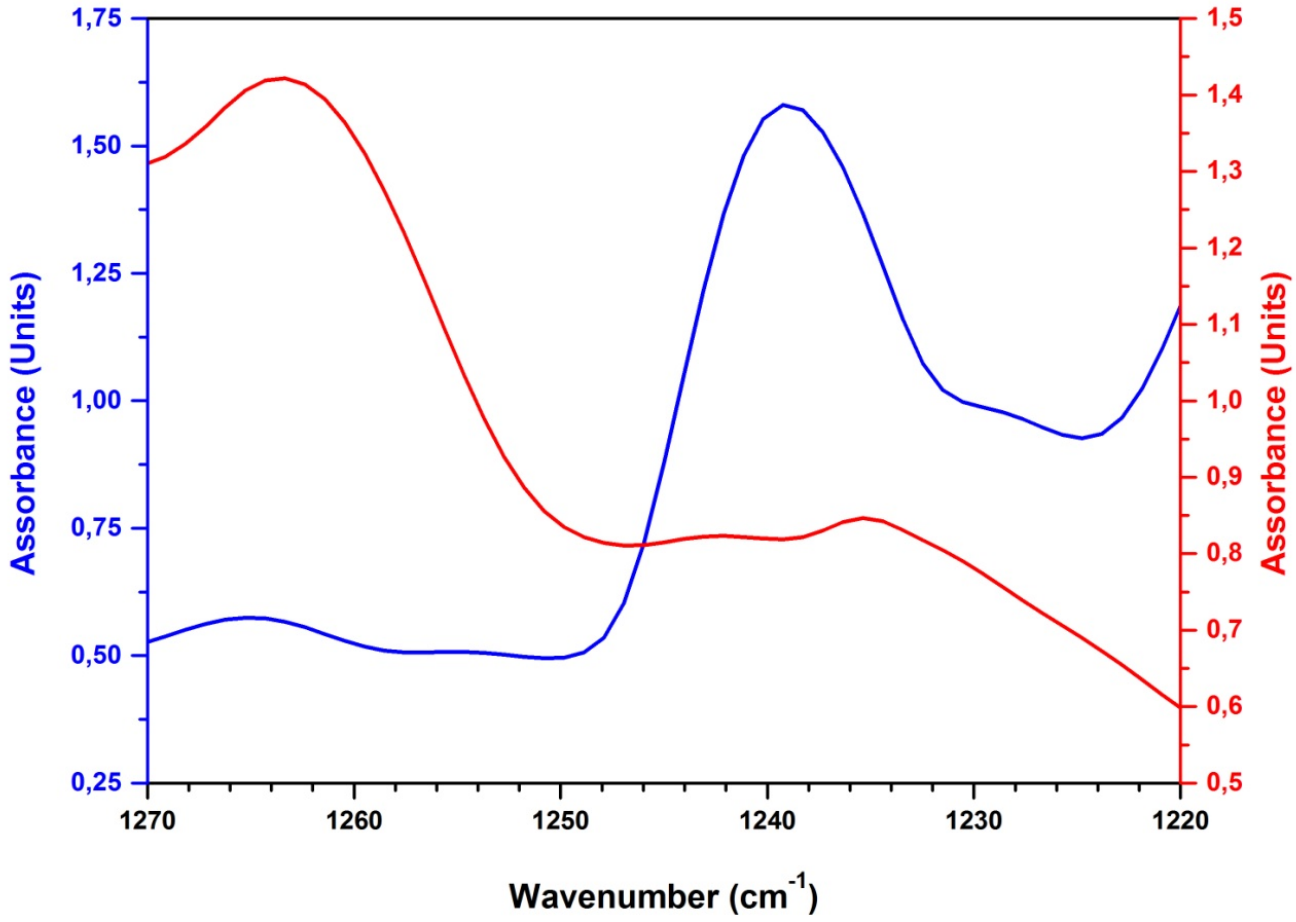

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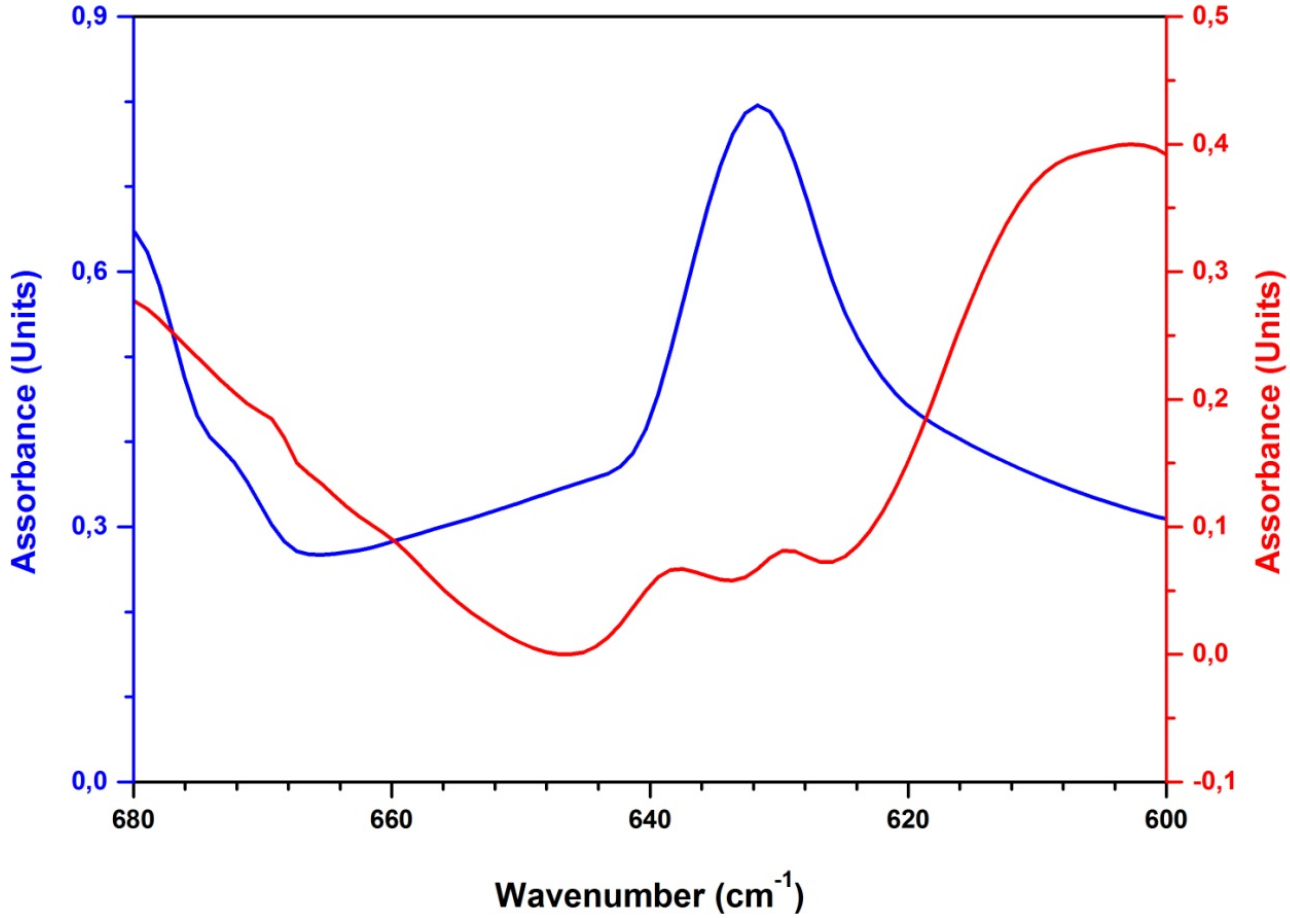

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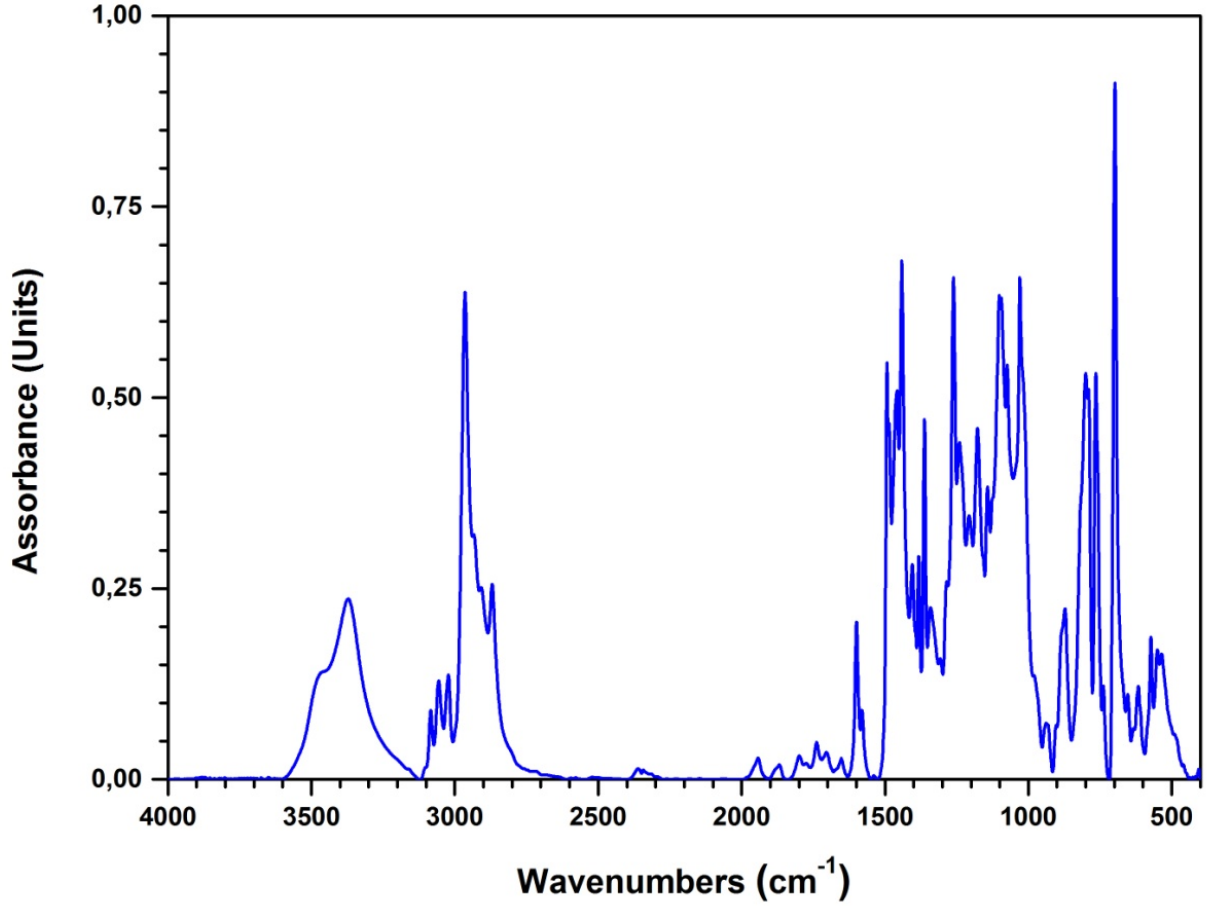


Figure S15. FT-IR spectrum of the pro-ligand $\mathbf{L}_{Cum}$ (KBr disk).

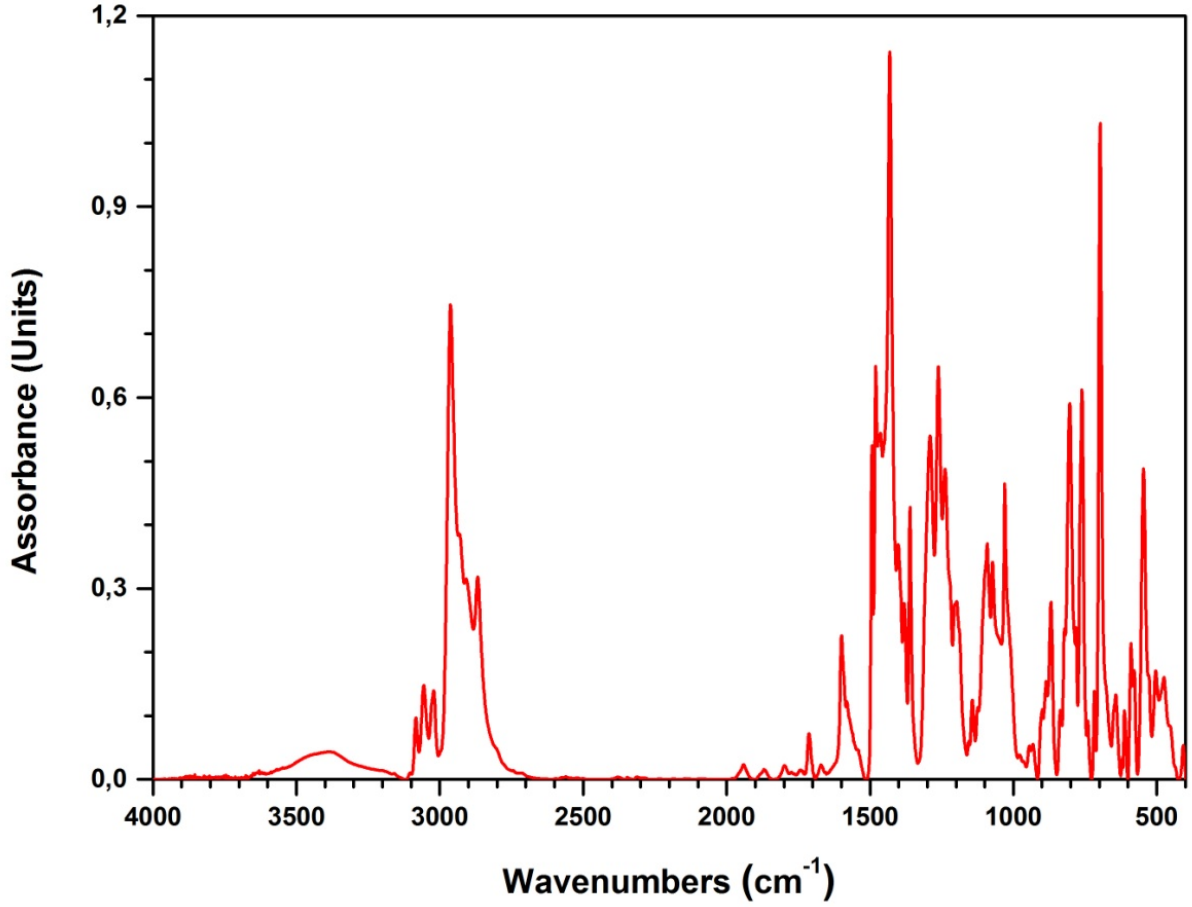


Figure S16. FT-IR spectrum of the complex $\mathbf{C}_{Cum}$ (KBr disk).

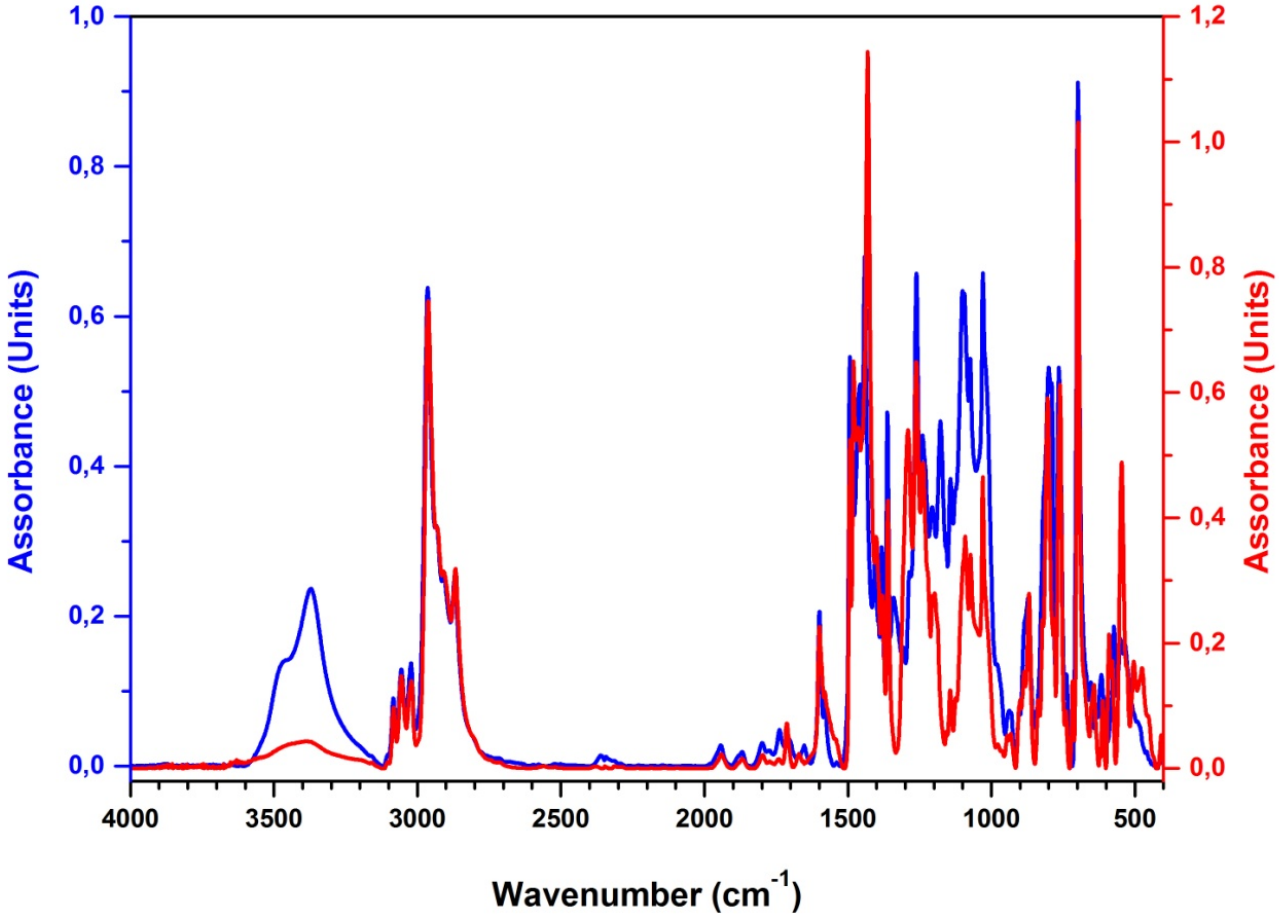


Figure S17. Comparison of the FT-IR spectra of the pro-ligand $\mathbf{L}_{Cum}$ (blue curve) and of the iron(III) complex $\mathbf{C}_{Cum}$ (red curve).

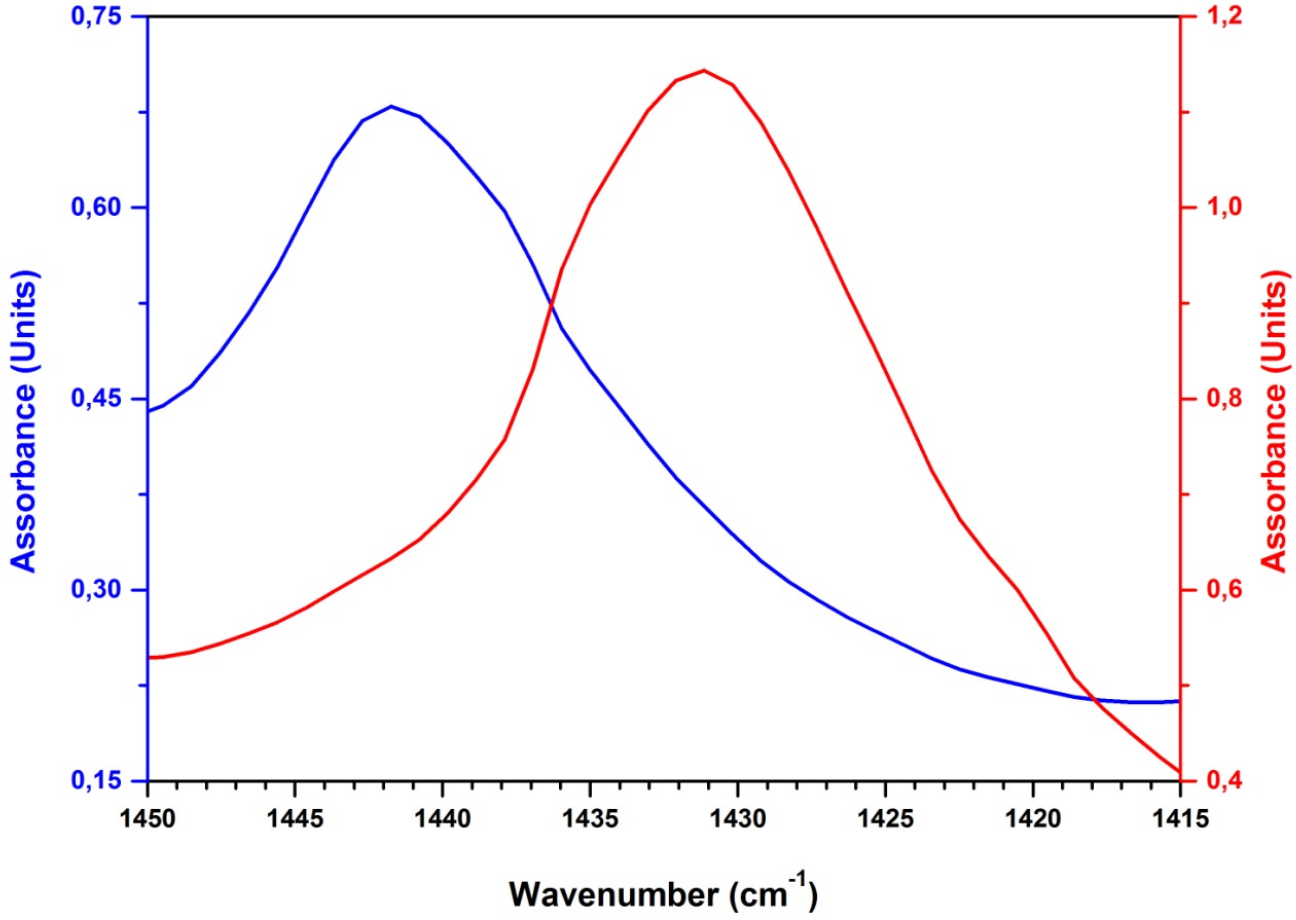
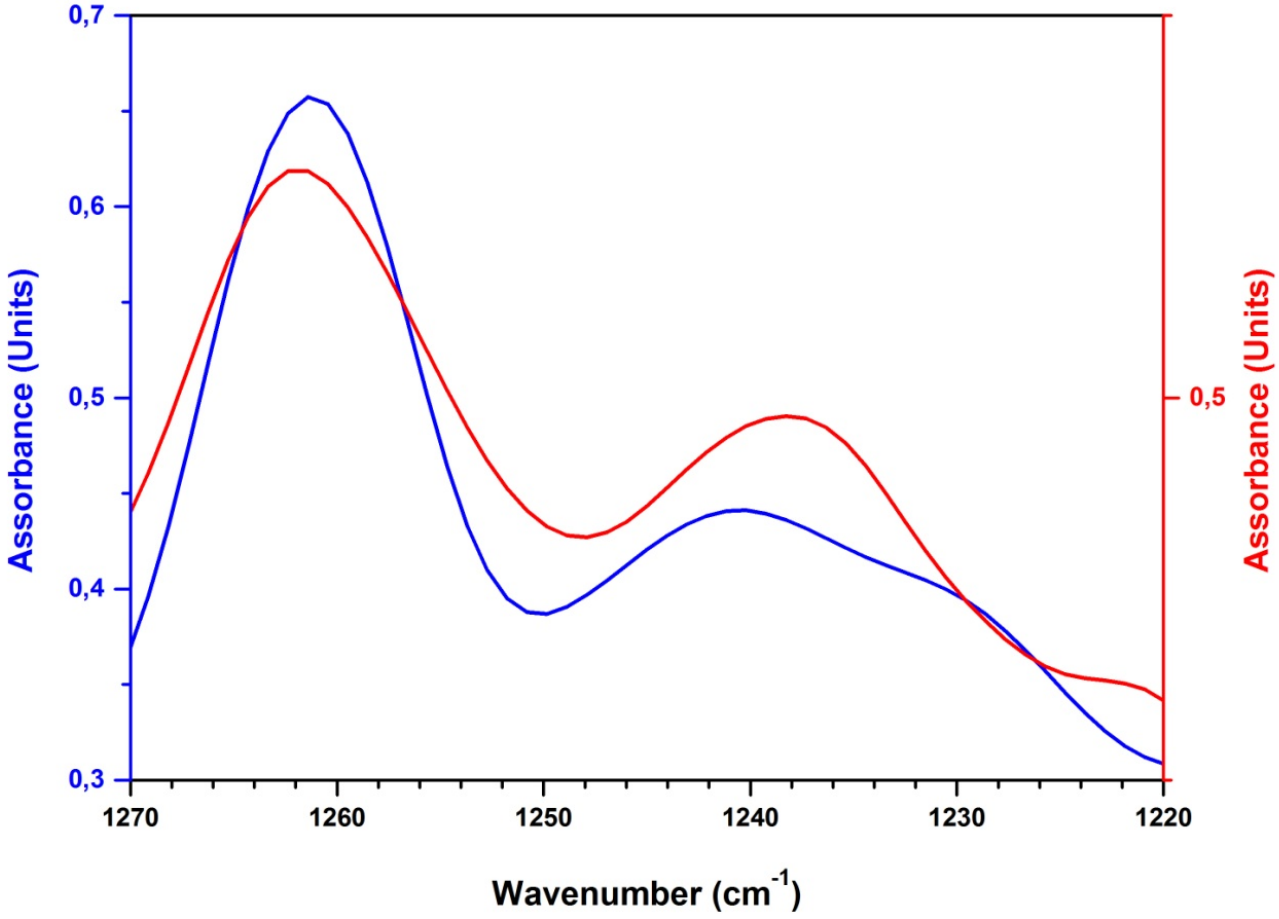


Figure S18. Magnification of the region 1450-1415 cm^{-1} (for the CH_2-S-C deformation)[1,2] of the FT-IR spectra of the pro-ligand $\mathbf{L}_{Cum}$ (blue curve) and of the iron(III) complex $\mathbf{C}_{Cum}$ (red curve).



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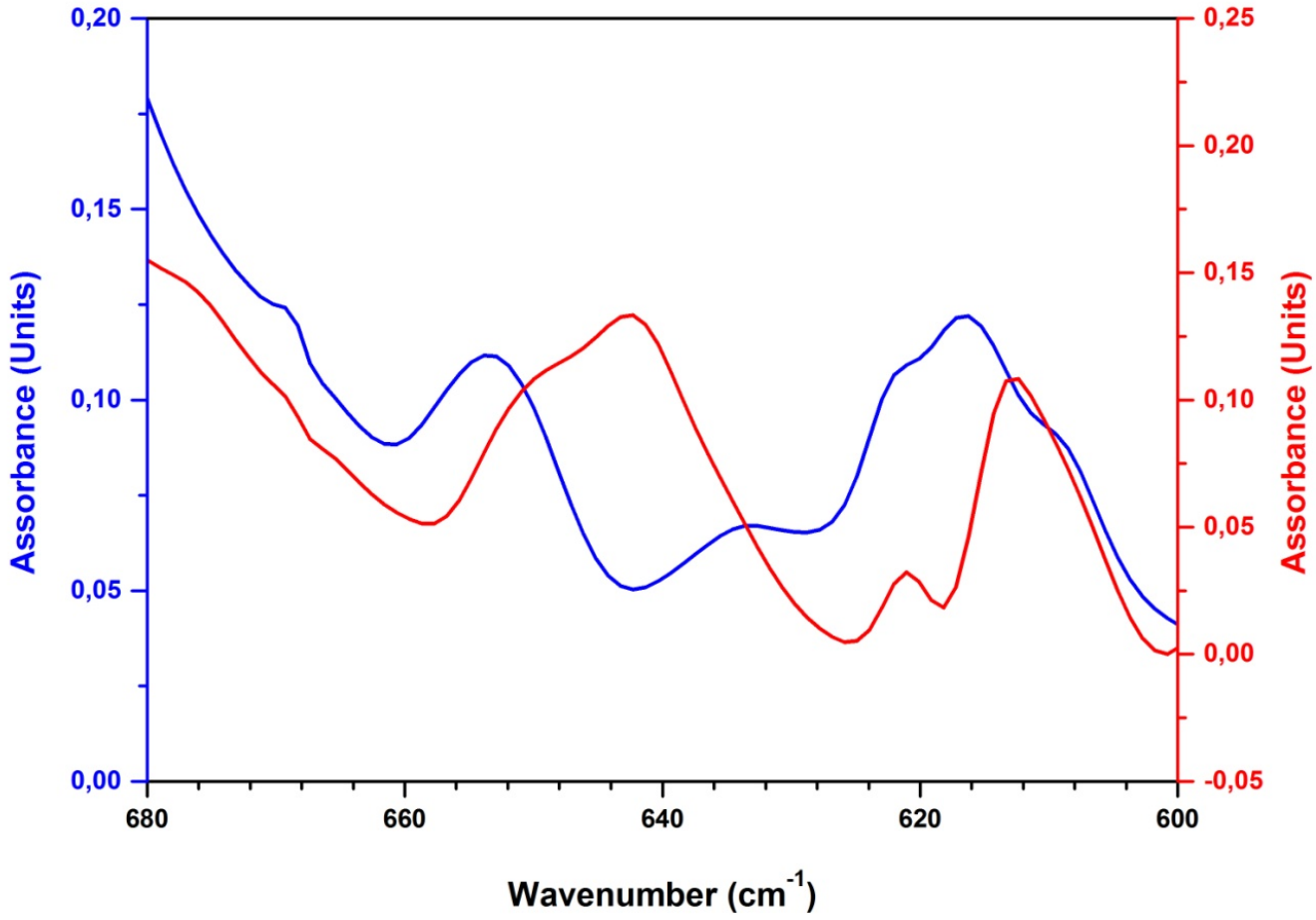

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UV-Vis Analysis.

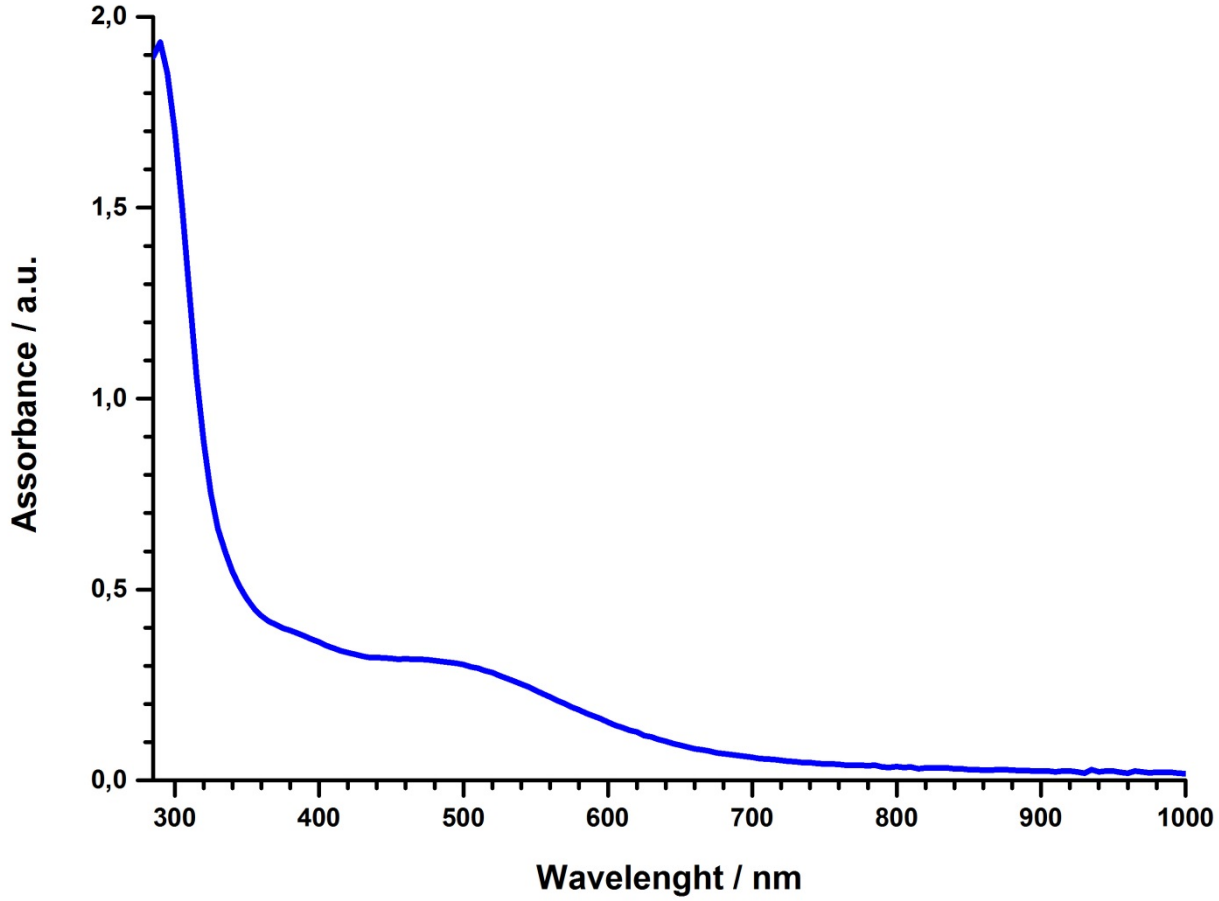

Figure S21. UV-Vis spectrum of the complex $\mathbf{C}_{\boldsymbol{H}}$ (1.07×10^{-4} M in toluene; $\varepsilon_{470} = 2804$ L mol^{-1} cm^{-1}).

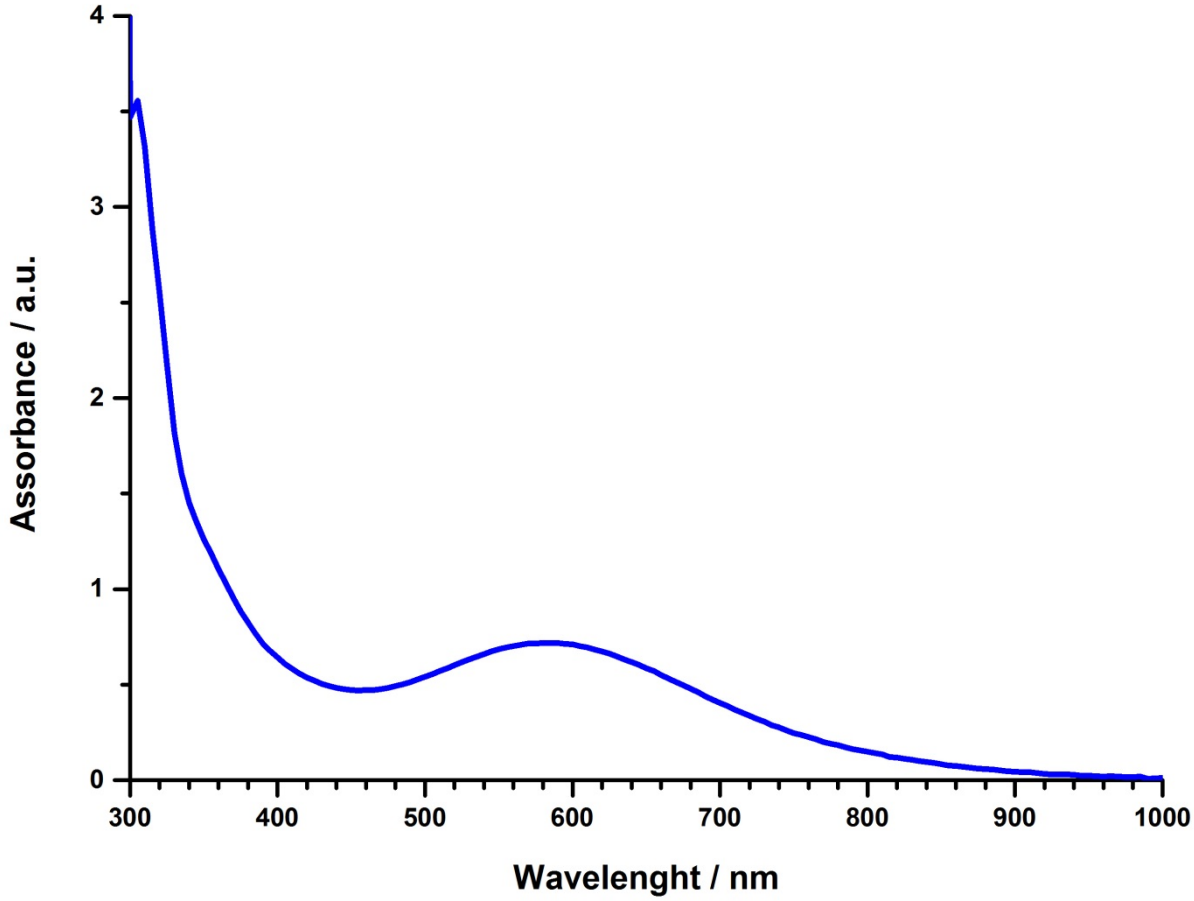

Figure S22. UV-Vis spectrum of the complex $\mathbf{C}_{\boldsymbol{Cum}}$ (1.07×10^{-4} M in toluene; $\varepsilon_{585} = 7188$ L mol^{-1} cm^{-1}).

References.

1. *The Sadtler handbook of infrared spectra*. ed. W. W. Simons, Sadtler Research Laboratories, Philadelphia, 1978.

2. *Interpreting Infrared, Raman, and Nuclear Magnetic Resonance Spectra*, ed. R. A. Nyquist, Academic Press, San Diego, 2001, pp. 65-83.