

Supplementary Information

Structure and properties of an Fe(III) complex containing a novel amide functionalized polyimidazole ligand.

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Physical Measurements:

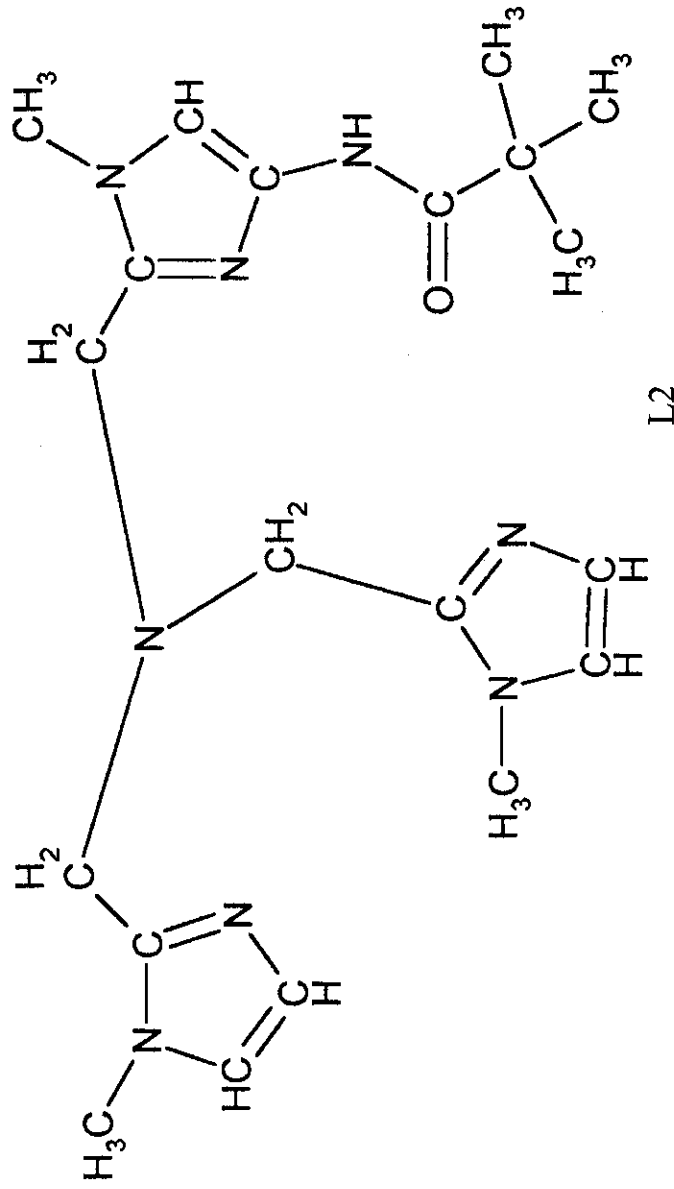
Compounds L1, L2, 1 and 2 have been characterized by elemental analysis (Midwest Analytical, Inc.) X-ray diffraction, ¹H, ¹³C NMR, UV-visible and FT-IR spectroscopies, electrospray mass spectrometry, and cyclic voltammetry.

Single crystal X-ray diffraction studies were performed using a Bruker Smart Apex diffractometer equipped with a cryoflex low-temperature apparatus, or on an Enraf-Nonius CAD4 diffractometer. Crystallographic data of compounds 1 and 2 were recorded at 293 and 100K, respectively.

¹H, ¹³C NMR spectra of L2 in CDCl₃ were recorded using a Varian Unity Inova 500 MHz NMR spectrometer at room temperature. UV-vis spectra of compounds 1 and 2 (1x10⁻⁴M in CH₃CN) were recorded using a Cary 50 Bio spectrophotometer. FT-IR spectrum of L2 was recorded using a Mattson Galaxy Series FTIR 5000 spectrophotometer. A chloroform solution of L2 was evaporated on Ag/AgCl plates prior to recording the spectrum. Positive ion mode electrospray mass spectra of compounds L2 and 1 were recorded using Micromass Mass Spectrometer Electrospray Triple Quadrupole Quattro LCZ.

Cyclic voltammograms of compounds 1 and 2 (1x10⁻³M in CH₃CN) containing 0.1 M TBAP were recorded using a standard three-electrode cell which included a glassy carbon working electrode, Pt-coil auxiliary electrode and a Ag/AgCl reference electrode. The electrochemical measurements were recorded using a PARC Model 175 programmer; Model 173 potentiostat/gavanostat and Houston 2000 X-Y recorder.

Structure and Formula



Molecular Weight 398.52

Molecular Formula C₂₀H₃₀N₈O

Elemental Analysis C₂₀H₃₀N₈O · H₂O

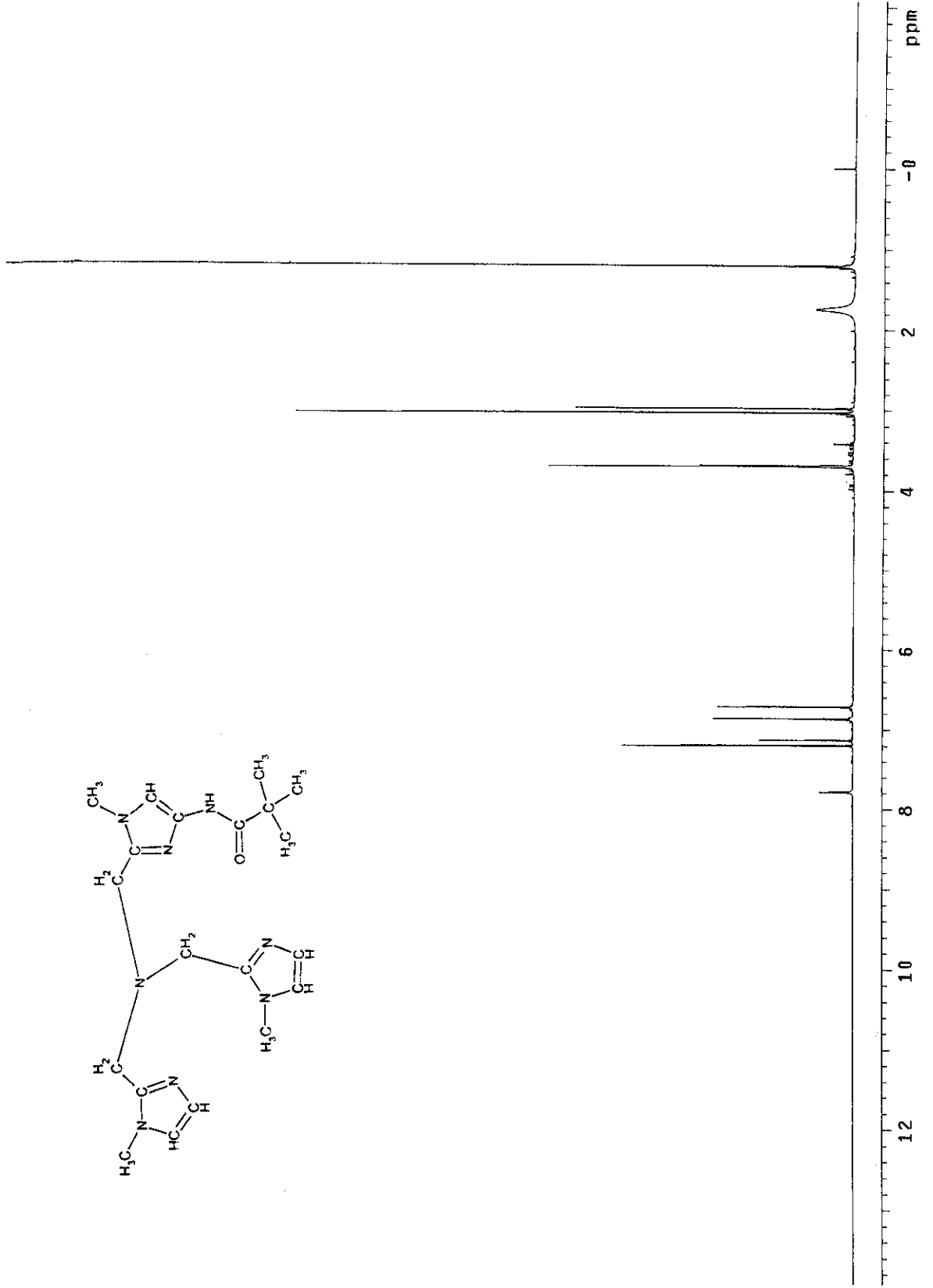
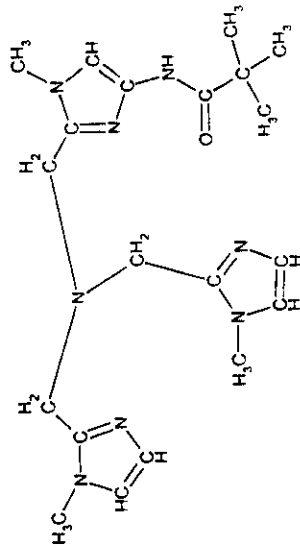
Calcd. : C 57.69, H 7.69, N 26.92

Found: C 58.00, H 7.94, N 27.04

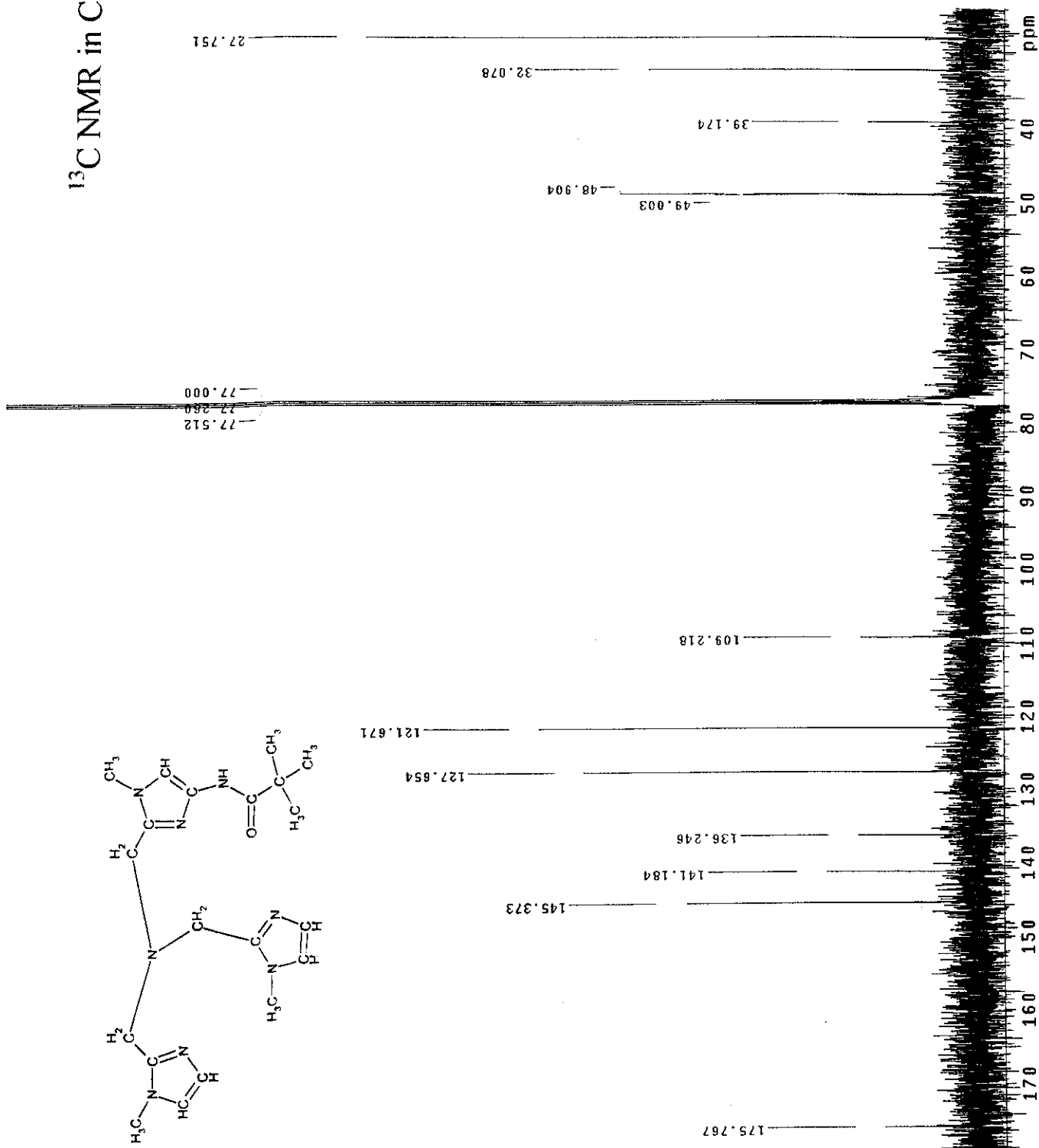
(water detected in proton spectrum of compound in CDCl₃)

ESI-MS 399.2 (M+H⁺)

¹H NMR in CDCl₃



^{13}C NMR in CDCl_3



NMR spectroscopic data

^1H NMR in CDCl_3

L2

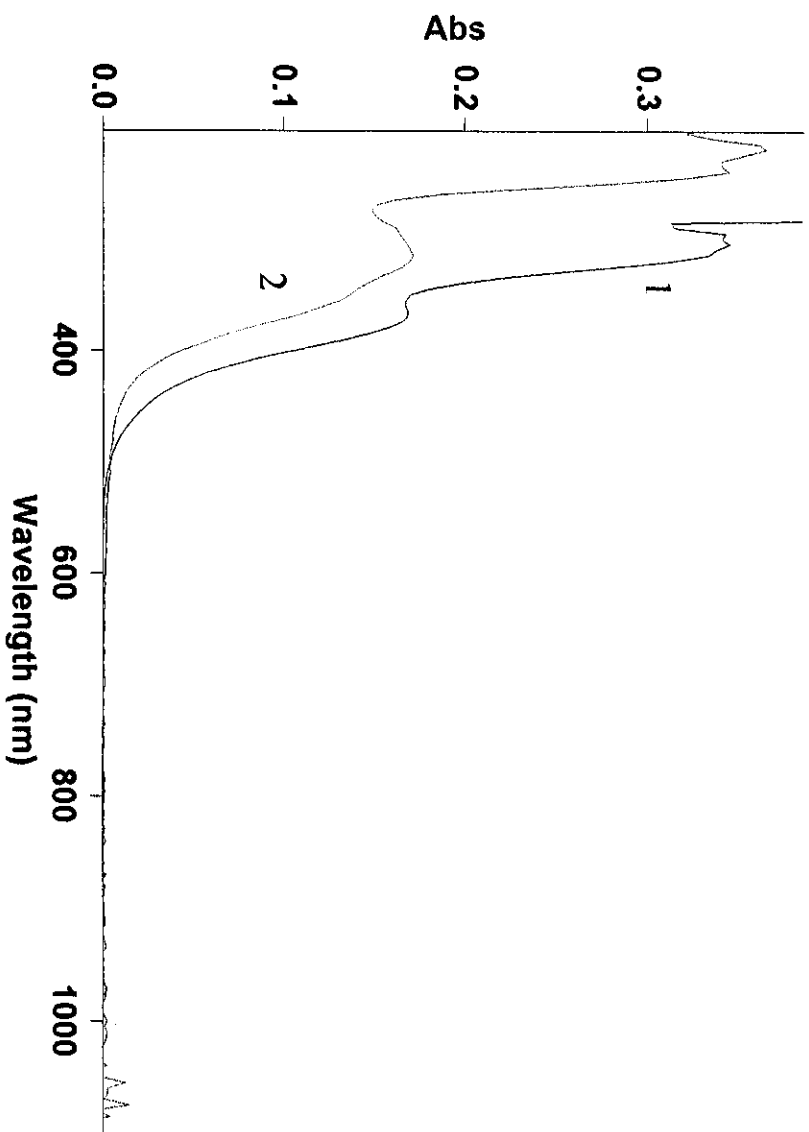
| ppm | Assignment | Integral | Multiplicity |
|------|---|----------|--------------|
| 7.8 | $^{\text{Am}}\text{Im}(-\text{NH}-)$ | 1 | s |
| 7.21 | $^{\text{Am}}\text{Im}(\text{C5-H})$ | 1 | s |
| 6.95 | $\text{Im}(\text{C5-H})$ | 1 | s |
| 6.8 | $\text{Im}(\text{C4-H})$ | 1 | s |
| 3.78 | $\text{Im}(-\text{CH}_2-)$ | 4 | s |
| 3.77 | $^{\text{Am}}\text{Im}(-\text{CH}_2-)$ | 2 | s |
| 3.11 | $\text{Im}(\text{N-CH}_3-)$ | 6 | s |
| 3.05 | $^{\text{Am}}\text{Im}(\text{N-CH}_3-)$ | 3 | s |
| 1.29 | $^{\text{Am}}\text{Im}(\text{tBu})$ | 9 | s |

^{13}C NMR in CDCl_3

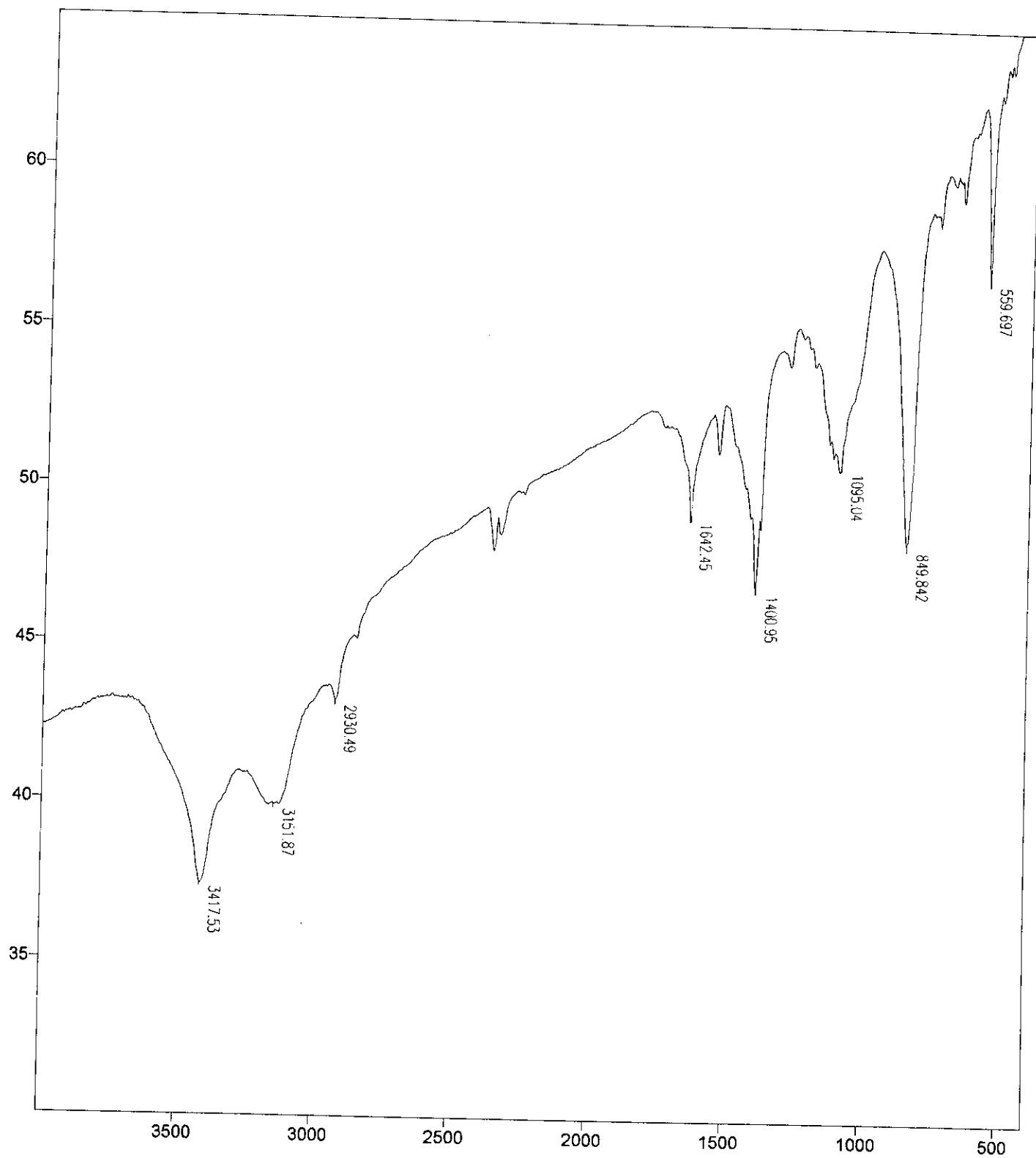
| ppm | Assignment |
|-------|---|
| 175.8 | $^{\text{Am}}\text{Im}(-\text{C}=\text{O})$ |
| 145.4 | $\text{Im}(\text{C2})$ |
| 141.2 | $^{\text{Am}}\text{Im}(\text{C2})$ |
| 136.3 | $^{\text{Am}}\text{Im}(\text{C4})$ |
| 127.7 | $\text{Im}(\text{C5})$ |
| 121.7 | $\text{Im}(\text{C4})$ |
| 109.2 | $^{\text{Am}}\text{Im}(\text{C5})$ |
| 48.9 | $\text{Im}(-\text{CH}_2-),$ $^{\text{Am}}\text{Im}(-\text{CH}_2-)$ |
| 39.2 | $^{\text{Am}}\text{Im}(\text{tBu-C})$ |
| 32.1 | $\text{Im}(\text{N-CH}_3-),$ $^{\text{Am}}\text{Im}(\text{N-CH}_3-)$ |
| 27.8 | $^{\text{Am}}\text{Im}(\text{tBu})$ |

$^{\text{Am}}\text{Im}$ corresponds to the amide functionalized imidazole ring

UV-visible Spectra of Compounds 1 and 2

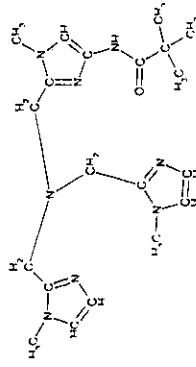


FT-IR Spectrum of L2

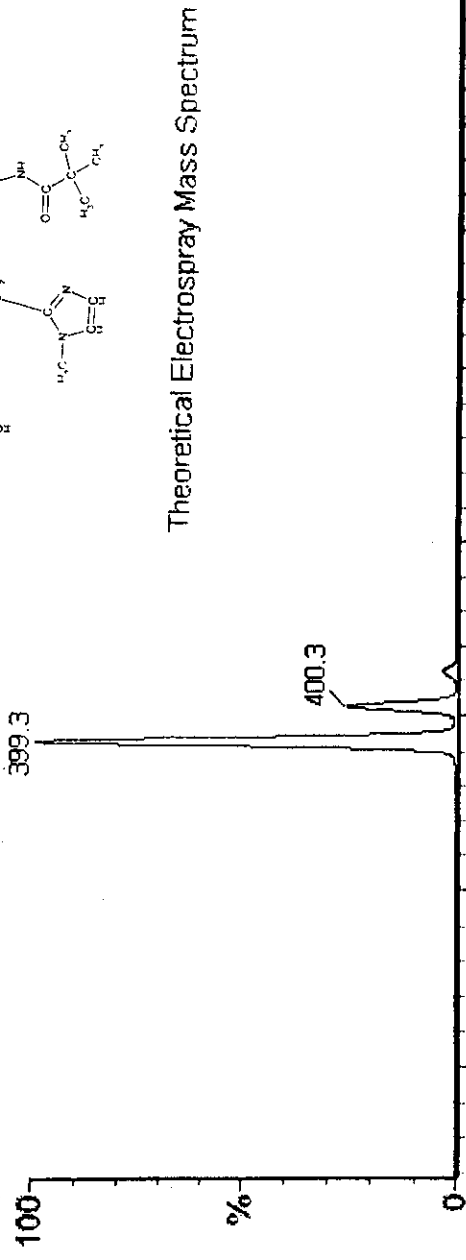


ESI-MS

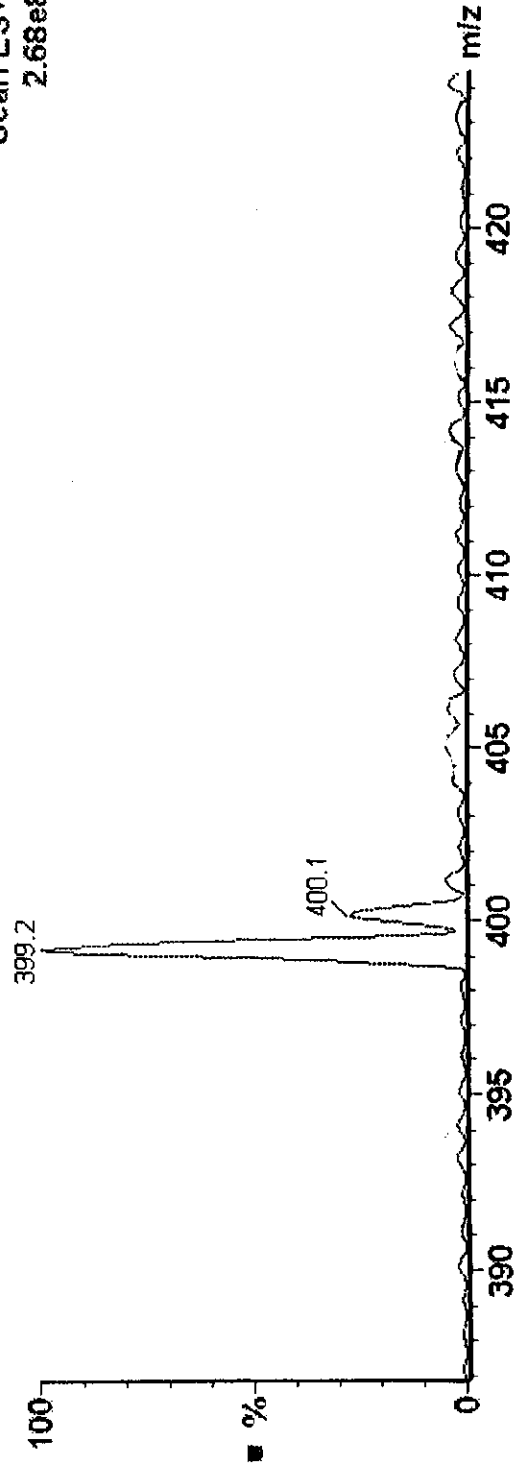
Molecular Ion

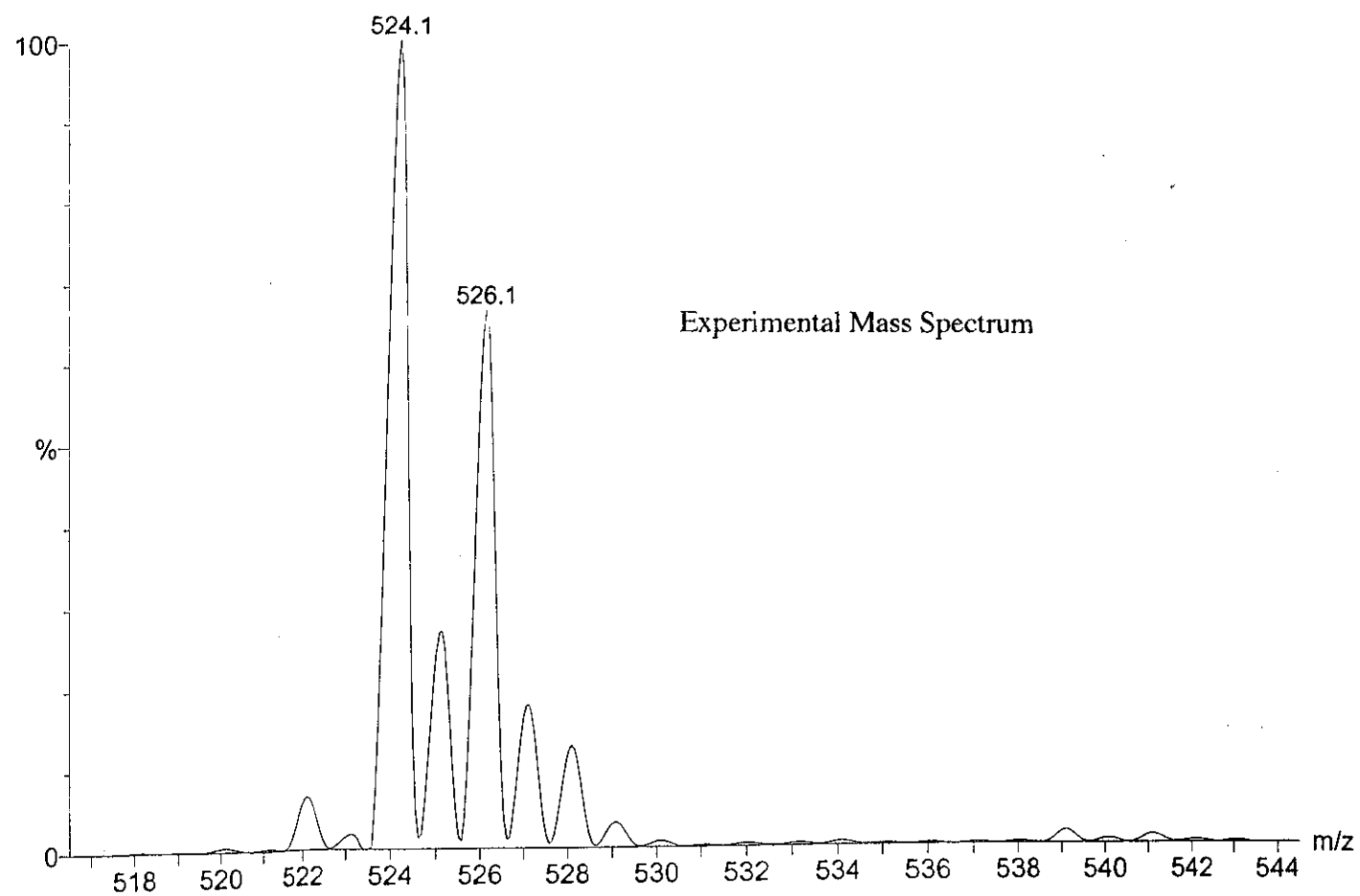
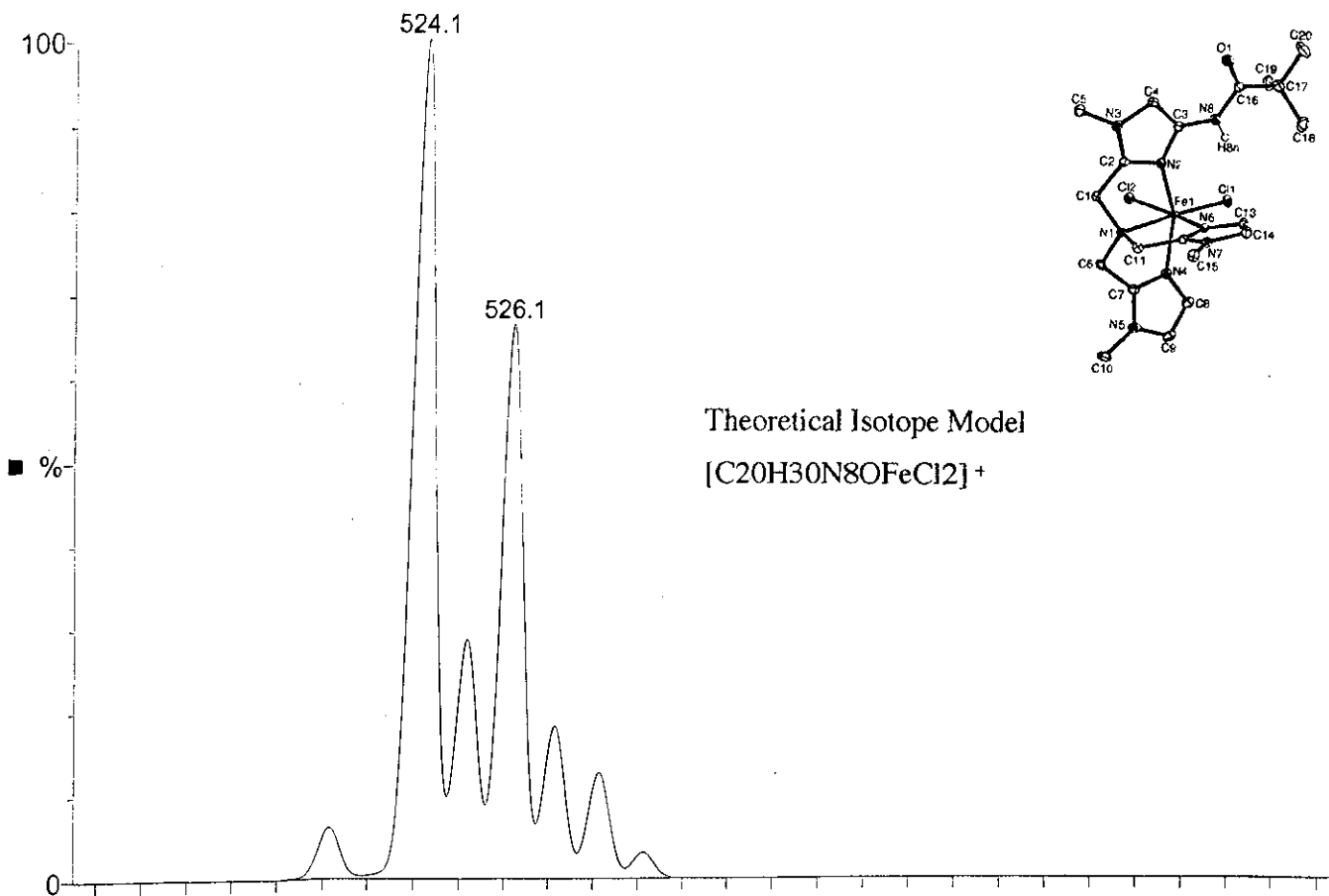


Scan ES+
7.73e12

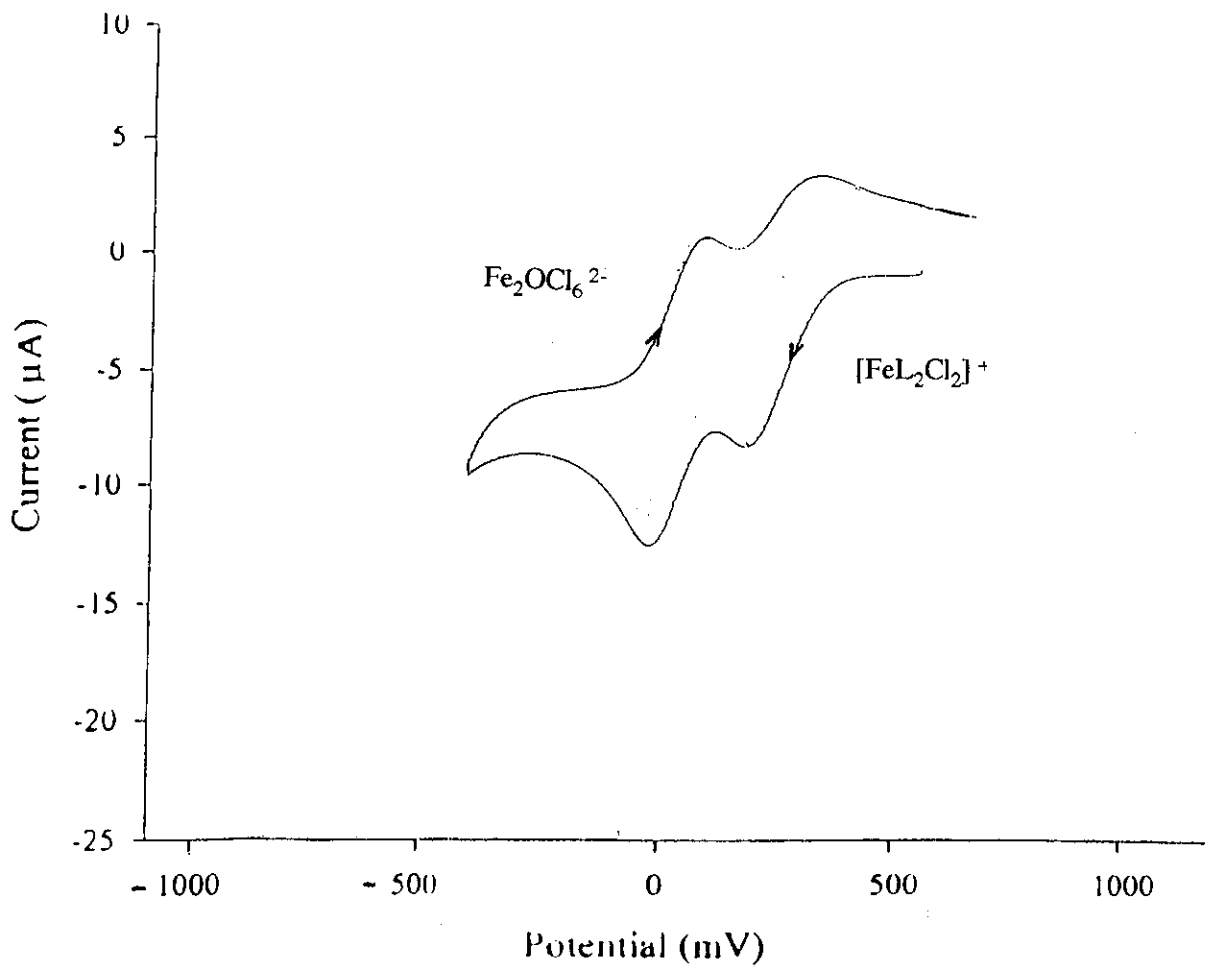
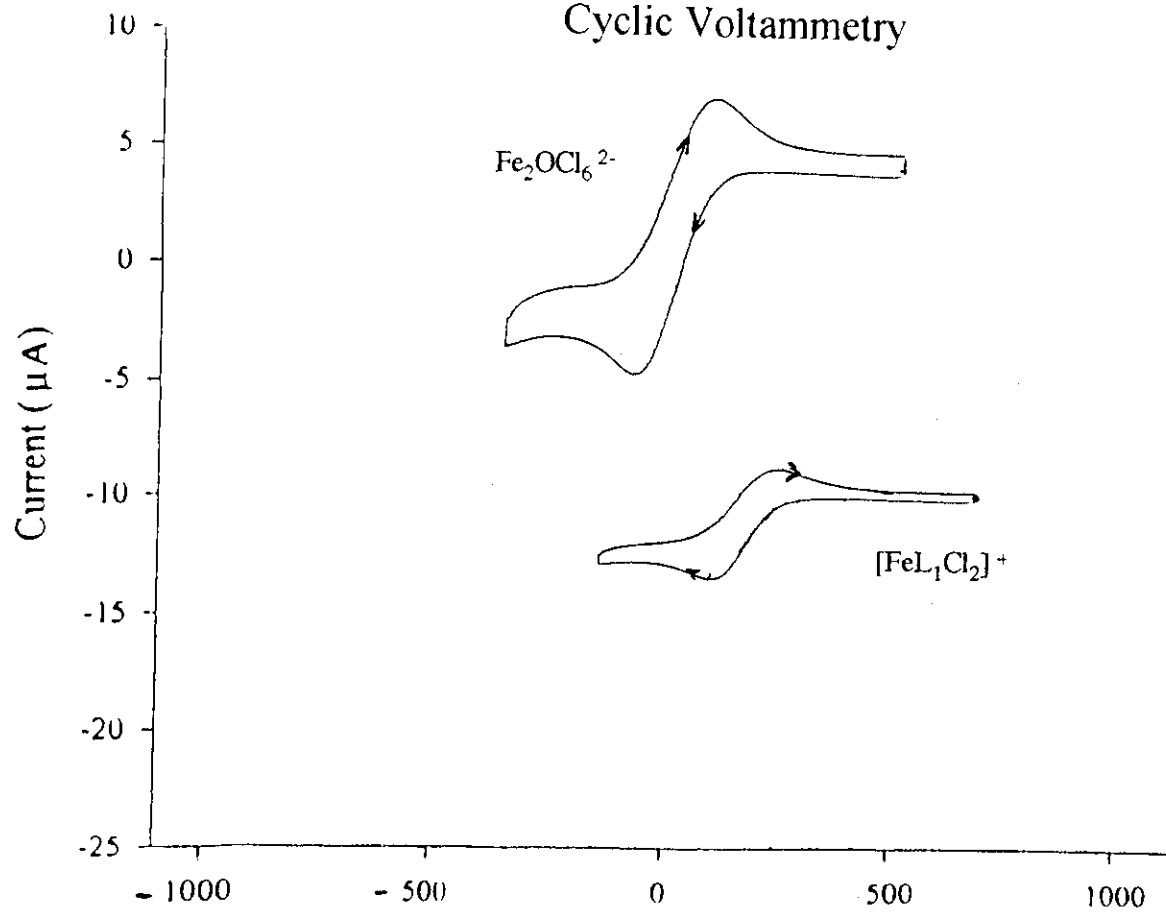


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2.68e8



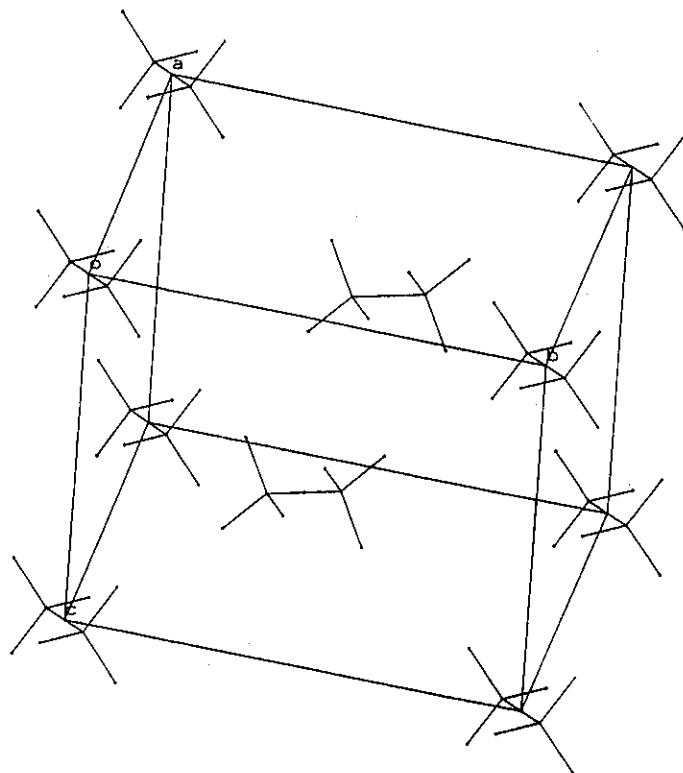


Cyclic Voltammetry



Packing diagrams

Packing diagram for the anionic species $\text{Fe}_2\text{OCl}_6^{2-}$



Packing diagram for the cationic species $\text{Fe}(\text{L}_2)\text{Cl}_2^+$

