Effective chiral recognition among ions in polar media

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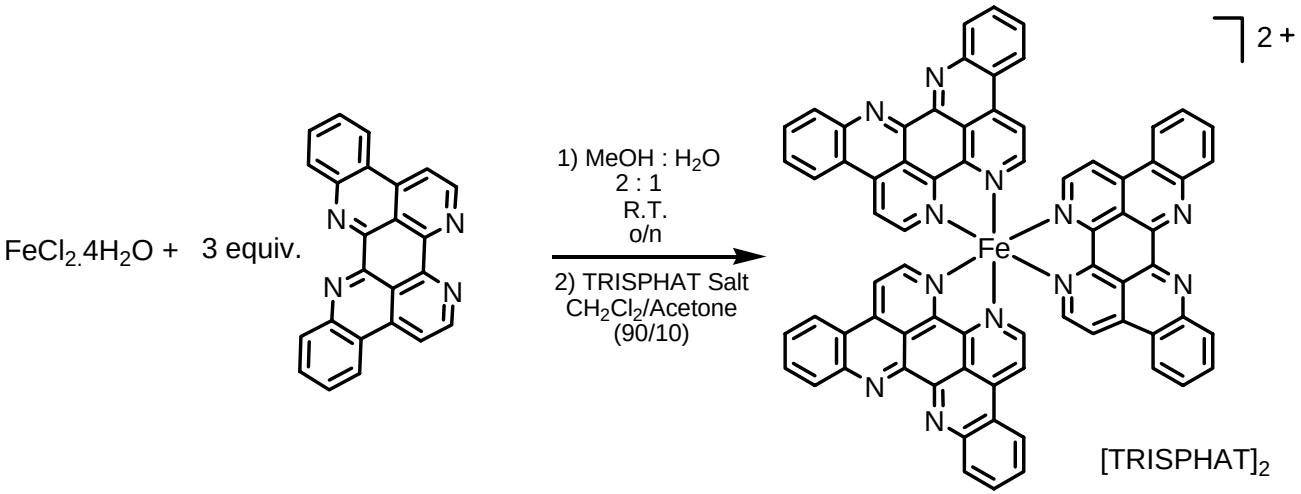
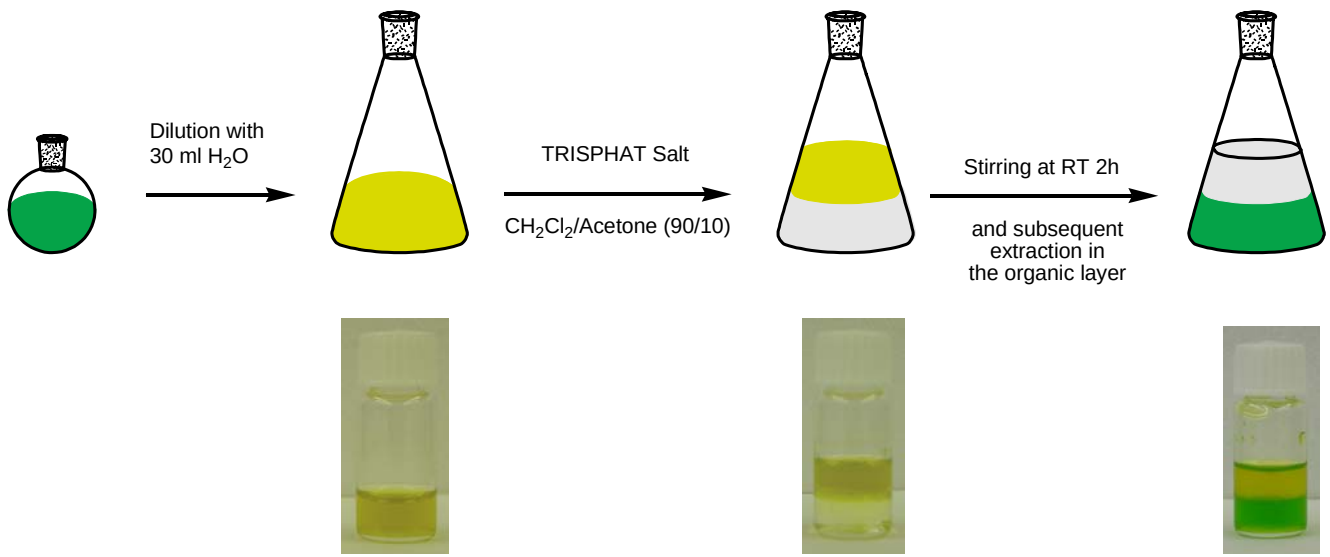
Supporting Information

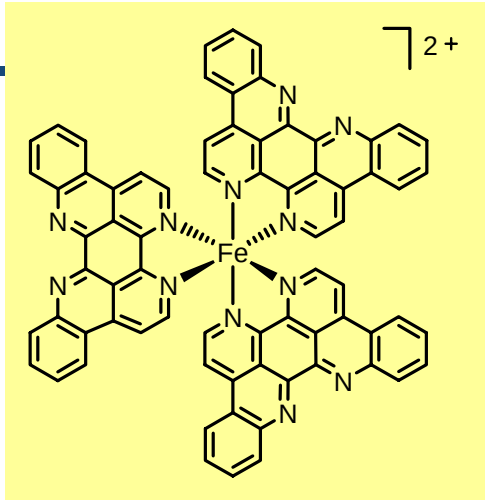
General Information. Solvents were dried and distilled prior to use. Chloroform (Fluka) and CD_2Cl_2 were filtered on basic alumina before use. Analytical thin layer chromatography was performed on Merck 0.25 mm silica gel plates. Visualization was accomplished with UV light. ^{1}H, ^{13}C, ^{19}F and ^{31}P NMR spectra were recorded on a Bruker AMX-500 spectrometer. Chemical shifts are given in ppm. ^{1}H chemical shifts were reported relative to Me_4Si. ^{31}P chemical shifts were reported relative to H_3PO_4. ^{19}F chemical shifts were reported relative to $CFCl_3$. Optical rotations were measured on a JASCO P-1030 polarimeter in a thermostated (20 °C) 10.0 cm long microcell with high pressure lamps of sodium and are reported as follows: $[\alpha]_{\lambda}^{20}$ (c (g/100 ml), solvent). UV spectra were recorded on a CARY 1 BIO spectrophotometer in a 1 cm quartz cell; λ_{max} were given in nm and molar adsorption coefficient ε in $mol^{-1}.L.cm^{-1}$. Circular dichroism spectra were recorded on a JASCO J-715 spectropolarimeter in a 1 cm quartz cell; λ were given in nm and molar circular-dichroic absorption $\Delta\varepsilon$ in $mol^{-1}.L.cm^{-1}$. FABMS were obtained on a VG-AutoSpec M250 mass spectrometer, in a *m*-nitrobenzyl alcohol matrix.

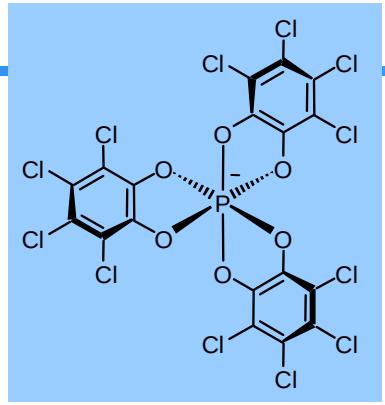




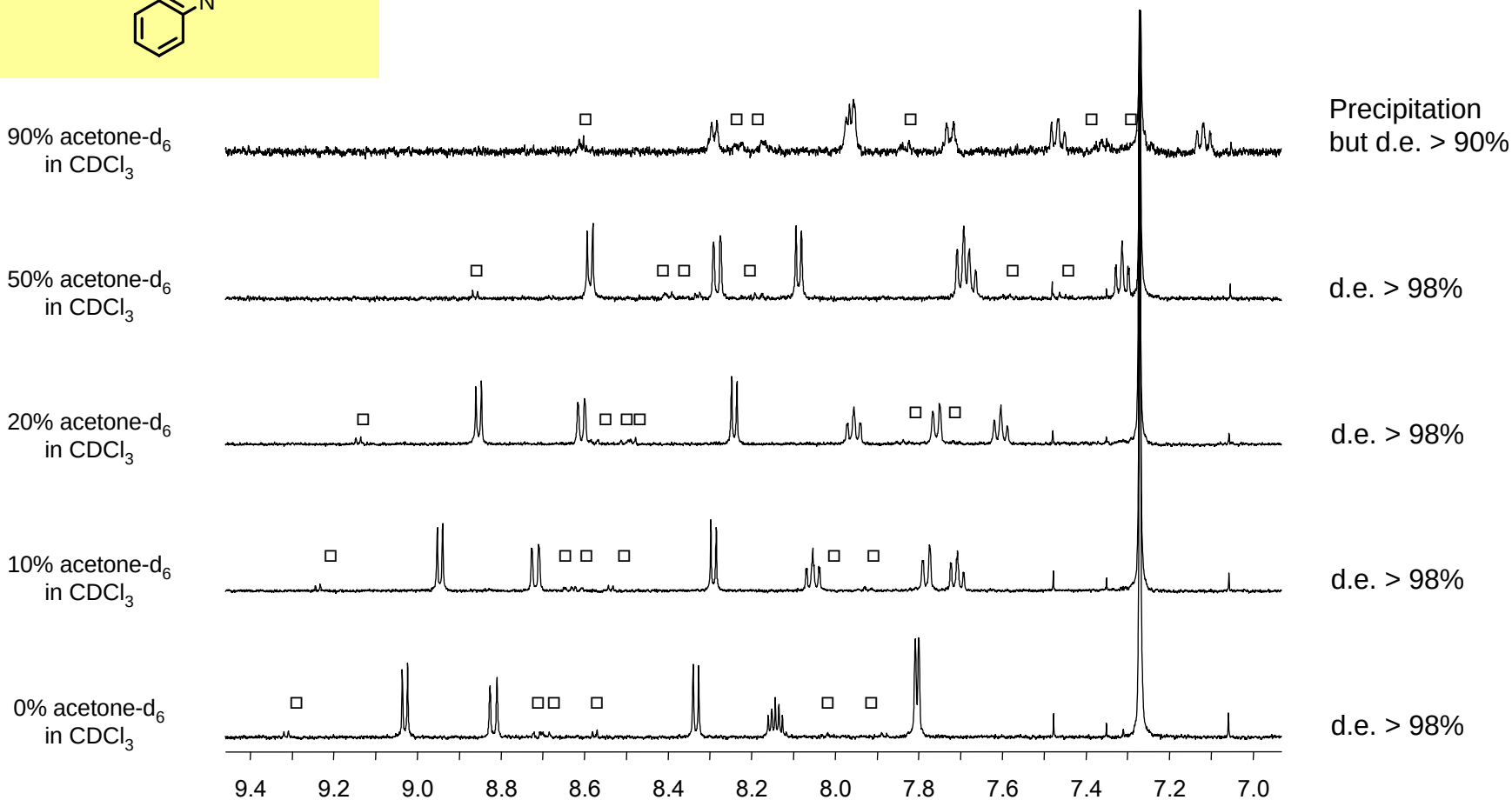
$[Fe(\mathbf{3})_3][\Delta\text{-}\mathbf{1}]_2$, Yield = 80 %; $[Fe(\mathbf{3})_3][\Lambda\text{-}\mathbf{1}]_2$, Yield = 70 %

^1H NMR (500 MHz)



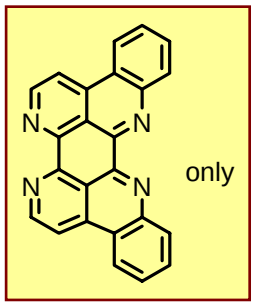


NO trace of the minor diastereomer
even in 90% acetone.
Only traces of free ligand □
see next page

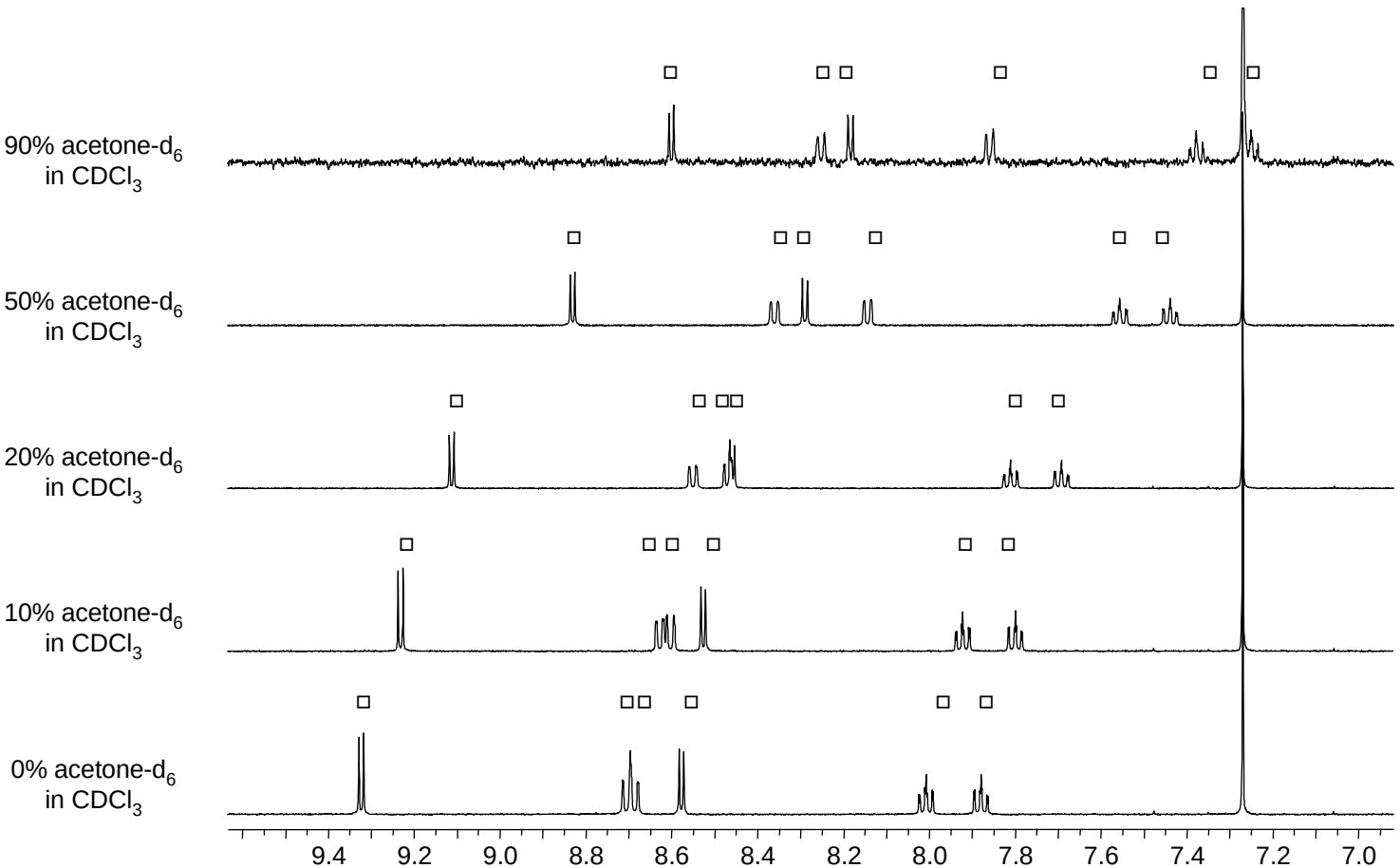


Conc. $5.4 \cdot 10^{-4}$ *M* except for the top spectrum

^1H NMR (500 MHz)

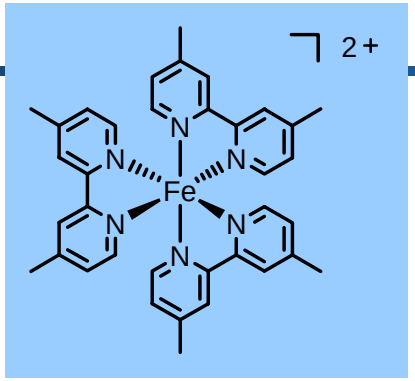


only

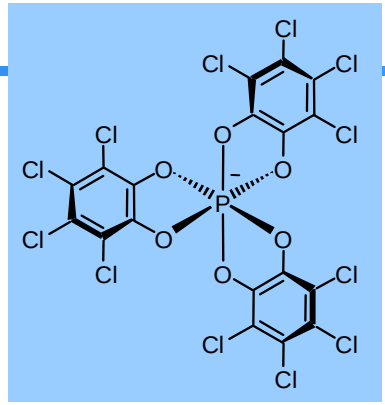


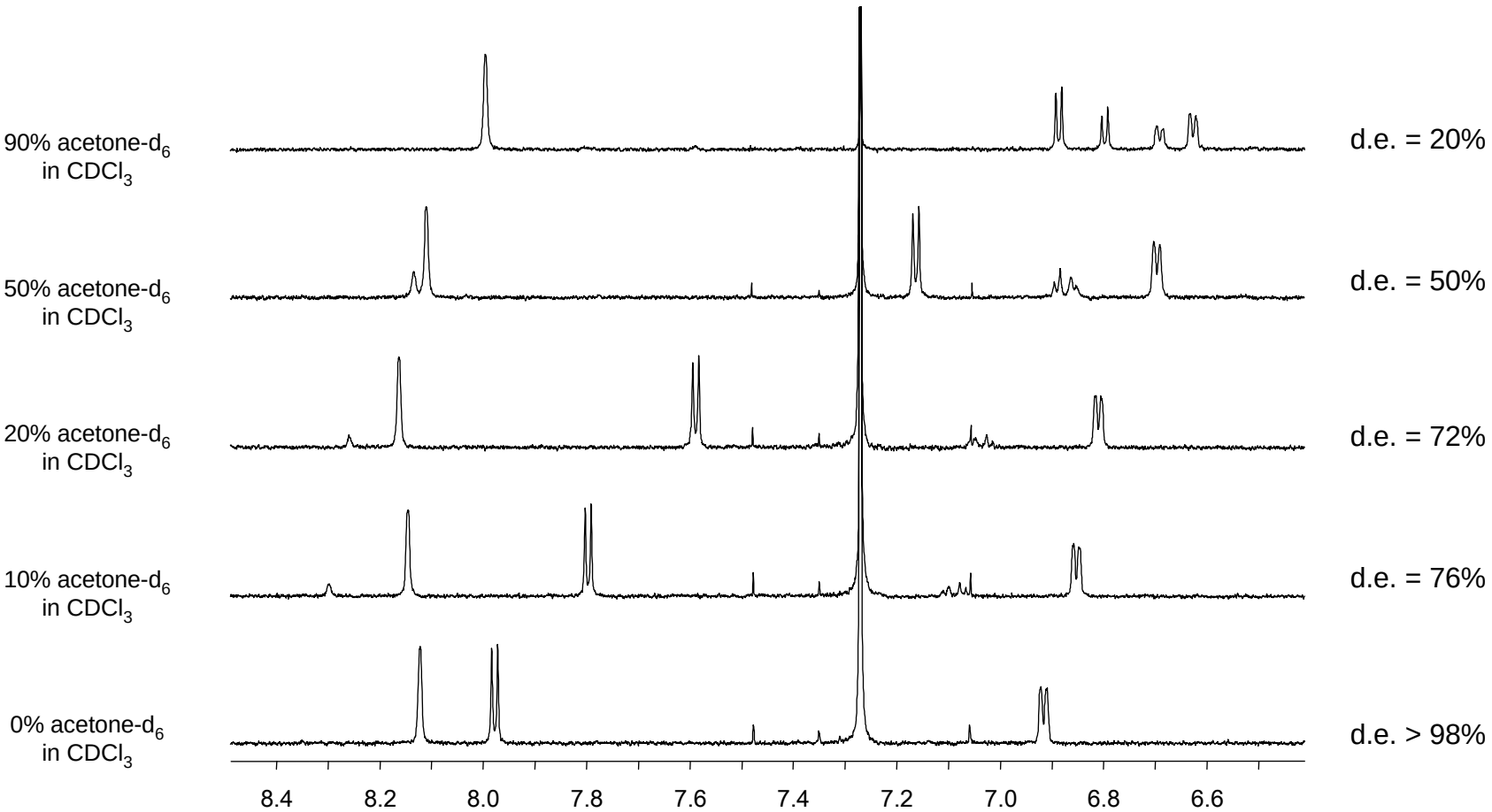
Precipitation

Conc. $5.4 \cdot 10^{-4}$ *M* except for the top spectrum

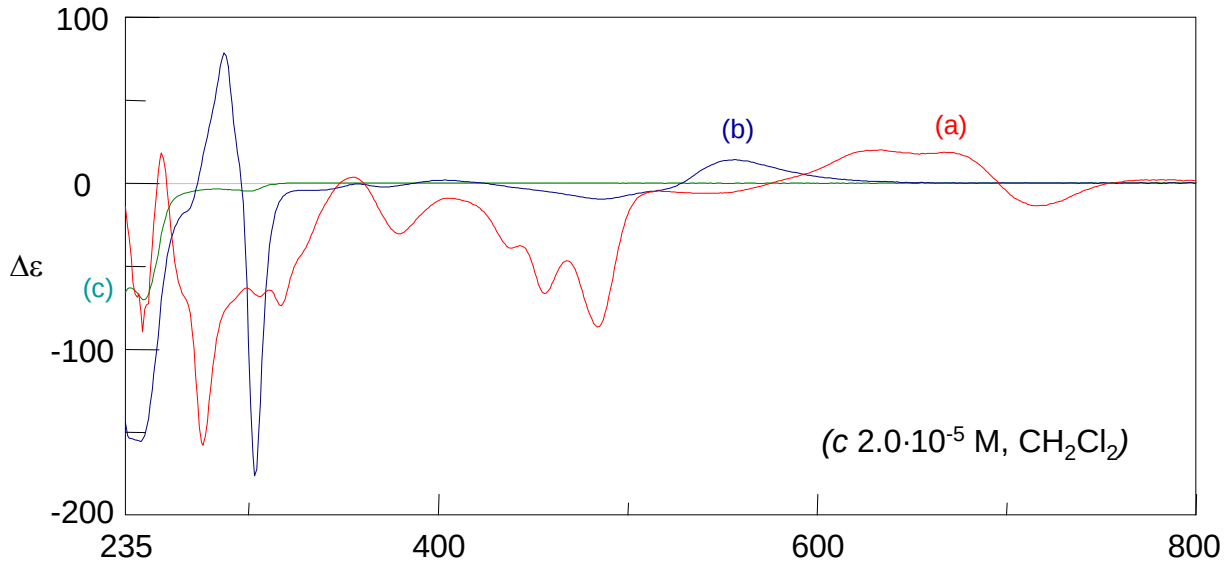


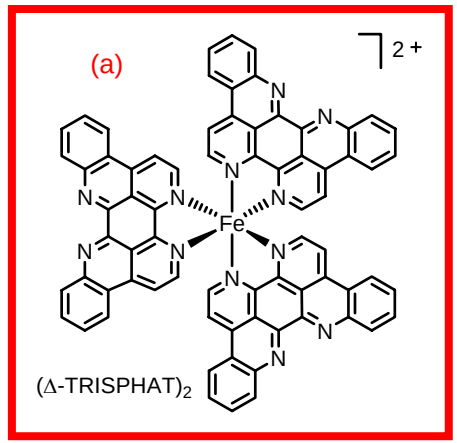
^1H NMR (500 MHz)

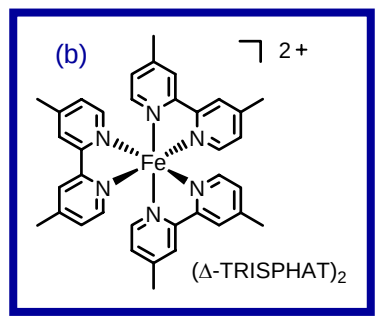


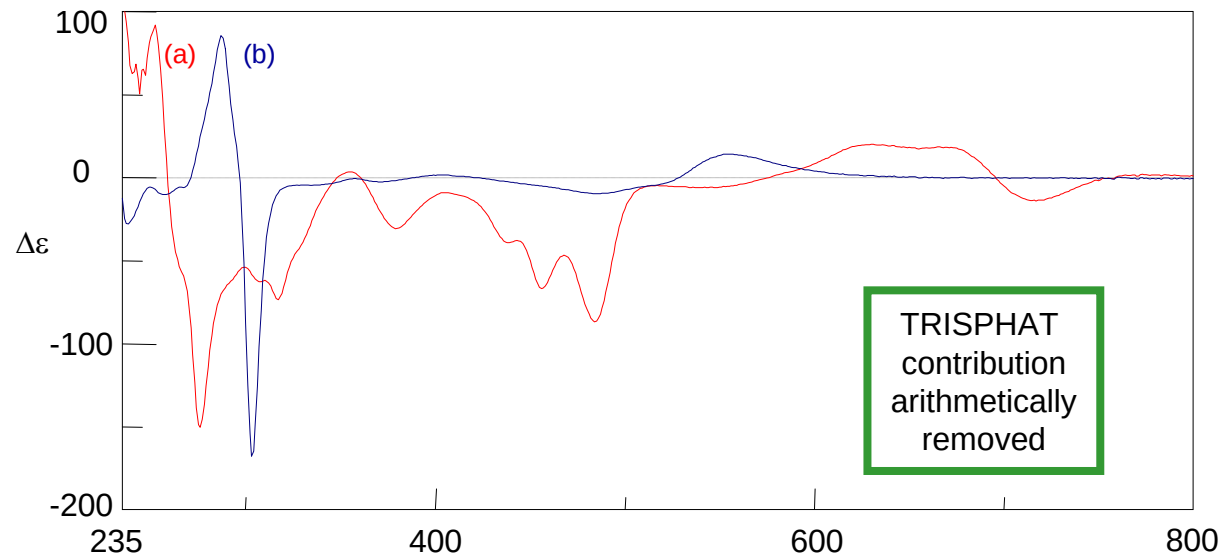


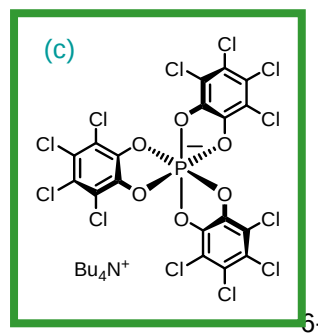
*Experimental and Calculated CD Spectra of [Fe(LL)$_3$][Δ-**1**]$_2$*

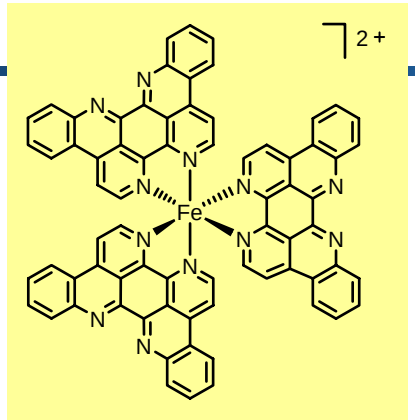


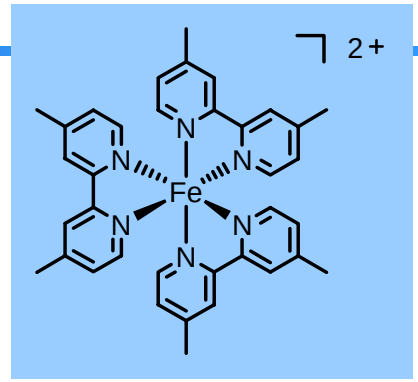


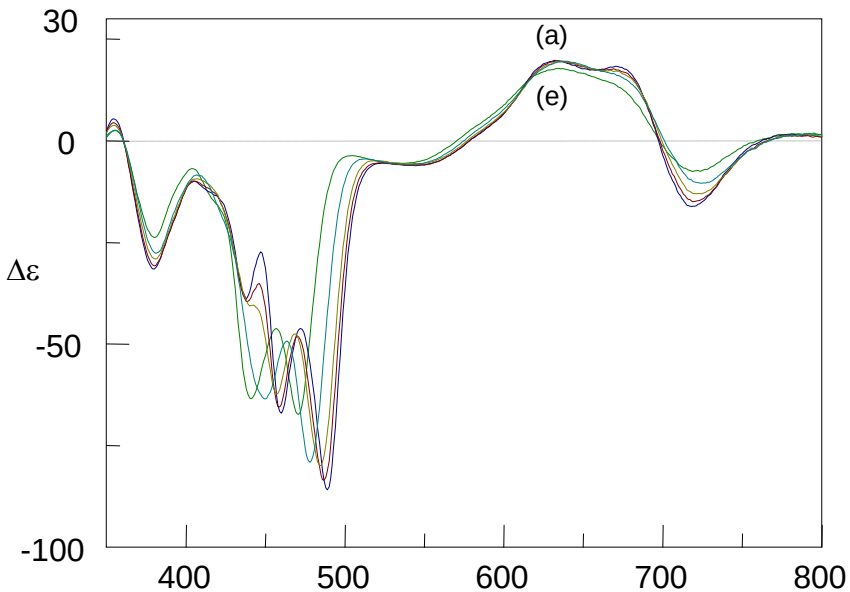


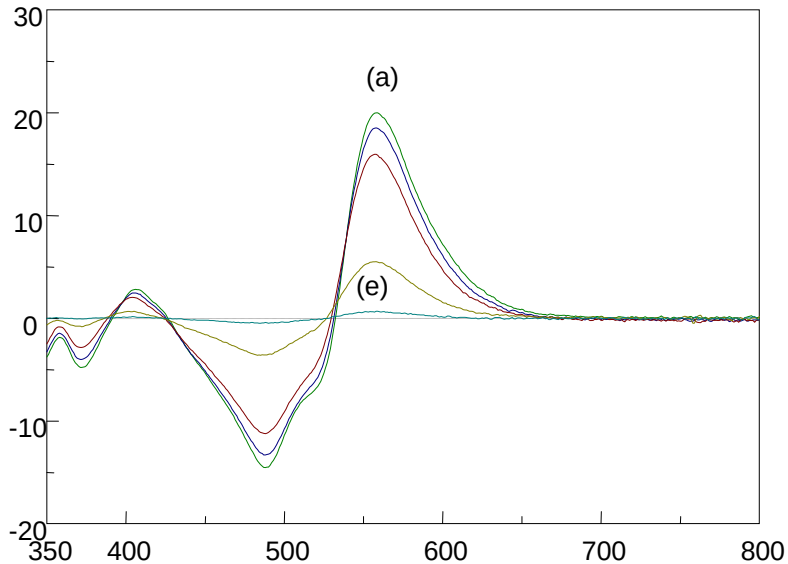












(a) 0% acetone-d_6 in $CDCl_3$ (b) 10% acetone-d_6 in $CDCl_3$ (c) 20% acetone-d_6 in $CDCl_3$ (d) 50% acetone-d_6 in $CDCl_3$ (e) 90% acetone-d_6 in $CDCl_3$