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Supporting Informations

for

Bis(acetonitrile)bis(acetylacetonato)ruthenium(III) mediated chemical transformations of coordinated 2-methylthioanilide

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Table S1. Solvent Effect on the position of the Long-Wavelength ν_{max} (cm^{-1}) of **1c** with dipole moment of the solvent

Solvent	ν (cm^{-1})	Dipole Moment (D)
n-Heptane	17513.1348511	0.00
n-Hexane	17513.1348511	0.00
Toluene	17574.6924428	0.37
Dichloromethane	18018.018018	1.60
Dimethylformamide	18018.018018	3.82
Dimethylsulfoxide	18148.8203266	3.96
Acetonitrile	18214.9362477	3.92

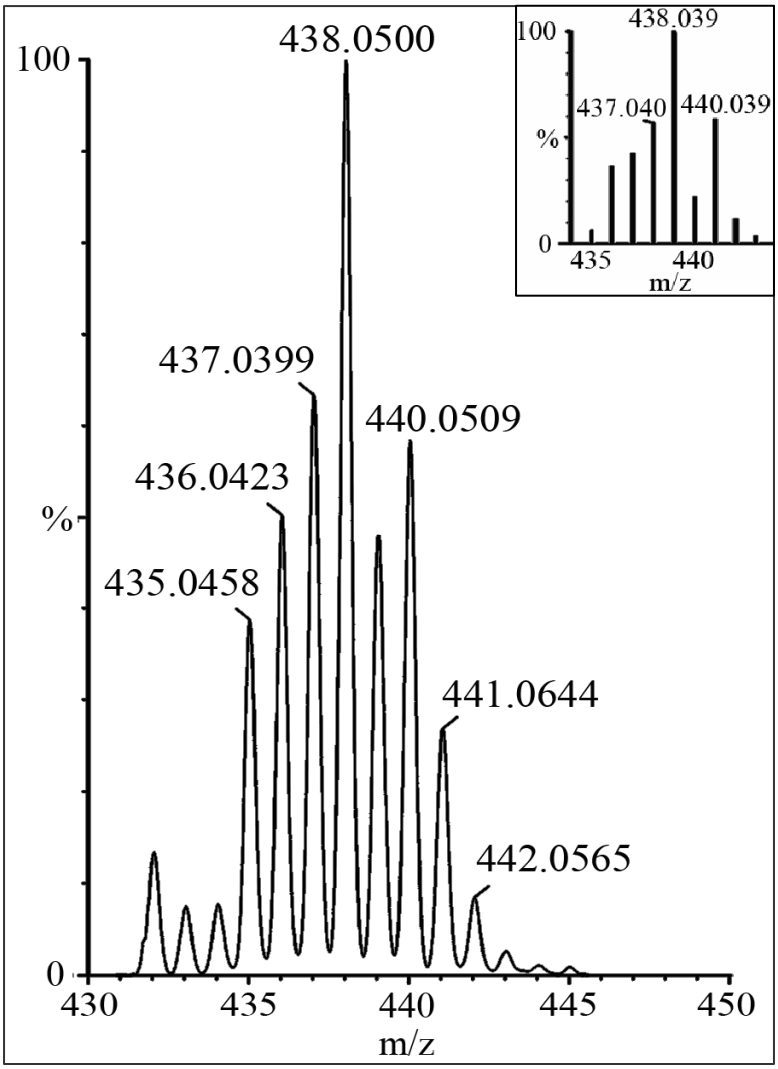

Figure S1. Experimental and simulated (inset) ESI mass spectra for the complex **1a**.

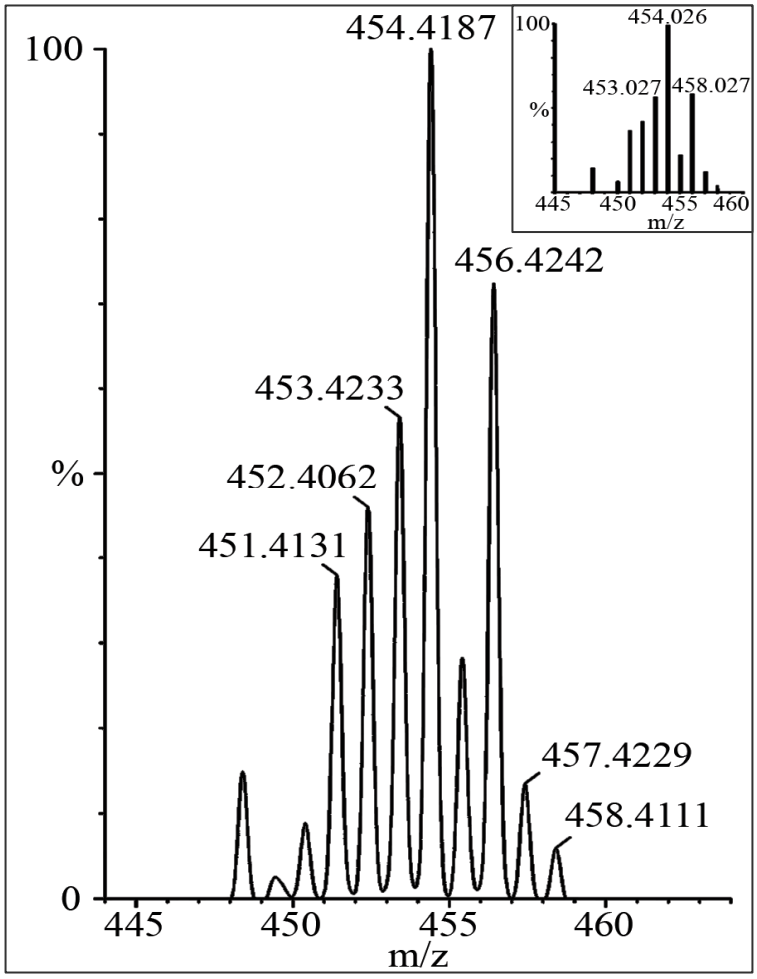

Figure S2. Experimental and simulated (inset) ESI mass spectra for the complex **1b**.

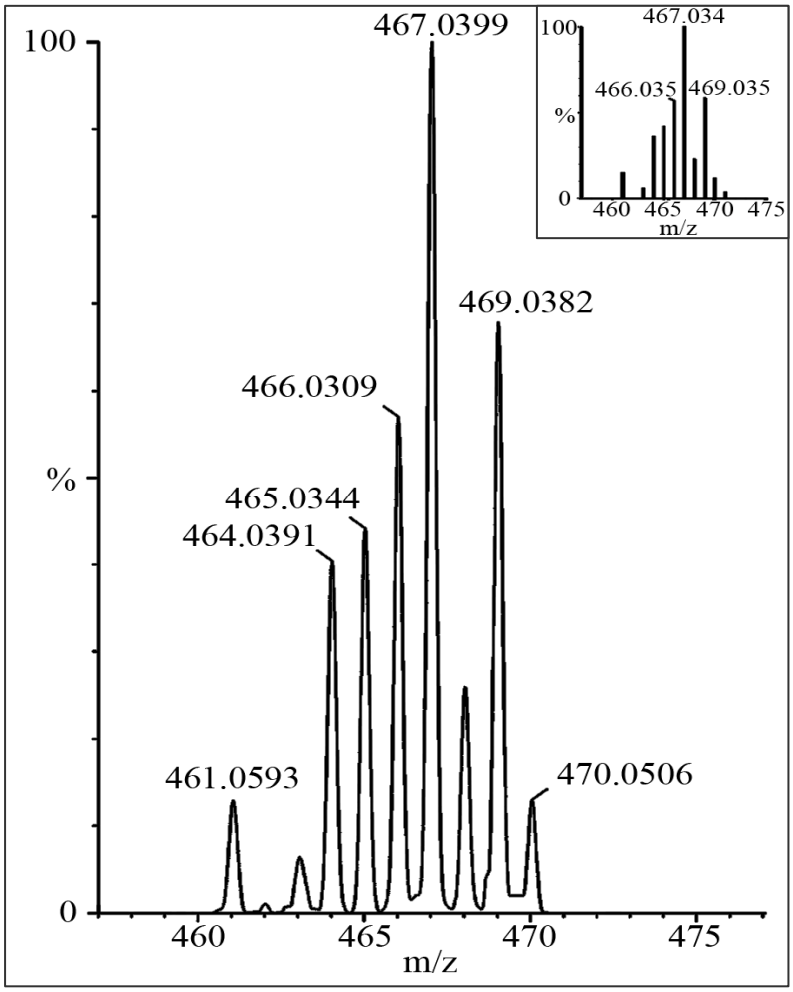

Figure S3. Experimental and simulated (inset) ESI mass spectra for the complex **1c**.

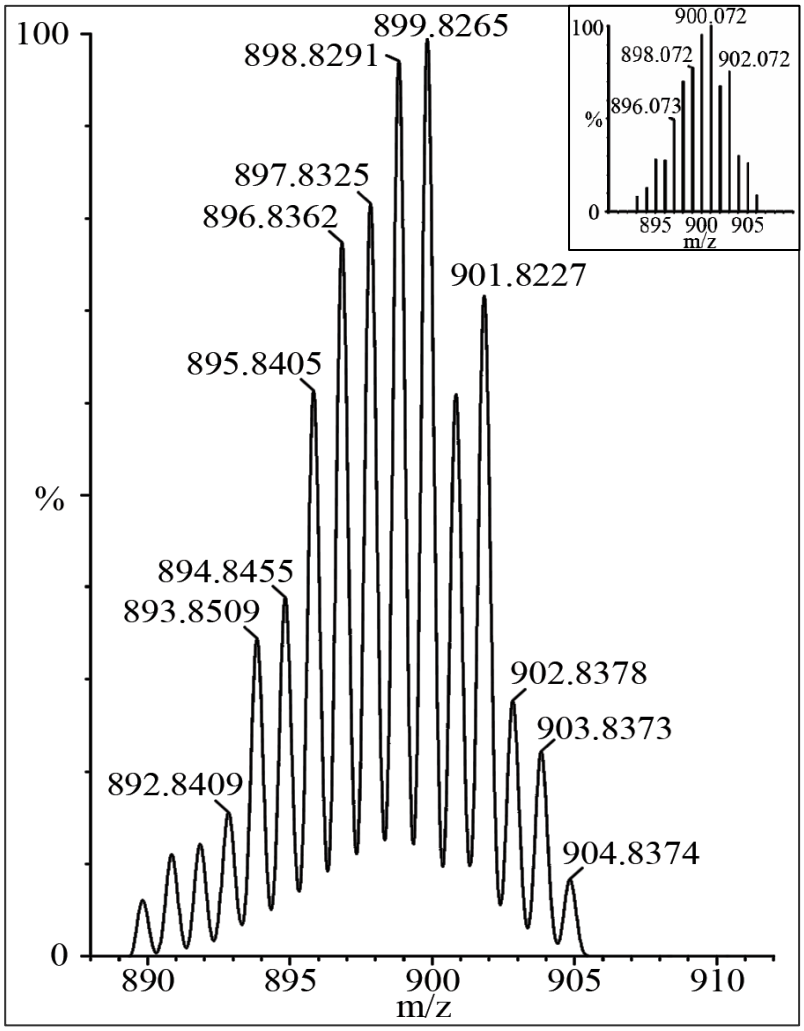

Figure S4. Experimental and simulated (inset) ESI mass spectra for **1d**.

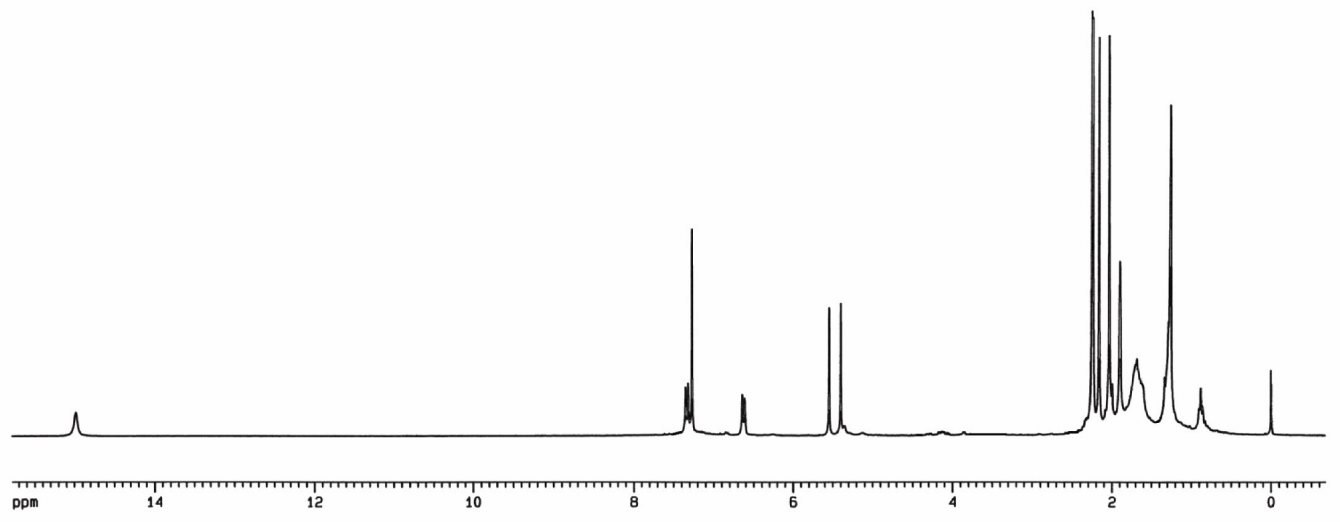

Figure S5. ^{1}H NMR spectrum of the complex **1b** in $CDCl_3$.

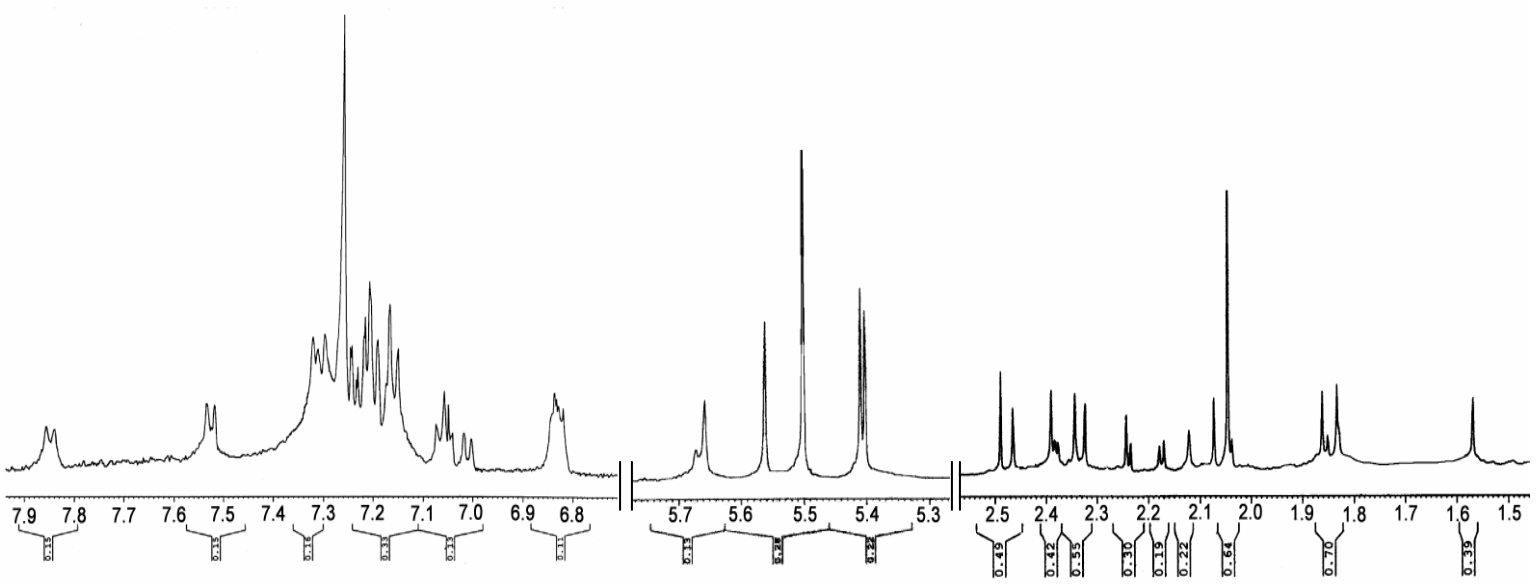

Figure S6. ^{1}H NMR spectrum of the complex **1d** in $CDCl_3$.

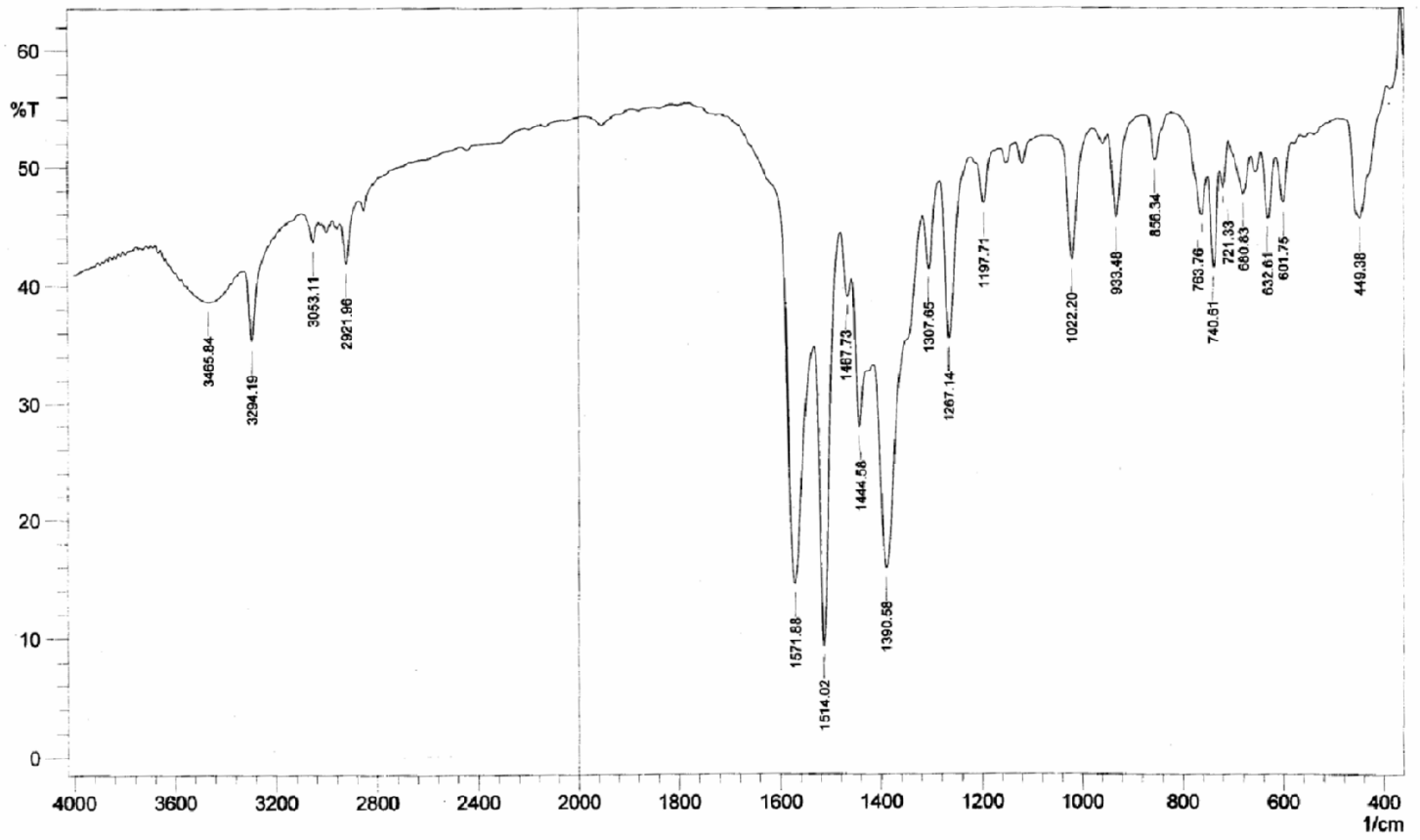

Figure S7. FT IR spectrum of the compound **1a**.

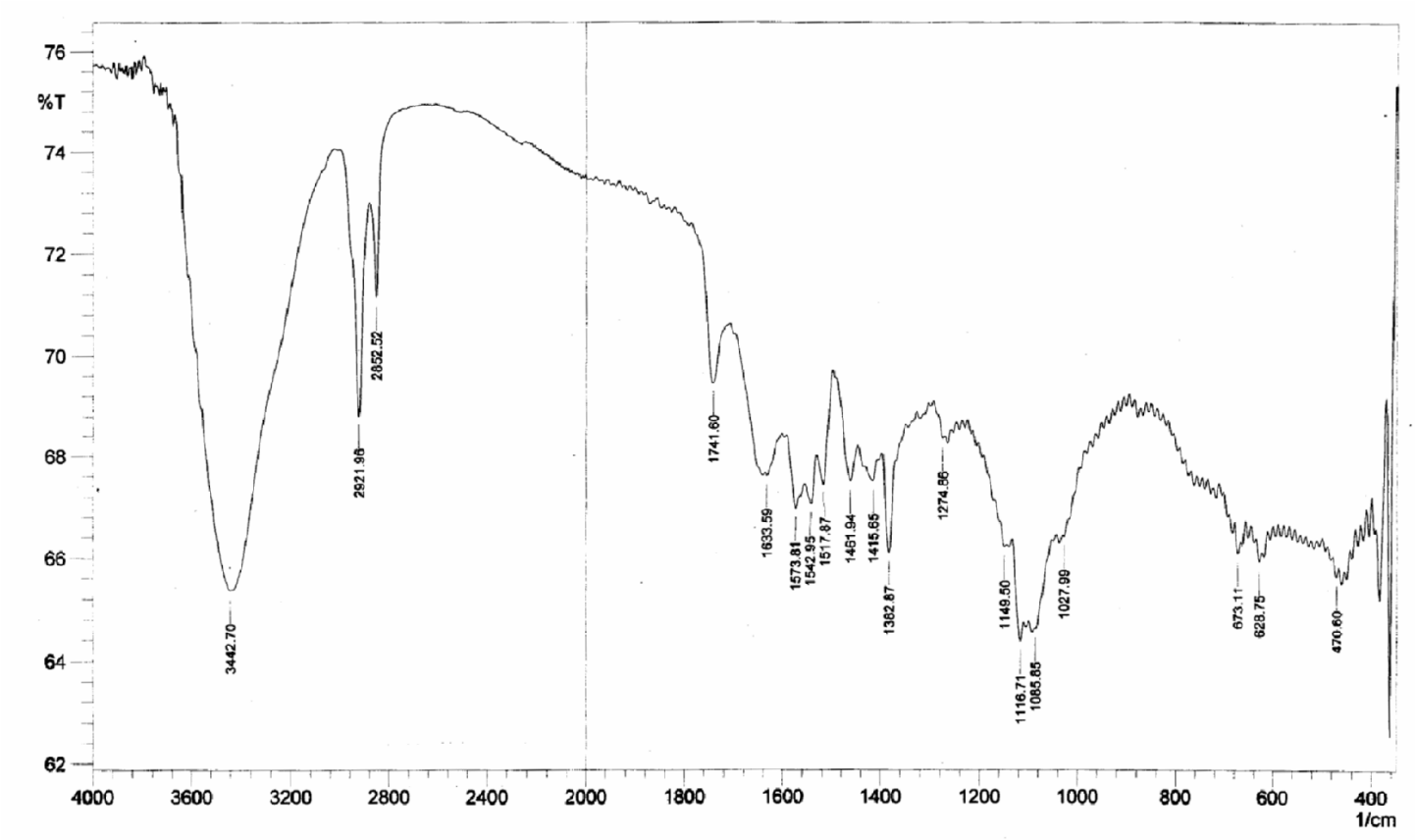

Figure S8. FT IR spectrum of the compound **1b**.

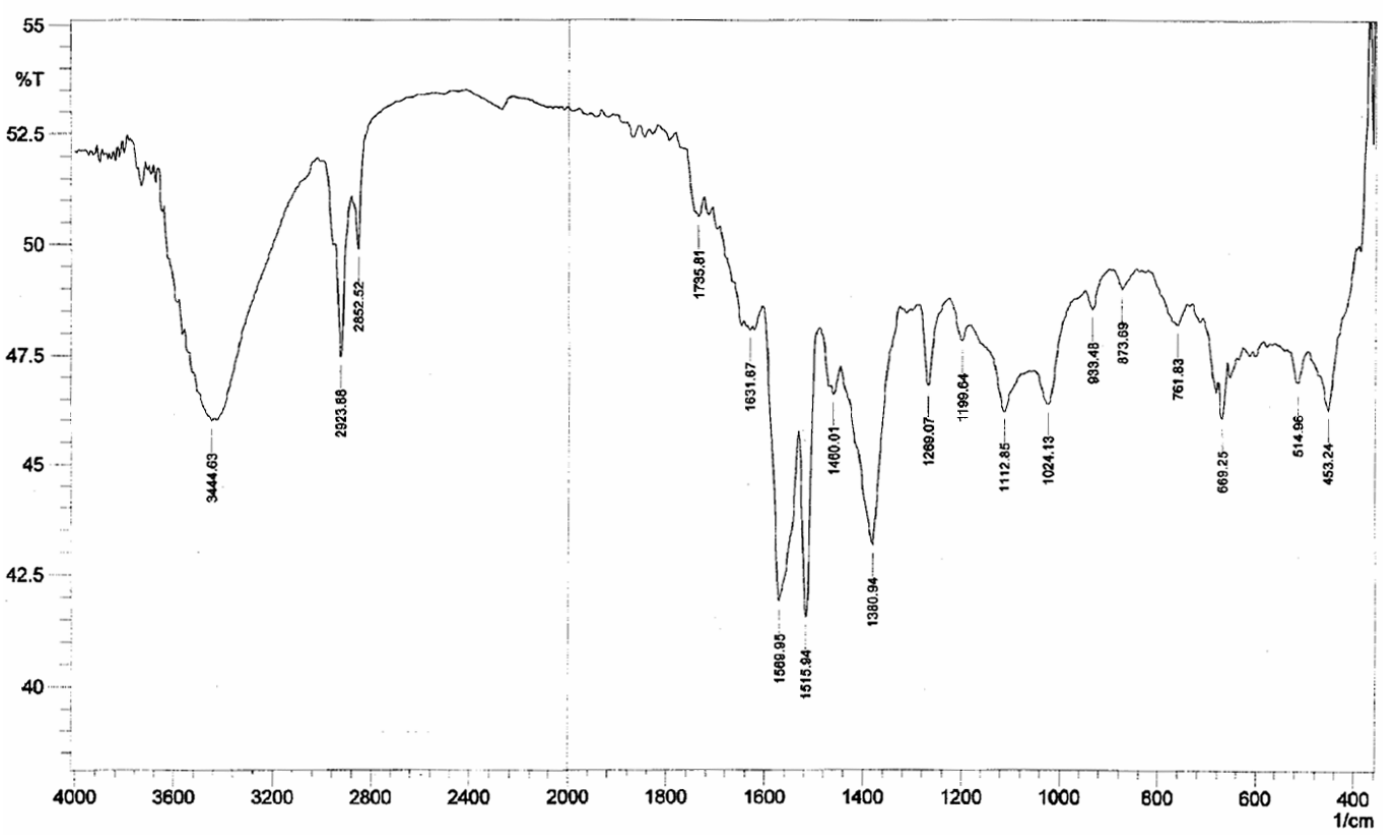

Figure S9. FT IR spectrum of the compound **1c**.

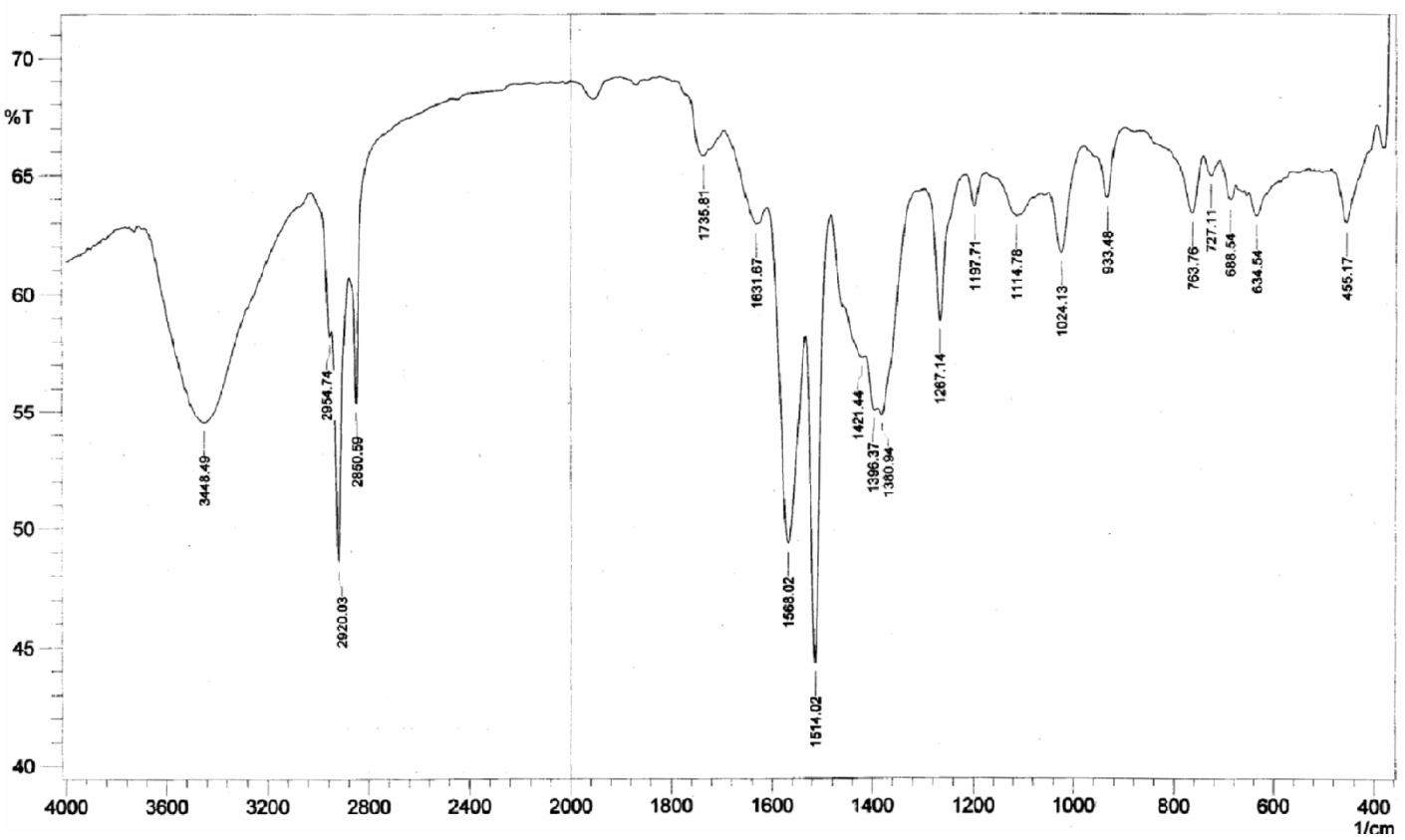

Figure S10. FT IR spectrum of the compound **1d**.

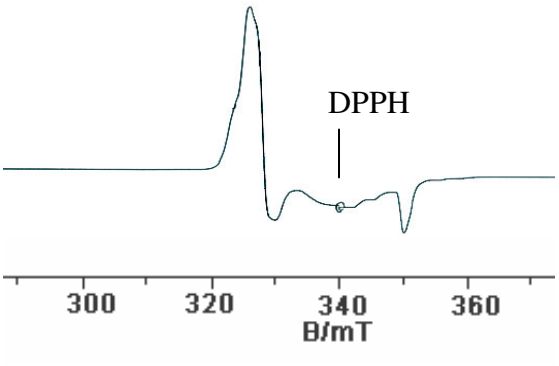

Figure S11. The X-band EPR spectrum of frozen CH_2Cl_2 solutions of **1a** at 140 K.

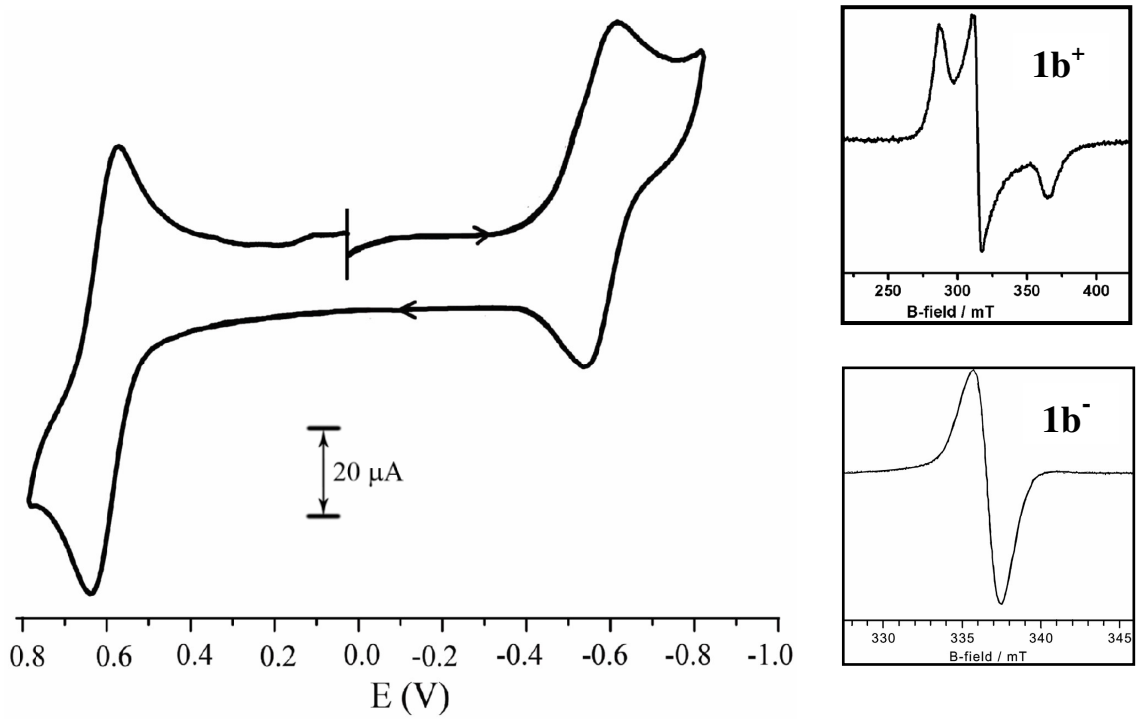

Figure S12. (a) Cyclic voltammogram of complex **1b** in CH_3CN containing 0.1 M NEt_4ClO_4 and the X-band EPR spectra of frozen CH_2Cl_2 solutions of $\mathbf{1b}^+$ and $\mathbf{1b}^-$.

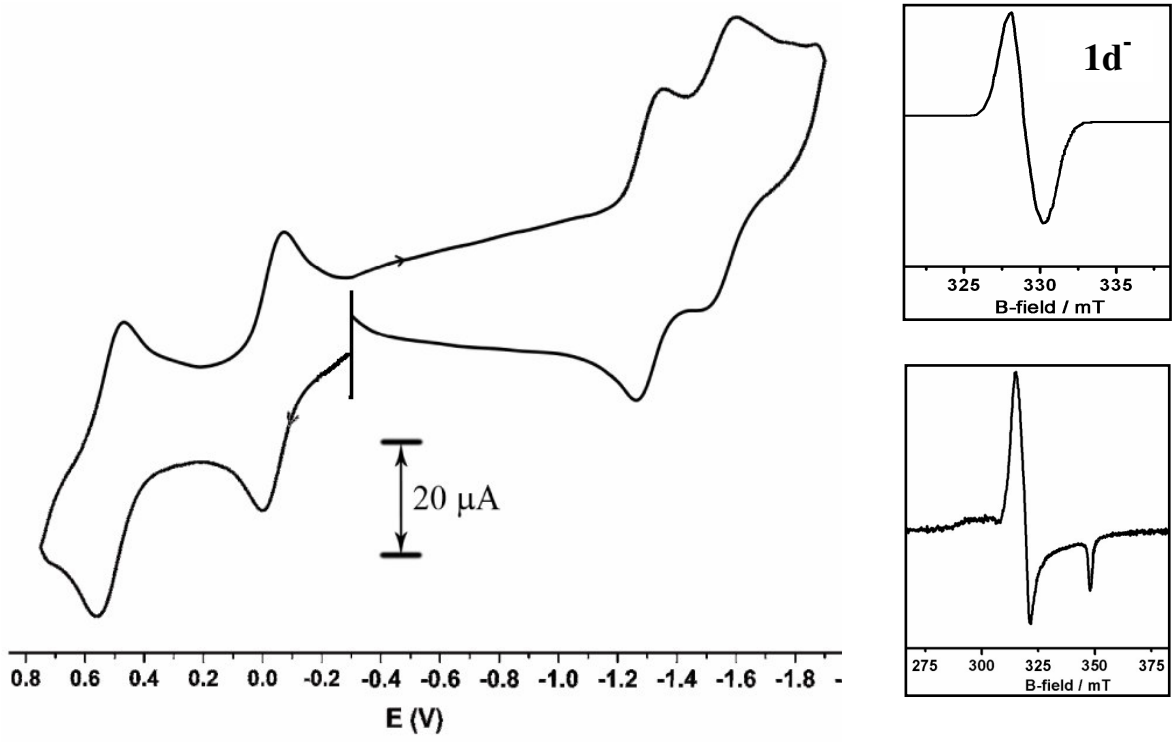

Figure S13. Cyclic voltammogram of complex **1d** in CH_3CN containing 0.1 M NEt_4ClO_4 and the X-band EPR spectra of frozen CH_2Cl_2 solutions of $\mathbf{1d}^+$ and $\mathbf{1d}^-$.

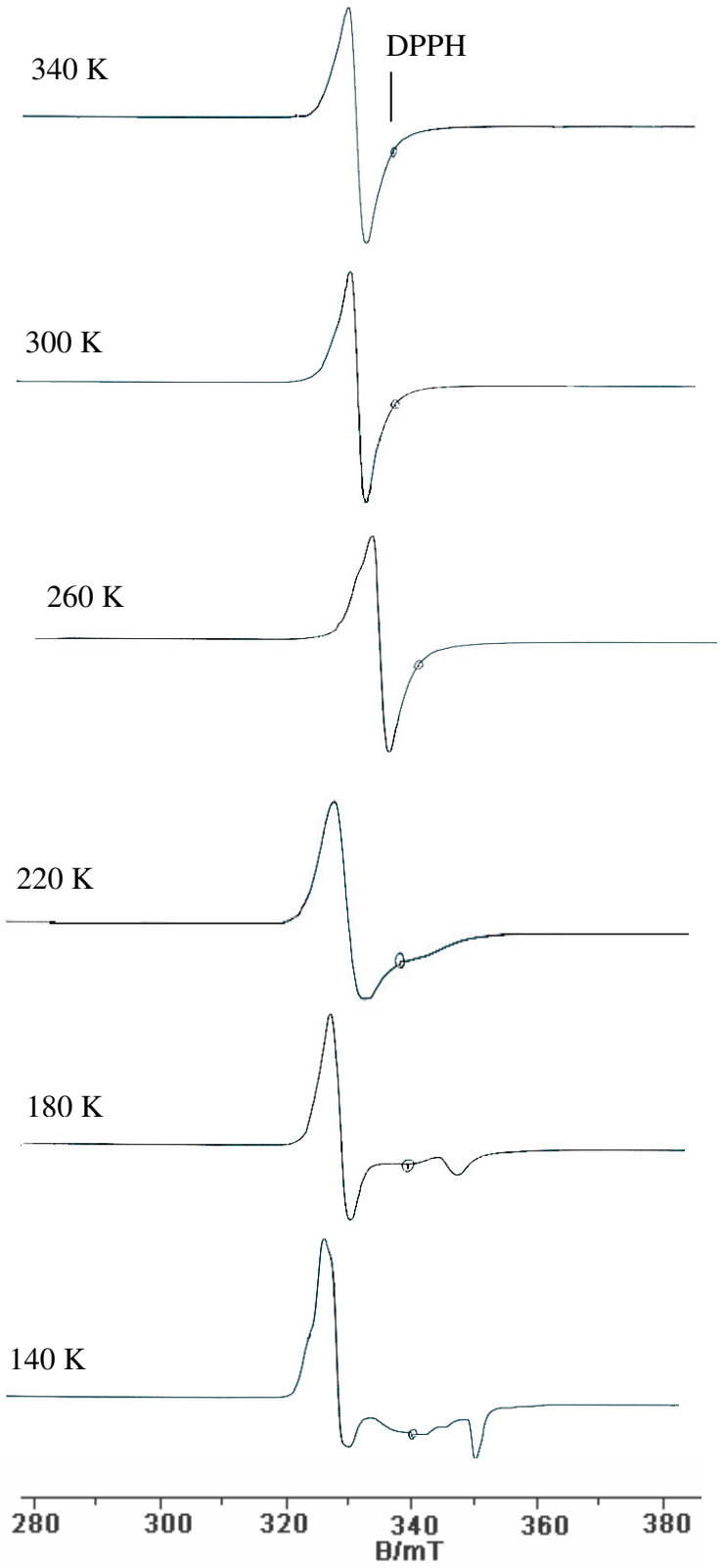

Figure S14. EPR spectra of **1a** illustrating the temperature dependent redox isomerism.

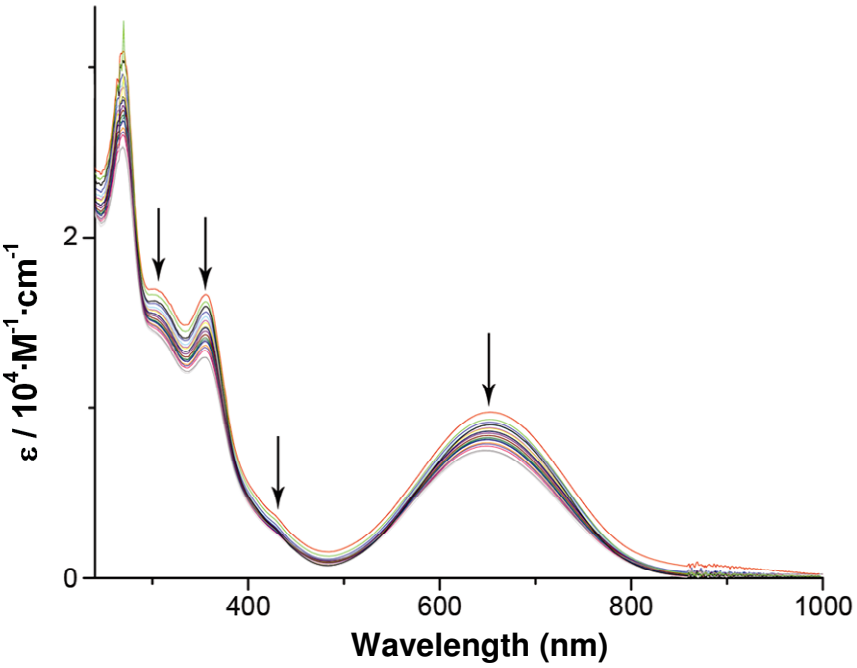

Figure S15. Temperature dependent spectral change for the complex **1a**.

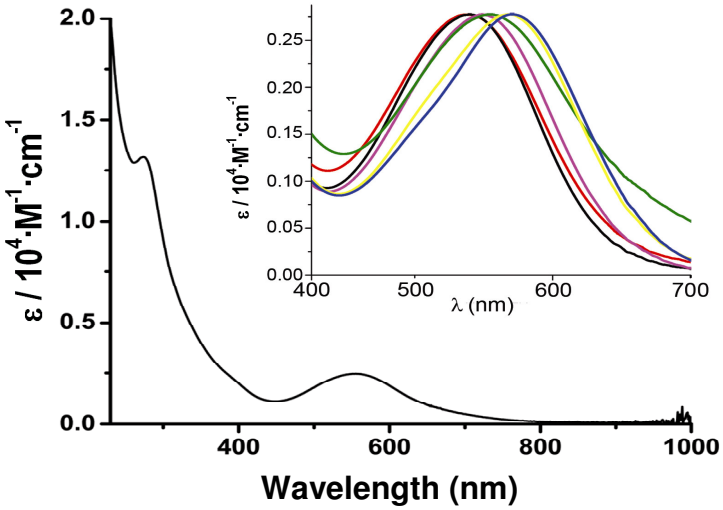

Figure S16. UV-visible spectrum of **1c** in dichloromethane. Inset: λ_{max} (nm) as a function of solvent (color code: ● Water, 537 nm; ● EtOH, 541 nm; ● CH_3CN, 549 nm; ● CH_2Cl_2, 555 nm; ● toluene, 569 nm; ● n-hexane, 571 nm).

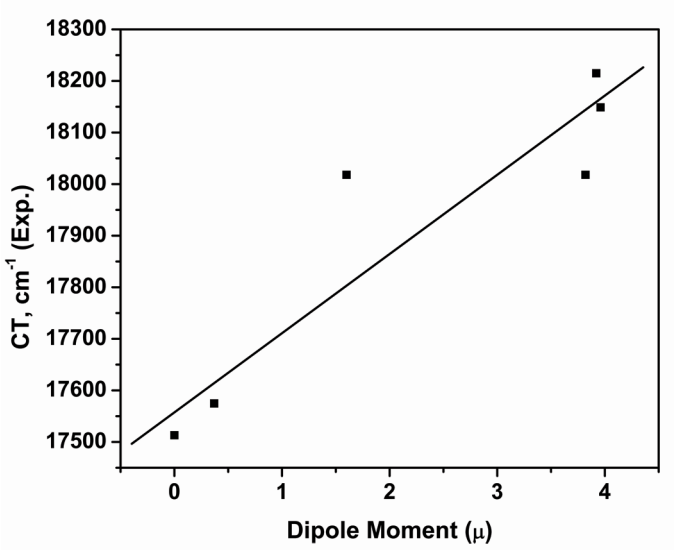

Figure S17. Correlation between the energy of the CT band and the dipole moment (μ) of the solvent ($E = 153.57153\mu + 17557.34741$).

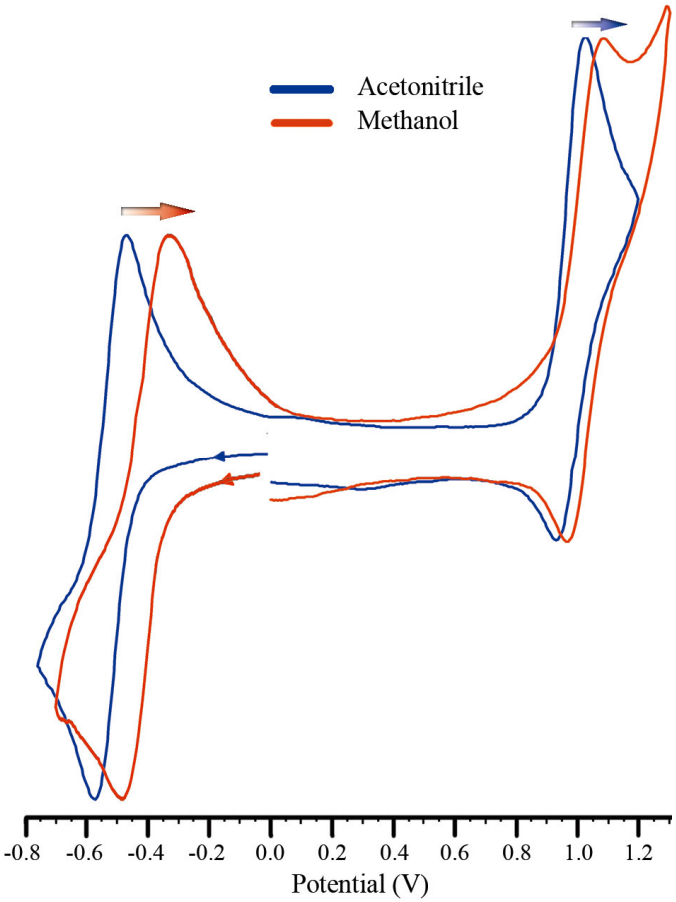

Figure S18. Segmented cyclic voltammogram (v = 1000 mV s^{-1}) of complex **1c** in CH_3CN and CH_3OH containing 0.1 M NEt_4ClO_4. Potentials are referenced to Ag/AgCl (satd. KCl).

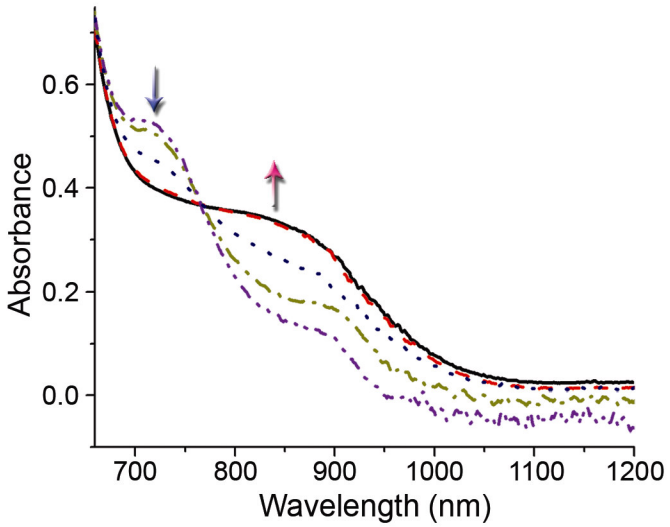

Figure S19. Concentration-dependent optical spectra of **1c** in CH_3CN solution. Arrows indicate changes in CT bands upon dilution from 5×10^{-5} to 1.5×10^{-3} M.

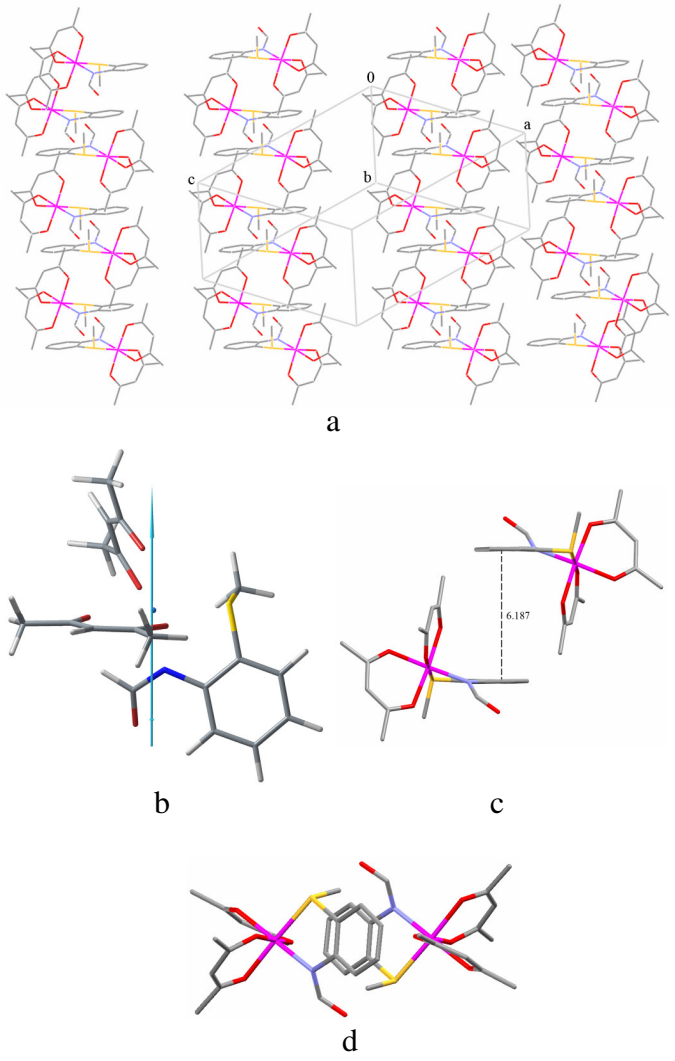

Figure S20. Crystal packing diagrams of **1c**. (a) View of the packing of the molecule in columns with a close and a more distant neighbor. (b) Direction of Dipole Moment (c) Distance between the aromatic backbones of two neighboring molecule. (d) Top view of the dimeric unit.