

Electronic Supplementary Information

Syntheses, characterization and redox properties of oxo-centered triruthenium cluster dimers and trimers linked by ortho-metallated polypyridyl ligands

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Table S1. ¹H NMR Chemical Shifts (δ) for Compounds **6**, **7**, **7a**, **9**, **11**, and **11a**.^a

	6	7	7a	9	11	11a
δ (acetate)	5.526 (6H)	5.543 (12H)	2.200 (24H)	10.688 (3H)	5.824 (12H)	2.122 (12H)
	5.066 (12H)	4.906 (24H)	2.125 (12H)	7.026 (3H)	4.954 (24H)	2.046 (24H)
				4.514 (3H)		
				2.837 (3H)		
				0.855 (3H)		
δ (N ligand)	8.877 (1H, g)	6.164 (2H, c)	10.084 (2H, a)	9.988 (1H, d)	8.573 (2H, d)	9.304 (2H)
	8.621 (1H, f)	1.288 (2H, b)	9.105 (2H, b)	5.872 (1H, f)	6.782 (2H, c)	8.781 (2H)
	8.549 (1H, d)	1.211 (2H, a)	8.821 (2H, c)	2.552 (1H, c)	2.863 (2H, b)	8.032 (2H)
	6.251 (1H, h)			1.288(1H, g)	1.291 (2H, a)	7.792 (2H)
	2.420 (1H, c)			-7.384 (1H, a)		
	0.897 (1H, a)					
δ (py')				9.497 (1H, α')		
				8.788 (2H, β')		
				7.431 (2H, γ')		
δ (py)	6.586 (2H, γ)	6.522 (4H, γ)	9.105 (8H, α)	6.405 (1H, γ)	6.308 (4H, α)	8.986 (8H)
	5.561 (4H, β)	5.468 (8H, β)	8.018 (4H, γ)	4.578 (2H, β)	5.304 (8H, β)	7.791 (4H)
	0.008 (4H, α)	-0.161 (8H, α)	7.755 (8H, β)	0.381 (2H, α)	-0.648 (8H, γ)	7.702 (8H)

^a ¹H NMR spectra (499.8 MHz) were recorded in CD₃CN at 298 K except for **7a** and **11a** in CD₂Cl₂.

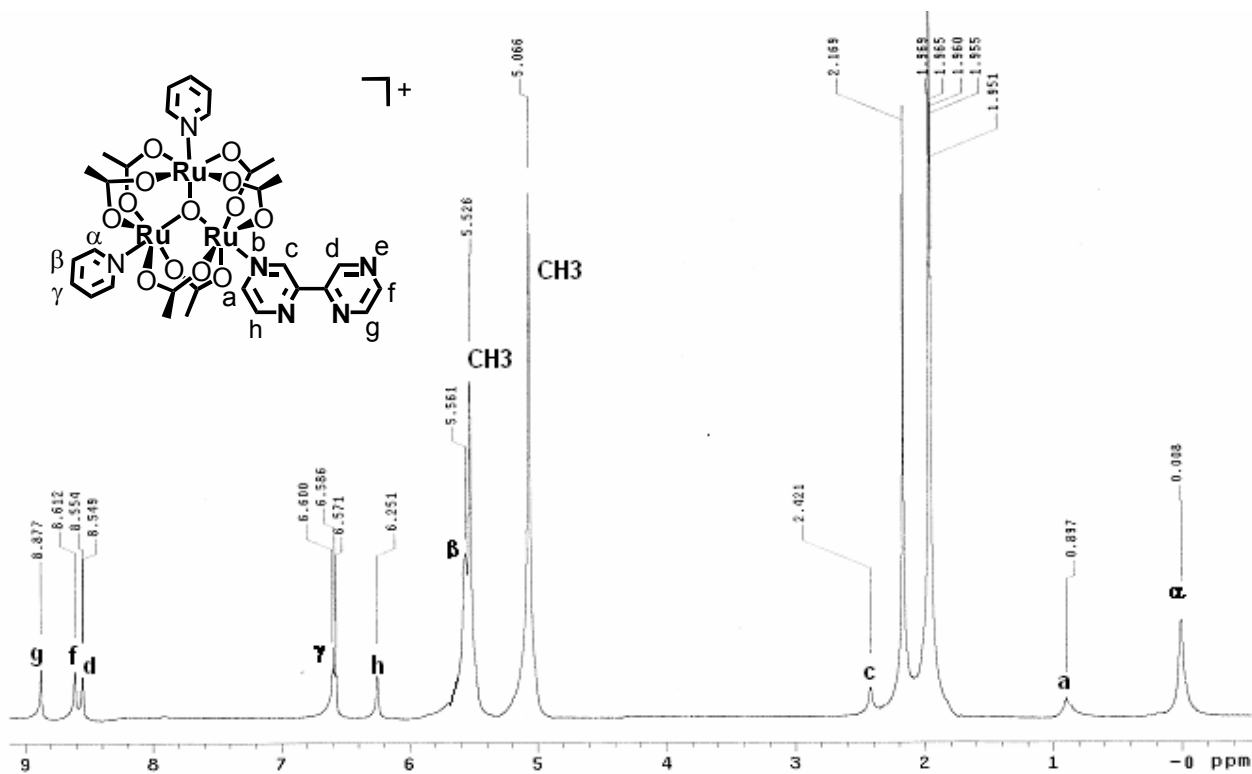


Fig. S1. ^1H NMR (499.8 MHz) spectrum of compound 6 in CD_3CN .

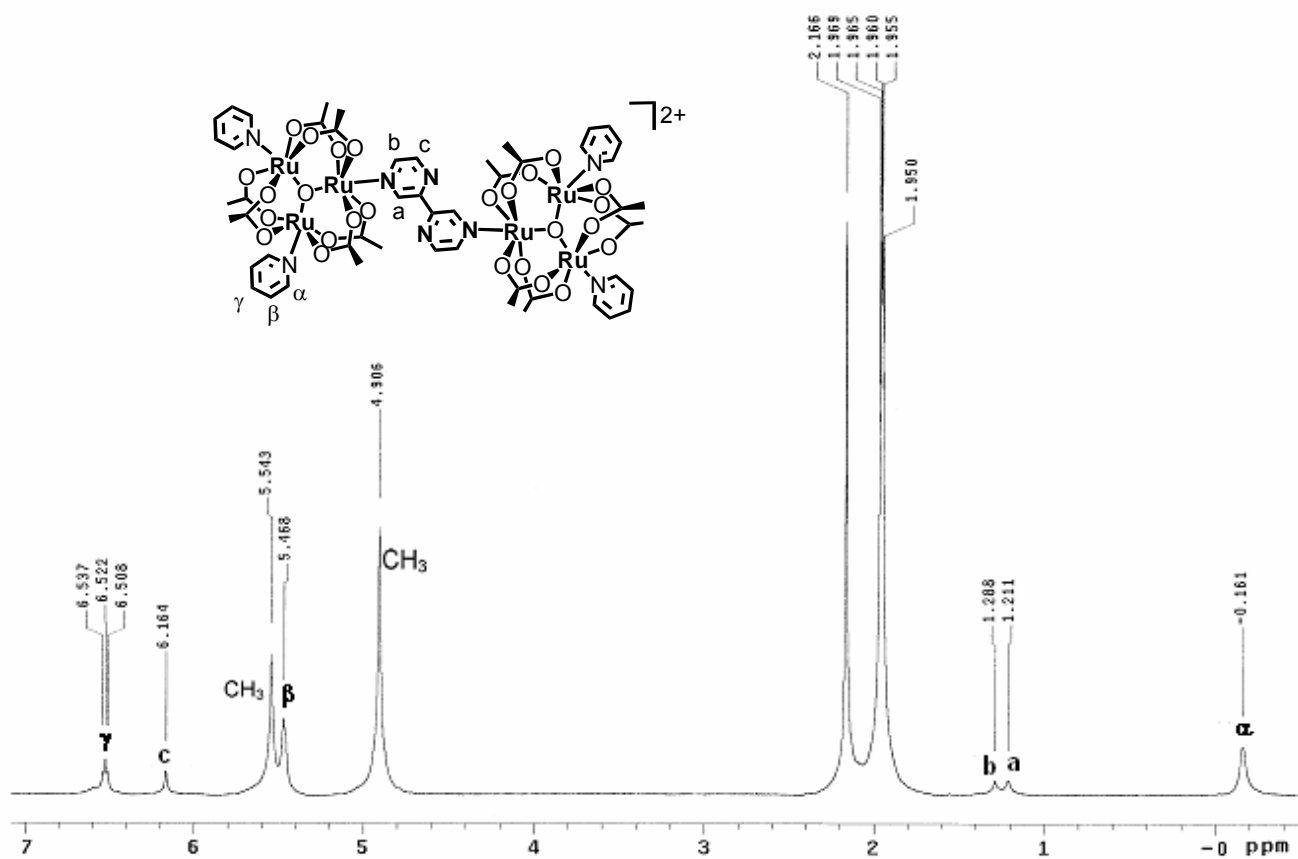


Fig. S2. ^1H NMR (499.8 MHz) spectrum of compound 7 in CD_3CN .

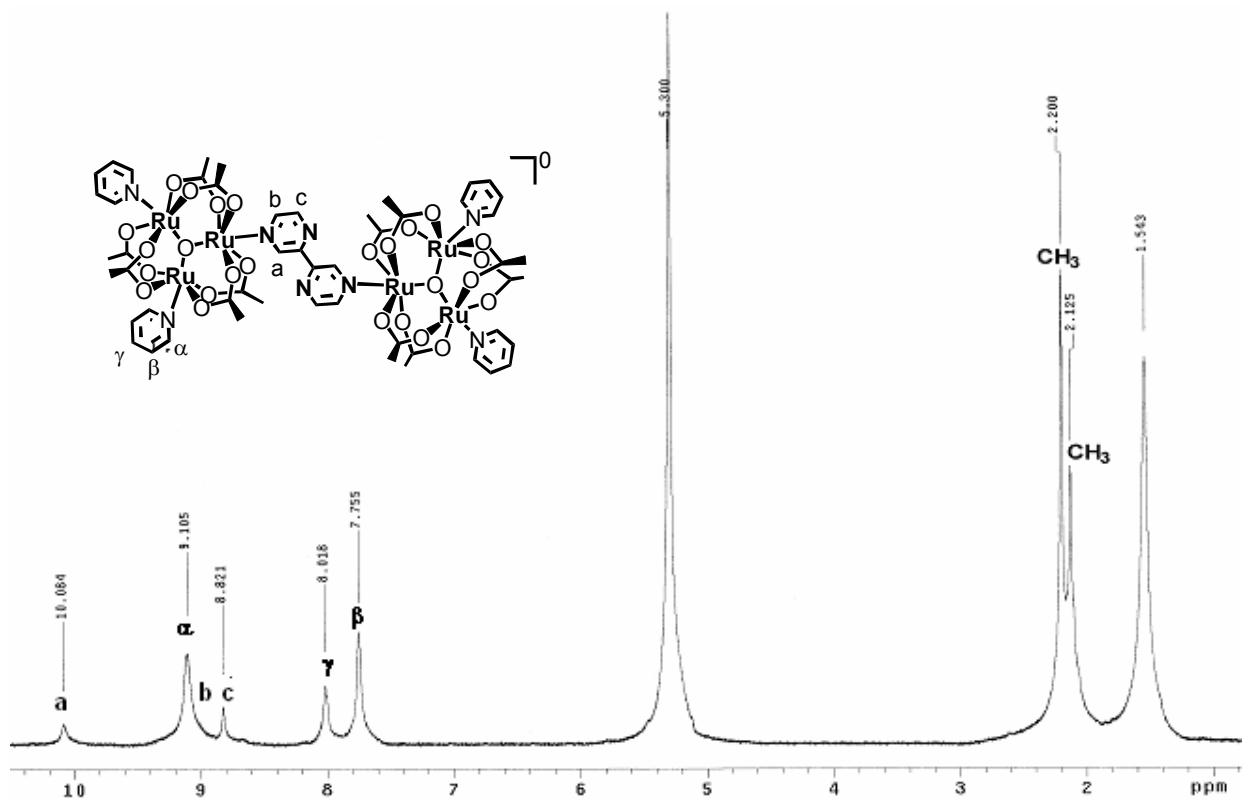


Fig. S3. ¹H NMR (499.8 MHz) spectrum of compound **7a** in CD₂Cl₂.

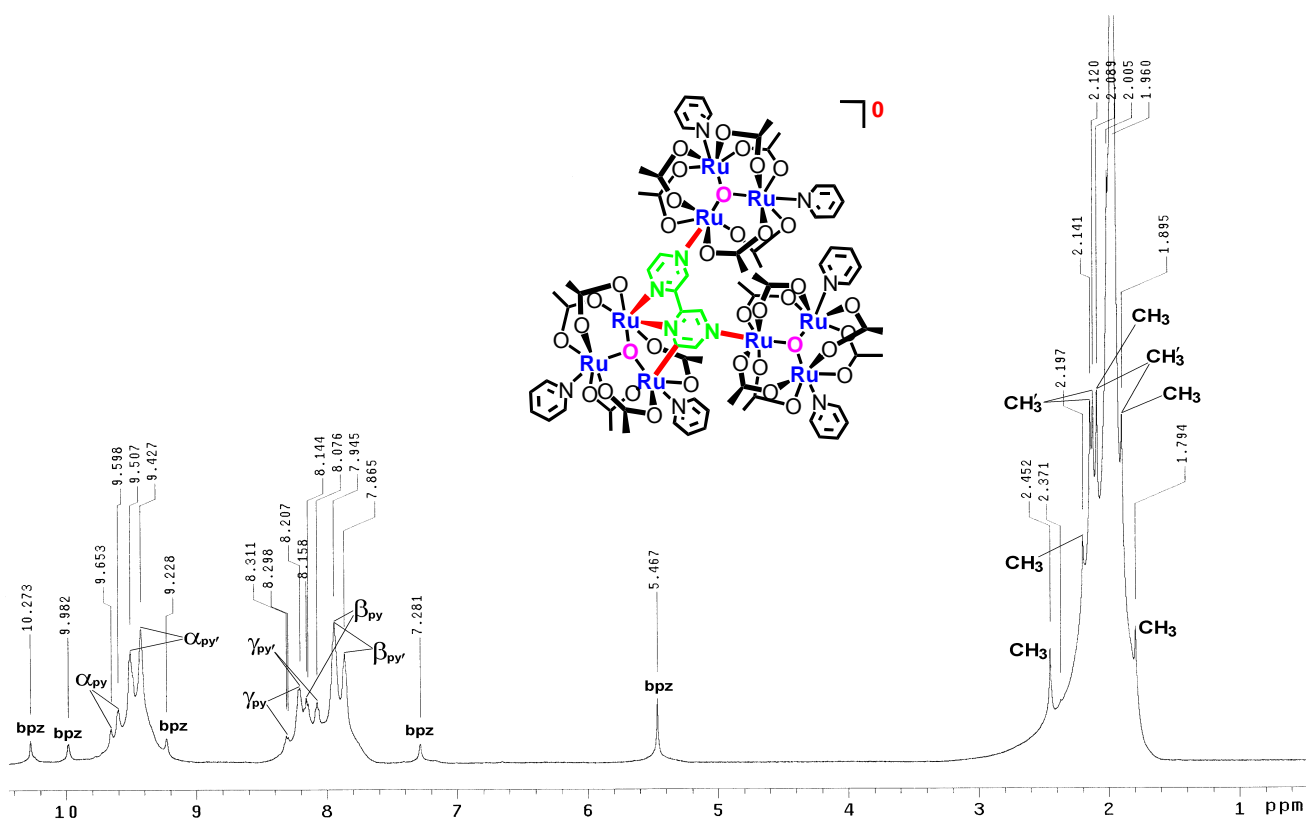


Fig. S4. ¹H NMR (499.8 MHz) spectrum of compound **8a** in CD₃CN.

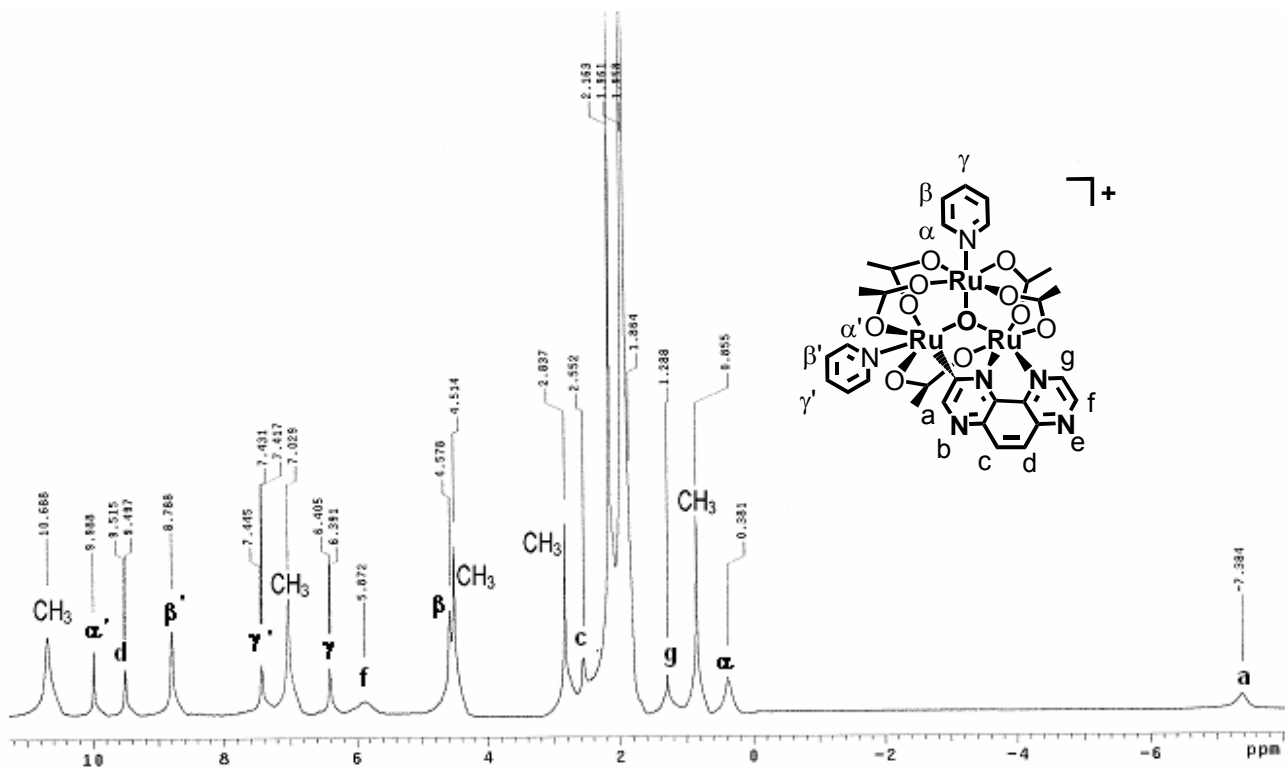


Fig. S5. ^1H NMR (499.8 MHz) spectrum of compound **9** in CD_3CN .

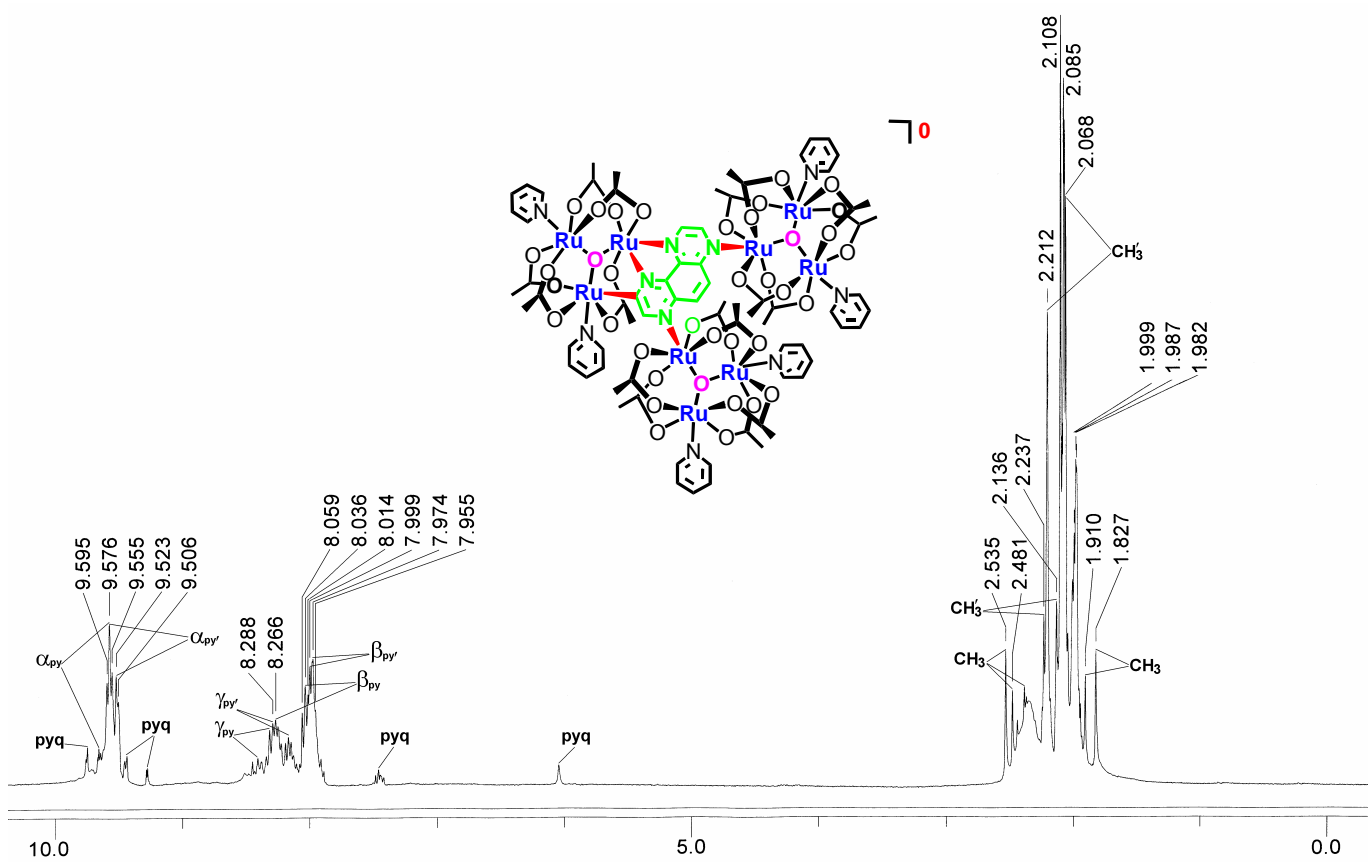


Fig. S6. ^1H NMR (499.8 MHz) spectrum of compound **10a** in CD_3CN .

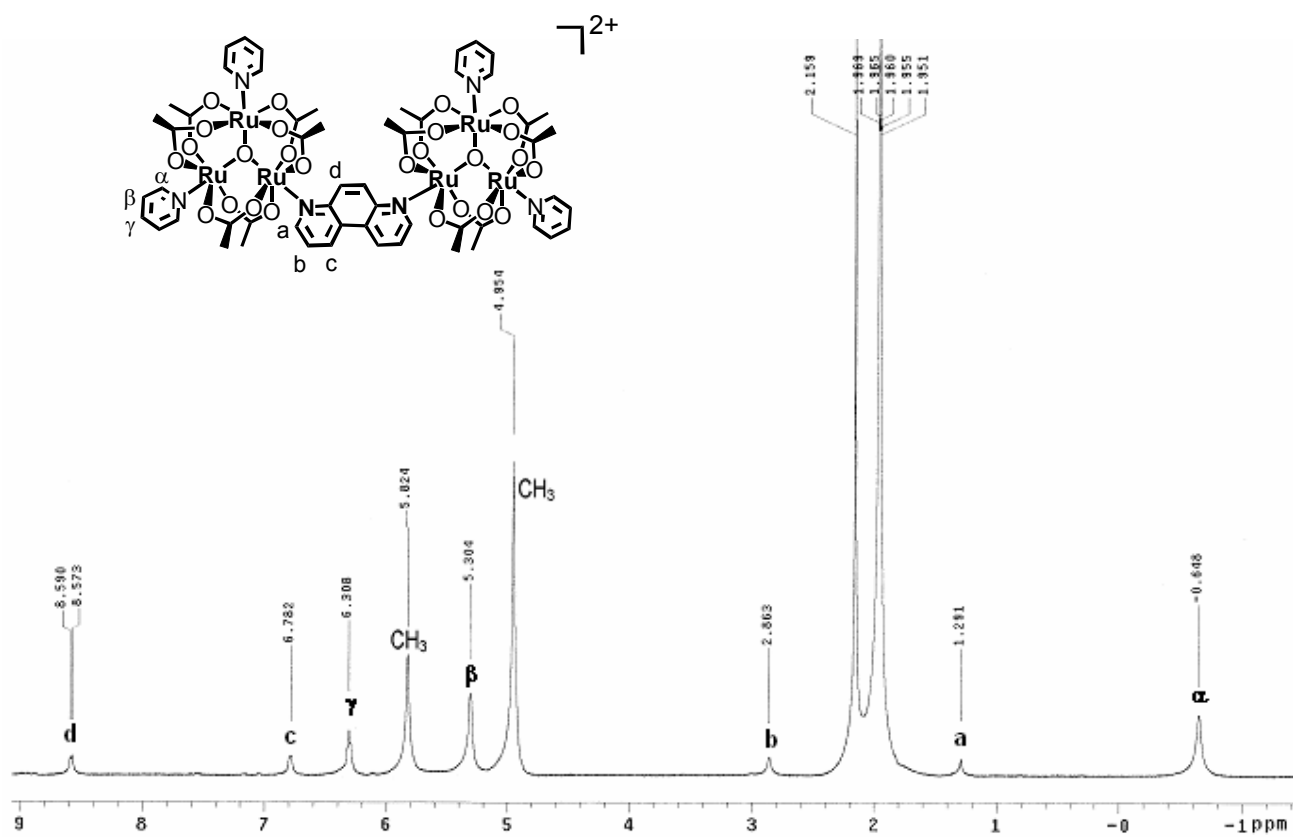


Fig. S7. ^1H NMR (499.8 MHz) spectrum of compound **11** in CD_3CN .

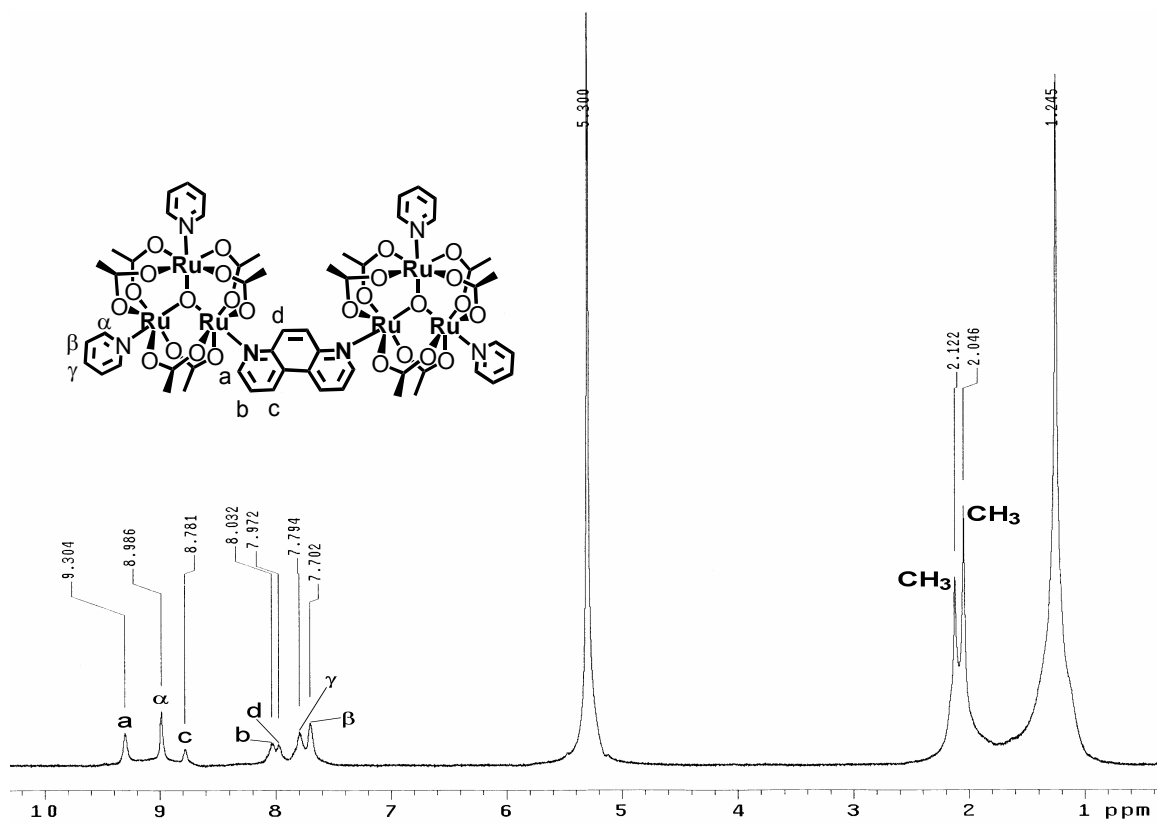


Fig. S8. ^1H NMR (499.8 MHz) spectrum of compound **11a** in CD_2Cl_2 .

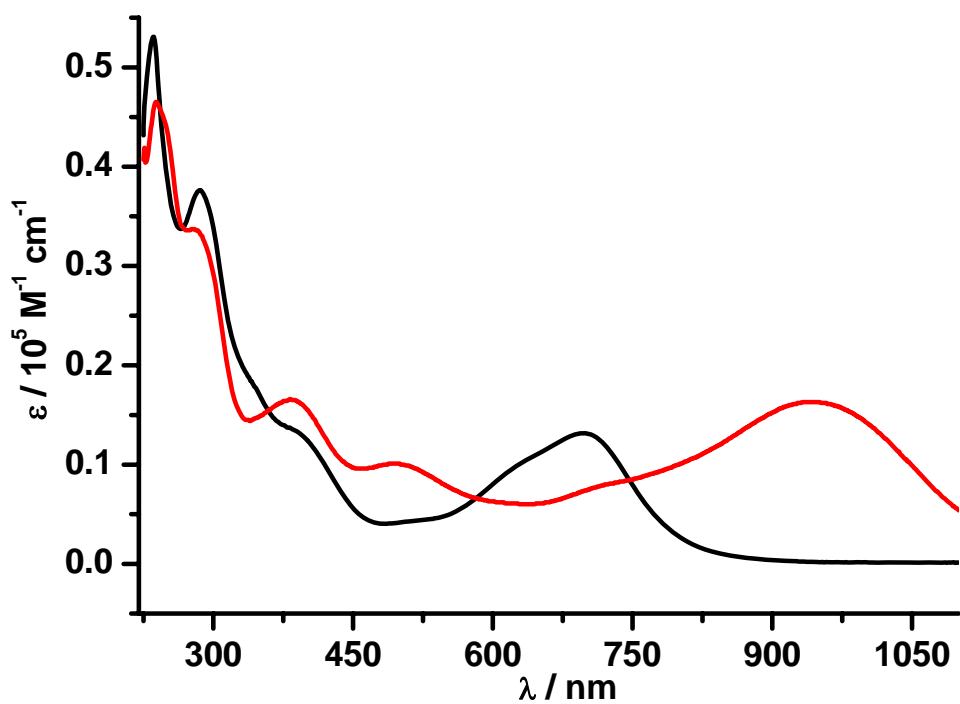


Fig. S9. Electronic absorption spectra of 2+ dimeric compound **7** (black line) and neutral compound **7a** (red line) in dichloromethane.

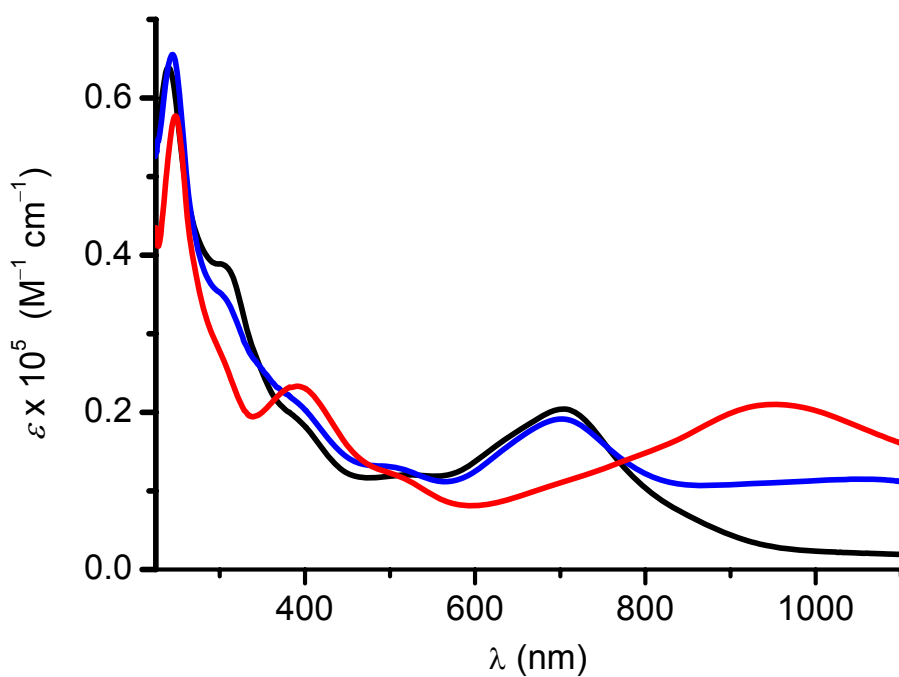


Fig. 10. Electronic absorption spectra of 3+ trimeric compound **8** (black line), neutral compound **8a** (red line) and 2+ compound **8b** (blue line) in dichloromethane.

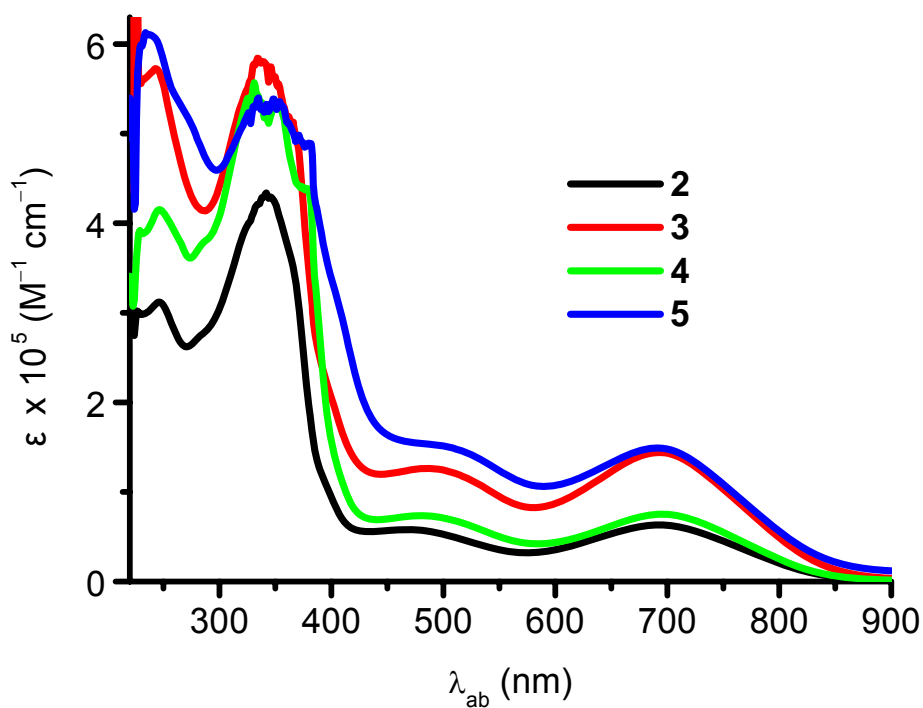


Figure S11. Electronic absorption spectra of compound 2(black), 3(red), 4(green), 5(blue) in dichloromethane.

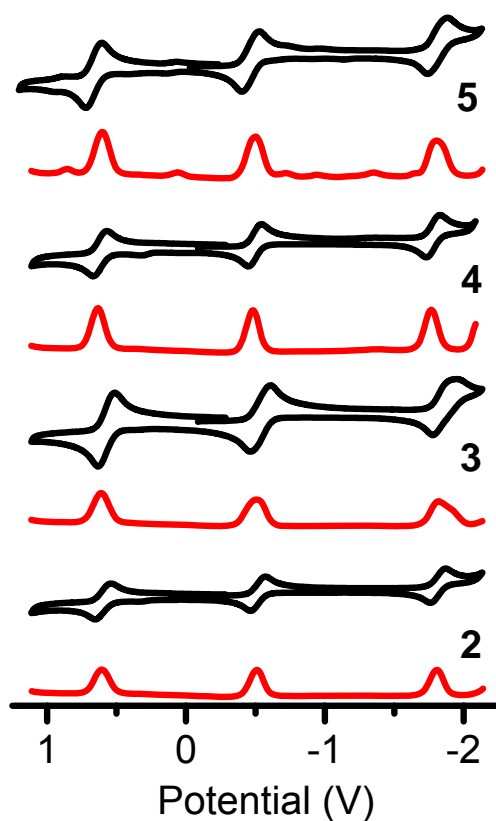


Fig. S12 Plots of cyclic and differential pulse voltammograms for compound 2-5 in 0.1 M dichloromethane solution of $(\text{Bu}_4\text{N})(\text{PF}_6)$. The scan rates are 100 mV s⁻¹ for CV and 20 mV s⁻¹ for DPV.

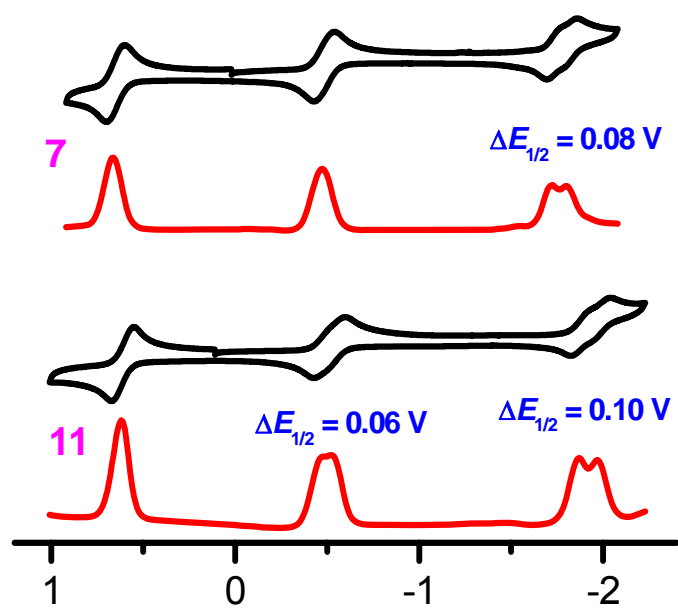


Fig. S13. Plots of cyclic and differential pulse voltammograms for bpz compound **7** and μ -4,7-phen compound **11** in 0.1 M dichloromethane solution of $(\text{Bu}_4\text{N})(\text{PF}_6)$. The scan rates are 100 mV s^{-1} for CV and 20 mV s^{-1} for DPV.