

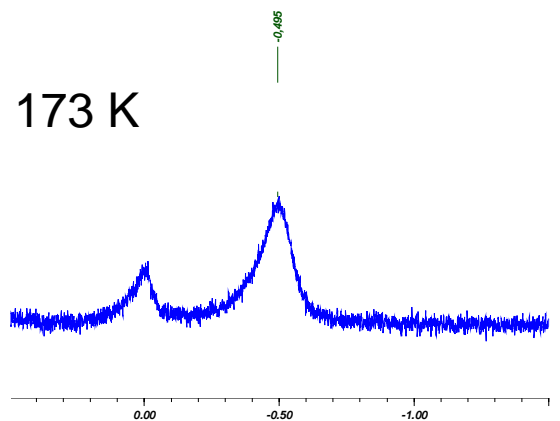
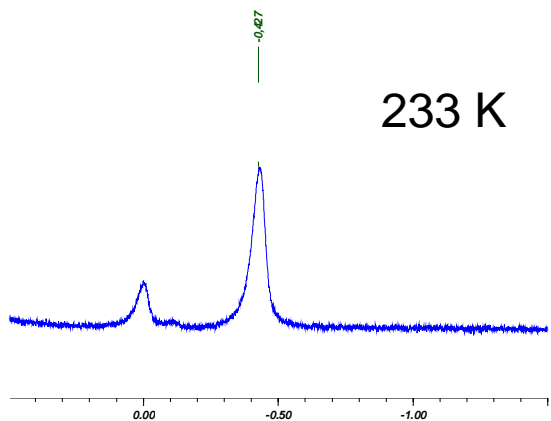
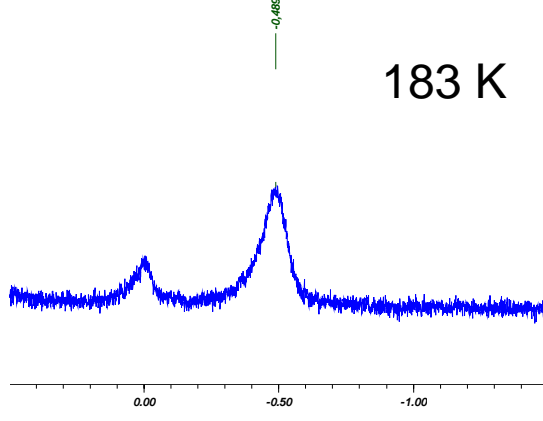
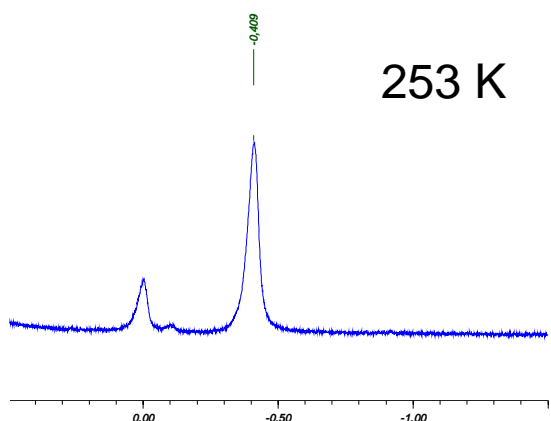
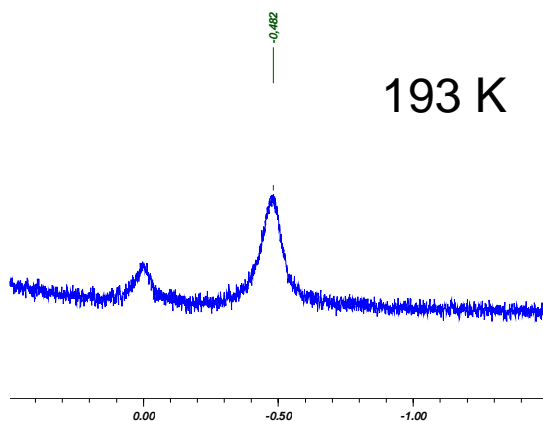
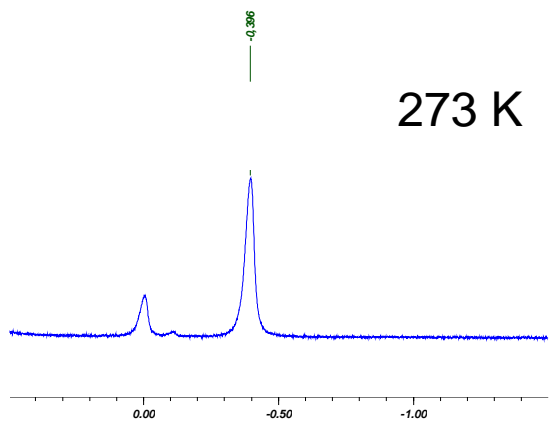
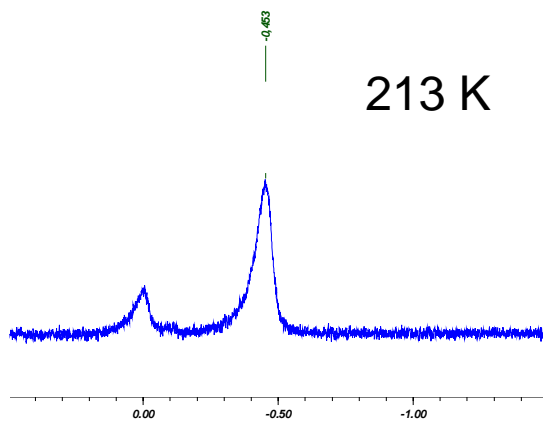
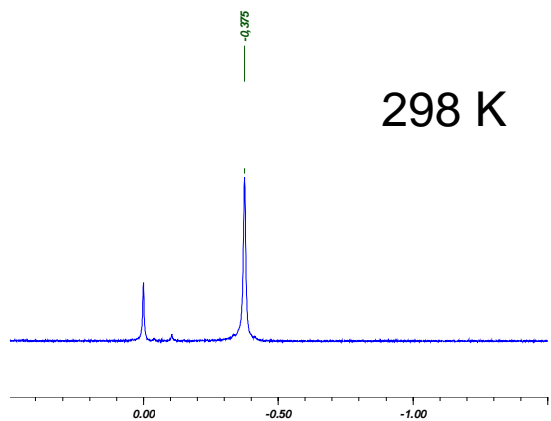
Supporting Information for Mixed-valence states formation in conformationally flexible metal-free 5,10,15,20-tetraferrocenylporphyrin and 5,10-bisferrocenyl-15,20-bisphenylporphyrin

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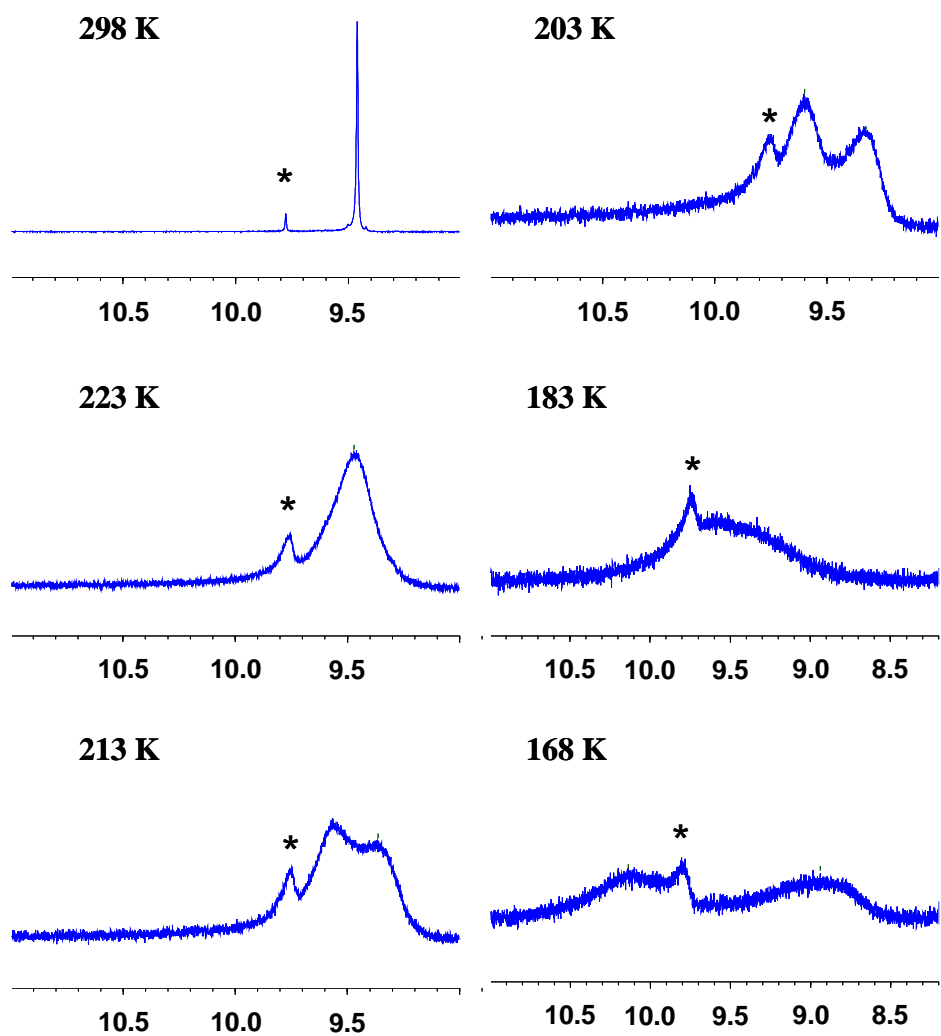
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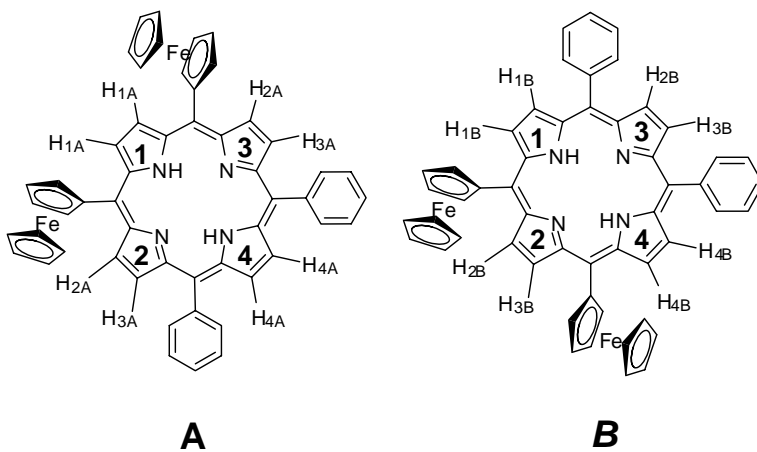
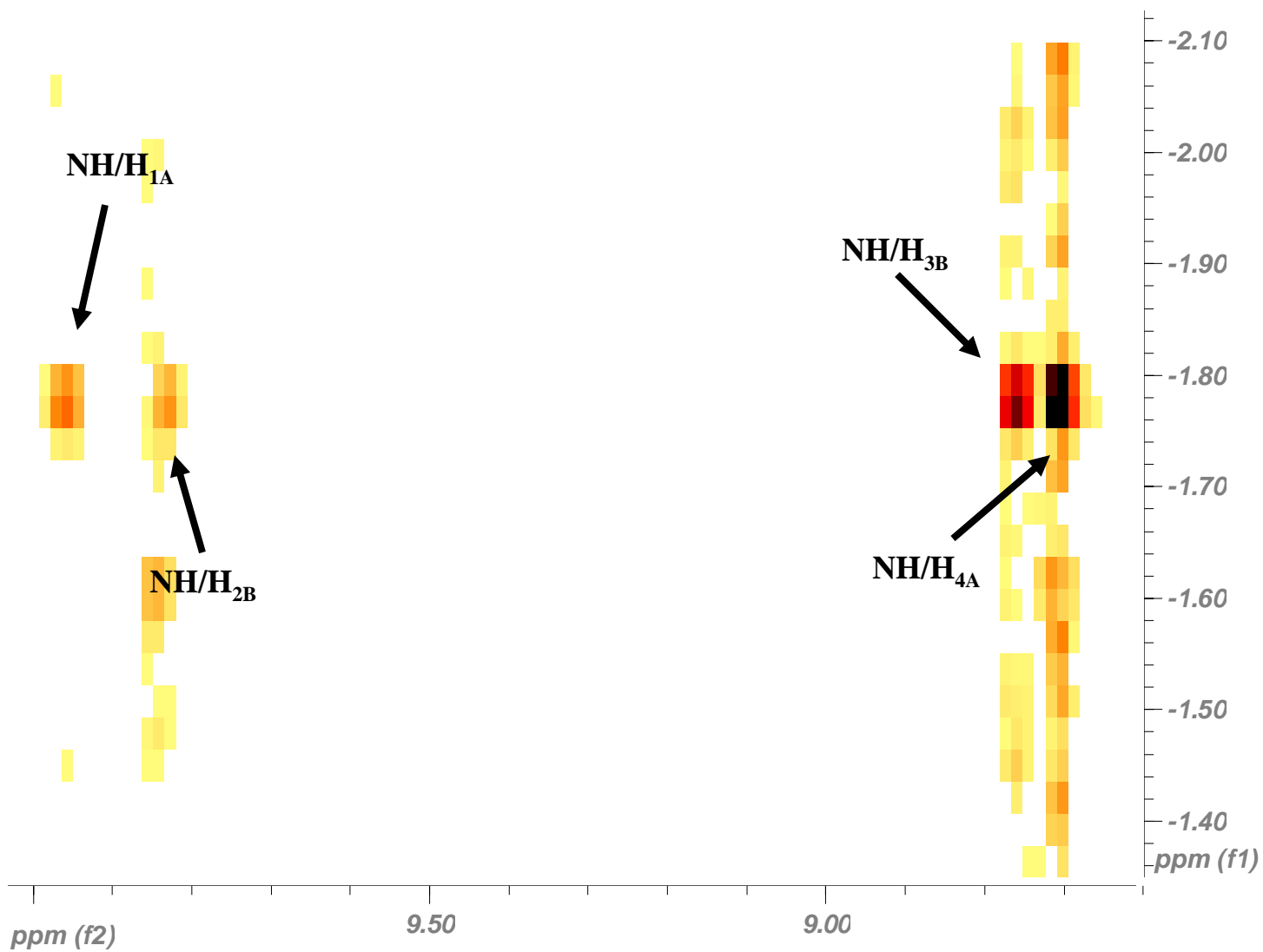


Variable-temperature ^1H NMR spectra of TFcPH_2 in the NH protons region in THF-d_8 .



Variable-temperature ^1H NMR spectra of TFCpH_2 in the β -pyrrolic protons region in THF-d_8 . Impurity labeled with asterisk.

Partial room-temperature COSY spectrum of *cis*-Fc₂Ph₂PH₂ representing weak NH / β-pyrrolic protons correlation



Predicted at DFT level charges, total spin densities (r) and principal components of electric field gradient for iron centers (labeled as 1 – 4) of TFcPZn (labeled as neutral) and [TFcPZn]²⁺ (labeled as oxidized)

	Charges		Oxidized	
	Neutral	Oxidized	ρ	V_{zz}
1	1.986	1.881	0.766	1.272
2	1.986	1.705	1.387	0.376
3	1.986	1.705	1.387	0.376
4	1.986	1.881	0.766	1.272