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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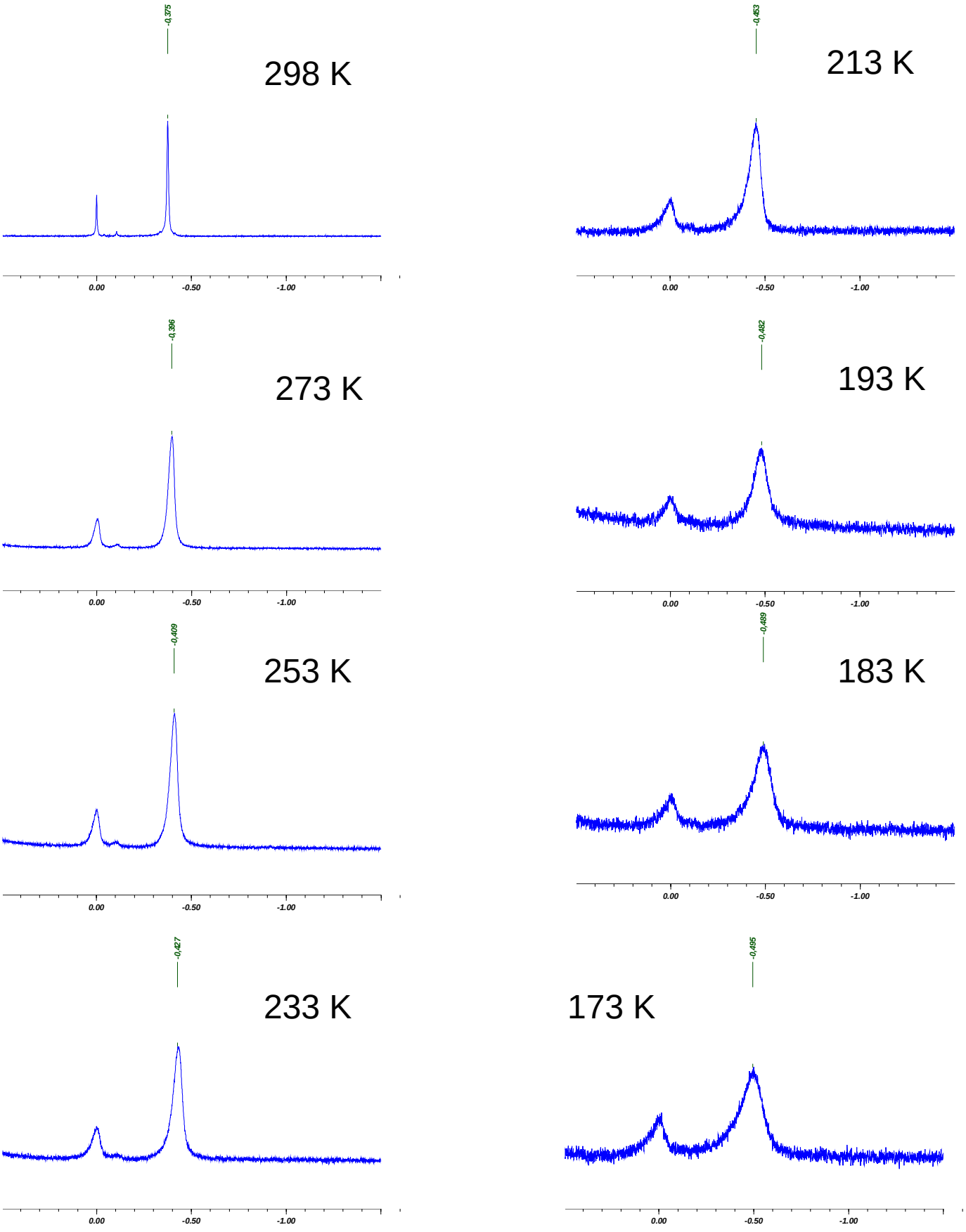
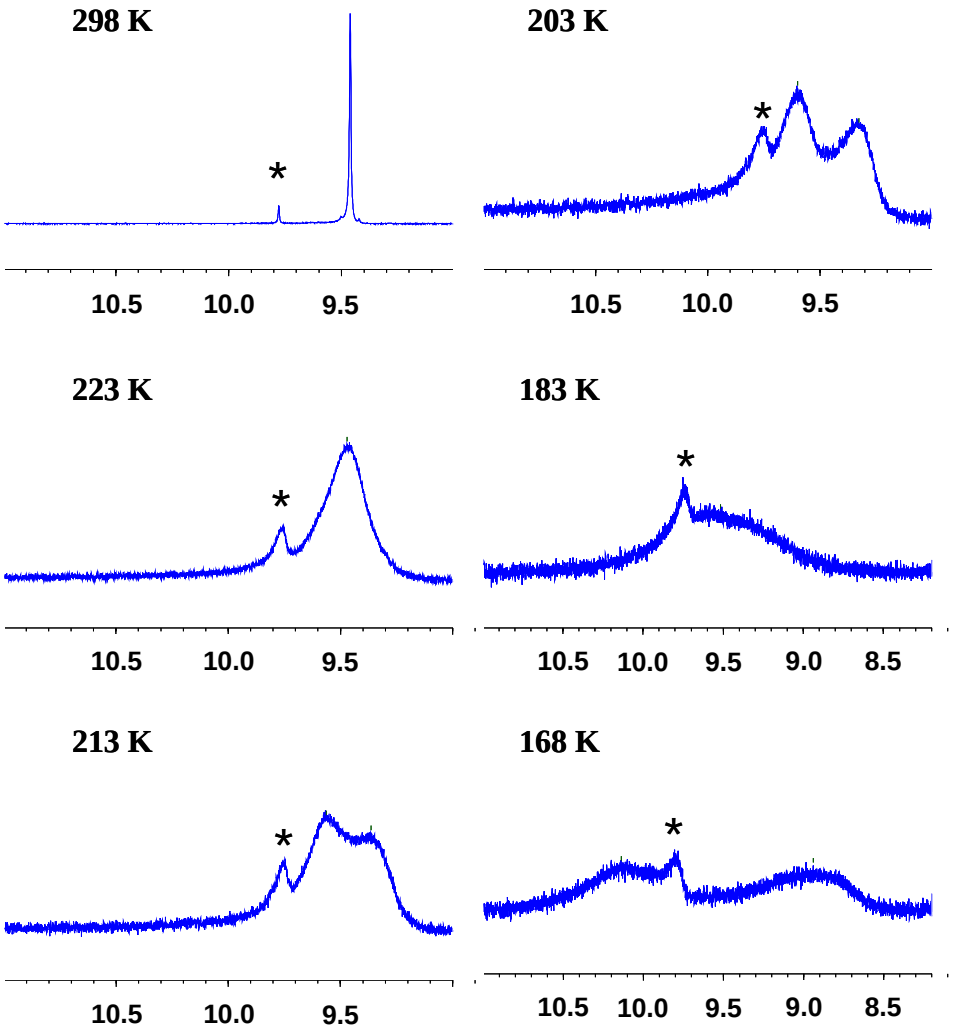
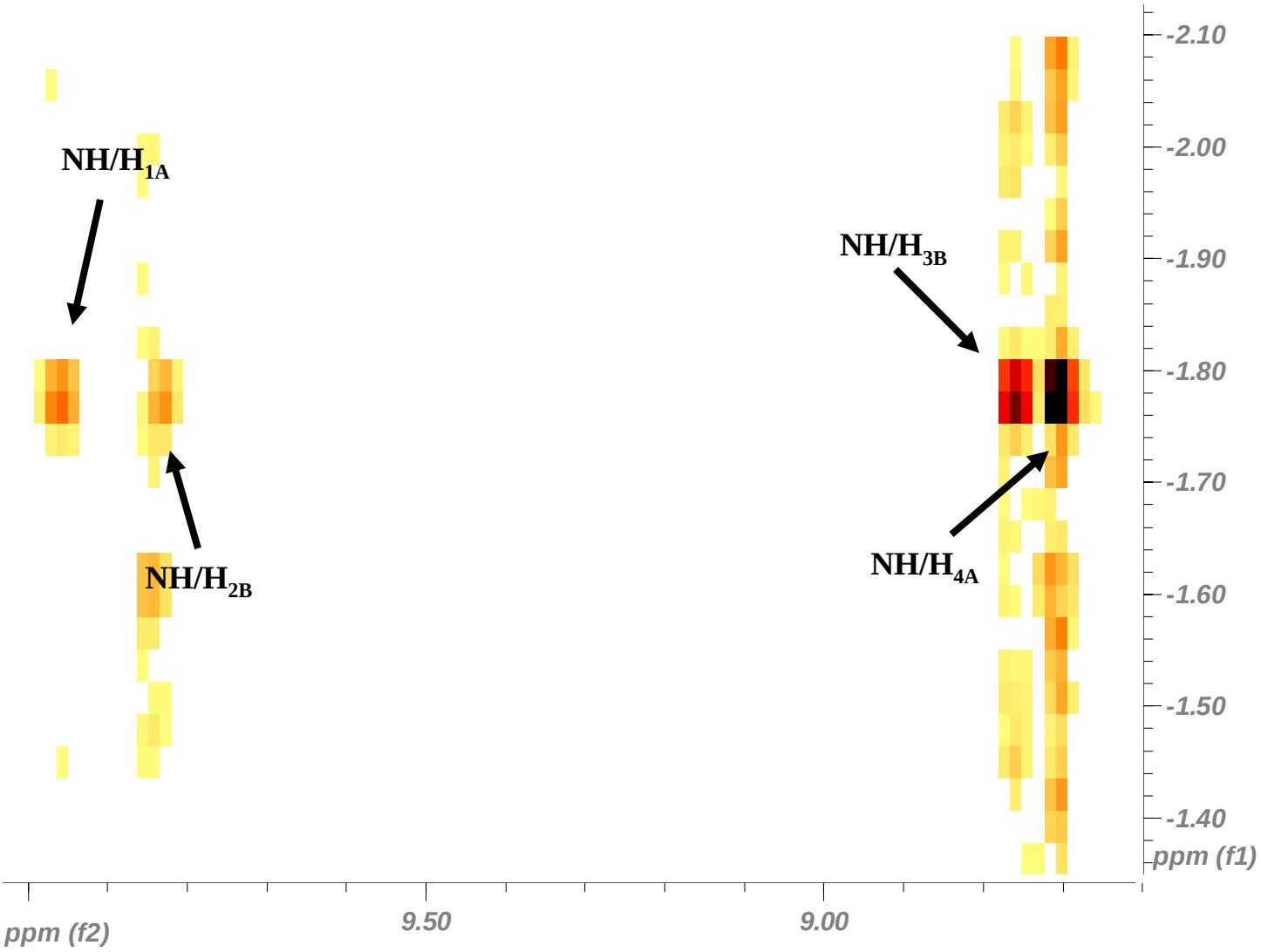


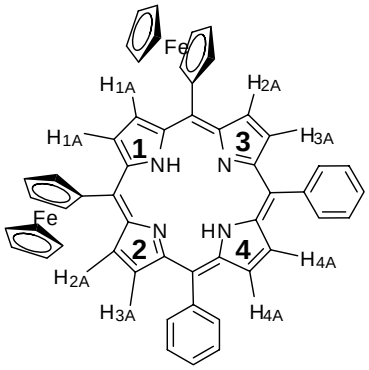
Variable-temperature ^{1}H NMR spectra of $TFcPH_2$ in the NH protons region in THF-d8.



Variable-temperature ^{1}H NMR spectra of $TFcPH_2$ in the β-pyrrolic protons region in THF-d8. Impurity labeled with asterisk.

Partial room-temperature COSY spectrum of *cis*-$Fc_2Ph_2PH_2$ representing weak NH / β-pyrrolic protons correlation





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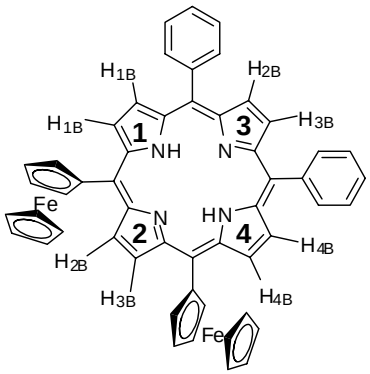

B

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