

Supporting Information

for

Thermodynamic and kinetic stabilization of divanadate in the monovanadate/divanadate equilibrium using a Zn-cyclene derivative: Towards a simple ATP synthase model

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⁵¹V NMR spectra and data fitting results

^{51}V NMR spectra

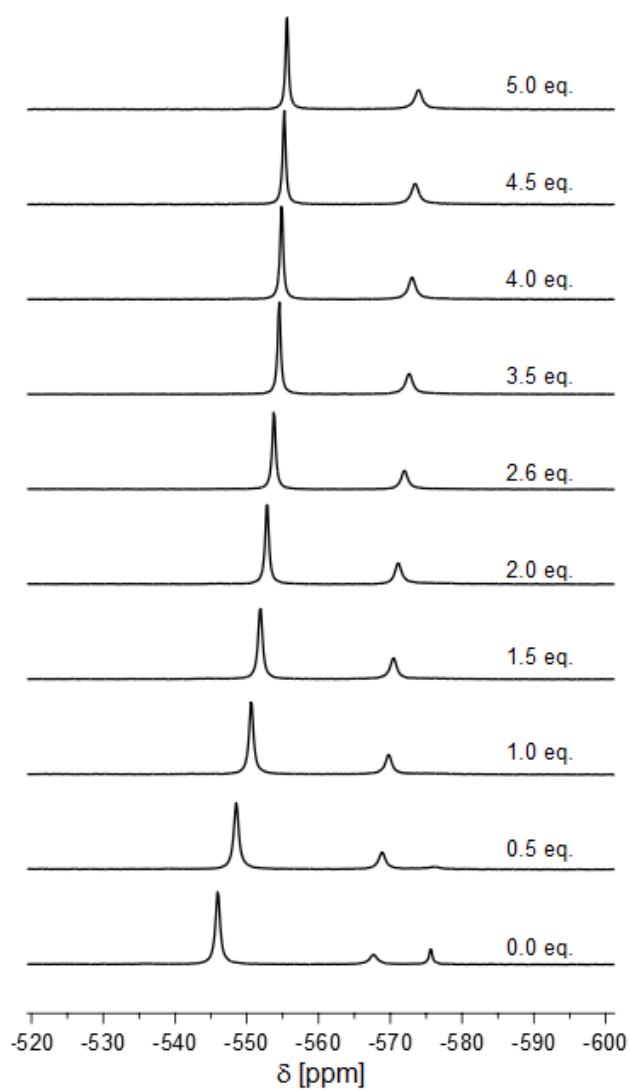


Figure ESI.1: ^{51}V NMR spectra of EPPS buffered solution (pH ~8.5) [100 mM EPPS; 1.5 mM $[\text{Na}_3\text{VO}_4]_t$; 25 °C].

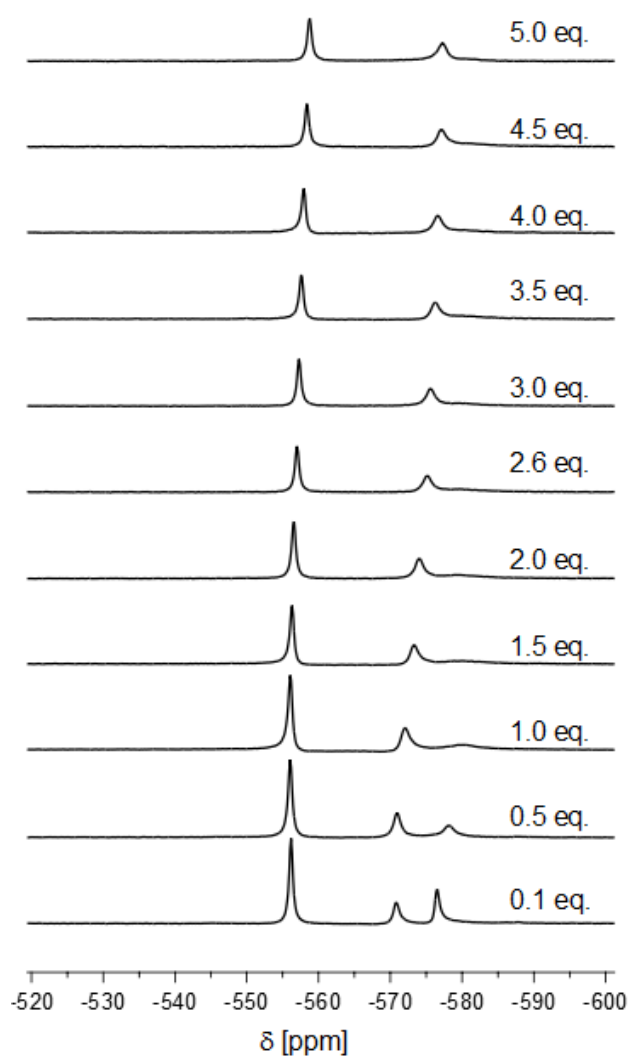


Figure S2: ^{51}V NMR spectra of HEPES buffered solution (pH \sim 7.6) [100 mM HEPES; 1.5 mM $[\text{Na}_3\text{VO}_4]_t$; 25 $^\circ\text{C}$].

Fits to experimental ^{51}V NMR data

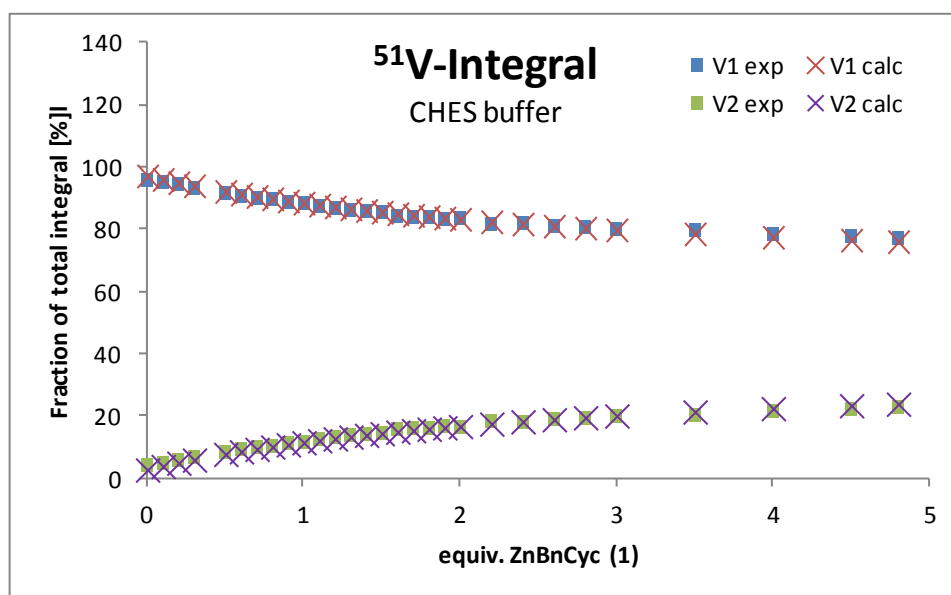


Figure S3: Fit to the ^{51}V NMR data of the titration in CHES buffered solution.

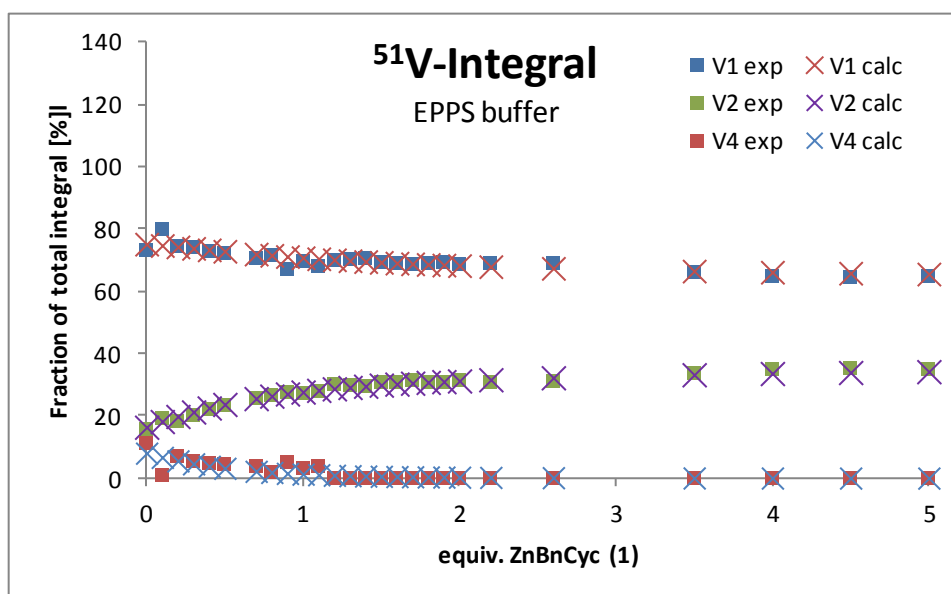


Figure S4: Fit to the ^{51}V NMR data of the titration in EPPS buffered solution.

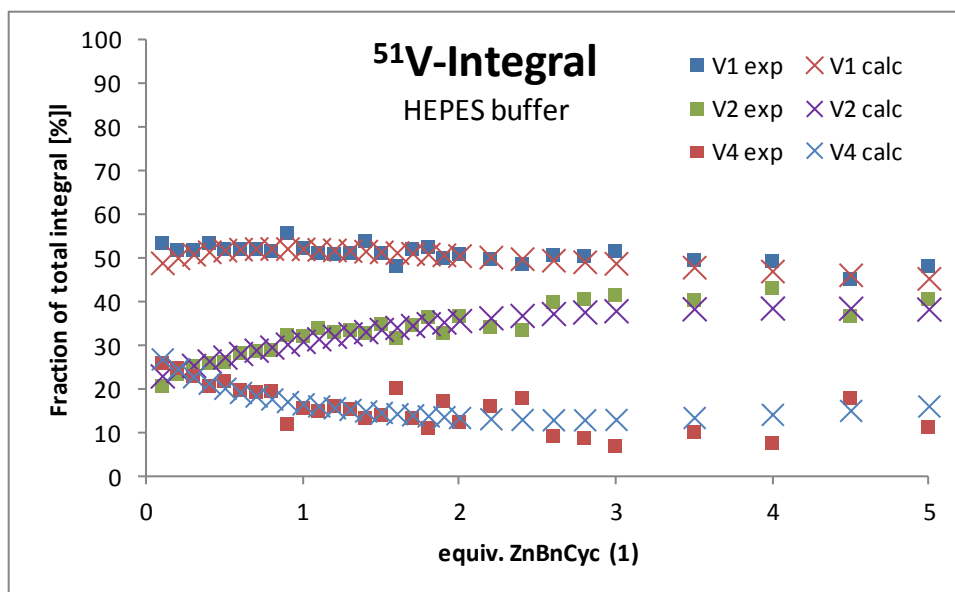


Figure S5: Fit to the ^{51}V NMR data of the titration in HEPES buffered solution.