



Figure S1: CW-EPR spectra (solid lines) and spectral simulations (dotted lines) for (a) reduced cytochrome *c* oxidase, and (b) reduced cytochrome *c* oxidase +cyanide. Data were collected on the Bruker E-680X EPR spectrometer in CW-mode using the Bruker 5mm dielectric resonator probe in a critically coupled configuration. Parameters used to collect EPR data were: sample temperature, 5 K; microwave frequency, 9.67 GHz (**A**) and 9.72 GHz (**B**); microwave power, 63 μ W; field modulation amplitude, 10 G; field modulation frequency, 10 kHz. Simulations were done using the XSOPHE program and the following parameters, for (a): microwave frequency, 9.67 GHz, $g = 2.00$, $D = 140$ G, $E/D = 0.20$, $a_{\text{iso}} = 96.5$ G, D -strain = 20G, E/D strain = .03 and intrinsic Gaussian linewidth = 8.0 G. For (b): microwave frequency, 9.72 GHz, $g = 2.00$, $D = 170$ G, $E/D = 0.20$, $a_{\text{iso}} = 96.5$ G, D -strain = 30G, E/D strain = .05 and intrinsic Gaussian linewidth = 8.0 G. 30 integration partitions were used in the simulations.