

Resonance Raman Spectra of Five-Coordinate Heme-Nitrosyl Cytochromes *c*: Effect of the Proximal Heme-NO Environment

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SUPPLEMENTARY INFORMATION

Table S1. pH-dependence of 5cNO RR frequencies (cm^{-1}) of wt and R124A AXCP at 100 K.

AXCP	pH	$\nu(\text{NO})$	$(\Delta^{15}\text{N}^{18}\text{O})$	$(\Delta^{15}\text{NO})$	$\nu(\text{FeNO})$	$(\Delta^{15}\text{N}^{18}\text{O})$
wt	5.0	1664	(-64)		530	(-15)
	7.0	1664		(-31)	531	(-16)
	9.5	1664	(-65)		533	(-17)
R124A	5.0	1669	(-66)		535	(-16)
	7.0	1671		(-32)	536	(-15)
	9.5	1673	(-69)		534	(-17)

Figure S1. RR spectra of 5cNO wt AXCP (100 K) at pH 9.5 (A and B) and pH 5.0 (C and D). Left panel: high frequency range; right panel: low-frequency range. Samples prepared with ^{14}NO (black traces) and $^{15}\text{N}^{18}\text{O}$ (magenta traces). Isotope difference spectra ($^{14}\text{NO} - ^{15}\text{N}^{18}\text{O}$, blue traces) identify $\nu(\text{NO})$ and $\nu(\text{FeNO})$ vibrations. Asterisks denote vibrations attributed to $\nu(\text{FeNO})$ from a minor 6cNO population.

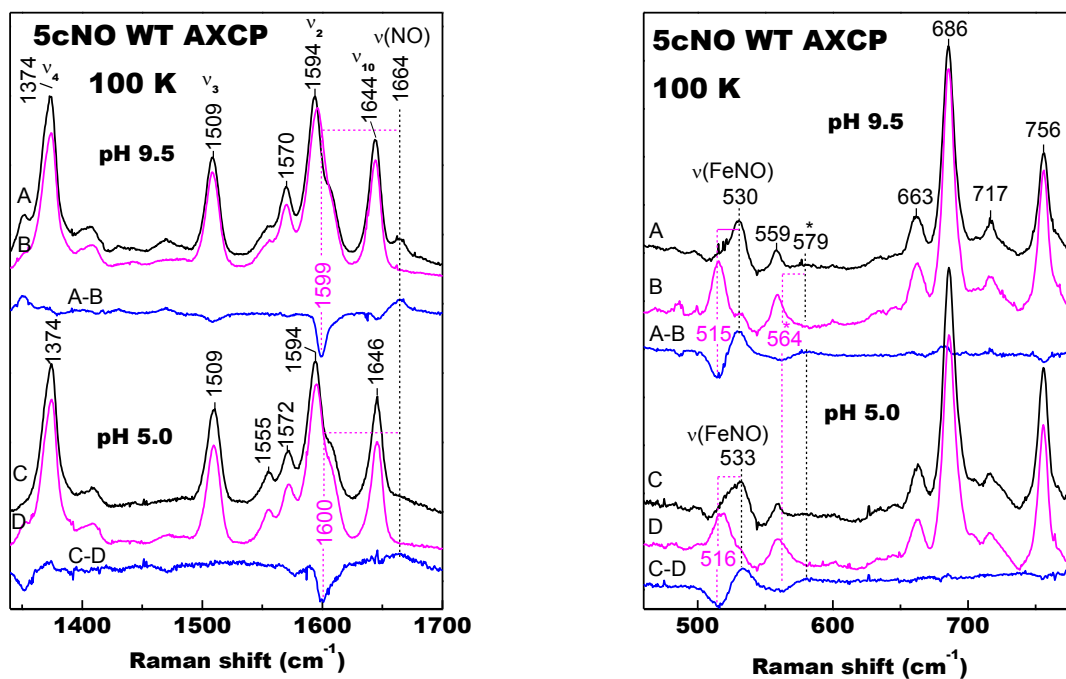


Figure S2. RR spectra of 5cNO R124A AXCP (100 K) at pH 9.5 (A and B) and pH 5.0 (C and D). Left panel: high frequency range; right panel: low-frequency range. Samples prepared with ^{14}NO (black traces) and $^{15}\text{N}^{18}\text{O}$ (magenta traces). Isotope difference spectra ($^{14}\text{NO} - ^{15}\text{N}^{18}\text{O}$, blue traces) identify $\nu(\text{NO})$ and $\nu(\text{FeNO})$ vibrations.

