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**Vibrational Dynamics of Ferric MbCN-A Revisit by  
Resonance Raman and Vibrational Coherence Spectroscopy<sup>1</sup>**

WEIQIAO ZENG, YUHAN SUN, ABDELKRIM BENABBAS, PAUL M. CHAMPION, Department of Physics and Center for Interdisciplinary Research on Complex Systems, Northeastern University, Boston, MA 02115 — Ultrafast pump-probe spectroscopy has indicated that there exists a photoproduct state following the excitation of ferric MbCN<sup>[1][2]</sup>. This excited state decays with a time constant of 3.6 ps<sup>[1]</sup>. Previous studies on this system have suggested that in this photoproduct state, the heme is either (i) still six-coordinated but vibrationally hot in the electronic ground state<sup>[1]</sup> or (ii) the proximal histidine residue (His93) is transiently dissociated, while CN<sup>-</sup> is still bound<sup>[2]</sup>. Recent resonance Raman measurements on ferric MbCN in static solution yield spectra that are very similar to ferric myoglobin, which has His93 and a water molecule as axial ligands. This indicates that a water molecule replaces CN<sup>-</sup> in ferric MbCN under continuous laser excitation. Photolysis of CN<sup>-</sup> from the heme iron is necessary to make this happen, which is not consistent with the above two suggestions. In this presentation we will revisit the dynamics of ferric MbCN with resonance Raman and vibrational coherence spectroscopy and try to explain how a water molecule competes with CN<sup>-</sup> in binding to the heme under photo excitation<sup>[3]</sup>.  
References: [1]Helbing J. et al., Biophys J, vol 87, 1881(2004) [2]Gruia F. et al., Biophys J, vol 94, 2252(2008) [3]Cao W. et al., Biochemistry, vol 40, 5728(2001)

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