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Vibrational Characterization of Myoglobin Compound II W. ZENG, A. BARABANSCHIKOV, Y. ZHANG, J.T. SAGE, Northeastern University, E.E. ALP, W. STURHAHN, J. ZHAO, Argonne National Laboratory — Compound II intermediates are essential to oxygen activation by heme proteins. The protonation status of the Fe^{IV} oxo fragment is controversial. EXAFS and Raman spectroscopy have long suggested an Fe^{IV}=O group, but recent crystal structures show a long Fe-O distance more consistent with a protonated Fe-OH. We use nuclear resonance vibrational spectroscopy (NRVS) to probe the motion of ^{57}Fe in compound II of horse heart myoglobin(Mb II). Although the NRVS signal is weaker than expected, we clearly identify the Fe-O stretch at 805 cm^{-1}, in addition to previously unobserved in-plane Fe vibrations near 360 cm^{-1}. Cryogenic Raman measurement on isotopically labeled Mb II reveals that the kinetic energy distribution (KED) of the Fe-O stretch is localized on the Fe-O fragment, with no significant involvement from the putative proton. Comparison with DFT vibrational predictions provide further insight into the character of the observed normal modes. We conclude that the oxo group is not protonated in Mb II.

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