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Quantitative Vibrational Dynamics of Iron in Porphyrins BOGDAN M. LEU, Northeastern University, Boston, MA, MAREK Z. ZGIERSKI, National Research Council of Canada, GRAEME R. A. WYLLIE, NATHAN SILVERNAIL, W. ROBERT SCHEIDT, University of Notre Dame, Notre Dame, IN, WOLFGANG STURHAHN, ERCAN E. ALP, Argonne National Laboratory, Argonne, IL, STEPHEN M. DURBIN, Purdue University, West Lafayette, IN, J. TIMOTHY SAGE, Northeastern University, Boston, MA, NORTHEASTERN UNIV. TEAM —
We compare quantitative experimental (nuclear resonance vibrational spectroscopy - NRVS) and theoretical (density functional theory - DFT) approaches to characterize the vibrational dynamics of the ^{57}Fe atom in CO-ligated porphyrins designed to mimic the active site of heme proteins. NRVS yields the frequencies, amplitudes, and directions of the Fe vibrations. These measurements confirm many aspects of the DFT predictions, suggesting that the latter provides a reliable description of the observed modes. We will discuss the character of normal modes for Fe(TPP)(1-MeIm)(CO), including a series of modes involving Fe motion in the plane of the heme, Fe-Im modes, Fe-ligand modes, and reactive modes.

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