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Vibrational Dynamics of Heme Model Compounds ALEXANDER BARABANSCHIKOV, Northeastern University, TIMOTHY SAGE, Northeastern University, MINORU KUBO, PAUL CHAMPION, Northeastern University, JIYONG ZHAO, WOLFGANG STURHAHN, ERCAN ALP, Advanced Photon Source, Argonne, IL — Synchrotron- and laser-based measurements supported by DFT calculations identify vibrational modes of the iron atom in Fe(P)(Cl) and Fe(P)(Br). These compounds are large enough to capture many essential aspects of heme geometry and vibrations. On the other hand, porphine models are small enough to simplify the vibrational spectrum and enable accurate analysis using DFT methods. Nuclear resonance vibrational spectroscopy (NRVS) and femtosecond coherence spectroscopy (FCS) provide a rare opportunity to identify both doming and Fe-halide stretching components of the reaction coordinate with confidence. Correlation analysis between 4-coordinate and 5-coordinate compounds suggests significant mixing between Fe-ligand and heme modes. Comparison with the larger model Fe(III)(OEP)(Cl) reveals the effect of peripheral group substitutions.

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