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**Investigations of the low frequency modes of Fe-porphyrin systems and perturbations induced by axial ligation** FLAVIU GRUIA, XIONG YE, PAUL CHAMPION, Northeastern University — We investigate the effect of a 2-methyl imidazole (2-MeIm) ligand on the low frequency ($<$250cm$^{-1}$) vibrational spectrum of iron protoporphyrin IX (Fe-PPIX). This compound is designed to mimic the active site of histidine ligated heme proteins. We use femtosecond coherence spectroscopy to probe the reduced species of Fe-PPIX with and without the 2-MeIm ligand. We notice important changes in the lowest frequency region ($<$50 cm$^{-1}$) of the spectrum, along with the expected disappearance of the 2-MeIm-Fe mode at 216cm$^{-1}$ (in the FePPIX model) when the 2-MeIm ligand is absent. Overall, these observations suggest that a low frequency mode observed near 20 cm$^{-1}$ is associated with the imidazole ligand and that the anharmonic heme doming mode, associated with the Fourier components in the power spectrum near 40 cm$^{-1}$ and 80 cm$^{-1}$, can be affected by axial ligation.

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