Low Frequency Reaction Dynamics in Biological Molecules

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Nuclear resonance vibrational spectroscopy (NRVS) extracts the complete vibrational spectrum of a Mossbauer nucleus from high-resolution X-ray measurements near the nuclear resonance. We determine the frequency, amplitude, and in some cases, the direction of Fe-57 vibrations in proteins and in small molecules designed to mimic Fe sites in proteins.

This rich set of quantitative data can be directly compared to theoretical predictions on an absolute scale. In particular, measurements on oriented single crystals of heme model compounds identify low frequency modes involving Fe motion perpendicular to the plane of the porphyrin.

Comparison with normal mode calculations identifies these motions with heme "doming", similar to the motion that takes place on oxygen binding in myoglobin and other heme proteins. The experimental data provide a direct estimate of the force constant for Fe motion normal to the heme plane, which does not depend on a specific normal mode interpretation. The result suggests that Fe displacement is an important element in protein control of ligand binding. Coupling with global protein vibrations can reduce the expected Fe signal from these reactive modes in the protein environment.