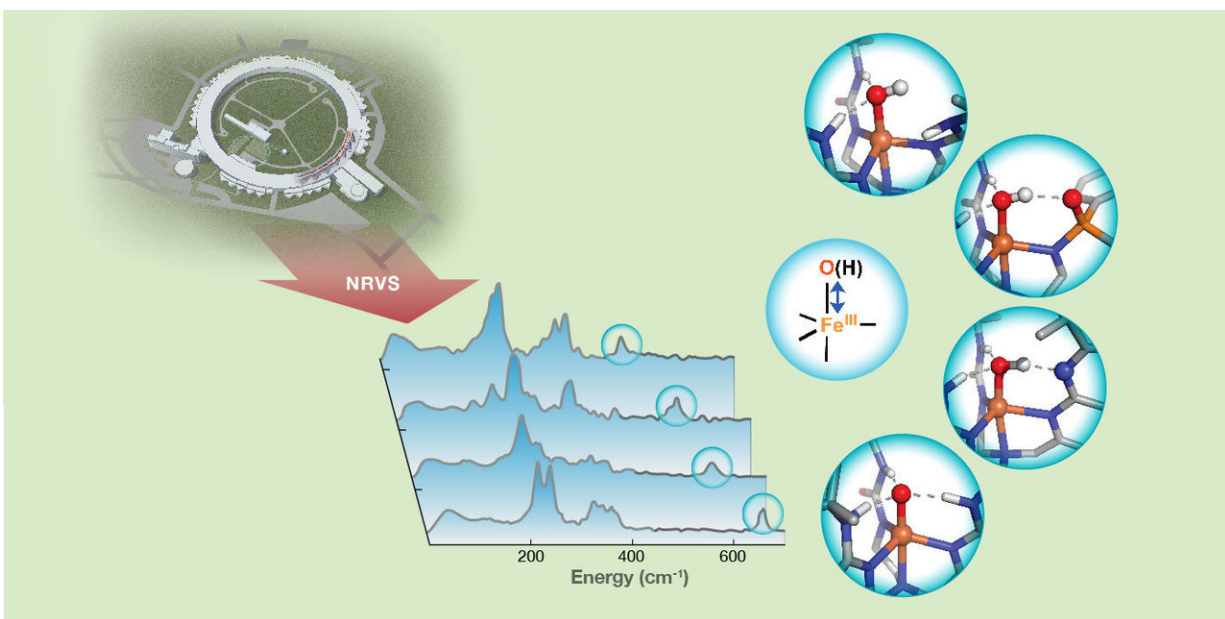


Researchers probe hydrogen bonds using new technique

December 7 2018



Hydrogen bond strength to iron(III)-oxido/hydroxido (FeIII-O/OH) units in nonheme iron complexes is revealed by FeIII-O/OH stretching vibrations detected with ^{57}Fe nuclear resonance vibrational spectroscopy (NRVS). Credit: Carnegie Mellon University

Researchers at Carnegie Mellon University have used nuclear resonance vibrational spectroscopy to probe the hydrogen bonds that modulate the chemical reactivity of enzymes, catalysts and biomimetic complexes. The technique could lead to the development of better catalysts for use

in a wide range of fields. The findings were published as a "[Very Important Paper](#)" in the Dec. 3 issue of *Angewandte Chemie* and featured on the journal's [back cover](#).

Hydrogen bonds are among the most fundamental interactions found in biology and chemistry. They are responsible for many of the chemically important properties of water, for the stabilizing the structures of proteins and nucleic acids, including those found in DNA and RNA, and contribute to the structure of natural and [synthetic polymers](#).

Research has shown that [hydrogen bonds](#) play an important role in tuning the reactivity of the metal centers of metalloenzymes and metal containing catalysts. However, little research has been done to experimentally demonstrate how systematic changes to [hydrogen](#) bonds within the secondary coordination sphere—molecules found in the vicinity of metal centers that do not have direct bonding interactions with the center—influence catalytic activity.

In catalysis, enzymes or synthetic catalysts spur on a chain of chemical reactions, which produce a number of intermediate structures or species. Understanding those structures and their [chemical properties](#) is key to understanding the entire reaction.

"Thoroughly understanding the chemical reactivity of the reactive intermediate is a key step to determining how to design highly efficient and selective catalysts for C-H functionalization," said Yisong Guo, assistant professor of chemistry at Carnegie Mellon and the study's lead author. "In the case of dioxygen-activating enzymes, the key intermediates of catalysis are iron-oxo (Fe-O) and iron-hydroxo (Fe-OH) species, which are involved in important biological processes, such as DNA biosynthesis, DNA and RNA repair, post-translational modification of proteins, biosynthesis of antibiotics and degradation of toxic compounds."

Guo and colleagues used ^{57}Fe nuclear resonance [vibrational spectroscopy](#) (NRVS), a newly developed [synchrotron radiation](#)-based technique, to detect the vibrational frequency of Fe-O and Fe-OH units of synthetic complexes that interact with the secondary coordination sphere through hydrogen bonds. Changes in the frequencies revealed valuable information about the [bond](#) strengths of these units and further provided a qualitative measure of hydrogen bond strength.

"This showed that NRVS is a sensitive technique to pick up very small changes in hydrogen bond strength, down to the changes of a single hydrogen bond. This provides us with a new method to connect changes in bond strength of Fe-O and Fe-OH units to their chemical reactivity," said Guo.

Guo says that this study is a proof-of-concept for using NRVS to probe hydrogen bonds. He plans to continue using this method to study more iron-oxo and iron-hydroxo species in both synthetic complexes and enzymes to build up the amount of available data to correlate chemical reactivity of these species with the changes of hydrogen bond interactions, with the hope that that information could be used to develop more efficient and effective catalysts.

More information: Andrew C. Weitz et al, Probing Hydrogen Bonding Interactions to Iron-Oxido/Hydroxido Units by ^{57}Fe Nuclear Resonance Vibrational Spectroscopy, *Angewandte Chemie International Edition* (2018). [DOI: 10.1002/anie.201810227](https://doi.org/10.1002/anie.201810227)

Provided by Carnegie Mellon University

Citation: Researchers probe hydrogen bonds using new technique (2018, December 7) retrieved 26 April 2024 from <https://phys.org/news/2018-12-probe-hydrogen-bonds-technique.html>

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.