

High Flux ^{57}Fe Nuclear Spectroscopy with a 25m ID

Ming-Hsi Chiang,^{§*#} Vladimir Pelmenschikov,^{€*#} Leland B. Gee,^{†#} Yu-Chiao Liu,[§] Chang-Chih Hsieh,[§] Hongxin Wang,[§] Yoshitaka Yoda,[¥] Hiroaki Matsuura,[‡] Lei Li,[¶] Martin Kaupp,[€] and Stephen P. Cramer^{§*}

[§] *Institute of Chemistry, Academia Sinica, Nankang, Taipei 115, Taiwan*

[€] *Institut für Chemie, Technische Universität Berlin, 10623*

[†] *Department of Chemistry, Stanford University, Stanford, California 94305, United States*

[§] *SETI Institute, Mountain View, CA 94043 USA*

[¥] *Research and Utilization Division, SPring-8/JASRI, 1-1-1 Kouto, Sayo, Hyogo 679-5198, JAPAN*

[‡] *RIKEN/SPring-8 Center, Advanced Photon Technology Division, Life Science Research Infrastructure Group, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5148, Japan*

We have been using the high flux available at BL19LXU for NRVS measurements on Fe-H and Fe-(H₂) complexes. Our goal has been to observe Fe-H and Fe-H₂ vibrational modes, some of which occur in the 1700-2000 cm⁻¹ region. These are relevant to future studies on [NiFe] and [FeFe] hydrogenase enzymes, which catalyze: $\text{H}_2 \rightleftharpoons 2\text{H}^+ + 2\text{e}^-$. Iron hydrogen chemistry is also relevant in its own right, since many Fe complexes and materials are being developed for fuel cell catalysts.

We observed Fe-H stretching modes at 1915 and 1957 cm⁻¹, along with an asymmetric Fe-H₂ stretch at 1773 cm⁻¹. Calculations suggest that even D-D stretching modes in Fe(D₂) should be observable above 2000 cm⁻¹. These are often hard to see in other spectroscopies. The rich information content in NRVS spectra continues to surprise.

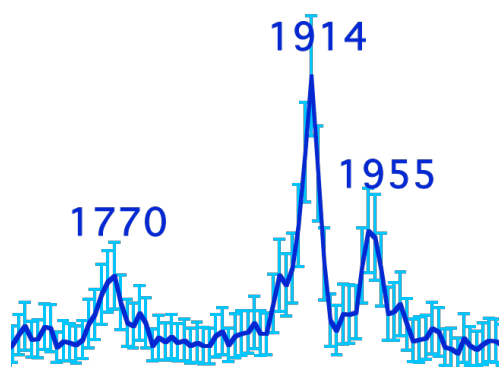


Figure. NRVS in the high frequency region for the classic complex *trans*-[⁵⁷Fe(η^2 -H₂)(H)(dppe)₂][BPh₄].