Submultiple Data Collection to Explore Spectroscopic Instrument Instabilities Shows that Much of the ''Noise'' is not Stochastic

Curtis W. Meuse^a, James J. Filliben^b, and Kenneth A. Rubinson^c

- ^a Institute for Bioscience and Biotechnology Research of the University of Maryland and the Biomolecular Measurement Division, National Institute of Standards and Technology, Rockville, MD 20850 USA
- ^b Statistical Engineering Division, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899
- ^c NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899 and Department of Biochemistry and Molecular Biology, Wright State University, Dayton, OH 45435

Contents:

Figures of a representative Raman autocorrelation and the Fourier transform of that autocorrelation



Figure S1. Autocorrelation of the 1000 submultiple points of the Raman spectrum at 1603 cm⁻¹ with the box showing the graph enlarged vertically and compressed horizontally.



Figure S2. A representative power function of the Raman autocorrelation functions. No clear pattern of lines in fixed positions is apparent between similar plots for various wavelengths. Note the frequency range is much narrower than the equivalent power spectra for IR and CD.

Acknowledgements

Thanks to Professor Faye Rubinson, Georgetown University, for acquisition of the Raman spectra. Support is acknowledged from the National Science Foundation MRI Program (NSF CHE-1429079) for purchase of the Raman instrument. We also wish to thank Dave Krile, Lee Richter, Veronika Szalai, and Jeff Hudgens for their critical reading of the typescript. We are grateful for comments by Sergey Shilov of Bruker Optics and Lindsey Graham of Applied Photophysics for discussions about the inner workings of their respective instruments.

⁺⁺Certain commercial equipment, instruments, chemicals, and software are identified in this paper to specify the experimental procedures adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.