
COLLOQUIUM

■ **SPEAKER**

Prof. Laurence A. Nafie (Department of Chemistry, Syracuse University)

■ **TITLE**

Vibrational Optical Activity: Chirality in Molecular Vibrations

■ **ABSTRACT**

Vibrational optical activity (VOA) consists of two major subfields, infrared vibrational circular dichroism (VCD) and vibrational Raman optical activity (ROA). VCD and ROA are measures of the difference in infrared (IR) absorption and Raman scattering for left circularly polarized (LCP) versus right circularly polarized (RCP) radiation. The first VOA measurements, ROA in 1973 and VCD in 1974, were reported and independently confirmed approximately 40 years ago.^{1,2} Since those early days, there have been many advances in instrumentation, theory, calculations and applications of VOA.^{3,4} In particular, the commercial availability of instrumentation for VCD in 1997 and ROA in 2003, followed by software for calculations of VCD in 1998 and ROA in 2003 opened the field VOA to a wide variety of scientists interested in molecular structure analysis of chiral molecules, including bio-molecules. In 2008 a series of VOA conferences began in Manchester, UK, followed Albany, New York, USA in 2010, Pisa, Italy in 2012 and now Baoding, China, 2014. Today, applications of VOA continue to widen as for example the widespread use of VCD for the determination of the absolute configuration of pharmaceutical and natural product molecules,⁵ the unusual sensitivity of VCD to the supramolecular structure of amyloid fibrils,⁶ and the enhanced sensitivity of ROA to higher-order protein structure where it is being used to assess the structural integrity of biopharmaceuticals and biosimilars.⁷ Given this wide-ranging global progress with over 100 new publications each year, VOA can now be regarded a mature field of molecular spectroscopy.

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2 Holzwarth, G.; Hsu, E.C.; Mosher H.S.; Faulkner, T.R.; Moscowitz, A. *J. Am. Chem. Soc.* 1974, 96, 252; Nafie, L.A.; Cheng, J.C.; Stephens, P.J. *J. Am. Chem. Soc.* 1975, 97, 3842..

3 Barron, L.D. *Molecular Light Scattering and Optical Activity*, second edition, Cambridge University Press, 2004.

4 Nafie, L.A. *Vibrational Optical Activity: Principles and Applications*. Wiley, Chichester, 2011.

5 He, Y.; Wang, B.; Dukor, R.K.; Nafie, L.A. *Appl. Spectrosc.* 2011 65, 699.

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- DATE AND VENUE

October 24, 2016 (Monday, 3:00–5:00 p.m.)

Seminar room 116, R&D Center