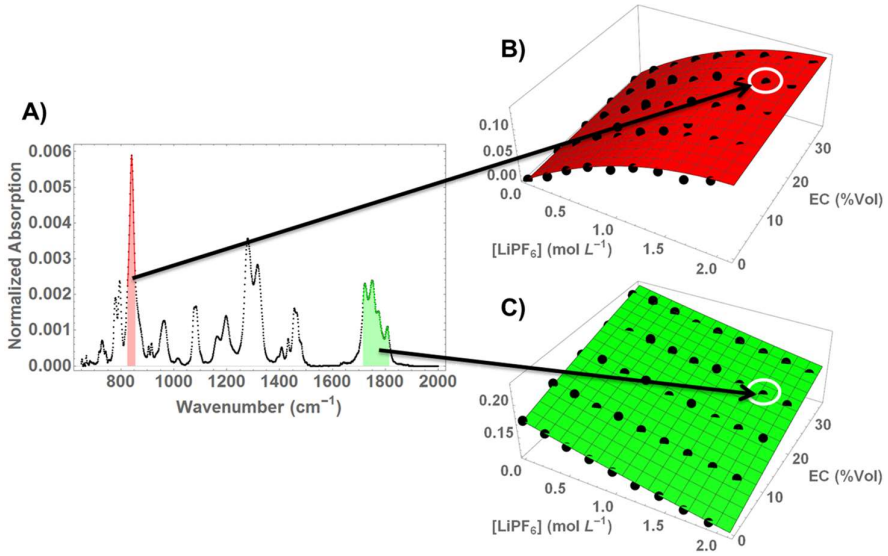
A New Method for Determining the Concentration of Electrolyte Components in Lithium-Ion Cells using Fourier Transform Infrared Spectroscopy and Machine Learning

L.D. Ellis [a], S. Buteau [b] Samuel G.C. Hames [b], L.M. Thompson[a], D.S. Hall [a], and J.R. Dahn [a,b]

[a] *Department of Chemistry, Dalhousie University, Halifax, B3H 4R2, Canada*
[b] *Department of Physics and Atmospheric Science, Dalhousie University, Halifax, B3H 4R2, Canada*

E-mail: jeff.dahn@dal.ca

A new method is introduced for determining unknown concentrations of major components in typical lithium-ion battery electrolytes. The method is quick, cheap, and accurate. Machine learning techniques are used to match features of the Fourier transform infrared (FTIR) spectrum of an unknown electrolyte to the same features of a database of FTIR spectra with known compositions. With this method, $LiPF_6$ concentrations can be determined with similar accuracy and precision as an inductively coupled plasma optical emission spectrometry (ICP-OES) method. The ratios of organic carbonate solvent species can be determined with more rapidity than gas chromatography (GC). This FTIR method is faster and less expensive than GC and ICP-OES, and has the added benefit of being able to determine $LiPF_6$ concentration and solvent fractions simultaneously. Application of this tool can facilitate electrolyte analysis of aged lithium-ion cells, and will help elucidate mechanisms for cell degradation.



A) FTIR spectrum of an electrolyte solution composed of 1.75 M $LiPF_6$, 25% (v) EC in DMC. Red highlights a prominent spectral feature that is strongly correlated with [$LiPF_6$]. Green highlights a prominent spectral feature that is correlated with [EC]. B) and C) show the variation of these spectral features over a range of electrolyte compositions.