SUPPORTING INFORMATION

2D Correlation Spectroscopy and Multivariate Curve Resolution in Analyzing pH-dependent Evolving Systems Monitored by FT-IR Spectroscopy – A Comparative Study

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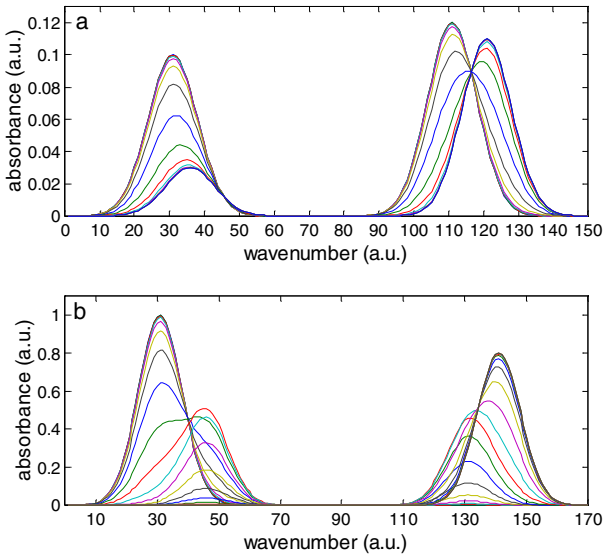

Figure S1. Simulated data sets. a) monoprotic model D1; b) diprotic model D3.

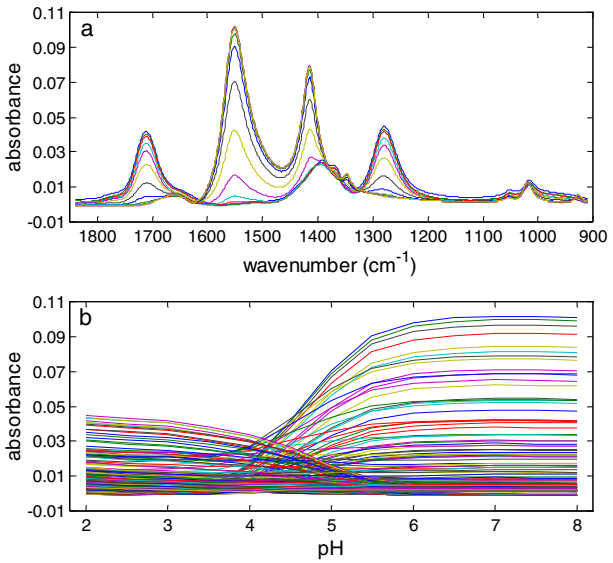

Figure S2. Acetic acid titration. a) spectra; b) wavenumber traces.

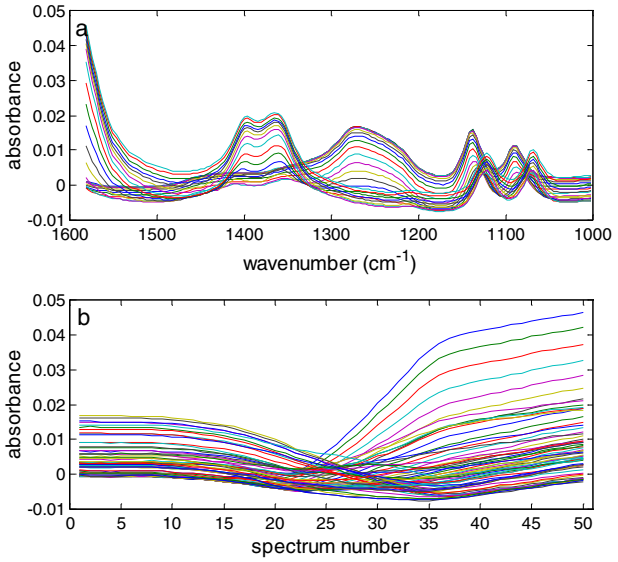

Figure S3. Tartaric acid titration. a) spectra; b) wavenumber traces.

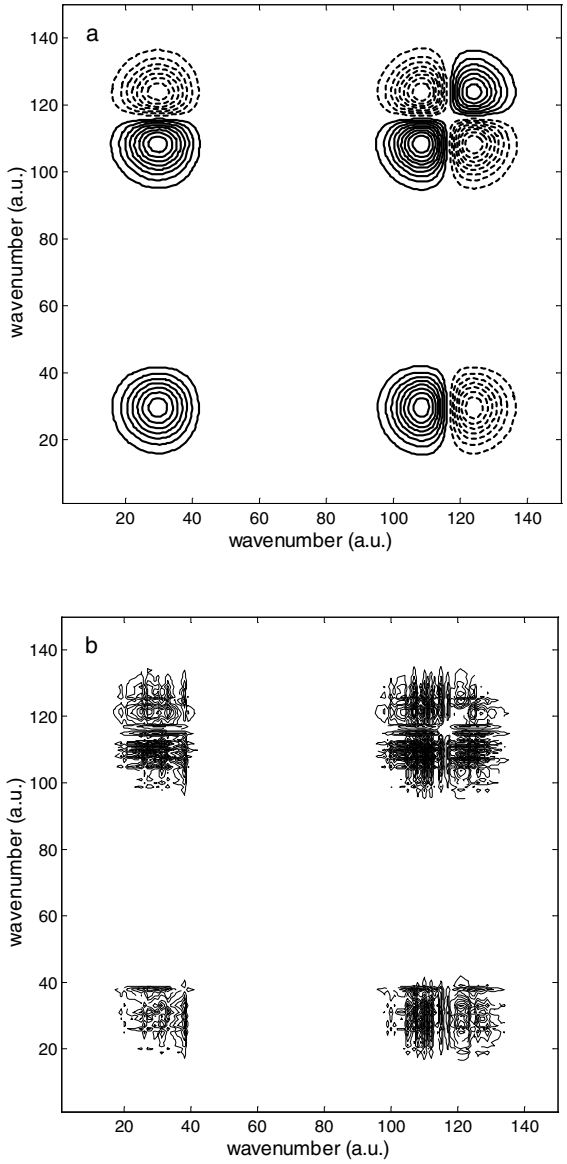

Figure S4. Wavenumber-wavenumber correlation of monoprotic model D1. Synchronous (a) and asynchronous (b) map. Intensities in (b) are at calculation noise level. Positive (solid) and negative (dashed) correlations.

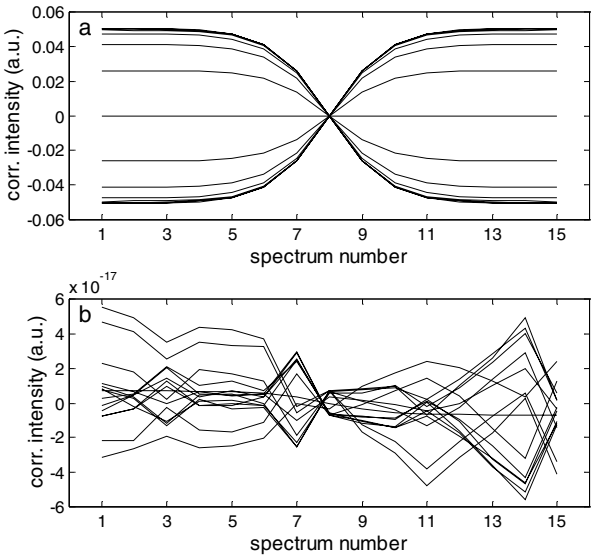

Figure S5. Sample-sample correlation of monoprotic model D1. Synchronous (a) and asynchronous (b) slice plot. Intensities in (b) are at calculation noise level.

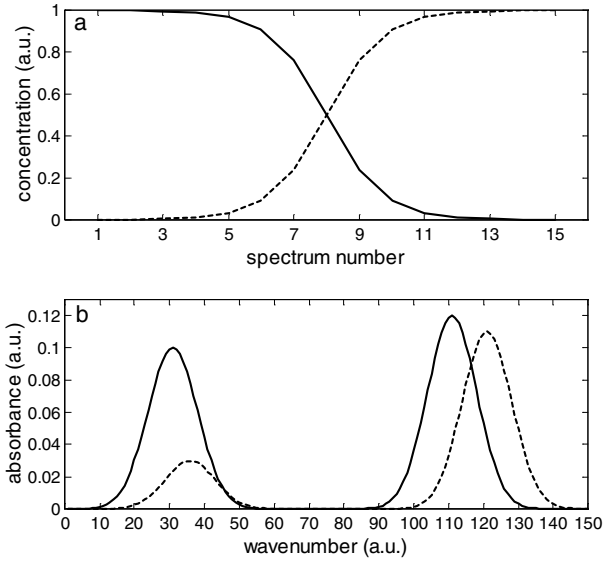

Figure S6. MCR results for monoprotic model D1. Concentration profiles (a) and spectra (b). HA^- (solid), A^- (dash).