

Experimental data associated with the article:

Inline Raman Spectroscopy and Indirect Hard Modeling for Concentration Monitoring of Dissociated Acid Species

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Author Contributions:

A.E.: Acquisition of inline Raman data for formic acid and citric acid titration; IHM calibration and application for quantitative analysis; MCR-ALS analysis; formulation of the parameter estimation problem; estimation of acid dissociation constants; evaluation of data; discussion on method and results; and preparation of the manuscript. C.M.: Acquisition of inline Raman data for acetic acid titration; analysis of aspects influencing the proposed analytical method; discussion on method and results; and preparation of the manuscript. A.M.: Design of the project; scientific support; formulation of the parameter estimation problem; advice on structure and presentation of this work; and reviewing and editing of the manuscript. J.V.: Design of the project; acquisition of inline Raman data for itaconic acid titration; scientific support, guidance, and discussion on method and results; advice on structure and presentation of this work; and reviewing and editing of the manuscript.

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Declaration of Conflicting Interests

The author(s) declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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Table of Content for Data Set:

The data set comprises Raman spectra as acquired with the respective spectrometer (RXN2 process analyzer, Kaiser Optical Systems, now Endress+Hauser AG) and operational software (HoloGRAMS ver. 3.2, Kaiser Optical Systems, now Endress+Hauser AG) in .spc-format (in case of triplicates, a mean spectrum in .mat-format is likewise provided). The Raman spectra are assigned to the composition data from sample preparation and titration experiments using Excel data tables. The following data sets are provided:

- 1) Acetic acid titration
 - a. Titration Raman spectra and associated preparation and experimental data.
 - b. Composition data based on calculation scheme of main article.
- 2) Citric acid titration
 - a. Titration Raman spectra and associated preparation and experimental data.
 - b. Composition data based on calculation scheme of main article.
- 3) Formic acid titration
 - a. Titration Raman spectra and associated preparation and experimental data.
 - b. Composition data based on calculation scheme of main article.
- 4) Itaconic acid titration
 - a. Titration Raman spectra and associated preparation and experimental data.
 - b. Composition data based on calculation scheme of main article.
- 5) Levulinic acid titration
 - a. Titration Raman spectra and associated preparation and experimental data.
- 6) Oxalic acid titration
 - a. Titration Raman spectra and associated preparation and experimental data.
- 7) Succinic acid titration (two separate titration experiments)
 - a. Titration Raman spectra and associated preparation and experimental data.