Supporting Information

PyMESpec: A Python Toolbox for Automated Modulation Excitation Spectroscopic Data Analysis and Transient Experiments

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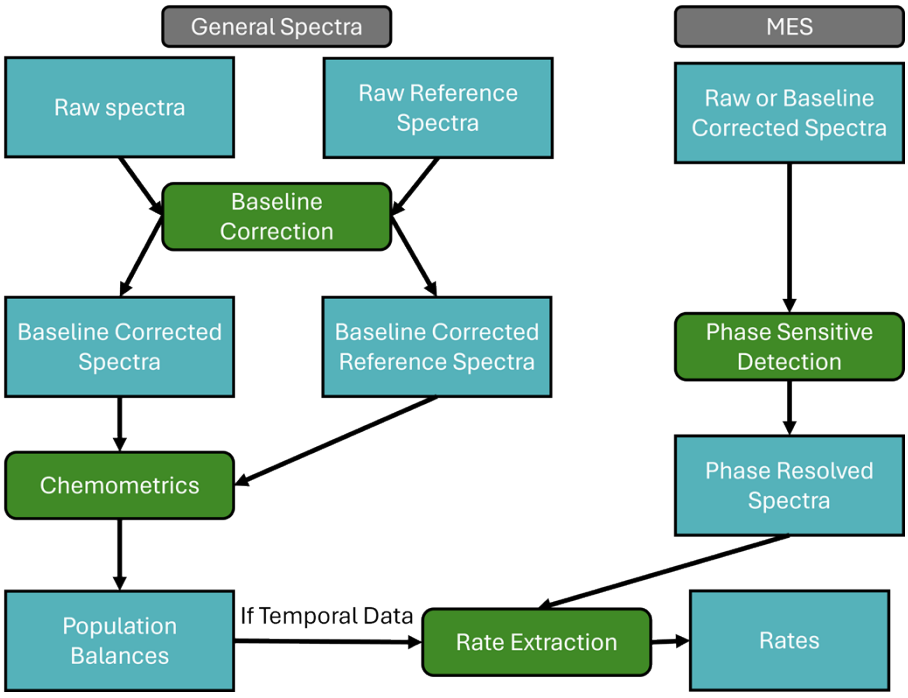

Figure S1*: A flowchart diagram detailing the general workflow of processing general or modulation excitation (MES) spectra to obtain quantities of interest. This is an example flow diagram; many processes can be performed out of order or omitted.*

S1. Correlating vanadium species compositions in UV-vis from NAP-XPS:

The NAP-XPS and UV-vis experiments were conducted in different reaction conditions (1 mbar and 60 mbar ethanol, respectively) due to equipment constraints in both cases. Despite the differences, both experiments show similar reduction trends (Figure S2). $4V/TiO_2$ reduction can be monitored with UV-vis by tracking absorbance at 600 nm, which corresponds to V^{4+} species.[1] The absorbance increases over 20 min before approaching a plateau, indicating the $4V/TiO_2$ cannot be reduced further by 60 mbar ethanol at 130 °C. Reduction in NAP-XPS is tracked by calculating V^{5+}, V^{4+}, and V^{3+} species compositions after XPS deconvolution. Although slower than in the UV-vis conditions, V^{5+} and V^{4+} change more rapidly when reduction starts before approaching a plateau as the $4V/TiO_2$ stops reducing further. V^{3+} increases slightly but is more stable than V^{5+} and V^{4+}. Since the samples start and end at the same degrees of reduction in both UV-vis and NAP-XPS, the $4V/TiO_2$ takes five times longer to stop reducing further. The difference in the time to reduce can be attributed to the difference in ethanol and Ar pressures between the UV-vis and NAP-XPS conditions.

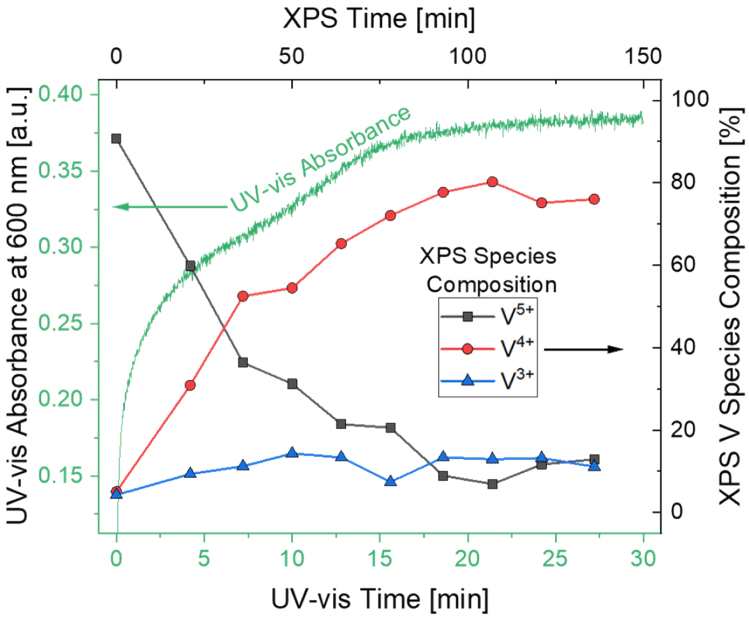

***Figure S2**: $4V/TiO_2$ reduction monitored by UV-vis and NAP-XPS. The 600 nm region in UV-vis corresponds to V^{3+} and V^{4+} species, so higher absorbance means greater reduction. The NAP-XPS data is displayed to be five times slower than UV-vis to match their reduction behaviors.*

S2. Explanation of the computation of pure components from composite spectra:

Given the known relative fractions of pure components in the UV-vis spectra, we solve for **B** in the equation **AB** = **C**, where **A**, **B**, and **C** are $m \times l$, $l \times n$, and $m \times n$ matrices, respectively. Here, l is the number of pure components, m is the number of spectra collected, and n is the number of wavenumber bins in UV-vis spectra. This results in an overdetermined problem, because we have three pure components and ten collected spectra, thus we solve by minimizing the residual error.

S3: Graphical user interface (GUI) details

The GUI can be activated by running python GUI.py from any IDE or the command line. The GUI enables the running of a simplified version with a subset of the functionality available in the PyMESpec Python toolbox. After a user has configured the analysis, they wish to perform, clicking the run button will perform the analysis, save the processed data files, and save a yaml configuration file for easy reloading of the same analysis settings for future data processing.

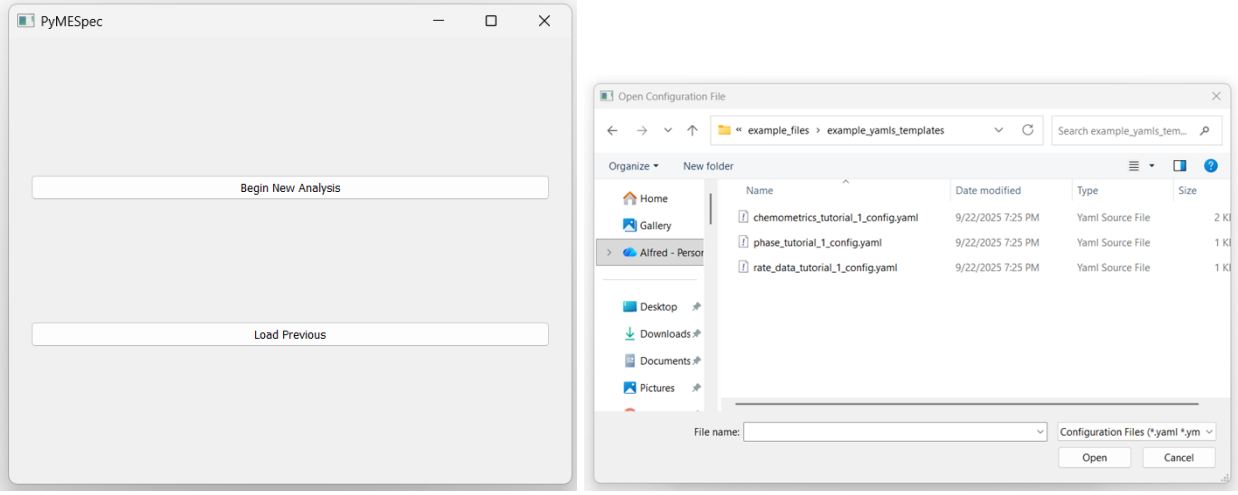

Figure S3*: (a) The GUI front page and (b) the interface for loading preexisting yaml configuration files for reproducible data processing.*

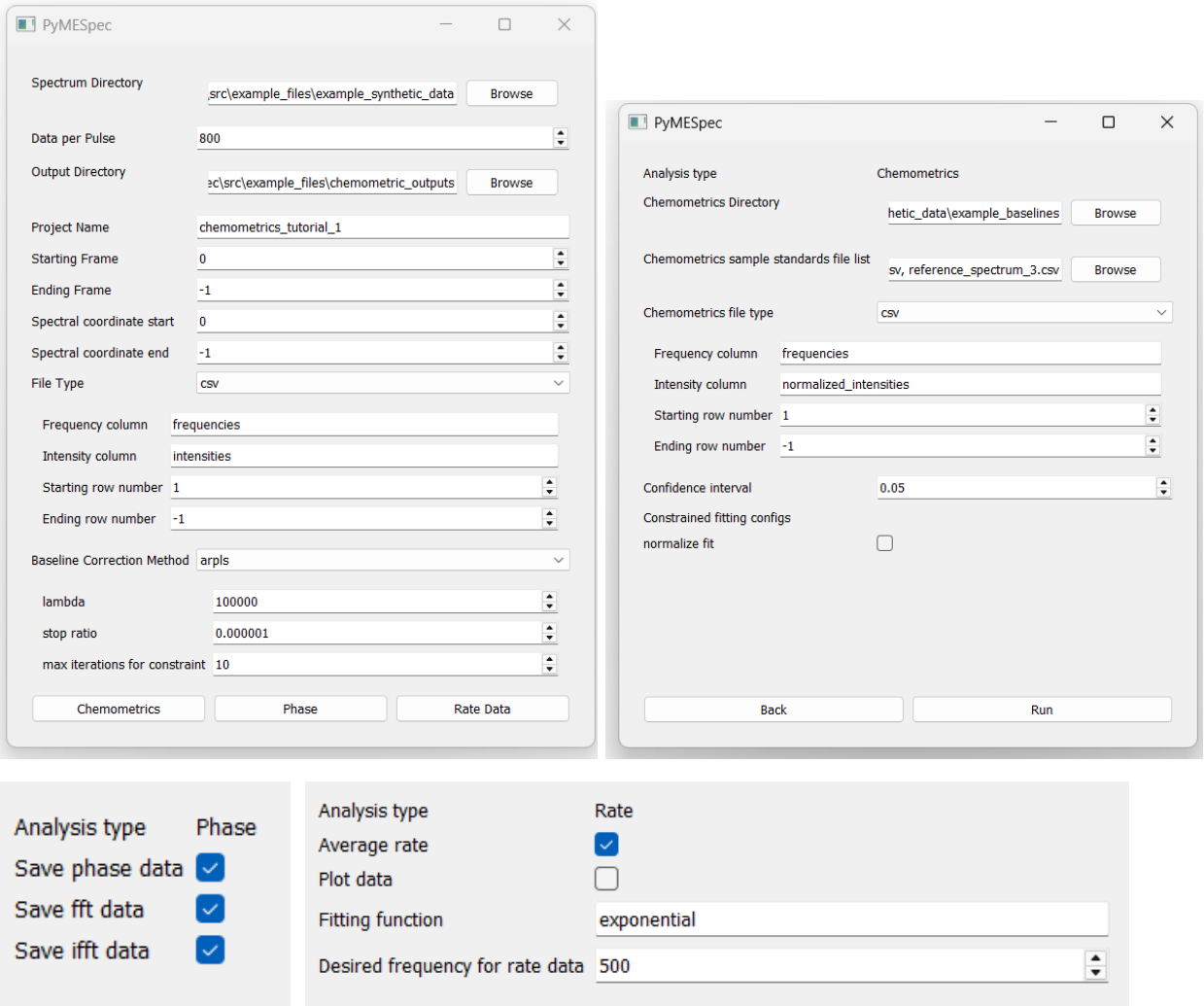

***Figure S4**: Example panels from the GUI for data processing functionalities of PSD, chemometrics, and rate extraction.*

References

1. D. W. Kwon, K. H. Park and S. C. Hong, *Appl. Catal., A*, 2015, **499**, 1-12.