

Diffraction Order Penalization to Improve Spectrometer Calibrations

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Calibration in diffracted spectroscopy typically depends on identifying strong, well-known lines in the recorded spectra and fitting a calibration function to them. We outline a novel method (order penalization) for improving spectroscopic calibrations by extending non-linear least squares fitting of the calibration curve. The method introduces an extra term into the minimized quantity that penalizes disagreement in the positions of spectral lines observed in multiple diffraction orders. The primary advantage of this method is that the lines used do not have to be identified, except for establishing the fact that they are different orders of the same line. This increases the number of constraints on the calibration curve, potentially in spectral regions where no regular calibration lines are available. The mathematical basis of this method is described, and the performance of this method is evaluated on simulated data and experimental data from the National Institute of Standards and Technology (NIST) Electron Beam Ion Trap. We demonstrate the effectiveness of the method on the spectra of highly charged Ag-like Re28+ and nearby charge state ions.