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Cautionary notes on the comparability of geothermometric data gained by Raman spectroscopy of carbonaceous material

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Raman spectroscopy of carbonaceous material (RSCM) is frequently used for geothermometric purposes. The Raman spectrum indicates the increase in structural order of the carbonaceous material by thermal overprint. The spectrum is usually processed by curve-fitting which gives peak-parameter ratios that express metamorphic temperature. The comparability of these results, however, is poor, especially in low metamorphic rocks, given at least three major sources which induce data variation. These sources are (1) the sample itself (for instance structural anisotropy, sample preparation), (2) the experimental setup which includes the Raman spectrometer configuration (e.g. excitation wavelength, spectral grating, and orientation of the sample to the laser) and (3) the spectral curve-fitting procedure (e.g. baseline function, degrees of freedom in the model and personal fitting strategy).

To investigate the impact of those sources on the RSCM results, a sample set covering low to high metamorphic conditions was investigated in an experimental series.

The experiments show that curve-fitting is strongly influenced by the applied fitting strategy and the degrees of freedom in the model which implies the need for a standardized procedure. Analyzing the same sample with different Raman spectrometers will generally give different or varying results due to the multitude of parameters (CCD, grating, excitation wavelength) and their combinations within the spectrometers. This implies that every Raman spectrometer used for geothermometry on CM needs its own calibration which demands a standard series that covers a wide range of temperatures, although sample heterogeneity will still induce variation even with a standard series. We conclude that the overall comparability of RSCM-data of different laboratories will be increased drastically when using a standard series combined with a standardized curve-fitting procedure.