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Title:Chemical identification and determination of sulfonamides in n-component solid mixtures within THz-region - Solid-state Raman spectroscopic and mass spectrometric study
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Abstract:The identification and quantitative determination of sulfonamidesin solid-state as n-component mixtures is performed. The limits of detection (LODs), accuracy, precision and repeatability are obtained and discussed, using the Raman spectra within 200-30 cm-1 region (6.00-0.9 THz). The excitations, corresponding to H-bonding deformations, lattice vibrations, as well as coupling modes are used for determination. The validation of the statistical and mathematical tools for procedure of the spectroscopic patterns is performed. The possibilities of baseline correction methods, smoothing procedures, and non-linear curve fitting method for quantitative analysis within THz-region for complex spectroscopic patterns of n-component mixtures (n = 1-5) are discussed. The hybrid HPLC tandem mass spectrometry (MS/MS) and powder XRD are applied as independent physical methods for analysis of the studied systems.
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