

ANALYSIS OF IONIC SPECIES IN NATURAL MINERAL WATERS STUDIED BY RAMAN SPECTROSCOPY

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Abstract: This contribution reports on the application of Raman scattering for qualitative and quantitative analyses of natural mineral waters. Polyatomic ions such as SO_4^{2-} , HCO_3^- and NO_3^- were measured down to concentrations of about 10^{-6} mol/L.

In the past, Raman scattering from aqueous electrolytic solutions has been proved to be a useful instrument for the analysis of the ion-water and ion-ion interaction. Contrary to IR measurements, the ionic vibrations are not as strongly masked by the water vibrations. However, most Raman investigations dealt with concentrated or moderate diluted solutions. Nowadays, spectrometers with high optical throughput and CCD detection enable measurements on highly diluted solutions [1] We have studied the possibilities of Raman scattering to analyse the content of polyatomic ions in highly diluted solutions. In particular, species in natural mineral waters were analysed qualitatively and quantitatively. Low concentrations, for instance, down to about 10^{-6} mol/L in the case of NaNO_3 , could be detected [2].

The Raman spectra were excited with 1.5 mW laser light power of an Ar^+ -laser working at the wavelength 514.5 nm. 90° geometry was used. The spectra were analysed by a Jobin-Yvon T64000 triple monochromator working in the subtractive mode of the gratings and detected by a cooled CCD. As an inner standard the deformation band of water at 1640 cm^{-1} was used. Prior to the fitting of the Raman spectra with Gauss-Lorentzian bands, the spectrum of triply distilled water was subtracted (this can be done because the solutions were very dilute). For calibration, solutions with known ionic concentrations were prepared and measured.)

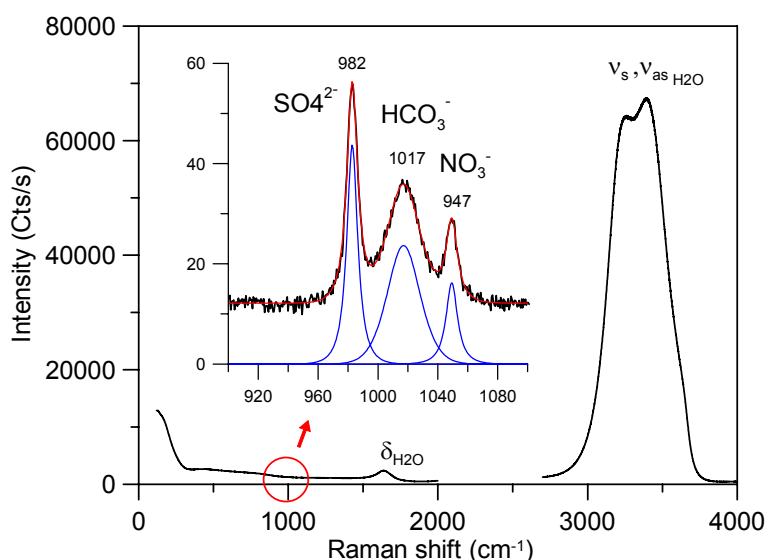


Fig. 1. Raman spectrum of a natural mineral water (Luna, Italy). The inset shows the fingerprint region after the pure water spectrum was subtracted.

As an example, Fig.1 shows the Raman spectrum of a commercially available mineral water (for a website of almost all commercially available mineral waters see [3]).

In Fig.2 the concentrations of several mineral waters obtained from our Raman measurements are compared with values taken from a data collection of about 2000 mineral waters, where the concentrations were determined with standard methods.

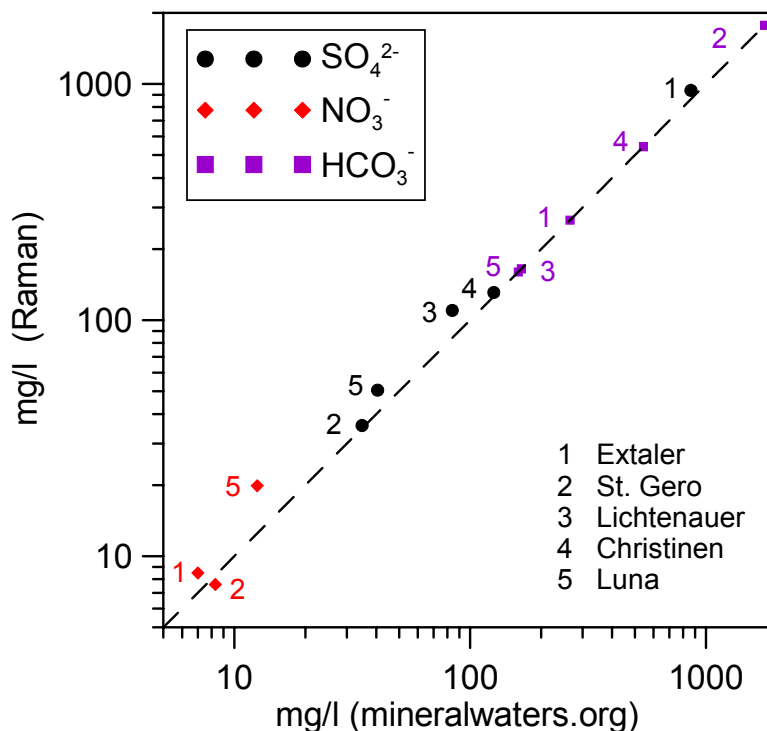


Fig. 2. Comparison of the concentrations obtained from the Raman measurements and published values measured with other methods.

The region between $900 - 1100 \text{ cm}^{-1}$, comprises the N-O stretching region of the anions (SO_4^{2-} , HCO_3^- , NO_3^-) and may be viewed as the fingerprint region for these anions. In addition to the anions we could also observe the vibrational modes for dissolved CO_2 in the gaseous mineral waters at 1276 cm^{-1} and 1384 cm^{-1} [4].

References:

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