

## WATER AS AN INTERNAL STANDARD IN THE RAMAN STUDY OF HYDROTHERMAL SYSTEMS

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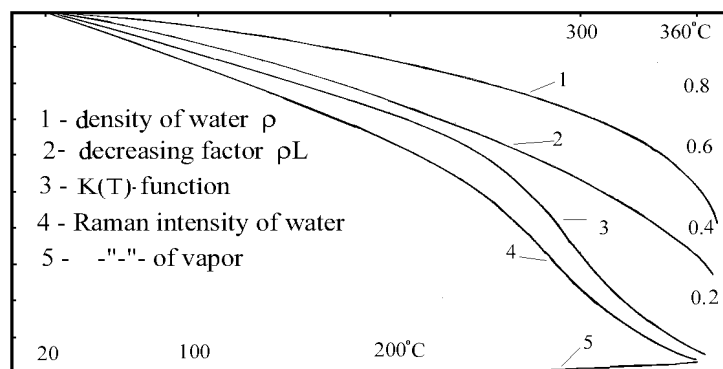
URL: [http://www.scgis.ru/russian/cp1251/h\\_dgggms/5-2000/hydroterm26.eng](http://www.scgis.ru/russian/cp1251/h_dgggms/5-2000/hydroterm26.eng)

The experimental study of hydrothermal systems by Raman spectroscopy is now broadly used. The highest temperatures and pressures are limited only by a firmness of the windows of the spectroscopic cell. In most cases the results of these study have a qualitative character.

But it turns to a quantitative tool if using the Raman scattering of the water as an internal standard. In this case Raman cross section of studied complex is assumed to be independent of the temperature, and

its concentration - to be proportional to Raman intensity.

Contrariwise the integral intensity of the band of water stretch vibrations ( $3000-3700\text{ cm}^{-1}$ ) decrease with a temperature faster then the density of the water as it depends also on the dielectric constant of the media  $n(T)^2$  after a Lorenz factor  $L(T) = [(n^2+2)/3]^4$ . The intensity depends on the number of hydrogen bonds in the structure of the water also.



The molal concentration of the  $i$ -th species in the solution at high temperature can be determined during next procedure. At first the scaling constant  $A_i = (I_{H_2O}^0 / I_i^0) \cdot m_i$ , where  $I$  is the intensity,  $m_i$  is the concentration of  $i$ -th species in mol/kg $H_2O$ , must be determined at the room temperature. The normalized values of the density and the intensity of the water as a function of the temperature  $K(T) = (I^T / I^0) \cdot (\rho^0 / \rho^T)$  are also required. The molal concentration of the  $i$ -th species is now expressed as:

$$m_i^T = A_i \cdot (I_i^T / I_{H_2O}^T) \cdot K(T)$$

The function  $K(T)$  is independent on the setup parameters, whereas the constant  $A_i$  depends on the scattering geometry, laser wavelength, spectral properties of the setup and thus is not a universal constant.

If the molal concentration of some volatile matter must be in a vapor phase determined then the calibration on the Raman line of a water vapor will be used. The intensity of this line is proportional to

vapor density up to  $360^\circ\text{C}$ , hence  $K(T) = 1$ . The constant  $A_i$  can be determined by using the Raman scattering cross section values published in [1] or to perform the calibration of the setup against the gas mixture including the water vapor of a known composition. For this purpose a solution with the known content of studied component is placed into the autoclave and then is heated up to complete evaporation of the liquid phase. The scaling constant is defined from the relation of the Raman lines areas already in gase phase.

1. V.M.Nemets, A.A.Petrov, A.A.Solov'ev. Raman spectroscopy of nonorganic gases // Zh. Prikl. Spectrosc. 1987. V.47. N4. P.536-549.