IR Fourier spectroscopy of water and H-containing defects in quartz

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The IR-spectroscopy, especially in connection to the appearance of modern Fourier-spectrometers, is the most effective method for studying the condition and structural position of water in quartz. IR spectrum of quartz in the field of fundamental valence vibrations of water (3000-3800 cm^{-1}) represents wide diffused band on which, narrow bands or so-called H-defects are imposed. The wide band is attributed to the molecular water which is found basically in the cracks and gas-liquid inclusions. Narrow bands are caused by vibrations of structurally related water which, first of all are related to hydroxyl groups, found in different structural environments.

For the detailed analysis of spectra of granulated quartz of Kuznechinskoe and Kishtimskoe deposits, modelling of "water" area (3000-3800 cm^{-1}) on superposition of 7 Gaussian lines is been done. It is stated, that the basic strips of 3220 and 3410 cm^{-1} belong, accordingly, to symmetric and antisymmetric valent vibrations of O-H links in water molecules. Small lines with maxima of 3198 and 3296 cm^{-1} are related to overtones and compound frequencies of the basic vibrations of Si-O link in a quartz lattice. The narrow band with a maximum of 3379 cm^{-1} is related to vibrations of Al-OH groupings formed during replacement of Si by Al in a lattice of SiO_4 tetrahedrons. Bands of 3600 and 3750 cm^{-1}, as a rule, are registered due to vibrations of O-H groups in finely dispersed hydrogenous mineral deposits in quartz [1, 2]. These bands are observed in spectra of micas which according to the mineral analysis, are widespread mineral inclusions in the studied samples of quartz. It is necessary to note, that in work [3] it is specified, that bands of 3600 and 3750 cm^{-1} may be related, accordingly, to symmetric and asymmetric vibrations of OH-groups in silanol groupings or in the isolated molecules of water.

In conformity with Bouguer-Lambert-Beer law, concentration of various H-defects has been calculated. The executed calculations have shown, that water in quartz of Kuznechinskoe and Kishtimskoe deposits is basically contained in the molecular form in cracks, channels, intergranular space and gas-liquid inclusions.

For determination of behaviour of water in quartz of Kuznechinskoe and Kishtimskoe deposit, experiments on high-temperature annealing were conducted in an interval of 100 - 1200 °C with spacing of 100 °C with registration of an infrared spectrum after every annealing. With the increase in temperature of annealing, intensity of wide bands of 3410 cm^{-1} decreases. At the temperature 1100 °C, the narrow band of 3378 cm^{-1} practically disappears, that specifies the dehydration of Al-OH groupings at this temperature.

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[1] Aines R.D., Rossman G.R. *Journal of Geophysical Research*. 1984. **89**. B6. 4059 [2] Kats A. Hydrogen in Alpha-quartz *Philips Research Reports*. 1962. **17** 201 [3] Kronenberg A.K. *Rev. Miner*. 1994. **29.** 123