

**Spectroscopic analysis of molecular water and hydroxyl groups content
in N–O–H ferriiferous silicate glasses by FTIR spectroscopy**

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The concentration of hydroxyl groups OH⁻ and molecular water H₂O dissolved in the quenched melt as a function of *f*O₂ was estimated by the method of Infrared Fourier pectroscopy.

Key words: experiment, silicate melt, dissolution, FTIR spectroscopy, hydroxyl groups, molecular water

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Studing the forms of dissolution of H, N and O volatiles in glasses – the quenching products of experiments in the system “silicate melt + fused metal Fe phase + Si₃N₄ (1, 3, 5 and 7 wt. %) + H₂» are continued at high pressure and temperature (4 GPa, 1550–1600°C) and low oxygen fugacity (by 2÷4 logarithmic units below the iron–wustite buffer equilibrium Δ*lgf*O₂ (IW)).

Table. Parameters for calculating the contents of hydroxyl groups OH⁻ and molecular water H₂O in L5–L8 albite samples

Run	NBO/T	Fugacity Δ <i>logf</i> O ₂ (IW)	Density ρ, g/cm ³	SiO ₂ , %***	Al ₂ O ₃ , %***	Na ₂ O, %***	FeO, % ***	H ₂ O, %***	Impurity							
									OH ⁻				H ₂ O			
									α, cm ⁻¹	ω, cm ⁻¹	ε*,	C ^{OH} , wt. %	α, cm ⁻¹	ω, cm ⁻¹	ε**	C ^{H₂O} , wt. %
L5 d=114 μ	0.384	-2.1	2.4892	63.43	15.87	8.64	9.40	2.66	650	3548	62.4	7.54	186	1632	(49 ± 2) liter/mol·cm	2.74
L6 96μ	0.359	-2.3	2.4725	64.38	15.70	8.78	8.61	2.53	475	3548	62.6	5.53	74	1632		1.10
L7 111μ	0.316	-2.9	2.3516	68.78	15.56	8.13	4.02	3.51	378	3548	63.3	4.58	104	1632		1.63
L8 94μ	0.303	-3.3	2.3143	69.97	15.47	8.45	2.43	3.67	185	3548	63.5	2.27	46	1632		0.73

α, cm⁻¹ – absorption coefficient (IR spectroscopic data)

d, μ – sample thickness

ω, cm⁻¹ – frequency

NBO/T – structural-chemical parameter describing a degree of melt polymerization

ε, liter/mol·cm – molar absorptivity

ε* – calculation according to [Mercier *et al.*, 2010] using our NBO/T data

ε** – according to [Dixon *et al.*, 1995]

C^{OH}, wt. % – OH⁻ content

C^{H₂O}, wt. % – H₂O content

$\Delta \log fO_2(IW)$ – oxygen fugacity below the iron–wüstite buffer equilibrium

*** - ion microprobe data

To estimate the concentration of hydroxyl groups OH^- and molecular water H_2O dissolved in the quenched melt as a function of fO_2 the method of infrared (IR) Fourier-spectroscopy is used. IR transmission spectra were recorded in the frequency region from 350 to 5000 cm^{-1} with a resolution of 2 cm^{-1} and a noise level not worse than 0.1 %.

The position and shape of a wide asymmetric absorption band at 3548 cm^{-1} corresponds to stretching vibrations of hydroxyl groups OH^- and molecules H_2O [Newman, et al., 1986, Kadik et al., 2004]. A sharp peak at 1632 cm^{-1} is a result of deformational (bending) vibrations of molecules H_2O [Dianov et al., 2005]. In both peaks a reduction of their intensity is observed with lowering fO_2 within the values of $\Delta \log fO_2(IW)$ from -2 to -4, so the content of oxidized hydrogen forms OH^- and H_2O decreases in glasses.

The absorption coefficient α of studied glasses has been calculated from thus obtained IR absorption spectra from the 3548 cm^{-1} and 1632 cm^{-1} bands corresponding to vibrations of hydroxyl groups OH^- and H_2O molecules. To calculate the extinction coefficient ϵ thereof we have used its empirical dependence on the structural parameter NBO/T obtained in [Mercier et al., 2010]. After all the OH^- and H_2O contents in glasses was calculated using the Lambert-Beer law [Stolper, 1982]: $C = \alpha \times 18.02 / \rho \times \epsilon$. Thus obtained results are listed in the Table.

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