

Chemical interdiffusion between Na-tephritic and phonolitic melts with different H₂O content, temperature, and oxygen fugacity

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SUPPLEMENTARY FIGURES AND TABLES

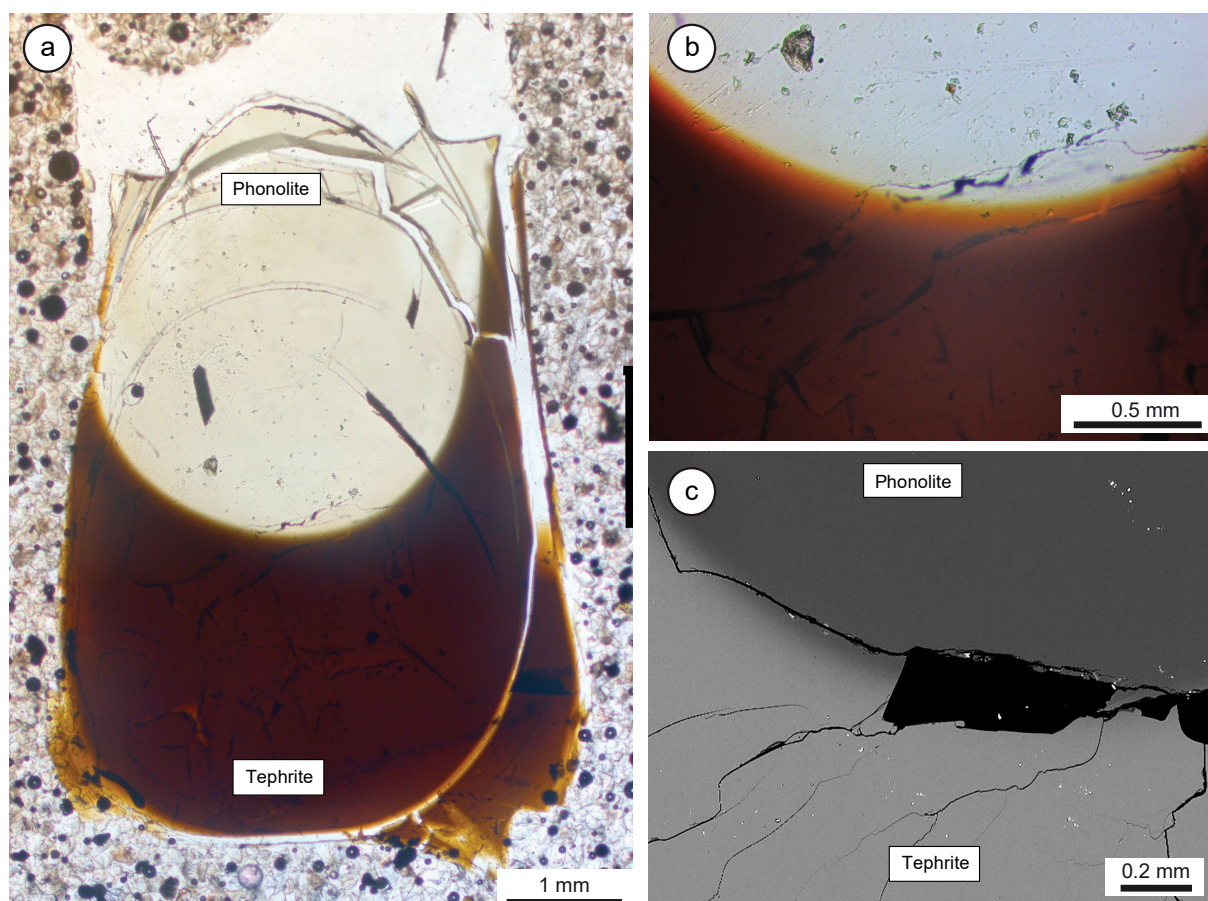


Figure S1. Zero-time experiment (DCB-01; 1200 °C, 0.3 wt% H₂O), run to check for dissolution quench crystals in the tephritic melt during experiment heat-up. (a) Transmitted light whole-experiment mosaic; (b) detail of the interface in transmitted light and (c) back-scattered electron (BSE) image from the electron microprobe.

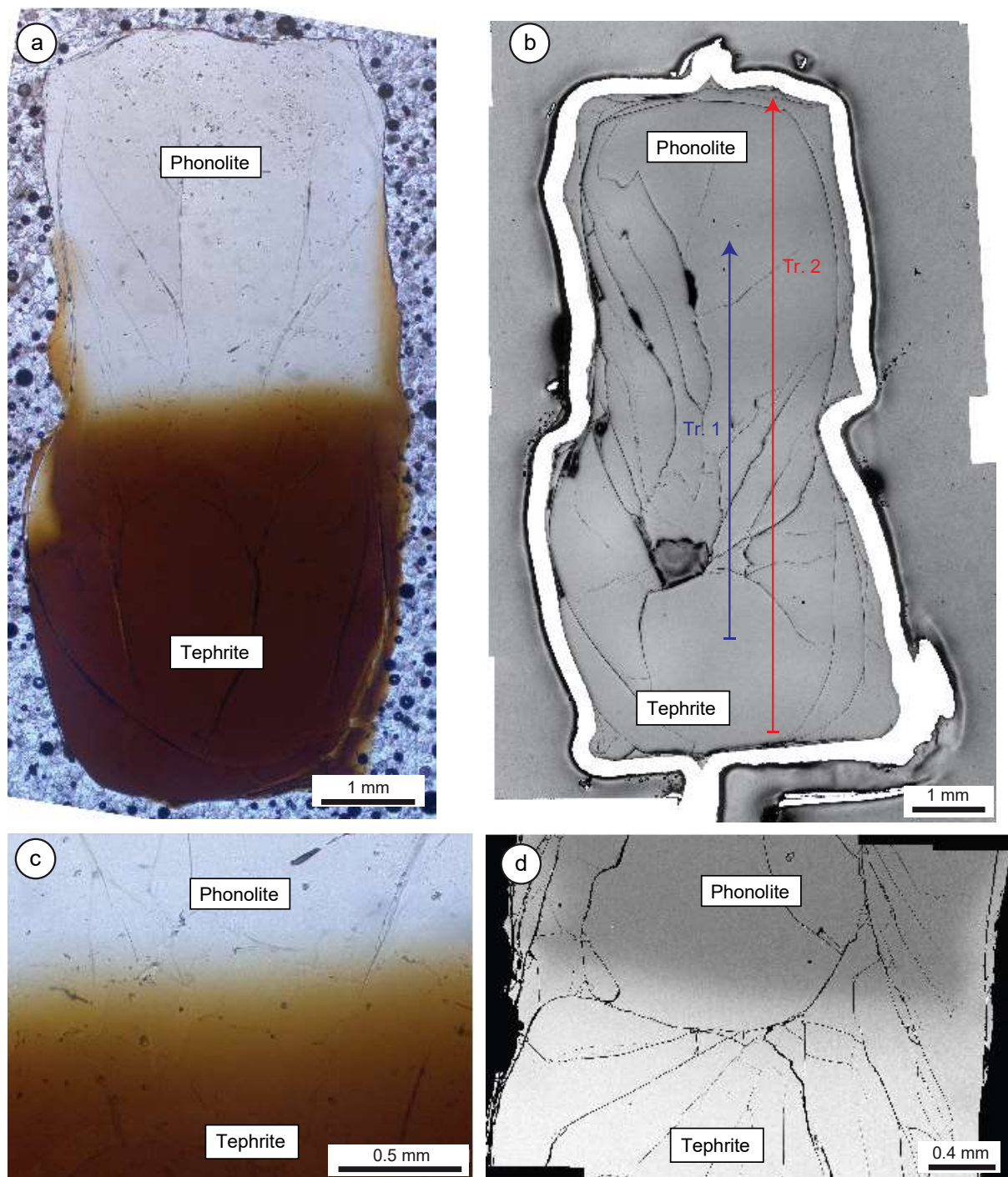


Figure S2. Example of a diffusion couple experiment. (a) Whole-run transmitted light mosaic from a double polished section (experiment DC-05); (b) reflected light mosaic of the same experiment mounted in epoxy, showing the approximate position of the short (Tr. 1) and long (Tr. 2) transects measured by the EPMA; (c) detail of the interface of the same experiment in transmitted light; and (d) BSE mosaic of the interface region of experiment DCB-02.

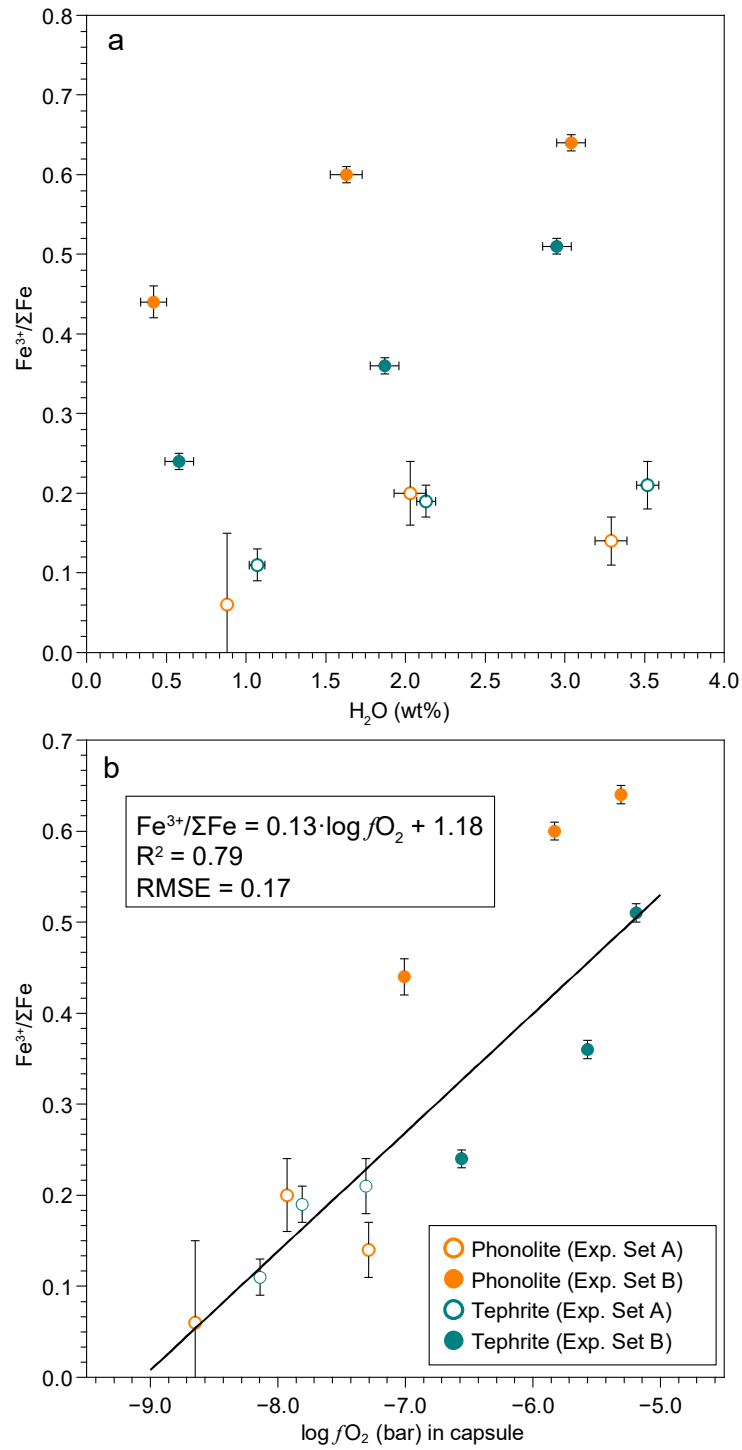


Figure S3. (a) Oxidation state of iron expressed as $\text{Fe}^{3+}/\Sigma\text{Fe}$ as a function of H_2O contents in synthesis runs, measured by wet chemistry (Schuessler et al. 2008) and Karl-Fischer Titration. Most data points are the average of two measurements. (b) Fe oxidation state as a function of estimated $\log f\text{O}_2$ in capsule (see text for details), fitted by a linear function.

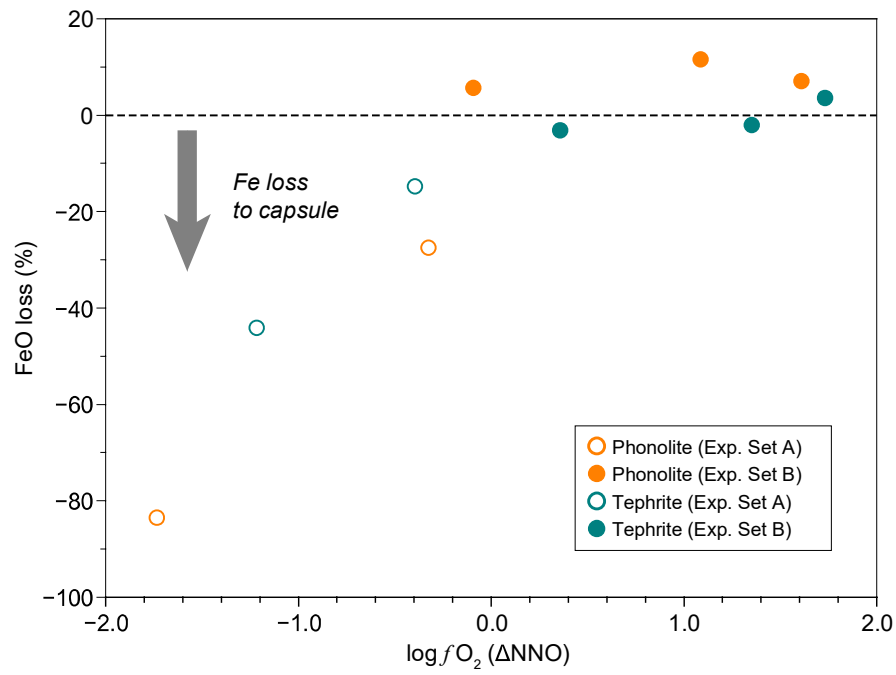


Figure S4. Fe loss to capsule walls (in % relative to starting value) in synthesis experiments as a function of estimated fO_2 . As chemical compositions were not measured in hydrous starting glasses, FeO values were obtained from the ends of the concentration-distance profiles of the corresponding diffusion couple experiments.

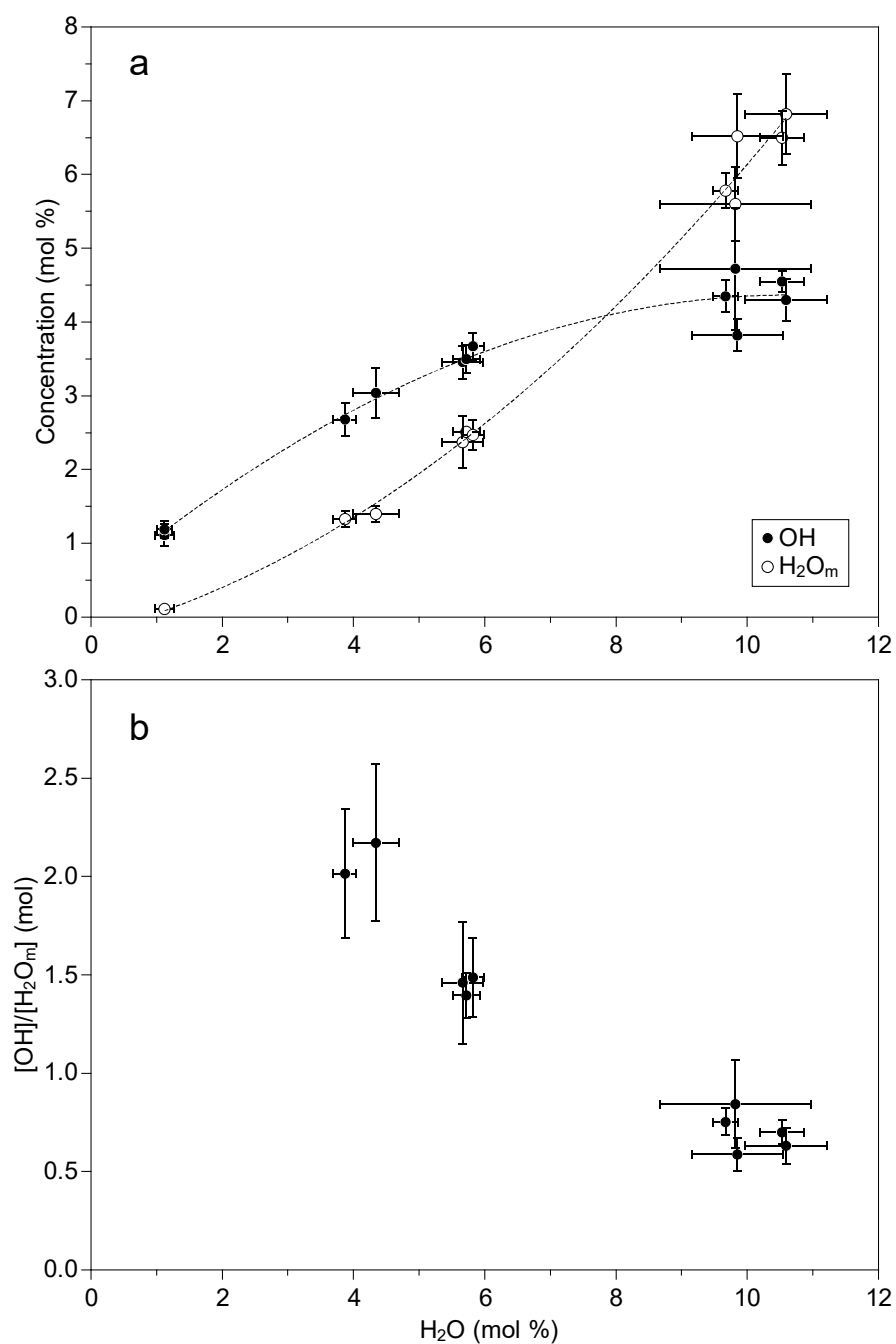


Figure S5. Estimated H₂O speciation in for the TP55 glass. (a) OH and H₂O_m (molecular water) as determined by FTIR in the diffusion couple experiments. (b) [OH]/[H₂O_m] ratio, excluding the 0.3 wt.% experiments, which yielded very high ratio errors due to low H₂O_m values.

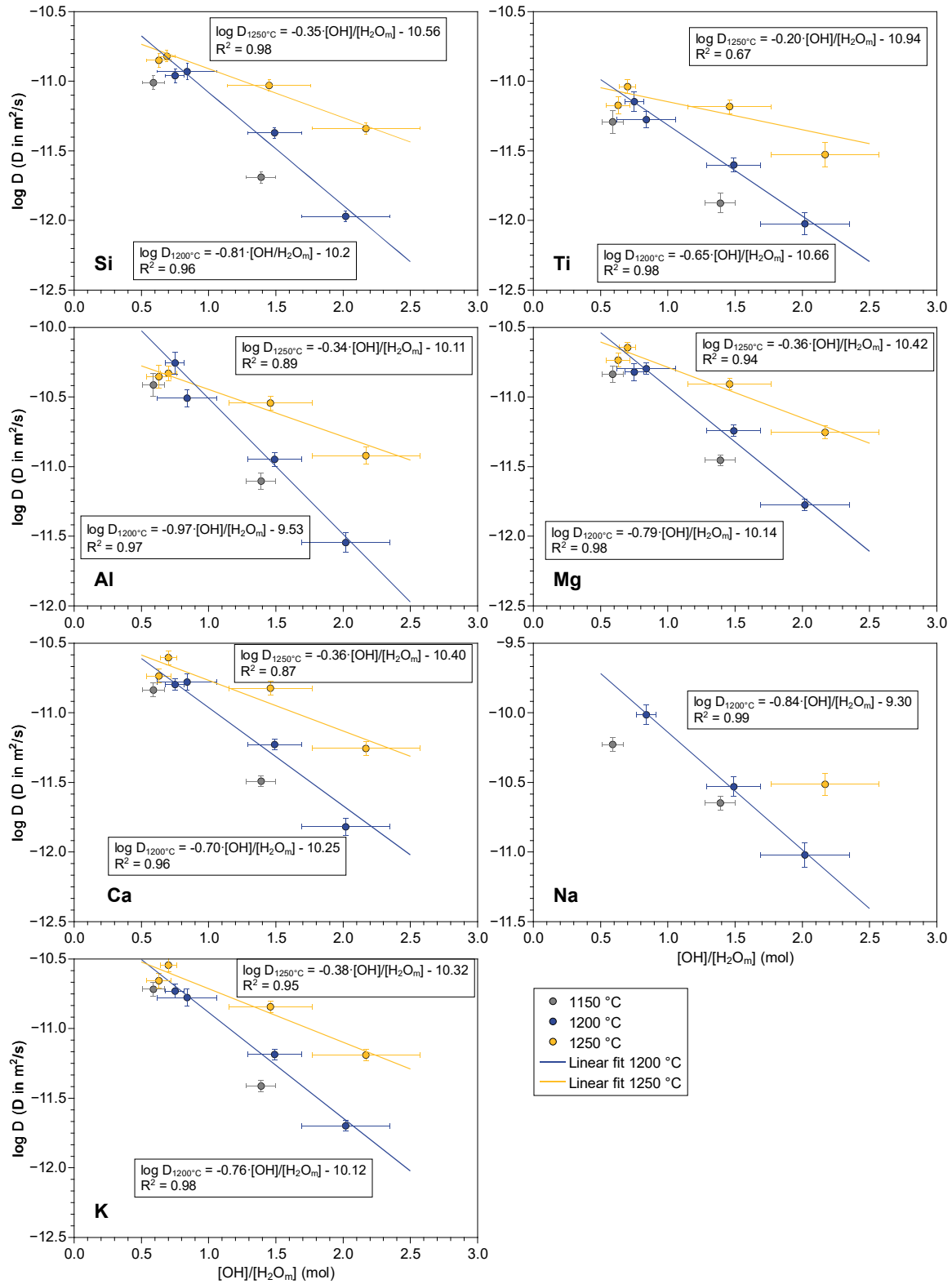


Figure S6. Relation between diffusion coefficients and the $[\text{OH}]/[\text{H}_2\text{O}_m]$ ratio, showing linear relationships for all major elements. Data at 0.3 wt.% H_2O was excluded due to the very high errors in the $[\text{OH}]/[\text{H}_2\text{O}_m]$ ratio.

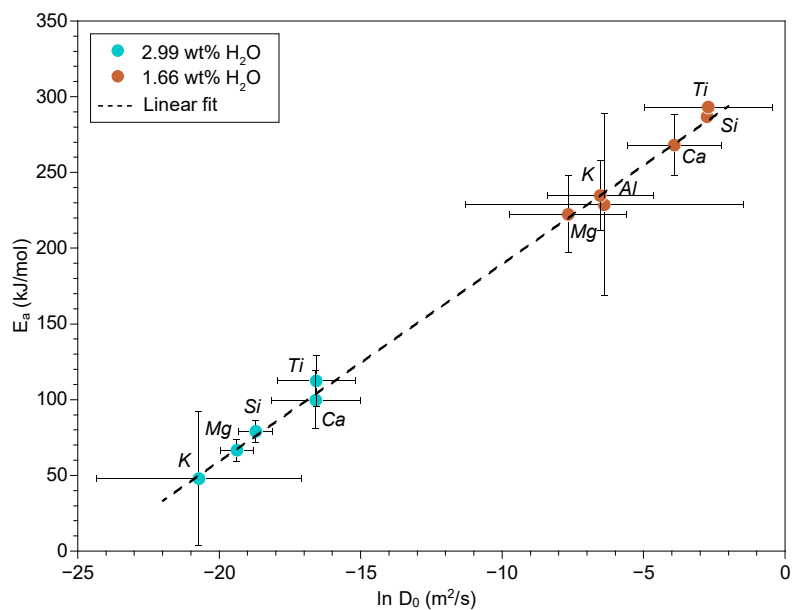


Figure S7. Plot of Arrhenius parameters $\ln D_0$ vs activation energy (E_a), showing that major elements plot (law of diffusion compensation) along the same linear fit for different H_2O contents.

Table S1. Synthesis run conditions.

Run #	Sample	Type	T (°C)	P (Mpa)	Target $f\text{O}_2$	H_2O KFT (wt%)	H_2O FTIR (wt%)	XH_2O^a	$\text{Fe}^{2+}/\Sigma\text{Fe}^b$	$\log f\text{O}_2$ capsule (bar) ^c	$\log f\text{O}_2$ capsule (ΔNNO)
Experiment Set A											
1	ABP-F-ND	Phonolite	1250	300	NNO		0.88 ± 0.02	0,14	0.94 ± 0.09	-8,65	-1.73
10	ABP-F-1.5	Phonolite	1250	300	NNO	2.07 ± 0.10	1.99 ± 0.02	0,30	0.80 ± 0.04	-7,93	-1.01
4	ABP-F-3	Phonolite	1250	300	NNO	3.34 ± 0.10	3.24 ± 0.03	0,48	0.86 ± 0.03	-7,29	-0.33
15	PF21-ND	Tephrite	1250	300	NNO	1.07 ± 0.05		0,10	0.89 ± 0.02	-8,14	-1.22
6	PF21-1.5	Tephrite	1250	300	NNO	2.13 ± 0.06		0,40	0.81 ± 0.02	-7,81	-0.90
13	PF21-3	Tephrite	1250	300	NNO	3.52 ± 0.07		0,51	0.79 ± 0.02	-7,31	-0.40
Experiment Set B											
18	ABP-F-ND	Phonolite	1250	300	NNO+2,3	0.5 ± 0.08	0.33 ± 0.02	0,06	0.56 ± 0.02	-7,01	-0.09
19	ABP-F-1.5	Phonolite	1250	300	NNO+2,3	1.7 ± 0.10	1.56 ± 0.02	0,25	0.40 ± 0.01	-5,83	+1.09
20	ABP-F-3	Phonolite	1250	300	NNO+2,3	3.13 ± 0.09	2.94 ± 0.03	0,45	0.36 ± 0.01	-5,31	+1.61
21	PF21-ND	Tephrite	1250	300	NNO+2,3	0.58 ± 0.09		0,11	0.76 ± 0.01	-6,56	+0.34
17	PF21-1.5	Tephrite	1250	300	NNO+2,3	1.87 ± 0.09		0,34	0.64 ± 0.01	-5,57	+1.35
27	PF21-3	Tephrite	1250	300	NNO+2,3	2.95 ± 0.06		0,52	0.49 ± 0.01	-5,19	+1.73

^a XH_2O calculated as $\text{H}_2\text{O}(\text{experiment})/\text{H}_2\text{O}(\text{saturation})$ in mol%, with $\text{H}_2\text{O}(\text{saturation})$ calculated using the MagmaSat model (Ghiorso and Gualda, 2015)

^b Fe speciation was obtained by a wet-chemical method (Schuessler et al., 2008). Each value is the average of two measurements.

^c $f\text{O}_2$ value inside the capsule was calculated from XH_2O by adding the term $2 \cdot \log(\text{XH}_2\text{O})$ to the intrinsic $f\text{O}_2$ value (see text).