



Supplement of

Experimental constraints on the stability of Mg-rich tourmaline and the boron concentration of hydrothermal fluids

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Supplementary Material

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S1. Experimental redox conditions

The NiO-NiPd sensors used for the determination of redox conditions behaved consistently across experiments to the other. The compositional evolution of the alloy phase of the sensor is summarized in graphical form in Figure S1 for all experiments except Run 5 (400°C). Results for Run 2, a moderately oxidizing experiment at 600°C (Table 2), are used as an example. The two analyzed pellets display a range of X_{Ni} , from 0.32 to 0.46 for one and from 0.2 to 0.27 for the other. We note the decrease in X_{Ni} for the pellet with initial $X_{\text{Ni}} = 0.5$ and the increase in X_{Ni} for the pellet with initial $X_{\text{Ni}} = 0.15$ with convergence toward $X_{\text{Ni}} \sim 0.3$ from both sides. This indicates that the sensor approached equilibrium although complete equilibration was not achieved. Using the minimum X_{Ni} of the reduced pellet (0.32) and the maximum X_{Ni} of the oxidized pellet (0.27), $f\text{O}_2$

is bracketed between NNO + 1.4 and NNO + 1.7 ($\Delta\text{NNO} = 1.4\text{-}1.7$) with the calibration of Pownceby and O'Neill (1994).

At the same temperature, the sensor in Run 1 (contained in Au rather than Pt capsule) yields an $f\text{O}_2$ range ($\Delta\text{NNO} = 1.1\text{-}1.9$), overlapping with results for Run 2. At 500°C (Run 3), the $f\text{O}_2$ interval ($\Delta\text{NNO} = 0.8\text{-}1.7$) is again similar but larger than at 600°C indicating less complete equilibration, despite the experiment being longer. Run 4 (500°C) equilibrated at $\Delta\text{NNO} = 1.8\text{-}2.6$, corresponding to more oxidizing conditions than in the other runs performed with 0.2 MPa initial $p\text{H}_2$. In Run 6 (600°C) performed without H_2 in the pressurizing gas, both pellets had experimental $X_{\text{Ni}} \leq 0.15$ implying a minimum ΔNNO of 2.7, the lowest X_{Ni} analyzed corresponding to a ΔNNO of 5.3 (Table 2). In Run 5 (400°C) which contained no solid sensor (see text), ΔNNO is estimated to lie between 0 and 2 on the basis of the sensor results in the 600 and 500°C experiments performed with a 0.2 MPa initial $p\text{H}_2$. ΔNNO values for all experiments are summarized in Table 2.

S2. Calculation of equilibrium constants

At given T and P, the log K of the tourmaline-forming reactions is of the form:

$$\text{Log}(K_{RT,P}) = \frac{-\Delta_r G^\circ_{T,P}}{RT \ln(10)} \quad (\text{Eq. S1})$$

where R is the ideal gas constant (= 8.3144 J/mol.K) and $\Delta_r G^\circ_{T,P}$ the Gibbs free energy change associated with the reaction considered. For reaction R1Mg:

$$\Delta_r G^\circ_{T,P, \text{R1Mg}} = 2\Delta_{\text{app}} G^\circ_{T,P, \text{Drv}} + 8\Delta_{\text{app}} G^\circ_{T,P, \text{Qtz}} + \Delta_{\text{app}} G^\circ_{T,P, \text{And}} + 5\Delta_{\text{app}} G^\circ_{T,P, \text{H}_2\text{O}_{(g)}} - (3\Delta_{\text{app}} G^\circ_{T,P, \text{Mg-Crd}} + 2\Delta_{\text{app}} G^\circ_{T,P, \text{Alb}} + 6\Delta_{\text{app}} G^\circ_{T,P, \text{B}(\text{OH})_3}) \quad (\text{Eq. S2})$$

where $\Delta_{\text{app}} G^\circ_{T,P,X}$ are apparent standard Gibbs free energies at T and P for component X (Helgeson et al., 1981; Tanger and Helgeson, 1988). Drv, Qtz, And, Mg-Crd, and Alb refer to the pure dravite,

quartz, andalusite, Mg-cordierite, and albite components respectively. $\Delta_{app}G^{\circ}_{T,P,X}$ is given by the equation:

$$\Delta_{app}G^{\circ}_{T,P,X} = \Delta_f G^{\circ}_{T^{\circ},P^{\circ},X} - (T - T^{\circ})S^{\circ}_{T^{\circ},P^{\circ},X} + \int_{T^{\circ}}^T Cp^{\circ}_{P^{\circ},X} \cdot dT - T \int_{T^{\circ}}^T \frac{Cp^{\circ}_{P^{\circ},X}}{T} \cdot dT + \int_{P^{\circ}}^P V^{\circ}_{T^{\circ},X} \cdot dP \quad (\text{Eq. S3})$$

where T° and P° are the reference temperature (298.15°K) and pressure (1 bar), respectively. The thermodynamic properties of the component X in Equation S3 are the standard Gibbs free energy of formation ($\Delta_f G^{\circ}_{T^{\circ},P^{\circ},X}$), the standard entropy, ($S^{\circ}_{T^{\circ},P^{\circ},X}$), the heat capacity ($Cp^{\circ}_{P^{\circ},X}$) and the molar volume ($V^{\circ}_{T^{\circ},X}$).

Calculation of the apparent standard Gibbs free energy of formation for the component X at elevated P and T involves the heat capacity equation:

$$Cp^{\circ}(T) = a + bT + cT^{-2} + dT^{-0.5} + eT^2 + fT^{-3} + gT^{-1} \quad (\text{Eq. S4})$$

and Equation S3 can be rewritten as:

$$\begin{aligned} \Delta_{app}G^{\circ}_{T,P,X} = & \Delta_f G^{\circ}_{T^{\circ},P^{\circ},X} - (T - T^{\circ})S^{\circ}_{T^{\circ},P^{\circ},X} + a \left((T - T^{\circ}) - T \ln \left(\frac{T}{T^{\circ}} \right) \right) + b \left(\frac{-(T - T^{\circ})^2}{2} \right) - \\ & c \left(\frac{(T - T^{\circ})^2}{2TT^{\circ 2}} \right) + 2d \left(\sqrt{T} - \sqrt{T^{\circ}} + \frac{T}{\sqrt{T}} - \frac{T^{\circ}}{\sqrt{T^{\circ}}} \right) + e \left(\frac{-T^3}{6} - \frac{T^{\circ 3}}{3} + \frac{TT^{\circ 2}}{2} \right) + f \left(-\frac{1}{6T^2} + \frac{1}{2T^{\circ 2}} - \frac{T}{3T^{\circ 3}} \right) + \\ & g \left(\ln \left(\frac{T}{T^{\circ}} \right) + 1 - \frac{T}{T^{\circ}} \right) + V^{\circ}_{T^{\circ},X} (1 + k_1(T - T^{\circ}) + k_2(T^2 - T^{\circ 2}))(P - P^{\circ}) \quad (\text{Eq. S5}). \end{aligned}$$

S3. Thermodynamic properties of H₃BO₃

In the present work, the HKF theory (Helgeson et al. 1981; Tanger and Helgeson 1988) was applied to calculate the standard thermodynamic properties of aqueous species at high pressure and temperatures. Different sets of HKF parameters are available for aqueous H_3BO_3 (Shock et al., 1989, used in SUPCRTBL, Zimmer et al. 2016; Pokrovski et al., 1995, used in Thermoddem, Blanc et al. 2012). To take into account the amphoteric behavior of aqueous boron, Shock et al. (1989) introduced the BO_2^- species, while Pokrovski et al. (1995) replaced BO_2^- by $\text{B}(\text{OH})_4^-$ and added $\text{NaB}(\text{OH})_4$. In addition to those studies, two other sets of HKF parameters for H_3BO_3 , based on the Pokrovski et al. (1995) experimental data, have been proposed more recently (Akinfiev et al., 2006; Wang et al., 2013). The four sets of HKF parameters were tested using PHREEQC in combination with the Thermoddem database (Fig. S6, S7). The Shock et al. (1989) parameters show the largest deviation with relative to the other simulations and experimental data at $T > 50^\circ\text{C}$ (Fig. S6). Results with the three other parameters are similar and in reasonable agreement with the experimental data. However, the simulation with the Wang et al. (2013) parameters begin to deviate from the two others at high temperatures (Fig. S7). The Akinfiev et al. (2006) parameters show the best overall reproduction and, the corresponding parameters were selected for our calculations. Apparent standard Gibbs free energies of aqueous H_3BO_3 calculated with the four sets of HKF parameters are summarized in Table S4.

S4. Extension to tourmaline solid solutions

Introduction of an activity term in Equation (1) leads to a shift of the calculated equilibrium constant according to:

$$\text{Log } K_{\text{R1Mg ss}} = \text{Log } K_{\text{R1 Mg}} + 2 \text{ Log } a_{\text{Dra in Tur}} \quad (\text{Eq. S6})$$

where $K_{R1Mg_{ss}}$ is the equilibrium constant of the R1Mg reaction for a tourmaline solid solution, K_{R1Mg} corresponds to the equilibrium constant for the R1Mg end-member reaction and $a_{Dra\ in\ Tur}$ is the activity of dravite in the tourmaline solid solution. Calculation of the shift for reaction R1Fe follows a similar equation involving $a_{Sch\ in\ Tur}$.

Activities in tourmaline solid solutions were calculated with a simple multi-site formulation, assuming random mixing on each crystallographic site:

$$a_{Dra\ in\ Tur} = Na^X \cdot [(Mg/(Mg+Fe+Mn+Ti+Al))^Y]^3 \cdot [(Si/(Si+Al))^T]^6 \text{ (Eq. S7)}$$

$$a_{Sch\ in\ Tur} = Na^X \cdot [(Fe/(Mg+Fe+Mn+Ti+Al))^Y]^3 \cdot [(Si/(Si+Al))^T]^6 \text{ (Eq. S8)}$$

where the cations refer to atomic concentrations (from structural formulae in Table 4) in the three different sites X, Y and T of tourmaline. The Z site was assumed to be fully filled and 4 OH groups and 3 B atoms were assumed per formula unit. Equation S7 and S8 were applied to the tourmaline compositions of Table 4. $\log K_{R1Mg_{ss}}$ and $\log K_{R1Fe_{ss}}$ were calculated at 500 and 600°C with Equation S6 and the equivalent equation for the R1Fe reaction, yielding two sets of calculated $[H_3BO_3]_{fluid_EQ}$ and $[B_2O_3]_{fluid_EQ}$ (wt%) for the experimental tourmaline compositions.

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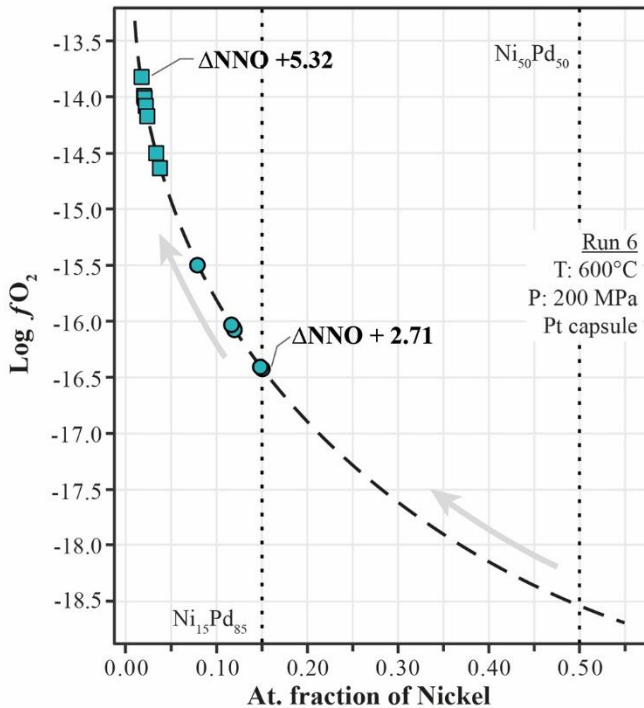
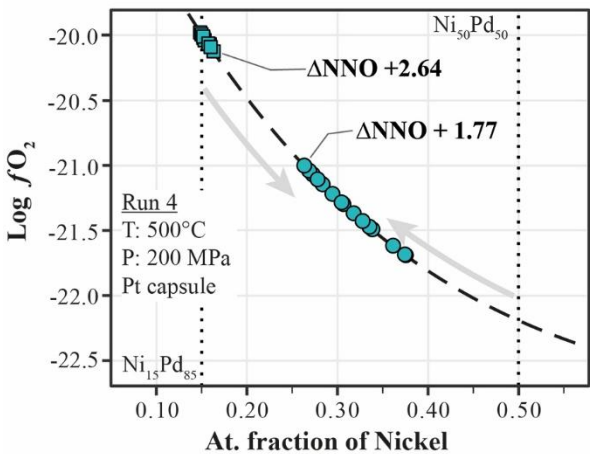
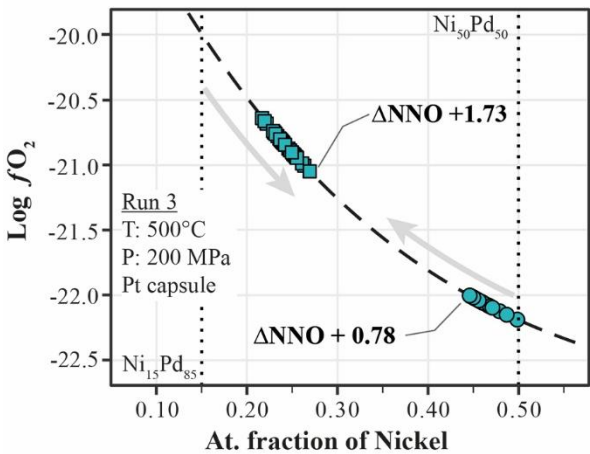
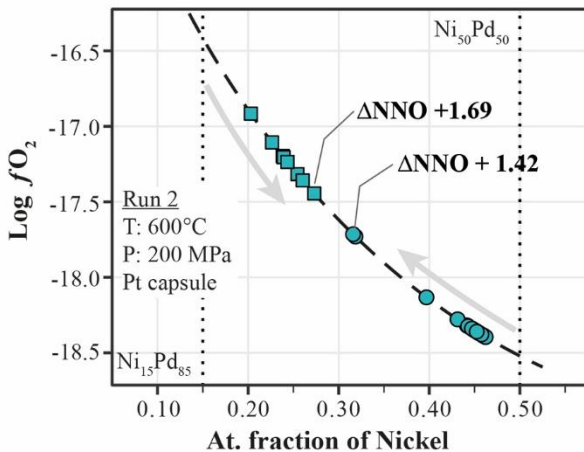
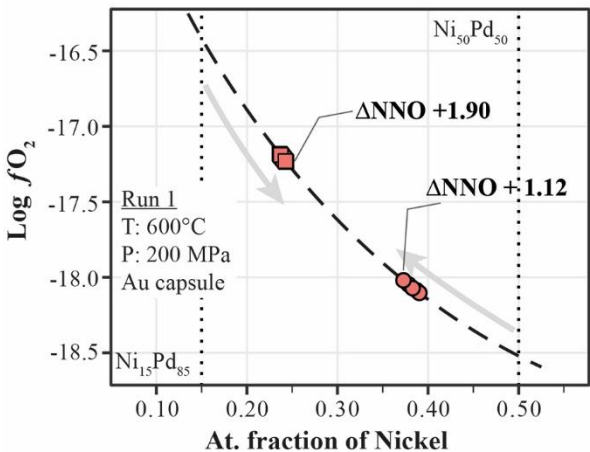
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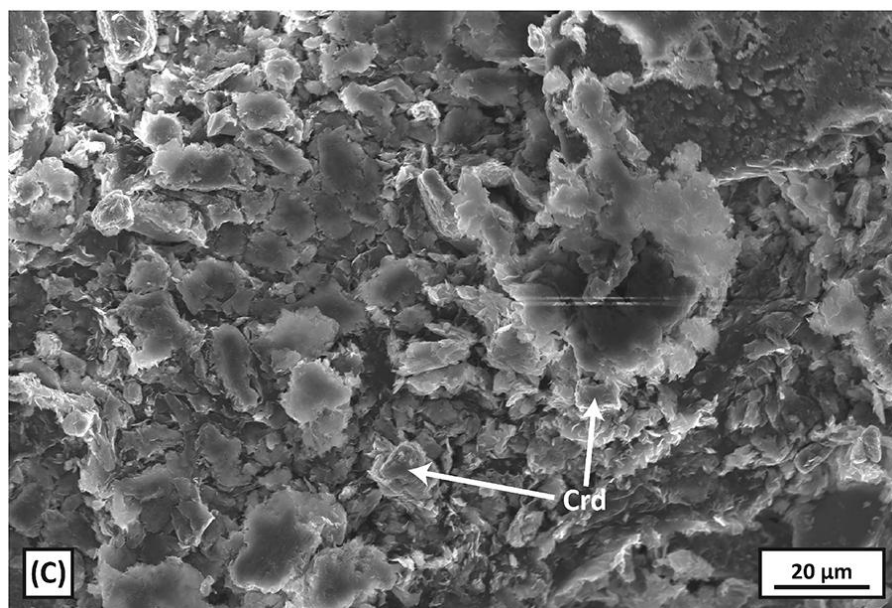
Supplementary Figures

Figure S1. Compositions of NiPd alloys in NiO-NiPd sensors for all 500 and 600°C experiments. Run conditions and capsule material are indicated. The dashed curves show the relation between X_{Ni} (atomic fraction of Ni in the alloy) and f_{O_2} at 600°C and 2 kbar as calibrated by Pownceby and O'Neill (1994). The two dotted vertical lines indicate the initial X_{Ni} in each pellet of the sensor. The final (measured) X_{Ni} are plotted as circles for the initially high Ni pellet (Ni₅₀Pd₅₀) and as squares for the initially high Pd pellet (Ni₁₅Pd₈₅). Arrows give directions of evolution of alloy compositions. For runs 1 to 4, the two alloys converge and the f_{O_2} bracket is calculated from

compositions closest to each other. In the highly oxidizing Run 6, alloys in both pellets migrated toward high Pd and the fO_2 range is determined from the entire spectrum of measured compositions.



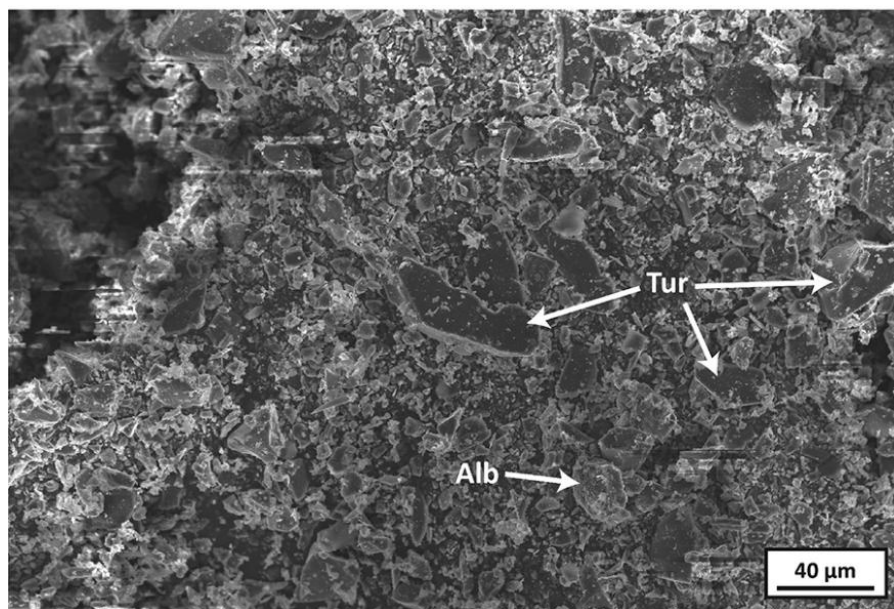
197 **Figure S2.** SEM image of charge S400-0Pt. Cordierite is destabilized, forming sheeted minerals
198 of the smectite group. Abbreviations as in Fig. 1.



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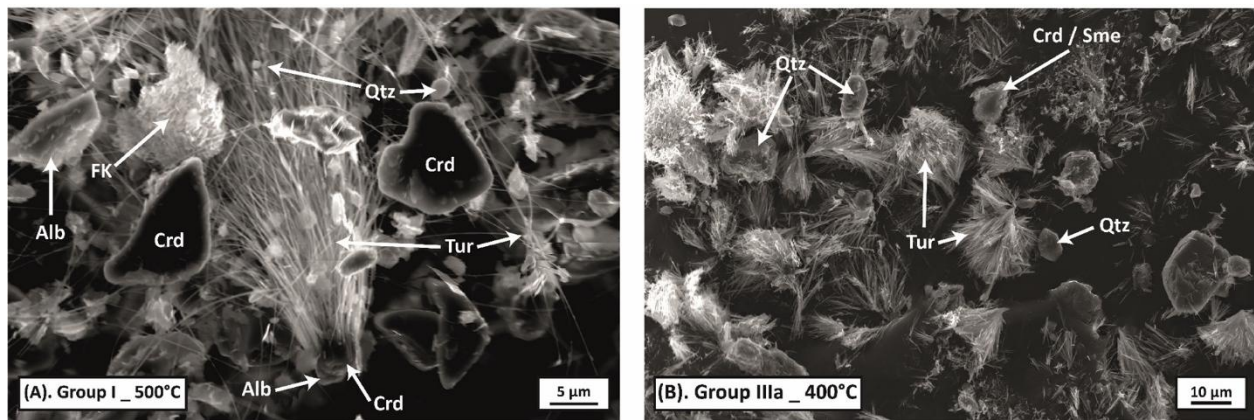
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201 **Figure S3.** SEM image of charge S600-Rev. In this reversal experiment, tourmaline remains
202 apparently unreacted, with sharp edges and no etching or dissolution features. Abbreviations as in
203 Fig. 1.

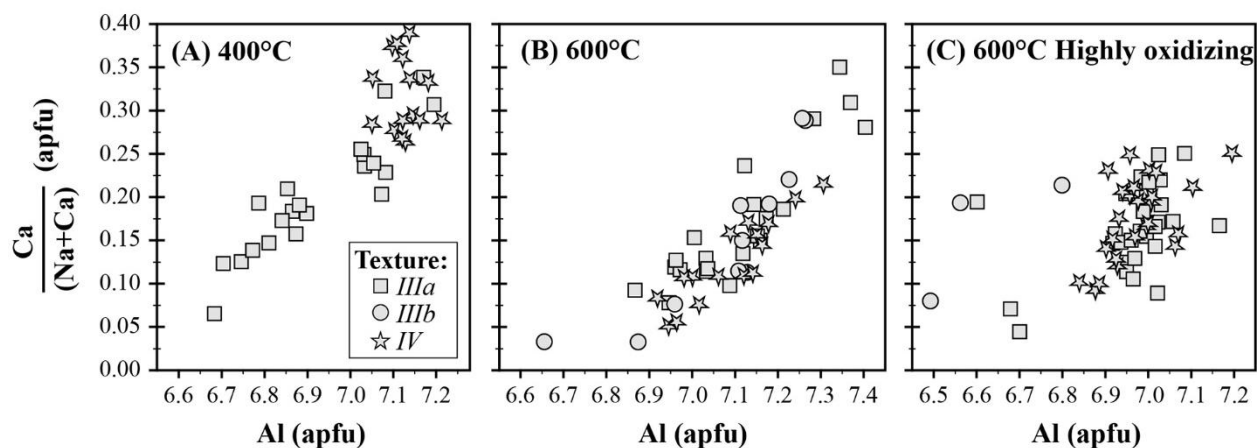


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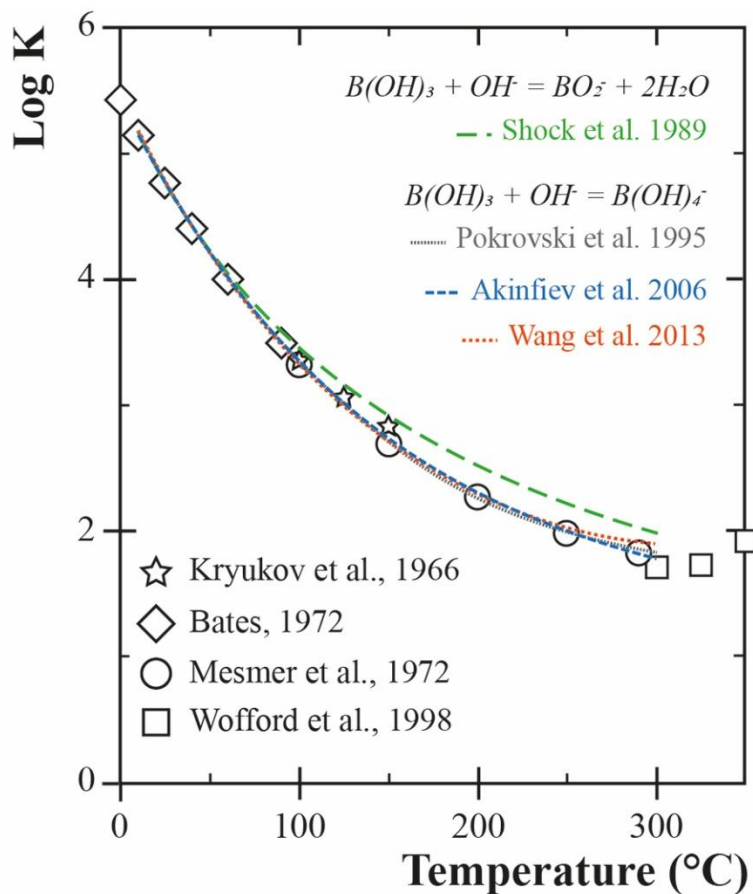
Figure S4. SEM image showing the textural evolution of Group I and Group IIIa tourmalines with temperature. (A) Charge S500-4. Group I tourmaline displays the same texture at 500 than as 600°C (Fig. 1B): tourmaline nucleates on cordierite and albite and the sheaves enclose platy K-feldspar and small quartz crystals. However, at 500°C, the tourmaline sheaves are thinner and also more numerous than at 600°C. (B) Charge S400-4Pt showing Group IIIa tourmaline aggregates texturally similar to those found at 600°C (Fig. 2D), but with a significantly smaller radius. Abbreviations as in Fig. 1.



213 **Figure S5.** Atomic Ca/(Na+Ca) (apfu) of tourmalines (Groups IIIa, IV, IIIb) plotted as a function
 214 of Al (apfu) at (A) 400°C (charges S400-6G), (B) 600°C (charges S600-10(G)) and (C) in the
 215 highly oxidizing experiment at 600°C (charge SOX-8(G)).

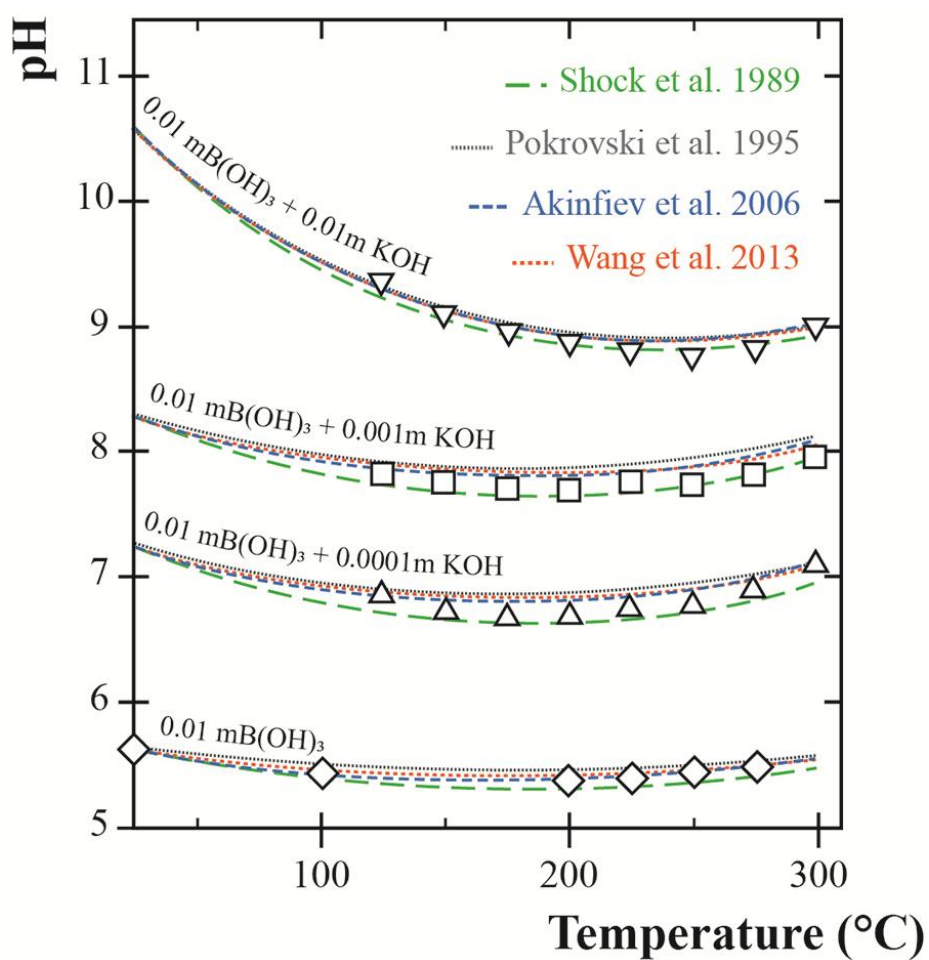


217 **Figure S6.** Temperature dependence of the equilibrium constant of the reaction $\text{H}_3\text{BO}_3 + \text{OH}^- \rightarrow$
 218 $\text{B}(\text{OH})_4^-$ (Shock et al., 1989) and of the equivalent reaction $\text{H}_3\text{BO}_3 + \text{OH}^- \rightarrow \text{BO}_2^- + 2\text{H}_2\text{O}$
 219 (Pokrovski et al., 1995; Akinfiev et al., 2006; Wang et al., 2013) between 10 and 300°C under
 220 saturated water vapor pressure. Experimental data from Kryukov et al. (1966), Bates (1972),
 221 Mesmer et al. (1972) and Wofford et al. (1998).



222

223 **Figure S7.** pH evolution of various H_3BO_3 / $\text{K}(\text{OH})$ solutions with temperature. Experimental
 224 points are from Macdonald et al. (1992), except for the pure H_3BO_3 solution (Macdonald et al.,
 225 1980). The pH curves are calculated by PHREEQC using different HKF parameters for H_3BO_3
 226 (Shock et al., 1989; Pokrovski et al., 1995; Akinfiev et al., 2006; Wang et al., 2013).



227

228

Supplementary Tables

229 Table S1. Average composition of starting cordierite, plagioclase and andalusite.

Starting product n	Cordierite				Plagioclase				Andalusite			
	23				32				14			
	<i>Mean</i>	<i>Sd</i>	<i>Min</i>	<i>Max</i>	<i>Mean</i>	<i>Sd</i>	<i>Min</i>	<i>Max</i>	<i>Mean</i>	<i>Sd</i>	<i>Min</i>	<i>Max</i>
SiO₂	49,49	(0.298)	49,00	50,10	67,91	(0.808)	64,22	69,08	36,21	(0.278)	35,82	36,82
TiO₂	0,08	(0.052)	0,05	0,12	0,02	(0.012)	0,01	0,04	0,06	(0.007)	0,05	0,06
Al₂O₃	33,45	(0.171)	33,15	33,74	19,76	(0.433)	18,12	20,60	63,38	(0.258)	62,91	63,69
FeO_{total}	3,21	(0.129)	2,91	3,46	0,10	(0.043)	0,06	0,15	0,28	(0.053)	0,21	0,38
MgO	11,06	(0.709)	10,35	12,11	<i>b.d.l</i>				0,05	(0.011)	0,03	0,07
MnO	<i>b.d.l</i>				0,05	(0.041)	0,00	0,09	<i>b.d.l</i>			
CaO	0,05	(0.021)	0,04	0,08	0,58	(0.262)	0,24	1,49	<i>b.d.l</i>			
Na₂O	0,18	(0.029)	0,12	0,25	10,79	(1.84)	0,85	11,85	<i>b.d.l</i>			
K₂O	0,06	(0)	0,06	0,06	0,67	(2.928)	0,05	15,90	<i>b.d.l</i>			
Total	97,60				99,89				99,97			
Si	5,02	(0.042)	4,95	5,08	2,98	(0.013)	2,94	3,00	0,98	(0.006)	0,97	0,99
Ti	0,01	(0.004)	0,00	0,01	0,00	(0)	0,00	0,00	0,00	(0)	0,00	0,00
Al	4,00	(0.021)	3,96	4,04	1,02	(0.015)	1,00	1,06	2,02	(0.008)	2,01	2,03
Fe	0,27	(0.011)	0,25	0,29	0,00	(0.002)	0,00	0,01	0,01	(0.001)	0,00	0,01
Mg	1,67	(0.099)	1,57	1,82	<i>b.d.l</i>				0,00	(0)	0,00	0,00
Mn	<i>b.d.l</i>				0,00	(0.002)	0,00	0,00	<i>b.d.l</i>			
Ca	0,01	(0.002)	0,00	0,01	0,03	(0.013)	0,00	0,06	<i>b.d.l</i>			
Na	0,04	(0.006)	0,02	0,05	0,93	(0.157)	0,08	1,03	<i>b.d.l</i>			
K	0,01	(0)	0,01	0,01	0,04	(0.166)	0,00	0,95	<i>b.d.l</i>			
Fe/(Fe+Mg)	0,14	(0.010)										
Ca/(Ca+Na)	0,14	(0.046)			0,03	(0.015)						

n = number of analyses. b.d.l. = below detection limit.

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231

232 Table S2. Average composition of starting tourmaline

Starting tourmaline^a	Core		Inner rim		Outer rim		Late	
n	41		53		55		12	
SiO₂	36,21	(0.49)	35,67	(0.6)	35,77	(0.52)	35,60	(0.29)
TiO₂	0,35	(0.15)	0,67	(0.11)	0,69	(0.11)	0,74	(0.16)
Al₂O₃	35,64	(0.43)	34,18	(0.4)	34,23	(0.3)	32,94	(0.55)
FeO	9,89	(0.7)	9,43	(0.52)	10,06	(0.49)	11,65	(0.79)
MgO	2,95	(0.3)	3,94	(0.38)	3,49	(0.21)	3,06	(0.52)
MnO	0,14	(0.01)	0,17	(0.04)	0,17	(0.03)	0,19	(0.05)
CaO	0,09	(0.07)	0,13	(0.08)	0,11	(0.03)	0,21	(0.09)
Na₂O	1,53	(0.1)	1,90	(0.1)	1,86	(0.06)	1,84	(0.08)
K₂O	0,08	(0.01)	0,07	(0.01)	0,09	(0.01)	0,11	(0.01)
B₂O₃^b	10,65		10,55		10,56		10,42	
H₂O^c	3,67		3,64		3,64		3,59	
Total	101,20		100,35		100,66		100,36	
Site T								
Si	5,91	(0.05)	5,88	(0.06)	5,90	(0.04)	5,94	(0.04)
Al	0,09	(0.05)	0,12	(0.06)	0,10	(0.04)	0,06	(0.04)
Site Z								
Al	6,00		6,00		6,00		6,00	
Site Y								
Al	0,76	(0.05)	0,53	(0.05)	0,54	(0.04)	0,41	(0.07)
Ti	0,04	(0.02)	0,08	(0.01)	0,09	(0.01)	0,09	(0.02)
Fe	1,35	(0.1)	1,30	(0.07)	1,39	(0.07)	1,62	(0.11)
Mg	0,72	(0.07)	0,97	(0.09)	0,86	(0.05)	0,76	(0.13)
Mn	0,00	(0.01)	0,00	(0)	0,00	(0.01)	0,00	(0.01)
Site X								
Ca	0,01	(0.01)	0,02	(0.01)	0,02	(0)	0,04	(0.02)
Na	0,48	(0.03)	0,61	(0.03)	0,59	(0.02)	0,60	(0.03)
K	0,00	(0)	0,00	(0)	0,00	(0.01)	0,01	(0.01)
[X]	0,50	(0.04)	0,37	(0.03)	0,38	(0.02)	0,36	(0.04)
B	3,00		3,00		3,00		3,00	
OH-	4,00		4,00		4,00		4,00	
Total Al	6,85	(0.06)	6,64	(0.07)	6,65	(0.06)	6,47	(0.08)
Fe/(Fe+Mg)	0,65	(0.04)	0,57	(0.04)	0,62	(0.02)	0,68	(0.05)
Ca/(Ca+Na)	0,02	(0.02)	0,04	(0.02)	0,03	(0.01)	0,06	(0.02)

(a) The zonation of the starting tourmaline has been simplified into three main zones, common to all observed sections. The Late tourmalines correspond to the filling of fractures intersecting the 3 other zonations. (b) B₂O₃ calculated assuming 3 apfu. (c) H₂O calculated assuming 4 apfu of OH⁻. n = number of analyses.

234 Table S3. Standard state properties (at 25°C, 1bar) for the species used in thermodynamic calculation.

	$\Delta_f G^\circ$	S°	V°	k1	k2	$C_p(T) = a + bT + cT^{-2} + dT^{-0.5} + eT^2 + fT^{-3} + gT^{-1}$ J/mol.K							Source
	J/mol	J/mol.K	J/mol	1/K	1/K ²	a (J)	b (J/K)	c (JK ²)	d (JK1/2)	e (J/K ²)	f (JK3)	g (JK)	
Minerals													
Dravite	- 1,56E+07	607,9	32,9	2,53E-05	-4,42E-09	2,20E+03	-6,45E-02	9,34E+06	2,56E+04	-	-	-	van Hinsberg and Schumacher, 2006
Schorl	- 1,44E+07	692,6	33,1	2,55E-05	-4,10E-09	2,22E+03	-4,27E-02	1,08E+07	2,58E+04	-	-	-	van Hinsberg and Schumacher, 2007
Magnesiofoitite	- 1,55E+07	588,5	33,2	2,12E-05	-3,50E-09	2,17E+03	-4,61E-02	8,76E+06	2,55E+04	-	-	-	van Hinsberg and Schumacher, 2007
Foitite	- 1,48E+07	644,9	33,0	2,14E-05	-3,29E-09	2,19E+03	-3,17E-02	9,76E+06	2,56E+04	-	-	-	van Hinsberg and Schumacher, 2007
Quartz (alpha)	- 9,11E+05	41,5	2,3	2,39E-05	0,00E+00	8,00E+01	0,00E+00	3,55E+06	2,40E+02	-	4,92E+08	-	Chatterjee et al., 1998
Andalusite	- 2,59E+06	91,4	5,1	2,34E-05	7,19E-10	2,77E+02	-6,59E-03	1,91E+06	2,27E+03	-	-	-	Chatterjee et al., 1998
Cordierite	- 9,16E+06	407,2	23,3	3,00E-06	1,80E-09	9,54E+02	-	2,32E+06	7,96E+03	-	3,70E+08	-	Chatterjee et al., 1998
Fe-Cordierite	- 8,47E+06	410,9	25,0	-	-	1,09E+03	-3,73E-01	1,32E+07	-	-	1,28E+10	-7,08E+04	Chatterjee 1989 in Saxena et al., 2013
Albite (low)	- 3,94E+06	207,4	10,0	1,10E-05	2,35E-08	3,94E+02	0,00E+00	7,89E+06	2,42E+03	-	1,07E+09	-	Chatterjee et al., 1998
Gas													
H2O	- 2,42E+05	188,84	-	0,00E+00	0,00E+00	2,71E+01	1,76E-02	2,77E+05	2,77E+01	- 2,51E-06	-	-	Chatterjee et al., 1998

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236 Table S4. Water fugacity and apparent standard Gibbs free energy of B(OH)₃ at T and 200 MPa
 237 used in the thermodynamic calculations.

P	T	$f_{\text{H}_2\text{O}}$ ^a	$\Delta_{\text{app}}G^\circ_{\text{B(OH)}_3}$ ^b			
			J/mol			
<i>bars</i>	<i>°C</i>	<i>bars</i>	<i>Shock et al.</i> <i>(1989)</i>	<i>Pokrovski et al.</i> <i>(1995)</i>	<i>Akinfiev et al.</i> <i>(2006)</i>	<i>Wang et al.</i> <i>(2013)</i>
2000	300	162,78	-1008593,325	-1019566,743	-1018342,128	-1015887,124
2000	350	271,26	-1018357,734	-1033025,278	-1031621,5	-1028910,995
2000	400	404,88	-1028295,53	-1046983,617	-1045385,872	-1042437,533
2000	450	556,61	-1038627,583	-1061597,701	-1059792,514	-1056637,527
2000	500	719,43	-1049310,548	-1076746,291	-1074718,641	-1071378,429
2000	550	886,31	-1060371,831	-1092383,908	-1090118,481	-1086611,034
2000	600	1050,21	-1071828,794	-1108471,973	-1105953,373	-1102294,172

(a) $f_{\text{H}_2\text{O}}$ values from Burnham et al. (1969). (b) $\Delta_{\text{app}}G^\circ_{\text{B(OH)}_3}$ were calculated by Thermo-ZNS, using the HKF parameters of the corresponding source.

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239 Table S5. Simplified average composition of experimental tourmaline (see Table 4).

T°C (charge)	Average composition						Simplified composition						Solid solution			[B ₂ O ₃] _{fluid EQ} calculated (wt%)
<i>Reaction</i>	X			Y			X			Y			X _{Drv}	X _{Mg-Fo}	X _{Srl}	
600°C (S600-10(G))	Na _{0.56}	Ca _{0.12}	□ _{X 0.32}	Mg _{1.57}	Fe _{0.38}	Al _{0.82}	Na _{0.64}	□ _{X 0.36}	Mg _{2.12}	Fe _{0.52}	Al _{0.36}	0,47	0,36	0,17	6,79	
500°C (S500-6)	Na _{0.60}	Ca _{0.08}	□ _{X 0.31}	Mg _{1.80}	Fe _{0.32}	Al _{0.68}	Na _{0.66}	□ _{X 0.34}	Mg _{2.26}	Fe _{0.4}	Al _{0.34}	0,53	0,34	0,13	3,26	
400°C (S400-6G)	Na _{0.44}	Ca _{0.11}	□ _{X 0.44}	Mg _{1.70}	Fe _{0.26}	Al _{0.82}	Na _{0.5}	□ _{X 0.5}	Mg _{2.17}	Fe _{0.33}	Al _{0.5}	0,39	0,50	0,11	0,22	

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