



Supplement of

In situ micro-FTIR spectroscopic investigations of synthetic ammonium phengite under pressure and temperature

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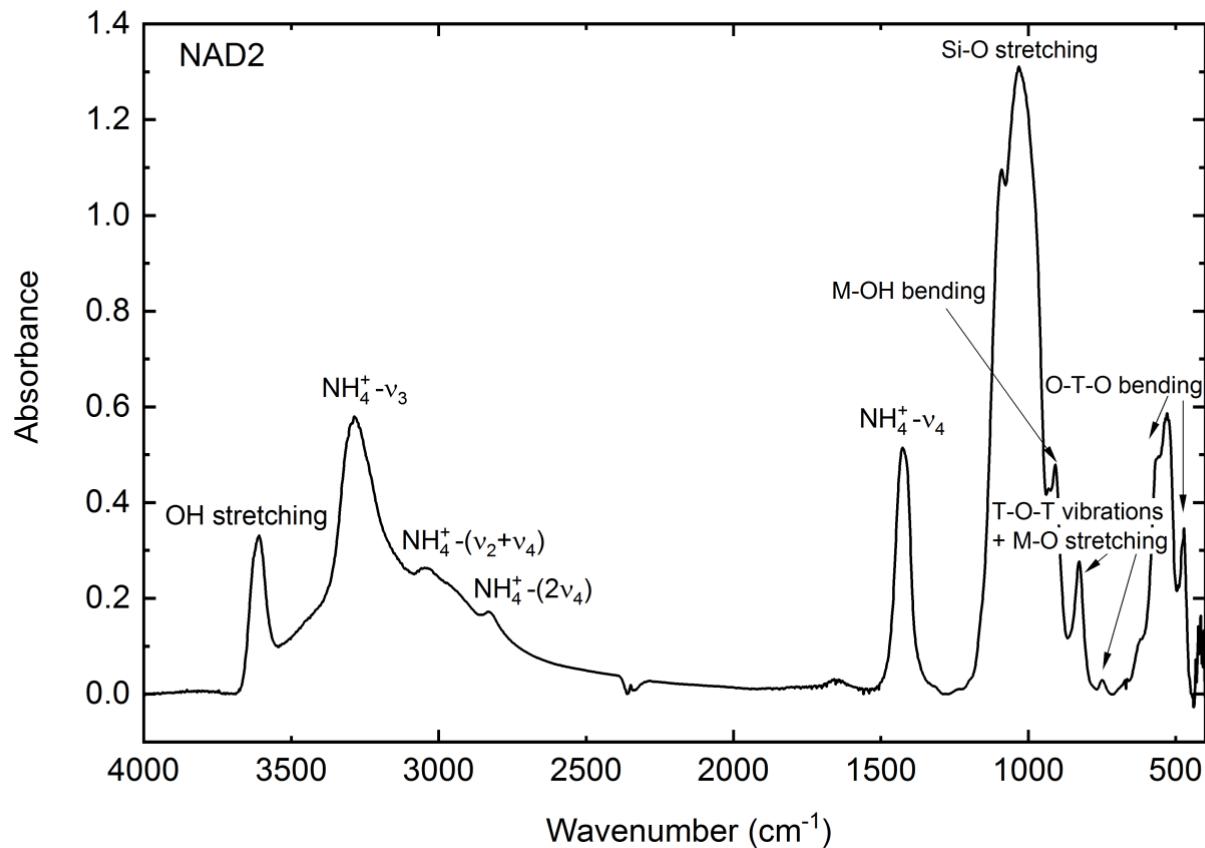
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Supplementary Table

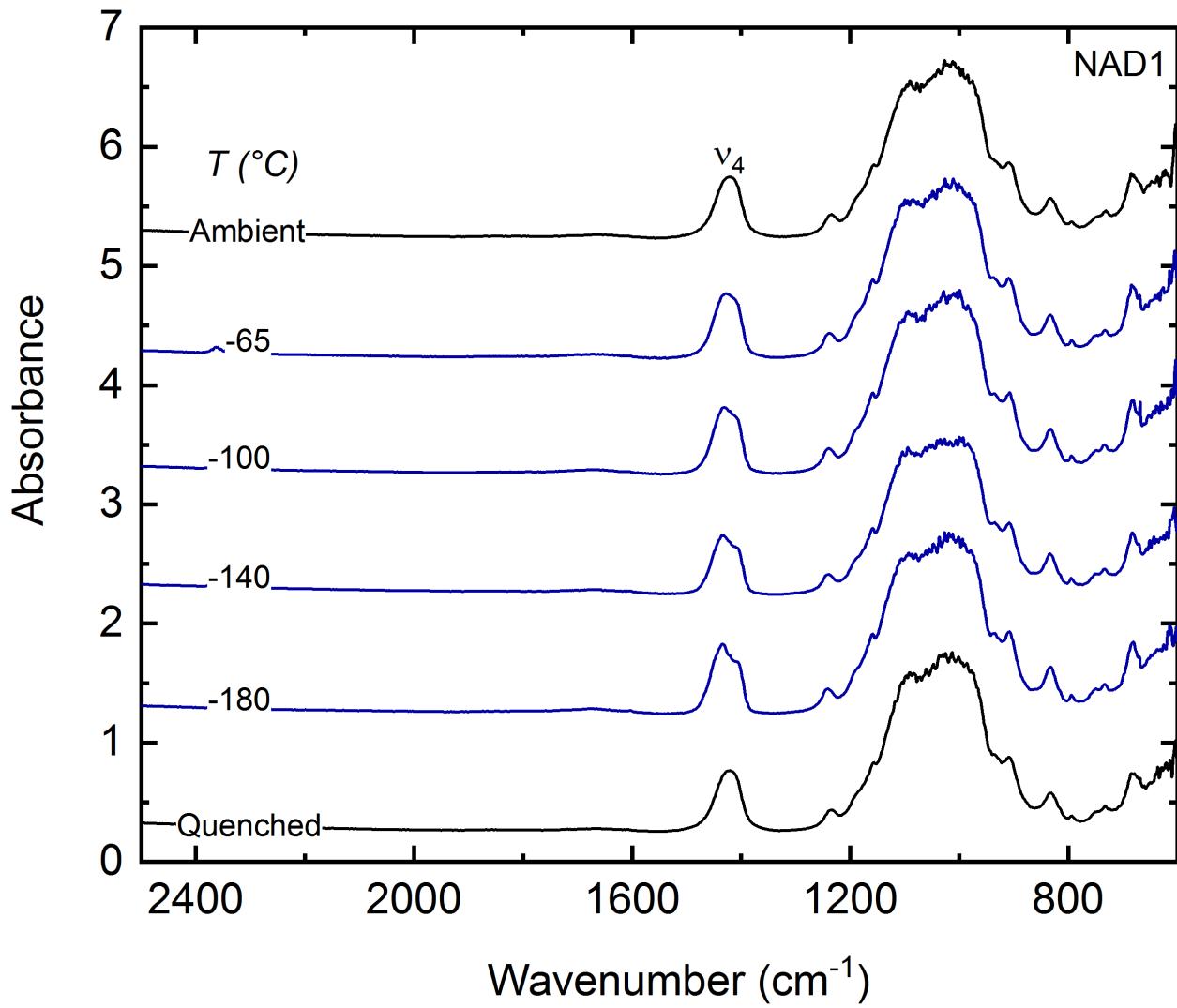
Table S1 Assignments of the observed IR bands at ambient conditions. Lattice vibrations are assigned according to McKeown et al. (1999), Velde (1978) and Zhang et al. (2010). M refers to octahedral site (Al or Mg) and T refers to tetrahedral site (Si or Al).

ν (cm ⁻¹)	Assignment	
3610	OH stretching vibration	NH_4^+ vibrations
3291	antisymmetric stretching vibration, triply-degenerate (ν_3)	
3036	a combination of symmetric and antisymmetric bending vibrations ($\nu_2+\nu_4$)	
2818	overtone of bending vibrations ($2\nu_4$)	
1430	antisymmetric bending vibration, triply-degenerate (ν_4)	
~1080	Si-O _{apical} stretching vibrations	lattice vibrations
~1000 & 1020	Si-O _{basal} stretching vibrations	
~910	M-OH bending vibrations	
830-750	T-O-T vibrations+ M-O stretching + tilting of the basis of the tetrahedron.	
~300-500	O-T-O bending	

Supplementary Figures



15 **Figure S1** FTIR spectrum at ambient conditions of synthesized run products of NAD2 showing OH stretching vibration, NH_4^+ vibrations: N-H antisymmetric stretching vibration (v_3), N-H antisymmetric bending vibration (v_4), the combination mode (v_2+v_4) and the overtone ($2v_4$) as well as the lattice vibrations. For more details see the main text. Additional peaks are observed at 2350 cm^{-1} for CO_2 , 1650 cm^{-1} for bending of H_2O whereas its stretching is hidden in the broad feature at 2800-3700 cm^{-1} .



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Figure S2 Low-temperature dependent FTIR spectra at ambient pressure of NAD1. Spectra are vertically offset for clarity. Blue spectra show cooling and black are quenched spectrum and spectrum at ambient conditions. The intense silicate stretching vibrations at ~ 950 - 1100 cm^{-1} are oversaturated.

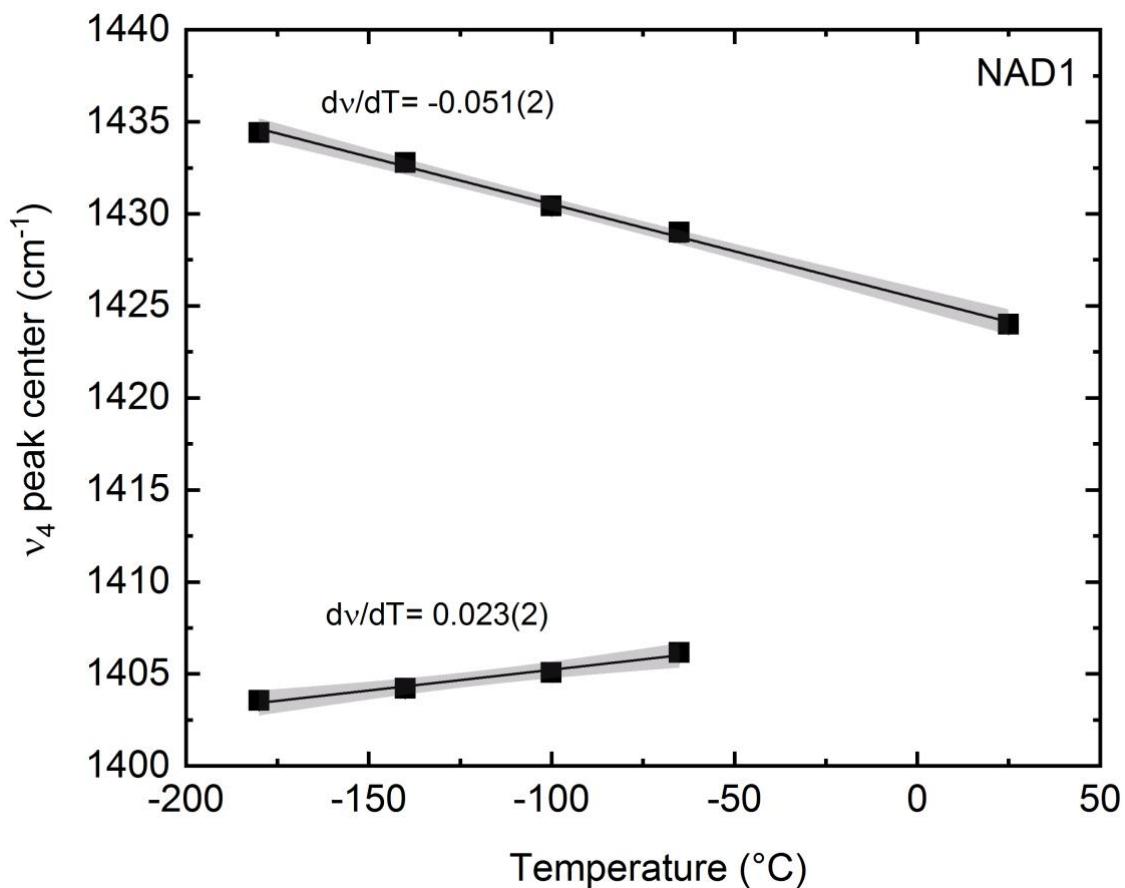


Figure S3 Peak splitting of the NH_4^+ - ν_4 bending vibration into two peaks with decreasing T. The error bars for the peak positions are smaller than the symbols. Black solid lines represent linear regression fit to the data. Grey shaded areas represent 95% confidence interval of the data. Changes in peak position with T, i.e., ($d\nu/dT$) values, are shown with esds of the last digit in parentheses.

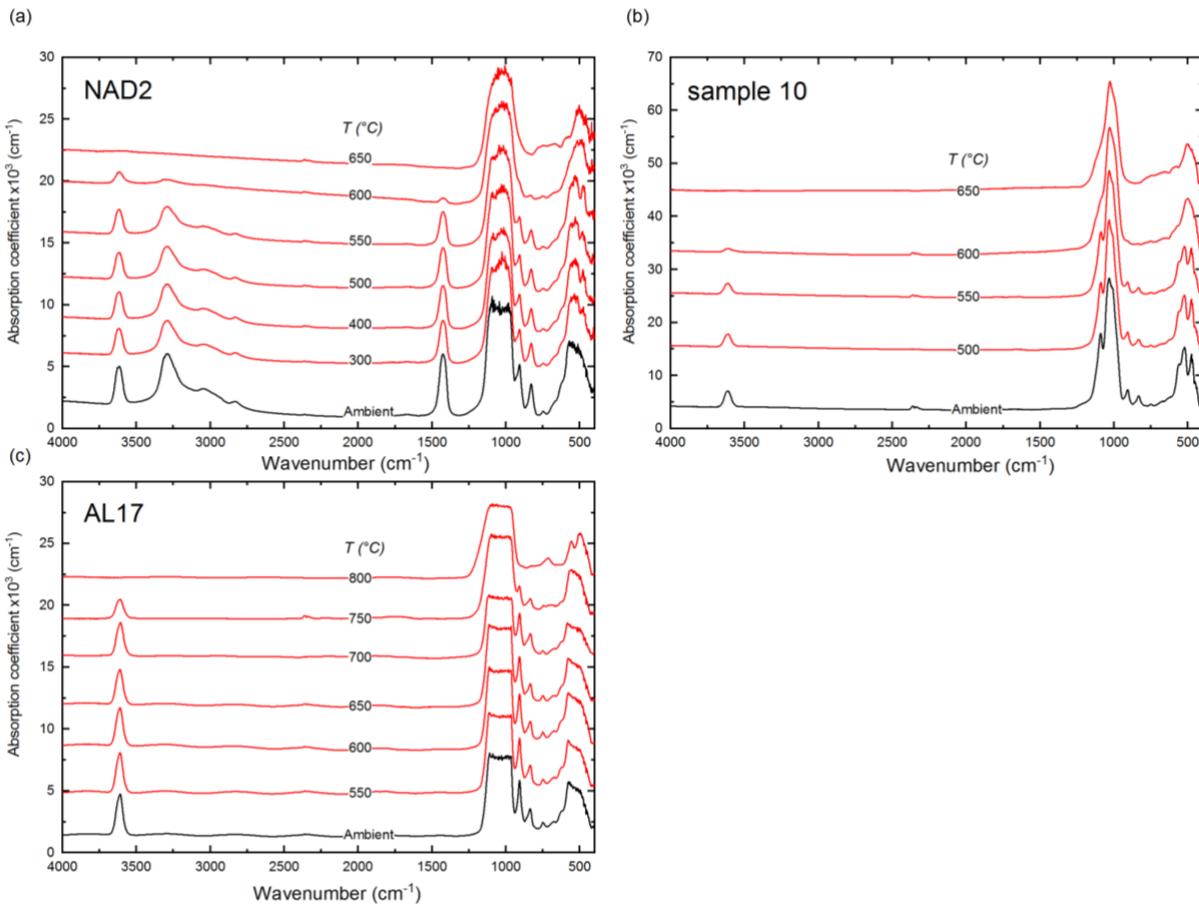


Figure S4 Calculated absorption coefficients in the $4000\text{-}400\text{ cm}^{-1}$ range of the quenched samples NAD2 (a), sample 10 (b) and AL17 (c) after 24 hours of annealing at each temperature. The difference between the spectra in (a) and (c) compared to (b) is the oversaturation of the band group around 1050 cm^{-1} due to a sample thickness of about $3\text{ }\mu\text{m}$ compared to about $1\text{ }\mu\text{m}$ for sample 10 in (b). Spectra are vertically offset for clarity.

References

McKeown, D. A., Bell, M. I., and Etz, E. S.: Vibrational analysis of the dioctahedral mica: 2M1 muscovite, *Am. Mineral.*, 84, 1041– 1048, <https://doi.org/10.2138/am-1999-7-806>, 1999.

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Zhang, M., Redfern, S. A., Salje, E. K., Carpenter, M. A., and Hayward, C. L.: Thermal behavior of vibrational phonons and hydroxyls of muscovite in dehydroxylation: In situ high-temperature infrared spectroscopic investigations, *Am. Mineral.*, 95, 1444–1457, <https://doi.org/10.2138/am.2010.3472>, 2010.