Supplementary Information for

Swelling Behaviour of Core-Shell Microgels in H_2O Analysed by Temperature-Dependent FTIR Spectroscopy

Lars Wiehemeier,[a] Marian Cors,[a,b] Oliver Wrede,[a] Julian Oberdisse,[b] Thomas Hellweg[a] and Tilman Kottke[a]*

[a] Physical and Biophysical Chemistry, Department of Chemistry, Bielefeld University, Universitätsstr. 25, 33615 Bielefeld, Germany, E-mail: tilman.kottke@uni-bielefeld.de

[b] Laboratoire Charles Coulomb (L2C), University of Montpellier, CNRS, 34095 Montpellier, France

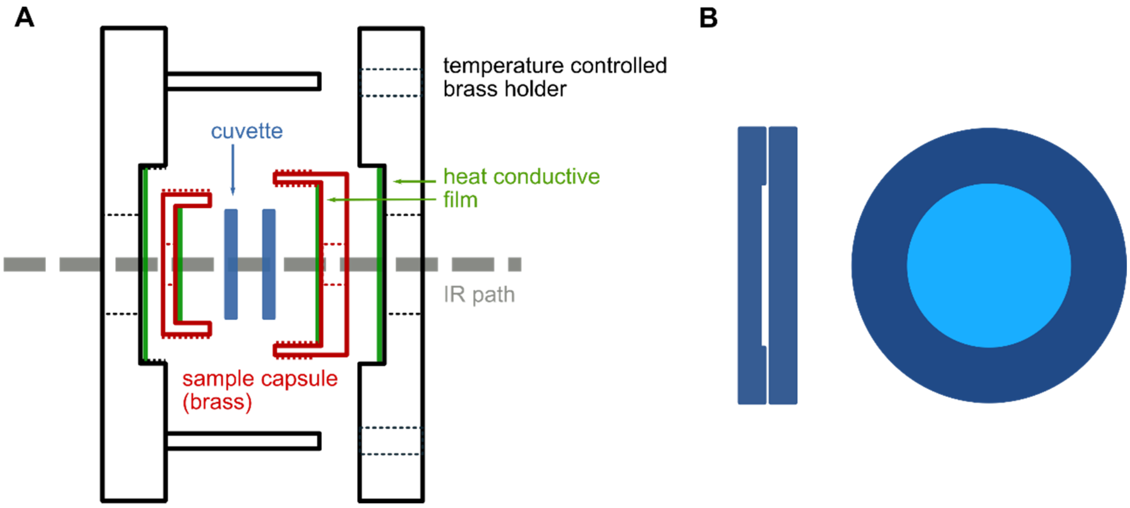

Figure S1: Sketch of the sample holder (A) and the BaF_2 cuvette (B).

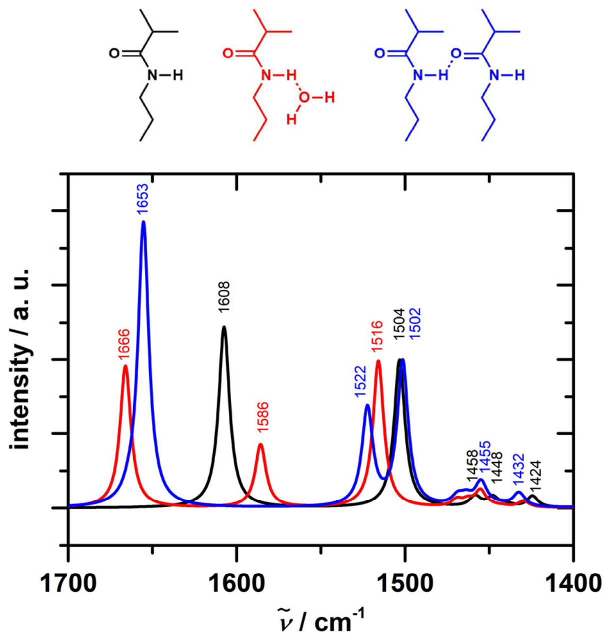

Figure S2: Calculated spectra of the model molecules for poly-NnPAM microgels shown above with different interactions to the NH group. The spectra were calculated using density functional theory and normalized to the intensity of the δ(NH) band at 1502, 1504 and 1516 cm^{-1}, respectively. An upshift in δ(NH) frequency by 12 cm^{-1} is observed upon binding of water (red). The interaction with a second monomer upshifts the band by 18 cm^{-1} (blue).

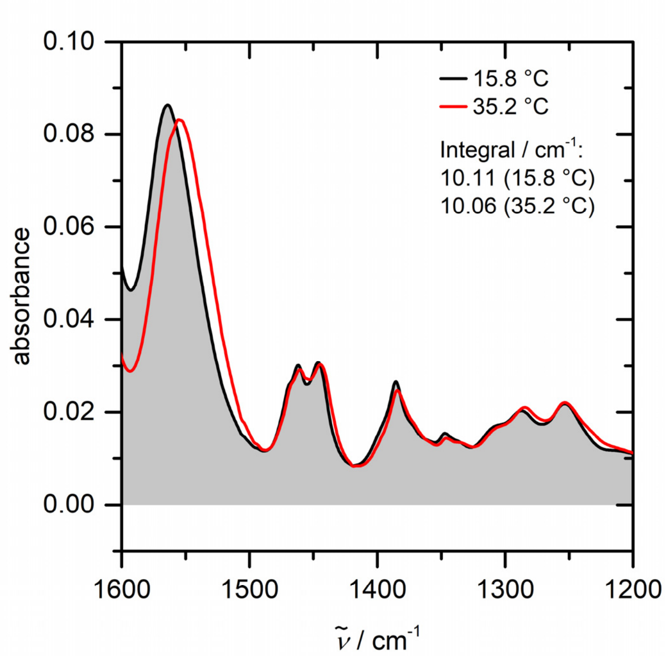

Figure S3: Comparison of FTIR spectra of a swollen and collapsed poly-NnPAM microgel at 15.8 °C and 35.2 °C in H_2O. The comparable integral absorbance at 1600 – 1200 cm^{-1} of swollen and collapsed microgel particles indicates that the entire particle is transmissive for infrared light even in the collapsed state and therefore contributes to the signal.

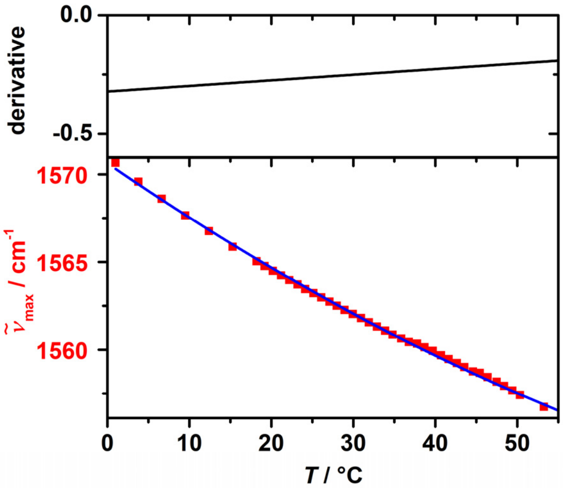

Figure S4: Temperature dependence of the frequency of the δ(NH)-band maximum for the model molecule Ni2MPA and the derivative of the fitted curve using equation (1).

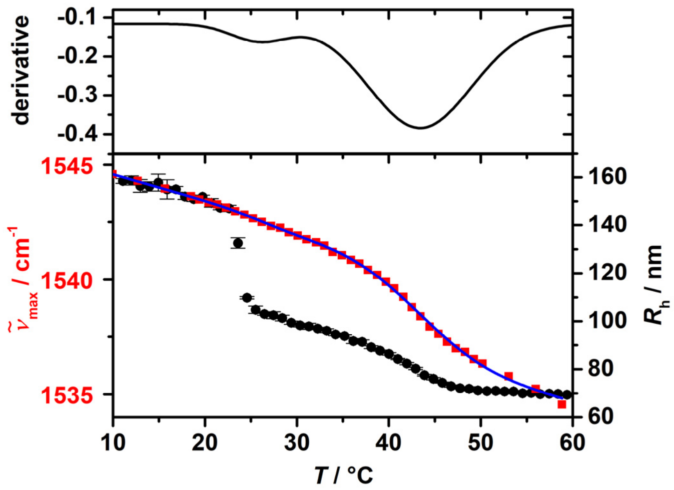

Figure S5: Investigation of a poly-NiPMAM-core poly-NnPAM-shell microgel with the shell synthesized at 35 °C, at which the core is in the swollen state. While the phase transition as seen by PCS (black circles) is dominated by the response of the shell, in FTIR spectroscopy (red squares) the phase transition of the NiPMAM core is clearly visible.