Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Table SI 1. Spectroscopically determined unfolding temperature and van´t Hoff enthalpy change (*) of GroEL, GroES and the GroEL-GroES complex (molar ratio of 1:2) in the absence and presence of different salts and cosolvents at ambient pressure. For GroES, two structural transitions (denoted 1, 2) could be observed.

	T_u / °C	$\Delta H_{vH,u}$ / kJ mol^{-1}
GroEL (buffer A)	69.1 ± 0.2	998 ± 61
GroEL (buffer A + 3 mM ADP)	67.8 ± 0.2	732 ± 89
GroEL (buffer B)	72.0 ± 0.6	821 ± 84
GroEL (buffer B + 3 mM ATP)	70.9 ± 0.5	788 ± 79
GroEL (buffer B + 3 mM ATP + 10 mM Mg^{2+})	70.6 ± 0.4	835 ± 37
GroEL (buffer B + 10 mM Mg^{2+})	71.8 ± 0.6	916 ± 77
GroEL (buffer B + 1 M ^{13}C-urea)	65.1 ± 0.3	917 ± 170
GroEL (buffer B + 1 M TMAO)	73.7 ± 0.6	732 ± 91
GroES (buffer B)	1) 82.1 ± 0.3 2) 87.1 ± 0.6	1) 691 ± 92 2) 669 ± 286
GroES (buffer B + 1 M ^{13}C-urea)	1) 80.0 ± 1.2 2) 83.5 ± 1.0	1) 829 ± 141 2) 1028 ± 245
GroES (buffer B + 1 M TMAO)	1) 84.8 ± 1.2 2) 87.8 ± 0.6	1) 822 ± 133 2) 671 ± 132
GroEL-GroES (buffer B)	71.4 ± 0.5	1007 ± 144
GroEL-GroES (buffer B + 3 mM ATP + 10 mM Mg^{2+} + 1 M ^{13}C-urea)	67.2 ± 0.4	863 ± 70
GroEL-GroES (buffer B + 3 mM ATP + 10 mM Mg^{2+} + 1 M TMAO)	75.9 ± 0.5	879 ± 61

Table SI 2. Spectroscopically determined unfolding pressures, p_u, and volume change of (partial) unfolding, ΔV_u, of GroES in the absence and presence of different cosolvents at 25 °C.

	p_u / bar	ΔV_u / cm^3 mol^{-1}
GroES (buffer B)	5395 ± 298	-52.9 ± 11.8
GroES (buffer B + 1 M TMAO)	5413 ± 321	-54.8 ± 7.8
GroES (buffer B + 1 M ^{13}C-urea)	3552 ± 85	-112.28 ± 14.6

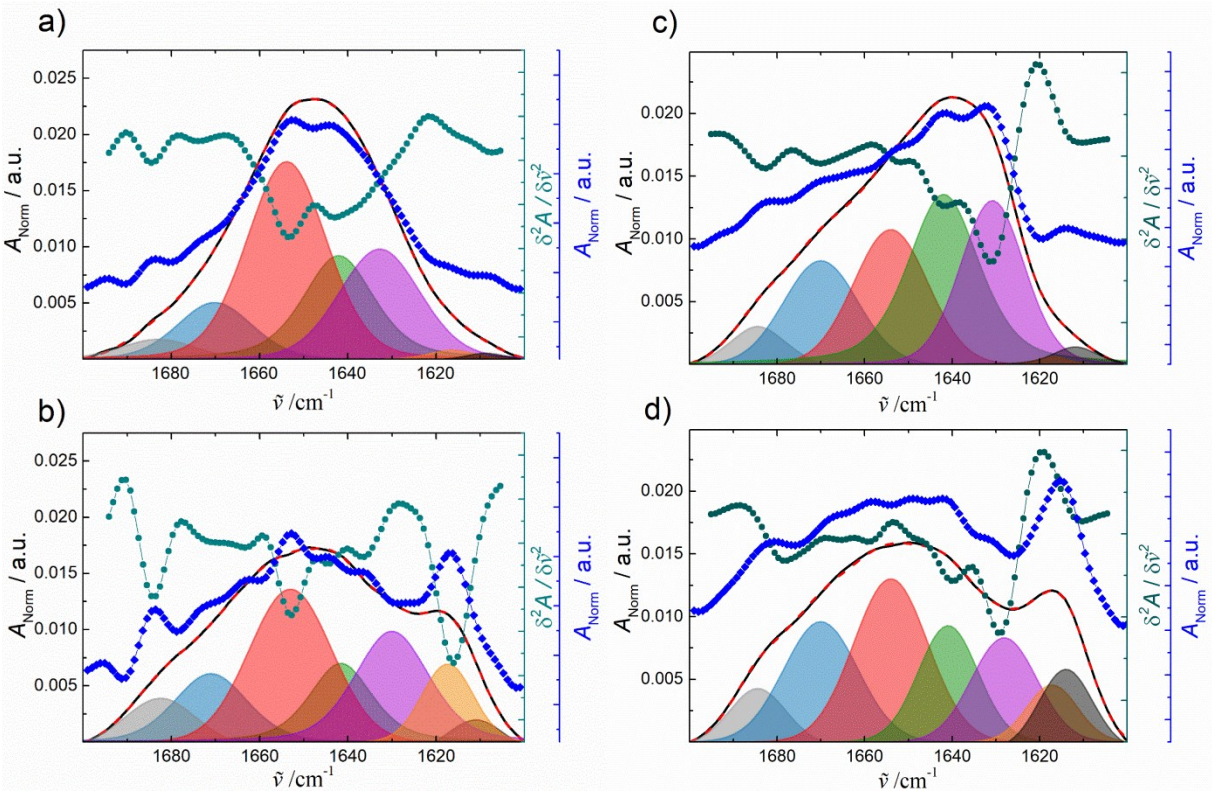

Figure SI 1. Curve fitting results of the temperature-dependent FTIR data of GroEL and GroES in neat buffer at ambient pressure: Amide I´ band region (black line), the corresponding fit (red dashed line), FSD (blue dotted (square) line) and 2nd derivative spectra (dark cyan dotted line) of GroEL for 25 °C (a) and 86 °C (b) at ambient pressure and of GroES at 25 °C (c) and 96 °C (d) at ambient pressure: intermolecular β-sheets (grey), turns and loops (blue), α-helices (red), random coils (green), intramolecular β-sheets (purple), intermolecular β-sheets (orange) and side chains (black).

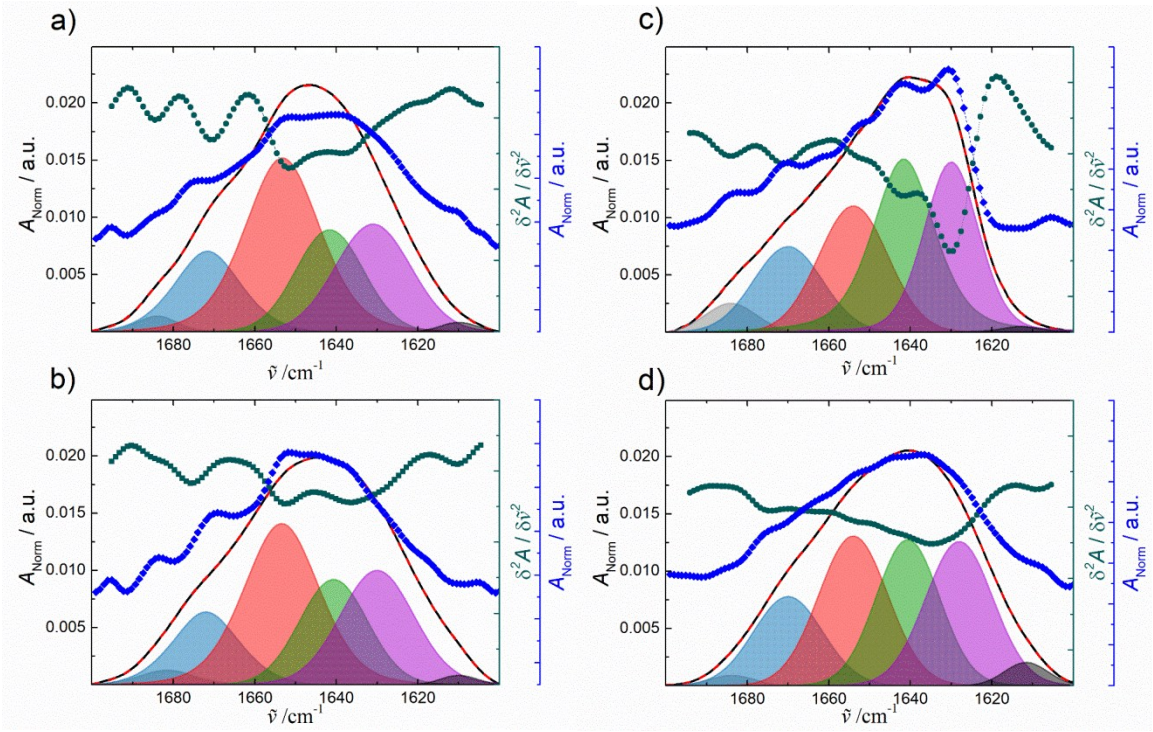

Figure SI 2. Curve fitting results of the pressure-dependent FTIR data of GroEL and GroES in neat buffer at 25 °C. Amide I´ band region (black line), the corresponding fit (red dashed line), FSD (blue dotted (square) line) and 2nd derivative spectra (dark cyan dotted line) of GroEL for 1 bar (a) and 10 kbar (b) at 25 °C and of GroES for 1 bar (c) and 10 kbar (d) at 25 °C: intermolecular β-sheets (grey); turns and loops (blue); α-helices (red); random coils (green); intramolecular β-sheets (purple) and side chains (black).

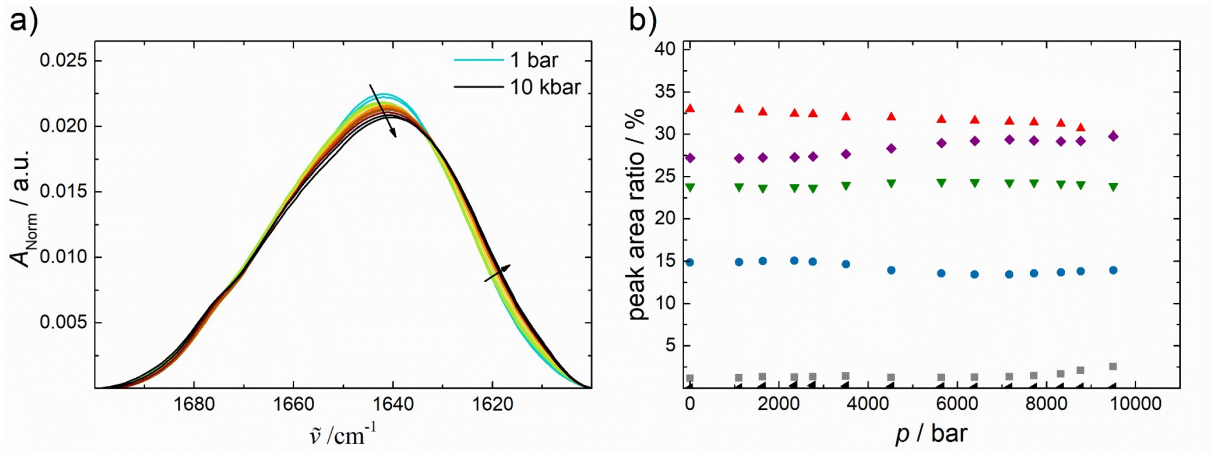

Figure SI 3. Pressure-dependent FTIR absorption data of the GroEL-GroES complex in neat buffer (buffer B + 3 mM ATP + 10 mM Mg^{2+}) at 25 °C. a) Pressure-dependent changes of the normalized amide I´ band region of the GroEL-GroES complex and b) corresponding changes in secondary structure elements by pressure: intermolecular β-sheets (1683 cm^{-1}, grey); turns and loops (1672 cm^{-1}, blue); α-helices (1653 cm^{-1}, red); random coils (1640 cm^{-1}, green); intramolecular β-sheets (1632 cm^{-1}, purple) and side chains (1610 cm^{-1}, black).