

Fig. 1S a)

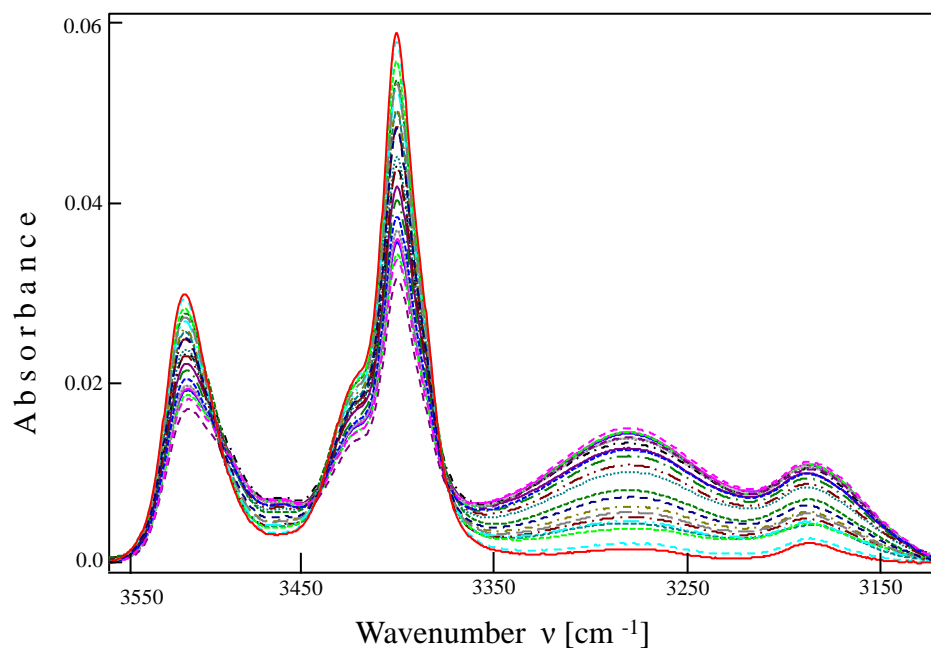


Fig. 1S b)

Fig. 1S Absorbance evolution as a function of concentration in the 3550-3100 cm^{-1} frequency range for a) N-butylurea (NBU); b) N-butylthiourea (NBTU) in dichloromethane solutions within the concentration (mol/dm^3).

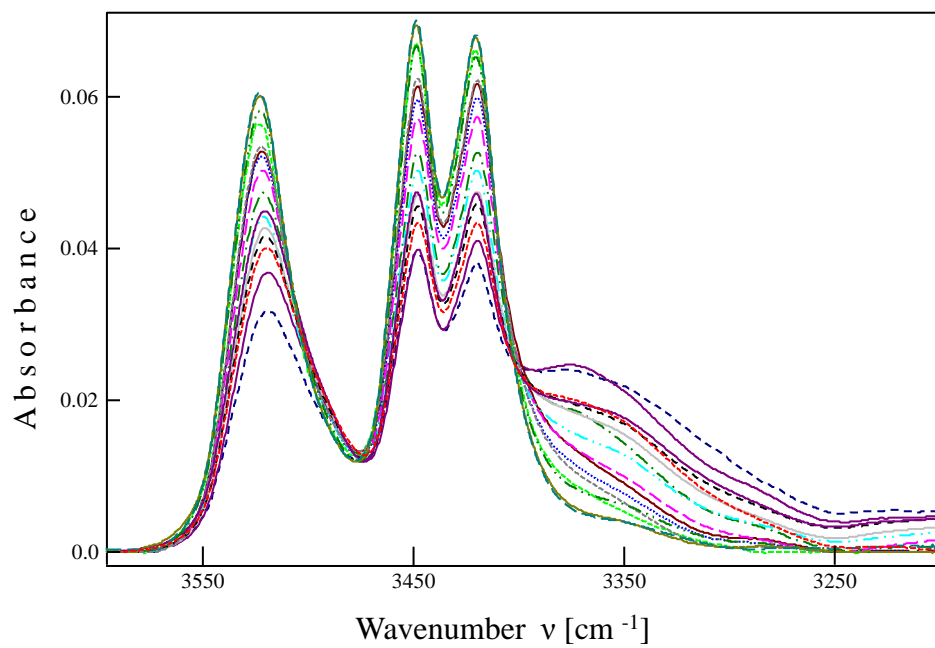


Fig. 2S a)

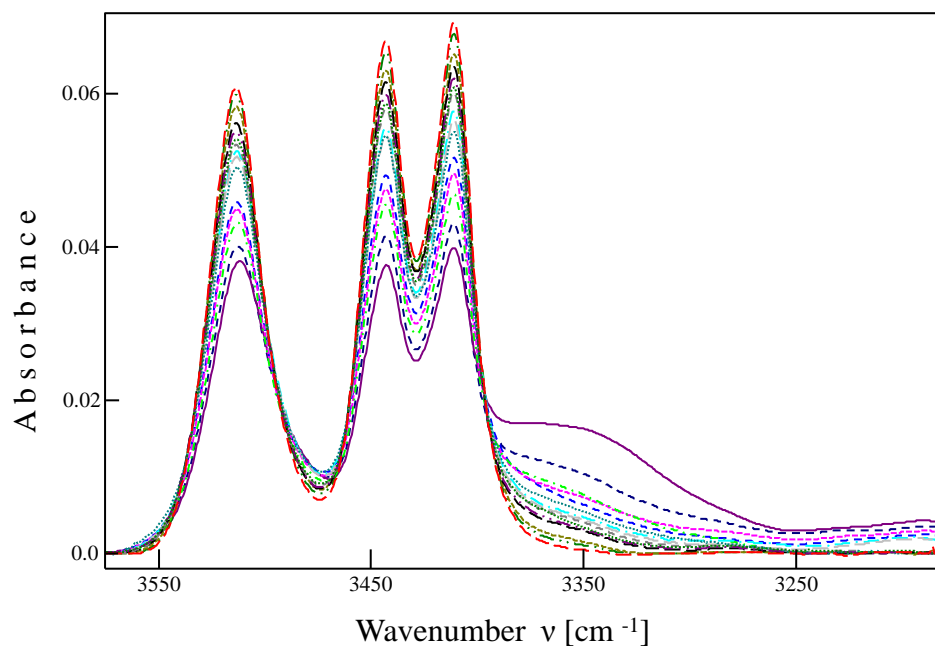


Fig. 2S b)

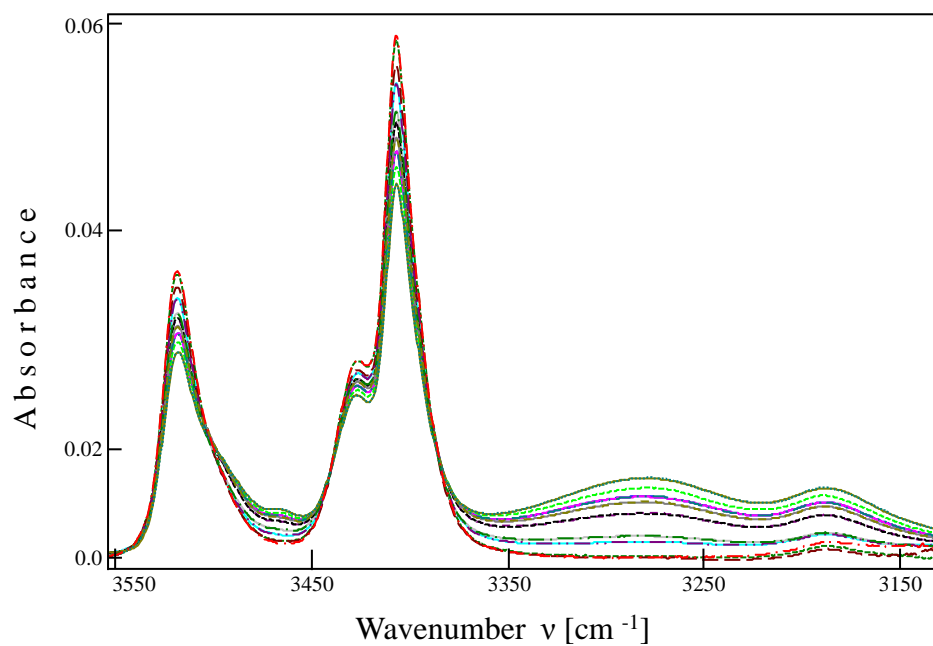


Fig. 2S c)

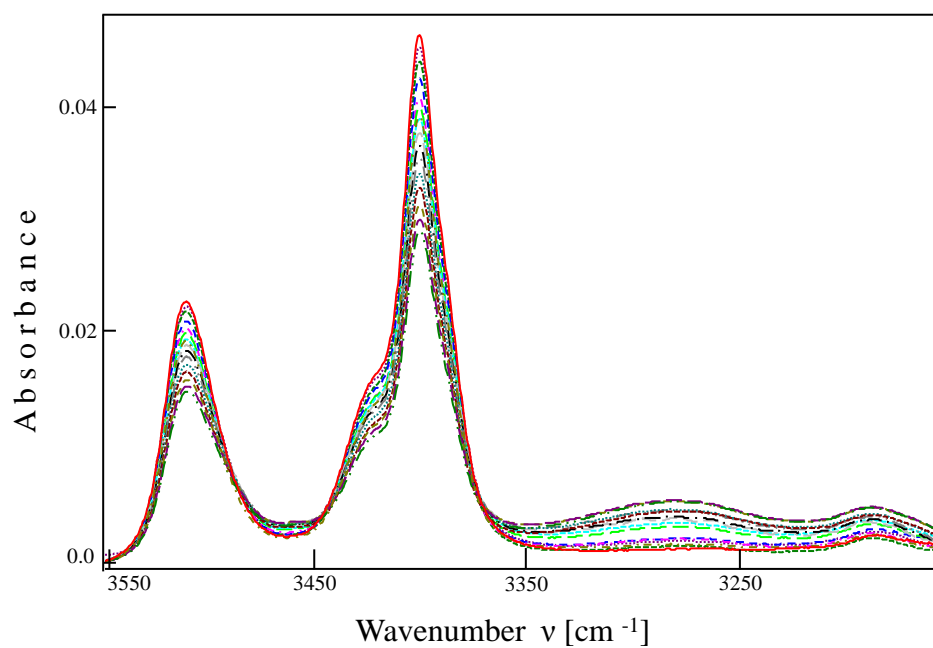


Fig. 2S d)

Fig. 2S Absorbance evolution as a function of concentration in the 3550-3100 cm^{-1} frequency range for a) N-propylurea (NPU); c) N-propylthiourea (NPTU) in chloroform and b) N-propylurea [NPU]; d) N-propylthiourea [NPTU] in dichloromethane solutions within the concentration (mol/dm^3).

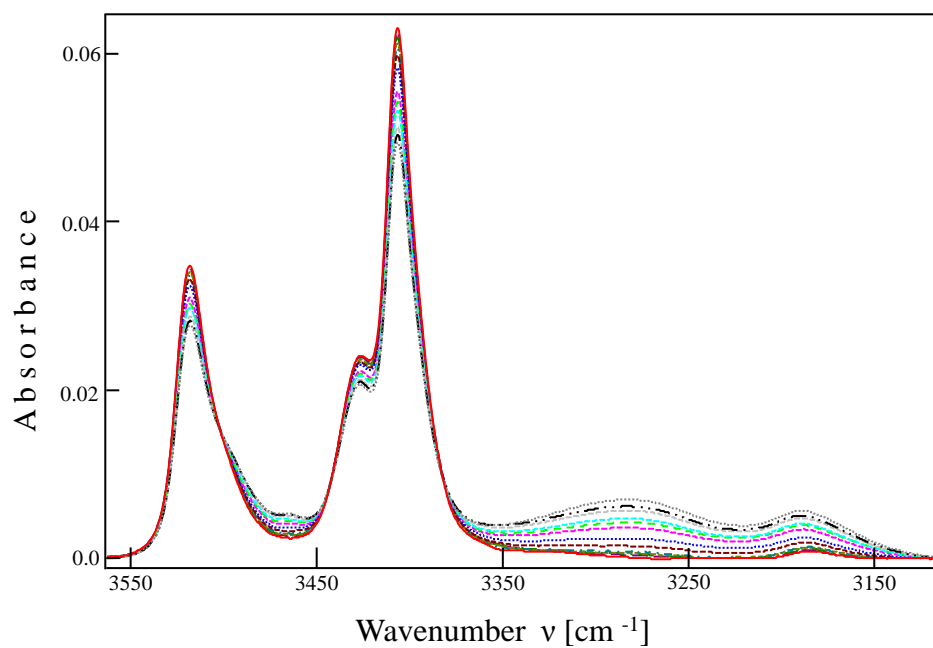


Fig. 3S a)

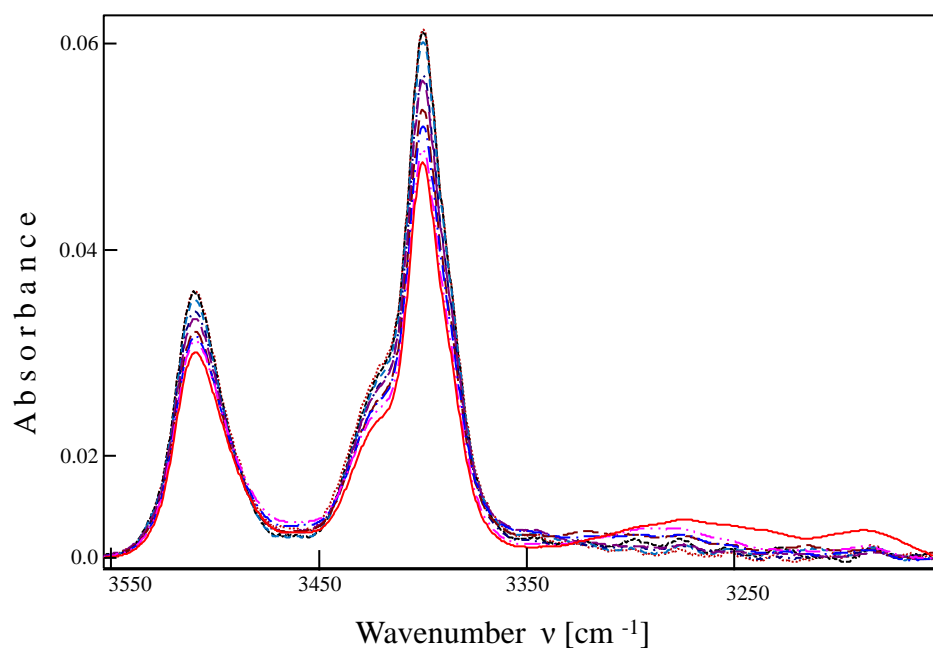


Fig. 3S b)

Fig. 3S Absorbance evolution as a function of concentration in the 3550-3100 cm⁻¹ frequency range for N-hexylthiourea (**NHTU**) in a) chloroform and b) dichloromethane solutions within the concentration (mol/dm³).

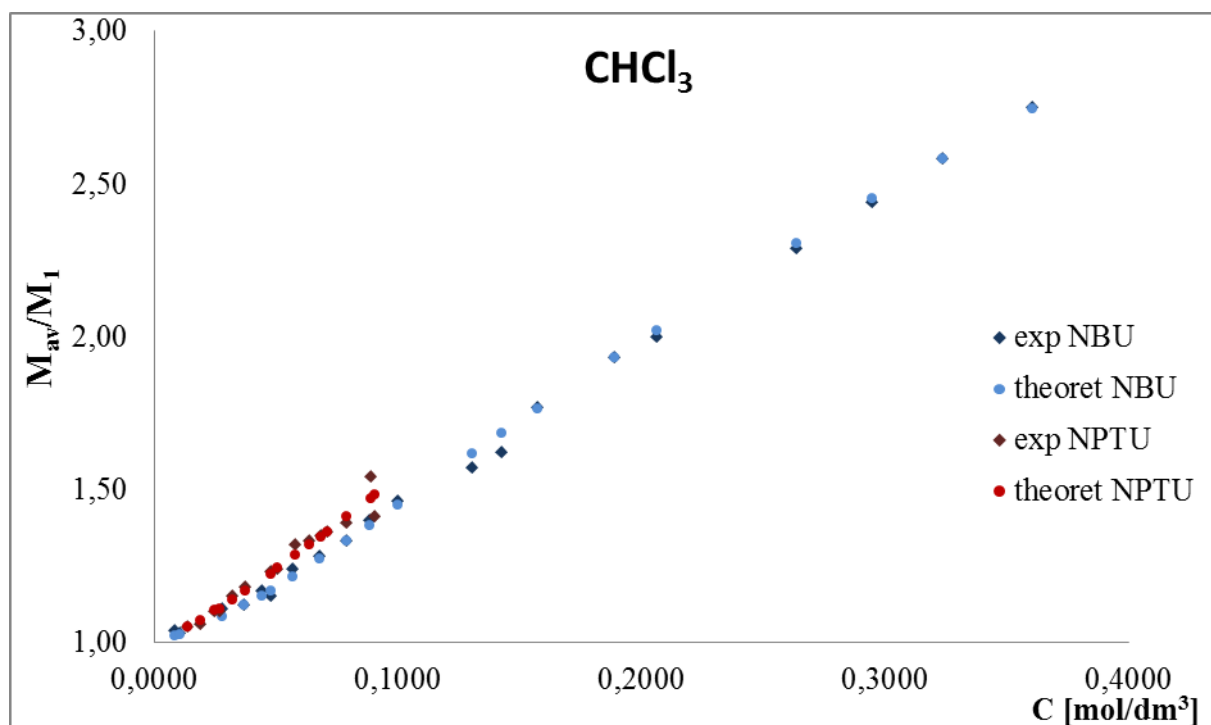


Fig. 4S Plots of average molecular weight versus c [mol/dm³] in chloroform for N-butylurea: experimental data (blue diamonds) and theoretical results (dark blue circles); N-propylthiourea experimental data (red diamonds) and theoretical results (dark red circles).

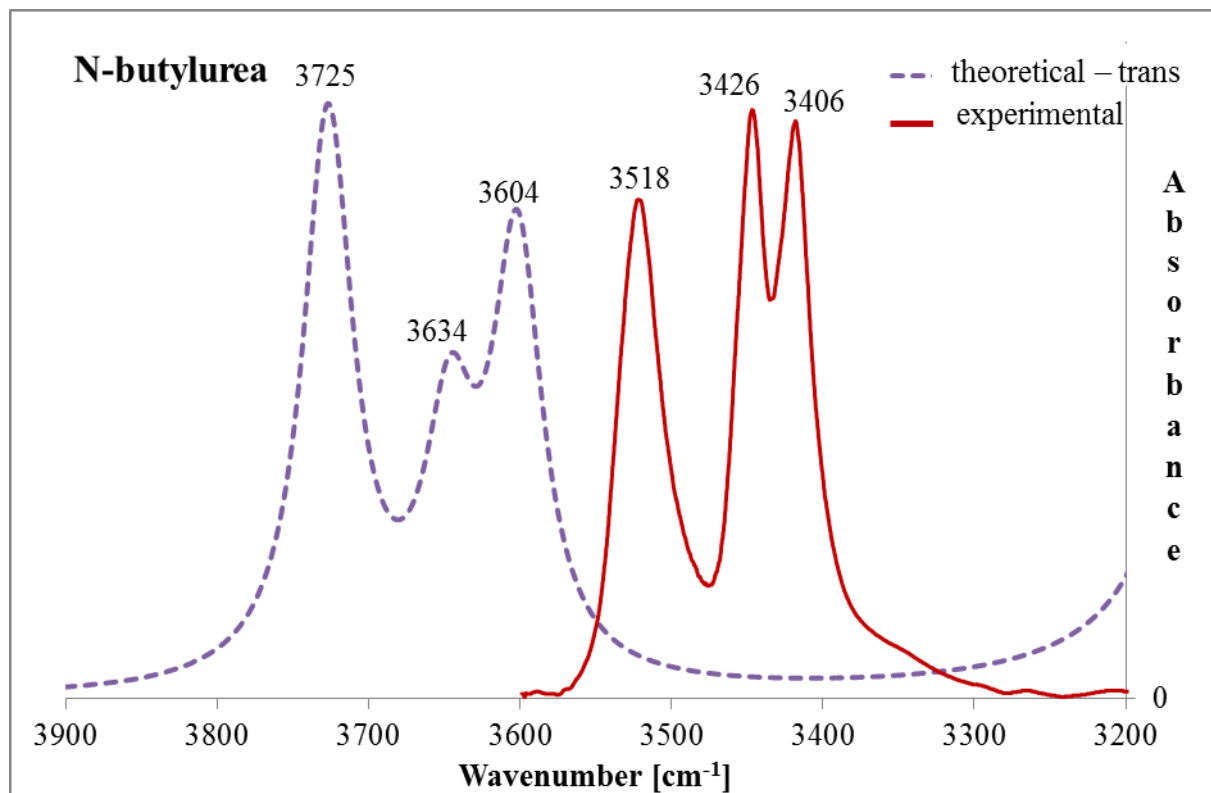


Fig. 5S Comparison of experimental and theoretical spectra of N-butylurea monomers. The difference in the position in the range of ν (NH) stretching bands is about 200 cm⁻¹.

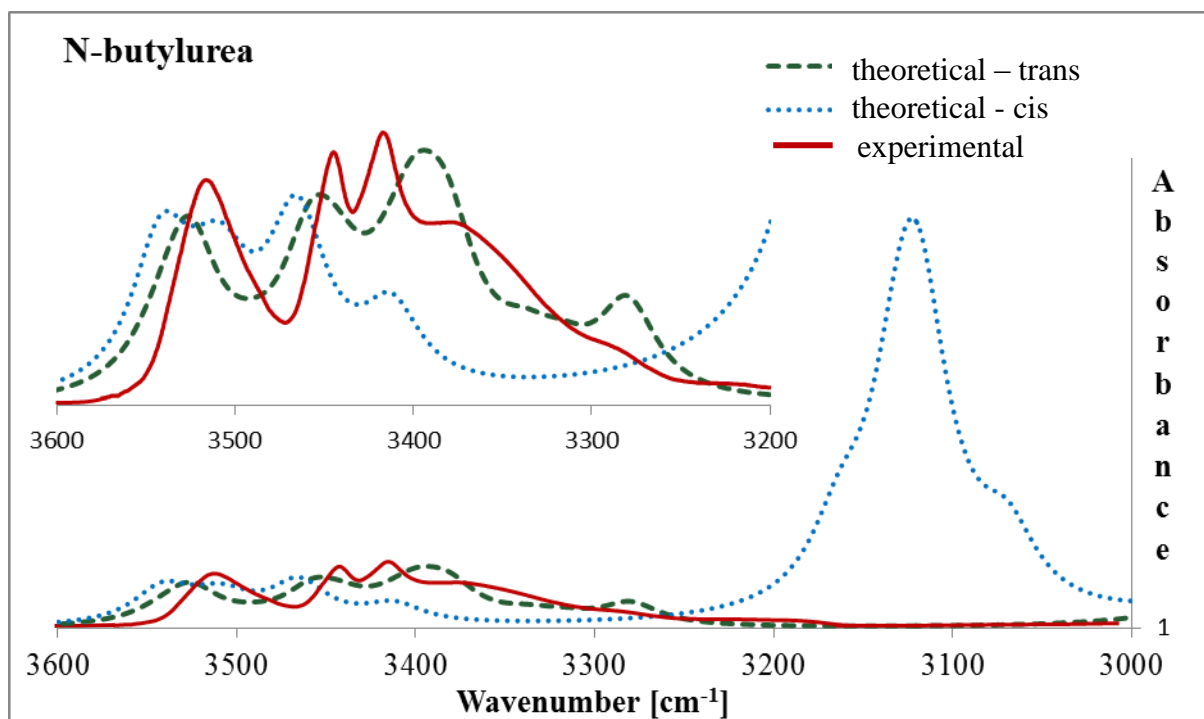


Fig. 6S Comparison of experimental and theoretical spectra of N-butylurea. Theoretical spectra are the sum of the spectra of monomers, dimers and trimers, multiplied by appropriate contribution coefficients of different forms, which are determined from association constant.

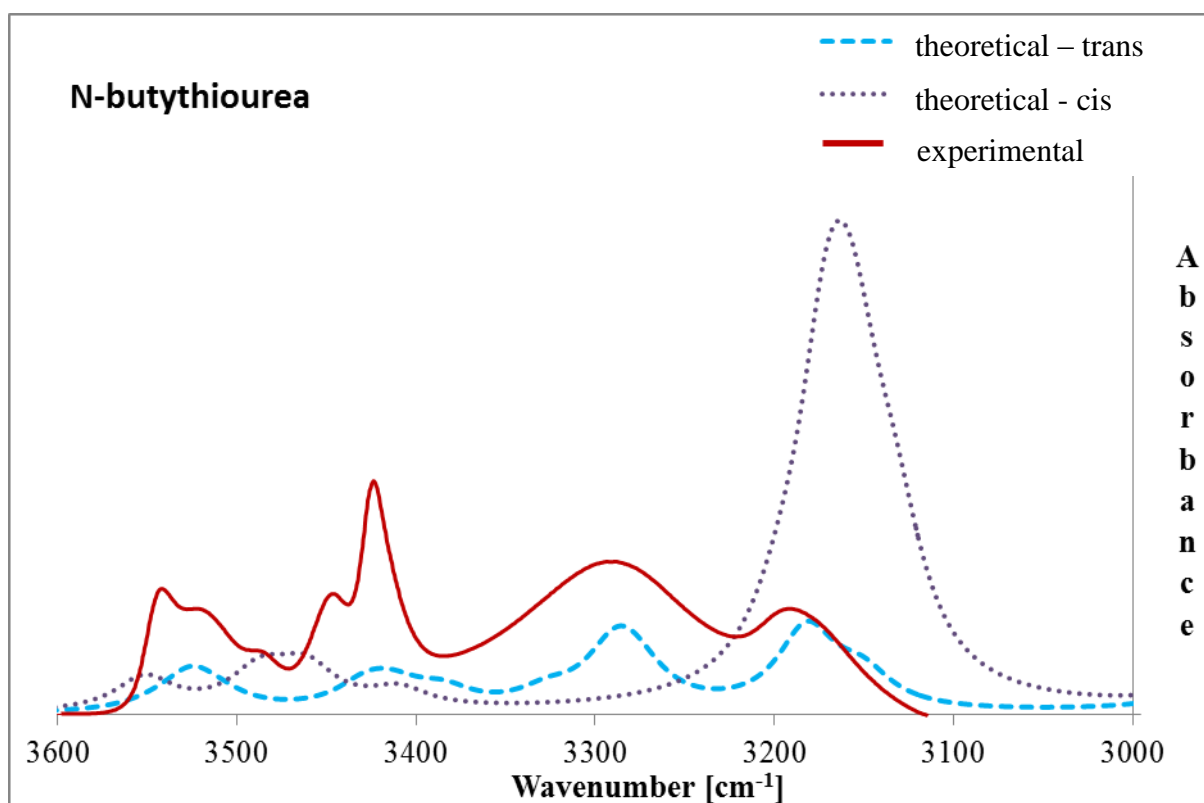


Fig. 7S Comparison of experimental and theoretical spectra of N-butylthiourea. Theoretical spectra are the sum of the spectra of monomers, dimers and trimers, multiplied by appropriate contribution coefficients of different forms, which are determined from association constant.