RSC Advances

Perturbation from temperature on hydrogen bonding in aqueous solutions for different urea concentrations†

Noushaba Nusrat Mafy,[a] Tanjina Afrin,[a] M. Muhibur Rahman,[b] M. Yousuf A. Mollah[a] and Md. Abu Bin Hasan Susan[a]*

[a]*Department of Chemistry, University of Dhaka, Dhaka 1000, Bangladesh*

[b]*University Grants Commission of Bangladesh, Agargaon, Dhaka 1207, Bangladesh*

Electronic supplementary information (ESI)

Fig. S1 FTIR spectrum of solid urea.

Fig. S2 ATR FTIR spectra of (a) pure water (b) aqueous urea solutions at different concentrations.

Fig. S3 NIR spectra of pure water at different temperatures.

Fig. S4 Difference spectra of (a) pure water (b) 6.0 M aqueous urea solution obtained with respect to the first spectrum measured at 20 ^{o}C.

Fig. S5 Second derivative spectra of pure water at different temperatures.

Fig. S6 Second derivative spectra of 1.5 M aqueous urea solution at different temperatures.

Fig. S7 Temperature dependent deconvoluted spectra of pure water.

Fig. S8 Variation of band position for (a) weak (b) third or moderate strength (c) normal or strong (d) strong hydrogen-bonded components resolved from the temperature dependent NIR spectra of pure water and aqueous urea solutions.

Fig. S9 Power spectra of three distinct groups of aqueous urea solutions.

Fig. S10 Variation of apparent molar volume with temperature and concentration.

Fig. S11 Variation of entropy with concentration of urea.

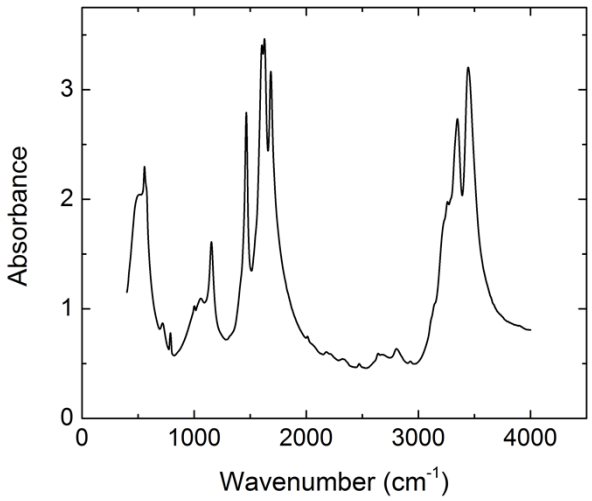

Fig. S1 FTIR spectrum of solid urea.

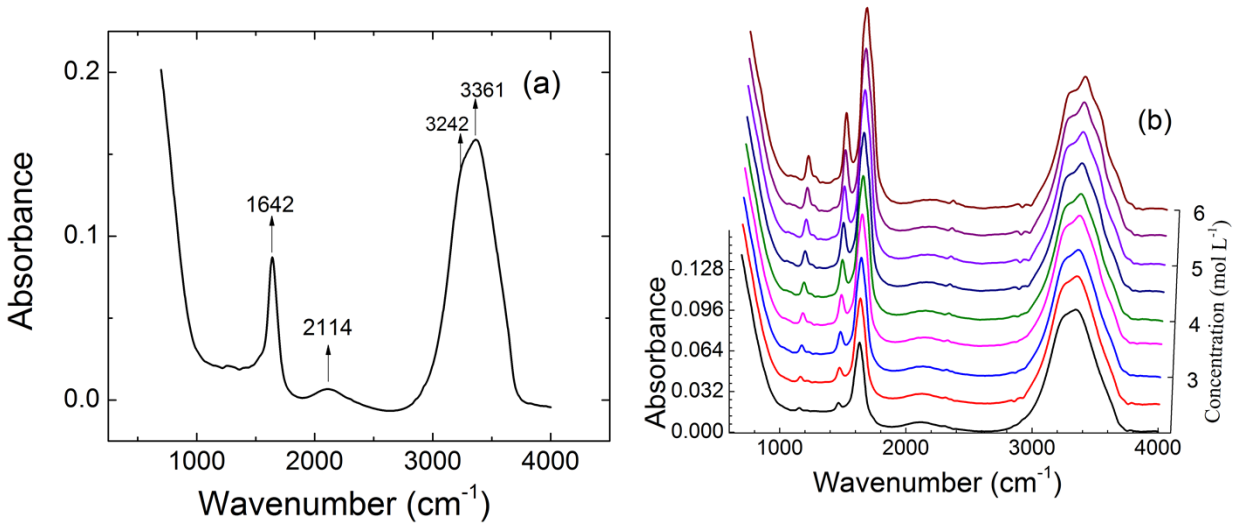

Fig. S2 ATR FTIR spectra of (a) pure water (b) aqueous urea solution at different concentrations.

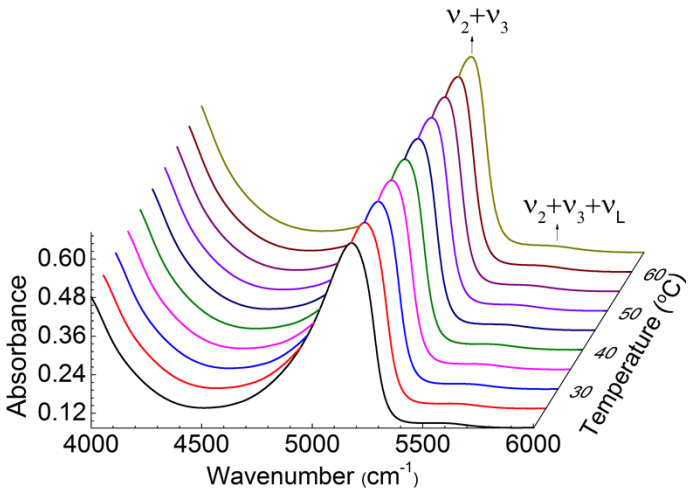

Fig. S3 NIR spectra of pure water at different temperatures.

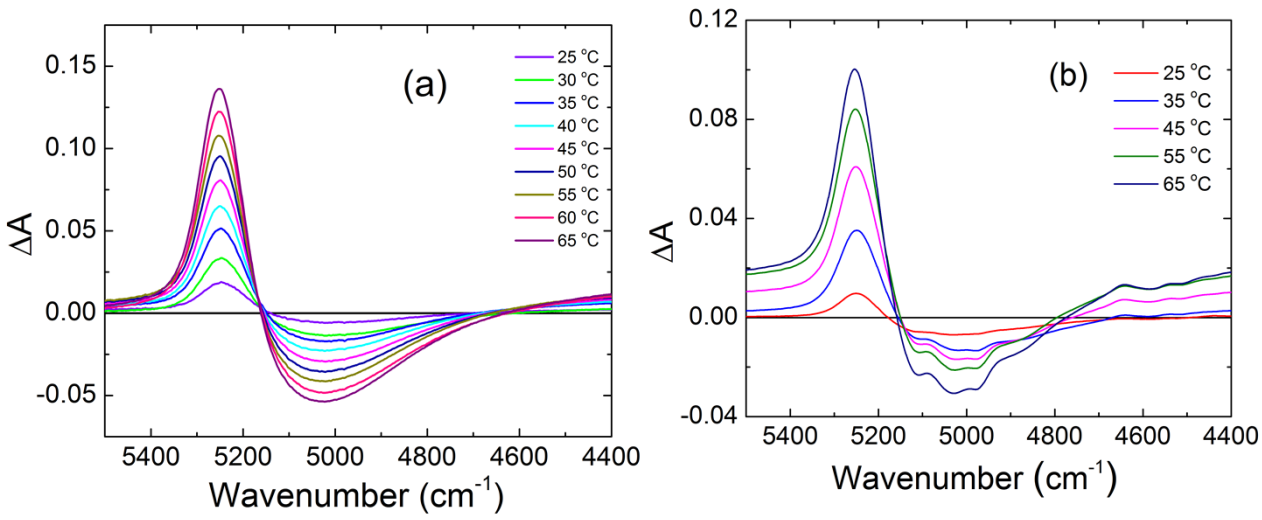

Fig. S4 Difference spectra of (a) pure water (b) 6.0 M aqueous urea solution obtained with respect to the first spectrum measured at 20 °C.

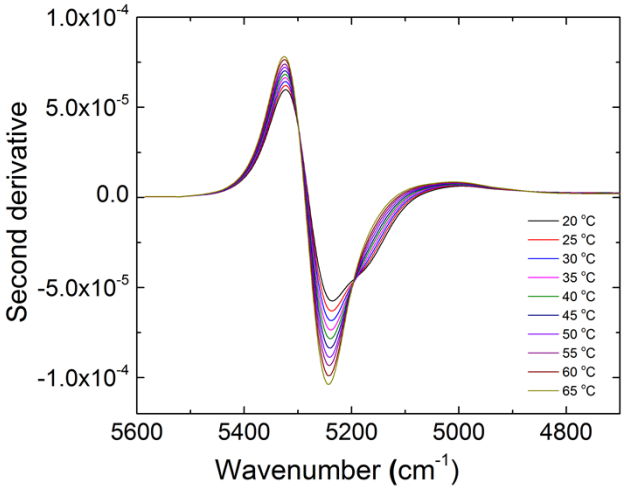

Fig. S5 Second derivative spectra of pure water at different temperatures.

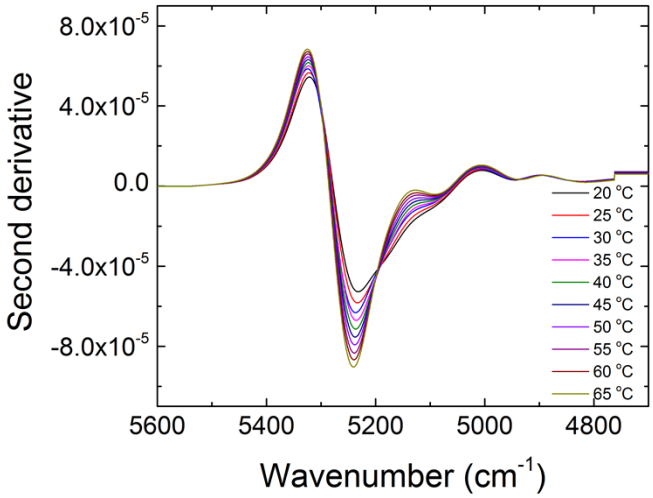

Fig. S6 Second derivative spectra of 1.5 M aqueous urea solution at different temperatures.

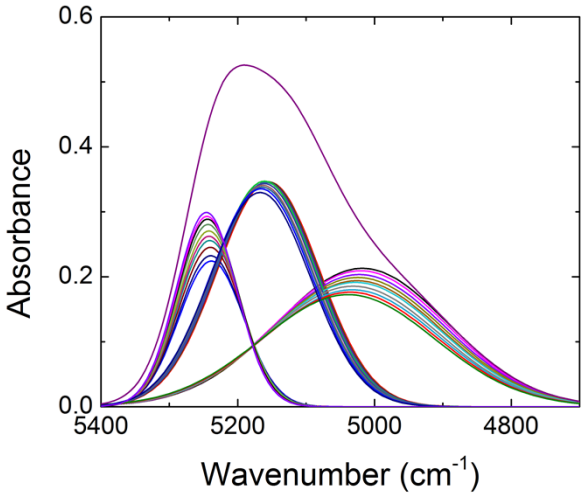

Fig. S7 Temperature dependent deconvoluted spectra of pure water.

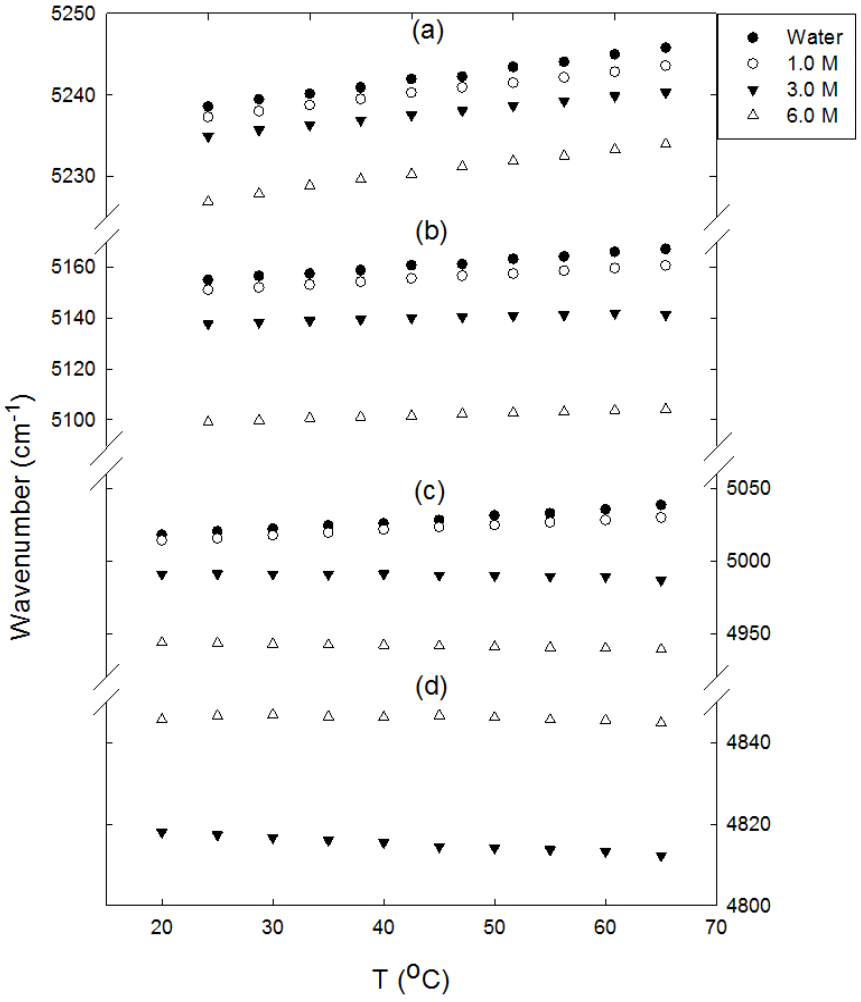

Fig. S8 Variation of band position for (a) weak (b) third or moderate strength (c) normal or strong (d) strong hydrogen-bonded components resolved from the temperature dependent NIR spectra of pure water and aqueous urea solutions.

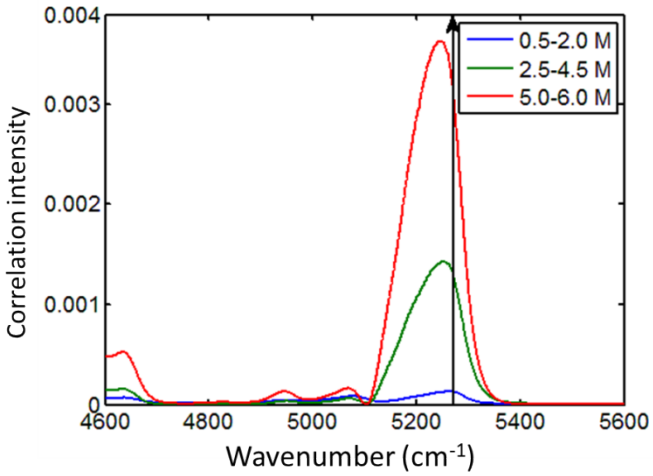

Fig. S9 Power spectra of three distinct groups of aqueous urea solutions.

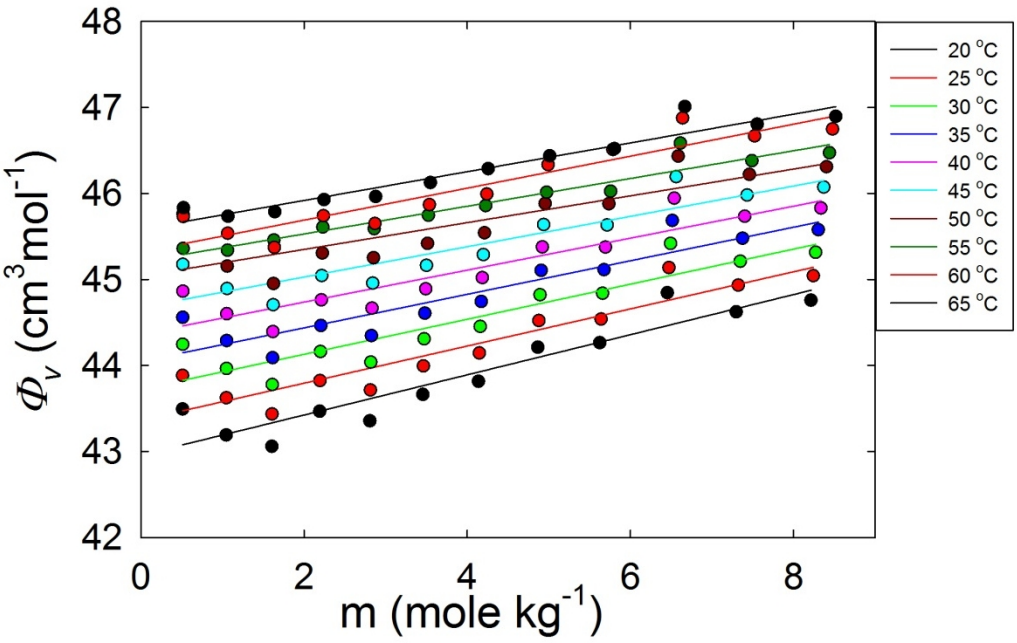

Fig. S10 Variation of apparent molar volume with temperature and concentration.

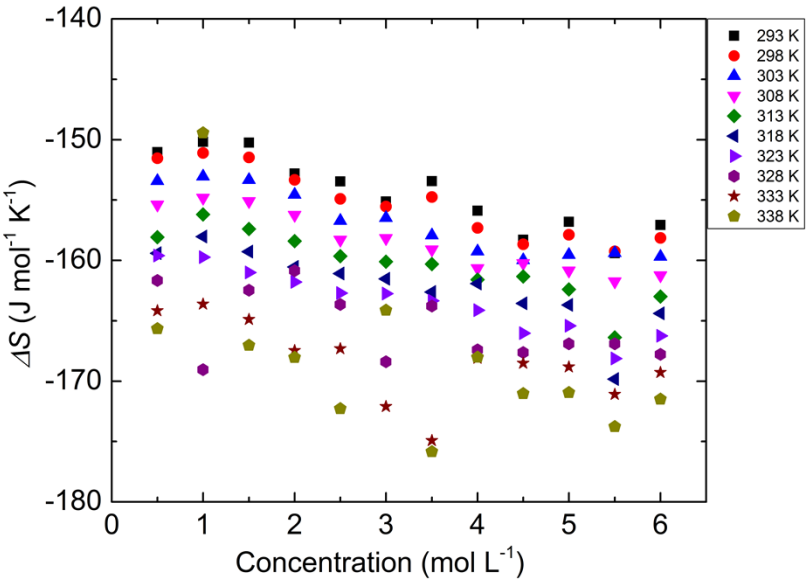

Fig. S11 Variation of entropy with concentration of urea.