Dynamics of Dihydrogen Bonding in Aqueous Solutions of Sodium Borohydride

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Supplementary Information

Figure S1 shows the plot of the base lined absorbance of 6 μm thick samples of 8:1 H_2O:$NaBH_4$ in pH14 solution made with pure H_2O and with a 5% HOD in H_2O solution. The major peaks have been labeled. Note that the presence of HOD leads to additional stretches at ~2500 cm^{-1} and 1450 cm^{-1}.

Figure S1

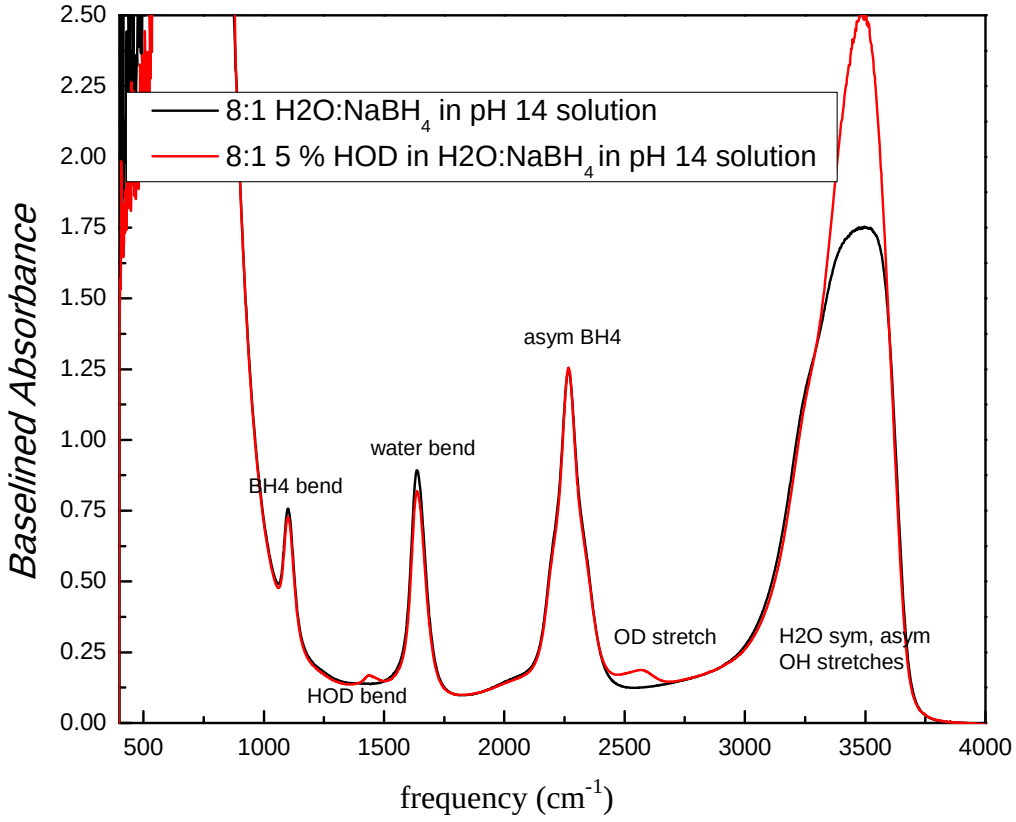

Figure S2 is the plot of the base lined absorbance of 12 μm thick samples of 50:1 H_2O:$NaBH_4$ in pH14 solution, and the pH14 solution by itself. Note that the presence of $NaBH_4$ leads to additional stretches at ~2260 cm^{-1} and 1100 cm^{-1}, the former being the asymmetric stretch and the later a bend.

Figure S2

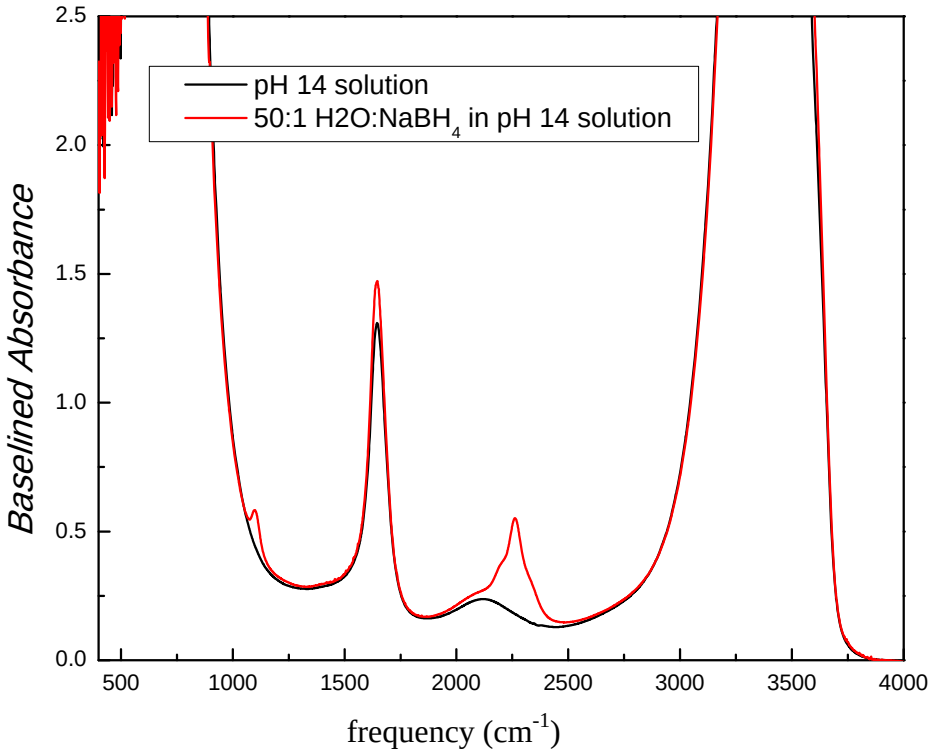

Figure S3 shows the 2D-IR spectra of the B-H stretch of 50:1 H_2O:$NaBH_4$ in pH 14 solution at a series of Tws. Even though the spectrum starts fairly spectrally diffused and rounded, it is possible to discern the change in peak shape from the more diagonally elongated spectrum at Tw=0.2ps to the more rounded spectrum at long time.

Figure S3

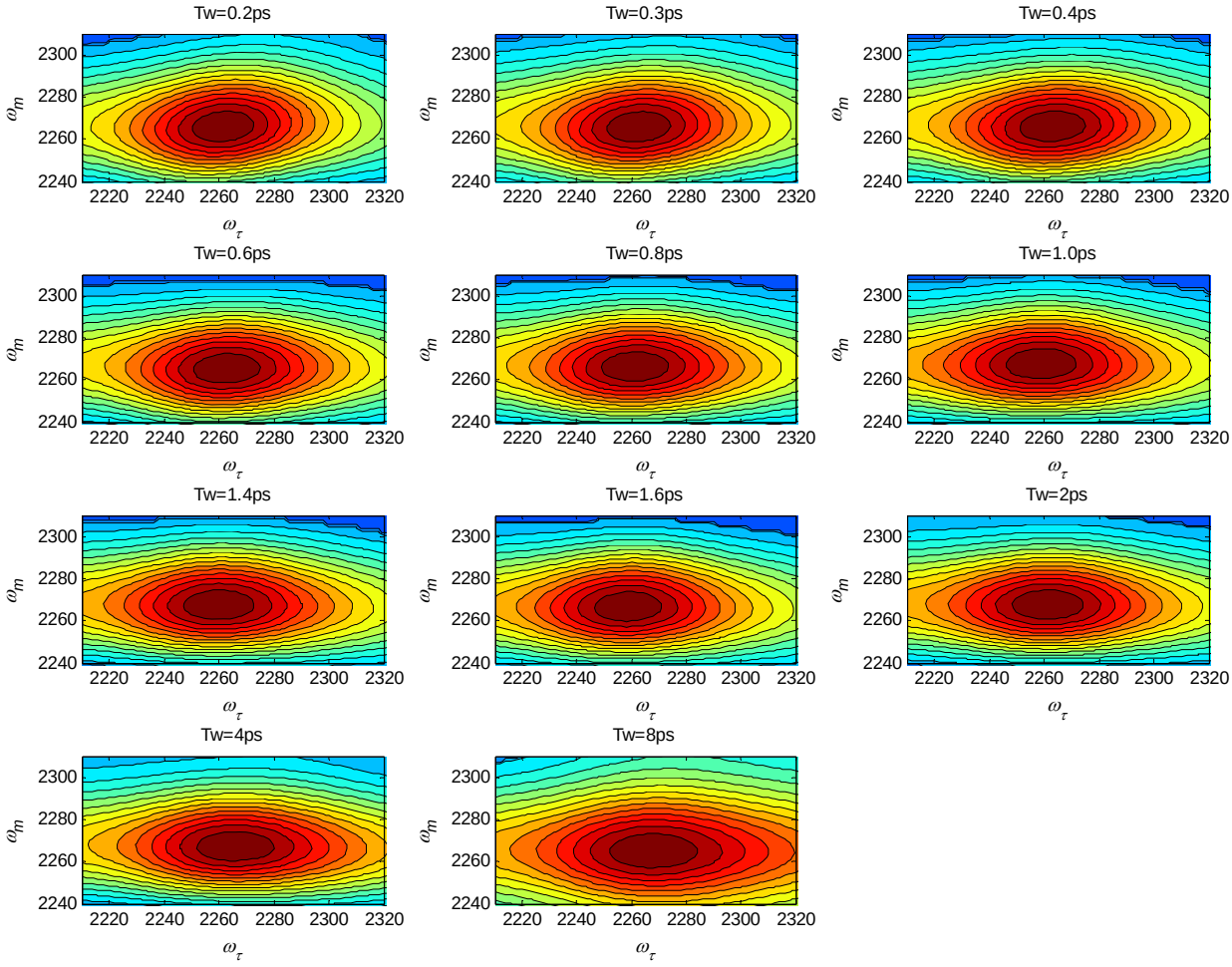

Figure S4 shows the 2D-IR spectra of 1M NaOH in a 5% HOD in H_2O solution. Figure S5 shows the 2D-IR spectra of the O-D stretch of 8:1 H_2O:$NaBH_4$ in pH 14 solution at a series of Tws. Note that the fairly elongated along the diagonal and compared to the NaOH spectra appears to have a second, blue-shifted peak along the diagonal which is lower in intensity. This smaller second peak consists of the borohydride-associated O-D's and is what we want to isolate utilizing subtraction. The subtracted spectra are shown in Figure S6.

Figure S4

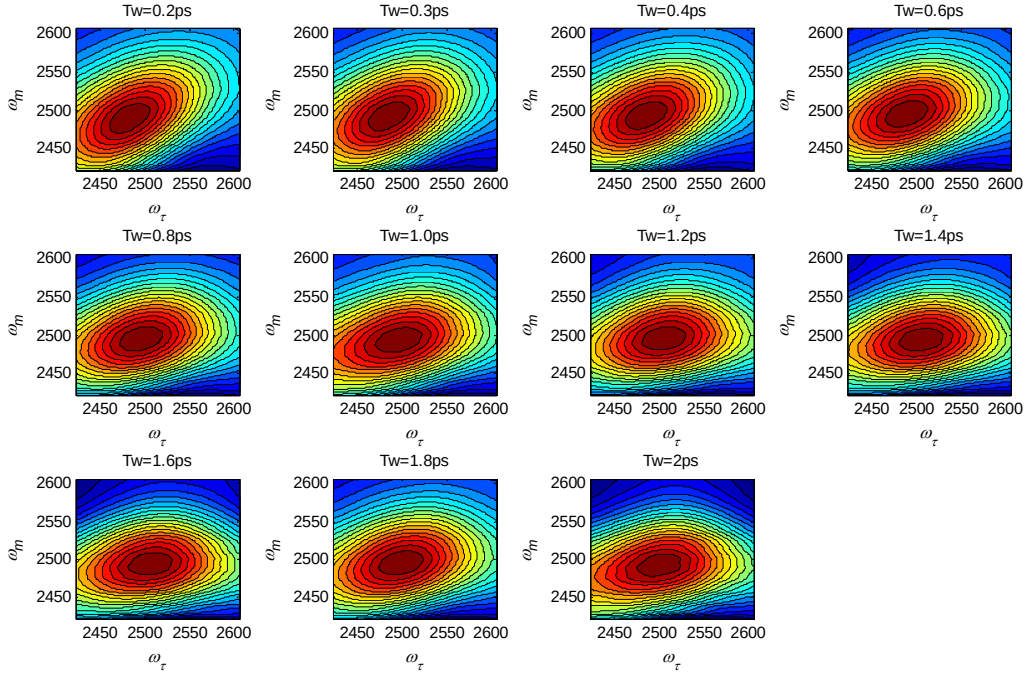

Figure S5

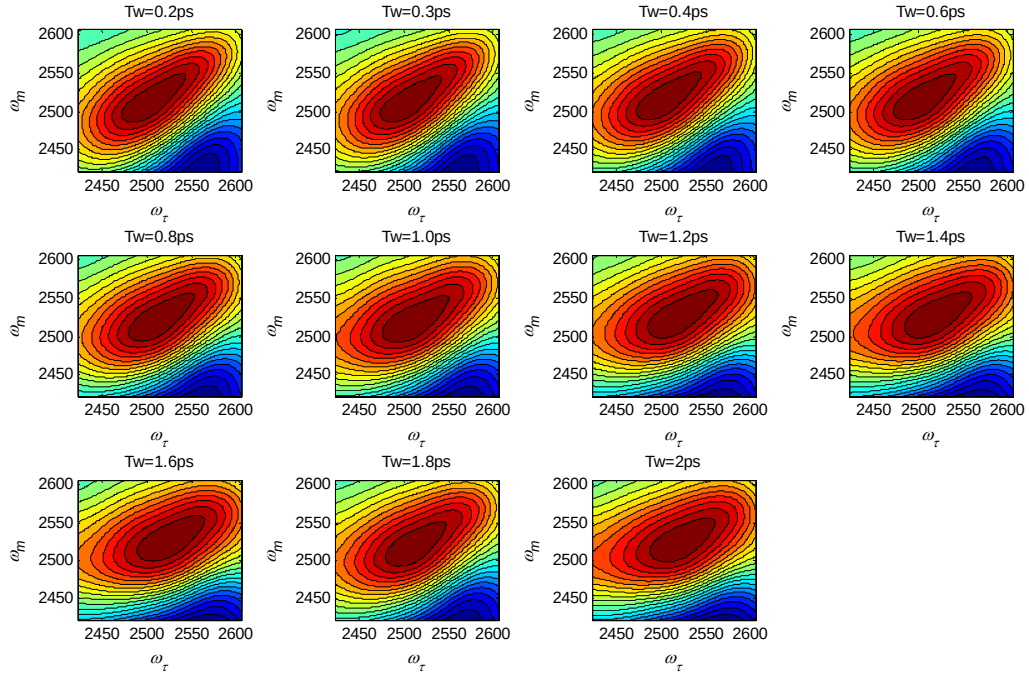

Figure S6