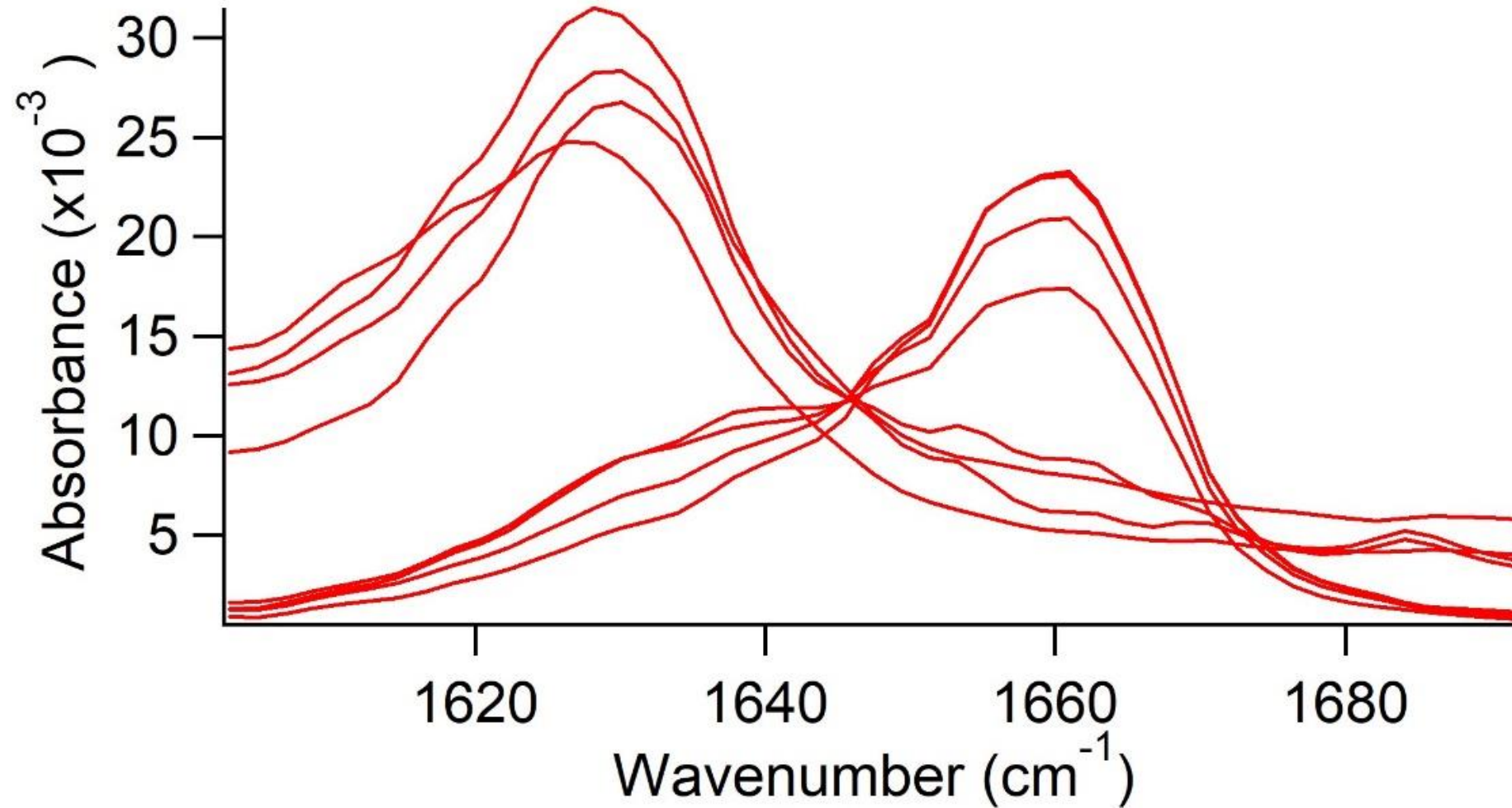


SVD fitting of FTIR data

Raw data plotted from 1600 to 1700  $\text{cm}^{-1}$



# SVD Background

Starting with a truncated data matrix that permits us to use the functional region of the spectrum that shows the effect of hydrogen bonding. SVD components do not always have a physical interpretation, but in fairly simple cases we can make sense of the data using these components.

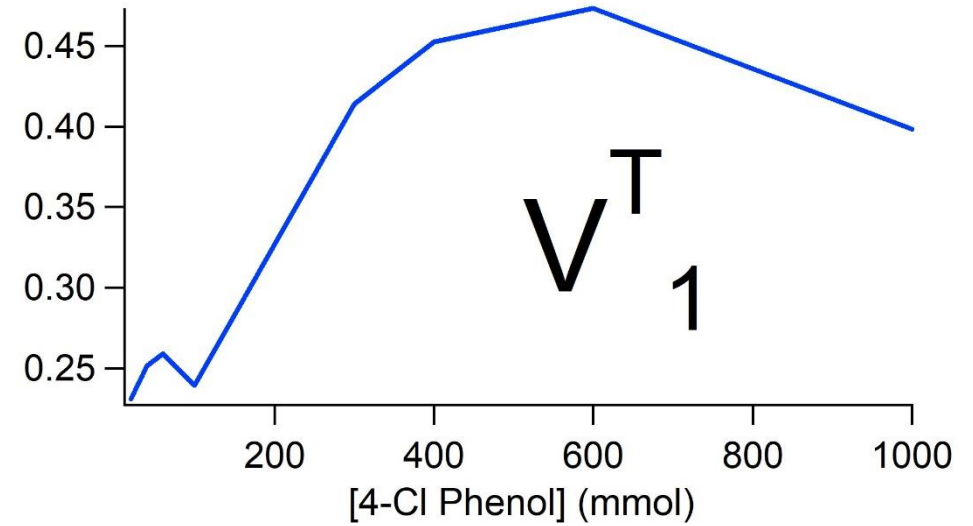
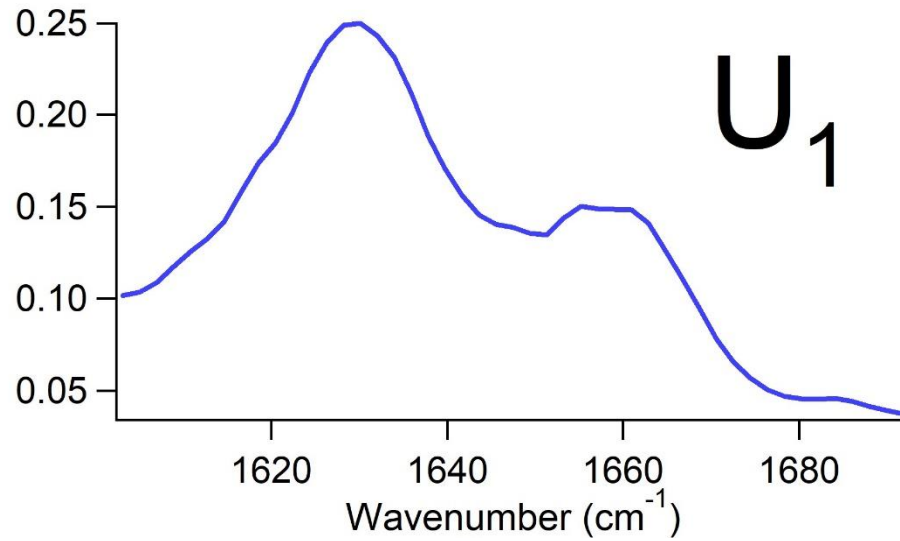
The first component is always the grand mean, the mean of all spectra.

The second component is a difference mean. This is the component that primarily corresponds to formation a hydrogen bond.

The third SVD component corresponds to a shift in the hydrogen-bonded band.

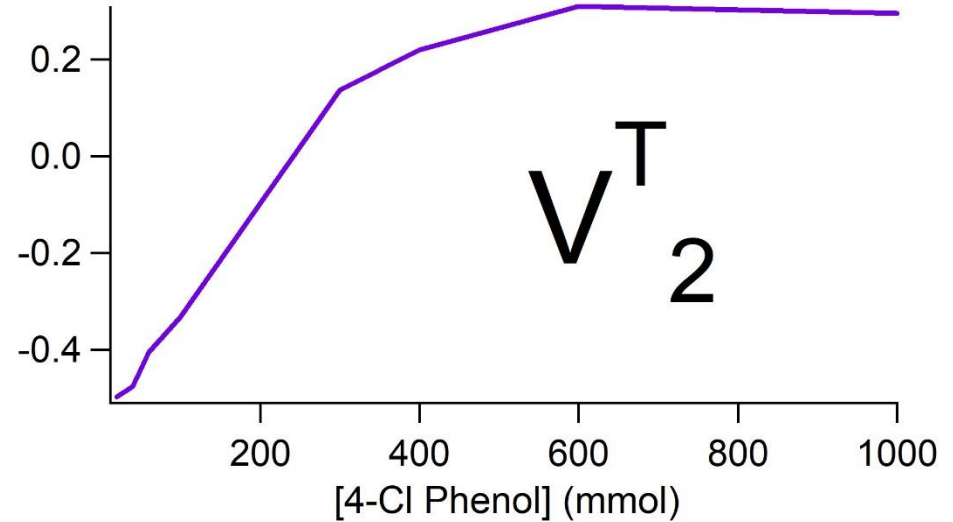
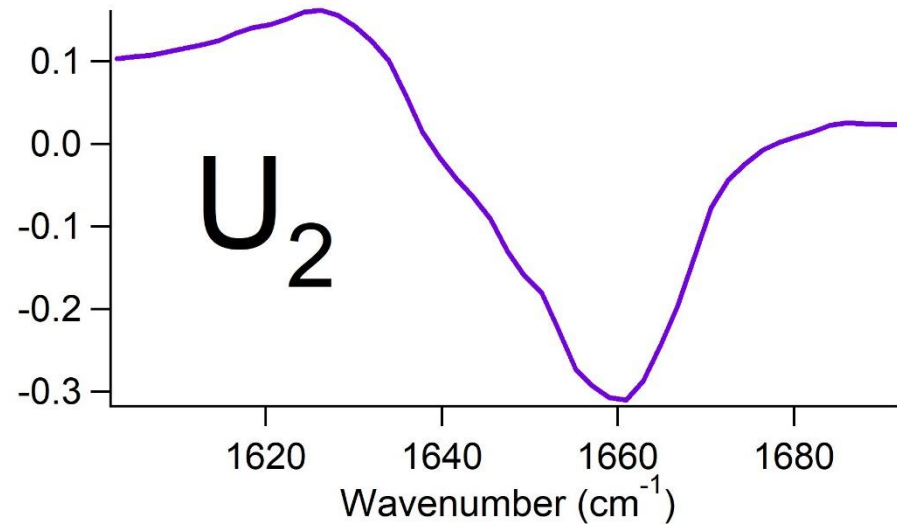
This may arise because of increased synergy of phenols binding to both lone pairs or other effects that strengthen the hydrogen bond.

## First SVD component (grand mean)



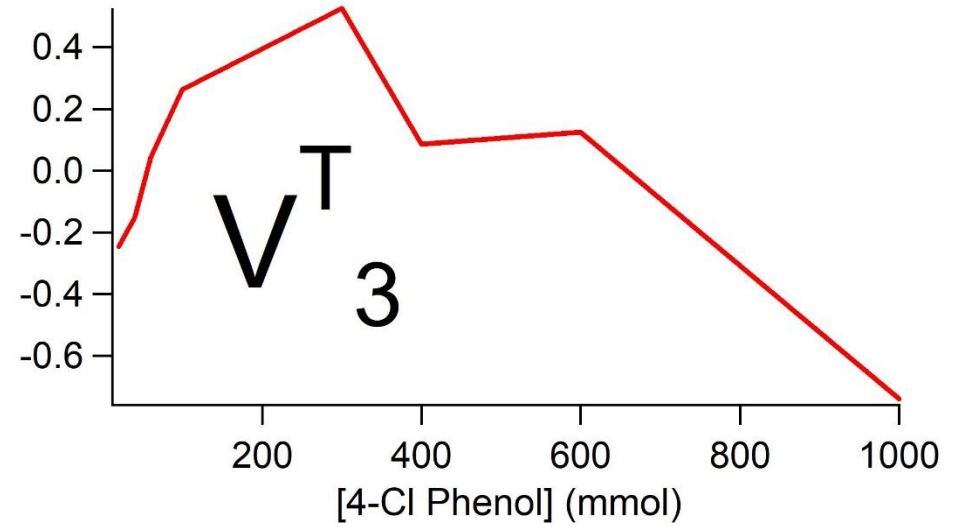
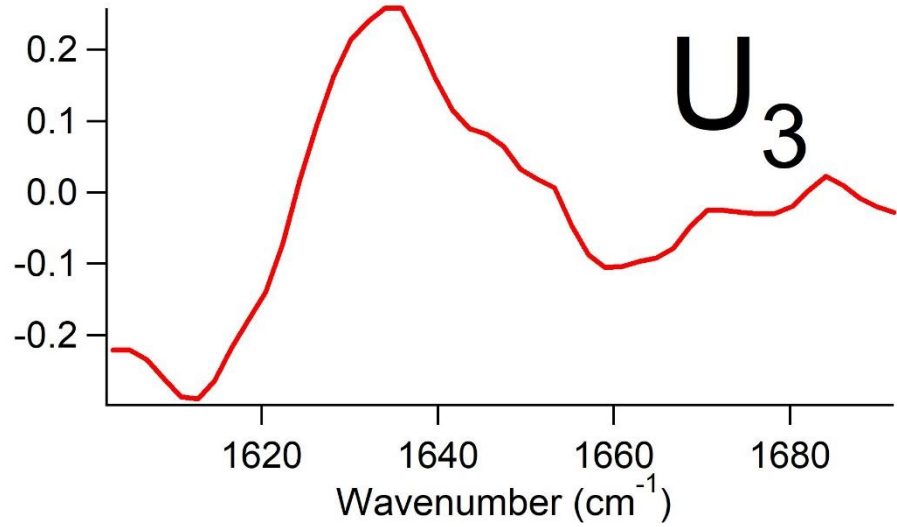
In these spectra the dependence of the transpose matrix is not easy to interpret.

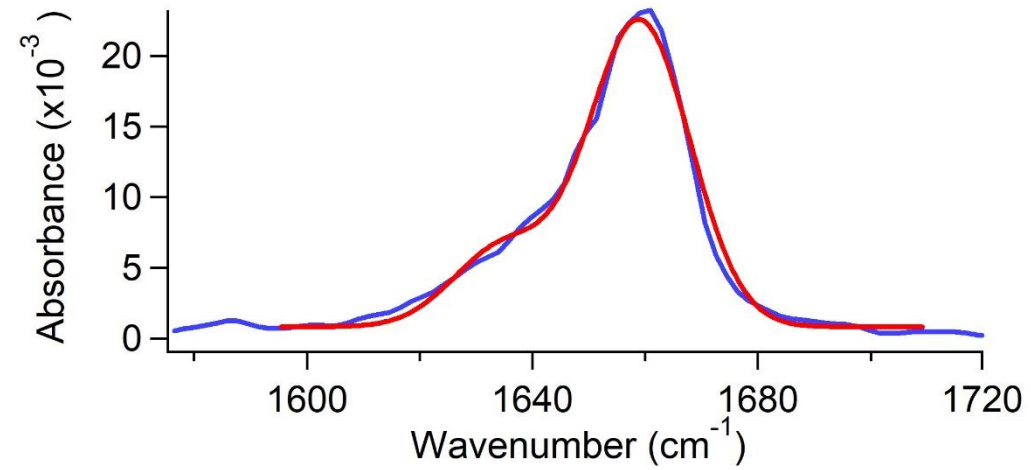
## Second SVD component (difference mean)



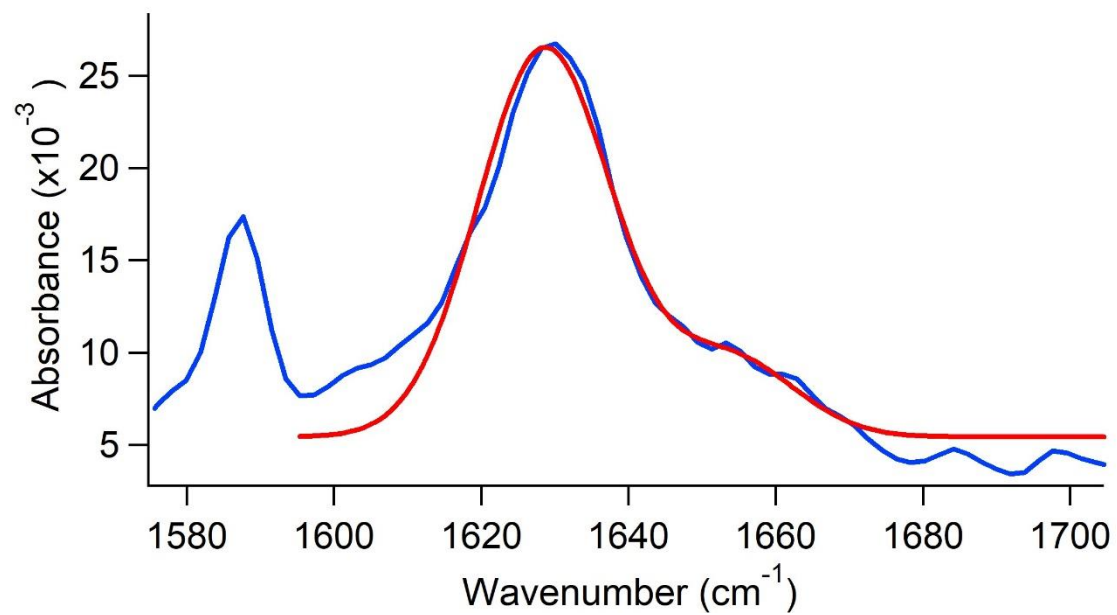
In this component we clearly see the decrease of the high wavenumber component and the increase of the low wavenumber component. The  $V_2^T$  trajectory has the appearance of a binding curve. It can be fit to a model for a binding curve to obtain the dissociation constant.

# Third SVD component (second difference mean)





w\_0 =  $0.48844 \pm 0.00615$   
w\_1 =  $1659 \pm 0$   
w\_2 =  $9 \pm 0$   
w\_3 =  $0.12775 \pm 0.00615$   
w\_4 =  $1635 \pm 0$   
w\_5 =  $9 \pm 0$   
w\_6 =  $0.00079766 \pm 0.000117$



w\_0 = 0.097397 ± 0.0154  
w\_1 = 1653.5 ± 1.88  
w\_2 = 9 ± 0  
w\_3 = 0.47441 ± 0.0154  
w\_4 = 1628.6 ± 0.386  
w\_5 = 9 ± 0  
w\_6 = 0.0054271 ± 0.000283