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## Two-dimensional infrared spectroscopy of antiparallel beta-sheet secondary structure

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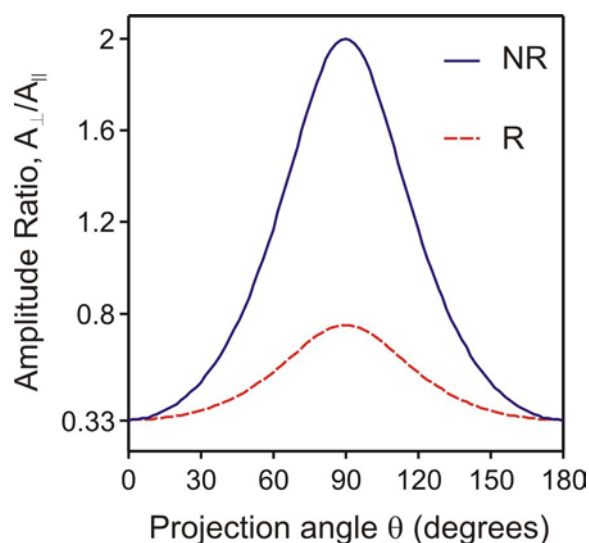
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## SUPPORTING INFORMATION

### Two-Dimensional Infrared Spectroscopy of Antiparallel $\beta$ -Sheet Secondary Structure

Nurettin Demirdöven, Christopher M. Cheatum, Hoi Sung Chung,  
Munira Khalil, Jasper Knoester and Andrei Tokmakoff

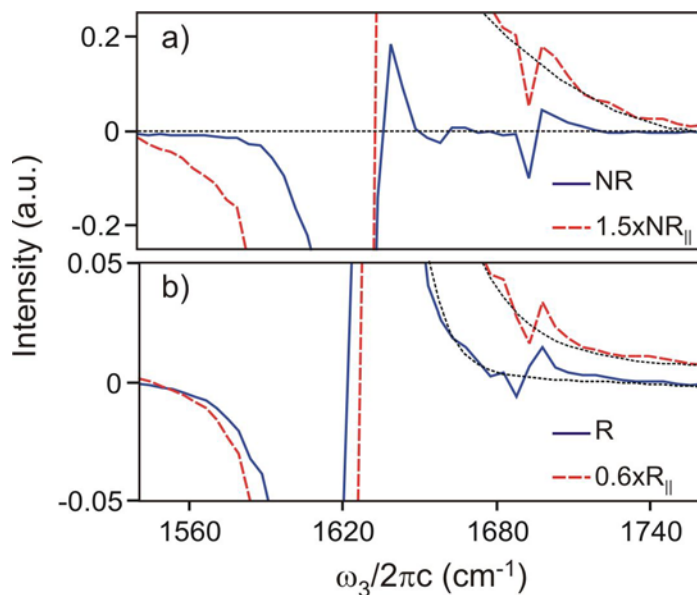
**Projection angle between modes  $\alpha^-$  and  $\alpha^+$  for Con A.** Our determination of the projection angle between the  $\alpha^-$  and  $\alpha^+$  transition dipole moments in Con A used the relative amplitude ratios of the cross peaks centered at  $(\omega_1, \omega_3)=(1630, 1698)$   $\text{cm}^{-1}$ . This cross peak shows relatively minor interference effects with diagonal features, whereas the other ( $\omega_1 > \omega_3$ ) cross peak interferes strongly with the  $\alpha^-$  diagonal peak. The cross-peak amplitude ratio between the parallel (ZZZZ) and perpendicular (ZZYY) spectra are compared separately for slices through the constituent rephasing (R) and nonrephasing (NR) spectra.<sup>1</sup> The dependence of the cross peak amplitude ratio  $A_{\perp}/A_{\parallel}$  on  $\theta$  is calculated as described in Ref. 1, and is given in Figure 1S.



**Figure 1S.** Cross-peak amplitude ratios  $A_{\perp}/A_{\parallel}$  as a function of the projection angle between two coupled vibrations for nonrephasing (NR, solid lines) and rephasing (R, dashed line) spectra.

Figure 2S shows two pairs of slices at  $\omega_1=1630$   $\text{cm}^{-1}$  taken from perpendicular and parallel nonrephasing and rephasing spectra of Con A. The ratio of the cross peak amplitudes,  $A_{\perp}/A_{\parallel} = 1.5 \pm 0.1$  for nonrephasing spectra (Fig. 1S.a) and  $A_{\perp}/A_{\parallel} = 0.6 \pm 0.05$  for rephasing spectra after correcting for interference with the sloping background signal. These values correspond to a projection angle of  $69^{\circ} \pm 4^{\circ}$  and  $65^{\circ} \pm 5^{\circ}$ , respectively. We therefore report an average value of  $67^{\circ} \pm 7^{\circ}$ . Note that errors in the determination of the

relative amplitudes reflect variation in baseline subtraction, experimental noise and phasing of the 2D spectrum.



**Figure 2S.** Anisotropy measurements used in the determination of the projection angle between modes  $\alpha^-$  and  $\alpha^+$  for Con A. Vertical slices corresponding to  $\omega_1=1630$  cm<sup>-1</sup> taken from perpendicular (solid blue lines) and parallel (dashed red line) polarized spectra. Nonrephasing (NR) spectra in (a) and rephasing spectra (R) in (b). Cross peak interfere with a sloping baseline (short dashed lines), which are subtracted prior to determination of the relative amplitudes. Note that the parallel slices in (a) and (b) are offset by a constant with respect to the perpendicular slices.

## REFERENCES

1. M. Khalil, N. Demirdöven, and A. Tokmakoff, *J. Phys. Chem. A* **107** (27), 5258 (2003).