Fermi Resonance as a Means to Determine the Hydrogen-Bonding Status of Two Infrared Probes

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Supporting Information

Figure S1. Normalized FTIR spectra of CP in the carbonyl stretching frequency region obtained in different solvents, as indicated.
**Figure S2.** 2D IR spectrum of the carbonyl stretching mode of CP in isopropanol at $T = 250$ fs. The appearance of off-diagonal peaks at this waiting time is indicative of coupled modes and supports the assignment of Fermi resonance.
Figure S3. Normalized FTIR spectra of 4-CI in the nitrile stretching frequency region obtained in different solvents, as indicated.
Figure S4. Dependence of the Fermi resonance coupling strength $W$ for 4-CI on the dielectric constant $\varepsilon$ of the aprotic solvents used in the current study.

Figure S5. Normalized FTIR spectra of 4-CI in low frequency region obtained in dichloromethane and cyclopentanone, as indicated.
Figure S6. Normalized FTIR spectra of 4-CI in methanol (MeOH) and ND-4-CI in deuterated methanol (MeOD), as indicated. The shoulders in the ND-4-CI spectrum likely arise from 4-CI, due to incomplete H/D exchange.