Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

Jeffrey M. Rodgers, Rachel M. Abaskharon, Bei Ding, Jianxin Chen, Wenkai Zhang, Feng Gai**

Supporting Information

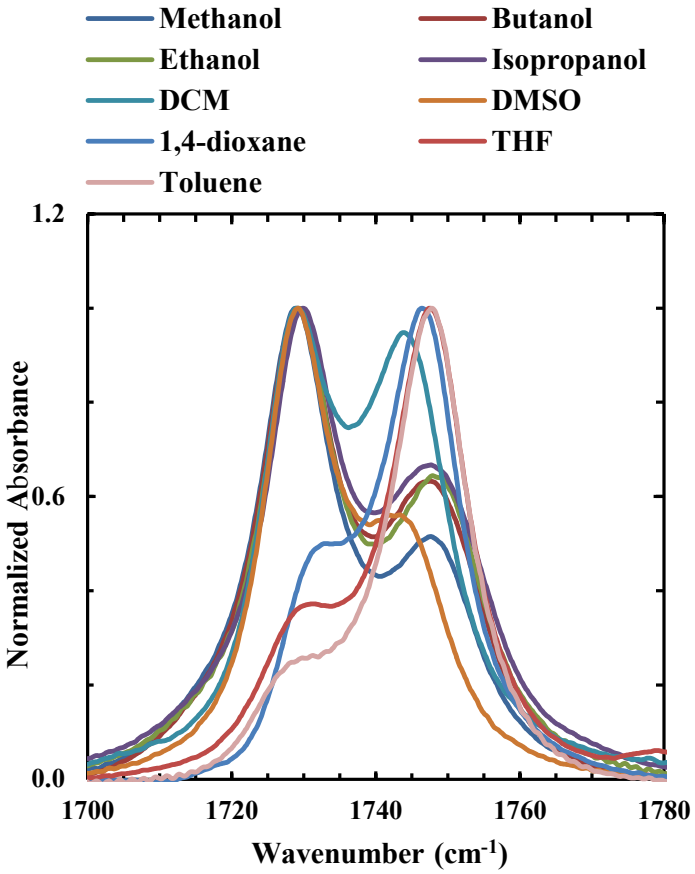

Figure S1. Normalized FTIR spectra of CP in the carbonyl stretching frequency region obtained in different solvents, as indicated.

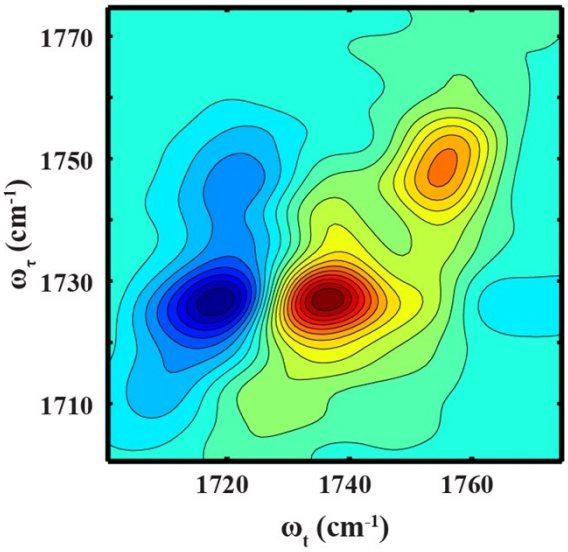

Figure S2. 2D IR spectrum of the carbonyl stretching mode of CP in isopropanol at T = 250 fs. The appearance of off-diagonal peaks at this waiting time is indicative of coupled modes and supports the assignment of Fermi resonance.

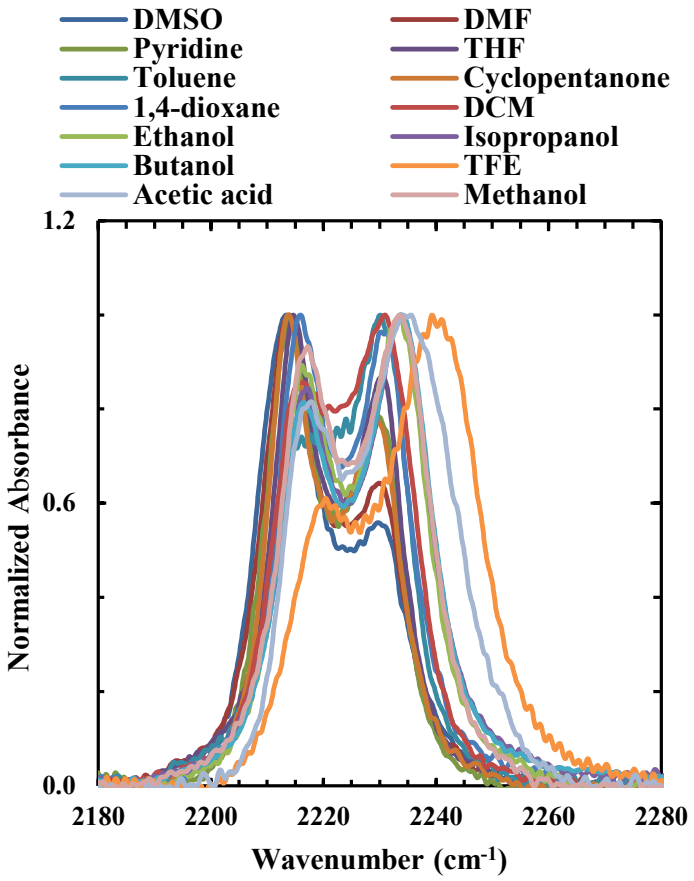

Figure S3. Normalized FTIR spectra of 4-CI in the nitrile stretching frequency region obtained in different solvents, as indicated.

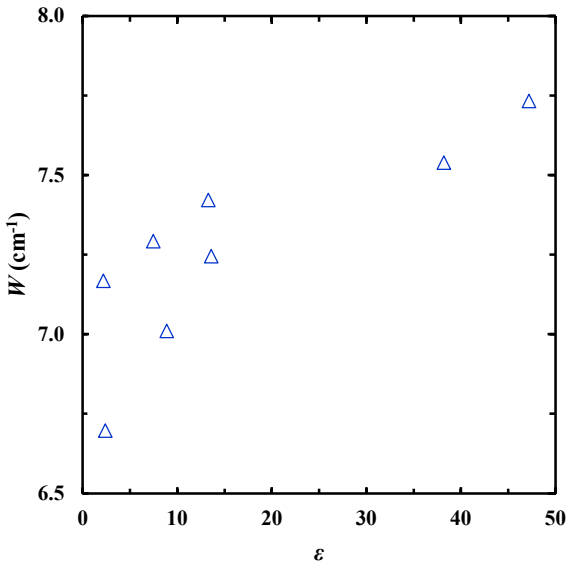

Figure S4. Dependence of the Fermi resonance coupling strength *W* for 4-CI on the dielectric constant ε of the aprotic solvents used in the current study.

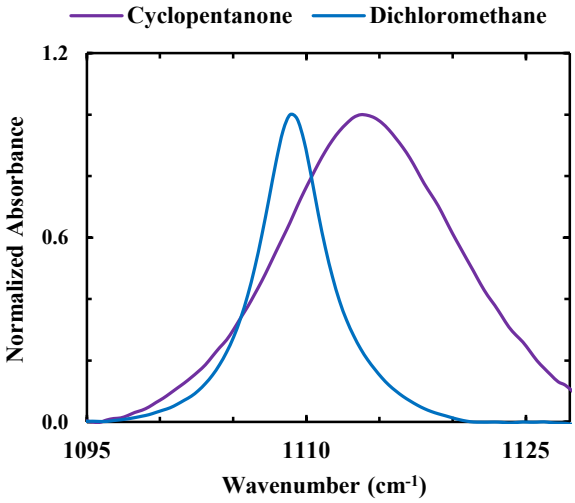

Figure S5. Normalized FTIR spectra of 4-CI in low frequency region obtained in dichloromethane and cyclopentanone, as indicated.

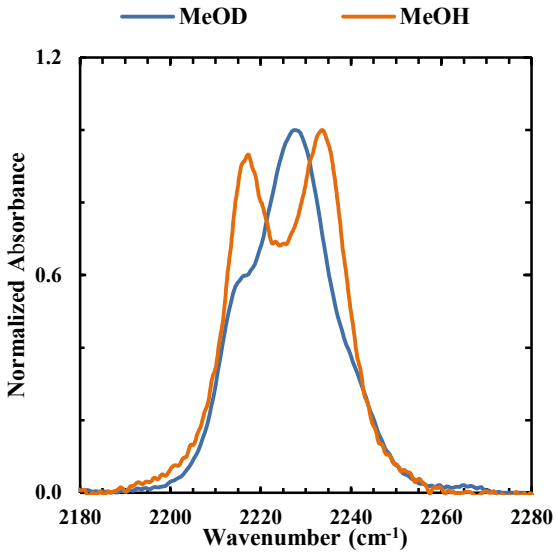

Figure S6. Normalized FTIR spectra of 4-CI in methanol (MeOH) and ND-4-CI in deuterated methanol (MeOD), as indicated. The shoulders in the ND-4-CI spectrum likely arise from 4-CI, due to incomplete H/D exchange.