Supporting Information

Vibrational Coupling on Stepwise Hydrogen Bond Formation of Amide I

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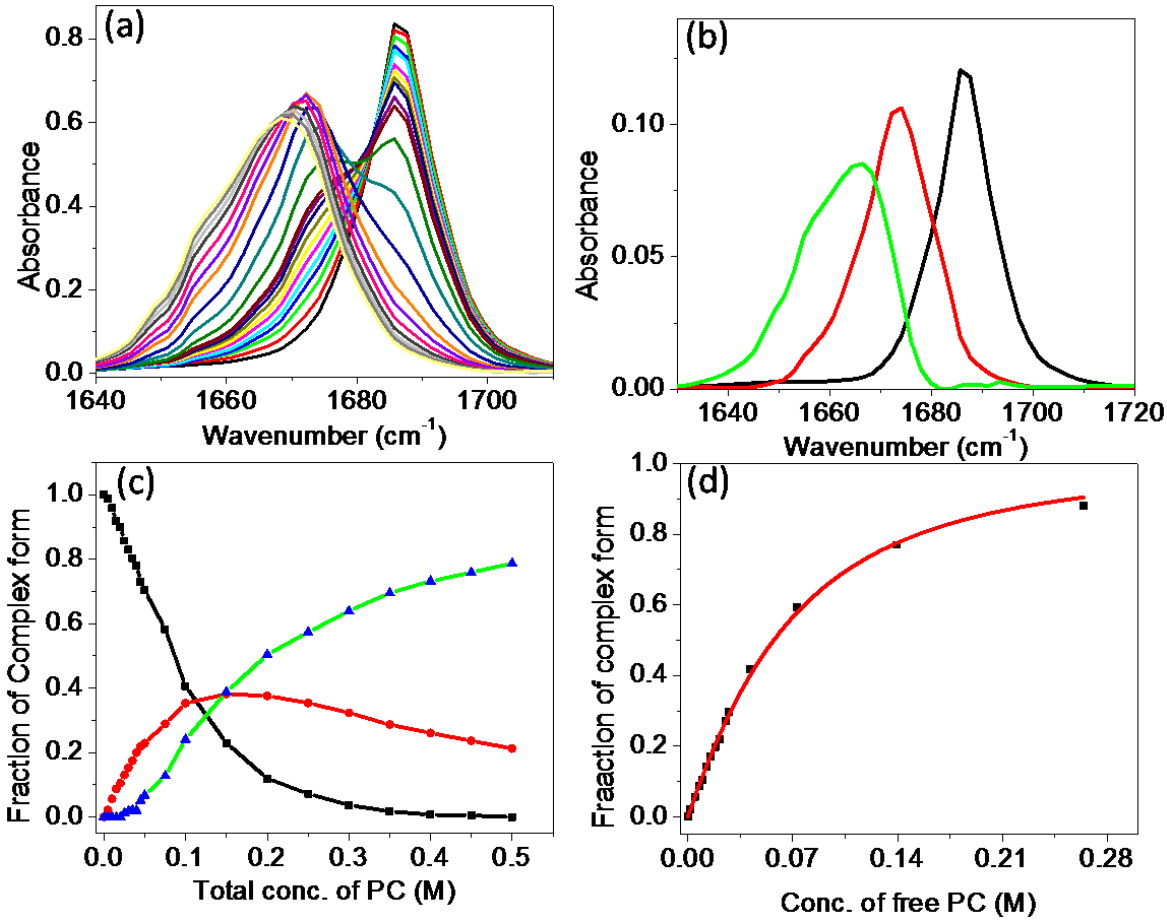

Figure S1: (a) IR absorption spectra of amide I transition of 0.1M solutions of DMF in carbon tetrachloride with increasing the concentrations of PC (0.000 M-black, 0.005 M-red, 0.010 M-green, 0.015 M-blue, 0.020 M-cyan, 0.025 M-magenta, 0.030 M-yellow, 0.035 M-dark yellow, 0.040 M-Navy, 0.045 M-purple, 0.050 M-wine, 0.0750 M-olive, 0.100 M-dark cyan, 0.15 M-royal, 0.20 M-orange, 0.25 M-violet, 0.30 M-pink, 0.35 M-dark gray, 0.40 M-L T gray, 0.45 M-gray, 0.50 M-L T yellow) (b) Individual line shapes of 0hb (black), 1hb (red), and 2hb (green) conformations of DMF. (c) The relative population of different H-bonded conformations for various concentrations of PC. The color code is the same as in (b). (d) The relative fraction of the H-bonded DMF plotted for various concentrations of free CP hydroxyl groups. The solid line shows a fit to the binding isotherm.

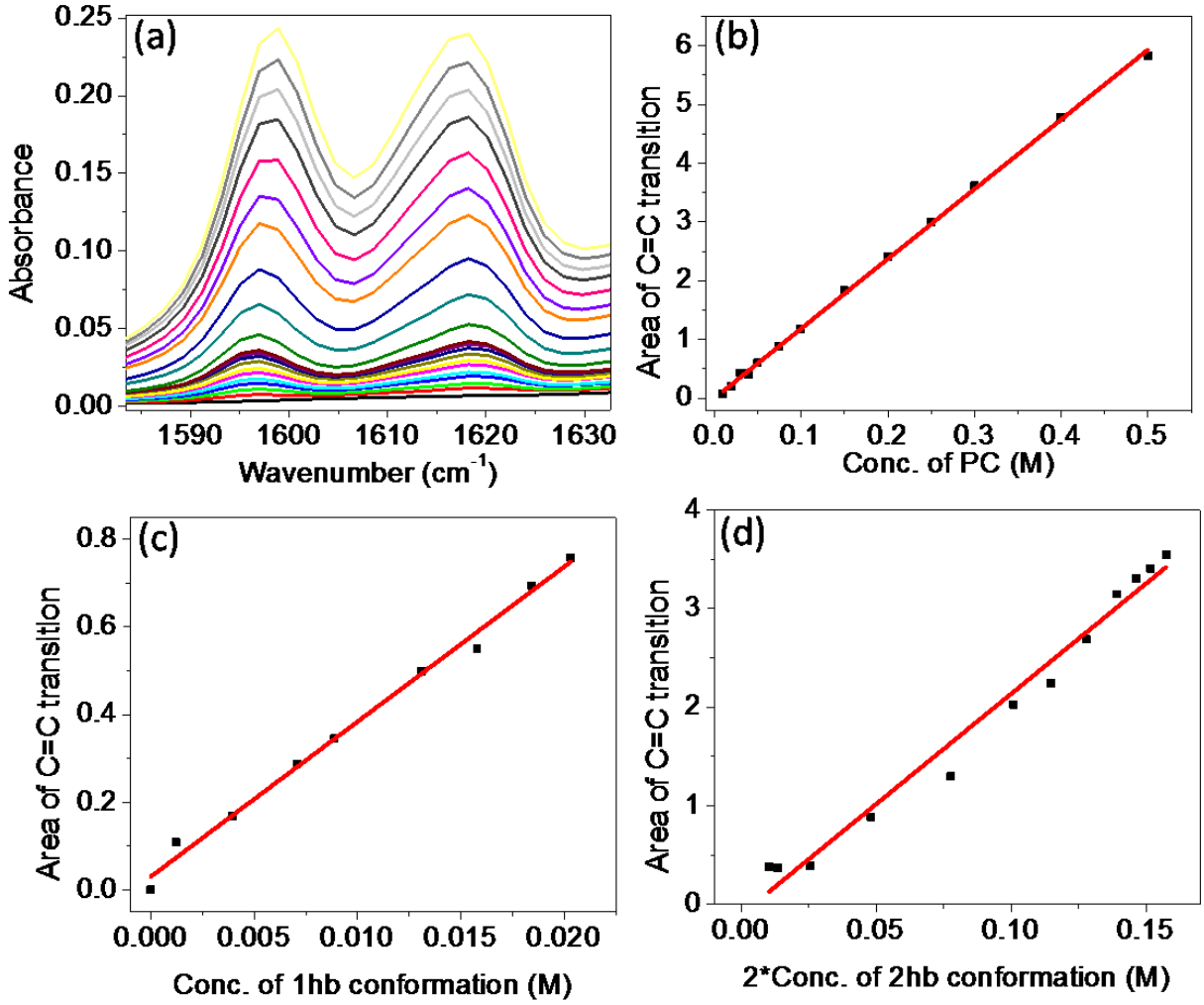

Figure S2: (a) Linear IR spectra of C=C transition of PC in different concentration (0.000 M-black, 0.005 M-red, 0.010 M-green, 0.015 M-blue, 0.020 M-cyan, 0.025 M-magenta, 0.030 M-yellow, 0.035 M-dark yellow, 0.040 M-Navy, 0.045 M-purple, 0.050 M-wine, 0.0750 M-olive, 0.100 M-dark cyan, 0.15 M-royal, 0.20 M-orange, 0.25 M-violet, 0.30 M-pink, 0.35 M-dark gray, 0.40 M-L T gray, 0.45 M-gray, 0.50 M-L T yellow) in presence of 0.1 M DMF (b) Plot of C=C IR absorbance area vs concentration of free PC (c) C=C IR absorbance area vs concentration of 1hb conformation (d) C=C IR absorbance area vs 2*concentration of 2hb conformation.

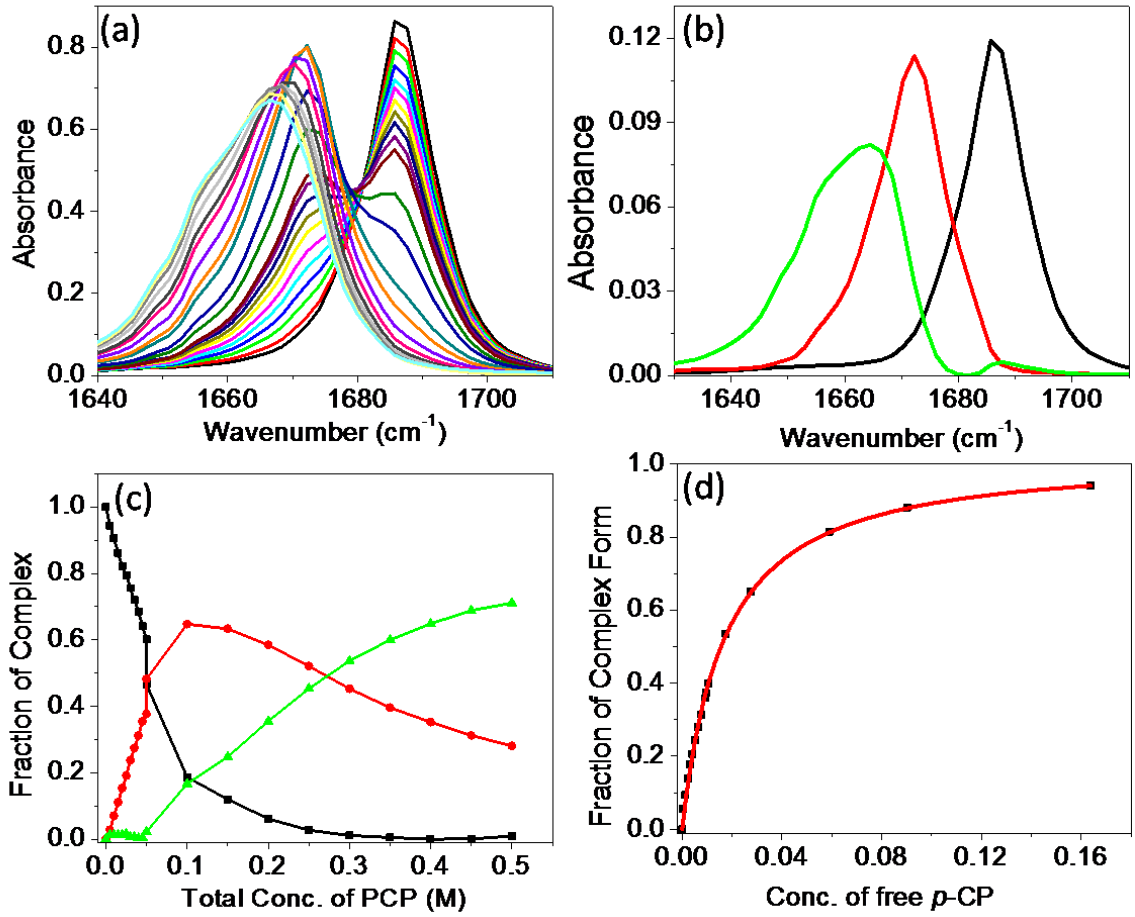

Figure S3: (a) Infrared absorption spectra of amide I transition of 0.1M solutions of DMF in carbon tetrachloride with increasing the concentrations of *p*-CP (0.000 M-black, 0.005 M-red, 0.010 M-green, 0.015 M-blue, 0.020 M-cyan, 0.025 M-magenta, 0.030 M-yellow, 0.035 M-dark yellow, 0.040 M-Navy, 0.045 M-purple, 0.050 M-wine, 0.0750 M-olive, 0.100 M-dark cyan, 0.125 M-royal, 0.15 M-orange, 0.20 M-violet, 0.25 M-pink, 0.30 M-dark gray, 0.35 M-L T gray, 0.40 M-gray, 0.45 M-L T yellow, 0.50 M-L T cyan) (b) Individual line shapes of 0hb (black), 1hb (red), and 2hb (green) conformations of DMF. (c) The relative population of different H-bonded conformations for various concentrations of *p*-CP. The color code is the same as in (b). (d) The relative fraction of the H-bonded DMF plotted for various concentrations of free *p*-CP hydroxyl groups. The solid line shows a fit to the binding isotherm.

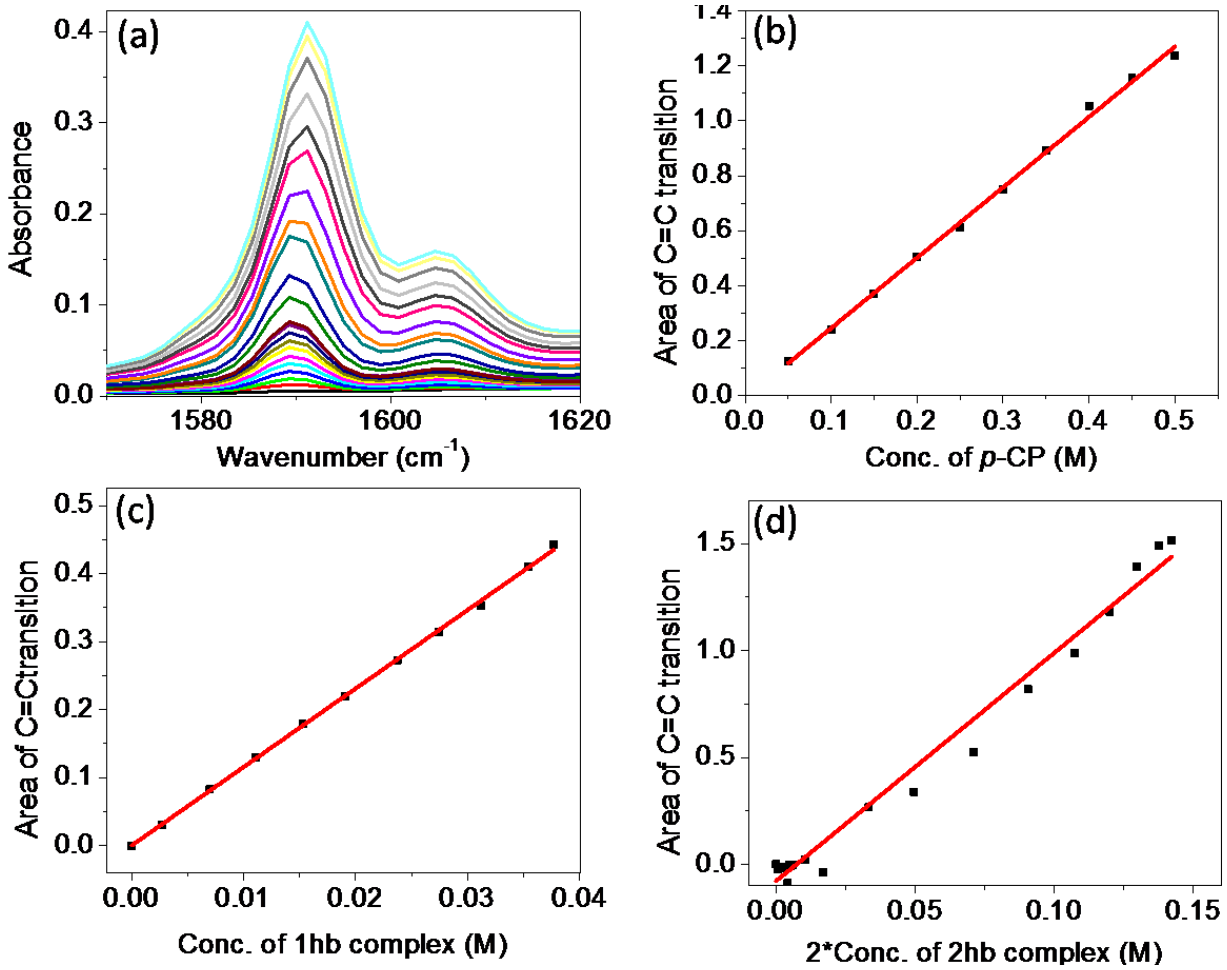

Figure S4: (a) Linear IR spectra of C=C transition of *p*-CP in different concentration (0.000 M-black, 0.005 M-red, 0.010 M-green, 0.015 M-blue, 0.020 M-cyan, 0.025 M-magenta, 0.030 M-yellow, 0.035 M-dark yellow, 0.040 M-Navy, 0.045 M-purple, 0.050 M-wine, 0.0750 M-olive, 0.100 M-dark cyan, 0.125 M-royal, 0.15 M-orange, 0.20 M-violet, 0.25 M-pink, 0.30 M-dark gray, 0.35 M-L T gray, 0.40 M-gray, 0.45 M-L T yellow, 0.50 M-L T cyan) in presence of 0.1 M DMF (b) Plot of C=C IR absorbance area vs concentration of free *p*-CP (c) C=C IR absorbance area vs concentration of 1hb conformation (d) C=C IR absorbance area vs 2*concentration of 2hb conformation.