Supplementary Information

Self Association of Acetic Acid in Dilute Deuterated Chloroform. Wide-Range Spectral Reconstructions and Analysis using FTIR Spectroscopy, BTEM and DFT.

Martin Tjahjono, Shuying Cheng, Chuanzhao Li and Marc Garland*

Institute of Chemical and Engineering Sciences, Agency for Science, Technology and Research (A*STAR), 1 Pesek Road, Jurong Island, Singapore 627833, Singapore

*Corresponding Author. Tel.: (65) 6796-3960; Fax: (65) 6316-6185

Email: martin_tjahjono@ices.a-star.edu

Figure S1. Comparison of BTEM spectral estimate of the monomer to several DFT infrared spectra predicted using B3LYP functional and basis sets (1) 6-31+g (2) 6-31++g (3) 6-31++g(d,p) (4) 6-31++g(2d,2p) (5) 6-311+g (6) 6-311++g (7) 6-311++g(d,p) (8) 6-311++g(2d,2p). Note: All calculations were carried out at room temperature (298.15 K) and IEFPCM method was used to account for the solvent model system (using chloroform as a solvent).

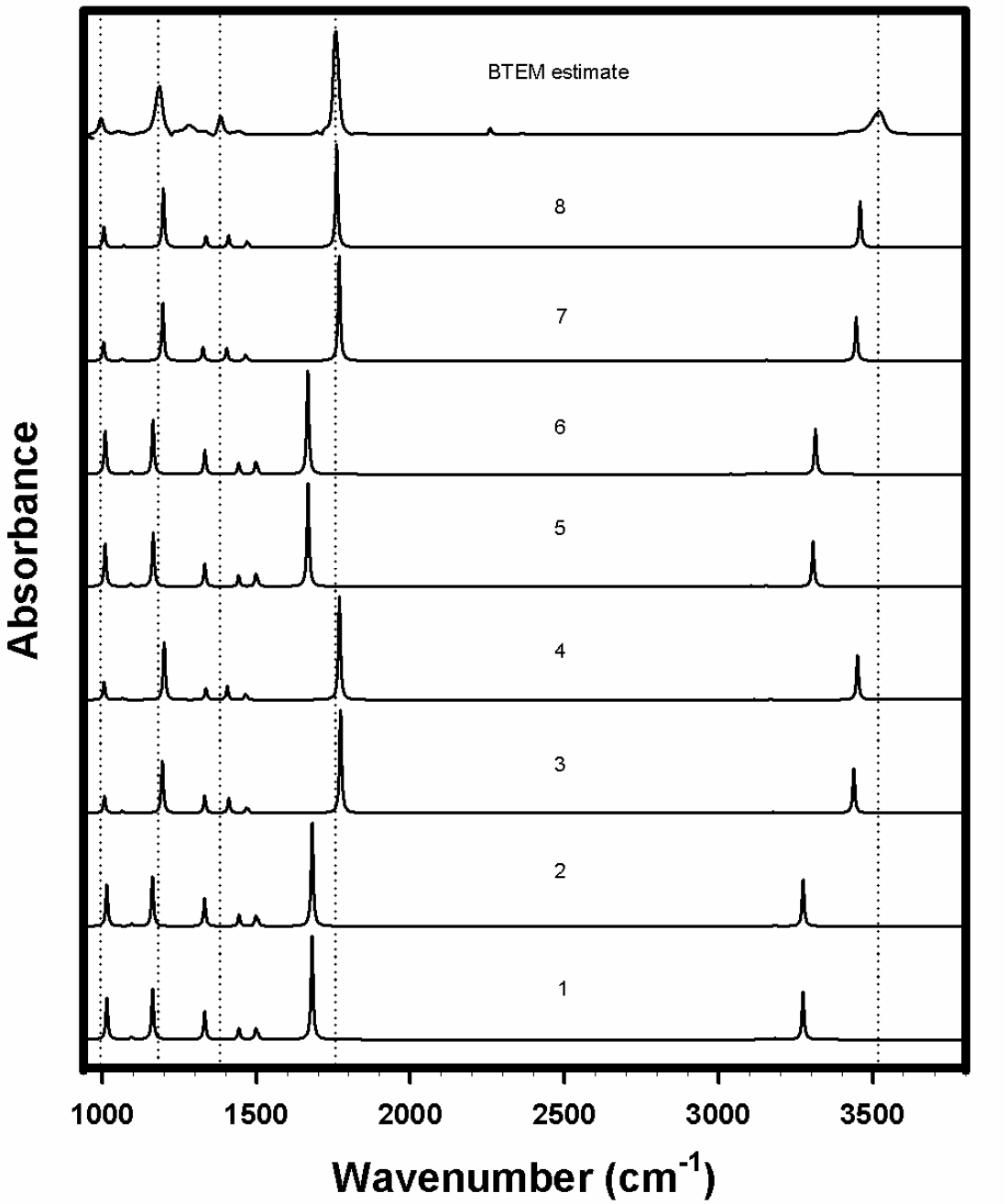


Figure S2. Comparison of BTEM spectral estimate of the cyclic dimer to several DFT infrared spectra predicted using B3LYP functional and basis sets of (1) 6-31+g (2) 6-31++g (3) 6-31++g(d,p) (4) 6-31++g(2d,2p) (5) 6-311+g (6) 6-311++g (7) 6-311++g(d,p) (8) 6-311++g(2d,2p). Note: All calculations were carried out at room temperature (298.15 K) and IEFPCM method was used to account for the solvent model system (using chloroform as a solvent).

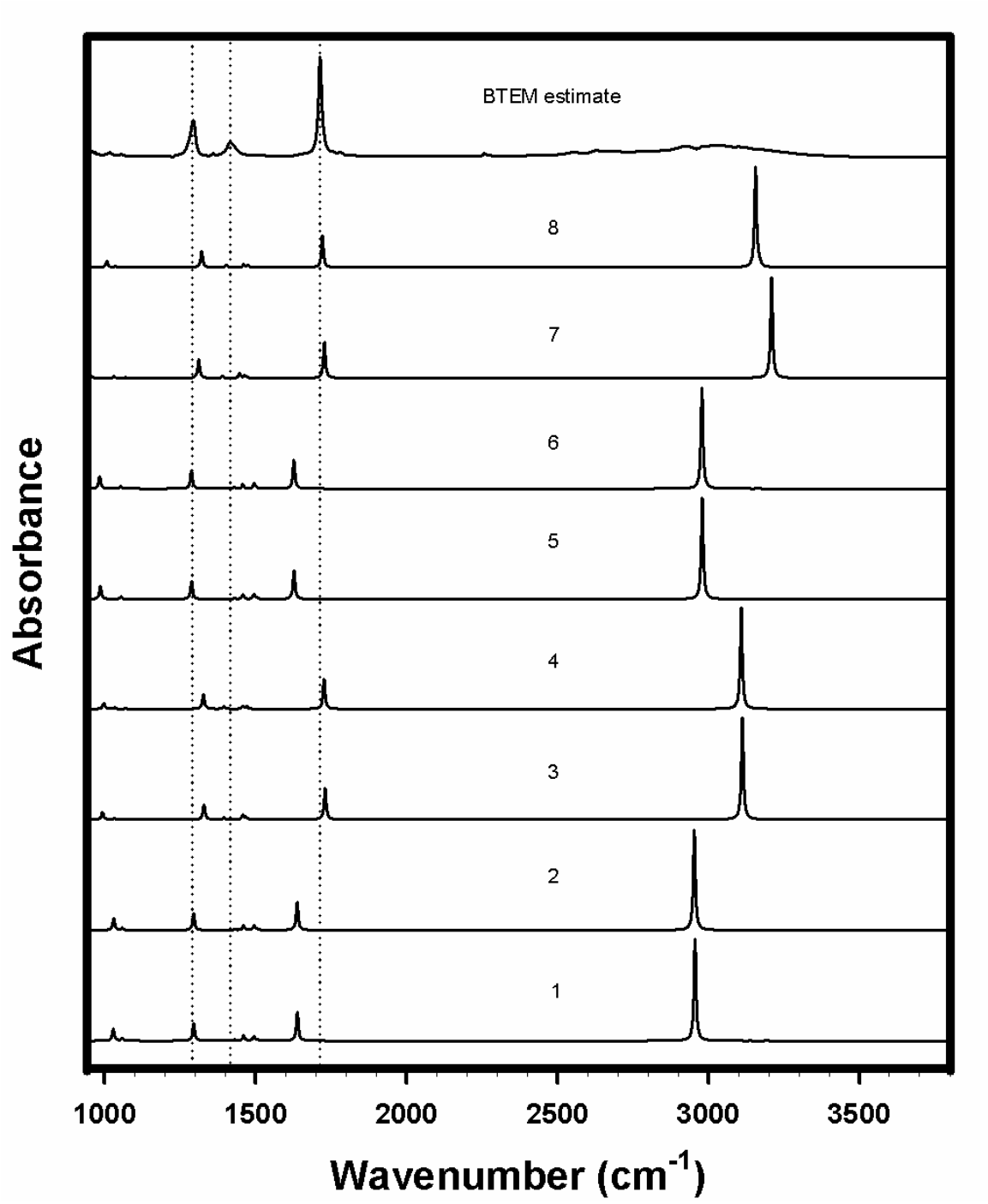
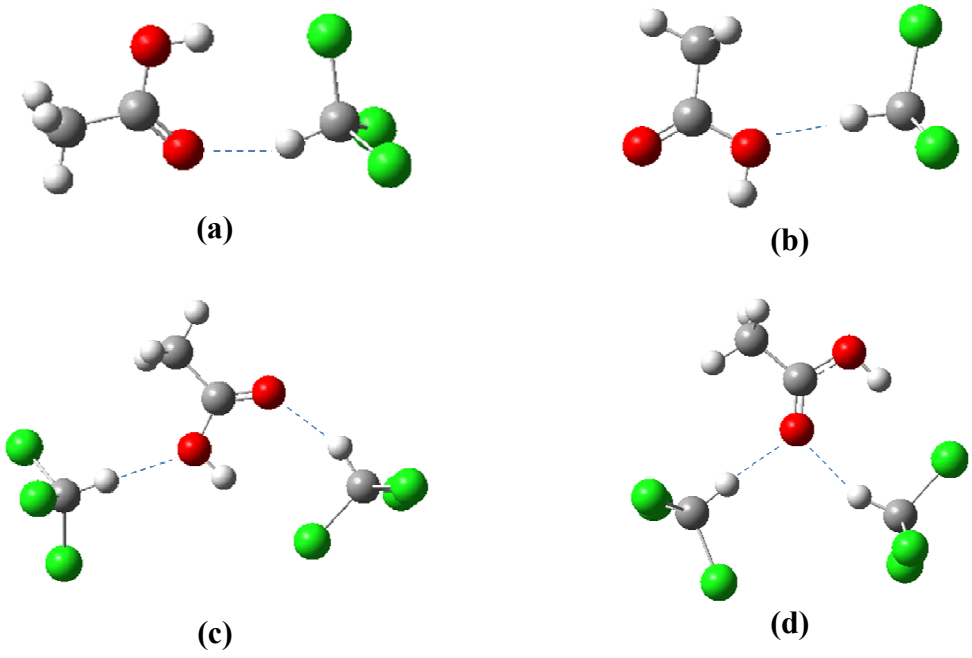
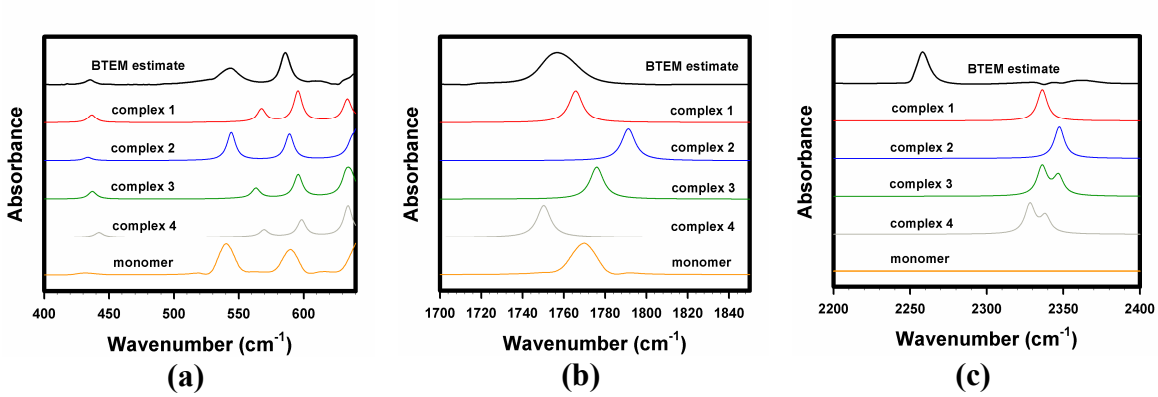


Figure S3. The optimized geometries of several acetic acid monomer-$[CDCl_3]_n$ (n=1 or 2) complexes. (a) complex 1 (b) complex 2 (c) complex 3 and (d) complex 4



(a) **(b)** **(c)** **(d)**

Figure S4. Comparison of BTEM spectral estimate of the acetic acid monomer in $CDCl_3$ to DFT infrared spectra of several acetic acid monomer-$CDCl_3$ complexes (see Figure S3) as well as the pure monomer. Note: DFT spectra are predicted using B3LYP functional and basis sets of 6-311++g(d,p). All calculations were carried out at room temperature (298.15 K) and IEFPCM method was used to account for the solvent model system (using chloroform as a solvent).



Please note that (1) the relative intensities of the low wavenumber vibrations of the monomer are inconsistent with the BTEM spectral estimate and there is no C-D vibration at circa 2250 cm^{-1} (2) the relative intensities of the low wavenumber vibrations of complex 2 are inconsistent with the BTEM spectral estimate and (3) complexes 3 and 4 are entirely inconsistent with the BTEM spectral estimate due to the splitting of the C-D vibration at circa 2340 cm^{-1}.