Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

TO PROBE THE STRUCTURE OF METHANOL AND AEROSOL OT (AOT) IN AOT REVERSE MICELLES BY FTIR MEASUREMENTS

Palash Setua, Debabrata Seth[+] and Nilmoni Sarkar*

Department of Chemistry

Indian Institute of Technology,

Kharagpur 721 302, WB, INDIA.

E-mail : nilmoni@chem.iitkgp.ernet.in; Fax : 91-3222-255303

[+]Indian Institute of Technology Patna, Navin Government Polytechnic Campus Patliputra Colony, Patna 800 013, Bihar, India.

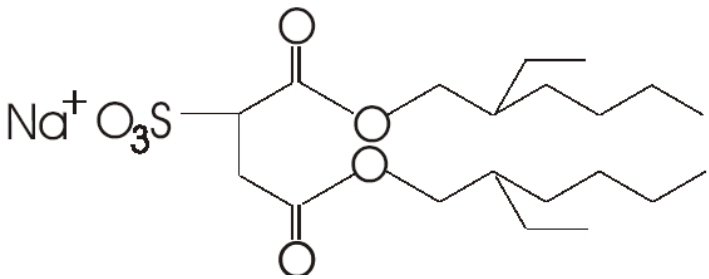

Fig. S1. Structure of AOT molecule.

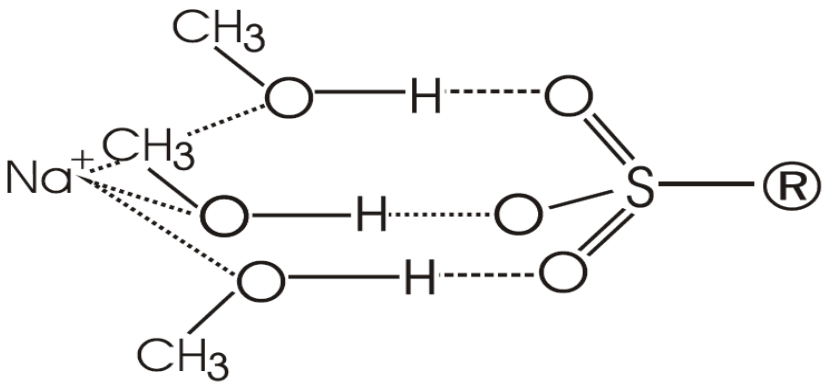

Fig. S2. Hydrogen bonded coordination structure of AOT molecule with Na^+ ion by bridging methanol molecule.

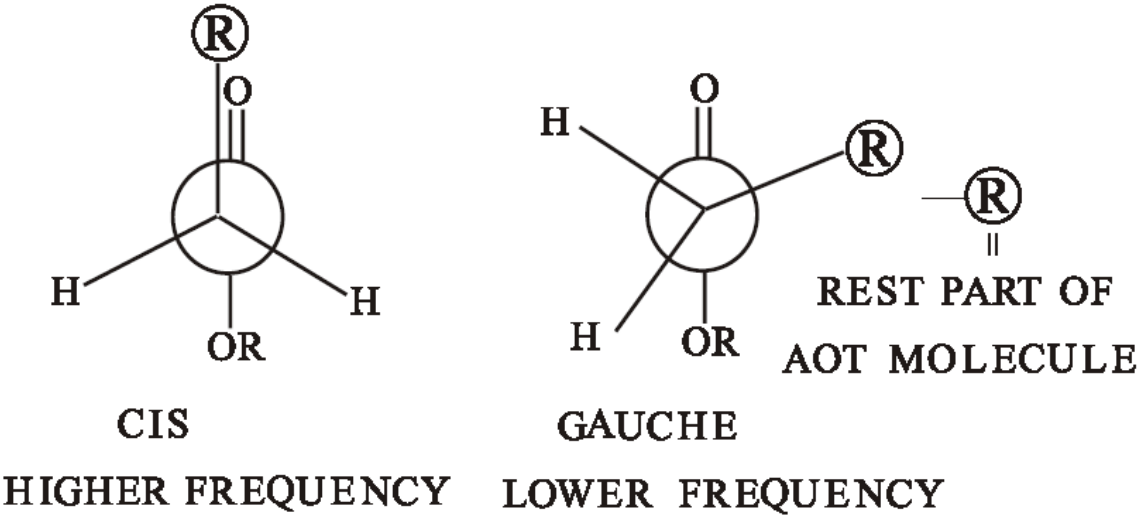

Fig. S3. Different infrared carbonyl stretches for different conformation along C(O)-C bond. Peak around 1718 cm^{-1} for gauche and 1738 cm^{-1} for the cis.

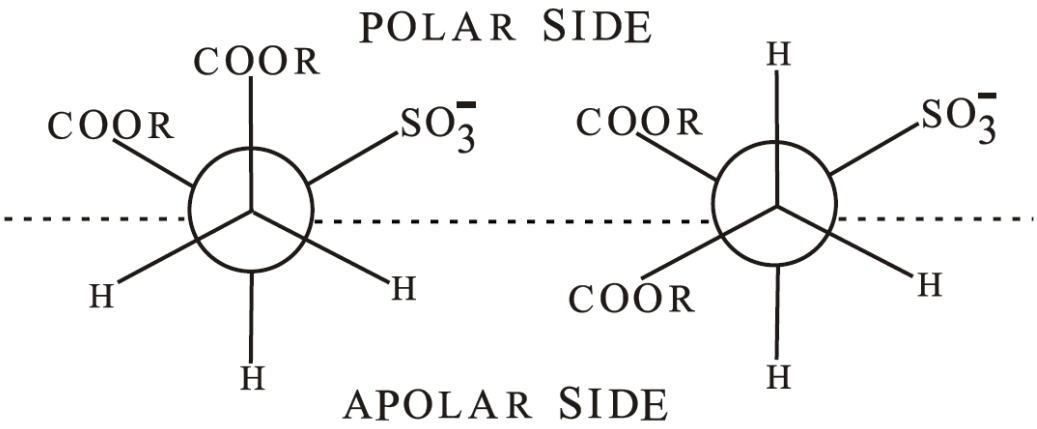

Fig. S4. Different possible stereospecific orientation of the three polar group at polar/apolar interface for different rotamers of AOT. Rotation is considered along the C-C bond of succinic acid skeleton.

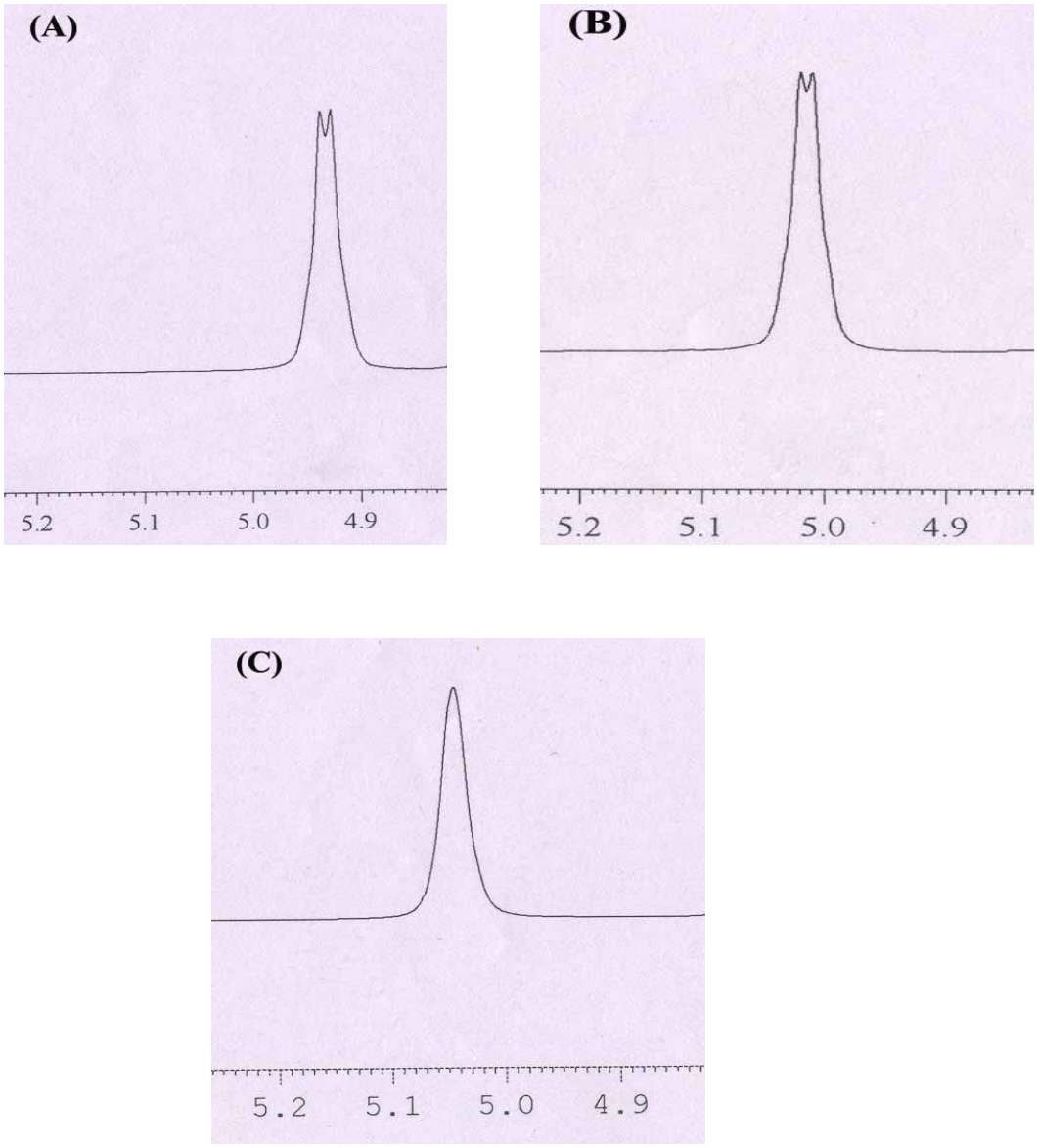

Fig. S5. ^{1}H-NMR spectra of methanol –OH proton in methanol/AOT/n-heptane reverse micellar medium where (A), (B) and (C) represent w=6, w=8 and w=9 respectively.

Peak position is shifting to higher ppm value with increasing w value. Splitting of the peak is observed up to $w \leq 8$. Probable reason for this may be higher percentage of methanol, which remain hydrogen bonded with the sulfonate head group.

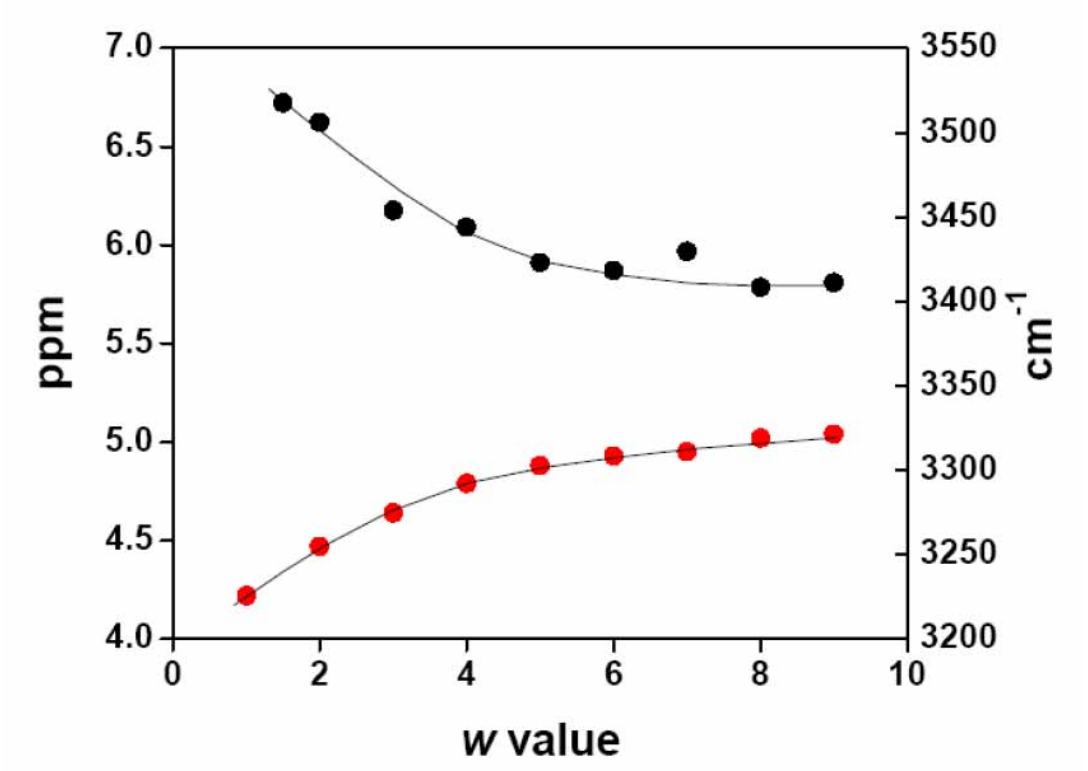

Fig. S6. Variation of O-H stretching frequency of methanol and NMR ppm value of OH proton in methanol/AOT/n-heptane reverse micellar system. Red points indicate the variation of ppm value and black points represent the O-H stretch variation. Black lines are drawn as the reference to eye.

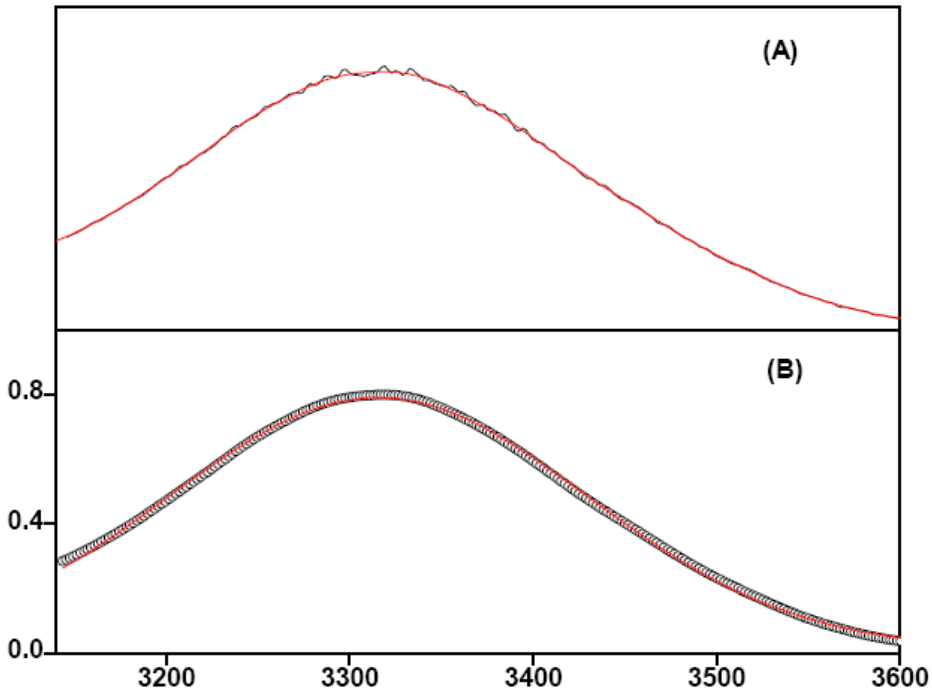

Fig. S7. Infrared spectra of –OH stretching frequency region of pure methanol. (A) Represent the smoothing of the spectra (black-original, red-fitted result) (B) Gaussian curve fitting to the O-H stretch (black circle smoothed spectra, red line single Gaussian curve fitting).

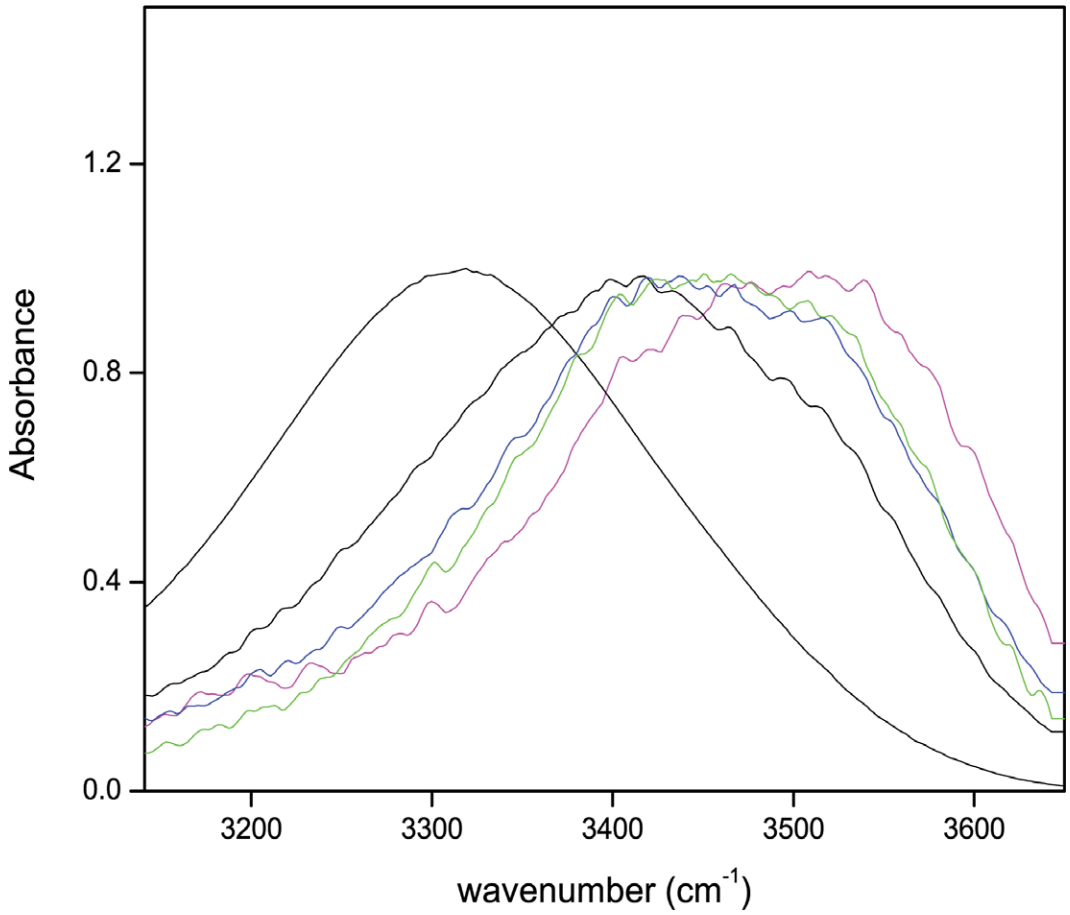

Figure S8. Raw spectra (not smoothed) of O-H stretching band of pure methanol(black) and methanol in methanol/AOT/n-heptane reverse micellar system at different *w* values, *w*=2(magenta), *w*=4(blue), *w*=7(green) and *w*=9(black).