Supporting Information

Can Trimethylamine-N-Oxide Act to Influence the Self-Aggregation of tert-Butyl Alcohol?

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FIG. S1: Water-water site-site radial distribution functions for different systems considered.
FIG. S2: TBA-water and TMAO-water selected site-site radial distribution functions. $CC_{tb}$ and $C_{tb}$ represent central carbon atom and methyl carbon of TBA and $N_{tm}$ and $C_{tm}$ are nitrogen atom and methyl carbon atom of TMAO respectively. $O_w$ refers to water oxygen.
FIG. S3: TBA-TMAO site-site radial distribution functions for different systems considered. O_{tm},
O_{tb} and H_{tb} refer to TMAO oxygen, TBA oxygen and TBA hydroxyl hydrogen respectively.
FIG. S4: TBA-TMAO methyl carbon-methyl carbon (C_{tb}–C_{tm}) site-site radial distribution functions for all systems considered.
FIG. S5: (a) The average number of different types of hydrogen bonds vs. mole fraction of TBA. W, TB, and TM refer to water, TBA, and TMAO and the subscripts D and A represent donor and acceptor respectively. Total$^{TB}$ is the total number of hydrogen bonds formed by a single TBA molecule. (b) The average energy (in kJ/mol of solution) of different types of hydrogen bonds vs. mole fraction of TBA.
FIG. S6: The time dependence of the correlation function $S_{HB}(t)$ of water-water hydrogen bonds for the lowest ($x_{tba} = 0.002$) and for the highest ($x_{tba} = 0.10$) mole fraction of TBA.
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