

Supporting Information

Structure and Aggregation Number of a Lyotropic Liquid Crystal: a Fluorescence Quenching and Molecular Dynamics Study

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Figure SI 1. Textures observed from the TDTMACl mesophase using polarized light microscopy. The textures are characteristics of lamellar structure.²²

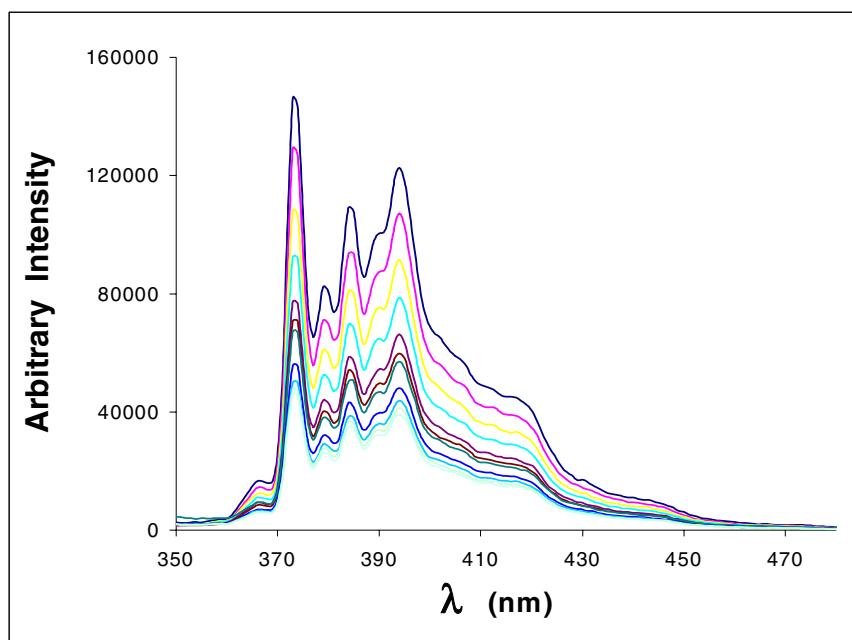


Figure SI 2. Series of fluorescence spectra of pyrene as a function of the concentration of quencher.

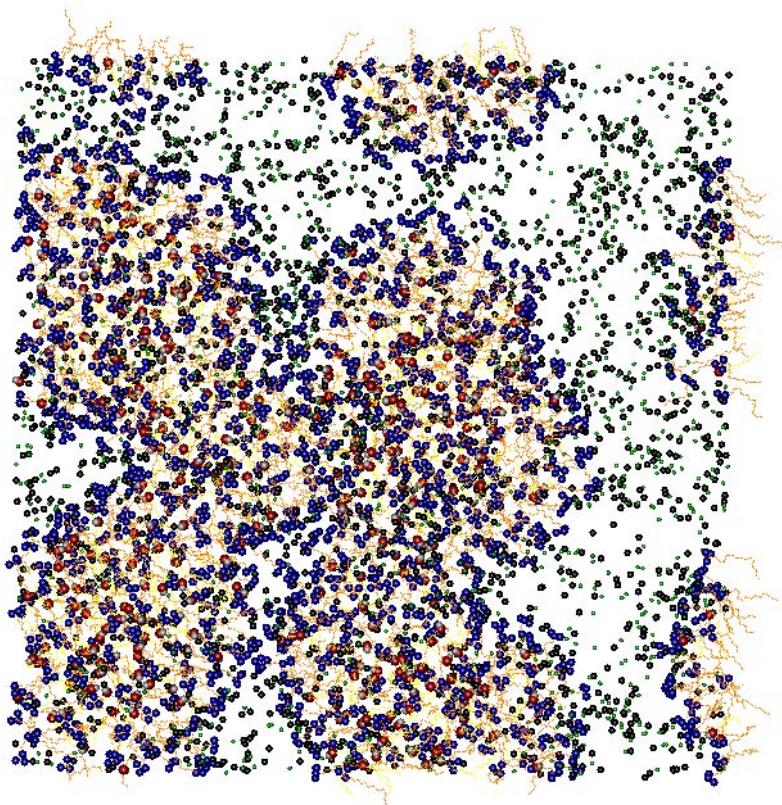


Figure SI 3. Snapshot of the large TDTMACl bilayer after 12.5 ns trajectory calculation. It clearly shows that it is dividing into 4 or 5 smaller fragments. Ammonium methyl groups are blue, oxygen from DeOH is red, hydrogen from DeOH is white, chains are yellow and orange for DeOH and TDTMA respectively. Sodium and chloride ions are green and black respectively. The solvent is not shown.

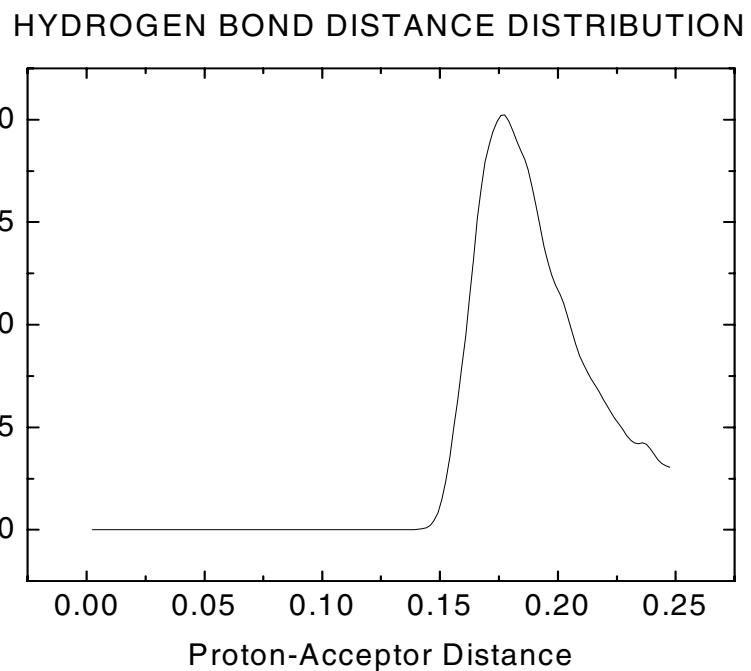


Figure SI 4. The hydrogen bond distance distribution between the oxygen of DeOH and protons from water. It shows the existence of a preferential O---H distance of 0.17 nm

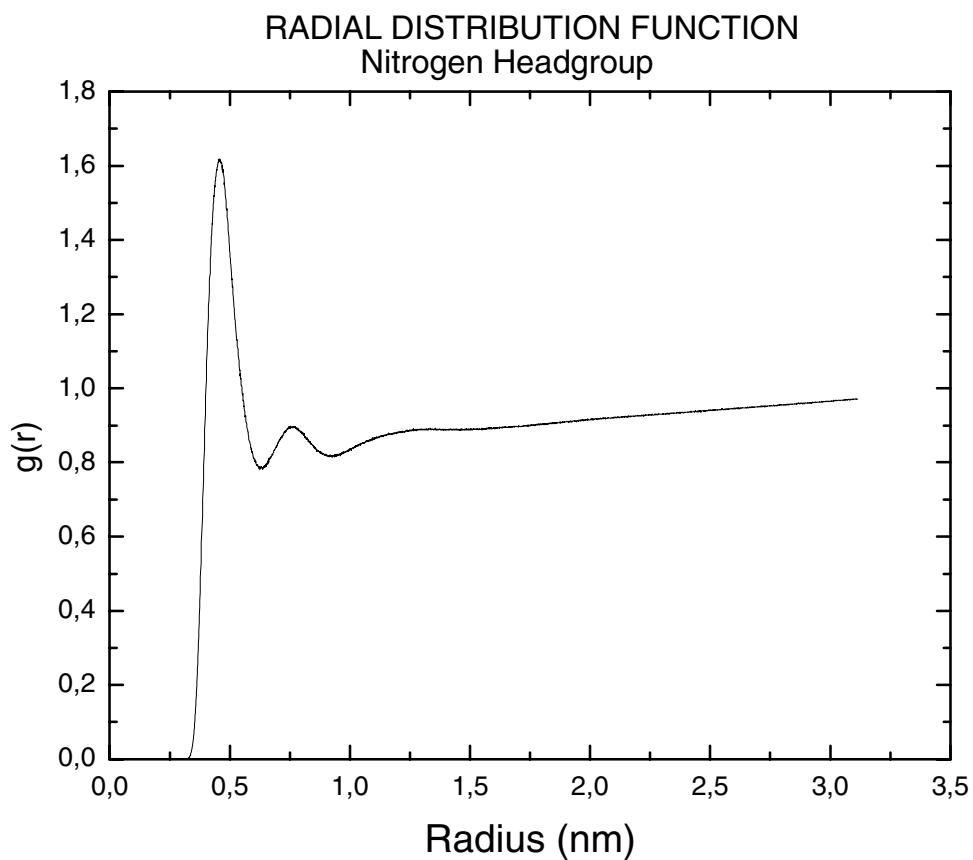


Figure SI 5. Radial distribution function of TDTMA^+ head-group with respect to the solvent. An estimate of the cumulative number indicates that there are 16 solvent molecules in the first solvation shell of the ammonium head-group.

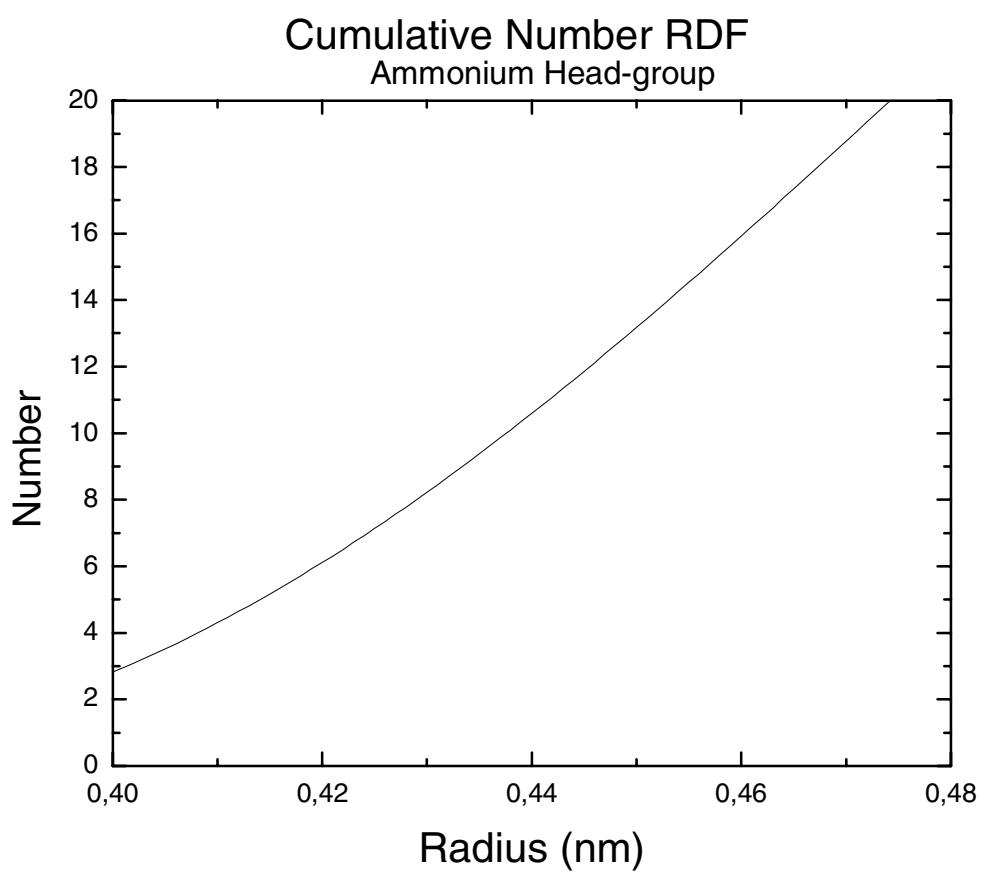


Figure SI 6. Cumulative number of the radial distribution function. It shows that there are 16 solvent molecules in the first solvation shell.

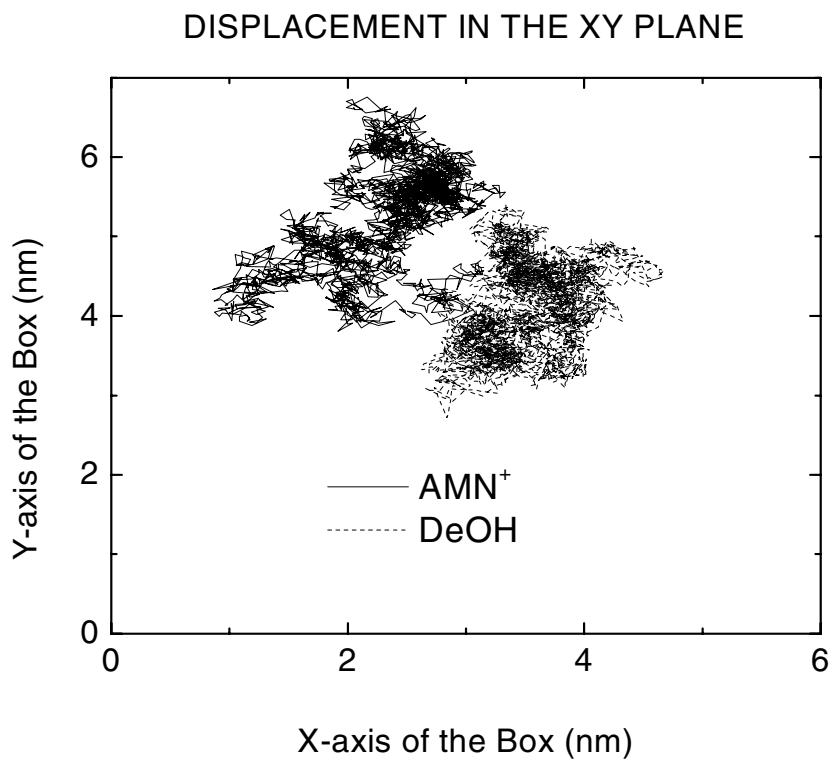


Figure SI 7. The displacement of the TDTMA⁺ and DeOH head-groups in the XY plane in 6 ns is about 2.5 nm. There is a random distribution of DeOH and TDTMA⁺ in the XY-plane after equilibration.