Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Investigation of small inhibitors effects on methane hydrate formation in carbon nanotube using molecular dynamic simulation

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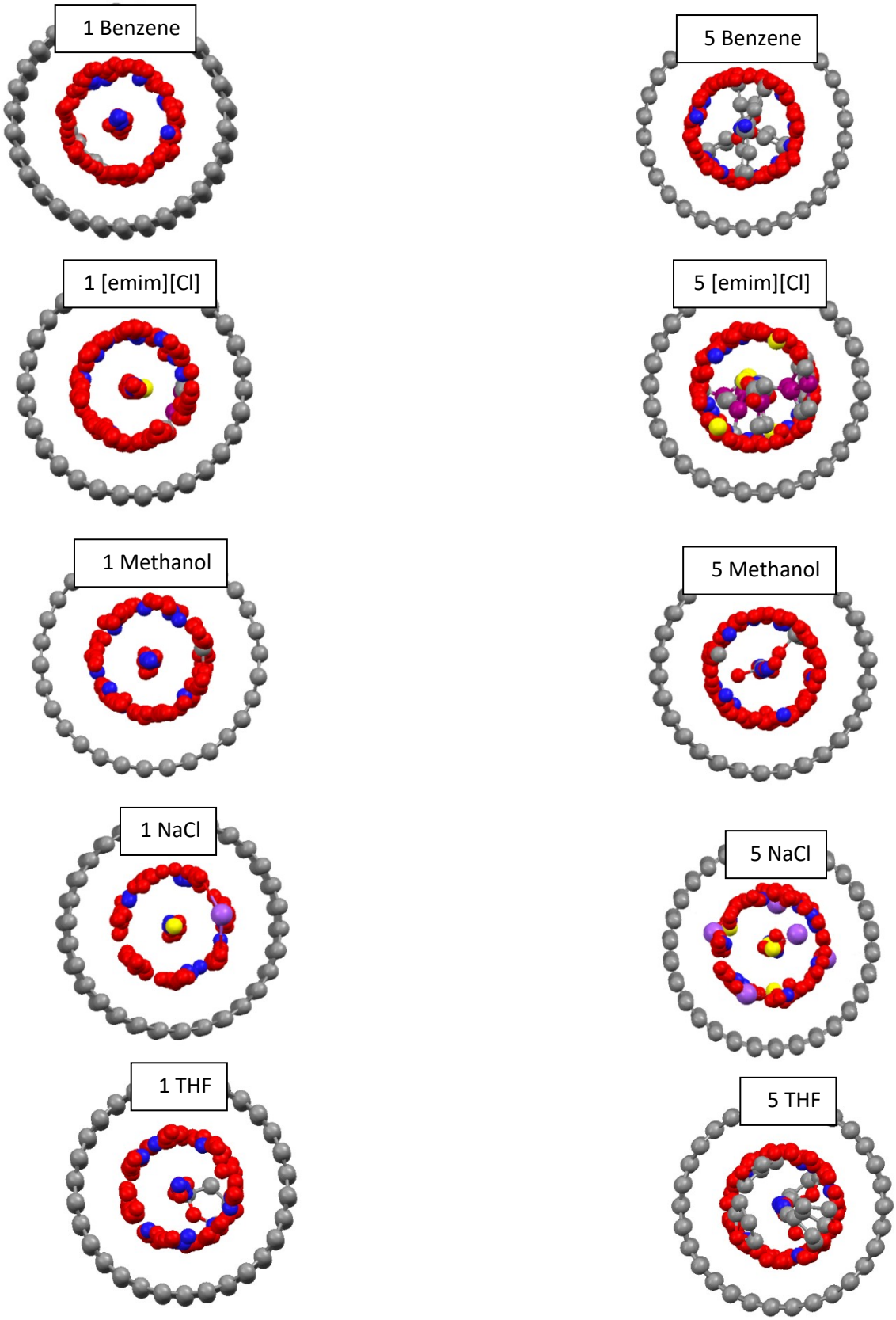

Fig. S1. One and five inhibitor molecules in the CNT containing methane clathrates. The O atoms are in red, carbon in gray, chlore in yellow, sodium in violet, nitrogen in purple, and CH_4 molecules are in blue.

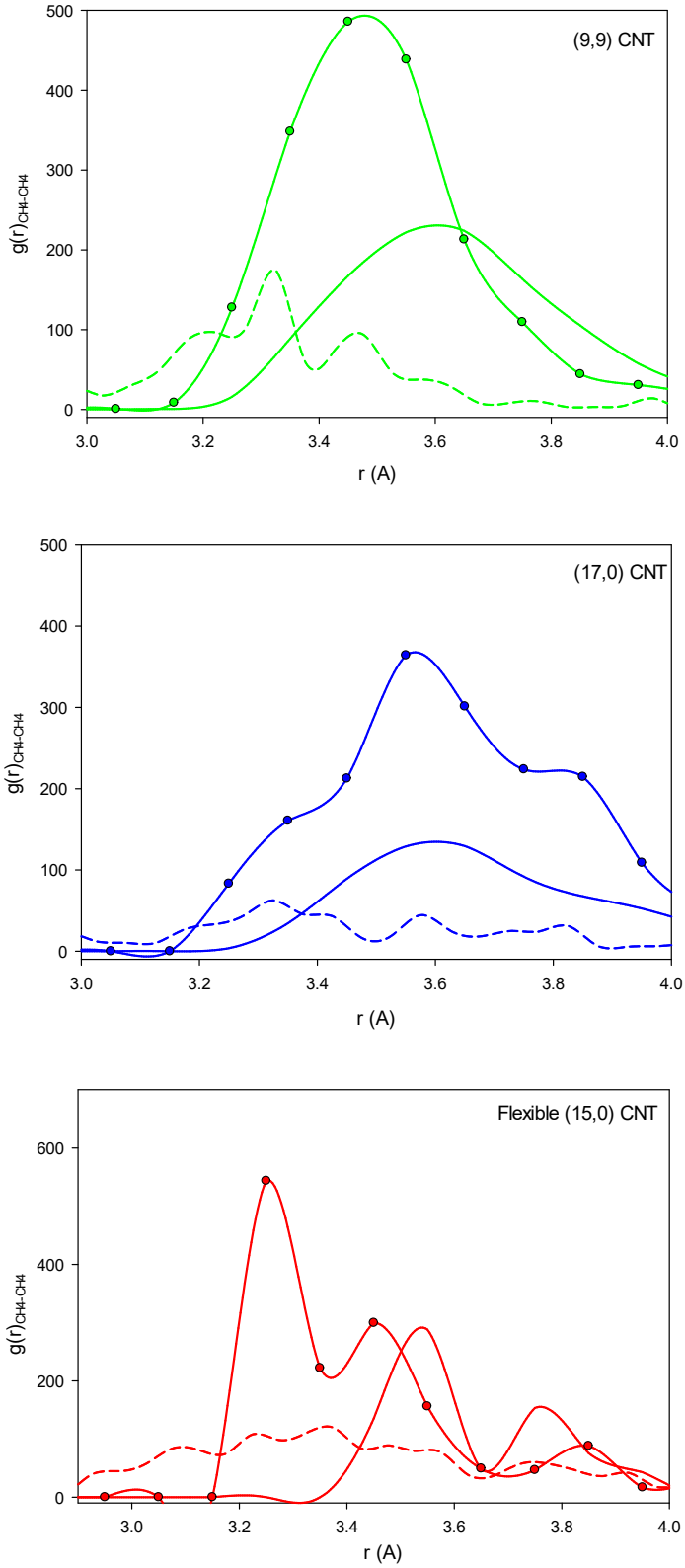

Fig. S2. The methane-methane RDFs for the different effects: The dashed lines are for the blank CNTs at the initial times of the simulations, the solid lines are for the blank CNTs at the end of simulations, and the dotted solid lines are for the (3.8 mol%) IL content CNTs at the end of simulations.

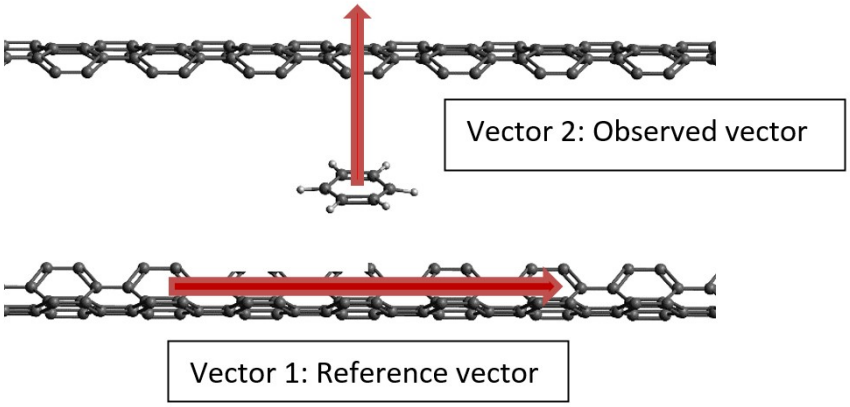

Fig. S3. The definition of the angle in the ADF function: the angle is defined between the vector along the CNT length (as the reference vector) and the vector perpendicular to the surface of the ring of the molecule (as the observed vector).