

Poster Presentations

[MS38-P08] Solvent Influence on Formation of C-H... π Interactions in Benzyltriethylammonium Chloride With Rac-1,1'-Bi-naphthol, Emmanuel Marfo-Owusu* and Amber L. Thompson

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Molecular interactions are of key importance to understanding supramolecular aggregation. The ability to examine solvent influence on generation of weak intermolecular interactions in supramolecular aggregates opens up new avenues for understanding some of the fundamental details of molecular recognition phenomena.

The crystal structure studies on benzyltriethylammonium chloride complex with rac-1,1'-bi-2naphthol (hereafter, BTEAC/BNP) grown in mixed solvents (ethyl acetate/ acetone) as well as in only methanol have revealed the effect of methanol influence on the formation of C-H... π interactions between the H-atoms of CH₃OH and C-atoms of one of the naphthol planes of BNP in the latter complex. The formation of the C-H... π interactions can be attributed to the contribution by the driving force of H-bonding network that places CH₃OH above the plane of one of the naphthol groups of an L-shaped BNP molecule, and thus enhances C-H...C contacts. The molecules of BTEAC/BNP grown in ethylacetate/acetone are held in their aggregates mainly by O1...Cl 3.089 (4) Å, O2...Cl 3.040 (6) Å intermolecular hydrogen bonds, while that of BTEAC/BNP grown in methanol are stabilized by O1...O3 2.665 (3) Å, O2...Cl 3.091 (2) Å, O3...Cl 3.072 (4) Å hydrogen bonds as well as C-H... π interactions. The observed C...H contact distances are within the range 2.834-2.879 Å, while the C...C contact distance observed is 3.332 (3) Å. In both complexes, the benzyl group is partially directed into the plane of a naphthol group in a fashion that does not promote any C-H... π interaction.