Supporting Information

Quantifying Dimer and Trimer Formation by Tri-n-butyl Phosphates in n-Dodecane: Molecular Dynamics Simulations

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Table S1. Lennard Jones Parameters and partial electric charges for TBP and n-dodecane molecules used in this study

Atom type	Partial charge (q)	σ (Å)	ε (kcal/mol)
TBP			
O2	- 0.8033	3.4945*	0.050*
P	1.5955	3.7418	0.2000
O	- 0.5665	3.0000	0.1700
C_a	0.1677	3.3997	0.1094
C_b	- 0.0834	3.3997	0.1094
C_c	- 0.0811	3.3997	0.1094
C_d	- 0.0921	3.3997	0.1094
H_a	0.0454	2.4714	0.0157
H_b	0.0564	2.6495	0.0157
H_c	0.0417	2.6495	0.0157
H_d	0.0348	2.6495	0.0157
n-dodecane			
C_a	- 0.0921	3.1324*	0.1444*
C_b	- 0.0804	3.1324*	0.1444*
C_c	- 0.0794	3.1324*	0.1444*
H_a	0.0317	2.6495	0.0157
H_b	0.0387	2.6495	0.0157
H_c	0.0397	2.6495	0.0157

Values marked by asterisk (*) were modified from the original GAFF. Partial charges were obtained using Antechamber package and AM1-BCC charge model.

Table S2. Average numbers of TBP species for all studied concentrations

Concentration (M)	**# of monomers**	**# of dimers**	**# of trimers**	**total # TBP molecules**
0.10	12.85	1.48	0.06	16
0.20	22.05	4.52	0.30	32
0.37	33.34	10.49	1.23	58
0.60	46.24	19.74	3.09	95
0.80	54.48	27.94	5.55	127
1.00	62.46	35.59	8.12	158

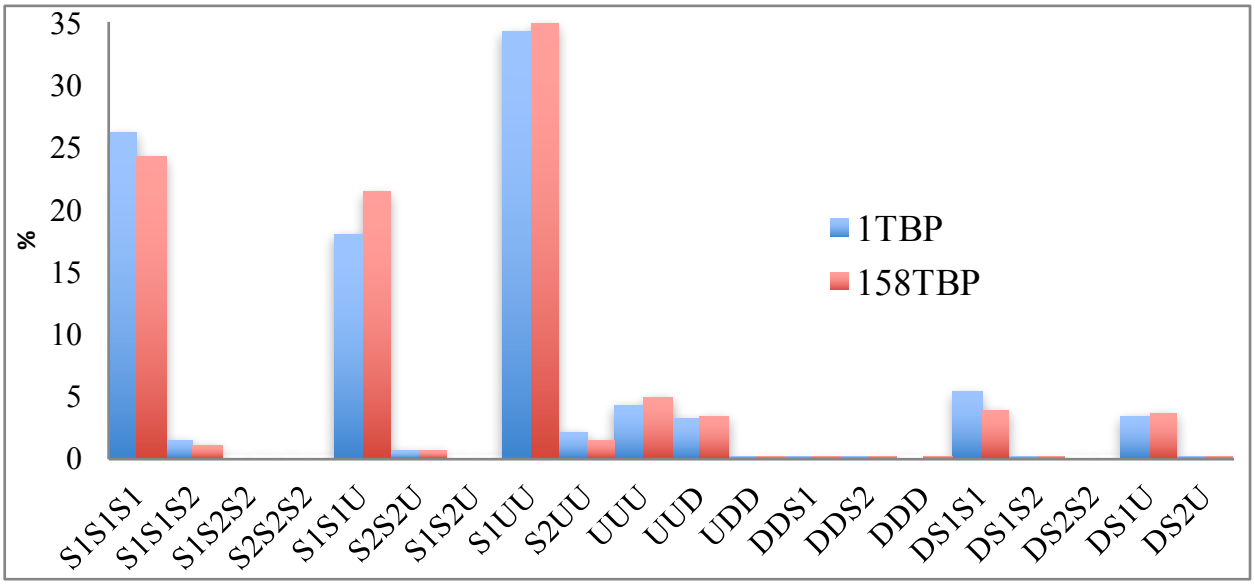

Figure S1. The percentage of various conformations of TBP molecules in n-dodecane solvent. 1TBP = 0.5 M TBP/n-dodecane mixture; 158TBP = 1.0 M TBP/n-dodecane mixture.