Supporting Information:

Solvatochromism of binary mixtures of 2, 2, 2-trifluoroethanol + Ionic Liquid [bmim][Tf$_2$N]: A comparative study with molecular solvents

Md Rabiul Islam$^\sharp$, Faiz Warsi$^\sharp$, Abbul Bashar Khan$^\¥$, Tasneem Kausar$^\sharp$, Imran Khan$^€$ and Maroof Ali$^\sharp\ast$

$^\sharp$ Department of Chemistry, Aligarh Muslim University Aligarh, U.P.-202002
India
$^\¥$ Department of Chemistry, Jamia Millia Islamia (Central University), New Delhi-110025, India
$^€$ Department of Chemistry, College of Science, Sultan Qaboos University, Al-Khod 123, Muscat, Oman

E-mail address: maroof.ch@amu.ac.in, mdmaroof@gmail.com

$^\ast$Corresponding author
Table S1. Experimental values of solvatochromic parameters of neat solvents used in this study. The value in parenthesis shows their corresponding literature values.

<table>
<thead>
<tr>
<th>Solvent</th>
<th>$E^N_T$</th>
<th>$\pi^*$</th>
<th>$\alpha$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TFE</td>
<td>0.90 (0.90)$^4$</td>
<td>1.22 (1.21)$^4$</td>
<td>0.98 (0.99)$^4$</td>
<td>0.01 (0.00)$^4$</td>
</tr>
<tr>
<td>IL</td>
<td>0.65 (0.64)$^2$</td>
<td>0.88 (0.98)$^2$</td>
<td>0.62 (0.61)$^2$</td>
<td>0.23 (0.24)$^2$</td>
</tr>
<tr>
<td>PEG-200</td>
<td>0.63 (0.63)$^1$</td>
<td>0.92 (0.93)$^1$</td>
<td>0.72 (0.62)$^1$</td>
<td>0.67 (0.67)$^1$</td>
</tr>
<tr>
<td>1-BuOH</td>
<td>0.57 (0.59)$^2$</td>
<td>0.56 (0.47)$^2$</td>
<td>0.75 (0.86)$^2$</td>
<td>0.73 (0.84)$^2$</td>
</tr>
<tr>
<td>DMF</td>
<td>0.39 (0.38)$^3$</td>
<td>0.88 (0.88)$^3$</td>
<td>0.15 (0.14)$^3$</td>
<td>0.69 (0.69)$^3$</td>
</tr>
</tbody>
</table>
Figure S1. Maximum wave number of various indicators (i.e., betaine dye 33, 4-nitroaniline, 4-nitroanisole and Nile Red) in TFE + 1-BuOH. Solid line represents fitting using preferential solvation model (eq 17).
Figure S2. Maximum wave number of various indicators (i.e., betaine dye 33, 4-nitroaniline, 4-nitroanisole and Nile Red) in TFE + DMF. Solid line represents fitting using preferential solvation model (eq 17).
Figure S3. Maximum wave number of various indicators (i.e., betaine dye 33, 4-nitroaniline, 4-nitroanisole and Nile Red) in TFE + IL [bmim][Tf$_2$N]. Solid line represents fitting using preferential solvation model (eq 17).
Figure S4. Maximum wave number of various indicators (i.e., betaine dye 33, 4-nitroaniline, 4-nitroanisole and Nile Red) in TFE + 1,4-dioxane. Solid line represents fitting using preferential solvation model (eq 17).
Figure S5. Maximum wave number of various indicators (i.e., betaine dye 33, 4-nitroaniline, 4-nitroanisole and Nile Red) in TFE + PEG-200. Solid line represents fitting using preferential solvation model (eq 17).
Figure S6. Variation in local mole fraction ($X^L_1$, $X^L_2$, and $X^L_{12}$) with bulk mole fraction ($X_2$) around solute molecule, betaine dye 33 (panel 1, left), and 4-nitroaniline (panel 2, right) for TFE-based binary systems.
Figure S7. Variation in local mole fraction (\(X^I_1\), \(X^I_2\), and \(X^I_{12}\)) with bulk mole fraction (\(X_2\)) around solute molecule, 4-nitroanisole (panel 1, left), and Nile Red (panel 2, right) for TFE-based binary systems.
Figure S8. Interaction between bmim and TFE in different parts of the simulation box. The intermolecular distance between C2H-F, C2H-HO, C2H-OH, C3H-F, and C3H-OH are given.
Figure S9. Interaction between Tf$_2$N and TFE in different parts of the simulation box. The intermolecular distances between SO---HO and N---HO are given.

References:

