

Electronic Supplementary information

Antimicrobial and Lubrication Properties of 1-Acetyl-3-hexylbenzotriazolium Benzoate / Sorbate Ionic Liquids

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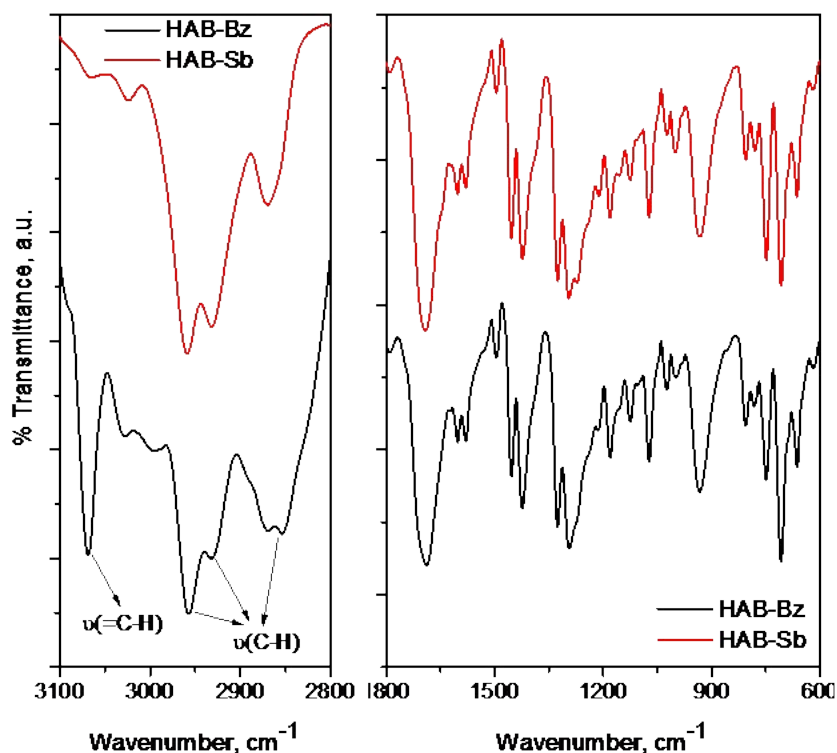


Figure S1: FTIR spectra of HAB-Bz and HAB-Sb ionic liquids.

Figure S1 shows the FTIR spectra of HAB-Bz and HAB-Sb ionic liquids. The vibrational signatures at 3066 and 3030 cm^{-1} are attributed to $=\text{C-H}$ stretches of aromatic ring in the HAB cation. The higher peak intensity of $=\text{C-H}$ stretch at 3030 cm^{-1} further confirmed the presence of additional aromatic ring component in the benzoate anion of HAB-Bz Ionic liquid. The presence of additional vibrational peaks at 1599, 1495, 1421 cm^{-1} are attributed to C-C stretches and several peaks in the range of 800-600 cm^{-1} are associated to the $=\text{C-H}$ (aromatic) bending and ring torsion modes, which confirmed the presence of di-substituted aromatic ring in the both ionic liquids. The strong vibrational modes in the range of 3000-2850 cm^{-1} owing to asymmetric and symmetric stretches of methylene and methyl units reveals the presence of hexyl chain in the HAB cation. The HAB-Sb ionic liquid exhibits a characteristic peak at 1642 cm^{-1} , overlapped with strong stretching mode (1690 cm^{-1}) of C=O functionality and was attributed to the C=C stretch of alkene moiety of sorbate anion. The presence of carboxylate group in both benzoate and sorbate anions of HAB-Bz and HAB-Sb ionic liquids was confirmed by appearance of two vibrational modes at 1573 and 1326 cm^{-1} , which are attributed to the asymmetric and symmetric

stretches of COO⁻ (carboxylate) group. These vibrational modes confirmed the presence of characteristics functionalities in the both ionic liquids.

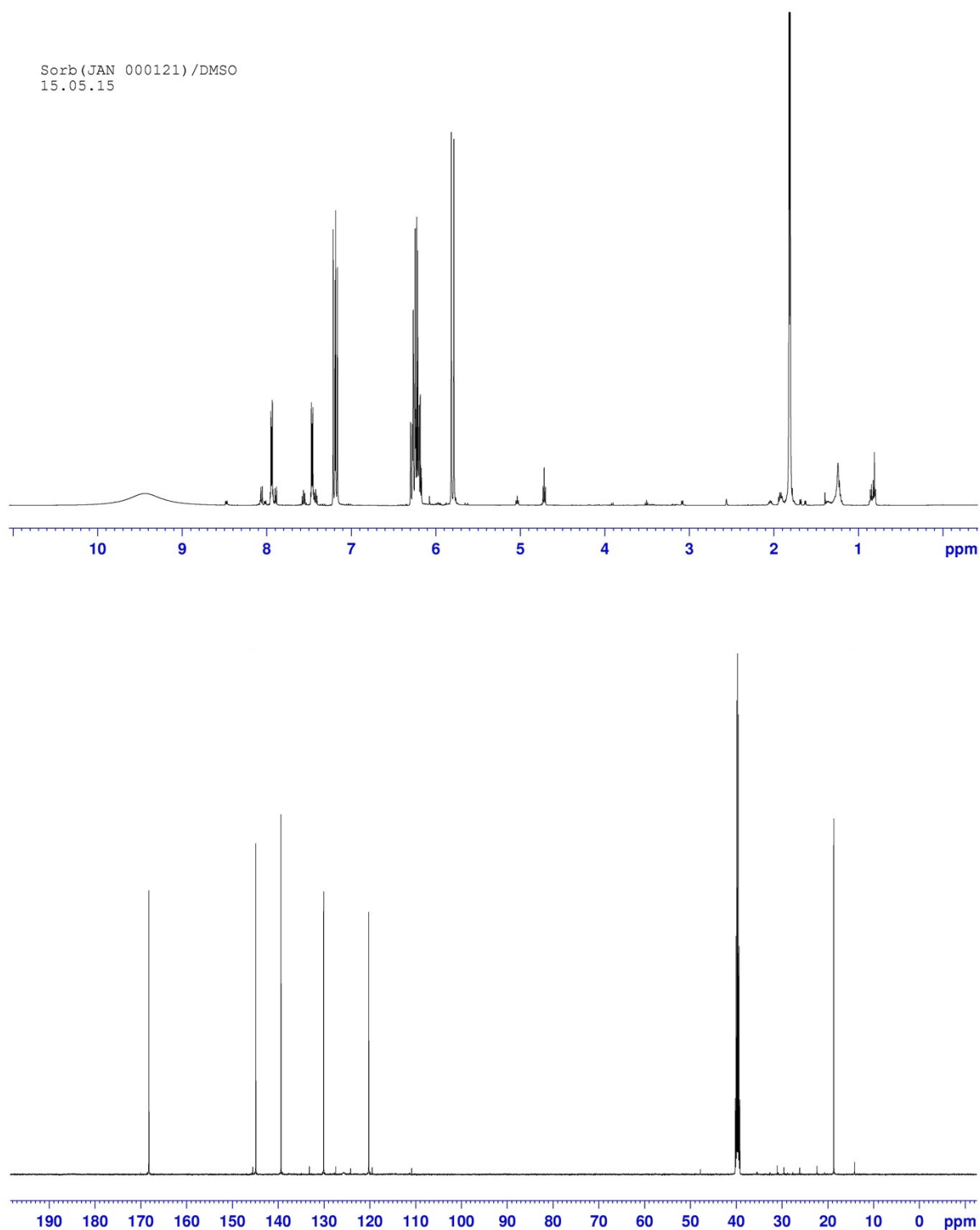


Figure S2: ¹H and ¹³C NMR spectra of HAB-Sb ionic liquid.

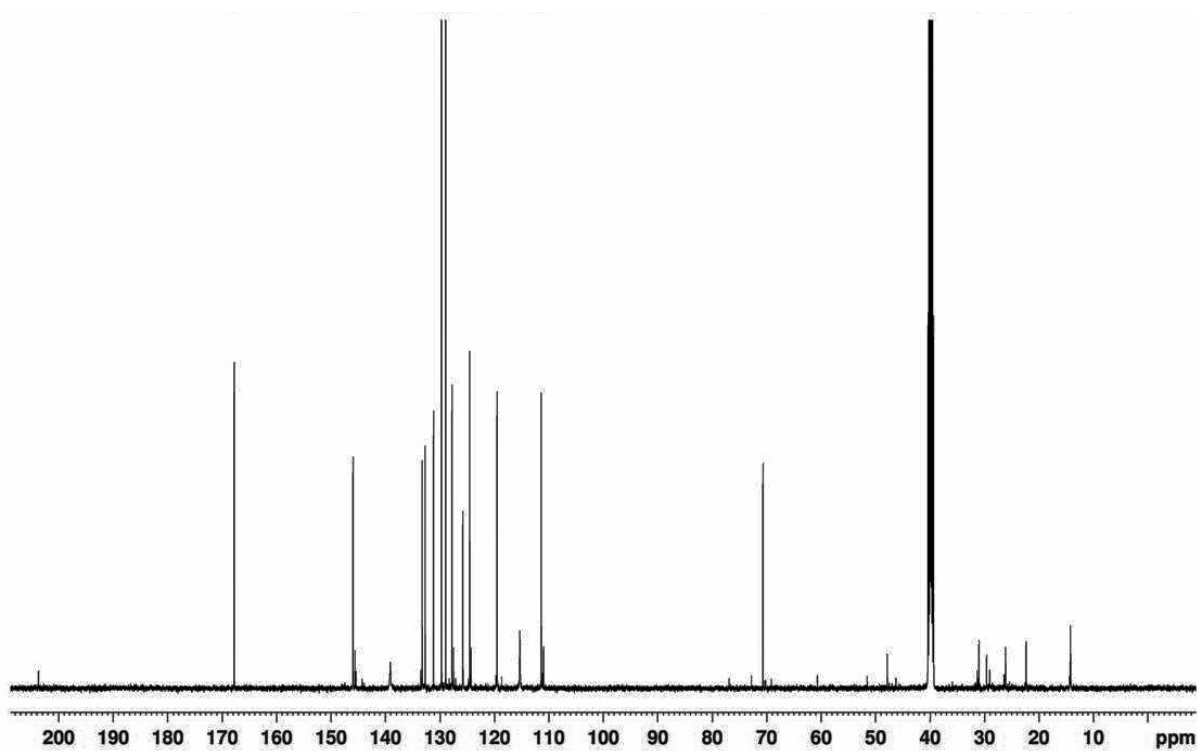
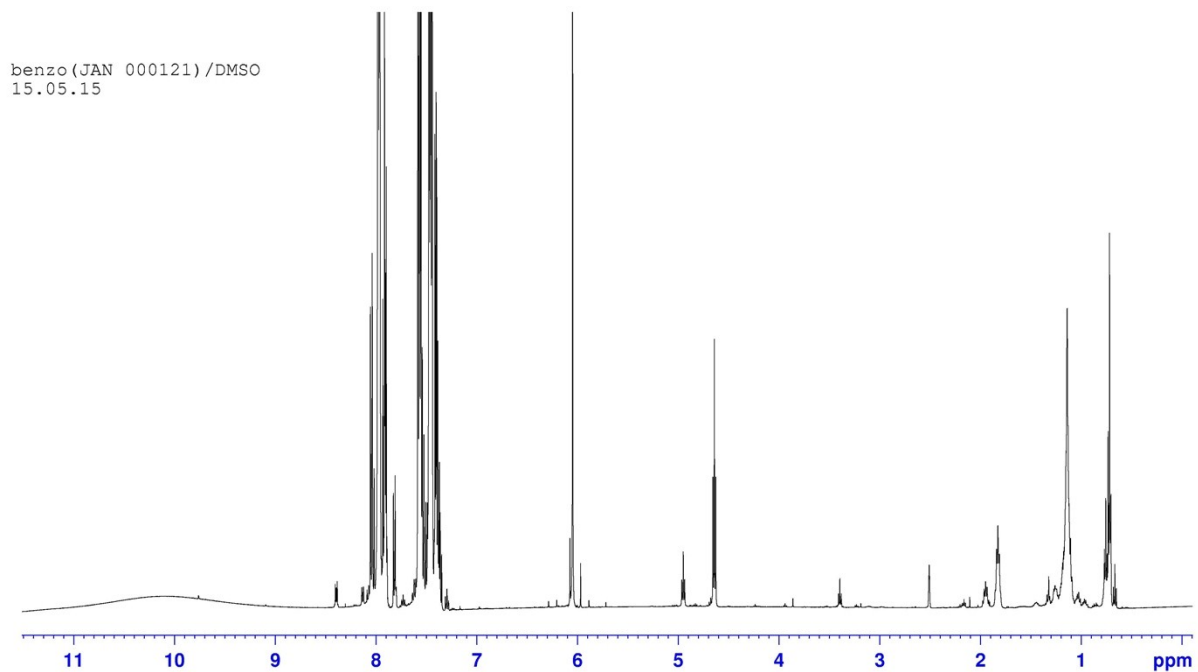


Figure S3: ^1H and ^{13}C NMR spectra of HAB-Bz ionic liquid.

Furthermore, the molecular structure of each ionic liquid is examined by both ^1H and ^{13}C NMR. The ^1H and ^{13}C NMR spectra of both ionic liquids are shown as Figure S2-S3. The terminal methyl group of each ionic liquid exhibited chemical shifts of ^1H and ^{13}C NMR at 0.7-0.86 ppm and ~ 14 ppm, respectively. The methylene protons, attached to cationic centre, exhibit proton shift at downfield position i.e. at ~ 3.3 - 3.5 ppm and corresponding carbon signal appeared at ~ 31 ppm due to de-shielding of electron density. An increasing distance of methylene units from cationic centre showed gradual upfield chemical shifts of proton NMR in the range of 1.21-1.85 ppm and corresponding carbon signals exhibit chemical shift in the range of 18-29 ppm. A methyl group directly bonded to C=O group of HAB cation is de-shielded by electronegative oxygen atom and showed characteristics ^1H and ^{13}C NMR shifts at ~ 2.5 and ~ 28 ppm, respectively. The ^1H and ^{13}C NMR chemical shifts at ~ 7.1 - 8.1 ppm and ~ 120 - 145 ppm are attributed to the aromatic character in the cationic and benzoate anion. The proton and carbon shifts at ~ 5.7 - 6.8 and 120 - 140 ppm, respectively, are attributed to the double bond (alkene) and confirms the sorbate anion in the HAB-Sb ionic liquid. The ^{13}C NMR signal owing to carboxylate group in both ionic liquids benzoate / sorbate anion shifts towards extreme downfield position because of two electronegative oxygen atoms. These oxygen atoms attract the electrons and influenced the electron density over the carbon and resultant carbon signals appeared at ~ 165 - 175 ppm. These characteristics NMR features along with FTIR spectra confirm the preparation of HAB-Bz and HAB-Sb ionic liquids.