Potentiometric Surfactant Sensor for Anionic Surfactants Based on 1,3-dioctadecyl-1*H*-imidazol-3-ium tetraphenylborate

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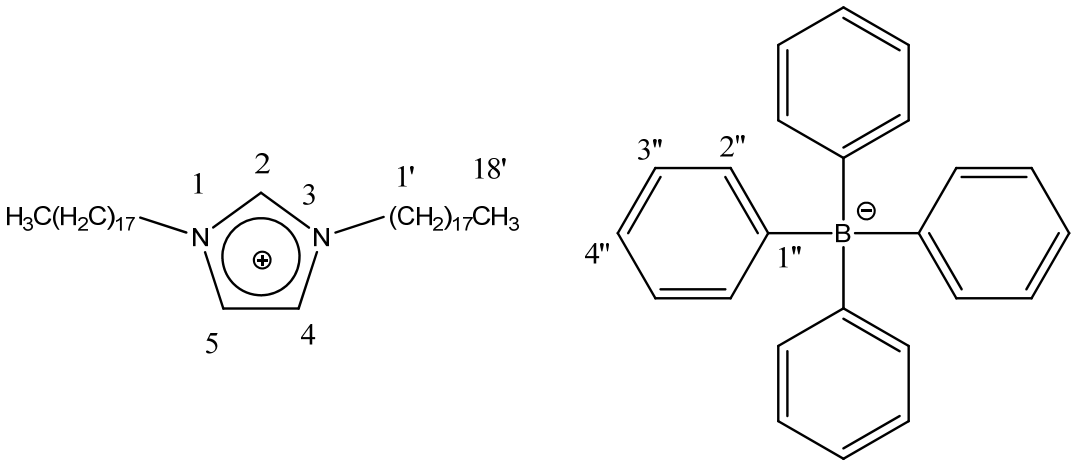
Figure S6. Charge distribution within the $DODI^+$ cation and the TPB^- anion.

1,3-dioctadecyl-1*H*-imidazol-3-ium tetraphenylborate (2).



Formula: $C_{63}H_{97}BN_2$, Mr = 893.27 g/mol, (mass of QAC^+ 574), Yield = 92.58%, White powder, m.p. = 81.4-83.9 °C, Elem. Anal. (calc.): C, 84.71; H, 10.95; B, 1.21; N, 3.14, Elem. Anal. (exp.): C, 82.29; H, 11.04; B N/A; N, 3.26.

^{1}H NMR (400 MHz; $CDCl_3$): δ 7.57-7.46 (8H, m, H-C(1'')), 7.00 (8H, t, J=7.4 Hz, H-C(2'')), 6.83 (8H, t, J=7.4 Hz, H-C(3'')), 6.24 (2H, brs, H-C(4), H-C(5)), 4.95 (1H, brs, H-C(2)), 3.21 (4H, t, J=7.4 Hz, H-C(1')); 1.39 (4H, quint, J=7.4 Hz, H-C(2')); 1.33-1.17 (56H, m, H-C(3')-H C(16')), 1.10 (4H, tq, J= 7.4, Hz, J=7.0 Hz, H-C(17')), 0.88 (6H, t, J=7.0 Hz, H-C(18'));

^{13}C NMR (100.613 MHz; $CDCl_3$): δ 164.0 (4C atoms, q, J= 49.0 Hz, C(1'')), 135.9, 134.9, 125.9, 121.9, 120.7, 49.4, 31.9, 29.8, 29.7 (8C atoms), 29.64 (4C atoms), 29.60, 29.4, 29.3 (4C atoms), 28.9, 26.1, 22.7, 14.1.

IR (KBr, cm^{-1}): 3450, 3100, 2900, 2850, 2050, 100, 1550, 1450, 1150

MS-CI (NH_3): 573, 491, 455, 395, 304, 219, 163, 122, 86.

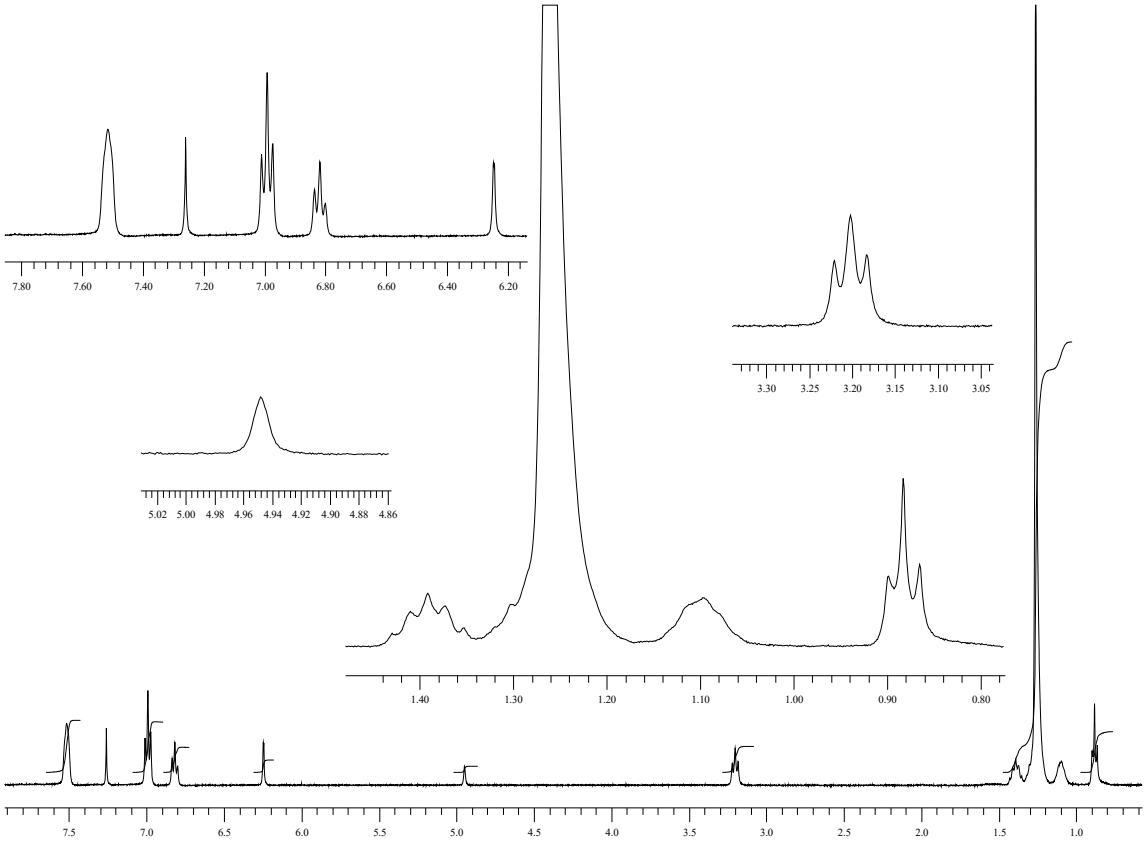


Figure S1. ^1H NMR (400 MHz; $CDCl_3$) of 1,3-dioctadecyl-1*H*-imidazol-3-ium tetraphenylborate (**2**).

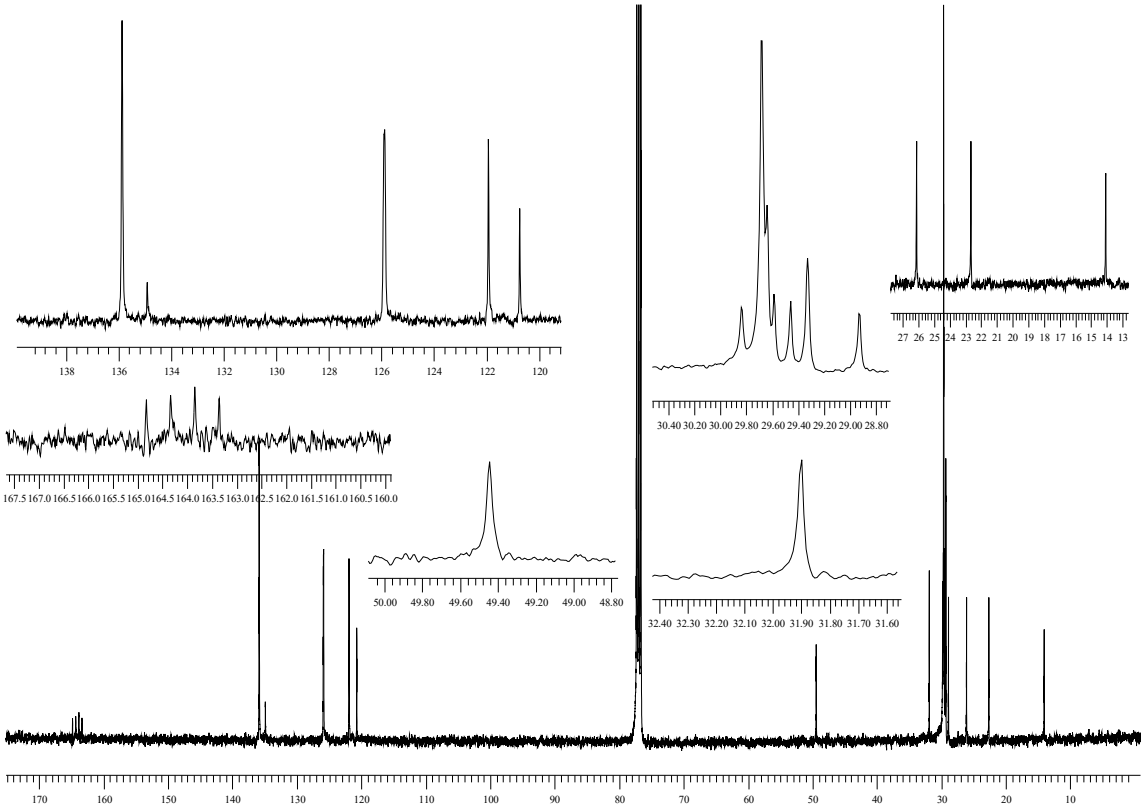


Figure S2. ^{13}C NMR (100.613 MHz; $CDCl_3$) of 1,3-dioctadecyl-1*H*-imidazol-3-ium tetraphenylborate (**2**).

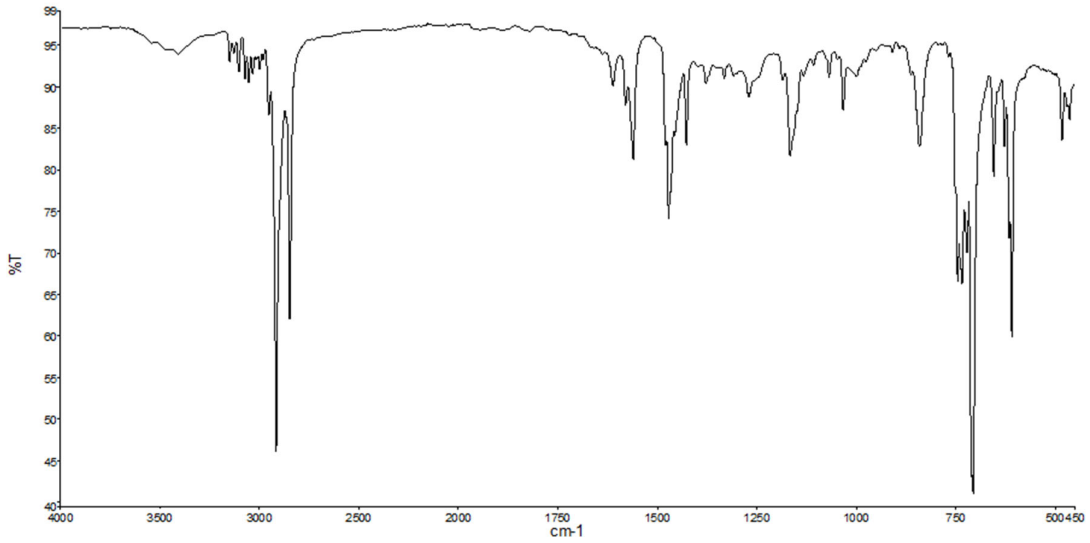


Figure S3. ATR-FTIR spectra of powder 1,3-dioctadecyl-1*H*-imidazol-3-ium tetraphenylborate (**2**).

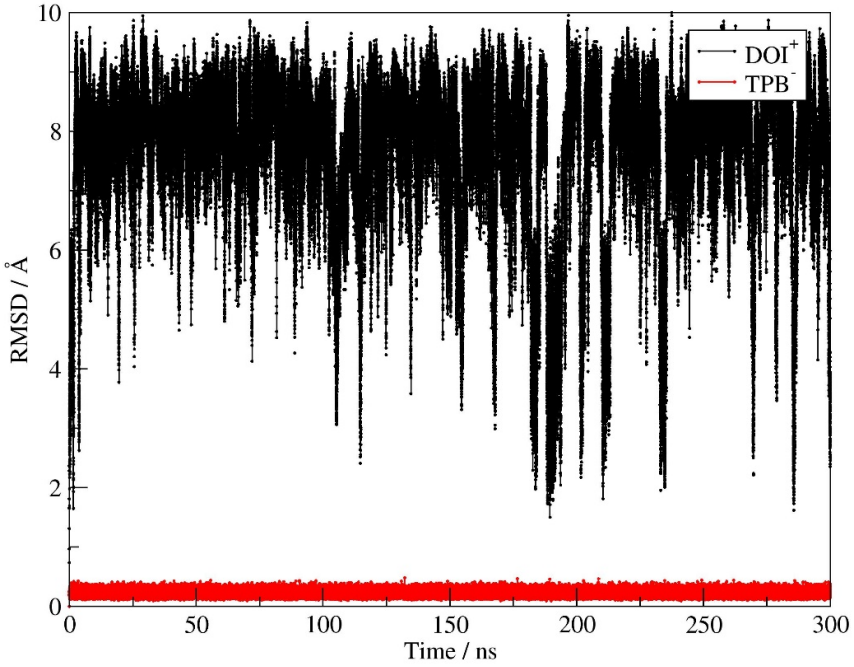


Figure S4. RMSD graphs during the molecular dynamics simulation of the $DODI^+$ cation (in black) and the TPB^- anion (in red) in the aqueous solution, revealing a much higher flexibility of the former.

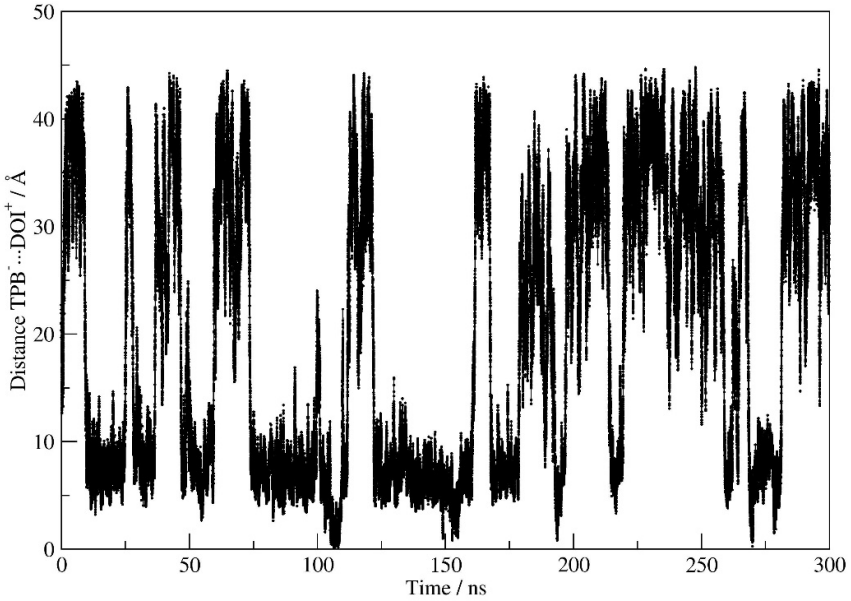
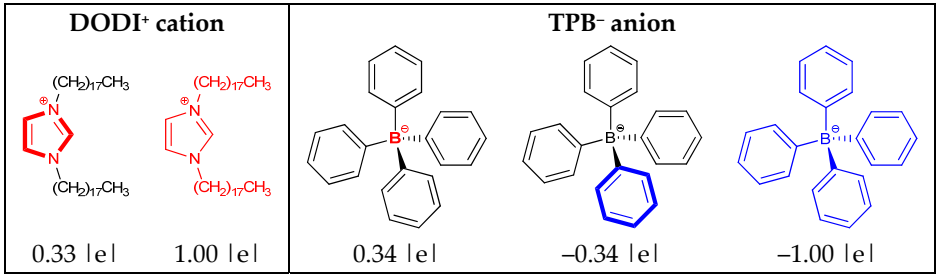


Figure S5. Time dependence of the distance between the boron atom in TPB^- and the nitrogen atoms in $DODI^+$ during the molecular dynamics simulation, indicating that the DODI–TPB complex formation is reversible and in the equilibrium with dissociated components.

ISOLATED COMPONENTS BEFORE THE COMPLEX FORMATION



COMPONENTS WITHIN THE DODI–TPB COMPLEX

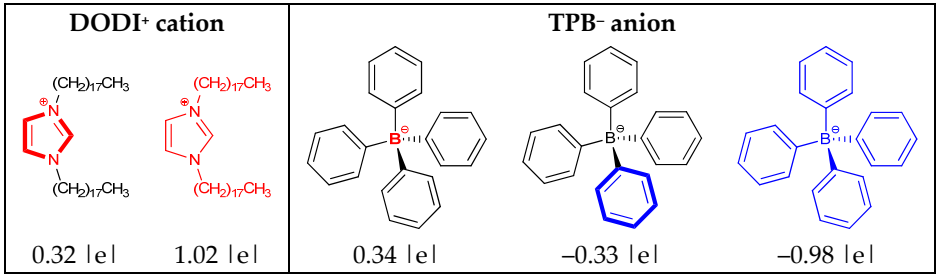


Figure S6. Charge distribution within the DODI$^+$ cation and the TPB$^-$ anion, either isolated or within the elucidated representative structure of the DODI–TPB complex, as obtained by the NBO analysis at the (SMD)/M06–2X/6–31+G(d) level of theory in water. Particular set of atoms considered for the analysis is denoted with a color and includes the attached hydrogen atoms as well. The results reveal that only 2% of the charge density is transferred among components following the DODI–TPB complex formation.