Supplementary Material (ESI) for New Journal of Chemistry

ELECTRONIC SUPPLEMENTARY INFORMATION

Ionic Liquids with Dual Biological Function: Sweet and Anti-microbial, Hydrophobic Quaternary Ammonium-based Salts

Whitney L. Hough-Troutman,[a] Marcin Smiglak,[a] Scott Griffin,[a] W. Matthew Reichert,[a] Ilona Mirska,[b] Jadwiga Jodynis-Liebert,[c] Teresa Adamska,[c] Jan Nawrot,[d] Monika Stasiewicz,[e] Robin D. Rogers,*[,a,f] and Juliusz Pernak.*[,e]

Benzalkonium saccharinate [BA][Sac]. White solid, yield 98%, δ_H(360 MHz; DMSO-d_6; Me_4Si) 0.85 (3H, t), 1.24 (20H, m), 1.77 (2H, m), 2.95 (6H, s), 3.24 (2H, m), 4.53 (2H, s), and 7.59 (9H, m); δ_C(90.6 MHz; DMSO-d_6; Me_4Si) 13.8, 21.7, 22.0, 25.7, 28.4, 28.6, 28.7, 28.8, 28.9, 31.2, 49.0, 63.4, 66.1, 118.9, 122.3, 128.0, 128.8, 130.1, 131.4, 132.8, 134.8, 145.2, and 167.7.

Didecyldimethylammonium saccharinate [DDA][Sac]. Viscous liquid, yield 95%, δ_H(360 MHz; DMSO-d_6; Me_4Si) 0.85 (6H, t), 1.24 (28H, m), 1.63 (4H, m), 3.00 (6H, s), 3.22 (4H, m), and 7.58 (4H, m); δ_C(90.6 MHz; DMSO-d_6; Me_4Si) 13.8, 21.6, 22.0, 25.6, 28.4, 28.6, 28.7, 28.8, 31.2, 49.9, 62.7, 118.9, 122.3, 130.8, 131.3, 134.8, 145.2, and 167.7.

Hexadecylpyridinium saccharinate [HEX][Sac]. White solid, yield 86%, δ_H(360 MHz; DMSO-d_6; Me_4Si) 0.85 (3H, t), 1.25 (26H, m), 1.89 (2H, m), 4.59 (2H, t), 7.57 (4H, m), 8.16 (2H, t), 8.61 (1H, t), and 9.11 (2H, d); δ_C(90.6 MHz; DMSO-d_6; Me_4Si) 13.8, 21.9, 25.2, 28.2, 28.6, 28.8, 28.9, 29.0, 30.6, 31.1, 60.6, 99.5, 118.9, 122.3, 127.9, 130.7, 131.3, 134.8, 144.6, 145.3, and 167.6.

Benzalkonium acesulfamate [BA][Ace]. White solid, yield 95%, δ_H(360 MHz; DMSO-d_6; Me_4Si) 0.85 (3H, t), 1.25 (20H, m), 1.78 (2H, m), 1.90 (3H, s), 2.95 (6H, s), 3.24 (2H, m), 4.53 (2H, s), 5.28 (1H, s), and 7.52 (5H, m); δ_C(90.6 MHz; DMSO-d_6; Me_4Si) 13.8, 19.3, 21.7, 22.0, 25.7, 28.4, 28.6, 28.7, 28.8, 28.9, 31.2, 49.0, 63.4, 66.1, 102.0, 128.0, 128.8, 130.1, 132.8, 159.5, and 167.6.

Didecyldimethylammonium acesulfamate [DDA][Ace]. Viscous liquid, yield 94%, δ_H(360 MHz; DMSO-d_6; Me_4Si) 0.86 (6H, t), 1.26 (28H, m), 1.63 (4H, m), 1.89 (3H, d), 2.99 (6H, s), 3.22 (m, 4H), and 5.26 (1H, q); δ_C(90.6 MHz; DMSO-d_6; Me_4Si) 13.8, 19.3, 21.6, 22.0, 25.7, 28.4, 28.6, 28.7, 28.8, 31.2, 49.8, 62.7, 102.0, 159.4, and 167.6.

Hexadecylpyridinium acesulfamate [HEX][Ace]. White solid, yield 88%, δ_H(360 MHz; DMSO-d_6; Me_4Si) 0.85 (6H, t), 1.23 (26H, m), 1.89 (5H, m), 4.58 (2H, t), 5.26 (1H, s), 8.15 (2H, t), 8.61 (1H, t) and 9.08 (2H, d); δ_C(90.6 MHz; DMSO-d_6; Me_4Si) 13.8, 19.3, 21.9, 25.2, 28.2, 28.5, 28.6, 28.7, 28.8, 28.9, 31.1, 60.6, 101.9, 127.9, 144.6, 145.3, 159.3, and 167.5

3-Hydroxy-1-octyloxymethylpyridinium acesulfamate [1-(OctOMe)-3-OH-Py][Ace]. Colorless crystals, yield 85%, mp 83-84 ^oC (visual, hot stage), δ_H(300 MHz; $CDCl_3$; Me_4Si) 0.87 (3H, t), 1.28 (10H, m), 1.6 (2H, q), 2.09 (3H, d), 3.60 (2H, t), 5.56 (1H, d), 5.76 (2H, s), 7.77 (1H, dd), 7.96 (1H, m), 8.21 (1H, d), 8.91 (1H, dd), 13.65 (1H, s); δ_C(75 MHz; $CDCl_3$; Me_4Si) 14.1, 20.1, 22.6, 25.7, 29.11, 29.12, 29.2, 31.7, 71.9, 89.4, 100.9, 128.0, 130.8, 131.5, 133.6, 159.2, 162.9, and 171.3.

3-Hydroxy-1-octyloxymethylpyridinium saccharinate [1-(OctOMe)-3-OH-Py][Sac]. Colorless crystals, yield 90%, mp 93-95 ^oC (visual, hot stage), δ_H(300 MHz; $CDCl_3$; Me_4Si) 0.87 (3 H, t), 1.28 (10H, m), 1.58 (2H, m), 3.60 (2H, t), 5.76 (2H, s), 7.61 (2H,

m), 7.80 (3H, dd), 8.06 (1H, m), 8.24 (1H, d), 8.99 (1H, s), 13.05 (1H, s); δ_C(75 MHz; $CDCl_3$; Me_4Si) 14.1, 22.6, 25.7, 29.11, 29.12, 29.2, 31.7, 71.9, 89.4, 119.9, 123.4, 128.0, 130.8, 131.4, 132.1, 132.3, 133.2, 133.6, 143.5, 159.2, and 170.1.

SUPPLEMENTARY FIGURES

Figure S1. ORTEP (50% probability thermal ellipsoids) of the asymmetric unit of [HEX][Ace].

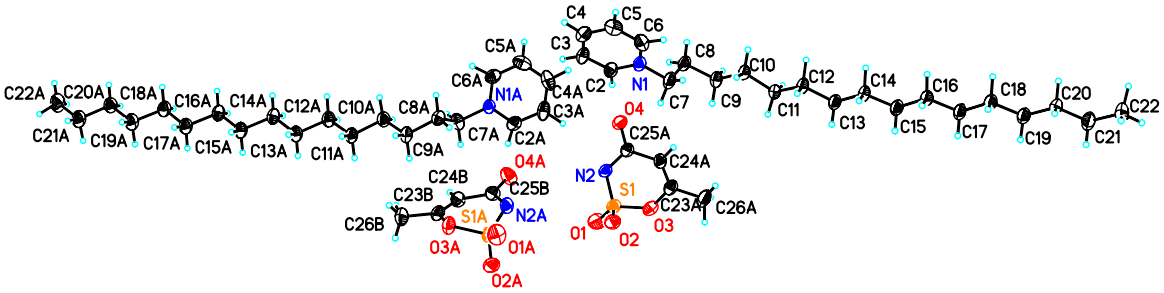

Figure S2. Close contacts around the cations in [HEX][Ace].

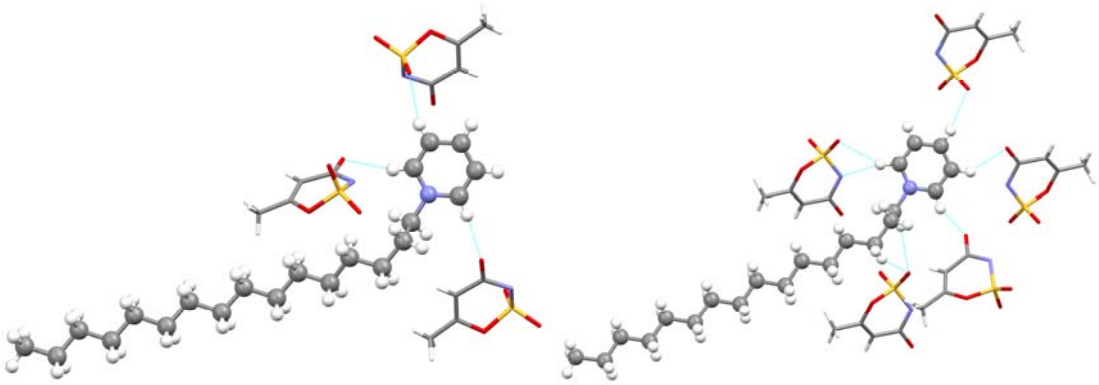

Figure S3. π-Stacking modes of the polymeric cation in [HEX][Ace]

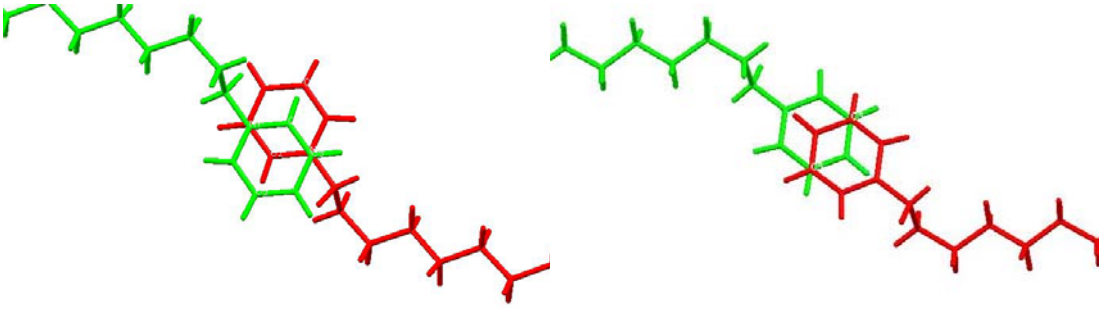

Figure S4. π-Stacking mode of the dimeric cation in [HEX][Ace]

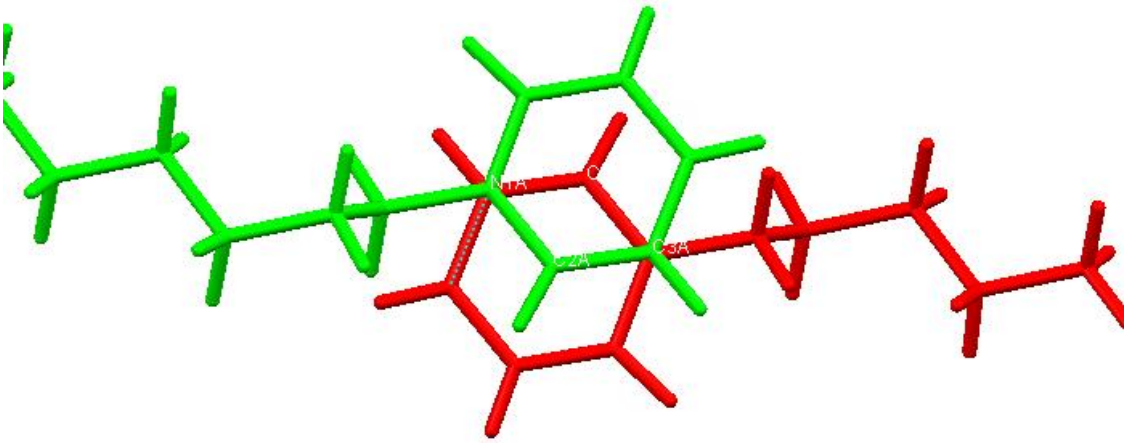

Figure S5. ORTEP (50% probability thermal ellipsoids) of the asymmetric unit of [1-(OctOMe)-3-OH-Py][Sac].