Supporting Information for

Characteristic Spectroscopic Features due to Cation-Anion Interactions Observed in the 700 – 950 cm^{-1} Range of Infrared Spectroscopy for Various Imidazolium-based Ionic Liquids

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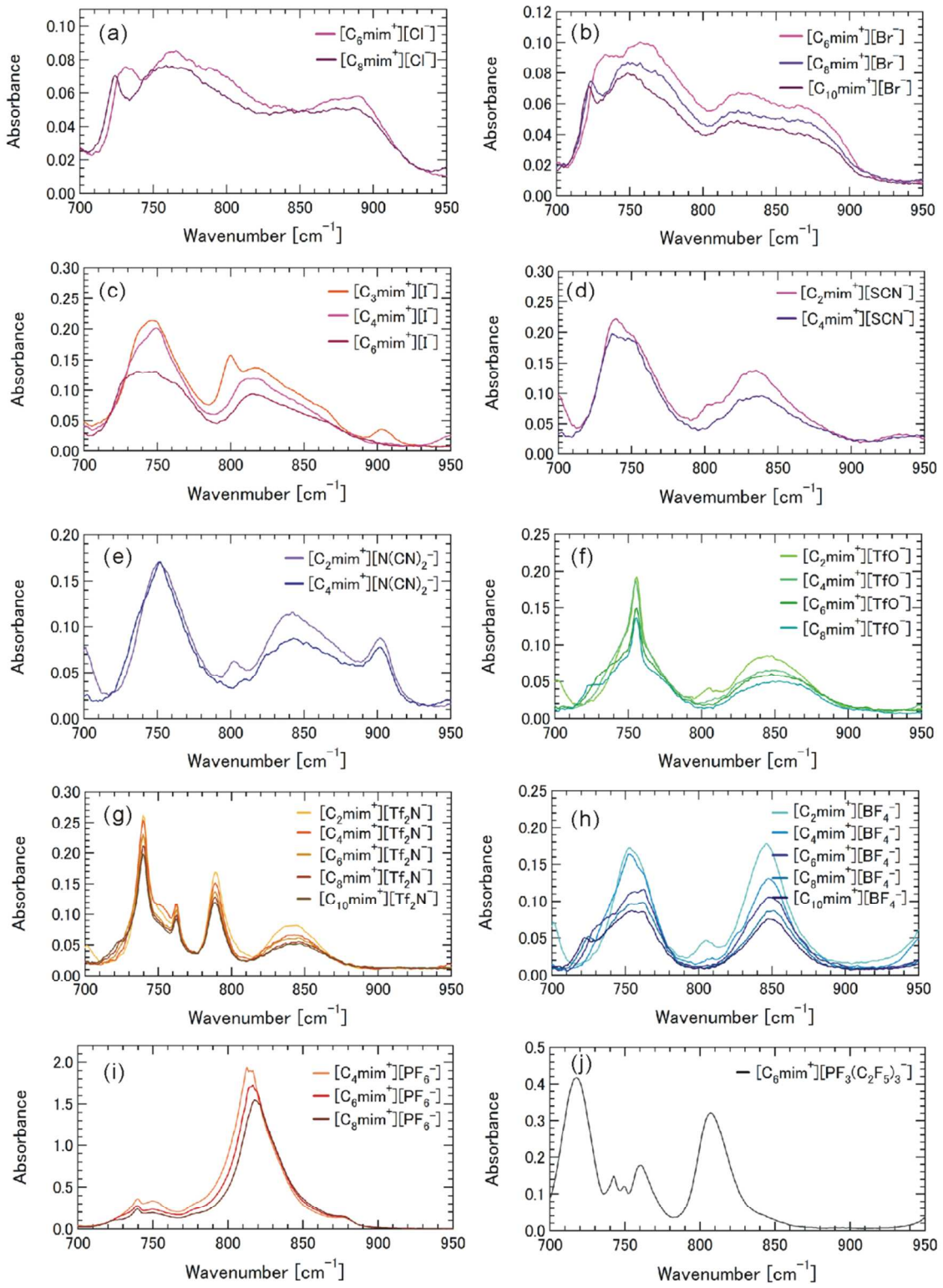

Figure S1. ATR-IR spectra in the 700 – 950 cm^{-1} range for (a) $[C_nmim^+][Cl^-]$ with n = 6, 8, (b) $[C_nmim^+][Br^-]$ with n = 6, 8, 10, (c) $[C_nmim^+][I^-]$ with n = 3, 4, 6, (d) $[C_nmim^+][SCN^-]$ with n =

2, 4, (e) $[C_nmim^+][N(CN)_2^-]$ with n = 2, 4, (f) $[C_nmim^+][TfO^-]$ with n = 2, 4, 6, 8, (g) $[C_nmim^+][Tf_2N^-]$ with n = 2, 4, 6, 8, 10, (h) $[C_nmim^+][BF_4^-]$ with n = 2, 4, 6, 8, 10, (i) $[C_nmim^+][PF_6^-]$ with n = 4, 6, 8, and (j) $[C_6mim^+][PF_3(C_2F_5)_3^-]$.

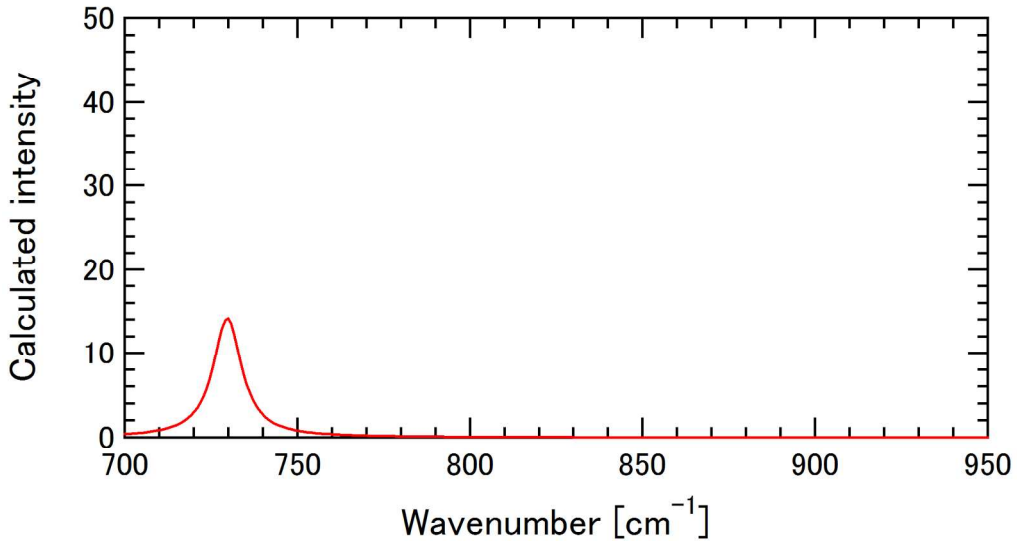

Figure S2. Calculated vibrational spectrum in the 700 – 950 cm^{-1} range for [SCN^{-}]. Density functional theory (DFT) calculations were performed. The geometry was optimized at the B3LYP/6-311+G(d,p) level of theory with a charge of –1, and then the infrared vibrational spectrum was calculated at the same level of theory. The absorption bandwidth was set at 5 cm^{-1} for the absorption bands to make them easily visible. The scale of the vertical axis is identical to that of Figure 2.

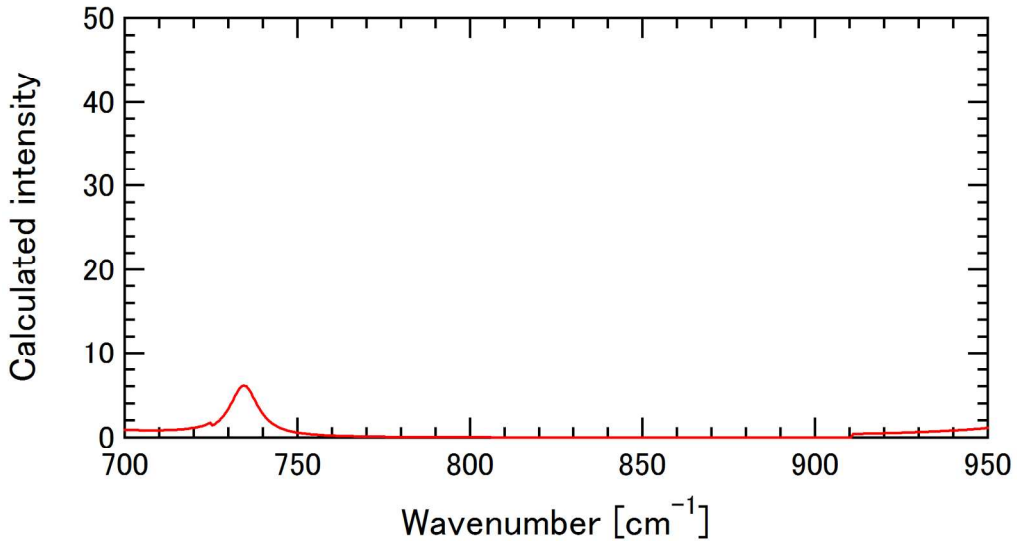

Figure S3. Calculated vibrational spectrum in the 700 – 950 cm^{-1} range for [TfO^{-}]. Density functional theory (DFT) calculations were performed. The geometry was optimized at the B3LYP/6-311+G(d,p) level of theory with a charge of –1, and then the infrared vibrational spectrum was calculated at the same level of theory. The absorption bandwidth was set at 5 cm^{-1} for the absorption bands to make them easily visible. The scale of the vertical axis is identical to that of Figure 2.

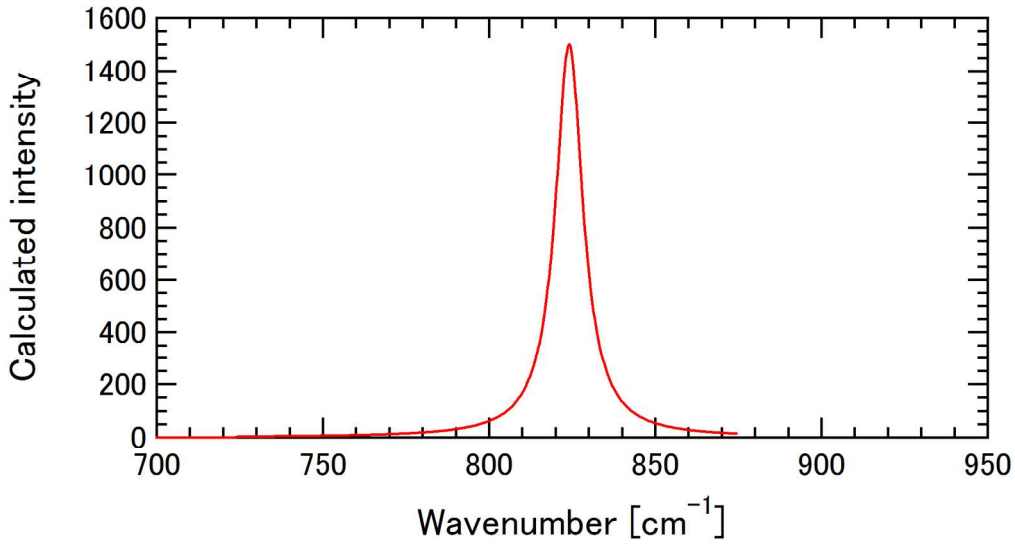

Figure S4. Calculated vibrational spectrum in the 700 – 950 cm^{-1} range for [PF_6^-]. Density functional theory (DFT) calculations were performed. The geometry was optimized at the B3LYP/6-311+G(d,p) level of theory with a charge of –1, and then the infrared vibrational spectrum was calculated at the same level of theory. The absorption bandwidth was set at 5 cm^{-1} for the absorption bands to make them easily visible. Note that the scale of the vertical axis differs significantly from that of Figure 2.

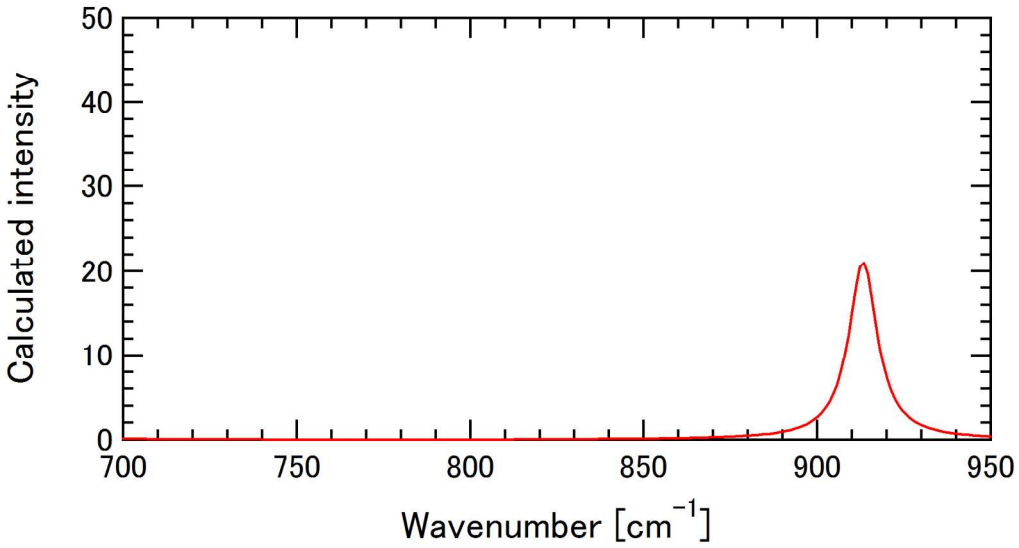

Figure S5. Calculated vibrational spectrum in the 700 – 950 cm^{-1} range for $[N(CN)_2^-]$. Density functional theory (DFT) calculations were performed. The geometry was optimized at the B3LYP/6-311+G(d,p) level of theory with a charge of –1, and then the infrared vibrational spectrum was calculated at the same level of theory. The absorption bandwidth was set at 5 cm^{-1} for the absorption bands to make them easily visible. The scale of the vertical axis is identical to that of Figure 2.