Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


# Supporting Information for the Self-Diffusion Coefficients of Emim-Acetate:Water mixtures

The self-diffusion coefficients of the anion and water for the Emim-Acetate:Water binary system were determined by monitoring the $CH_3$ protons and the $H_2$ protons of the acetate and water molecules respectively. For the cation, self-diffusion coefficients of each magnetically non-equivalent protons of the cation were determined. They are listed in the table in the order H2,H4,H5,H6,H8 and H7. (Please refer to the following figure for atom labeling). The self-diffusion coefficients of all the protons of the cation are almost similar except for the H2 proton, especially at 373K, which might be due to its exchange with acetate or water due to its acidic nature. All the self-diffusion coefficients values for the cation reported in the main text are an average of all the protons of the cation except the acidic H2 proton.

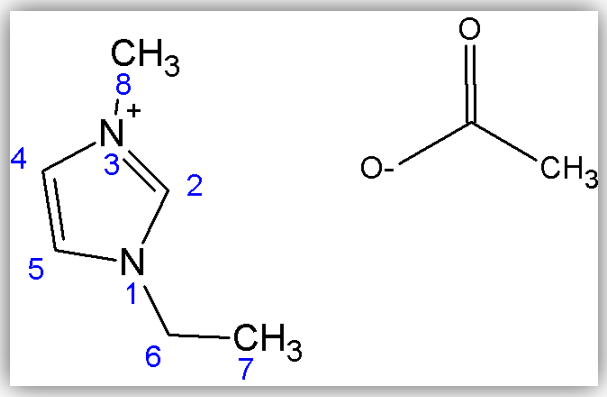


**Table: Self-diffusion coefficients of Cation, Anion and Water of Emim Acetate with varying water content**

| % of water | Temperature (K) | Self-Diffusion Coefficients ($m^2/s$) | | | |
|---|---|---|---|---|---|
| | | Cation | Anion | Water | |
| | | | | | |
| | | | | | |
| Neat Emim acetate | 313 | 2.33E-11 | 2.00E-11 | | H2 |
| | | 2.31E-11 | | | H4 |
| | | 2.31E-11 | | | H5 |
| | | 2.30E-11 | | | H6 |
| | | 2.29E-11 | | | H8 |
| | | 2.30E-11 | | | H7 |
| | | | | | |
| | 373 | 2.09E-10 | 1.77E-10 | | H2 |
| | | 1.91E-10 | | | H4 |
| | | 1.90E-10 | | | H5 |
| | | 1.89E-10 | | | H6 |
| | | 1.93E-10 | | | H8 |
| | | 1.90E-10 | | | H7 |
| | | | | | |
| 11% | 313 | 2.72E-11 | 2.40E-11 | - | H2 |

| | | | | | |
|---|---|---|---|---|---|
| | | 2.72E-11 | | | H4 |
| | | 2.72E-11 | | | H5 |
| | | 2.71E-11 | | | H6 |
| | | 2.70E-11 | | | H8 |
| | | 2.71E-11 | | | H7 |
| | | | | | |
| | 373 | 2.42E-10 | 1.90E-10 | 2.64E-10 | H2 |
| | | 2.06E-10 | | | H4 |
| | | 2.06E-10 | | | H5 |
| | | 2.04E-10 | | | H6 |
| | | 2.06E-10 | | | H8 |
| | | 2.04E-10 | | | H7 |
| | | | | | |
| 21% | 313 | 3.00E-11 | 2.65E-11 | 5.35E-11 | H2 |
| | | 2.89E-11 | | | H4 |
| | | 2.88E-11 | | | H5 |
| | | 2.88E-11 | | | H6 |
| | | 2.89E-11 | | | H8 |
| | | 2.88E-11 | | | H7 |
| | | | | | |
| | 373 | 2.95E-10 | 2.01E-10 | 3.05E-10 | H2 |
| | | 2.12E-10 | | | H4 |
| | | 2.12E-10 | | | H5 |
| | | 2.12E-10 | | | H6 |
| | | 2.11E-10 | | | H8 |
| | | 2.11E-10 | | | H7 |
| | | | | | |
| 35% | 313 | 3.71E-11 | 3.53E-11 | 8.70E-11 | H2 |
| | | 3.68E-11 | | | H4 |
| | | 3.67E-11 | | | H5 |
| | | 3.66E-11 | | | H6 |
| | | 3.66E-11 | | | H8 |
| | | 3.66E-11 | | | H7 |
| | | | | | |
| | 373 | 3.97E-10 | 2.64E-10 | 4.23E-10 | H2 |
| | | 2.70E-10 | | | H4 |
| | | 2.70E-10 | | | H5 |
| | | 2.66E-10 | | | H6 |
| | | 2.68E-10 | | | H8 |
| | | 2.67E-10 | | | H7 |
| | | | | | |
| 42% | 313 | 4.19E-11 | 3.80E-11 | 7.58E-11 | H2 |
| | | 3.82E-11 | | | H4 |
| | | 3.82E-11 | | | H5 |
| | | 3.81E-11 | | | H6 |
| | | 3.82E-11 | | | H8 |

| | | | | | |
|---|---|---|---|---|---|
| | | 3.82E-11 | | | H7 |
| | | | | | |
| | 373 | 4.22E-10 | 2.57E-10 | 4.19E-10 | H2 |
| | | 2.55E-10 | | | H4 |
| | | 2.55E-10 | | | H5 |
| | | 2.54E-10 | | | H6 |
| | | 2.55E-10 | | | H8 |
| | | 2.54E-10 | | | H7 |
| | | | | | |
| 50% | 313 | 4.79E-11 | 4.83E-11 | 1.15E-10 | H2 |
| | | 4.73E-11 | | | H4 |
| | | 4.73E-11 | | | H5 |
| | | 4.72E-11 | | | H6 |
| | | 4.72E-11 | | | H8 |
| | | 4.72E-11 | | | H7 |
| | | | | | |
| | 373 | 5.38E-10 | 3.24E-10 | 5.65E-10 | H2 |
| | | 3.20E-10 | | | H4 |
| | | 3.20E-10 | | | H5 |
| | | 3.17E-10 | | | H6 |
| | | 3.19E-10 | | | H8 |
| | | 3.18E-10 | | | H7 |
| | | | | | |
| 70% | 313 | 7.50E-11 | 7.97E-11 | 1.88E-10 | H2 |
| | | 7.40E-11 | | | H4 |
| | | 7.43E-11 | | | H5 |
| | | 7.41E-11 | | | H6 |
| | | 7.44E-11 | | | H8 |
| | | 7.43E-11 | | | H7 |
| | | | | | |
| | 373 | 8.80E-10 | 4.97E-10 | 9.35E-10 | H2 |
| | | 4.74E-10 | | | H4 |
| | | 4.79E-10 | | | H5 |
| | | 4.79E-10 | | | H6 |
| | | 4.79E-10 | | | H8 |
| | | 4.79E-10 | | | H7 |
| | | | | | |
| 91% | 313 | 3.30E-10 | 3.42E-10 | 7.86E-10 | H2 |
| | | 3.30E-10 | | | H4 |
| | | 3.32E-10 | | | H5 |
| | | 3.33E-10 | | | H6 |
| | | 3.33E-10 | | | H8 |
| | | 3.32E-10 | | | H7 |
| | | | | | |
| 92% | 313 | 3.57E-10 | 3.70E-10 | 8.45E-10 | H2 |
| | | 3.59E-10 | | | H4 |

| | | | | | |
|---|---|---|---|---|---|
| | | 3.59E-10 | | | H5 |
| | | 3.60E-10 | | | H6 |
| | | 3.60E-10 | | | H8 |
| | | 3.57E-10 | | | H7 |
| | | | | | |