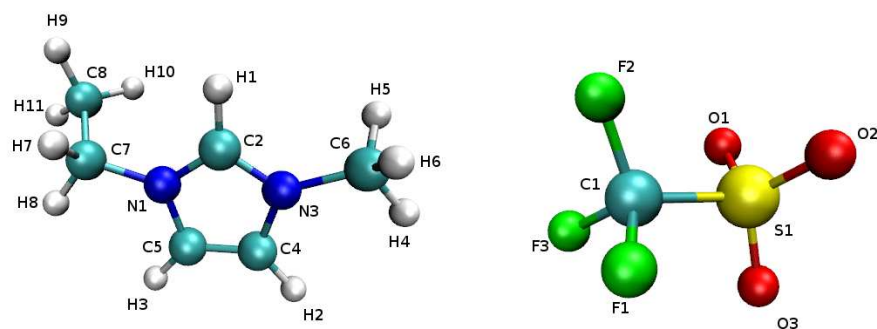
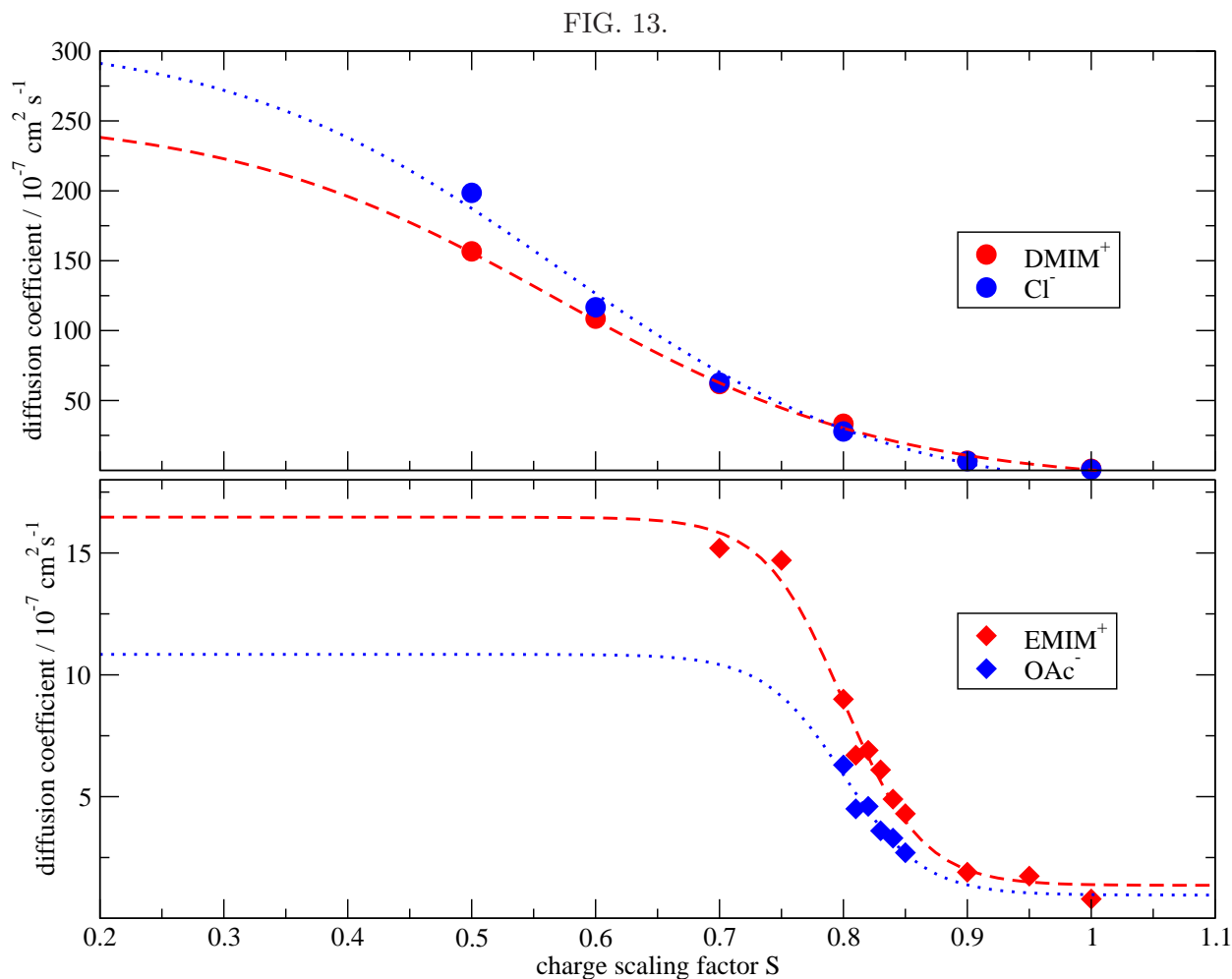


## SUPPLEMENTARY MATERIAL



| atom | partial charges $q_{i\beta}$ of the cation / e |   | polarizability $\alpha_{i\beta}$ / $\text{\AA}^3$ |
|------|--|---|---|
|      | charge-scaled system ( $S^{\text{eff}}=0.74$ ) | polarizable system ( $\alpha = 100\%$ ) |   |
| C6   | 0.09176  | 0.12400                                 | 1.28860   |
| H4   | 0.04736  | 0.06400                                 | (0.41342)   |
| H5   | 0.04736  | 0.06400                                 | (0.41342)   |
| H6   | 0.04736  | 0.06400                                 | (0.41342)   |
| N1   | -0.19758                                       | -0.26700                                | 0.97157   |
| C2   | 0.30118  | 0.40700                                 | 1.28860   |
| N3   | -0.19758                                       | -0.26700                                | 0.97157   |
| C4   | 0.07770  | 0.10500                                 | 1.28860   |
| C5   | 0.07770  | 0.10500                                 | 1.28860   |
| H1   | 0.07178  | 0.09700                                 | (0.41342)   |
| H2   | 0.06956  | 0.09400                                 | (0.41342)   |
| H3   | 0.06956  | 0.09400                                 | (0.41342)   |
| C7   | 0.09620  | 0.13000                                 | 1.28860   |
| H7   | 0.04070  | 0.05500                                 | (0.41342)   |
| H8   | 0.04070  | 0.05500                                 | (0.41342)   |
| C8   | -0.04366                                       | -0.05900                                | 1.28860   |
| H9   | 0.03330  | 0.04500                                 | (0.41342)   |
| H10  | 0.03330  | 0.04500                                 | (0.41342)   |
| H11  | 0.03330  | 0.04500                                 | (0.41342)   |
| sum  | 0.74000  | 1.0000                                  |   |

| atom | partial charges $q_{i\beta}$ of the anion / e  |   | polarizability $\alpha_{i\beta}$ / $\text{\AA}^3$ |
|------|--|---|---|
|      | charge-scaled system ( $S^{\text{eff}}=0.74$ ) | polarizable system ( $\alpha = 100\%$ ) |   |
| C1   | 0.25900  | 0.35000                                 | 1.28860   |
| F1   | -0.11840                                       | -0.16000                                | 0.44475   |
| F2   | -0.11840                                       | -0.16000                                | 0.44475   |
| F3   | -0.11840                                       | -0.16000                                | 0.44475   |
| S1   | 0.75480  | 1.0200                                  | 2.47445   |
| O1   | -0.46620                                       | -0.63000                                | 0.85197   |
| O2   | -0.46620                                       | -0.63000                                | 0.85197   |
| O3   | -0.46620                                       | -0.63000                                | 0.85197   |
| sum  | -0.74000                                       | -1.0000                                 |   |



**Fig. 13:** Diffusion coefficients of molecular ionic liquids from Ref. 75 and 56.

|                   | $A_0$ | $A$    | $k$   | $\alpha_0$ |
|-------------------|-------|--------|-------|------------|
| DMIM <sup>+</sup> | 254   | -264   | 7.46  | 0.57       |
| Cl <sup>-</sup>   | 311   | -332   | 7.46  | 0.57       |
| EMIM <sup>+</sup> | 16.47 | -15.11 | 31.25 | 0.80       |
| OAc <sup>-</sup>  | 10.84 | -9.88  | 31.25 | 0.80       |

TABLE II. Fit parameters of the logistic function for the above displayed diffusion coefficients. Please note, that the prediction of diffusion coefficients for DMIM chloride above a scaling factor  $\gg 1.0$  leads to wrong results due to  $A_0 < |A|$ .