Predicting Sigma-Profile for Ionic Liquids Using COSMO. Supporting information

A. COSMO calculation from Material Studio. Results.
B. Sigma profiles
C. Python codes

A. COSMO calculation from Material Studio. Results.

Materials Studio requires the following code to perform COSMO calculations:

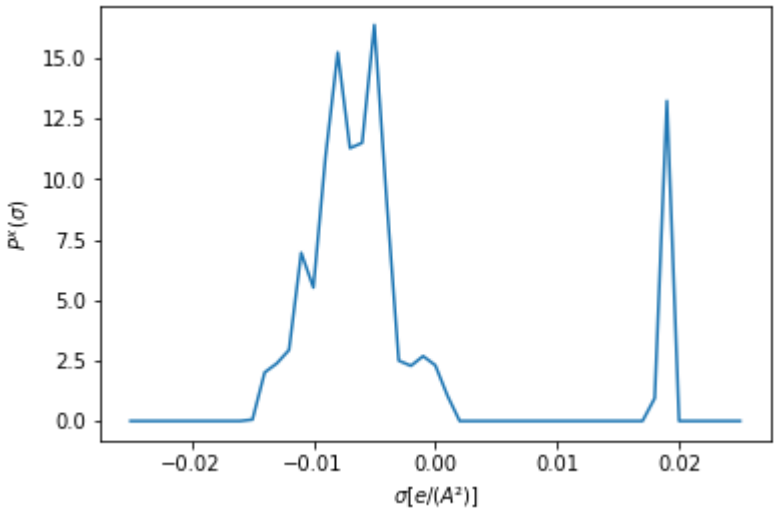
```
Basis_Version     v4.0.0

# Environment Keywords
Cosmo                     on
Cosmo_Grid_Size           1082
Cosmo_Segments            92
Cosmo_Solvent_Radius      1.300000
Cosmo_A-Matrix_Cutoff     7.000000
Cosmo_Radius_Incr         0.000000
Cosmo_A-Constant          1.882190
Cosmo_B-Constant          0.010140
Cosmo_RadCorr_Incr        0.150000
Cosmo_Atomic_Radii
1         1.300000
6      2.000000
7         1.830000
8         1.720000
9         1.720000
15        2.120000
16        2.160000
17        2.050000
35        2.160000
53        2.320000
```

COSMO calculation results are attached in .txt files for every cation and chloride anion.

B. Sigma profiles

The sigma profiles are generated with our first code by introducing any cation.txt file and chloride.txt file.

As example, [MMIM][Cl] sigma profile:



C. Python codes

We divided our work in four separately Python codes to make it understandable:

1. Sigma profile and net charge generation code:

We developed a code to generate sigma profiles for ionic liquids by computing the results coming from Material Studio COSMO analysis. The remaining net charge of those sigma profiles are also determined by using this code.

2. Regression code:

This code manages the generated sigma profiles by ascribing their tendency to a second order polynomial regression.

3. Sensitivity analysis code:

One-at-time approach, scatter plots and Morris method sensitivity analysis are generated by this code.

4. Activity coefficient code:

This code reports the activity coefficients for binary mixtures with different mole fractions and temperatures. However, the code requires long time to generate the activity confident and its accuracy was not validated by comparing with literature results.