How to generate SDFs with TRAVIS

This document is written to explain how to draw spatial distribution of anions in the first shell around a cation by using $[N_{1444}][NTf_2]$ (Fig. 1) as an example.

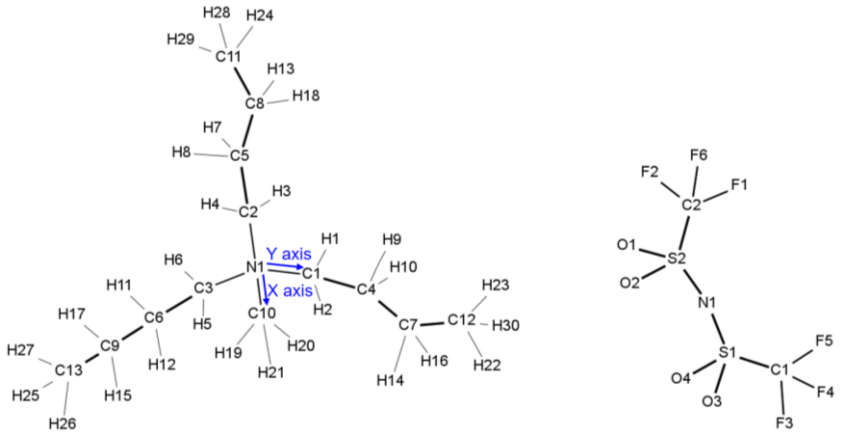


Fig. 1 Structure of $[N_{1444}][NTf_2]$

1. Create a new directory and put HISTORY file there.
   *HISTORY file is so huge that it takes much time to copy. It is recommended to make a link from the original location by executing “ln -s (Original location)/HISTORY HISTORY” in the created directory.

2. Execute “travis HISTORY” in the created directory, and answer the displayed questions based on your model (and preference). Default answers are shown in brackets and when you choose the default answers, just type Enter. Questions and answers shown below are based on $[N_{1444}][NTf_2]$.

```
Do you want to assign atom data to them (y/n)? [yes]
Automatically rename all atoms to corresponding elements (recommended) (y/n)? [yes]
```

```
Does your system really contain "Cs" atoms (y), or are these "C" atoms (n)? [no]

  Renaming 768 "Cs" atoms to "C"...

Does your system really contain "Nb" atoms (y), or are these "N" atoms (n)? [no]

  Renaming 256 "Nb" atoms to "N"...

Does your system really contain "Sb" atoms (y), or are these "S" atoms (n)? [no]
```

```
Use the advanced mode until the analysis selection menu (y/n)? [no]
```

```
Use these values (y) or enter different values (n)? [yes]
Update cell geometry in every time step (i.e., NPT ensemble) (y) or use fixed cell (n)? [yes] n
```

Usually, NVT ensemble is used for production run.

```
Create images of the structural formulas (y/n)? [no] y
```

After answering “Create images of the structural formulas?”, press “Ctrl” and “c” at the same to quit once. Then, execute “ls -l”, and you will find “.dot” files.

```
dot0.log
HISTORY -> ../Run1/HISTORY
input.txt
mol1_C2F6NO4S2.dot
mol2_C13H30N.dot
mol2_C13H30N_no_H.dot
travis.log
```

3. Execute “neato -Tpng mol1_****.dot -o mol1_***.png”.
   (In $[N_{1444}][NTf_2]$ example, execute “neato -Tpng mol1_C2F6NO4S2.dot -o mol1_C2F6NO4S2.png”.)
   Then, execute “neato -Tpng mol2_****.dot -o mol2_***.png”.
   (In $[N_{1444}][NTf_2]$ example, execute “neato -Tpng mol1_C13H30N.dot -o mol1_C13H30N.png”.)
   *If you cannot execute the command, visit https://www.graphviz.org/download/ and download Graphviz.

4. When you execute “ls -l”, you will find two png files. After sending these png files to your local machine, open them and confirm the structure.
   (In $[N_{1444}][NTf_2]$ example, you will find the structure shown in Fig 1.)

5. Then, return to the directory created in Step 1, and execute “travis HISTORY”. Restart answering the questions again. When you face “Create images of the structural formulas?”, answer no (just type Enter) this time, and keep answering.

```
Accept these molecules (y) or change something (n)? [yes]
Which functions to compute (comma separated)? sdf
Use the advanced mode for the main part (y/n)? [no]

Which of the molecules should be the reference molecule (C2F6NO4S2=1, C13H30N=2)? 2
Please enter three comma-separated reference atoms (e.g. "C1,H2,O1"): N1,C10,C1
The first reference atom will be put into the center.
The 2nd reference atom will be put onto the positive X axis.
The 3rd reference atom will be put into the X-Y plane with positive Y values.

Observation 1 >>>

Perform this observation intramolecular (within the reference molecule) (0) or intermolecular (1)? [1]

Which molecule should be observed (C2F6NO4S2=1, C13H30N=2)? 1
Which atoms to observe (e.g. "C1,C3-5,H", "*"=all)? [#2] *
Please enter radius of this SDF in pm: [2700.0] 800
Please enter binning resolution of this SDF per dimension: [100]

Add a condition to this observation (y/n)? [no]

End of Observation 1 <<<

Add another observation (y/n)? [no]

Map a quantity to the surface of the SDF (y/n)? [no]
Up to which degree should the SDFs be smoothened (0=not at all)? [2]
Calculate SDF values in nm^-3 (n) or relative to uniform density (y)? [no]

In which time step to start processing the trajectory? [1]
How many time steps to use (from this position on)? [all]
Use every n-th time step from the trajectory? [1]
```

Type “sdf” to obtain SDF.

In this case, C13H30N (cation) is used as the reference molecule.

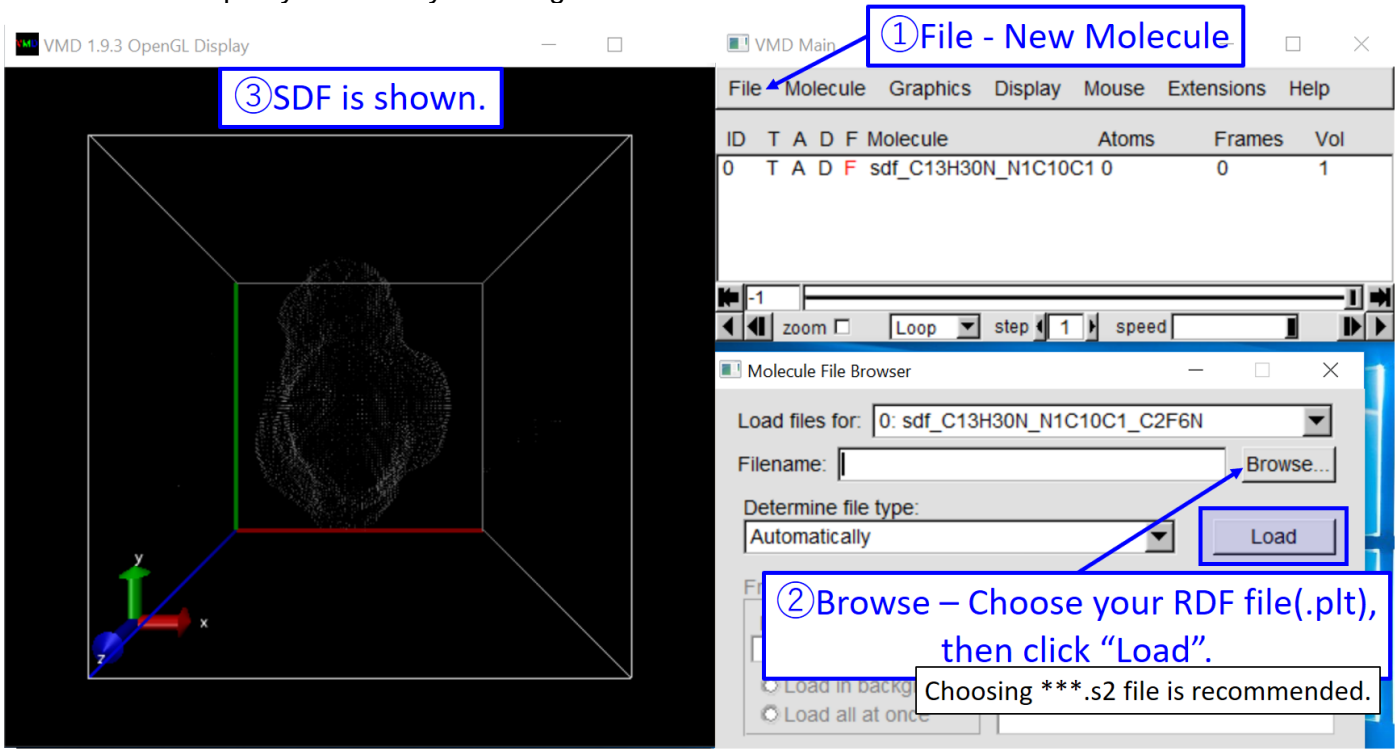
You should decide each atom based on the png files obtained in Step 4.

In this case, all atoms in C2F6NO4S2 (whole anion) is observed.

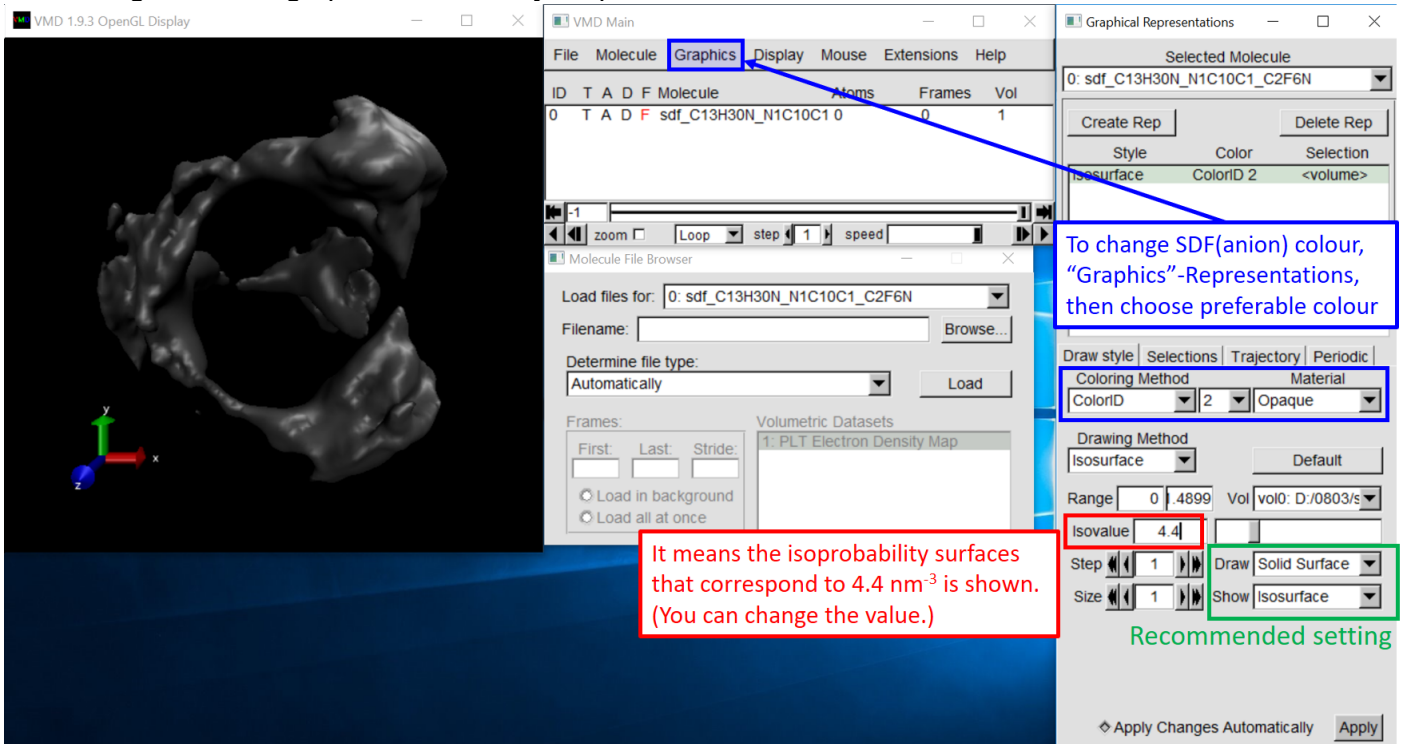
```
*** The End ***

[scarf686@ui3 travis_analysis]$ ls -l
total 49200
lrwxrwxrwx 1 scarf686 cseg       15 Mar  6 16:47 HISTORY -> ../Run1/HISTORY
-rw-r--r-- 1 scarf686 cseg     2082 Mar  7 09:59 input.txt
-rw-r--r-- 1 scarf686 cseg     1635 Mar  7 09:59 ref_c13h30n_n1_c1_c10.xyz
-rw-r--r-- 1 scarf686 cseg 10347415 Mar  7 09:59 sdf_C13H30N_N1C1C10_C2F6NO4S2_#2.cube
-rw-r--r-- 1 scarf686 cseg  4000044 Mar  7 09:59 sdf_C13H30N_N1C1C10_C2F6NO4S2_#2.plt
-rw-r--r-- 1 scarf686 cseg 10623243 Mar  7 09:59 sdf_C13H30N_N1C1C10_C2F6NO4S2_#2.s1.cube
-rw-r--r-- 1 scarf686 cseg  4000044 Mar  7 09:59 sdf_C13H30N_N1C1C10_C2F6NO4S2_#2.s1.plt
-rw-r--r-- 1 scarf686 cseg 10731648 Mar  7 09:59 sdf_C13H30N_N1C1C10_C2F6NO4S2_#2.s2.cube
-rw-r--r-- 1 scarf686 cseg  4000044 Mar  7 09:59 sdf_C13H30N_N1C1C10_C2F6NO4S2_#2.s2.plt
-rw-r--r-- 1 scarf686 cseg    34570 Mar  7 09:59 travis.log
```

After answering all questions, SDF files are created.
SDF files(.plt) and ref file should be sent to your local machine.

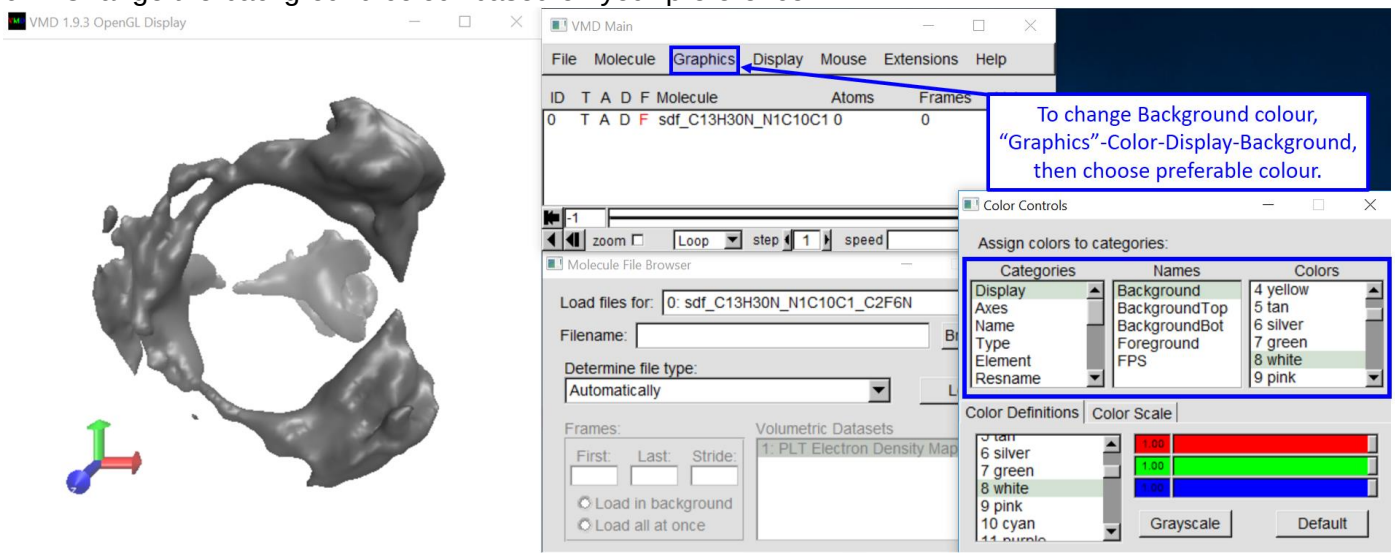
6. Start VMD. Open your SDF by following the instruction below.



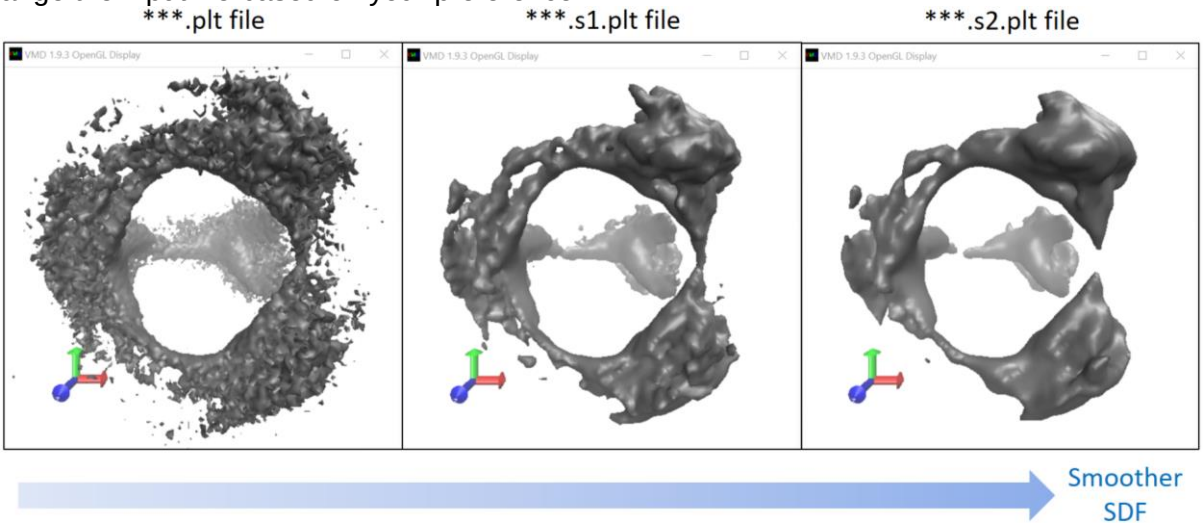
6-1. Change the SDF graphics based on your preference.



6-2. Change the background colour based on your preference.



6-3. Change the input file based on your preference.



7. Insert the reference molecule (cation) by following the instruction below.