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***IMoS (Ion Mobility Software)***

***User Guide***

***Version 1.0***

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## 2 INTRODUCTION

Welcome to the IMoS software guide. This guide is a thorough explanation of the basics of the IMoS software, such as how to use the interface and non-interface versions of the program with several examples of calculations. This manual is not intended to describe the insides of the code. However, included in the IMoS downloadable package, there are several manuscripts (Explanation folder) that describe the insides of the program in detail. If a refresher on the different possible methods available in IMoS to calculate ion mobility and Collision Cross Sections (CCS), section 3 gives some detail. Refer to appropriate literature for a better understanding. If you are familiar with the calculation of ion mobilities, you may skip to section 4. Section 4 describes the installation procedure of IMoS. IMoS may be downloaded from [www.imospedia.com](http://www.imospedia.com) and requires the Matlab Compiler Runtime (check version used). Section 5 lists the files downloaded with IMoS and their purpose. When IMoS is first run, it will create additional files and folders within its main folder. Do not tamper with the IMoSXXX\_mcr folder as it may corrupt the installation. Section 6 establishes how to create a structure file compatible with IMoS. Section 7 describes a process to generate a Density Functional Theory Structure using the freely available software “Avogadro”. Section 8 is the program overview where the interface and governing file IMoS.cla are explained in detail. For the program to run, a coordinate file is required. Section 9 offers a range of examples of how to use the interface and non-interface parallelized versions.

### 2.1 PURPOSE AND TERMS OF USE

The purpose of this manual is to cover the basic understanding of how to calculate ion mobility and collision cross sections of charged molecules in gas phase using the IMoS program (application). IMoS v1.10 is a piece of software created to validate experimental results using numerical models. The author takes no accountability or responsibility for any damages caused due to incorrect usage of the program or due to defects in the application. The application is free of spyware, trojan horses, virus or any malware at the time of download and the application works as described in this user guide; at least to the authors’ best knowledge. This is a licensed software that is made available to the public solely for research purposes. By downloading the application from imospedia.com or by accessing it you indicate that you agree to be bound by all the terms and conditions herein. Any attempt of using this product for profit by anyone without the author or authors expressed agreement is considered a breach of usage terms and may be subject to prosecution and damages. If there are any questions or requests, please contact the author/authors. Sit back and enjoy.

### 2.2 CHANGES FROM PREVIOUS VERSIONS

#### +IMoS v1.10

- The User interface is now much more practical since it has been parallelized for the most common calculations (PA, EHSS/DHSS, TDHSS, TMLJ with and without quadrupole).
- The output file has been modified and cleaned. A copy of the IMoS.cla file and a copy of the coordinate file have both been included in the output file in order to reproduce the results.
- An error where the mobility of other gases that were not diatomic nitrogen was incorrectly provided due to an error in the density calculation. The CCS has not been affected by this.
- Added a Repeat Seed value so that the same seed can be used within the same calculation for different molecules.

#### +IMoS v1.09

- The subroutines have been modified making the program run 20-40% percent faster when using the Trajectory Method.
- Small bugs

## 2.3 ABBREVIATION TABLE

Most common abbreviations used are provided below

Abbreviation	Definition
CCS	Collision Cross Section
DFT	Density Functional Theory
DTM	Diatomic Trajectory Method
DHSS	Diffuse Hard Sphere Scattering
EHSS	Elastic Hard Sphere Scattering
IMoS	Ion Mobility Software
L-J / LenJon	Lennard Jones
MCR	Matlab Compiler Runtime
MC	Monte Carlo
PA	Projection Approximation/Projected Area
PDB	Protein Data Bank
QPol	Quadrupole
SMILES	Simplified Molecular-Input Line-Entry System
SAS	Solvent Accessible Surface
TDHSS	Trajectory Diffuse Hard Sphere Scattering
TM	Trajectory Method
TM	Trajectory Method
TMLJ	Trajectory Method Lennard Jones
TS / TSA	Travelling Salesman
VdW	Van der Waals

## 2.4 VARIABLES TABLE

Most common variables are provided below

Variable	Definition
$K$	Ion mobility
$ze$	Charge of the ion
$n$	Gas density
$\mu$	Reduced mass
$m$	Mass of the gas
$M$	Mass of the ion/nanoparticle
$k_b$	Boltzmann constant
$T_{eff}$	Effective temperature
$\bar{\Omega}_{T_{eff}}$	Collision cross section at effective temperature
$v_d$	Drift velocity
$T$	Environment Temperature
$\zeta$	Correction factor
$\Omega$	Collision cross section
$\Delta p$	Momentum transfer
$\vec{g}_i$	Initial relative velocities
$\vec{g}_f$	Final relative velocities
$N_t$	Number of gas molecules
$\tau_t$	Total time that $N_t$ gas molecules take to collide with the ion
$\vec{F}_D$	Total drag force of the ion
$\vec{E}$	Electrical field
$\Phi$	potential
$r_i$	the relative distance between each of the n atoms (and/or charges) and the gas molecule
$\alpha$	The polarizability of the buffer gas
$\epsilon$	Lennard-Jones(L-J) gas-atom parameters to well-depth
$\sigma$	Lennard-Jones(L-J) gas-atom parameters to zero potential crossing
$k$	Thermal conductivity
$p$	pressure
$K_{eff}$	Effective ion mobility
$K_0$	Reduced mobility



### 3 METHODS

The calculation of ion mobility that IMoS performs is based on Mason-Schamp's first approximation of the two-temperature theory[3]:

$$\langle K \rangle_I = \frac{3}{16} \frac{ze}{n} \left( \frac{2\pi}{\mu k_b T_{eff}} \right)^{\frac{1}{2}} \frac{1}{\bar{\Omega}_{T_{eff}}(1,1)}$$

Here  $ze$  is the charge of the ion,  $n$  is the gas density,  $\mu = mM / (m + M)$  is the reduced mass, with  $m$  the mass of the gas and  $M$  the mass of the ion/nanoparticle,  $k_b$  is the Boltzmann constant,  $T_{eff}$  is the effective temperature and  $\bar{\Omega}_{T_{eff}}(1,1)$  is the Collision Cross Section (CCS). The effective temperature takes into account the effects of strong fields and is calculated as:  $T_{eff} = T + mv_d^2/3k_b$ . Under most instances, i.e. when the electric field is low, the second term of  $T_{eff}$  accounts for less than 1% in the calculation.

The most important part of the code involves calculating  $\bar{\Omega}_{T_{eff}}(1,1)$  directly, or a related quantity using different approximations, obtaining the mobility only once the solution for the CCS is obtained. The CCS is a very complicated parameter that measures the interaction between the charged nanoparticle and the gas molecules in the free molecular regime. This interaction can depend on the size of the gas molecule compared to the charged nanoparticle, their mass, their relative velocity and the potential interaction between them. In what follows, a brief explanation of the most important CCS calculations performed in IMoS is presented, including the Projection Approximation (PA), the Elastic/Diffuse Hard Sphere Scattering (EHSS/DHSS), and the Trajectory Method (TM)[2, 4-8]. The degree of accuracy of the calculation is directly proportional to the computational time.

#### 3.1 PROJECTION APPROXIMATION (PA)

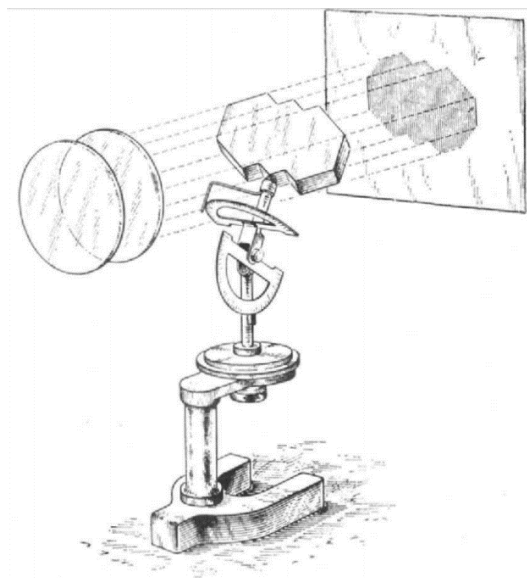


Fig. 5.

Figure 3.1 Mack's projection Area Apparatus.[1]

the name suggests, CCS is directly related to area of interaction between gas and ion. In its most simple definition, this area is equivalent to the projected area of the combination of gas and ion. In short, the gas ion footprint is projected at random angles onto a plane and the area of the shadow is calculated [8, 9]. The average area over all orientation is then calculated and is directly related to the CCS of the ion in the gas of choice as shown in Figure 3.1. For this calculation to work, the Van der Waals (VdW) radii of the atoms in the molecule as well as radii of the gas have to be provided. The area of the all-atom structure with the addition of the gas molecule is calculated either using a Monte Carlo algorithm or a Travelling Salesman (TS) algorithm. The PA method gives rough estimates of CCS for all but the smallest ions in very light gases. The error varies, generally being below 40%, but could be as high as 300% for small highly charged ions in very polarizable gases such as CO<sub>2</sub> or N<sub>2</sub>. The 40% value comes from the general assumption of diffuse reemission for heavy gases like N<sub>2</sub> and CO<sub>2</sub>. This was already studied by Millikan[9] and Epstein[10] who suggested for larger ions an asymptotic value of 1.36\*PA for the CCS. This value maybe augmented by the ion-induced dipole interaction. In the limit of polarization, a minimum mobility is established regardless of the physical PA of the ion. This could effectively increase

the CCS to 2-3 times over PA[11]. If the reason for the deviation from experimental results is known, e.g. due to diffuse reemission, one can attempt to multiply the resulting value of PA value by a correction factor,  $\xi$ , to obtain a more accurate

result  $\Omega = \xi \cdot \text{PA}$ . The PA has the advantage of being the most efficient calculation. In IMoS, the only method that is parallelized is the Monte Carlo algorithm while TS is reserved for plotting.

### 3.2 ELASTIC/DIFFUSE HARD-SPHERE SCATTERING (EHSS/DHSS)

The calculation involving the mobility and  $\bar{\Omega}_{T_{eff}}(1,1)$  corresponds to a calculation of the momentum exchange (momentum transfer) or drag force, i.e. how much does the buffer gas restrict the motion of an ion that is accelerated due to the presence of an electric field. In order to calculate that momentum exchange, the algorithm simulates the trajectories of different gas molecules and calculates the momentum transfer,  $\Delta p$ , of each as:

$$\Delta p \sim m(\vec{g}_f - \vec{g}_i),$$

where  $\vec{g}_i$  and  $\vec{g}_f$  are the initial and final relative velocities. Correcting for the effect of the reduced mass on the algorithm, and knowing the total time  $\tau_t$  that  $N_t$  gas molecules take to collide with the ion, one can calculate the total drag as[12]:

$$\vec{F}_D = \left(1 + \frac{m}{M}\right)^{-\frac{1}{2}} \frac{N_t m}{\tau_t} (\vec{g}_f - \vec{g}_i)$$

Finally, the drag is related to the mobility through the drift velocity, the field and charge,

$$ze\vec{E} = \vec{F}_D \rightarrow KE = KF_D/ze = v_d$$

or

$$K = \frac{ze}{F_D} v_d$$

The calculation is repeated for 3 perpendicular orientations. The final result is then averaged, and the mobility obtained with the above formula. The CCS can then be inferred through the Mason-Schamp approximation. While this calculation slightly differs from other types of ion mobility calculations, it yields equivalent results. Given that initial and final relative velocities are not assumed equal, an advantage of using this approach is that it allows for the study of inelastic collisions.

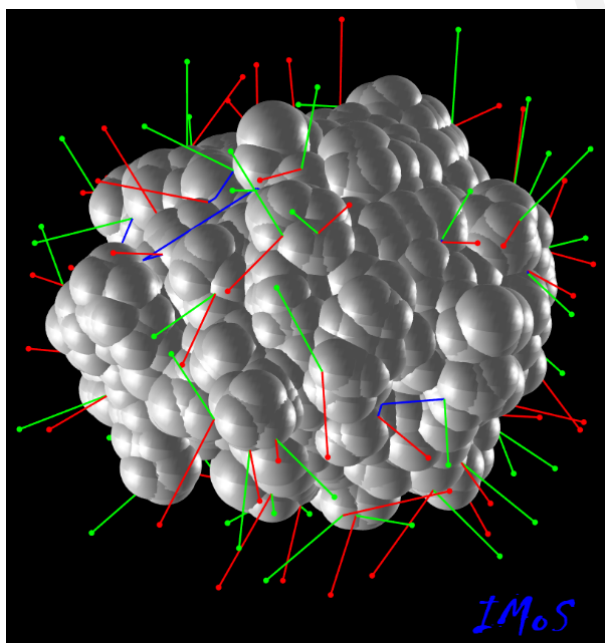


Figure 3.2 EHSS/DHSS of Cytochrome C ion. Red are incoming gas molecules; green are re-emitted gas molecules and blue are partially scattered molecules that collide more than once with the ion.

The EHSS/DHSS method calculates the trajectories as if they were rectilinear not considering any interaction potential and thus using the VdW of gas and ion to study the collision, i.e. using a hard sphere potential. Upon collision with the ion, the gas molecule is re-emitted, checks for secondary collisions (scattering) until the gas molecule leaves the domain and the momentum transfer is calculated. An schematic of the process is shown in Figure 3.2. The original Exact Hard Sphere Scattering only allowed elastic and specular collisions to occur[13]. However, IMoS allows the user to choose an accommodation parameter that specifies that a portion of the collisions maybe regarded as inelastic and may be re-emitted diffusely. The program works as follows. The accommodation parameter has a value between 0 and 1[4, 5]. This parameter only establishes the percentage of gas molecules that are accommodated. For example, choosing 0.9 establishes that 90% of the gas molecules will be accommodated while 10% will follow an elastic and specular collision. The selected 90% may be chosen to be re-emitted diffusely or not using a secondary parameter, labeled diffuse. When diffuse is chosen, the gas molecules are re-emitted at a random angle within a semi-sphere at the point of contact. The re-emission speed of the 90% accommodated molecules may also be chosen. The program allows for plenty of different choices for this velocity, including being

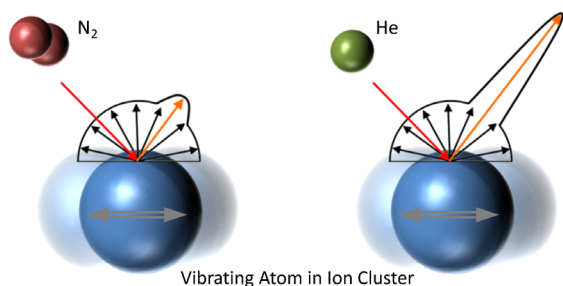


Figure 3.3 A cartoon of the expected reemission mechanisms for two different gases. On the left, for a diatomic gas molecule heavier than most organic atoms, a more diffuse collision is expected with a very small contribution of specular collisions. On the right, for a spherical light gas molecule like He, the expectancy is that the collision will be mostly specular although scattering events and potential interactions might lead to some diffuse reemission[2].

negligible contribution from interaction potentials. Even under diatomic nitrogen, the  $1.36 \cdot PA$  will not hold for very small ions where it seems that the collisions become slightly more elastic. At the same time, for those small sizes, the ion-induced dipole potential becomes quite important and may increase the CCS value even by a factor of two. For these cases, a trajectory method should be employed.

### 3.3 TRAJECTORY METHOD / DIATOMIC TRAJECTORY METHOD (TM/DTM)

The trajectory method follows the logic of the EHSS/DHSS but allows interaction potentials between atoms/charges and the gas molecules. IMoS allows many different types of potentials to be used. Among the different trajectory methods there are two that are the most important, the Trajectory Diffuse Hard Sphere Scattering (TDHSS) which utilizes a  $(4-\infty)$  potential and the Trajectory Method Lennard Jones (TMLJ) which uses a  $(4-6-12)$ .

The TDHSS method is very similar to EHSS/DHSS but adds an ion-induced dipole potential between charges and the gas molecule. Since the gas and ion are hard spheres, one can add inelastic/diffuse collisions to TDHSS in the same way as they are done in the EHSS/DHSS and therefore VdW's radii for atoms and gas must still be provided. For TDHSS, the reemission velocity for those gas molecules that are accommodated should come from a distribution rather than the mean of the distribution. The main reason for this choice is that since there is an attraction potential, lower velocities will lead to more scattering than higher velocities which affects the overall result. TDHSS works well for nanoparticles in diatomic nitrogen gas, in particular for those that are heavily charged. For ions that are smaller than 1.3nm in diameter, TDHSS performs poorly as it seems that smaller ions undergo more elastic collisions (accommodation should be lower). A good estimate for ions in the 0-300Å<sup>2</sup> range of CCS is to set the accommodation coefficient to 0.48 to yield a value close to the TMLJ.

The TMLJ composes the set of algorithms that employ a 4-6-12 potential. It follows the same principles as previous trajectory methods, but the potential is now given by [14]:

$$\Phi(x, y, z) = 4\epsilon \sum_{i=1}^n \left[ \left( \frac{\sigma}{r_i} \right)^{12} - \left( \frac{\sigma}{r_i} \right)^6 \right] - \frac{\alpha}{2} \left( \frac{ze}{n} \right)^2 \left[ \left( \sum_{i=1}^n \frac{x_i}{r_i^3} \right)^2 + \left( \sum_{i=1}^n \frac{y_i}{r_i^3} \right)^2 + \left( \sum_{i=1}^n \frac{z_i}{r_i^3} \right)^2 \right]$$

$r_i = (x_i, y_i, z_i)$  is the relative distance between each of the  $n$  atoms (and/or charges) and the gas molecule, with  $\alpha$  being the polarizability of the buffer gas, and  $\epsilon$  and  $\sigma$  are the Lennard-Jones(L-J) gas-atom parameters corresponding to well-depth and zero potential crossing, respectively. The aforementioned potential is then used to calculate the acceleration of the gas molecule and its trajectory until the gas molecule leaves the domain and the angle of deflection recorded for each gas

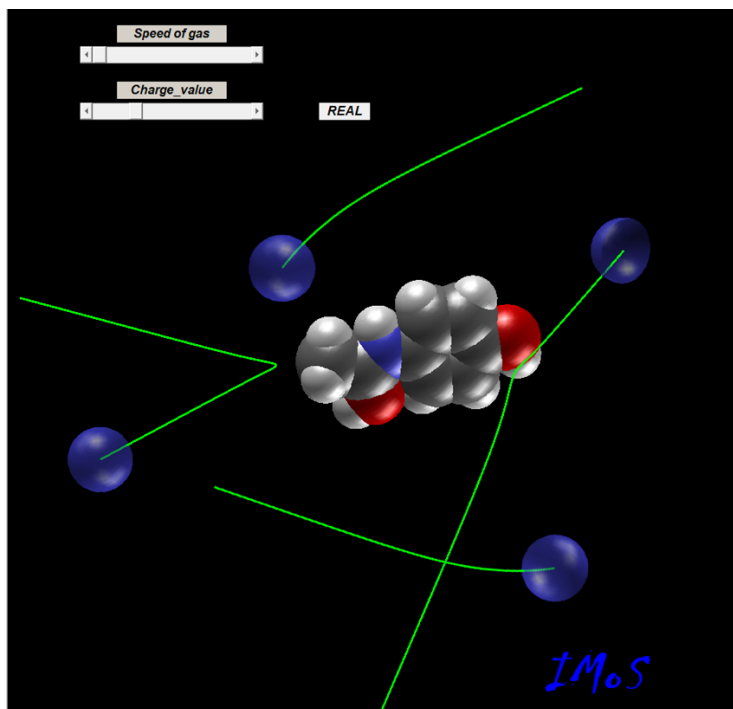


Figure 3.4 IMoS cartoon of the TMLJ 4-6-12 potential interaction.

molecule. If the L-J potentials are optimized correctly, TMLJ yields some of the most accurate results available for numerical CCS and mobility. The optimization of L-J parameters can be done straightforward if empirically accurate information is available. IMoS allows to change the L-J parameters quite easily through a tabulated table. Each different gas requires a different set of L-J parameters. IMoS includes optimized parameters for C, H, O, N and F in He and N<sub>2</sub> and has general values for other atoms. Even when L-J parameters are not exactly known for a small fraction of the atoms, the calculations may still be reliable for large ions, in particular when the unknown atoms are not on the surface. The error is approximately 2% on average for TMLJ calculations in N<sub>2</sub> and He with optimized L-J parameters. A cartoon of the soft interaction when using an all-energy interaction 4-6-12 potential is shown in Figure 3.4.

or N<sub>2</sub> gas, IMoS offers the possibility of adding an ion quadrupole potential together with gas orientation averaging. The quadrupole moment is obtained by placing one negative charge of 0.4825e on each nitrogen and one

positive charge of 0.965e in the center of the molecule. In such a way, the quadrupole potential can be expressed as[15]:

$$\Phi_{IQ}(x, y, z) = \sum_{j=1}^3 \sum_{i=1}^n z_i z_j e^2 / r_{ij}^3$$

The index j denotes three different N<sub>2</sub> charges (where 2 is the center charge) and index i indicates the charges on the ion. The orientation of the N<sub>2</sub> molecule is taken into account by assuming that the interaction potential may be averaged over the rotational degrees of freedom. This assumption arises from the expectation that molecular rotation of N<sub>2</sub> is not quenched and that only partial locking may occur. The ion quadrupole potential could have an effect on very small molecules. Given the high computational cost of adding the ion-quadrupole potential, the ion quadrupole should be considered only if its effect has the same order of magnitude as the rest of the potential interaction and may not be embedded in the L-J potentials directly.

A final method considered in IMoS is that of the diatomic trajectory method (DTM)[6]. This method takes into account the moment of inertia of the N<sub>2</sub> molecule together with a 4-∞ potential and conserves not only linear momentum but also angular momentum of the gas molecule. Similarly to TDHSS, the re-emission may be chosen to be elastic/inelastic and specular/diffuse depending on the choice of accommodation. The results from DTM follow the same trend as those of TDHSS although the resulting CCS may be larger due to augmented effective size of the gas molecule. Rotation and scattering effects due to the diatomic nature seem to be increasingly important for very small ion sizes (in particular, smaller than the gas molecule). The DTM subroutine is not parallelized and hence its performance falls behind the other subroutines specified above.

A table is provided in the next section outlining the different methods, characteristics of the methods with advantages and disadvantages. A benchmark comparison is also provided using the TMLJ method. Refer to the table for speed comparisons to other methods.

### 3.4 CALCULATION METHODS TABLE

A table describing possible methods.

Method	Definition	Advantages	Disadvantages	Speed Comparison
<b><i>PA</i></b>	Projection Approximation	Most Efficient. Result may be analytically adjusted to accommodate other effects: $\Omega = L \cdot \xi \cdot PA$	It lacks any kinetic theory behind it. Results could be up to 300% wrong. Adjusting parameters might be difficult to calculate for all ions	Approximately 40-100 times faster than TMLJ assuming 500 orientations are calculated.
<b><i>EHSS /DHSS</i></b>	Exact Hard Sphere Scattering with specular/diffuse, elastic/inelastic reemission	Second Most efficient. Very fast and useful for very large molecules and nanoparticles. Takes into account the $\xi$ scattering parameter. The accommodation parameters can be adjusted to any gas.	Does not take into account any potentials. Setting accommodation coefficient to 90% for small molecules in N2 is ill-advised and disagrees with results from TMLJ	Approximately 10-20 times faster than TMLJ assuming the same number of gas collisions.
<b><i>TDHSS</i></b>	Trajectory Method with $4 - \infty$ potential and specular/diffuse, elastic/inelastic reemission	Trajectory method that takes into account the ion-induced dipole potential. Fastest out of all TM methods.	Accommodation parameter is complicated to set for all ions.	Approximately 20% faster than TMLJ when partial charges are present and up to 50% faster without partial charges.
<b><i>TMLJ</i></b>	Trajectory Method with $4 - 6 - 12$ potential	Most well-rounded method. Gold standard in terms of accuracy.	Slower compared to other methods. Requires optimized L-J parameters for all gases which are difficult to obtain	See benchmark graph in section 3.5.
<b><i>TMLJ qpol</i></b>	Trajectory Method for Nitrogen that includes the ion quadrupole potential	Adds the ion quadrupole potential to the N2 calculations.	Slow compared to TMLJ. Requires optimized L-J parameters different from those of TMLJ.	Approximately 5-7 times slower than TMLJ.
<b><i>DTM</i></b>	Diatomic trajectory method with $4 - \infty$ potential	Add two rotational degrees of freedom to the N2 molecule and accounts for the ion induced dipole potential.	Very slow and not optimized. Requires an accommodation coefficient that is different from TDHSS. Not parallelized.	On a single core, it is an order of magnitude slower than TMLJ.



### 3.5 BENCHMARK COMPARISON.

Benchmark comparison using a set of atoms ranging from 17 to 720 atoms for the TMLJ Method for 3 orientations and 900000 total number of gas molecules (300000\*3). The benchmark was done using a TimeStep of 100, on a 3.6Ghz computer using 6 physical cores. Use this result as an approximation as speed varies from computer to computer.

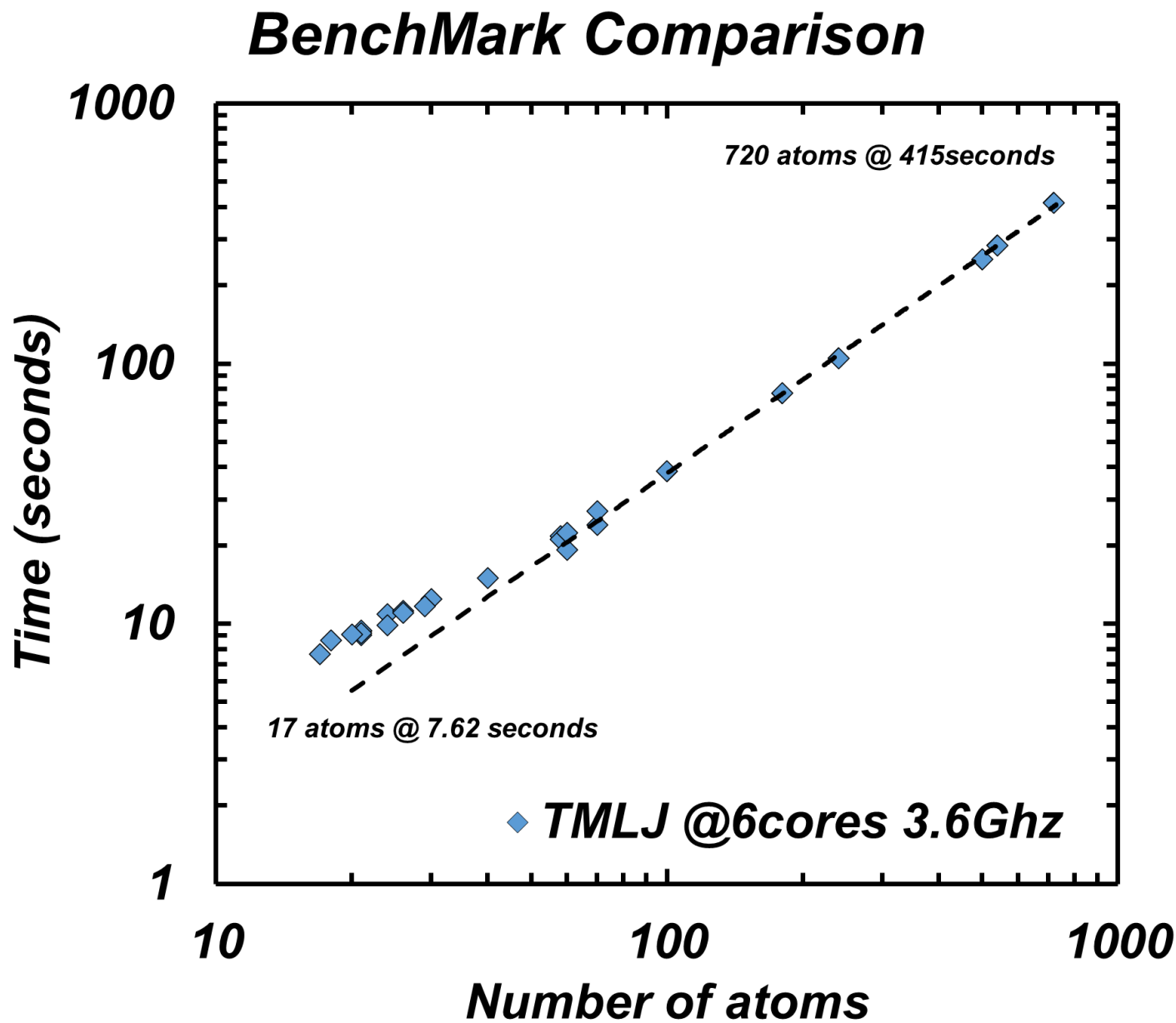


Figure 3.5 Benchmark comparison for the TMLJ method.

## 4 INSTALLATION AND SETUP

### 4.1 WINDOWS INSTALLATION

In order to run IMoS, Matlab Compiler Runtime (MCR) version 9.5 (check if different) must be installed. Navigate to the link below (or to the Mathworks website if required) to download the appropriate runtime files.

<http://www.imospedia.com/imos/download-area/>

Once downloaded, run the MCR executable and follow the prompts. Administrator privileges will be required for installation. You may also download the IMoSv110\_install.exe that will install the software as an app.

Next, the IMoS files will be downloaded. Navigate to the link below and download the desired version of the IMoS software.

<http://www.imospedia.com/imos/download-area/>

Extract the files to a directory that does not require administrator privileges to write to. Once extracted, open the IMoSXXX.exe file. There is no installation required but note that the first run may take longer than usual, as initial files/directories are created. Follow the examples below to run the code appropriately.

### 4.2 LINUX INSTALLATION

1.) In order to run IMoS, Matlab MCR version 9.8 (Check if different) must be installed. Navigate to the link below to download the appropriate runtime files.

<https://www.mathworks.com/products/compiler/matlab-runtime.html>

2.) Once downloaded, write down the filepath of the runtime folder. Next, the IMoS files will be downloaded. Navigate to the link below and download the desired version of the IMoS software.

<http://www.imospedia.com/imos/download-area/>

3.) Extract the files to a directory and allow the appropriate permissions. Once extracted, follow the instructions located in the “readme.txt” file. One has to add the Library Path to the MCR prior to executing IMoS. To do so, execute the following two commands:

```
export
```

```
LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/PATHTOMCR/MCR/v98/runtime/glnxa64:/PATHTOMCR/MCR/v98/bin/glnxa64:/PATHTOMCR/MCR/v98/sys/os/glnxa64:/PATHTOMCR/MCR/v98/extern/bin/glnxa64
```

```
export XAPPLRESDIR=/PATHTOMCR/MCR/v98/X11/app-defaults
```

Here substitute “PATHTOMCR” for the path to MCR in your comp (normally usr/local/matlab/). Also change “v96” for the appropriate version of MCR if needed. Once the library paths have been added, you can run the shell script:

- `./run_IMoSXXXL64.sh /PATHTOMCR/MCR/v98`

to run IMoS. The above commands can be (and should be) added to your batch or profile files in order to not have to execute them every time you run IMoS.

4.) **Submit a JOB to a QUEUE in a Super-Computer using IMoS.** The Linux version comes with an example, runimos2, of how to submit a job queue. It is a general version of a queue submission for IMoS and details of how to submit a proper queue to your super-computer of choice should be addressed with IT personnel.

### 4.3 MAC INSTALLATION

The Mac version of IMoS is available and its installation follows closely to that of Linux. Make sure you understand how shell scripting works in Unix systems before attempting the installation. Follow Matlab documentation on standalone application to learn how to run the application properly. A summary of how to install and run is provided below:

If installing IMoS as an application, the installation process will install the appropriate MCR. If only the distribution files are installed, install the appropriate MCR version (currently v9.9).

- 1) Download the appropriate files.

<http://www.imospedia.com/imos/download-area/>

- 2) Install.

- A) If the application file is downloaded, click on it and follow the process of installation. It is recommended that the installation folder is a folder you have easy access to. The process will ask you to install the MCR. Take note of the folder where the MCR is installed.
- B) If only the files are downloaded, place them on a folder of easy access and extract them. Download and install the appropriate MCR (v 9.9 as of now) from:

<https://www.mathworks.com/products/compiler/matlab-runtime.html>

Take note of the location where the MCR is installed.

- 3) Once installed, open a terminal and go to the folder where IMoS has been installed. Make sure you provide writing access to this folder. To provide access to write in the folder (and subfolders) use the command “chmod -R 777 foldernamendpath”.
- 4) From the terminal, run: “./run\_IMoS110Mac64.sh /Applications/MATLAB/MATLAB\_Runtime/v99”  
If the MCR is installed in a custom folder, substitute the path “/Applications/MATLAB/MATLAB\_Runtime/v99” for the appropriate path. If the version is different than v99, also choose the appropriate version.



## 5 FILE EXPLANATIONS

The following table lists the different files that are provided with IMoS. While the number of files may change from version to version, most of the files should be similar to the ones that appear here.

Title	Description
<b>Root</b>	
Readme.txt	"Readme" file detailing the installation process.
IMoSXXWin64.exe	IMoS V1.10 executable. The version and platform may change as well as the extension.
IMoSXXWin64.ctf	Component technology file. This file will create a folder with some of the files required to run MCR. If the program becomes corrupt. You may delete the _mcr folder completely and the .ctf file will recreate a new one. Make sure that you have permission to write in the folder where IMoS is installed.
Icon.ico	Icon file.
Splash.png	Splash screen picture.
<b>IMoS.cla</b>	Master configuration / input file. Edit with a text editor to change inputs to IMoS.
<b>IMoS2.cla</b>	Input file to run interface parallel computations. NOT the master configuration.
LJtable.xlsx	Excel file defining the Lennard Jones parameters for multiple gasses. Use sheet 8 to enter custom values when needed.
IonColor.xlm	Excel file defining the plot colour of all atoms.
Vdwimos.xlsx	File contains the Van der Waals radii of the atoms. It also contains the masses of the atoms to be used if necessary. This may be altered at will.
<b>Filefolder</b>	
1IGY.pdb	Humanin Protein pdb file.
Anallainb.xlsx	16 DFT structures provided from ref. [16].
Anthracene_pop.mfj	Mobcal .mfj type file that can be run with IMoS.
C60positions.xlsx	Several fullerene structures.
NaI_coors.xlsx	Several DFT calculations of Sodium Iodide Clusters.
N-Ethylaniline_pop.mfj	Mobcal .mfj type file that can be run with IMoS.
pdby32mod12.pdb	Humanin molecule with different models.
xtal-fix-charge6-cytoc.pdb	Crystal structure of Cytochrome C directly taken from PDB database.
Spheretest.xlsx	Sphere to test Millikan and Epstein's 1.36 value.
Smallions.xlsx	DFT of small ions to test High Fields and Effective temperatures
<b>Explanations Folder</b>	
IMoSManualv110.pdf	This Manual.
LarribaJPCA2013.pdf	The explanation folder contains multiple published works that explain how the different subroutines of IMoS work as well as how to optimize LJ parameters.
LarribaJCP2013.pdf	More computational aspects of IMoS.
LarribaJoChemPhys2014.pdf	Diatomic version of the code
LarribaPCCP2015.pdf	Difference between N2 and He gases. Why is one more diffuse and the more specular?
ShrivastavASMS2017.pdf	Test of IMoS vs. Mobcal results.
WuJPCMS2018.pdf	Optimization of Lennard-Jones potentials.
<b>savefolder</b>	
saveme.txt	Results file example created with IMoS.

saveme.cla	CLA file, created with IMoS. Includes all input parameters used for the associated results file. Can be used to quickly re-run calculations when needed.
<b>SPEED folder</b>	
speed.exe	File used to transform Gaussian outputs into excel files to be used with IMoS.
<b>Optimizer folder</b>	
Savefolder	Folder specific to L-J optimization. Any optimization results will be saved here.
Optinput.txt	Contains inputs to run the optimizer. “interface 0 1” will run the optimizer as well the appropriate checkbox in the interface.
LJTable.csv	These are the LJ parameters that the optimizer will use and modify. For convenience, default csv values are also provided in different csv tables.
Vdwimos.csv	VdW radii that the optimizer will use and modify. For convenience, default values are also included.
ResultsoptX.txt	Results output from optimization calculation.
<b>Workhorse folder</b>	
Different coordinate files	“interface 0 2” option or “interface 1 0” with appropriate checkbox will run all .xls, .pdb or .mfj files contained in this folder.
<b>Workmulecla folder</b>	
Different IMoS.cla files	“interface 0 3” option or “interface 1 0” with appropriate checkbox will run all .cla files contained in this folder
<b>Platform only files</b>	
Msvcrl20.dll	Visual C file required to run some C code subroutines. Most Windows platforms already have this file, but some do not.
Run_IMoSXXL64.sh	Shell Script required to run IMoS from the command line or when submitted to a queue.

## 6 STRUCTURE FILES

This section deals with the creation of a structure file to be used with IMoS. IMoS supports the use of .xlsx, .mfj and .pdb files. IMoS only has compatibility with Mobcal .mfj files but please refer to the authors of Mobcal on how to write .mfj files.

### 6.1 STRUCTURE FILE FOR EXCEL

Excel maybe used to create and store structure files to be used in IMoS. One can write a different structure per excel sheet so that many structures can be organized within a single file. Figure 6.1 shows an example of a sheet file. The structure file contains 4 to 7 “Data” columns. The first 4 are required to use PA and EHSS/DHSS methods. Columns 1-5 are required to run TDHSS and TDM algorithms and columns 1-5 and 7 are required for TMLJ with or without qpol.

<i>X, Y and Z Coord</i>			<i>VdW radii</i>	<i>P. Charge</i>		<i>Atom label</i>	
A	B	C	D	E	F	G	H
0.149	0.31	-0.331	1.7	0.350817	TOTAL z	12	
-0.424	-0.914	-0.694	1.7	-0.27724	1	12	
-0.628	1.343	0.197	1.7	-0.23731	Totalmass	12	
-1.784	-1.116	-0.499	1.7	-0.19007	152	12	
-1.993	1.142	0.388	1.7	-0.27805	Crossectio	12	
-2.575	-0.089	0.043	1.7	0.420172		12	
-3.889	-0.356	0.201	1.52	-0.56208		16	
1.563	0.544	-0.568	1.55	-0.60237		14	
2.557	-0.024	0.074	1.7	0.684439		12	
2.383	-0.951	1.221	1.7	-0.41605		12	
3.808	0.196	-0.264	1.52	-0.50018		16	
1.789	1.195	-1.319	1.1	0.391226		1	
0.182	-1.699	-1.136	1.1	0.1892		1	
-0.177	2.293	0.467	1.1	0.191966		1	
-2.255	-2.054	-0.77	1.1	0.20297		1	
-2.601	1.94	0.805	1.1	0.186204		1	
-4.371	0.399	0.567	1.1	0.447165		1	
2.526	-1.981	0.874	1.1	0.186273		1	
1.392	-0.859	1.664	1.1	0.149795		1	
3.163	-0.744	1.959	1.1	0.195939		1	
3.941	0.776	-1.034	1.1	0.467198		1	

Figure 6.1 Structure File for Excel

#### 6.1.1 Letter Label Column

An atom label column maybe used as the first column of the file (see for example NaI\_coors file). In it, one can label the atoms using letters for convenience. This column is, in general, ignored unless TMLJ is run and “Data” column number 7 is missing. If that is the case, then IMoS will attempt to use Column 1 as a guide to give L-J parameters to the atoms based on their atom label. The atom label (e.g. Na for sodium) commonly used by IMoS can be taken in in vdwimos file.

#### 6.1.2 Coordinate Columns

The first 3 data columns correspond to the x, y, and z coordinates of the center of the atom. Their values are given in Angstroms.

### 6.1.3 VdW Radii Column

The 4<sup>th</sup> data column corresponds to the VdWs radii of the atoms given in Angstroms. This column may not be blank but if the value of the first row is set to -1, it will ignore the rest of the column and instead pick the VdW values directly from the vdwimos file.

### 6.1.4 Partial Charge Column

The 5<sup>th</sup> data column is reserved for charges and partial charges. One can choose to give partial charges to all atoms or just set particular charges in different atoms of choice. The total sum of the charges in this column must be equivalent to the charge set in column 5 or to the charge set in the imos.cla file or at the interface. The sum of all partial charges must be within 0.8% of an integer. The column may be left blank. If this is the case and a Trajectory Method is selected, the charge in column 5 will be set at the geometrical center of the molecule prior to the calculation starting.

### 6.1.5 Total Charge Column/Total Mass Column

In the 6<sup>th</sup> data column, one may set the total charge (integer) and total mass in Da of the ion on the second and fourth row respectively. The values set on this column override any other value in either the imos.cla or the interface if it is used. This is very useful when running several structures in a batch as there will be no need to change the mass and charge on each and every ion. The column may be left blank and the values of charge and mass will be taken from either the imos.cla file or the interface. If a -1 is set as the total mass, IMoS will read the masses from vdwimos file.

### 6.1.6 Atom Number Label Column

The 7<sup>th</sup> data column is used to assign the L-J potential parameters (as well as the color for plotting) used in TMLJ. The values that must be used for each particular atom can be taken from the vdwimos file but they, in general, correspond to the rounded mass of the ion. Some atoms have the same rounded atomic number (e.g. Ar and Ca). In such cases, check the file (Ca is set to 40 and Ar is set to 41). The corresponding L-J parameters for the particular gas of choice will be selected from the LJtable.xlsx file.

## 6.2 STRUCTURE FILE FOR PDB

The structure file for .pdb is basically the structure file that can be taken from the Protein Data Bank. A few changes can be made to the file to add partial charges and or different models. In what follows, a few explanations of how IMoS treats the .pdb files are explained.

### 6.2.1 Skipping Headers. Reading Coordinates, atom labels and integer charges.

IMoS will skip any headers and look for rows with that start with ATOM to start reading coordinates. It reads the coordinates in the respective pdb columns for coordinates and then reads the atom label in column 78-79. IMoS then attempts to read column 80 to look for charges. If no charges are specified in this column, it will take the value from imos.cla or the interface and center it.

### 6.2.2 Removing Water Adducts

IMoS will try to remove any water adducts that exist in the structure prior to starting the calculation. IMoS looks for the lines that start with HETAM and ignore those values. The command window will specify whether or not water molecules were subtracted from the molecule. Check the mAb IIGY protein file to see how it works.

### 6.2.3 Adding Partial Charges to pdb files.

IMoS allows the possibility of reading partial charges from the .pdb if the charges are there. This can only be done from imos.cla no-interface routine. To allow partial charges, the parameter "partialc" should be set to 1 within the imos.cla file. Note that the partialc parameter may be hidden. If the partialc value has been set to 1, IMoS will look for a second parameter labeled "chargelines". The parameter chargelines has two inputs the beginning and end column of the pdb file where the partial charges are located (e.g. chargelines 55 62). IMoS will then look for values between columns XX and YY of the pdb

file to assign the partial charges to every atom. If chargelines does not exist in the imos.cla file but partialc is set to 1, IMoS will take 55 and 62 as the default beginning and end of the partial charge value in every row of the pdb file.

#### 6.2.4 Adding Different Models of the Same molecule to a pdb file and running them separately.

IMoS can run different models within the pdb file as long as the models are separated correctly. In order to do so, the following must be met:

- 1) You must have a TER line to terminate a chain in your model.
- 2) You must have an ENDMDL line to terminate your model.
- 3) You must have a MODEL line that starts your new model with a number.

Example from Humanin (file : pdb1y32mod12.pdb)

```
ATOM  390 HB1 ALA A 24    1.791  10.249 -16.257 1.00  0.00    H
ATOM  391 HB2 ALA A 24    0.371   9.436 -16.916 1.00  0.00    H
ATOM  392 HB3 ALA A 24    1.609   8.504 -16.072 1.00  0.00    H
TER   393           ALA A 24
ENDMDL
MODEL   13
ATOM    1 N    MET A  1    8.093  -8.495  15.332 1.00  0.00    N
ATOM    2 CA   MET A  1    6.757  -8.803  15.906 1.00  0.00    C
ATOM    3 C    MET A  1    5.730  -7.748  15.511 1.00  0.00    C
```

#### 6.2.5 Adding Different Chains a pdb Model.

If a pdb file has different chains, the interface version it will ask whether or not you want to consider the next chain combined to the previous or by itself. This cannot be used to run CCS calculations but just to visualize different chains. In order for IMoS to ask for different chains, a TER input must be in place in the pdb file followed directly by an ATOM and not by an ENDML.

### 6.3 STRUCTURE FILE FOR MOBCAL

IMoS allows .mfj files to be loaded into IMoS and run. Please refer to the Mobcal's for how to create these files. It is possible to have more than one structure in an .mfj file. IMoS will warn the user if there is more than one structure in the .mfj file.

## 7 DFT CALCULATIONS

DFT or Density Functional Theory is an “ab initio” method used to calculate of the structure of atoms, molecules, crystals, surfaces, and their interactions in quantum mechanics. For IMoS, it is used to find the molecular structure used in the process of calculating the mobility and CCS. To get the equilibrium molecular the structure, a preprocessor – Avogadro– and solver – Gaussian– may be used as explained below. Avogadro<sup>1</sup> or Gaussian<sup>2</sup>[17] are not part of IMoS in any way and the tutorial here described is but a means to obtain a structure that is recommended to be used with the optimized L-J potentials that exist in IMoS. You may use any other suitable software to obtain or create your structures.

### 7.1 AVOGADRO

Avogadro is an advanced molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It offers flexible high-quality rendering and a powerful plugin architecture. The program can be obtained from the web at <https://avogadro.cc/>. A manual can also be obtained from the same website. Avogadro works as a preprocessor for many solvers. It is used to approximate the structure of a neutral molecule or to establish an initial guess for the position of the atoms. Avogadro is then used to create an input file for Gaussian.

#### 7.1.1 Import in Avogadro

User can create the molecule by drawing on the dashboard or it can be imported using its chemical name or by an input using Simplified molecular-input line-entry system (SMILES). The imported structure for the neutral molecule is, in most cases, already optimized. To obtain a file from the web, go to File, Import and Fetch by chemical name. To create a molecule using SMILES, go to Build, Insert, SMILES....

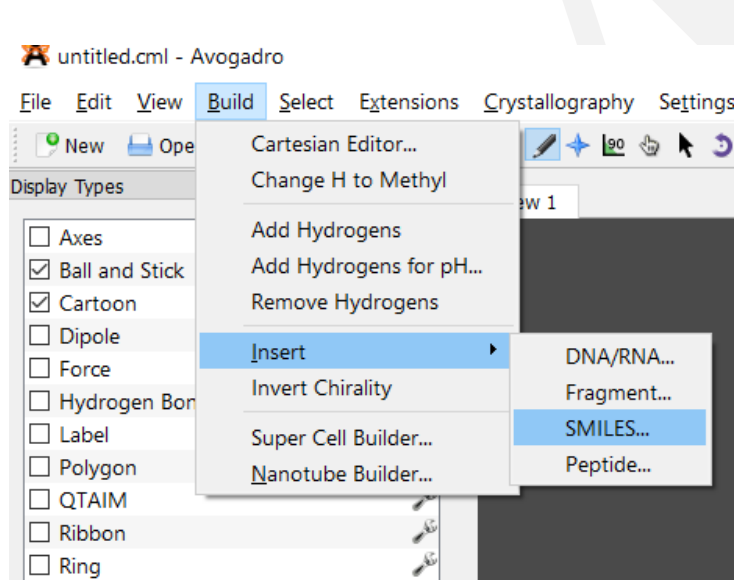


Figure 7.1 - Import molecular structure using SMILES

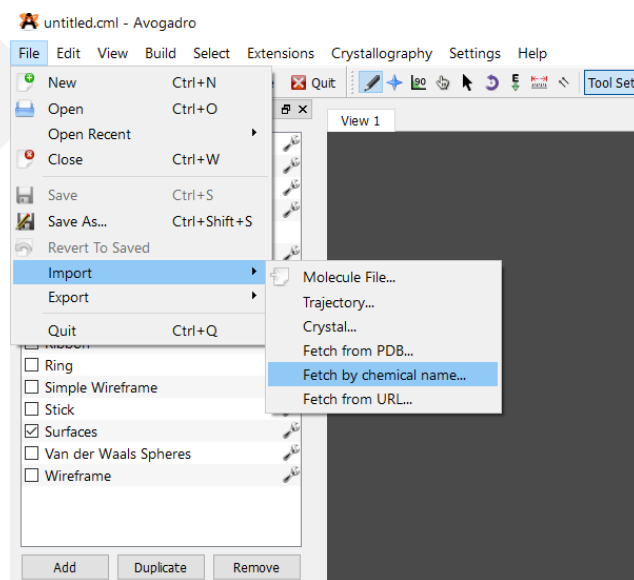


Figure 7.2 - Import molecular structure using name

<sup>1</sup> Avogadro: an open-source molecular builder and visualization tool. Version 1.2.

<sup>2</sup> Gaussian/GaussView is a program owned by Gaussian Inc. . IMoS and its authors have no competing interest.

### 7.1.2 Force Field Minimization

When using Avogadro, further shape optimization of a neutral molecule can be done using different force field optimization. This step might reduce iterations required in Gaussian. In order to use a Force Field minimization, go to the Energy Minimization icon (shown in Figure 7.3), click on the force field of choice and press start. Once the minimization is run, the structure is ready to be optimized using Gaussian.

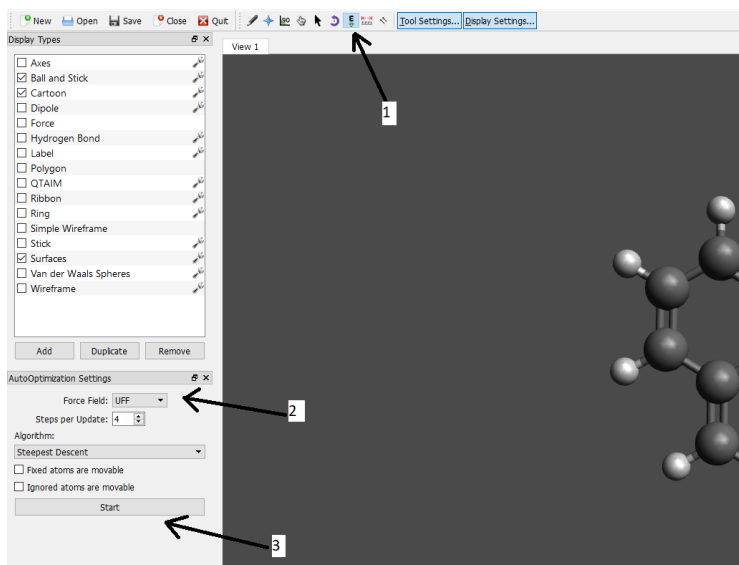


Figure 7.3 - Force Field Optimization

### 7.1.3 Create Gaussian Input File

In order to create a Gaussian input file, go to extensions and click on Gaussian. In the following figures, the pyrene molecule will be used as an example for obtaining the Gaussian input file. Once Gaussian is clicked, a Gaussian dialog box appears where atom coordinates appear together with several calculation choices (See Figure 7.5). The input parameters are described in following lines. After applying the desired parameters, the file can be edited manually as well.

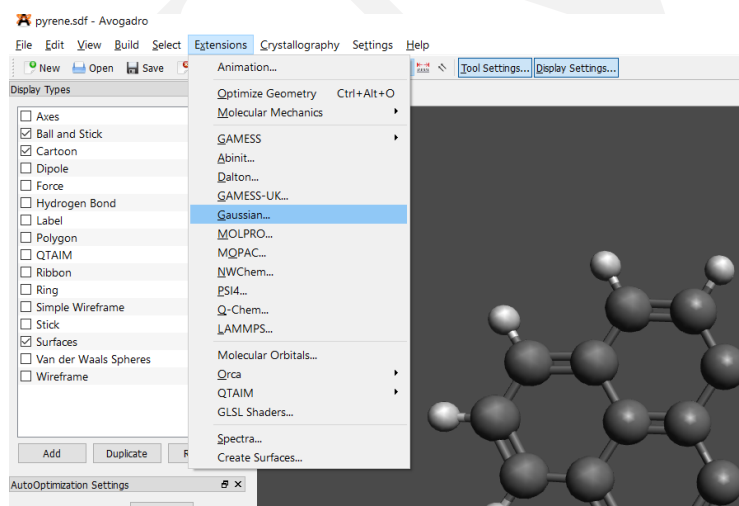


Figure 7.4 - Gaussian in Avogadro

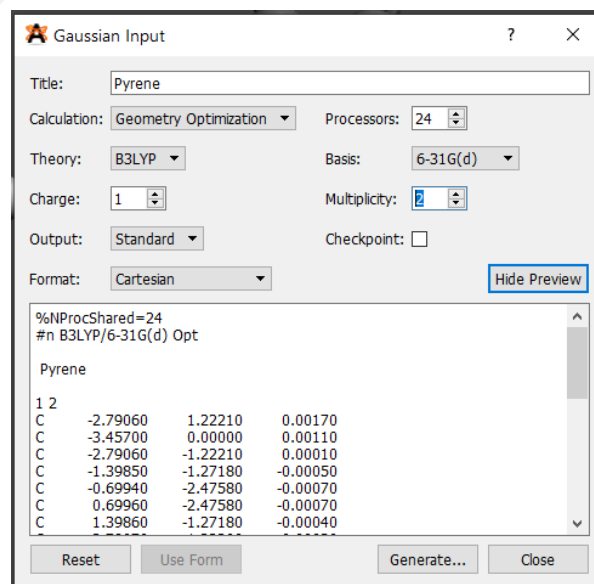


Figure 7.5 - Gaussian dialog box



### 7.1.3.1 Title

Name of Job (Pyrene).

### 7.1.3.2 Calculation

Type of calculation (i.e. optimize geometry).

### 7.1.3.3 Processors

Maximum number of cores to be assigned to job.

### 7.1.3.4 Theory and Basis

There are different Theories and related Basis for ab initio methods. A description of some of the methods may be found at which is described [here](#)<sup>3</sup>. According to our observations, the final answer of collision cross section with L-J potentials only is almost the same regardless of the basis used. B3LYP/6-31G(d) is one commonly used.

### 7.1.3.5 Charge

The charge applied on molecule (can be positive or negative but an integer).

### 7.1.3.6 Multiplicity

Spin multiplicity after applying the charge. The spin multiplicity is the number of possible orientations of the spin angular momentum corresponding to a given total spin quantum number for the same spatial electronic wave-function.

### 7.1.3.7 Output

Type of partial charge/dipole moment listed in output. Standard output gives Mulliken charges only. By adding 'pop=cm5', at the end of 2<sup>nd</sup> line, user can get Hirshfeld partial charges too.

### 7.1.3.8 Checkpoint

If during the n<sup>th</sup> iteration, the calculation stops and/or gets cancelled, the calculation can be started by taking values from checkpoint file. Checkpoint (.chk) file is a backup file of parameters and values of the (n-1)<sup>th</sup> iteration. To create checkpoint file, the checkbox is marked and the name of (.chk) file must be provided. To use the previously created checkpoint file, 'Opt = restart' should be added to a new file as shown in Figure 7.6

```
Format: Cartesian Hide Preview
%NProcShared=24
%Chk=Pyrene_backup.chk
#n B3LYP/6-31G(d) Opt=restart pop=cm5
Pyrene
1 2
C -2.79060 1.22210 0.00170
C -3.45700 0.00000 0.00110
C -2.79060 -1.22210 0.00010
C -1.39850 -1.27180 -0.00050
C -0.69940 -2.47580 -0.00070
C 0.69960 -2.47580 -0.00070
Reset Use Form Generate... Close
```

Figure 7.6 - Manually edited Gaussian file

### 7.1.3.9 Generate

Finally, click on Generate.. to produce a Gaussian (.com) file.

<sup>3</sup> <https://barrett-group.mcgill.ca/tutorials/Gaussian%20tutorial.pdf>



## 7.2 GAUSSIAN

Gaussian is used to obtain the optimized structure to be used with IMoS. Refer to the Gaussian website and videos at <https://gaussian.com/videos/>.

### 7.2.1 Running Gaussian

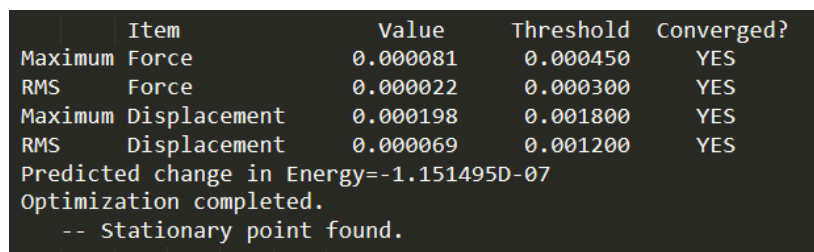
To run Gaussian on a Linux cluster, please load gaussian and then run Gaussian (e.g. Gaussian 16) from the command line by specifying the input molecule and output file. If Pyrene.com is the input file and Pyrene.txt is the output file.

```
>> module load gaussian
```

```
>> g16<Pyrene.com>&Pyrene.txt
```

### 7.2.2 Output File

Once the calculation is done, you should look in the output file to make sure that geometry and frequency got optimized. All four conversion criteria in Figure 7.7 should have converged on the last iteration.



	Item	Value	Threshold	Converged?
Maximum	Force	0.000081	0.000450	YES
RMS	Force	0.000022	0.000300	YES
Maximum	Displacement	0.000198	0.001800	YES
RMS	Displacement	0.000069	0.001200	YES
Predicted change in Energy=-1.151495D-07				
Optimization completed.				
-- Stationary point found.				

Figure 7.7 - Conversion criteria

If the structure has converged, find the optimized coordinates as well as the dipole moments and Mulliken and/or Hirshfeld partial charges. This will be used to create the structure files as shown in Section 6. The IMoS folder has certain tools to create the excel files using the outputs from Gaussian. Please see Speed.exe below.

## 7.3 MAKE IMoS INPUT FILE FROM GAUSSIAN OUTPUT FILE

The locations of atoms and Mulliken/Hirshfeld partial charges which are calculated using Gaussian needs to be arranged in certain format given in 'anallainb.xlsx'. Since the calculations are iterative, only the last iterated value should be selected. To simplify the process, an executable file "speed.exe" is made available with the IMoS package which parses the Gaussian result file (.txt) and puts it in a .xlsx file.

### 7.3.1 Speed.exe

To use speed.exe, place all Gaussian input (.com) and output files (.txt) inside a folder with speed.exe. Make sure that the input and output files have the same name (different extension). Then run speed.exe. It will ask user for the name of resultant .xlsx file. Input the name without extension. Speed.exe will get the name of .txt files from .com file names.

## 8 PROGRAM OVERVIEW

The program overview is meant for beginners to learn how to use IMoS and explains the basics of the program with and without the User Interface. In version 1.10, the interface has been parallelized and works in a very similar manner to the non-interface version. Section 8.2 deals with the use of the interface while section 8.3 with the use of imos.cla file.

### 8.1 SELECTING INTERFACE/NON-INTERFACE VERSIONS

IMoS is controlled through the use of the IMoS.cla file. To bring the interface up, change the interface parameter to “*interface 1 0*”. To use the no-interface version, change the interface parameter to “*interface 0 0*”. If the interface is invoked when executing IMoS, the program ignores the rest of the parameters in the IMoS.cla file.

### 8.2 INTERFACE WINDOWS/LINUX

The screenshot displays the IMoS interface window, which is divided into several sections:

- File:** Contains a 'Data Path' field set to 'E:\IMoS Program Files' and a list of files including 'Anallainb.xlsx', 'C60positions.xlsx', 'IonColor.xlsm', 'LJtable.xlsx', 'Nal\_coors.xlsx', 'mouseover\_locations.xlsx', and 'vdwimos.xlsx'. Below the list are 'From:' and 'To:' checkboxes, an 'Excel sheet' field set to '5', and 'Simplify all?' and 'Plot all?' radio buttons. 'Load File' and 'Plot Figure' buttons are at the bottom.
- Status:** A text area with the message: 'Welcome to IMoS!. Please choose and load a file with an.xlsx, .pdb or other extension.'
- Calculation Parameters:** A section with input fields for 'N. Orientations' (500), 'N. Total / Orient.' (300000), 'Accommodation' (0.0), 'Timestep' (150), 'Diffuse?' (1), 'Reemission vel' (Elastic(mean)), 'Other(Specify):' (m/s), and 'SASsimplify?' (Simplify). It also includes 'SaveSASName' and 'SaveSAS' buttons.
- Gas and molecule parameters:** A section with 'Gas' (N2), 'Red Coeff.' (1), 'Charge' (1), 'LJ Table', 'Gas Radius' (1.5), 'Mgas' (28.00), 'VdW Table', 'Pressure' (101325), 'Mweight' (256000), 'Color Table', 'Temperature' (304), and 'Polarization' (1.7). It includes a 'ReloadColor' button.
- Calculation:** A section with radio buttons for 'Projected Area', 'EHSS/DHSS', 'Trajectory M.', and 'TM Diatomic'. It also includes 'Traveler Salesman' and 'PA MonteCarlo' options, 'Parallel Options' (Threads: 7, Seed: 13), 'Plotting: OFF', 'Save File?' checkbox, and a 'File' field set to 'Saveme.txt'. A large 'Calculate' button is at the bottom right.

Red labels with white text are overlaid on the image to identify specific sections: 'File and Status Window' (pointing to the top right), 'Gas and Molecule Parameters' (pointing to the middle right), 'Calculation Parameters' (pointing to the bottom left), and 'Method and Plotting Options' (pointing to the bottom right).

Figure 8.1 - Interface Window Labels

When the IMoS executable file is run with interface 1 0, the interface will show up consisting of an interface window (as shown in Figure 8.1) and a plotting window. The interface window is broken down into the four different sub-panels depending on their purpose. The following sections will go into more detail for each option available in these panels.

## 8.3 FILE AND STATUS PANEL

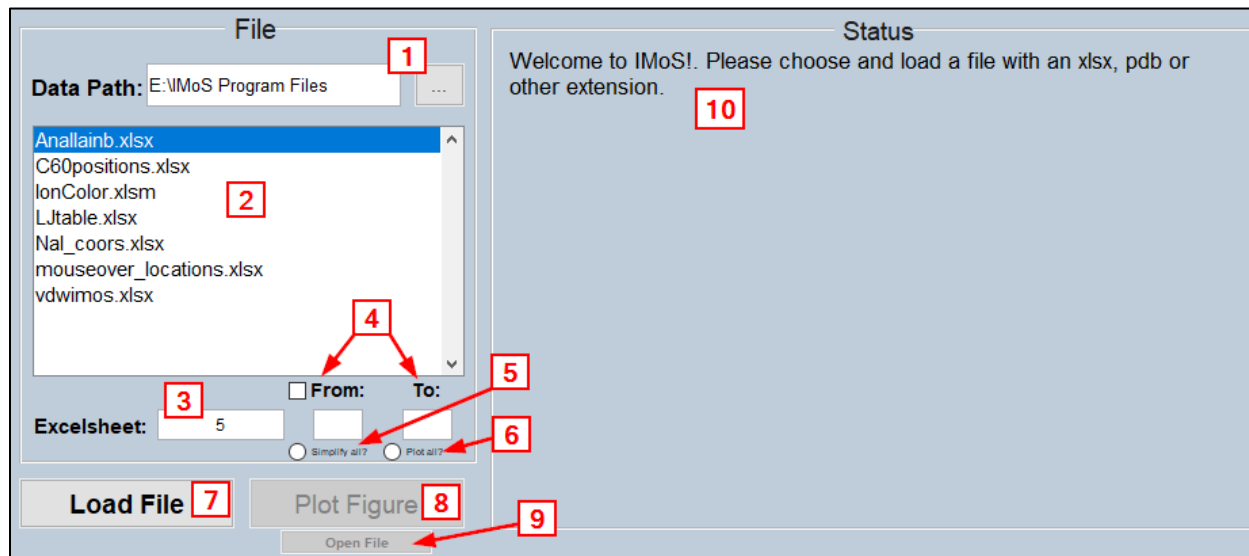


Figure 8.2 - File and Status Window

The file and status panel allow you to select, load and plot a structure file. Among the different files to load, one can choose excel files, MOBCAL type .mfj files and .pdb files. Excel, .mfj and .pdb files also allow you to choose different excel sheets and/or models and you can run more than one molecule at a time.

### 8.3.1 #1 - Data Path and Browse Button

The data path field shows the currently selected file directory. This directory populates the file window below. When using the browse button, ensure that a folder is selected, as opposed to closing the file browser without making a selection.

### 8.3.2 #2 - File window

All .xlsx, .mfj and .pdb files found in the selected directory are displayed in the file window list. Ensure the desired file is selected when loading the molecule.

### 8.3.3 #3 – Excelsheet/ModelNumber

This field determines the model number or excel sheet number that is chosen when the molecule is loaded. This field is only used when a single molecule is being loaded. If the *From:* checkbox is checked, then this field is ignored. If a .pdb or .mfj file is selected from the file window, this field is ignored.

### 8.3.4 #4 - From / To Options

This section determines the range of excel sheets or models that are chosen when multiple molecules are being run through the program. When the *From* box is checked, all excel sheets between (and including) the *From* and *To* fields will be loaded and calculations from the method panel applied. Sheets are loaded as the program begins calculations on that particular molecule.

### 8.3.5 #5 – Simplify all?

This option ensures that the *SASsimplify* option will be applied to all molecules loaded in a from-to batch, simplifying their structures by eliminating interior atoms speeding up the calculations but have little to no effect on the collision cross-sectional area and mobility (see Calculation Pannel). This option is only allowed on calculations that do not use 6-12 potential (TMLJ). When using a 6-12 potential, all atoms (including the interior ones) will contribute to the gas angular deflection so simplifying the structure might lead to errors.

### 8.3.6 #6 - Plot all?

When multiple sheets are selected (to-from batch), this option ensures all the molecules are plotted prior to calculation. Without this option selected, each molecule will need to be manually plotted during calculations.

### 8.3.7 #7 – Load File

This button loads the selected file and sheet number (if excel file) selected.

### 8.3.8 #8 – Plot Figure

This button plots the molecule loaded. It is recommended to plot the molecule prior to running calculations with plotting turned on, to ensure the visualization method will be shown. Some large molecules (>1000 atoms) may take some time to plot. Note that plotting the molecule is available even when using the *Plotting:OFF* option (See method Panel).

### 8.3.9 #9 – Open file

This opens the file selected in the file window.

### 8.3.10 #10 – Status Window

This window displays relevant information and results during calculation. Only the results from the most recent molecule and method ran will be shown. It is recommended to save the results in a file in order to ensure that all the results can be reviewed. The bottom of the status window contains the mouseover information for all the options in the interface with guidelines to explain some of the values.

## 8.4 CALCULATION PARAMETERS PANEL

The screenshot shows the 'Calculation Parameters' dialog box. It contains several input fields and buttons, each with a red numbered callout:

- 1**: N. Orientations: 500 (PA), 3 (EHSS/DHSS), 3 (TM/DTM)
- 2**: N. Total / Orient.: 300000 (EHSS/DHSS), 300000 (TM/DTM)
- 3**: Accommodation: 0.0
- 4**: Timestep: 150
- 5**: Diffuse?: 1
- 6**: Reemission vel: Elastic(mean) ...
- 7**: Other(Specify): m/s
- 8**: SASsimplify?: Simplify
- 9**: Connolly (selected) / Recolored
- 10**: SaveSASname / SaveSAS

Figure 8.3 - Calculation Parameters

### 8.4.1 #1 – Number of Orientations

Total number of orientations for each method. The option for EHSS/DHSS and TM/DTM is three and should not be modified. It represents the number of perpendicular directions explored. PA randomly orients the projection instead of only doing 3 perpendicular orientations. For this reason, 50-500 or more is recommended for Projected Area. Default should be 500 although 100 is sufficient for a good estimate.

### 8.4.2 #2 – Total / Orientation

This parameter sets the number of gas molecules per orientation. For EHSS/DHSS and TM methods. If for example 300000 gas molecules are chosen, the program will run  $300000 \times 3 = 900000$  gas molecules total. Default values are 300000 for both. Increase for better accuracy. Decrease for faster output.

### 8.4.3 #3 – Accommodation

Accommodation coefficient. Percentage of the number of accommodated gas molecules. 1 for full accommodation, and 0 for fully elastic. Only valid for EHSS/DHSS, TDHSS and DTM methods. This parameter only establishes the percentage of gas molecules that are accommodated. For example, choosing 0.9 establishes that 90% of the gas molecules will be accommodated while 10% will follow an elastic and specular collision. The remaining 90% may be chosen to be reemitted diffusely or not using the parameter diffuse (see below). When diffuse is chosen, the gas molecules are reemitted at a random angle within a semi-sphere at the point of contact. The speed of the 90% accommodated molecules may also be chosen through the reemission velocity parameter. There are plenty of different choices including being reemitted elastically or being reemitted at the surface temperature. The reemission velocity may be chosen randomly from a Maxwellian distribution or it may be chosen to always be the mean of the particular distribution chosen. For example, if accommodation is chosen to be 0.91 with diffuse reemission at the Maxwell surface temperature, the resulting value for a sphere would be the expected to be the characteristic 1.3573 from the Millikan oil experiments. Do to scattering of the 9% that undergo specular and elastic collisions, a better approximation for non-spherical ions is to choose an accommodation of 1 and a velocity coming from a distribution at 92% of that of Maxwell which more closely yields the 1.36 value for non-spherical ions.

### 8.4.4 #4 – Timestep

Timestep coefficient for TM and Diatomic methods. 150-450 are normal values. Higher values, longer timesteps. Adjust only if results seem inaccurate.

### 8.4.5 #5 – Diffuse?

Specifies whether an accommodated molecule (only the percentage that is accommodated) is reemitted diffusely or specularly. 1 for diffuse, 0 for specular. No intermediate values.

### 8.4.6 #6 – Reemission Velocity

Reemission velocity for accommodated gas molecules. Only works with EHSS/DHSS, TDHSS and DTM methods. The re-emitted gas molecules may be assumed to be re-emitted using a distribution of velocities or using the mean value of a particular distribution. When trajectories are rectilinear, the mean value should always be used (e.g. with EHSS/DHSS). However, when trajectory methods are used (e.g. TDHSS, DTM), one should use the distribution as trajectories may drastically change depending on the reemitted velocity. The following choices exist:

- 1) **Elastic(mean).** The accommodated gas molecules will be reemitted at the average velocity of the incoming molecules. With accommodation 1, this is equivalent on a spherical ion to  $\xi = 1.44$  or  $\text{CCS} = 1.44\text{PA}$  when using EHSS/DHSS.
- 2) **Elastic.** The accommodated gas molecules will be reemitted using the same distribution that was used to establish the initial velocity of the gas molecules into the control domain. The average of this distribution is Elastic(mean).
- 3) **Distributed Maxwell.** The accommodated gas molecules are reemitted using a Maxwell distribution at the surface temperature of the ion. The surface temperature of the ion is the same as the gas temperature (see Other if you want to use a different temperature).

- 4) **Maxwell.** The accommodated gas molecules are reemitted at the mean value of Distributed Maxwell. With accommodation 1, this is equivalent on a spherical ion to  $\xi = 1.39$  or CCS=1.39PA when using EHSS/DHSS.
- 5) **Distributed 92% Maxwell.** The accommodated gas molecules are reemitted using a Maxwell distribution with 92% of the energy of a Maxwell distribution.
- 6) **92% Maxwell.** The accommodated gas molecules are reemitted using the mean value of 92% Distributed Maxwell. With accommodation 1, this is equivalent on a spherical ion to  $\xi = 1.36$  or CCS=1.36PA when using EHSS/DHSS.
- 7) **Distributed Other (Specify Mean).** The accommodated gas molecules are reemitted using a Maxwell distribution (3D normal distribution) with the mean velocity specified in the Other dialog. Based on the description of the mean velocity of a 3D Maxwell distribution, one can infer a given velocity through the choice of a particular surface temperature.
- 8) **Other (Specify Mean).** The accommodated gas molecules are reemitted using the mean value specified in the box below. This represents a mean velocity for a momentum flux (not the mean velocity of the distribution). For this reason, the elastic mean value is  $\sqrt{\frac{128kT}{9\pi m}}$ , that of Maxwell is  $\sqrt{\frac{18\pi kT}{16m}}$  and that of Maxwell 92% is  $\sqrt{\frac{3kT}{m}}$ .

#### 8.4.7 #7 – Other

Specify the reemitted velocity if other (Specify) was chosen as the reemission velocity.

#### 8.4.8 #8 – SASsimplify

Solvent Accessible Surface (SAS). Simplifies the structure by eliminating atoms that are not on the surface for a **particular gas radius**(see **Gas and Molecule panel**). Only valid for PA, EHSS/DHSS, and TDHSS methods. As shown in Figure 8.4, this may represent a very large amount in particular when large spherical ions are chosen.

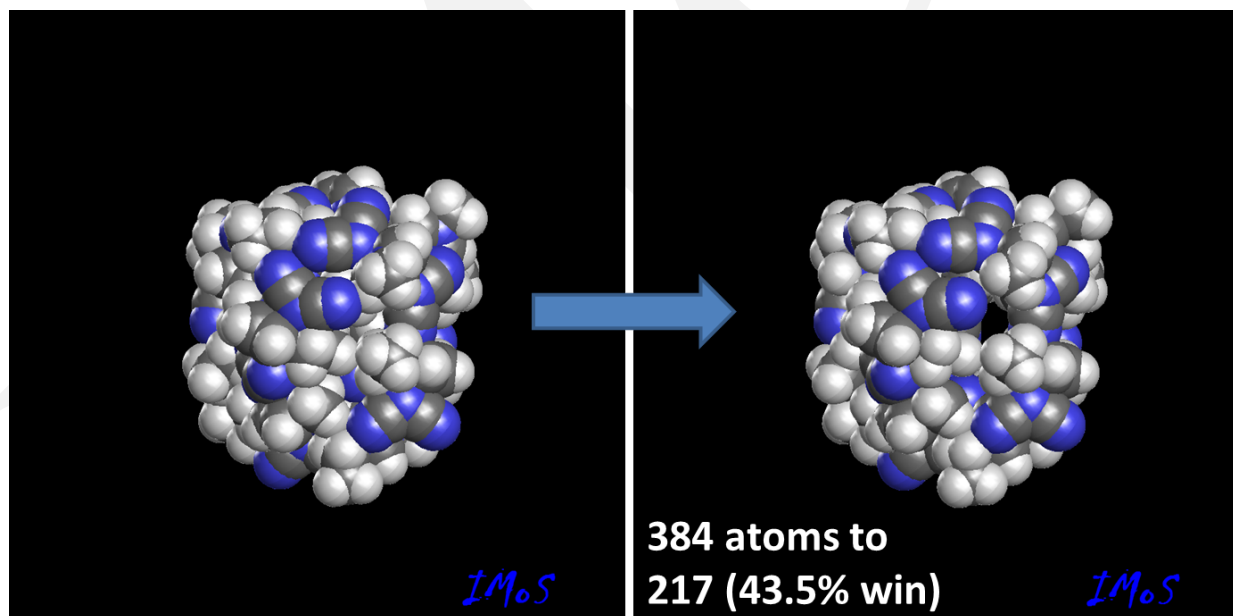


Figure 8.4 – Molecule reduced from 384 atoms to 217 through Solvent Accessible Surface simplify algorithm.

#### 8.4.9 #9 – Connolly and Recolored

- *Connolly Surface:* When on, atoms are drawn with Van der Waals radii. When off, the gas molecule radius is added to the atom radius. **Only works after SASsimplify has been executed.**
- *Recolored:* Colors the surface atoms white when selected. **Only works after SASsimplify has been executed.**

### 8.4.10 #10 – SaveSAS

Saves the simplified version of the molecule to an excel file after *SASsimplify* has been run. Enter the desired file name in the text field. Saved to the “savefolder” directory. You can later load the simplified structure.

## 8.5 GAS AND MOLECULE PARAMETERS PANEL

Gas and Molecule Parameters panel. When some parameters are modified, reload the molecule so that they are considered when plotting.

The screenshot shows a panel titled "Gas and molecule parameters" with various input fields and buttons. Red boxes with numbers 1 through 13 are placed over specific elements:

- 1: Gas dropdown menu (showing N2)
- 2: Red Coeff input field (showing 1)
- 3: Charge input field (showing 1)
- 4: Gas Radius input field (showing 1.5 A)
- 5: Mgas input field (showing 28.00 Da)
- 6: Pressure input field (showing 101325 Pa)
- 7: Mweight input field (showing 256000 Da)
- 8: Temperature input field (showing 304 K)
- 9: Polarization input field (showing 1.7 A<sup>3</sup>)
- 10: LJ Table button
- 11: VdW Table button
- 12: Color Table button
- 13: ReloadColor button

Figure 8.5 - Gas and Molecule Parameters

### 8.5.1 #1 - Gas

Selects the gas to be used for the study. If the gas that is needed is not listed, you can select *Custom* from the list and add the required gas by editing the eighth sheet (labeled Custom) of the “LJTable.xlsx” file.

### 8.5.2 #2 – Reduction Coefficient

Reduces/Enlarges the structure by the given ratio (>1 to reduce).

### 8.5.3 #3 – Charge

Number of centered charges (only if not designated in the excel file. You must select the charge for other files).

### 8.5.4 #4 Gas Radius

Gas Molecule Equivalent Van der Waals radius (1.5 for N2).

### 8.5.5 #5 – Mgas

Molecular mass of the gas molecule in Da.

### 8.5.6 #6 – Pressure

Gas Pressure in Pa.

### 8.5.7 #7 – Mweight

Molecular mass of the ion in Da (only if not designated in the excel file. You must select the mass here for other files).

### 8.5.8 #8 – Temperature

Experiment gas Temperature in K.



### 8.5.9 #9 – Polarization

Gas Polarizability in cubic Angstroms (N<sub>2</sub> 1.7) (He 0.2073).

### 8.5.10 #10 – LJ Table

Opens the “LJTable.xlsx” excel file. This contains the L-J parameters for different gases. IMoS only reads the first two columns. Each sheet is labeled accordingly to the gas and or method used. You may modify these values. Note that most ions do not have optimized Lennard-Jones parameters.

### 8.5.11 #11 – VdW Table

Opens the “vdwimos.xlsx” excel file. Lists the VdW radii used if first row of 4<sup>th</sup> data column is set to -1. The table also incorporates the atom labels used on the 7<sup>th</sup> data column for L-J values.

### 8.5.12 #12 – Color Table

Opens the “Ioncolor.xlsm” excel file. You can modify colors of the atoms here.

### 8.5.13 #13 – ReloadColor

Reloads the atom colors. This should be used if the colors are updated in the “Ioncolor.xlsm” file to update the colors in the plot.

## 8.6 METHOD AND PLOTTING OPTIONS PANEL

This sets the different calculations to be performed using IMoS. Note that you can run more than one calculation at a time. You can also select TM TDHSS and TM LJ simultaneously.

Figure 8.6 - Method and Plotting Parameters

### 8.6.1 #1 – Projected Area

Calculates the average projected Area using two possible methods. 500 orientations are in general more than enough. Fastest method.

### 8.6.2 #2 – EHSS/DHSS

Elastic/Diffuse Hard Sphere Scattering. Momentum transfer with no potentials. Choose accommodation, diffuse and any reemission velocity and number of gas molecules per orientation (max 3).

### 8.6.3 #3 – Trajectory Method

Verlet Algorithm is employed to calculate the effect of potentials.



- TDHSS:  $4 - \infty$  potential. The reemission is chosen depending on your choice of accommodation.
- LenJon: Lennard Jones 4-6-12 potential is used. Parameters specified in LJtable.xlsx
- QPol: Ion induced quadrupole potential is now added to 4-6-12 potential. Only in  $N_2$ . Cannot be used with plotting turned on (Kim, H., et al. Anal. Chem. 80, 1928–1936 (2008))[15].

#### 8.6.4 #4 – TM Diatomic

Diatomic Trajectory Method. Incorporates a Rotational Maxwell Distribution to the Trajectory Method.

#### 8.6.5 #5 – Travelling Salesman and PA Monte Carlo

- Travelling Salesman Method: Inaccurate for point contact particles with point contact gas molecules. Used for Plotting. Not parallelized in v. 1.10.
- PA Monte Carlo: General Projected Area Method. Calculates the area from random shooting. Parallelized, and not available when using the plotting option.

#### 8.6.6 #6 – Save File

The results are saved to a text file in the directory chosen. Default save directory is the “savefolder” folder. Enter the desired file name in the text field. If the directory typed into the text field isn’t found, it will be created. If the save file already exists, a prompt will ask if the user wishes to overwrite the existing file. If you do not want to overwrite, the calculation will still run and will be saved in “Notsaved.txt” file.

#### 8.6.7 #7 – Threads

Determines the number of threads to be used for parallel computation. It is recommended to leave at least one thread available for other user tasks while calculating.

#### 8.6.8 #8 – Seed & Repeat Seed (RS)

Seed is the pseudo random number. Use 0 to use the computer clock for a seed. Repeat Seed (RS) is a convenient way to test results for different molecules and methods. Even if one chooses a seed, the seed is not re-started automatically as long as the program is open. So, for example, if you run a method twice without closing the program, the second result will be different from the first. RS allows the seed to be restarted. When set to 0, the seed is not restarted. When set to 1, the seed is set to be restarted for every molecule (if submitted in a batch). If set to 2, the seed is restarted for every call to calculate but not for every molecule (if submitted in a batch).

#### 8.6.9 #9 – Plotting

Switches between the parallelized and plotting options (See Examples). The button changes color and text when toggled, to indicate the current state. Several options in the interface are available only in one or the other and will be enabled/disabled as necessary. Note that default values for several parameters will be written in when swapping between the two options.

**PLOTTING OPTIONS SHOULD ONLY BE USED FOR TEACHING PURPOSES.**

#### 8.6.10 #10 - Calculate

Calculate button to begin calculations. This button will only be enabled once a file is loaded.

## 9 NON-INTERFACE VERSION AND THE IMOS.CLA FILE

IMoS can be run without the need of the interface which is many times convenient, such as for example when submitting a job to supercomputer queue. All the existing parameters in the interface may also be changed in the imos.cla file.

### 9.1 HEADER OF IMOS.CLA FILE

The header can only be two lines. The first one is not read but there must be some characters on it. The second line states the file that you are going to be using (either .xls(x), .mfj or .pdb), the save file for the output and the gas that is being used. **They must be separated by spaces (NO TABS)**. Possible gases that may be used are N2, He, Argon, CO2, SF6, Air, Other. The code is case sensitive in this case so be careful. The selection of the gas here only affects which LJtable.xlsx sheet is used for the Lennard-Jones parameters. An example of an imos.cla header looks like this:

File	Savefile	Gas
\filefolder\pdb1y32mod12.pdb	\savefolder\Saveme.txt	N2

### 9.2 BODY OF IMOS.CLA FILE

```

excelfile      Savefile      Gas
/filefolder/AnalIainb.xlsx /savefolder/savefile.txt  N2

interface 0 0
fromvalue 1
tovalue 5
Charge 1
Mgas 28
radgas 1.5
Polarizability 1.7
Pressure 101325
Mweight 55000
Temperature 301

NrotationsPA 500
NgastotalEHSS 300000
NgastotalTM 300000
Acommodation 0
reemvel 6

PA 0
EHSS/DHSS 0
TM 1

LennardJones 1
qp01 0
TDHSS 0

Numthreads 11
seed 17
Repeatseed 1
  
```

**Input File**  
**Output File**  
**Gas (L-J table)**

**Models to calculate (excelsheets,...)**

**Gas & Ion Parameters**

**Mobility Calculation Parameters**

**Calculation Methods**

**Trajectory Method Options**

**Random Seed and Number of Threads**

Figure 9.1 IMoS.cla file parameters

The body of the imos.cla file contains a list of parameters to run IMoS. Figure 9.1 shows the imos.cla file with some of the most common parameters. These set of parameters is sufficient to run IMoS. When the interface is set to 0 0, just execute the program and it will run without the interface. Check the interface explanation to find the explanation for most of these parameters. If other parameters are needed or for additional information, please contact the authors. In the next section, some additional parameters are added, and some are explained.

### 9.3 EXPLANATIONS AND HIDDEN PARAMETERS OF THE IMOS.CLA FILE.

Explanations of some of the hidden parameters of IMoS. More parameters do exist but these are the most common. Email authors if other options are needed.

#### 9.3.1 [redcoef]

*redcoef* reduces the size of the structure by the percentage applied in this coefficient. A value of 1.2 will reduce the dimensions of the distance to the geometric center and the radii of the atoms by 20%. Default is 1.

#### 9.3.2 [Diffuse?]

*Diffuse* has a value of 0 or 1 and will state you if the number of gas molecules given by [accommodation] will be reemitted as diffuse (Diffuse? 1) or only as specular (Diffuse? 0).

#### 9.3.3 [reemvel]

The reemission velocities can be taken from a Maxwell distribution (distributed Maxwell, distributed 92% Maxwell, distributed Other) or they can be taken as the mean values of such distributions which is recommended only for EHSS/DHSS (Maxwell, 92% Maxwell, Other). Choosing elastic means that you will re-emit with the same velocity as the gas molecule impinged and choosing elastic(mean) tells you that your gas molecules will be re-emitted with the mean of the incoming velocities taken from a skewed Maxwellian distribution. The [reemvel] is a numerical value. These are the corresponding velocities to the numbers used: 1 Elastic(mean), 2 Elastic, 3 Maxwell, 4 92%Maxwell, 5 Maxwell Distrib, 6 92% Maxwell Distrib, 7 Other, 8 Other Distrib.

#### 9.3.4 [other]

Other is used when reemvel is set to 7 or 8 to establish the mean value of the velocity for the momentum flux.

#### 9.3.5 [Simplify]

Setting Simplify 1 will simplify your structure so that you can get rid of all the internal atoms that will not affect Hard Sphere collision. Default is set to 0. It is very recommended that this value is set to 1 unless [LennardJones] is set to 1 for TM methods.

#### 9.3.6 [PATSA]

*PATSA* establishes which version of the PA algorithm is used. If [PATSA]=1, (PATSA 1) a Travelling Salesman(TSA) type of calculation is performed. If [PATSA]=0 a Monte Carlo(MC) approach is used. TSA is faster on a single core but it is not parallelized. If TSA causes problems or there are passable holes in the structure, the MC approach should be used instead.

#### 9.3.7 [partialc]

*partialc* is used to let IMoS knows that a pdb file contains partial charges. If *partialc* is set to 1, IMoS looks for the variable *changethelines* which has two values. If *changethelines* does not exist, IMoS will look for the partial charge values between columns 55 and 62 (inclusive) of the pdb file. Default is 0.

#### 9.3.8 [changethelines]

*Changethelines* has two values (*changethelines* XX XX). They correspond to the first and last column that contain the partial charges in the pdb file. Is only read if partial is set to 1. Default is *changethelines* 55 62.

#### 9.3.9 [Repeatseed]

*Repeatseed* allows the seed to be restarted. When set to 0 (default), the seed is not restarted. When set to 1, the seed is set to be restarted for every molecule (if submitted in a batch).

#### 9.3.10 [DTM]

*DTM* is the calculation option for Diatomic Trajectory Method. If set to 1, it will run the DTM method. Not recommended as it is slow and not parallelized.

#### 9.3.11 [HandB]

If Happel and Brenner's or Landau's way of averaging the tensor to calculate CCS and mobility is required or wanted set *HandB* 1. IMoS will give both HandB and regular. Default is 0.

#### 9.3.12 [Timestep]

The timestep in IMoS varies depending on the strength of the force applied to the gas molecule. One can affect the timestep through this variable. It is set to 100 by default. Higher values means more accurate (recommended is 100-450) but slower.

## 9.4 L-J/VDW OPTIMIZER OPTION

### 9.4.1 Optimize a L-J epsilon sigma pair (or vdw radii) for a particular set of atoms.

IMoS can be used to optimize L-J potentials for a particular set of atoms and temperature ranges. To run the Optimizer *interface 0 1* must be set (or the appropriate check box pressed in the interface version). The Optimizer folder contains a file labeled *Optinput.txt*. This file is the master configuration for L-J optimization.

```
efrom 0.55
eto 0.95
ejump 0.05
sfrom 3.1
sto 3.9
sjump 0.1
vdwfrom 1
vdwto 1
vdwjump 0.5
atom 2
structures 2
Temp 300 350
result 10
expected 213.10 231.40 115.80 131.10
```

The order may not be changed!! The Optimizer folder also contains the *LJtable.csv* and *vdwimos.csv*. These are the tables that the program will use to test different LJ-parameter and vdw radii values.

When executed, the Optimizer will take the *IMoS.cla* file (or interface options) to obtain which parameters to use for the calculation and which calculations to perform, will take the L-J parameters (or vdw radii) from the csv tables and commence the run by changing the appropriate values provided by *Optinput.txt*. Once completed, the result will be given in the *resultsopt\_.txt* file and also plotted if done from the interface. See Examples in section 10. The optimization routine will look for the minimum of the function (vdw is changed for epsilon and sigma if vdw is the option selected):

$$F_{opt}(\epsilon, \sigma) = \sum_{i=1}^{N_{CCSexp}} \left( 1 - \frac{\Omega_{cal}(\epsilon, \sigma)}{\Omega_{Exp}} \right)^2$$

At least 2 expected values (either two temperatures for one structure or two structures) are necessary to optimize the values of a sigma and epsilon. More are recommended as an overdetermined system is more likely to give more accurate results.

#### 9.4.1.1 *efrom, eto, ejump, sfrom, sto, sjump, vdwfrom, vdwto and vdwjump variables.*

The first 9 variables correspond to the range of the parameters used for the calculations. *xfrom* and *xto* variables correspond to the interval ranges of the calculation while *xjump* corresponds to the jump between values. *e* and *s* stand for the epsilon and sigma values and the units are 1e-21J and angstroms respectively. The vdw units are in Angstroms. Only either LJ or vdw radii optimization is performed on a single run. If *vdwfrom* variable is the same as *vdwto* variable (as in the case above), then the LJ parameters will be optimized. If they are different, then vdw radii optimization will occur and epsilon sigma ranges will be omitted.

#### 9.4.1.2 *atom variable.*

The *atom* variable selects the atom number that will be optimized from the csv table. For example, if a L-J parameter run is done using *atom 2*, with the following *LJtable.csv*:

```
Var1,Var2,Var3
H,0.4806,2.3
C,0.95,3.9
```

O,0.68886,3.5  
N,0.92916,4.2  
F,0.19224,3.4  
Cs,0.5814,4.20081  
Na,0.41677632,3.5  
Cl,0.41677632,3.5...

then the Carbon atom will be selected for optimization. Note that you will have to change the csv table to the appropriate gas parameters prior to running the Optimizer.

#### 9.4.1.3 *structures, Temp and expected variables*

The *structures* variable has to be the same number of structures as the *fromvalue tovalue* (From to checked in the interface). The *Temp* range can be an array of different temperatures for which experimental conditions are known (please see examples). The *expected* variable contains the experimental collision cross sections separated by spaces. The *expected* variable array has to be the size of *structures\*Temp*. The order of *expected* is structures CCS per temperature. So for example if there are two structures and two temperatures, the *expected* variable order is 1<sup>st</sup> Temp 1<sup>st</sup> structure, 1<sup>st</sup> Temp 2<sup>nd</sup> structure 2<sup>nd</sup> Temp 1<sup>st</sup> structure, 2<sup>nd</sup> Temp 2<sup>nd</sup> structure. If the expected value is not the correct size, the program will still run but will not do any optimization. The optimization will have to be done manual with the results from the results file.

#### 9.4.1.4 *result variable*

The *result* variable is an integer number that will appear at the end of the *resultsopt\_.txt* file. If 9 for example is chosen, the result file will be appear as *resultsopt9.txt*.

## 9.5 WORKHORSE AND WORKMULE OPTIONS

### 9.5.1 Run all analyte files from a folder

IMoS can be used to run all available files (of supported format) contained in a folder. To use the all file analyzer, change the interface parameter to *interface 0 2* (or the appropriate check box pressed in the interface version).. Place all analyte files in the *Workhorse* folder and put that folder in the directory of IMoS110W64.exe (for Windows) or ImoS110W64.sh (for Linux). Sequentially, all files available in the folder will be analyzed and the result files will be saved in the savefolder with the name (and extension) of the analyte file itself.

### 9.5.2 Run all .cla files from a folder

To run all the .cla files from a folder, change the interface parameter to *interface 0 3*(or the appropriate check box pressed in the interface version).. Place all .cla files in the *Workmulecla* folder and put that folder in the directory of ImoS110W64.exe (for Windows) or ImoS110W64.sh (for Linux). Sequentially, IMoS will copy the content from .cla files to IMoS.cla and analyze accordingly.

## 10 EXAMPLES

The idea of this part of the manual is to get accustomed to IMoS regardless of whether using the interface or not. While most of the examples here use the interface, the result file contains the imos.cla file that can be used to produce the same result (except perhaps for the seed), just using the non-interface version. The first portion of the examples use the plotting option to visualize some of the techniques used to calculate mobility and CCS in IMoS.

### 10.1 PLOTTING: ON

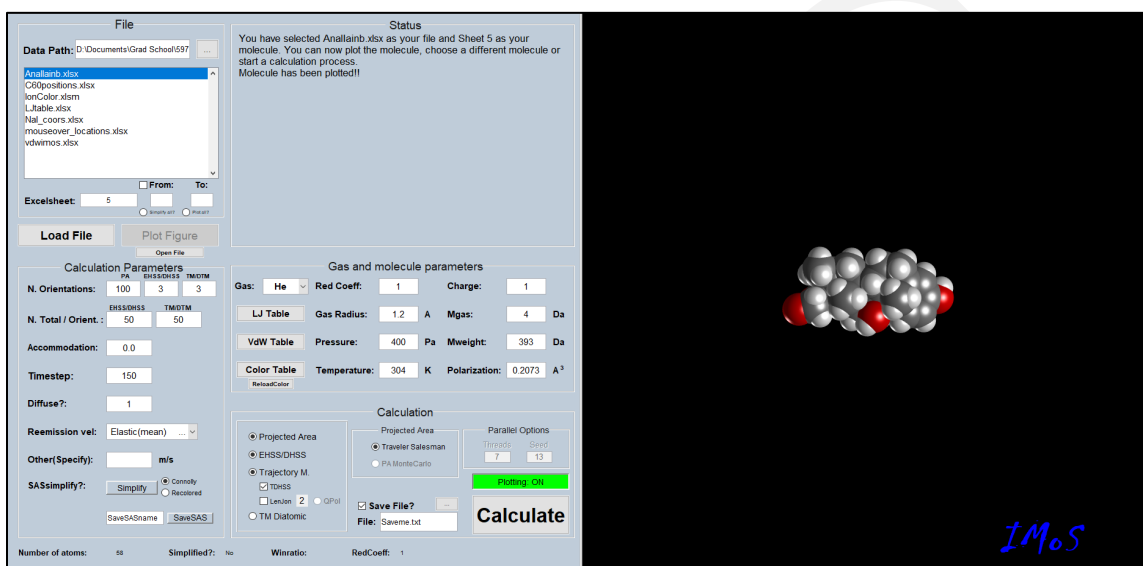


Figure 10.1 - Plotting Example (File Loaded)

This example showcases the plotting options for all four methods.

1. Open the program and select the “anallainb.xlsx” from the list. If this file is not in the list, click the browse button next to the data path and select the *filefolder* directory. Type as an example the number “5” into the Model Number option to select the molecule located on the fifth sheet of the selected excel file (Figure 10.1).
2. Certain parameters from the *Gas and molecule parameters* may be edited prior to loading the file. For this example, select Helium from the *Gas* list.
3. Click *Load File* and *Plot Figure* to import the data into the program and plot the molecule.
4. Click the *Plotting: OFF* button to swap to the plotting enabled, non-parallelized version of the program. The button should turn green to indicate the plotting version is enabled. Note that several options that are only available on the parallelized version are disabled.
5. For this example, Projected Area, EHSS/DHSS, Trajectory Method and DTM will be ran. You can either run all methods together or separately. For visualization, it is better to run very few gas molecules. For that reason, the number of gas molecules was changed to 50.
6. Click the *Calculate* button. All three methods will plot their results while calculating. Once completed, the most recently run method’s results will be shown on the *Status* window. To view the results from all methods, open the save file from the Examples folder created. This text file includes the results from each method, as well as the parameters used for the calculations.
7. Figures of the different plotting options are shown below. Note that results are not saved, and this is meant for visualization purposes only.



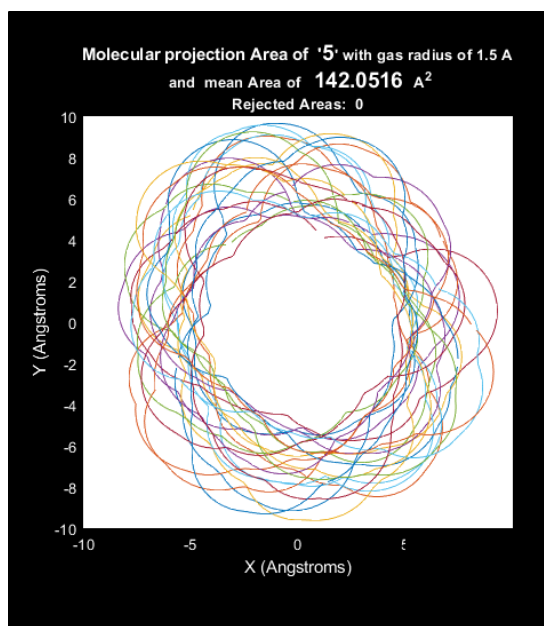


Figure 10.2 - Projected Area Plotting

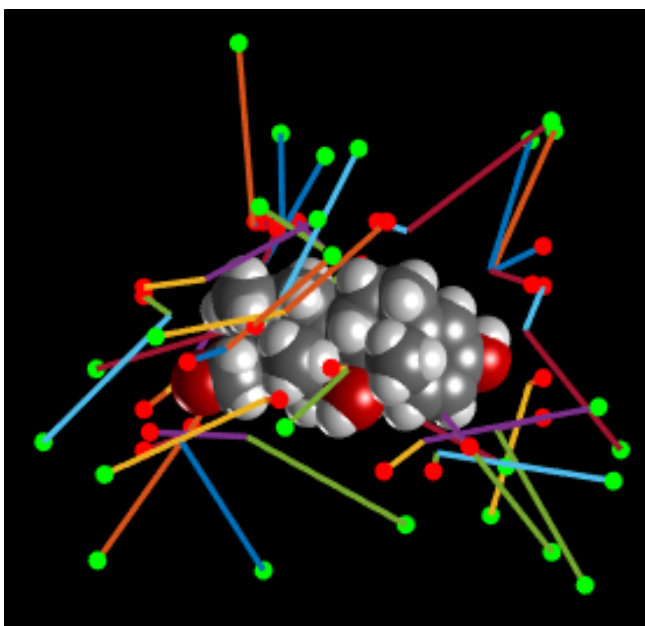


Figure 10.3 - EHSS/DHSS Plotting

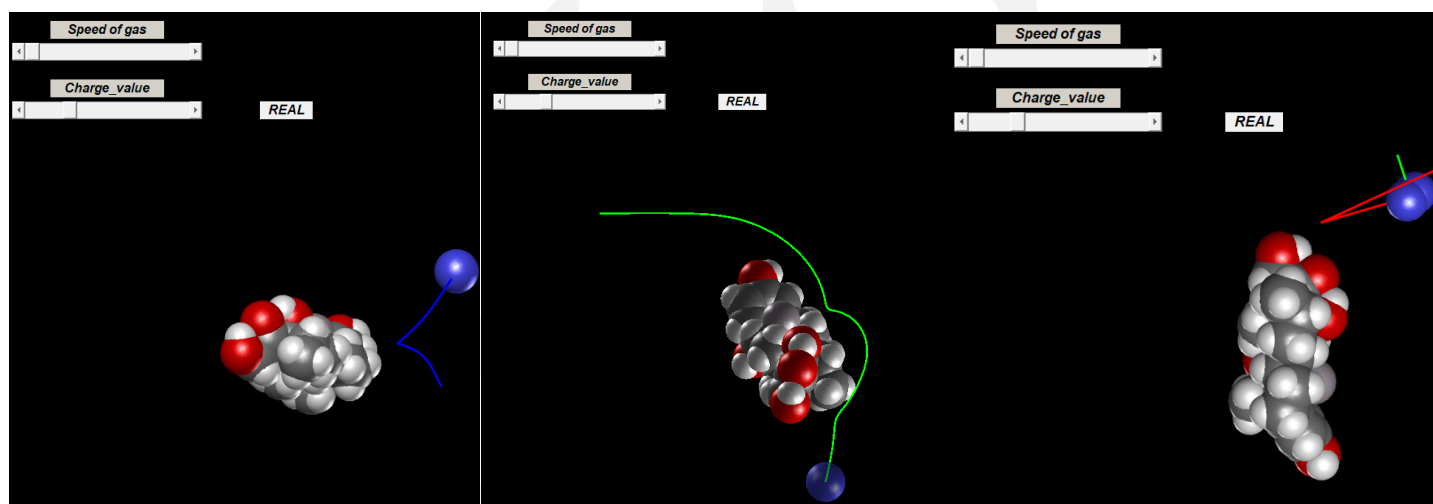


Figure 10.4 - Trajectory Method Plotting. Left TDHSS, middle LJTM, right DTM

## 10.2 PARALLELIZED (INTERFACE)

This example showcases the faster parallelized option, using the interface.

1. For this example, a PDB file will be used as opposed to an excel file. Open the program and click browse next to the data path. Select “filefolder” from the folder list.
2. Click “xtal-fix-charge6-cytoc.pdb” from the list and click load. A dialog box will open, stating that there are multiple chains that can be loaded for this molecule. For this example, only the first chain will be loaded. Click *No* on the dialog box. Note that some PDB files may have multiple models. In this case, the program will step through the available models until the user chooses a model to load.

3. Click *Plot Figure*. Note that the number of atoms shown in the bottom of the window is 1668. Due to the large size of this molecule, plotting may take some time.
4. Once the figure is plotted, click and drag on the plot to rotate the molecule. It is easy to see that there are many atoms in the interior of the molecule that will have little to no effect methods that only require surface atoms to calculate the cross-sectional area and mobility. Click “Simplify” to simplify the structure by eliminating the interior atoms. It may take a minute or so to re-plot after simplifying. Once re-plotted, click and drag the molecule to see the changes in the number of atoms on the interior of the molecule. Also note the reduction in number of total atoms on the bottom left-hand side of the program. Keep in mind that using this simplification is only applicable for Projected Area, EHSS/DHSS, DTM and TDHSS.
5. Type “Example2” into the *SaveSAS* text field and click *SaveSAS*. This will save an excel sheet with the new structures coordinates in the “savefolder” folder.
6. To keep calculation times low for this example, change the number of gas molecules per orientation to 30,000 for EHSS/DHSS and TM/DTM. Default values are 300,000.
7. Since using a simplified structure is not applicable to Lennard Jones, ensure only TDHSS is checked under the Trajectory Method options.
8. Type “\Examples\par1.txt” into the save file location.
9. Change the *Threads* to a number appropriate for the machine this example is being run on. It is recommended to leave at least one core available for other computing tasks while calculating.
10. Change *Seed* to 0. This will choose a pseudo-random number for calculations using the computer clock.
11. Ensure the plotting button is set to *Plotting: OFF*.
12. Click *Calculate*.
13. The parallel-interface version of the program works by creating an imos.cla file with the options chosen by the interface and calling the parallelized non-interface version of the code. During this process, the program saves a copy of this CLA file with the save file chosen. This allows for the same calculations run in the interface to be run in the non-interface version. It also allows for a review of all the parameters chosen.

### 10.3 PARALLELIZED (NON-INTERFACE)

This example showcases the faster parallelized option, without using the interface.

1. Save a back-up of the existing CLA file. Open the “IMoS.cla” file with an editor (Notepad++/Wordpad or Emacs is recommended if available).
2. On the second line, ensure the “Anallainb.xlsx” file is typed in first, followed by at least a single space. Only use spaces. Do not use tab.
3. Next, change the directory and filename (including file extension) for the results file, followed by at least a single space. For this example, the directory will be “/savefolder/Examples/par2.txt”.
4. Ensure nitrogen is the chosen gas. “N2” should be typed after the save file directory with at least one space
5. Ensure line 3 is blank.
6. Line 4 determines whether the interface is loaded. Since this example will not be using the interface, ensure both values to the right of “interface” are zeros.
  - a. “interface 0 0” = no interface
  - b. “interface 1 0” = use interface
7. For this example, multiple molecules will be run through the program. Change the “fromvalue” to 1 and the “tovalue” to 4. This will ensure the molecules found on sheets 1 through 4 of the selected excel file will be run through the program.
8. Change “NgastotalTM” to 30000. Note that if any of the items in this example are not found in your CLA file, you can simply add the title and value chosen for the example.
9. For this example, we will only run the Trajectory Method. Ensure the “PA” and “EHSS/DHSS” options are set to 0.



10. Set “*LennardJones*” to 1, and “*qpol*” to 1. Ensure “*TDHSS*” is set to 0.
11. Select an appropriate number of threads for the “*Numthreads*” option. Select any integer for a “*Seed*”. If one would like to use the same seed for all molecules, add “*Repeatseed*” 1 to the end of the file.
12. At this point, the CLA file should look similar to Figure 10.5 below.
13. Save and close the CLA file. Click the IMoS executable file, and calculations should begin. As with the other examples, you can navigate to the chosen save file directory to view the results.

```

1  excelfile          Savefile          Gas
2  AnalIainb.xlsx /savefolder/Examples/par2.txt  N2
3
4  interface 0 0
5  fromvalue 1
6  tovalue 4
7  Charge 1
8  Mgas 28
9  radgas 1.5
10 Polarizability 1.7
11 Pressure 101325
12 Mweight 55000
13 Temperature 301
14
15 NrotationsPA 500
16 NgastotalEHSS 300000
17 NgastotalTM 30000
18 Accommodation 0
19 reemvel 6
20
21 PA 0
22 EHSS/DHSS 0
23 TM 1
24
25 LennardJones 1
26 qpol 1
27 TDHSS 0
28
29 seed 500
30 Numthreads 7

```

Figure 10.5 – No Interface Example (Edited CLA file)

## 10.4 RESULTS FOR A SPHERE USING EHSS/DHSS. ARRIVING AT MILLIKAN’S 1.36

This example uses a simple sphere to explain how the accommodation coefficient and diffuse reemission work.

1. Load *spheretest.xlsx* and model number 1 either onto the interface or select the appropriate path on the *imos.cla* file. *Spheretest* consists of a single atom that has a radius so that its projected area is 1 Å<sup>2</sup>.
2. Select the *gas radius (radgas)* to be 0. *Temperature* to 304K (Temperature will not change the result but will be used to interpret the velocities used). *Seed* is 13 for the runs below. *Repeatseed* is 1.
3. Select the PA as well as the EHSS/DHSS methods. Select *NrotationsPA* 500 and *NgastotalEHSS* to be 300000.
4. For the first run, select *Accommodation* to be 0 (can also be misspelled *Acommodation*). Select your savefile and run the calculation. The result for the CCS for PA and EHSS should be equals to 1 in this case. For EHSS, the calculation states that the 100% of the molecules will be reemitted specularly and elastically.

The average collision cross section for Sheet1 is 1.0004 Å<sup>2</sup> and the Mobility is 223.3518 cm<sup>2</sup>/Vs.  
Time taken is a mere 0.58686 seconds

5. For the next runs we will be modifying the accommodation coefficient, diffuse option and reemission velocities. Deselect the PA option as it will always yield the same result.
6. Select *Accommodation 1, diffuse? 1 and Elastic* or Elastic (mean) as your velocity. This calculation states that 100% of your gas molecules will be reemitted elastically and diffuse. Epstein calculated this value to be 1.444\*PA. The result for IMoS is:

The average collision cross section for Sheet1 is 1.4445 Å<sup>2</sup> and the Mobility is 154.6756 cm<sup>2</sup>/Vs.  
Time taken is a mere 0.59565 seconds

7. Select *Accommodation 1, Diffuse? 1 and Maxwell* or Distributed Maxwell. This calculation states that 100% of your gas molecules will be reemitted diffusely but accommodated at the gas temperature. Epstein calculated this value to be 1.39\*PA. The result for IMoS is:

The average collision cross section for Sheet1 is 1.3927 Å<sup>2</sup> and the Mobility is 160.4256 cm<sup>2</sup>/Vs.  
Time taken is a mere 0.57402 seconds

8. Select *Accommodation 0.91, Diffuse? 1 and Maxwell*. This calculation states that 91% of the gas molecules will be reemitted diffusely but accommodated at the gas temperature. The remaining 9% are reemitted specularly and elastically. This was the choice of Epstein to match Millikan's 1.357~1.36 result. IMoS yields:

The average collision cross section for Sheet1 is 1.3572 Å<sup>2</sup> and the Mobility is 164.6316 cm<sup>2</sup>/Vs.  
Time taken is a mere 0.60444 seconds

9. Select *Accommodation 1, Diffuse? 1 and 92% Maxwell*. This calculation states that 100% of the gas molecules will be reemitted diffusely but accommodated at 92% of the energy of the Maxwell Distribution. This is equivalent to Epstein and Millikan's 1.36 result but has the advantage that the 9% reemitted specularly will not be specularly diffuse due to scattering. IMoS yields:

The average collision cross section for Sheet1 is 1.3618 Å<sup>2</sup> and the Mobility is 164.0676 cm<sup>2</sup>/Vs.  
Time taken is a mere 0.61382 seconds

10. As a last example. Let us understand the use of Other. Select Accommodation 1, diffuse? 1 and Other (mean) to the values below. The average momentum flux velocity for each Elastic is value is  $\sqrt{128kT/9\pi m}$ , that of Maxwell is  $\sqrt{18\pi kT/16m}$  and that of Maxwell 92% is  $\sqrt{3kT/m}$ . For 304K, these velocities correspond to 639.11, 564.70 and 520.269 m/s (8% less) respectively. The results (respectively) are:

The method used is: EHSS/DHSS (parallel)  
The mean collision cross section for Sheet1 is 1.4445 Å<sup>2</sup> and the Mobility is 158.3608 cm<sup>2</sup>/Vs.  
Time taken is a mere 0.56265 seconds

Calculations complete!

The method used is: EHSS/DHSS (parallel)  
The mean collision cross section for Sheet1 is 1.3927 Å<sup>2</sup> and the Mobility is 164.241 cm<sup>2</sup>/Vs.  
Time taken is a mere 0.57679 seconds

Calculations complete!

The method used is: EHSS/DHSS (parallel)  
The mean collision cross section for Sheet1 is 1.3618 Å<sup>2</sup> and the Mobility is 167.9696 cm<sup>2</sup>/Vs.  
Time taken is a mere 0.58433 seconds

Calculations complete!

## 10.5 RESULTS COMPARISON (LENNARD JONES AND LENNARD JONES QPOL)

This example showcases the accuracy of the results from the Lennard Jones calculations. Note that the calculation time for this example will be much longer than the previous examples.

1. Open the IMoS program and select the “Anallainb.xlsx” file from the file window. Type in 1 and 16 into the *From* and *To* boxes, to run calculations on the first 16 sheets of the excel file. Be sure to check the *From* checkbox to enable running multiple files.
2. Ensure Nitrogen is selected from the *Gas* list and click *Load File*.
3. Ensure the plotting option is turned off.
4. For this example, the results for Lennard Jones and Lennard Jones QPol will be compared to experimental values. Uncheck the *Projected Area* and *EHSS/DHSS* options under the *Calculations* section.
5. For the first part of the calculations, only the Lennard Jones method will be used. Check *LenJon*, ensuring that *QPol* is not checked. Uncheck *TDHSS*.
6. Make sure the number of Gas Molecules is set to at least 300000.
7. Ensure the file save option is enabled and select an appropriate file name and location.
8. Choose the appropriate *Threads* value for the machine this example is being run on.
9. For the results shown below, a *Seed* of 13 was used.
10. Click *Calculate*.
11. Once calculations are completed, choose a new save file name to ensure the previous results are not overwritten.
12. Check the *QPol* option, enabling the ion induced quadrupole potential.
13. Click *Calculate*.
14. Once calculations are complete, open the results text file for review.

Shown below is an excerpt from the first round of calculations. The first section of the results lists several parameters chosen for calculations. The bottom two lines in the excerpt below show the resulting molecular cross-sectional area and mobility for the first sheet ran. The following sections of the results file show all the remaining sheets results in the same format.

```
IMoS v1.10 RESULTS FILE

File: \filefolder\Anallainb.xlsx and excel sheet(if available): 1

Number of atoms: 30
Is it simplified?: 0

Molecular Weight:    228.00 Da
Total Charge: 1

Method used: Trajectory Method
n_rotations: 3
Gas molecules per rotation: 300000
Lennard-Jones?(1 for yes): 1
Cutoff?(1 for yes): 0
TMSimplified?: 1
The mean molecular cross sectional area for Model 1 is 144.4152 Å^2 and the Mobility is 1.5841 cm^2/Vs.
Time taken is a mere 32.7539 seconds
```

Figure 10.6 - IMoS Results File (Molecule)

After each molecule's results are shown, the results file lists additional parameters chosen for the calculations. Included among these is the Lennard Jones parameters used, from the LJTable excel file. Since Nitrogen was used for this example, the Lennard Jones parameters from the first sheet of the LJTable file was used and printed in the results file. The next section is a summary and lists the molecular cross-sectional areas and mobilities of all molecules in a format that makes copying/pasting into excel easier.

PARAMETERS USED:	Lennard Jones parameters (if used)			SUMMARY
	Atom	eps (J*10 <sup>21</sup> )	sigma (Å)	
Gas: N2	H	0.4806000000	2.3000000000	COLLISION CROSS SECTION (Å <sup>2</sup> )
Reduction Coef: 1.000	C	0.7449300000	3.5000000000	
Molecular mass of Gas: 28.00 Da	O	0.6888600000	3.5000000000	
Alpha polarization: 1.70 Å <sup>3</sup>	N	0.9291600000	4.2000000000	
Radius of gas: 1.50 Å	F	0.1922400000	3.4000000000	
Temperature: 304 K	Cs	0.5814000000	4.2008100000	
Pressure: 101325 Pa	Na	0.4167763200	3.5000000000	
Accommodation coefficient: 0	Cl	0.4167763200	3.5000000000	
Diffuse Scattering?: 1	I	0.6300000000	5.4000000000	
Reemission_vel(mean): 639.11 m/s Elastic (mean)	K	0.4167763200	3.5000000000	
Timestep: 150	Rb	0.4167763200	3.5000000000	
Boxdomain(one charge): 16 Å	P	0.4167763200	3.5000000000	
	Ca	0.4167763200	3.5000000000	
	Li	0.4167763200	3.5000000000	
	S	0.4167763200	3.5000000000	
	Other	0.4167763200	3.5000000000	
				MOBILITY (cm <sup>2</sup> /Vs)
				144.415218
				119.879310
				189.785923
				129.486112
				189.335627
				1.584121
				1.996963
				1.177415
				1.814429
				1.180215

Figure 10.7 - IMoS Results File (Parameters)

The remainder of the results file is a print-out of all excel sheets ran (if an excel file is used) and the CLA file used. To ensure columns are aligned correctly, be sure to use a monospaced font (courier, fixedsys, etc.) in whatever program being used to read the results file.

AnalIainb.xlsx - Sheet #1					
x	y	z	Radius	Charge	Atom
-0.037000	2.847000	0.000000	1.70000	-0.2335540000	12
0.878000	3.424000	0.000000	1.10000	0.1696540000	1
-1.241000	3.538000	0.000000	1.70000	0.0164670000	12
-1.236000	4.623000	0.000000	1.10000	0.1477940000	1
-2.472000	2.840000	0.000000	1.70000	-0.1059910000	12
-3.409000	3.388000	0.000000	1.10000	0.1617550000	1
-2.471000	1.468000	0.000000	1.70000	-0.1649070000	12

Figure 10.8 - Results File - Excel Sheet

The results from this example can be summarized below, compared to the experimental values obtained from Campuzano et al. Analytical Chemistry (2012)[16]. The results from the Lennard Jones calculations have an average percent error of approximately 1.05%. For the calculations utilizing the ion induced quadrupole potentials, the average error is slightly higher at 1.14%.

	Exp. CCS	IMoS CCS	Error	IMoS	Error
	(Å <sup>2</sup> )	(Å <sup>2</sup> )	(%)	Qpol CCS	(%)
				(Å <sup>2</sup> )	
Tryphenylene	143.30	144.42	0.78%	145.94	1.84%
Nethylaniline	124.50	119.88	3.71%	122.55	1.57%
Dexamethasone	190.70	189.79	0.48%	190.00	0.37%
Acetaminophen	131.10	129.49	1.23%	130.82	0.22%
Betamethasone	189.60	189.34	0.14%	188.55	0.56%
Anthracene	129.60	130.95	1.05%	133.43	2.96%
Choline	115.40	113.63	1.54%	115.63	0.20%
Phenanthrene	129.10	131.68	2.00%	132.95	2.98%
Acetylcholine	127.80	127.47	0.26%	127.78	0.02%
C60	213.10	212.17	0.44%	213.40	0.14%
C70	231.40	230.80	0.26%	230.44	0.41%
Naphtalene	115.80	115.88	0.07%	118.45	2.29%
Paracetamol2	131.10	130.38	0.55%	131.75	0.49%
Pyrene	135.00	136.00	0.74%	137.45	1.82%
TtEA	122.20	121.86	0.27%	120.41	1.46%
TMA	107.40	103.79	3.36%	106.39	0.94%
<b>Error Avg(%)</b>			<b>1.05%</b>		<b>1.14%</b>

Figure 10.9 - IMoS Results Comparison

## 10.6 RUN IMoS AT SEVERAL DIFFERENT TEMPERATURES

The following section validates the ability of IMoS to simulate mobility at different temperatures. Here, the L-J parameters for carbon and experimental data for C60 are taken from Mesleh's work[14]. The results will also be compared to those of this work.

This can be done from the interface or directly from the IMoS.cla file.

1. Interface.
  - a. Open interface. Load any molecule from file: Anallainb.xlsx.
  - b. Check the From: To: box in the File parameters. In the From box, choose 10, in the to box choose 10. This will run molecules C60.
  - c. Select only the Trajectory M. LenJon option in He.
  - d. It is recommended to choose the same seed (13 for example) for all runs to lower variability. Choose Repeatseed (RS 1) equals 1.
  - e. In the Workbatch group, check the Optimize LJ box.
  - f. Open the Optinput file in the Optimizer folder. Set the parameters to:

```
efrom 0.214668
eto 0.214668
ejump 0.05
sfrom 3.068
sto 3.068
sjump 0.1
vdwfrom 1
vdwto 1
vdwjump 0.5
atom 2
structures 1
Temp 80.51 87.67 95.06 102.50 114.7666 129.2572 151.1708 181.1045 209.11 245.16 273.1217 301.09
329.70 376.60
result 11
expected 175.2523424 172.8743668 167.1750739 163.8699468 158.5039306 152.2930377 145.8644951
138.528596 134.1387114 130.1639879 126.727528 124.3742918 122.6727138 119.5136
```

The *expected* values correspond to the experimental CCS for the C60 at given temperature while *atom 2* corresponds to Carbon in the LJTable.csv list (H is 1, C is 2, O is 3,...)

- g. Set the LJ parameters in LJTable.csv for which the simulation needs to run.
  - h. Press Calculate and wait for completion.
2. No Interface.
  - a. Open IMoS.cla and choose *interface 0 1*. Fill out the rest of the parameters in the IMoS.cla making sure that only structures 10 (*fromvalue 10 tovalue 10*) is run.
  - b. Make sure that only the TMLJ (*TM 1 LennardJones 1*) is the only method selected to run.
  - c. Open the *Optinput.txt* file in the Optimizer folder. These will be the parameters to set:

```
efrom 0.214668
eto 0.214668
ejump 0.05
sfrom 3.068
sto 3.068
sjump 0.1
vdwfrom 1
vdwto 1
vdwjump 0.5
atom 2
structures 1
Temp 80.51 87.67 95.06 102.50 114.7666 129.2572 151.1708 181.1045 209.11 245.16 273.1217 301.09
329.70 376.60
result 11
expected 175.2523424 172.8743668 167.1750739 163.8699468 158.5039306 152.2930377 145.8644951
138.528596 134.1387114 130.1639879 126.727528 124.3742918 122.6727138 119.5136
```

The *expected* values correspond to the experimental CCS for the C60 at given temperature while *atom* 2 corresponds to Carbon in the LJTable.csv list (H is 1, C is 2, O is 3,...)

- d. Set the LJ parameters in LJTable.csv for which the simulation needs to run. In this particular example, the C60 He parameters are set on the *Optinput.txt* file.

- e. Run IMoS110(platform) executable.

The mobility at the effective temperature will be printed in *resultsopt8.txt*. It needs to be converted to reduced mobility ( $K_0$ ) through the equation:  $K_0 = \frac{p}{101325} \frac{273.15}{T} K$ . The pressure value is 101325Pa. Thus, the equation becomes  $K_0 = \frac{273.15}{T}$ . In this case, the effect of field is negligible in the equation of  $T_{eff}$ . Thus, the gas temperature is considered  $T_{eff}$  and the  $E/n$  is zero.

The following graph represents the simulated Vs experimental reduced mobility at different temperature.

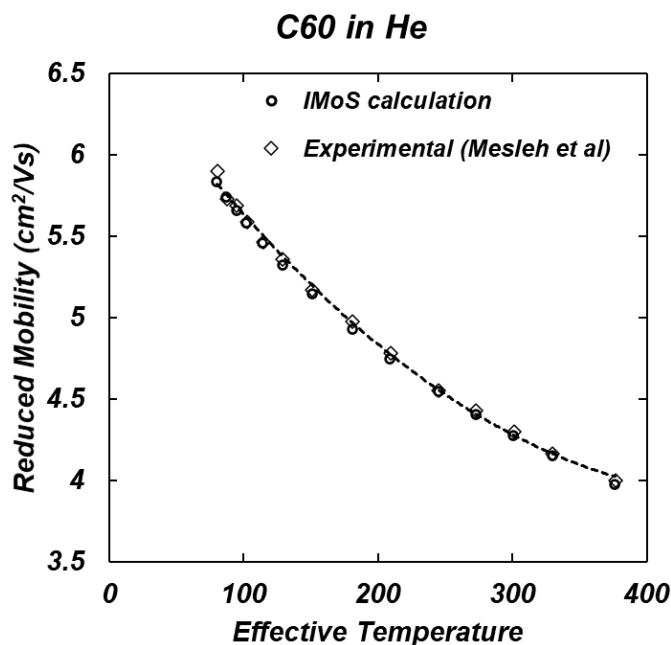


Figure 10.10 C60 at different temperature (experiment vs simulation) based on Mesleh's manuscript.

## 10.7 USING IMoS AS AN APPROXIMATION FOR HIGHER FIELDS. EFFECTIVE TEMPERATURE.

The following example shows the validity of the two-temperature approximation used in IMoS to calculate the CCS and mobility as a function of  $E/n$ . This result is only an approximation, but it is relatively accurate for gases like He. The process is to select a Temperature that will be higher than the assumed gas temperature thus imitating an effective temperature. The mobility calculation in IMoS calculates  $n$  using a perfect gas assumption ( $n = p/k_b T$ ) with  $p$  being the pressure. Since you will be choosing a higher temperature than that of the gas for the CCS, this will have to be corrected later.

1. Choose the smallions.xlsx file and the first 4 molecules (From 1 to 4). The molecules chosen are  $H_3^+$ ,  $O^+$ ,  $CH_5^+$ , and  $NO_2^-$ .
2. Make sure that He is selected as the gas and that TMLJ method is selected.
3. We will consider that the gas is at 298K. Select the Pressure to be 101325 and record this value. The Pressure may be any value and will not affect the end result of the calculation.
4. Run and save the calculation for different Temperatures. For example, 298K (zero field), 300, 305, 315, 350, 400, 500, 600, 800, 1000, 1300, 1600, 2000K. These are effective temperatures. Record the mobility. This is  $K_{eff}$ .
5. In order to do a comparison with experimental calculations, one needs to express the mobility as reduced mobility, and calculate the field from the effective temperature compared to the gas temperature.
6.  $n$  was calculated by IMoS using  $T_{eff}$ . First correct the mobility to the appropriate  $n$ . To do so:

$$K = K_{eff} \frac{n_{eff}}{n} = K_{eff} \frac{T}{T_{eff}}$$

7. Now calculate the reduced mobility  $K_0$  ( $p$  and  $T$  are in this case 101325 and 298K):

$$K_0 = \frac{p}{101325} \frac{273.15}{T} K$$

8. To calculate  $E/n$ , we use the corrected value of mobility and the definition of  $T_{eff} = T + mv_d^2/3k_b$  and  $v_d = KE$ :

$$\frac{E}{n} = \frac{1}{Kn} \left( \frac{3k_b(T_{eff} - T)}{m} \right)^{1/2}$$

9. The final results can then be calculated and compared to Lindinger et al. J Chem. Phys from 1975[18].

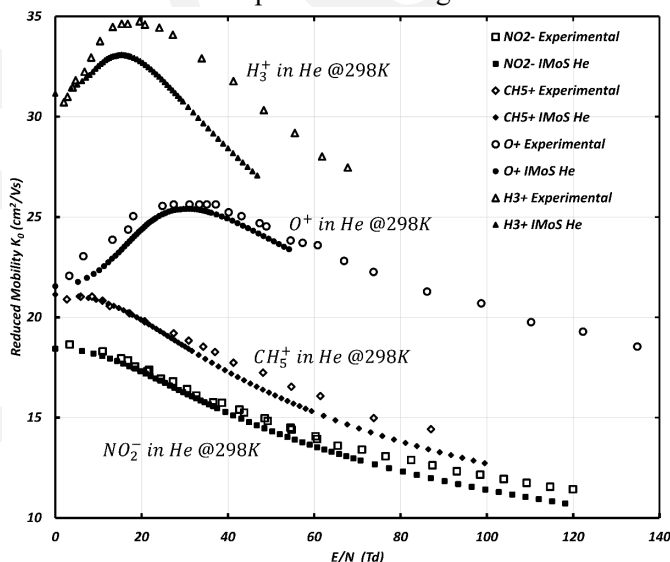


Figure 10.11 High Field Using IMoS and Effective Temperature



## 10.8 OPTIMIZING L-J PARAMETERS AT CONSTANT TEMPERATURE.

To optimize L-J parameters, please follow reference [19]. Here we will showcase an example using 4 different structures to optimize the Carbon atom in N2 at 300K. We will choose 4 structures from the Analaiinb.xlsx file. This can be done from the interface or directly from the IMoS.cla file.

1. Interface.
  - a. Open interface. Load any molecule.
  - b. Check the From: To: box in the File parameters. In the From box, choose 10, in the to box choose 13. This will run molecules C60, C70, Naphtalene and Paracetamol2.
  - c. Select only the Trajectory M. LenJon option in N2. **Only this one.**
  - d. Make sure Temperature is set to 300K and all other parameters are correct. It is recommended to choose the same seed (13 for example) for all runs to lower variability. Choose Repeatseed (RS 1) equals 1.
  - e. In the Workbatch group, check the Optimize LJ box.
  - f. Open the *Optinput.txt* file in the Optimizer folder. These will be the parameters to set:

```

|efrom 0.55
eto 0.95
ejump 0.05
sfrom 3.1
sto 3.9
sjump 0.1
vdwfrom 1
vdwto 1
vdwjump 0.5
atom 2
structures 4
Temp 300
result 10
expected 213.10 231.40 115.80 131.10

```

The *expected* values correspond to the experimental CCS for the 4 structures while *atom 2* corresponds to Carbon in the LJTable.csv list (H is 1, C is 2, O is 3,...)

- g. Copy LJTableN2default.csv to LJTable.csv. If the LJ parameters for the other atoms are different from default, customize as appropriate. **The order must remain the same.**
- h. Press Calculate and wait for completion. Note that these calculations could take several hours if too many calculations are required.
- i. The output will be printed in *resultsopt10.txt* and the program will try to plot the results on the interface as well. Result is shown in the figure below. Note that under some cases, the minimum result might not be the most physically correct due to a mathematical relation that exists between  $\epsilon$  and  $\sigma$  (like below).

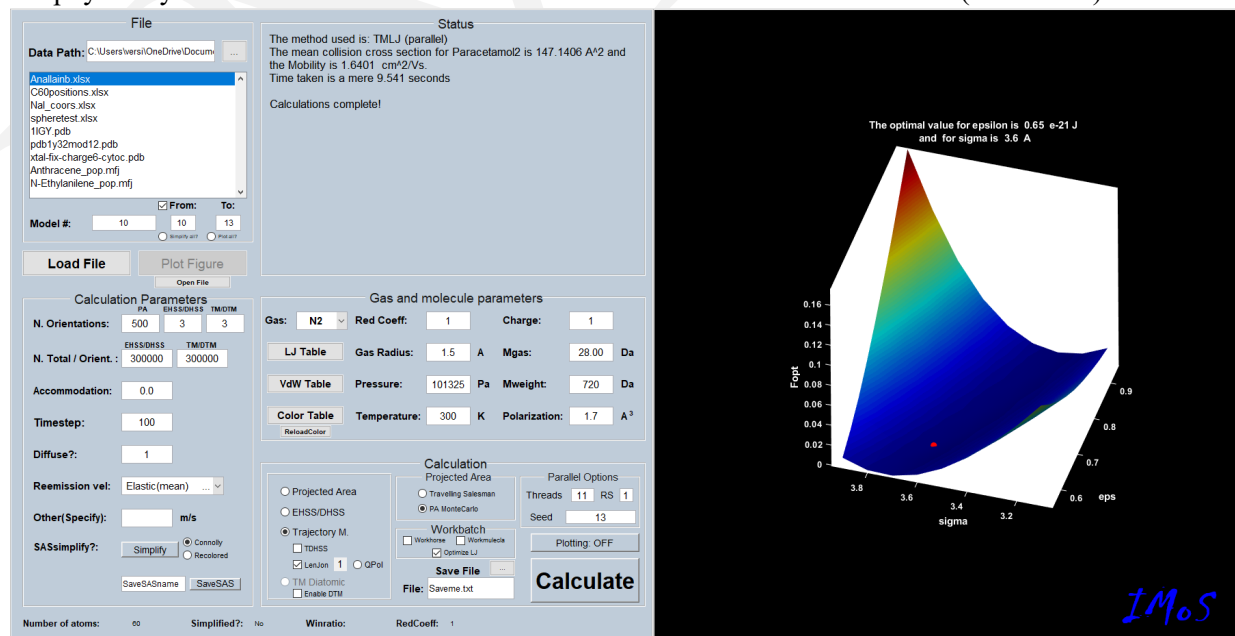


Figure 10.12 Optimization of Carbon L-J parameters using IMoS Optimizer

## 2. No Interface.

- Open IMoS.cla and choose *interface 0 1*. Fill out the rest of the parameters in the IMoS.cla making sure that only structures 10 through 13 (*fromvalue 10 tovalue 13*) are run.
- Make sure that only the TMLJ (*TM 1 LennardJones 1*) is the only method selected to run.
- Open the Optinput file in the Optimizer folder. These will be the parameters to set:

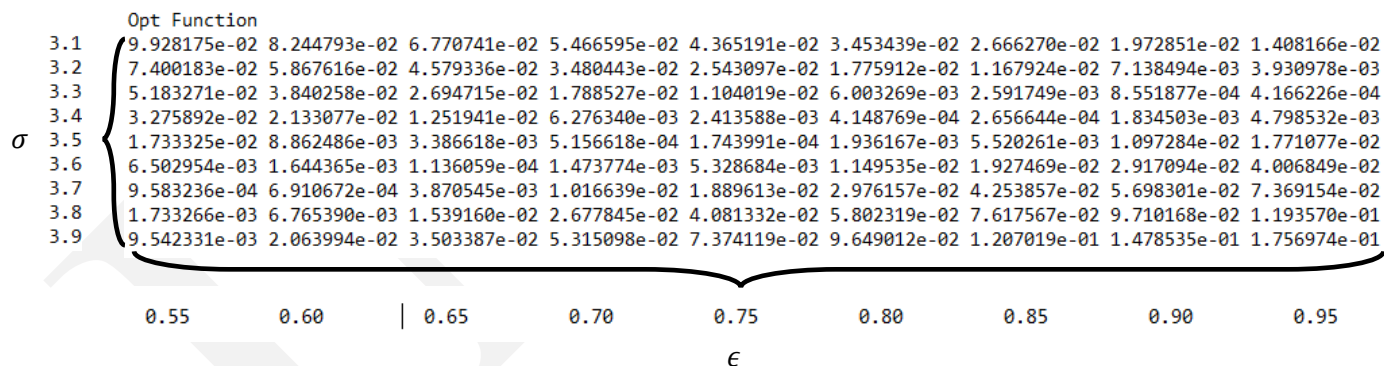
```

efrom 0.55
eto 0.95
ejump 0.05
sfrom 3.1
sto 3.9
sjump 0.1
vdwfrom 1
vdwto 1
vdwjump 0.5
atom 2
structures 4
Temp 300
result 10
expected 213.10 231.40 115.80 131.10

```

The *expected* values correspond to the experimental CCS for the 4 structures while *atom 2* corresponds to Carbon in the LJTable.csv list (H is 1, C is 2, O is 3,...)

- Copy LJTableN2default.csv to LJTable.csv. If the LJ parameters for the other atoms are different from default, customize as appropriate. **The order must remain the same.**
- Run IMoS110(platform) executable. The output will be printed in *resultsopt10.txt*. The program will attempt to find a minimum, but one should plot  $F_{opt}$  vs epsilon and gamma to verify the result. Note that under some cases, the minimum result might not be the most physically correct due to a mathematical relation that exists between  $\epsilon$  and  $\sigma$  (like below).
- In the results file,  $F_{opt}$  is printed with rows pertaining to changes in sigma and columns pertaining to changes in epsilon. As captured below:



## 10.9 OPTIMIZATION OF L-J PARAMETERS AT DIFFERENT TEMPERATURES

Here we will showcase an example of optimizing parameters for Carbon in Helium gas using 1 structure at different temperatures. We will choose structure of C60 from the Analiainb.xlsx file. This can be done from the interface or directly from the IMoS.cla file. The experimental values are taken from (Mesleh) paper.

1. Interface.
  - a. Open interface. Load any molecule from file: Anallainb.xlsx.
  - b. Check the From: To: box in the File parameters. In the From box, choose 10, in the to box choose 10. This will run only C60 molecule.
  - c. Select only the Trajectory M. LenJon option in He.
  - d. Make sure all parameters related to gas are correct. It is recommended to choose the same seed (13 for example) for all runs to lower variability. Choose Repeatseed (RS 1) equals 1.
  - e. In the Workbatch group, check the Optimize LJ box.
  - f. Open the Optinput file in the Optimizer folder. These will be the parameters to set:

```
efrom 0.1
eto 0.3
ejump 0.02
sfrom 2.70
sto 3.30
sjump 0.05
vdwfrom 1
vdwto 1
vdwjump 0.5
atom 2
structures 1
Temp 80.51263411 87.67177152 95.0691201 102.5048751 114.7665782
129.2572246 151.1708239 181.1045043 209.113292 245.1586208
273.1216866 301.0902391 329.7016416 358.6134372 376.6022673
result 8
expected 5.900290791 5.732036431 5.692172637 5.592394845 5.464138016
5.358729571 5.173514666 4.976973301 4.783264408 4.552551626
4.43016892 4.299227071 4.165439033 4.063037947 4.000462934
```

The *expected* values correspond to the experimental CCS for the C60 structure at different temperature while *atom 2* corresponds to Carbon in the LJTable.csv list (H is 1, C is 2, O is 3,...)

- g. Copy LJTableHedefault.csv to LJTable.csv. If the LJ parameters for the other atoms are different from default, customize as appropriate.
- h. Press Calculate and wait for completion. Note that these calculations could take several hours if too many calculations are required.
- i. The output will be printed in *resultsopt8.txt* and the program will try to plot the results on the interface as well. Result is shown in the figure below. Note that under some cases, the minimum result might not be the most physically correct due to a mathematical relation that exists between  $\epsilon$  and  $\sigma$ .

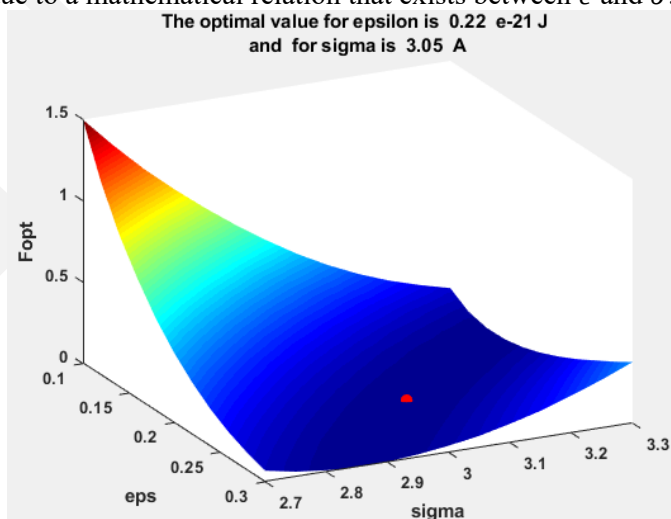


Figure 10.13 Optimization of Carbon L-J parameters using IMoS Optimizer (Temperature and LJ change)

## 1. No Interface.

- Open IMoS.cla and choose *interface 0 1*. Fill out the rest of the parameters in the IMoS.cla making sure that only structures 10 (*fromvalue 10 tovalue 10*) is run.
- Make sure that only the TMLJ (*TM 1 LennardJones 1*) is the only method selected to run.
- Open the Optinput file in the Optimizer folder. These will be the parameters to set:

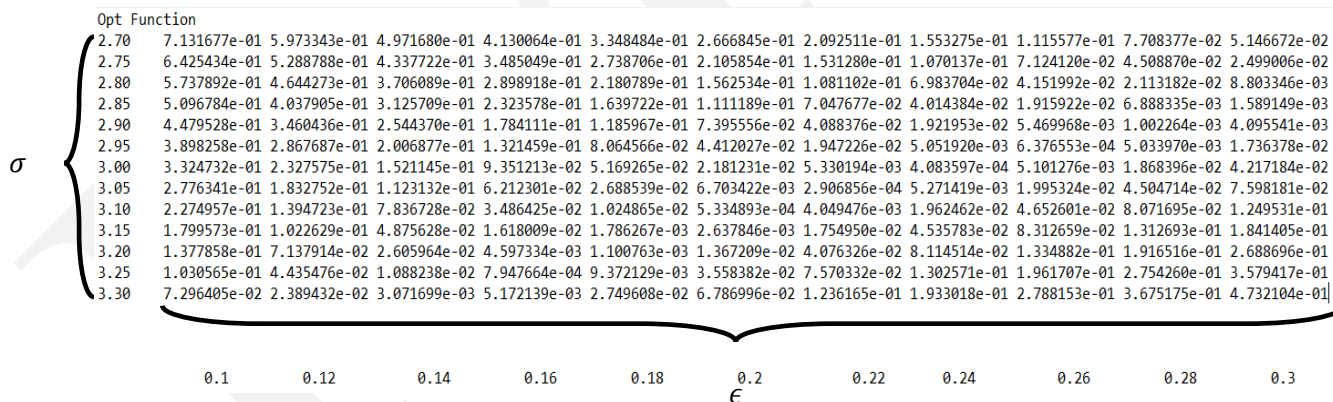
```

efrom 0.1
eto 0.3
ejump 0.02
sfrom 2.70
sto 3.30
sjump 0.1
vdwfrom 1
vdwto 1
vdwjump 0.5
atom 2
structures 1
Temp 80.51 87.67 95.06 102.50 114.7666 129.2572 151.1708 181.1045 209.11 245.16 273.1217
301.09 329.70 376.60
result 8
expected 175.2523424 172.8743668 167.1750739 163.8699468 158.5039306 152.2930377 145
.8644951 138.528596 134.1387114 130.1639879 126.727528 124.3742918 122.6727138 119.5136

```

The *expected* values correspond to the experimental CCS for the C60 structure at different temperature while *atom 2* corresponds to Carbon in the LJTable.csv list (H is 1, C is 2, O is 3,...)

- Copy LJTableHedefault.csv to LJTable.csv. If the LJ parameters for the other atoms are different from default, customize as appropriate. **The order must remain the same.**
- Run IMoS110(platform) executable. The output will be printed in *resultsopt8.txt*. The program will attempt to find a minimum, but one should plot  $F_{opt}$  vs epsilon and gamma to verify the result. Note that under some cases, the minimum result might not be the most physically correct due to a mathematical relation that exists between  $\epsilon$  and  $\sigma$ .
- In the results file,  $F_{opt}$  is printed with rows pertaining to changes in sigma and columns pertaining to changes main epsilon. As captured below:



## 10.10 USING IMoS TO RUN ALL COORDINATE FILES FROM WORKFOLDER OR ALL CLA FILES FROM WORKMULE

This example showcases the option to run all analyte files from a folder, without using the interface.

- Put files in the Workhorse folder.
  - Files in the folder could be: Anthracene\_pop.mfj, NEthylaniline\_pop.mfj, Anallainb.xlsx, C60positions.xlsx, ch3.xlsx, CH4.xlsx, pdb1y32mod12.pdb, and xtalfixcharge6cytoc.pdb, pdb1y32mod12twomodelonly.pdb, Anthracene\_pop2.mfj
  - .pdb files will run for the number of models. The program searches for the variable NUMMDL to set the number of models to run. Example pdb1y32mod12twomodelonly.pdb will run two models while pdb1y32mod12.pdb will run all 14. If there is no NUMMDL variable in the pdb file, only one structure is assumed.
  - .mfj files may have more than one model as well. The second-row value in the .mfj file is used to establish how many structures to run. The example Anthracene\_pop2.mfj has two structures.
- The Workhorse can be run with or without the interface:
  - No interface. Change IMoS.cla parameter *interface* to *interface 0* 2. Execute IMoS110(platform) executable. The parameters are selected from IMoS.cla.
  - Within the interface, check the workhorse checkbox. Choose parameters to run within the interface (From to box is not taken into account, program will run all structures within the Workhorse folder. Press calculate. It will print a SUMMARY.txt file on the Workhorse folder with all the CCS and mobility results.
- Result files are available in savefolder with the analyte names and extension

Similarly, to run all .cla files, change the interface parameter to *interface 0* 3 and provide appropriate folder name. Sequentially, IMoS will copy the content from .cla files to IMoS.cla and analyze accordingly.

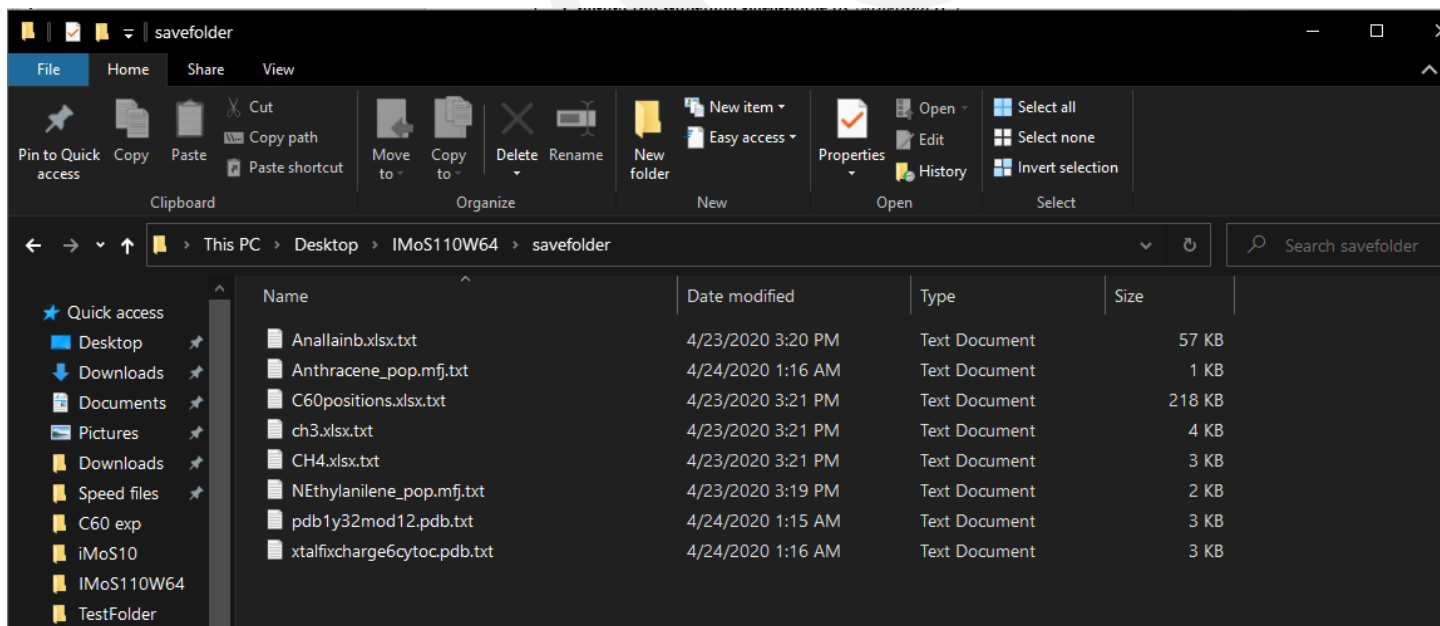


Figure 10.14 savefolder after analysis

## 11 EXAMPLE OF A COMPLETE OUTPUT FILE

For completeness, a result file is printed here for comparison using AnalIainb.xlsx with the first 2 structures and PA, EHSS/DHSS, TDHSS and TMLJ (no qpol) using N<sub>2</sub>. **Note the use of accommodation=0.48 to match TMLJ.**

### IMoS v1.10 RESULTS FILE

File: AnalIainb.xlsx                      Molecule: Tryphenylene

Number of atoms: 30  
Molecular Weight:    228.00 Da  
Total Charge: 1

Method used: Projected Area MC  
Number of Orientations: 500  
Gas molecules per orientation: 0  
The average collision cross section for Tryphenylene is 106.1366 Å<sup>2</sup> and the Mobility is 2.2286 cm<sup>2</sup>/Vs.  
Time taken is 0.14571 seconds

Method used: EHSS/DHSS  
Number of Orientations: 3  
Gas molecules per orientation: 300000  
Accommodation coefficient: 0.48  
Diffuse Scattering?: 1  
Reemission\_vel(mean): 520.27 m/s 92% Maxwell Distributed  
The average collision cross section for Tryphenylene is 125.9964 Å<sup>2</sup> and the Mobility is 1.8155 cm<sup>2</sup>/Vs.  
Time taken is a mere 0.64151 seconds

Method used: Trajectory Method  
Number of Orientations: 3  
Gas molecules per orientation: 300000  
  
The TM Method used is TMLJ(4-6-12 potential)  
The average collision cross section for Tryphenylene is 144.1563 Å<sup>2</sup> and the Mobility is 1.6409 cm<sup>2</sup>/Vs.  
Time taken is a mere 16.2106 seconds

The TM Method used is TDHSS(4-inf with reemission choice)  
Accommodation coefficient: 0.48  
Diffuse Scattering?: 1  
Reemission\_vel(mean): 520.27 m/s 92% Maxwell Distributed  
Timestep: 150  
Reemvel(not used if LJ=1): 92% Maxwell Distributed  
The average collision cross section for Tryphenylene is 144.8035 Å<sup>2</sup> and the Mobility is 1.6335 cm<sup>2</sup>/Vs.  
Time taken is a mere 11.2002 seconds

File: AnalIainb.xlsx                      Molecule: NEthylaniline

Number of atoms: 21  
Molecular Weight:    122.00 Da  
Total Charge: 1

Method used: Projected Area MC  
Number of Orientations: 500  
Gas molecules per orientation: 0

## IMoS V1.10

The average collision cross section for NEthylaniline is 79.7605 Å<sup>2</sup> and the Mobility is 3.1033 cm<sup>2</sup>/Vs.  
Time taken is 0.12702 seconds

Method used: EHSS/DHSS

Number of Orientations: 3

Gas molecules per orientation: 300000

Accommodation coefficient: 0.48

Diffuse Scattering?: 1

Reemission\_vel(mean): 520.27 m/s 92% Maxwell Distributed

The average collision cross section for NEthylaniline is 95.3955 Å<sup>2</sup> and the Mobility is 2.5092 cm<sup>2</sup>/Vs.

Time taken is a mere 0.83098 seconds

Method used: Trajectory Method

Number of Orientations: 3

Gas molecules per orientation: 300000

The TM Method used is TMLJ(4-6-12 potential)

The average collision cross section for NEthylaniline is 120.7086 Å<sup>2</sup> and the Mobility is 2.0506 cm<sup>2</sup>/Vs.

Time taken is a mere 14.1277 seconds

The TM Method used is TDHSS(4-inf with reemission choice)

Accommodation coefficient: 0.48

Diffuse Scattering?: 1

Reemission\_vel(mean): 520.27 m/s 92% Maxwell Distributed

Timestep: 150

Reemvel(not used if LJ=1): 92% Maxwell Distributed

The average collision cross section for NEthylaniline is 123.8953 Å<sup>2</sup> and the Mobility is 1.9979 cm<sup>2</sup>/Vs.

Time taken is a mere 9.9488 seconds

## PARAMETERS USED:

Gas: N2

Reduction Coef: 1.000

Molecular mass of Gas: 28.00 Da

Alpha polarization: 1.70 Å<sup>3</sup>

Radius of gas: 1.50 Å

Temperature: 304 K

Pressure: 101325 Pa

## Lennard Jones parameters

Atom	eps(J*10 <sup>21</sup> )	sigma(Å)
H	0.4806000000	2.3000000000
C	0.7449300000	3.5000000000
O	0.9000000000	4.0000000000
N	1.3500000000	3.8400000000
F	0.1922400000	3.4000000000
Cs	0.5814000000	4.2008100000
Na	0.4167763200	3.5000000000
Cl	0.4167763200	3.5000000000
I	0.6300000000	5.4000000000
K	0.4167763200	3.5000000000
Rb	0.4167763200	3.5000000000
P	0.4167763200	3.5000000000
Ca	0.4167763200	3.5000000000
Li	0.4167763200	3.5000000000
S	0.4167763200	3.5000000000
Other	0.4167763200	3.5000000000



## SUMMARY

COLLISION CROSS SECTION (Å <sup>2</sup> )	MOBILITY (cm <sup>2</sup> /Vs)
106.136605	2.228642
125.996388	1.815495
144.156333	1.640861
144.803491	1.633527
79.760548	3.103348
95.395536	2.509217
120.708570	2.050598
123.895256	1.997855

AnalIainb.xlsx - Sheet #1

x	y	z	Radius	Charge	Atom
-0.037000	2.847000	0.000000	1.70000	-0.2335540000	12
0.878000	3.424000	0.000000	1.10000	0.1696540000	1
-1.241000	3.538000	0.000000	1.70000	0.0164670000	12
-1.236000	4.623000	0.000000	1.10000	0.1477940000	1
-2.472000	2.840000	0.000000	1.70000	-0.1059910000	12
-3.409000	3.388000	0.000000	1.10000	0.1617550000	1
-2.471000	1.468000	0.000000	1.70000	-0.1649070000	12
-3.421000	0.953000	0.000000	1.10000	0.1626630000	1
-2.478000	-1.456000	0.000000	1.70000	-0.1645830000	12
-3.426000	-0.936000	0.000000	1.10000	0.1626320000	1
-2.487000	-2.828000	0.000000	1.70000	-0.1060860000	12
-3.426000	-3.371000	0.000000	1.10000	0.1617320000	1
-1.259000	-3.531000	0.000000	1.70000	0.0156690000	12
-1.259000	-4.617000	0.000000	1.10000	0.1479830000	1
-0.051000	-2.847000	0.000000	1.70000	-0.2313680000	12
0.860000	-3.429000	0.000000	1.10000	0.1689700000	1
2.504000	-1.391000	0.000000	1.70000	-0.1004450000	12
2.535000	-2.473000	0.000000	1.10000	0.1490260000	1
3.721000	-0.705000	0.000000	1.70000	-0.0896240000	12
4.653000	-1.261000	0.000000	1.10000	0.1586980000	1
3.725000	0.687000	0.000000	1.70000	-0.0888260000	12
4.659000	1.238000	0.000000	1.10000	0.1585220000	1
2.511000	1.379000	0.000000	1.70000	-0.1036130000	12
2.547000	2.461000	0.000000	1.10000	0.1500950000	1
0.008000	1.442000	0.000000	1.70000	0.1410250000	12
-1.249000	0.719000	0.000000	1.70000	0.0847350000	12
-1.252000	-0.713000	0.000000	1.70000	0.0837650000	12
0.000000	-1.442000	0.000000	1.70000	0.1406790000	12
1.267000	-0.713000	0.000000	1.70000	0.0017150000	12
1.271000	0.707000	0.000000	1.70000	0.0054210000	12

AnalIainb.xlsx - Sheet #2

x	y	z	Radius	Charge	Atom
0.601000	1.113000	-0.531000	1.70000	-0.2353780000	12
1.915000	1.267000	-0.082000	1.70000	-0.0368450000	1
0.028000	-0.155000	-0.479000	1.70000	0.1903190000	12
2.625000	0.166000	0.404000	1.70000	-0.1136680000	122
0.716000	-1.269000	-0.003000	1.70000	-0.1924850000	12
2.028000	-1.098000	0.442000	1.70000	-0.0650150000	12

## IMoS V1.10

-1.373000	-0.332000	-0.948000	1.55000	-0.4801540000	14
-2.441000	-0.504000	0.143000	1.70000	0.1944770000	12
-2.604000	0.753000	0.978000	1.70000	-0.3500800000	12
0.049000	1.968000	-0.913000	1.10000	0.1692130000	1
2.381000	2.246000	-0.117000	1.10000	0.1510160000	1
3.646000	0.291000	0.749000	1.10000	0.1582860000	1
0.254000	-2.253000	0.018000	1.10000	0.1709160000	1
2.583000	-1.954000	0.811000	1.10000	0.1542010000	1
-1.414000	-1.146000	-1.570000	1.10000	0.3599880000	1
-3.360000	-0.767000	-0.387000	1.10000	0.0664830000	1
-2.119000	-1.360000	0.739000	1.10000	0.0747850000	1
-1.686000	1.013000	1.512000	1.10000	0.1380680000	1
-2.922000	1.608000	0.372000	1.10000	0.1182840000	1
-3.384000	0.572000	1.722000	1.10000	0.1467120000	1
-1.630000	0.474000	-1.527000	1.10000	0.3808760000	1

## IMoS.cla

```
-----
excelfile      Savefile      Gas
AnalIainb.xlsx \savefolder\ResultFile.txt  N2
```

```
interface 1 0
fromvalue 1
tovalue 2
red_coef 1
Charge 1
radgas 1.5
Mgas 28
Pressure 101325
Mweight 228
Temperature 304
Polarizability 1.7
NrotationsPA 500
NrotationsEHSS 3
NrotationsTM 3
NgastotalEHSS 300000
NgastotalTM 300000
Accommodation 0.48
Timestep 150
Boxdomain 16
Diffuse? 1
reemvel 6
Other 564.7014
Simplify 0
PA 1
EHSS/DHSS 1
TM 1
TDHSS 1
qp01 0
LennardJones 1
DTM 0
PATSA 0
SimplifiedTM 1
seed 13
Numthreads 11
Repeatseed 1
```

## 12 AUTHOR, ACKNOWLEDGEMENTS AND REFERENCES

### 12.1 AUTHOR

Carlos Larriba-Andaluz is the author and owner of the program IMoS. He can be contacted through email [clarriba@iupui.edu](mailto:clarriba@iupui.edu) or [versiera@gmail.com](mailto:versiera@gmail.com).

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### 12.3 REFERENCES

The following references may be consulted to understand how IMoS works. Some of them are included with the IMoS software.[2, 4-8, 19]

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