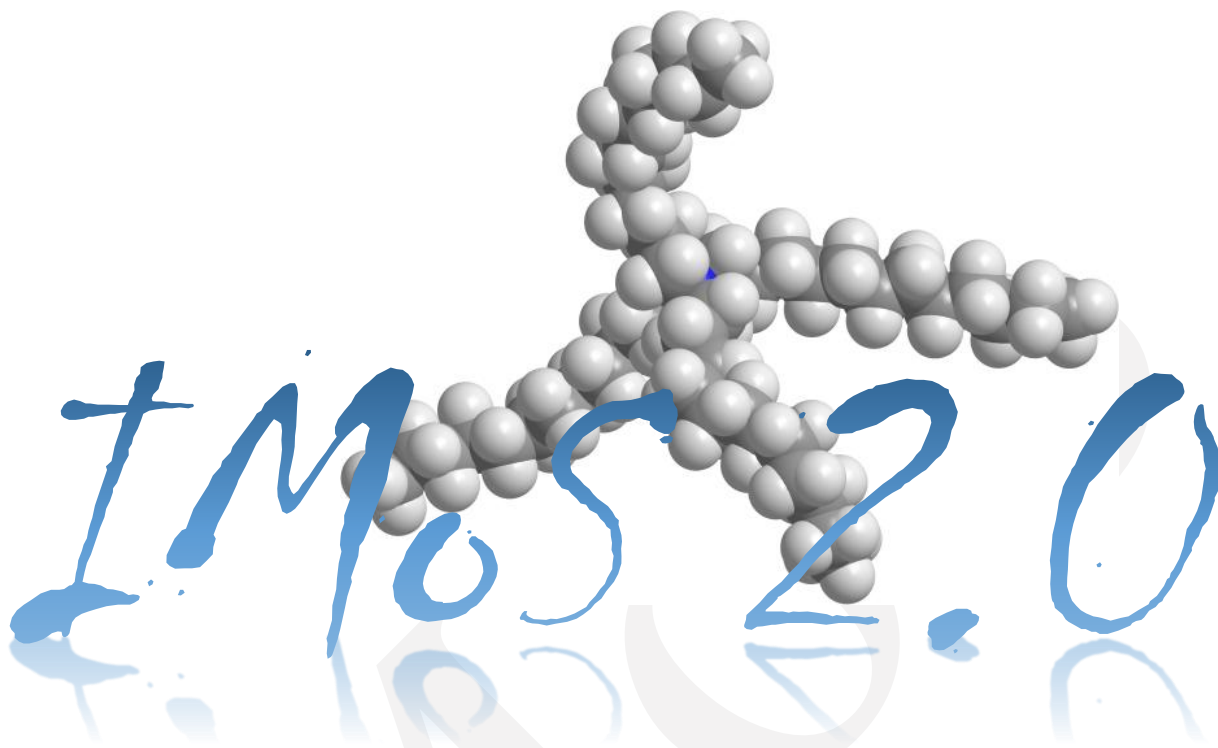




IMoS 2(Ion Mobility Software)

User Guide

Version 0.9

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2 INTRODUCTION

Welcome to the IMoS 2 software guide. This guide is a thorough explanation of the basics of the IMoS 2 software. 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. IMoS 2 may be downloaded from www.imospedia.com and requires the Matlab Compiler Runtime (check version used). Section 5 lists the files downloaded with IMoS 2 and their purpose. Section 6 establishes how to create a structure file compatible with IMoS 2. Section 7 describes a process to generate a Density Functional Theory (DFT) Structure using the freely available software “Avogadro”. It also shows how to do the calculation in Gaussian (paid software) and ORCA (free software). Section 8 is the program overview where the input file DSMCinput.txt are explained in detail. For the program to run, a coordinate file is required. Section 9 explores the possibility of using the program without the interface. Section 10 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 2 program (application). IMoS 2 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 at 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 2 v0.9

Linux version

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
μ	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
ξ	Correction factor
Ω	Collision cross section
Δp	Momentum transfer
$\vec{g}_i$	Initial relative velocities
$\vec{g}_f$	Final relative velocities
N_t	Number of gas molecules
τ_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
Φ	potential
r_i	the relative distance between each of the n atoms (and/or charges) and the gas molecule
α	The polarizability of the buffer gas
ϵ	Lennard-Jones(L-J) gas-atom parameters to well-depth
σ	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
α_i	Coefficients of higher order terms
β	Energy correction term

3 METHODS

The calculation of ion mobility that IMoS 2 performs is NOT based on Mason-Schamp's first approximation of the two-temperature theory[3]:

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

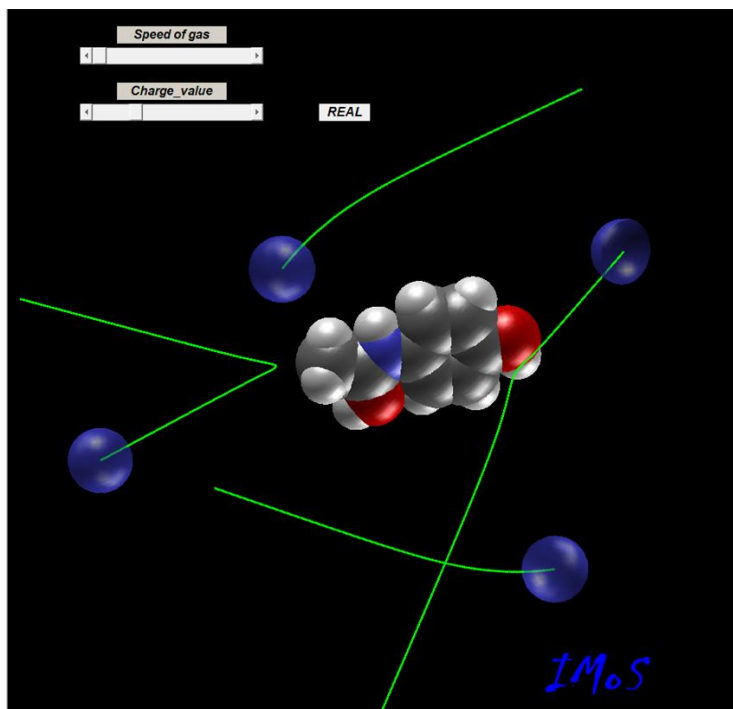


Figure 3.1 IMoS cartoon of the TMLJ 4-6-12 potential interaction.

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: $T_{eff} = T + mv_d^2/3k_b$ (See corrections for high field effects below). 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.

MoS 2.0 models a single ion and its immediate surrounding neutral environment within an NVT ensemble, tracking momentum exchange through discrete collisions. The algorithm includes ion-neutral interactions based on a 4-6-12 potential[2, 4-8] and accounts for energy and momentum exchange across translational, internal, and rotational degrees of freedom. While rotational contributions such as center of mass location and moment of inertia are not expected to play a dominant role in the relaxation behavior of small organic analytes, they remain essential for systems involving isotopomers or structural isomers, and are fully supported by the code. The results are quantitatively

equivalent to those of IMoS Trajectory Method, taking into account the appropriate differences.

3.1 TRAJECTORY METHOD (TM)

The trajectory method allows interaction potentials between atoms/charges and the gas molecules. IMoS 2 only uses the Trajectory Method Lennard Jones (TMLJ) which employs a (4-6-12) potential.

The TMLJ composes a 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 α being the polarizability of the buffer gas, and ϵ and σ 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 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 straightforwardly 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 N₂ 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 N₂ 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.

4 INSTALLATION AND SETUP

4.1 WINDOWS INSTALLATION

1.) In order to run IMoS, Matlab MCR version 24.1 (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/>

Next, the IMoS files will be downloaded. Navigate to the same link above and download the desired version of the IMoS software. Extract the files to a directory that does not require administrator privileges to write to. Once extracted, open the DSMCXX.exe to execute the 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 24.1 (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 “v98” 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.

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
Root	
<code>readme.txt</code>	"Readme" file detailing the installation process.
<code>IMoS2vXXXX</code>	IMoS 2 executable. The version and platform may change as well as the extension.
<code>Icon.ico</code>	Icon file.
<code>Splash.png</code>	Splash screen picture.
<code>LJtable.xlsx</code>	Excel file defining the Lennard Jones parameters for multiple gasses. Use sheet 8 to enter custom values when needed.
<code>IonColor.xlm</code>	Excel file defining the plot colour of all atoms.
<code>Vdwimos.xlsx</code>	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.
<code>DSMCH2input.txt</code>	Configuration file
<code>runimos5</code>	Sbatch queue file example
<code>password.txt</code>	File with the password required to run the program. Please contact the author to get a password.
<code>fieldmat.txt</code>	Matrix with space and time values for the electric field.
Files for running examples	
<code>Anallainb.xlsx</code>	16 DFT structures provided from ref. [16].
<code>Smallions.xlsx</code>	DFT of small ions to test High Fields and Effective temperatures
Explanations Folder	
<code>IMoS2_UserManual_09.pdf</code>	This Manual.
<code>LarribaJPCA2013.pdf</code>	The explanation folder contains multiple published works that explain how the different subroutines of IMoS work as well as how to optimize LJ parameters.
<code>LarribaJCP2013.pdf</code>	More computational aspects of IMoS.
<code>LarribaJoChemPhys2014.pdf</code>	Diatomic version of the code.
<code>LarribaPCCP2015.pdf</code>	Difference between N ₂ 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.
Gandhi2022FourthApproximationexplanation.pdf	Two-temperature theory explanation in detail.
Gandhi2022SupplInfo.pdf	Calculation of Matrix elements and other formulas for two-temperature theory
File save examples	
saveme.txt	Results file example created with IMoS 2.
Ionpath_1.txt	Saves the ion path if prompted in this file. The _1 can change depending on the number of ions run.
Ionvelocity_1.txt	Saves the ion velocity in this file if prompted.
Angularvelocity_1.txt	Saves the ion angular velocity.
Platform only files	
Msvcr120.dll	Visual C file required to run some C code subroutines. Most Windows platforms already have this file, but some do not.
Run_DSMC4DtrialFieldparforFigure.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 2. IMoS 2 only supports the use of .xlsx files.

6.1 STRUCTURE FILE FOR EXCEL

Excel may be used to create and store structure files to be used in IMoS 2. 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.

X, Y and Z Coord			VdW radii	P. Charge	Atom label		
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	Crosssectic	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	

► ... Anthracene Choline Phenanthrene Acetylcholine C60 C70 Naphtaler

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 4th 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 5th 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 6th 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 7th 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.

7 DFT CALCULATIONS

DFT or Density Functional Theory is an “ab initio” method used to calculate 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 structure, a preprocessor – Avogadro¹– and solver – Gaussian²– may be used as explained below. Avogadro¹, Orca[17] or Gaussian²[18] 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

Users 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). 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....

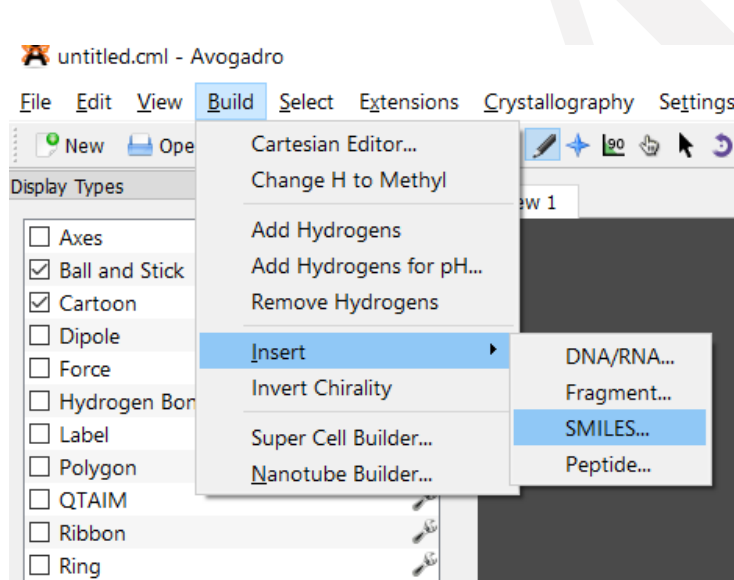


Figure 7.1 - Import molecular structure using SMILES

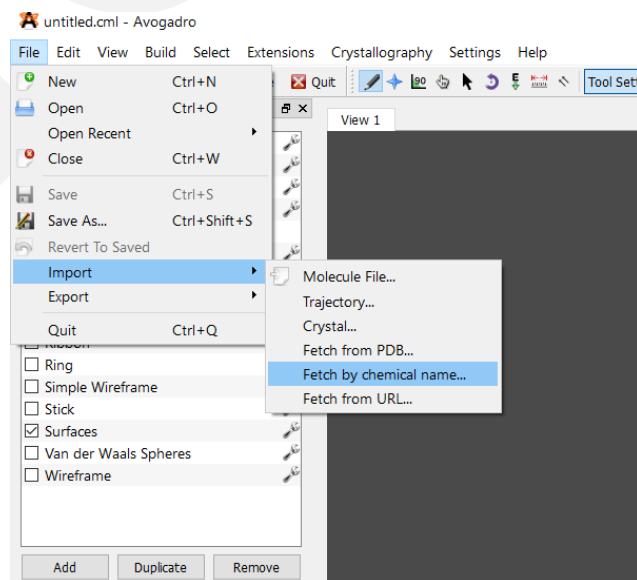


Figure 7.2 - Import molecular structure using name

¹ Avogadro: an open-source molecular builder and visualization tool. Version 1.2.

² 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 during the geometry optimization process in the computational chemistry software. 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.

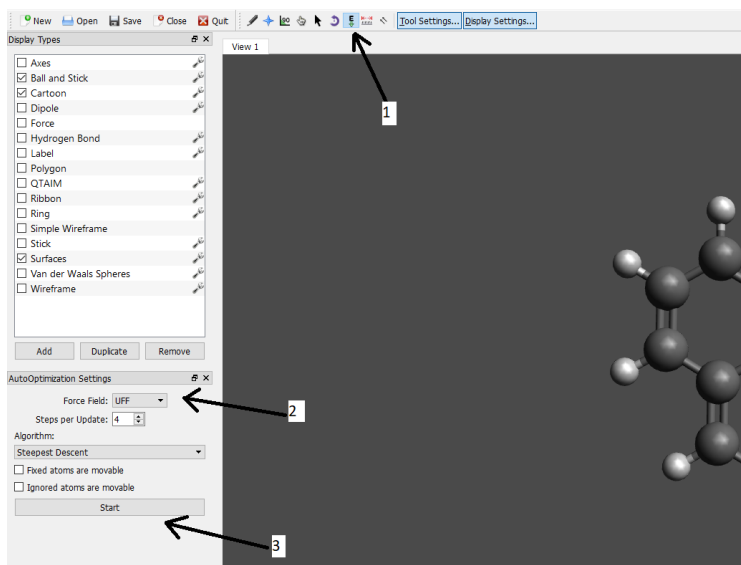


Figure 7.3 - Force Field Optimization

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 the following lines. After applying the desired parameters, the file can be edited manually as well.

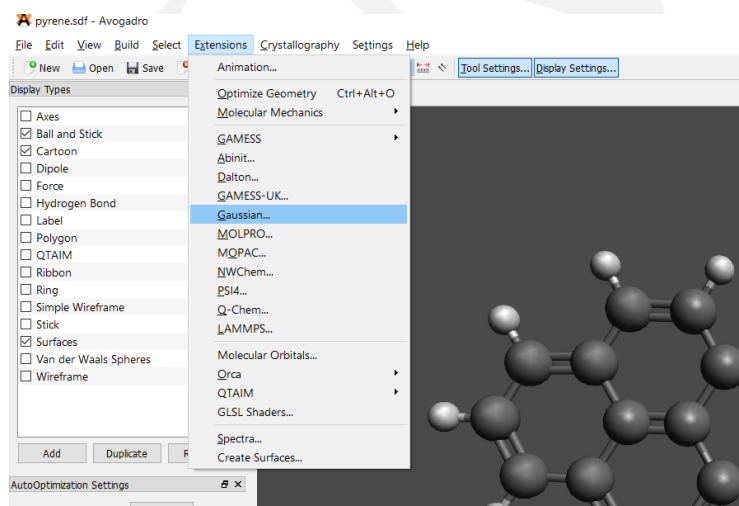


Figure 7.4 – Gaussian in Avogadro

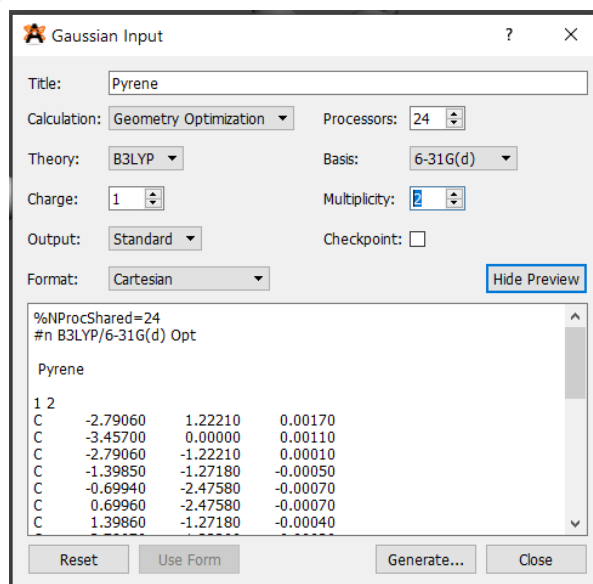


Figure 7.5 – Gaussian dialog box

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 and described [here](#)³ and [here](#)⁴. 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

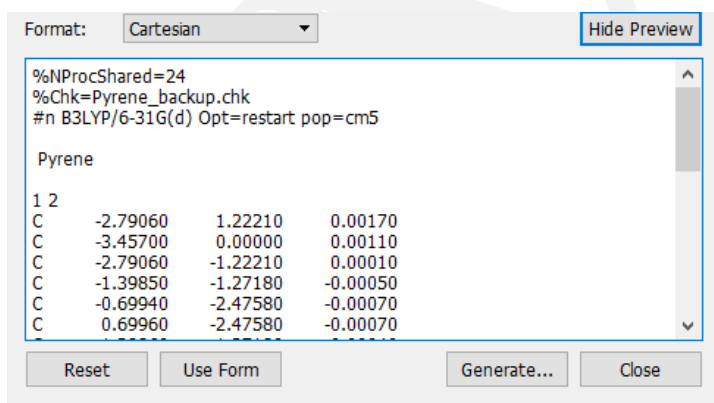
Spin multiplicity after applying the charge. The spin multiplicity is the number of possible orientations of the spin angular momentum corresponding to a given total spin quantum number for the same spatial electronic wave-function.

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 2nd line, user can get Hirshfeld partial charges too.

7.1.3.8 Checkpoint

If during the nth 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)th 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.

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

⁴ <https://sites.google.com/site/orcainputlibrary/basis-sets>

7.2 GAUSSIAN

Gaussian is one of the programs 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

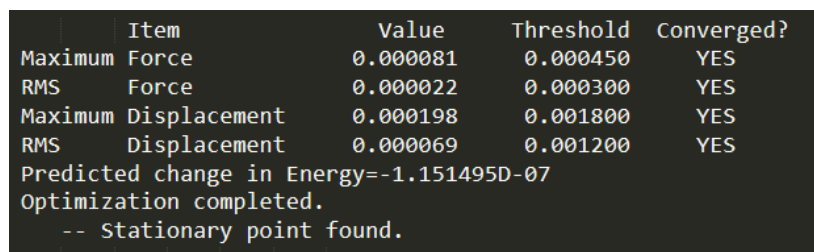
To run Gaussian on a Linux cluster, please load gaussian and then run Gaussian (e.g. Gaussian 16) from the command line by specifying the input molecule and output file. If Pyrene.com is the input file and Pyrene.txt is the output file.

```
>> 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.

7.2.3 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.

7.2.4 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.

7.3 ORCA

ORCA is the second options to obtain the optimized structures to be used in ImoS. Refer to the Orca website at https://www.orcasoftware.de/tutorials_orca/

a. Create Orca Input File

To create an Orca input file, go to extensions and click on Orca -> Generate Orca Input. In the following figures, the pyrene molecule will be used as an example for obtaining the Orca input file. Once Generate Orca Input is clicked, an Orca dialog

box appears where atom coordinates appear together with several calculation choices (See Figure 7.9). The input parameters are described in following lines. After applying the desired parameters, the file can be edited manually as well.

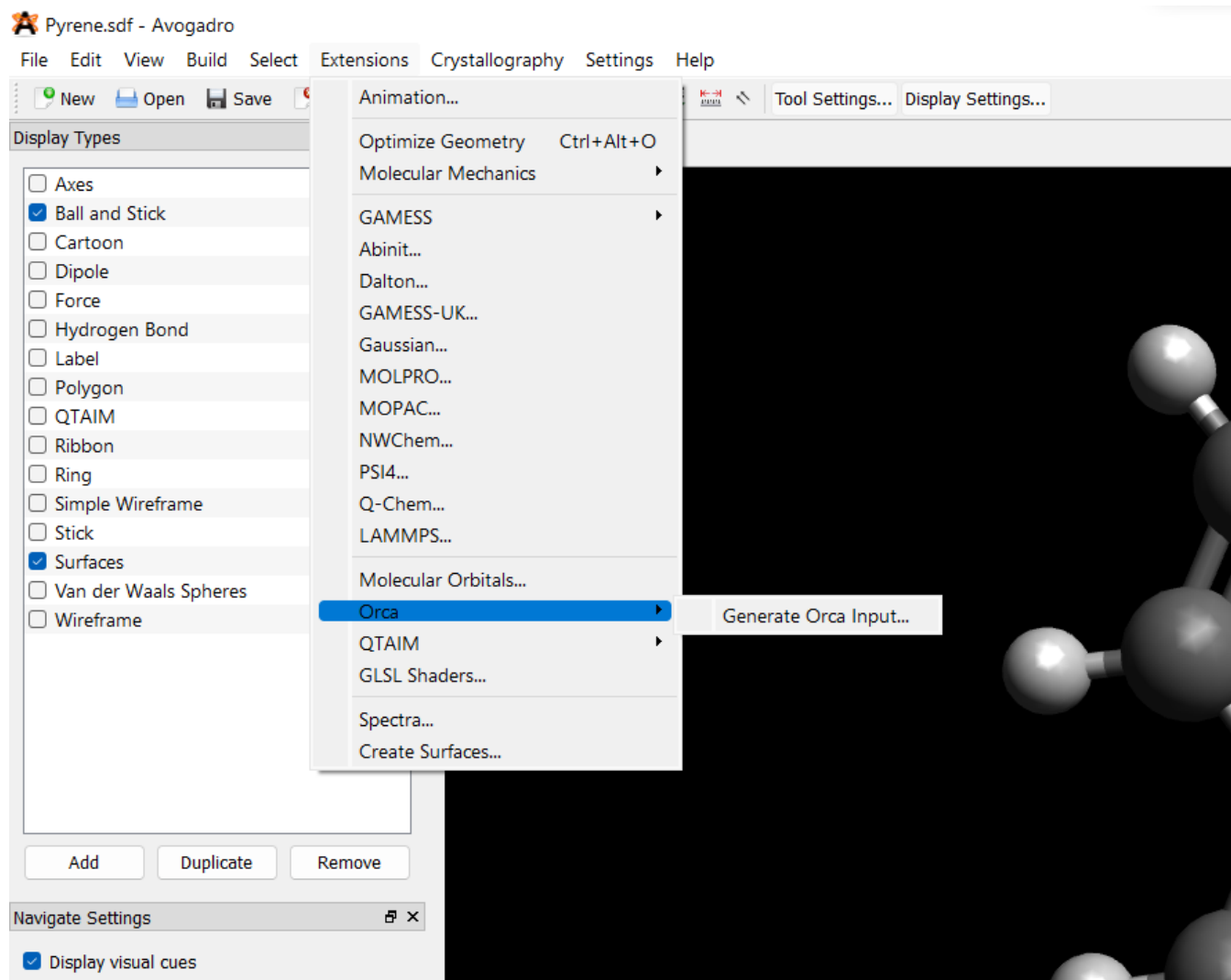


Figure 7.8 – ORCA in Avogadro

7.3.1.1 Calculation

Type of calculation (i.e., Geometry optimization).

7.3.1.2 Method

Different methods favor different calculation objectives. For geometry optimization, DFT is preferred.

7.3.1.3 Basis set

There are different Theories and related Basis for ab initio methods.

7.3.1.4 Charge

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

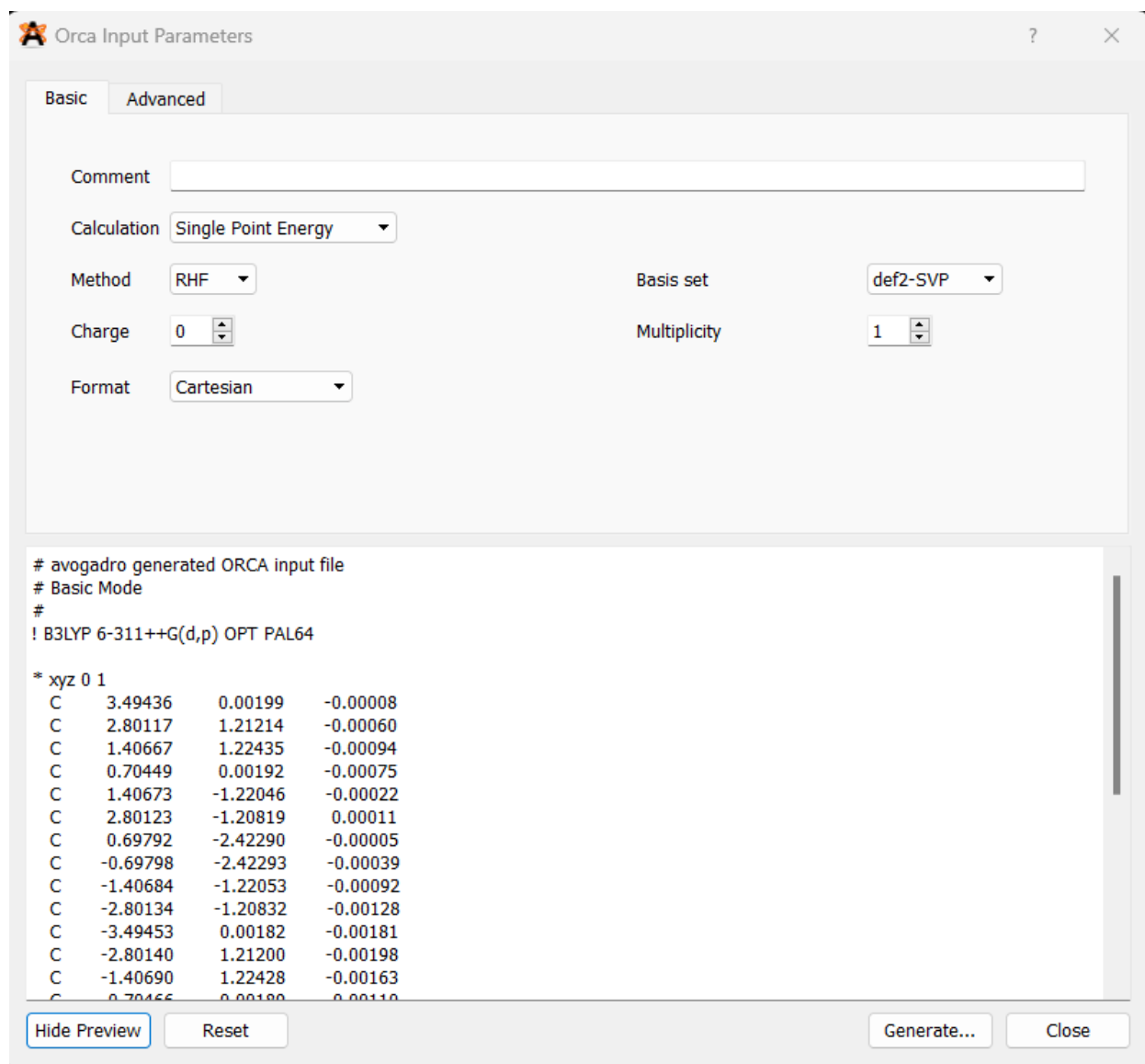


Figure 7.9 – Orca dialog box (functional and the basis set are edited manually)

7.3.1.5 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.

7.3.1.6 Multi-processors

Orca can be used on multiple processors by adding a keyword PALxx (where xx is the number of cores. e.g., 64 in case of Figure 7.9). Avogadro doesn't have an option to add the keyword.

7.3.1.7 Generate

Finally, click on Generate... to produce an Orca (.inp) file.
(Note that Orca doesn't have a feature to restart the geometry optimization in case of an abrupt calculation halt. This has to be done manually by taking the last set of coordinates and start a new calculation from there.)

7.3.2 Running Orca

To run Orca on a Linux cluster or a Windows machine, write the following commands in the terminal of your OS:

```
D:\setups\orca5\orca Pyrene.inp > Pyrene.out
```

Orca installation directory input file result file

7.3.3 Output file

Once the calculation is done, you should look in the output file (.out) to make sure that the geometry and the energy has converged (the energy can be close to convergence, as shown in Figure 7.10), and Orca terminated normally. If the structure has converged, find the optimized coordinates as well as the dipole moments and Mulliken and/or Loewdin partial charges (the coordinates can be found in the .xyz file as well). This will be used to create the structure files as shown in Section 6.

```

-----|Geometry convergence|-----
Item          value          Tolerance      Converged
-----|-----|-----|-----
Energy change -0.0000440316          0.0000050000      NO
RMS gradient   0.0000617730          0.0001000000      YES
MAX gradient   0.0002710295          0.0003000000      YES
RMS step       0.0006167456          0.0020000000      YES
MAX step       0.0017944072          0.0040000000      YES
.....
Max(Bonds)    0.0005      Max(Angles)  0.06
Max(Dihed)    0.10      Max(Improp)  0.00
-----

```

Everything but the energy has converged. However, the energy appears to be close enough to convergence to make sure that the final evaluation at the new geometry represents the equilibrium energy. Convergence will therefore be signaled now

```

*****HURRAY*****
***      THE OPTIMIZATION HAS CONVERGED      ***
*****

```

```

Geometry Relaxation ... 2.527 sec (= 0.042 min)
***ORCA TERMINATED NORMALLY***
TOTAL RUN TIME: 0 days 0 hours 25 minutes 59 seconds 329 msec

```

Figure 7.10 – Orca output file for a successful run

8 PROGRAM OVERVIEW

The program overview is meant for beginners to learn how to use IMoS 2 and explains the basics of the program.

9 NON-INTERFACE VERSION AND THE DSMCH2INPUT.TXT 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 DSMCH2INPUT.TXT 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 (.xls(x)), 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. If two gases are used, a second gas can be added to the header section. The selection of the gas here only affects which LJtable.xlsx sheet is used for the Lennard-Jones parameters. An example of an DSMCH2input.txt header looks like this:

DSMCH2 VALUES CONFIG

\filefolder\Analiainb.xlsx \savefolder\Saveme.txt N2 He

9.2 BODY OF DSMCINPUT.TXT FILE

```
DSMCH2 VALUES CONFIG
Analiainb.xlsx Saveme.txt N2 He
interface 0 0 0
n 800
pr 101325
Te 300
ttotal 10
fromv 1
tov 1
Particlevguess 160.06
Enlargedomain 1.0
threadc 31
seed 129
enhance 0
field 1e6
charge 1
mgas 28.013
mgas2 4.006
alpha_pol 1.7
alpha_pol2 0.2073
dgas 3.1
timestep 1e-9
mixture 1
fraction 0.1
EHSS 0
draw 0
to_surface 1
maxvel 7000
velpotincrease 1.02
printvelocity 1
printangvelocity 1
printionpath 1
```

Figure 9.1 DSMCH2input file parameters

The body of the file contains a list of parameters to run IMoS 2. Figure 9.1 shows the file with some of the most common parameters. This set of parameters is sufficient to run IMoS 2. In the next section, these parameters and some additional parameters that can be added are explained. The output should have the file to be generated and used.

9.3 EXPLANATIONS OF PARAMETERS OF THE DSMCH2INPUT.TXT 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 [interface]

Interface has no use at this time, but it needs to be there for the program to work.

9.3.2 [n]

n is the number of gas molecules in the NVT ensemble. Default is 800.

9.3.3 [pr]

pr is the pressure for a given NVT ensemble. The pressure, unlike in IMoS 1, is a very important parameters as it affects the number of collisions per unit time. Default is 101325 Pa.

9.3.4 [Te]

Te is the gas temperature. Default is 100.

9.3.5 [ttotal]

ttotal is the number of timesteps that are used to record the data and get statistically significant results, without recording an immense amount of data. Typical values range from 10000 to several million.

9.3.6 [fromv]

fromv refers to the first excel sheet that will be calculated this run from the excel file (not necessarily 1) and has a integer value.

9.3.7 [tov]

tov refers to the last excel sheet that will be calculated this run from the excel sheet. Has to be larger than or equal to *fromv*.

9.3.8 [Enlargedomain]

Enlargedomain is only used in general to better visualize collisions between ions and gas and enlarges the sphere of influence surrounding the ion. Default is 1.

9.3.9 [Kappaval]

Kappaval is the ratio of the average Kinetic to Potential Energy on the surface of the sphere of influence and follows the same logic as IMoS 1. And serves to establish the cutoff of the potential interaction between gas molecules and ion. Default is 0.01.

9.3.10 [threadc]

Threadc is the number of cores that the program will use simultaneously. If the program is run on a personal computer, the recommendation is to choose 1 core less than your personal computer has, to allow active work on your computer. Choose the maximum available if sent to a supercomputer. Default is 1.

9.3.11 [seed]

Seed is the rng number used for the program to run. It is recommended to use the same seed for ions which are being compared. Default is 121.

9.3.12 [enhance]

Enhance establishes the use of the dipole moment on the molecules. If set to 1, the dipole is calculated and the ion will suffer its torque. Default is set to 0 (no dipole considered).

9.3.13 [field]

field is the value of the constant field in V/m used by the program when *Twave* is set to 0, i.e., when constant field is applied. The default value is $\text{pressure}/101325 \times 1e5$, which would yield 1e5 V/m at atmospheric pressure.

9.3.14 [charge]

Charge sets the charge of the ion when and only when it is not specified in the file. Its use is not recommended. Default value is 1.

9.3.15 [mgas] and [mgas2]

It is the mass in daltons of the first gas and second gas (if a mixture is used) respectively. Default values are 28.013 and 4.006 respectively.

9.3.16 [alpha_pol] and [alpha_pol2]

Alpha_pol and *alpha_pol2* correspond to the ion-induced dipole polarizability in Angstroms cubed for gases 1 and 2 respectively. The Default values are 1.7 and 0.2073 Å³.

9.3.17 [timestep]

timestep is the timestep used to record instances of the code and it is not the timestep that the code uses internally. The Default is set to 1e-9. It is recommended that it is not smaller than this value as it creates massive amounts of data and it might create issues with other internal timesteps.

9.3.18 [mixture] and [fraction]

If you would like to use a mixture of two gases, set *mixture* to 1. Fraction represents the percentage of the second gas. For example setting *mixture* 1 and *fraction* to 0.1, will provide 10% concentration of the second gas.

9.3.19 [maxvel]

To avoid issues with numerical errors, the code has a maximum set velocity. This by Default is set to 7000 m/s.

9.3.20 [velpotincrease]

Since the sphere of influence has a cutoff, *velpotincrease* sets a percentage increase in kinetic energy that would correspond to the increase in velocity due to the interaction from infinity to the radius of the sphere of influence. Default value is set to 1.02.

9.3.21 [printvelocity] and [printangvelocity] and [printionpath]

To record the values of the ion velocity, ion angular velocity and ion path at each time step, give a value of one to the above parameters. For example, setting *printvelocity* to 1, will record the x, y and z velocities at each timestep. Default value is 0. Recording these values takes up a lot of disk space. Typical files may take 1Gb of data.

9.3.22 [Twave] and [frequency] and [wavelength] and Ecomp

Twave establishes whether to use varying fields. If this value is set to 1, the program will look for the file *fieldmat.txt* that has electric field values as a function of time (rows wise) and space (column wise). The parameter *frequency* establishes the inverse of the whole period for time. For example setting a *frequency* of 1e7 establishes that the program will visit all the row values in 1e-7 seconds. Similarly, *wavelength* establishes the length of the full wave which will be equally distributed between all the column values of *fieldmat.txt*. Default values are 5e6Hz and 8e-3 m for *frequency* and *wavelength*. The default value for *Twave* is 0. See FAIMS example below. *Ecomp* shifts the *fieldmat.txt* values by a constant amount.

9.3.23 [vgas]

This value establishes the velocity in m/s of the gas in the y direction (perpendicular to the field). This value is used to propagate the ions perpendicularly as it would be done for FAIMS. See FAIMS example. Default is 0.

10 EXAMPLES

The idea of this part of the manual is to get accustomed to IMoS 2. The examples are rather simple and are not meant to be exhaustive study. An interface will be available soon.

10.1 GETTING ACCUSTOMED TO THE PROGRAM.

To make sure that everything is running correctly, or to get the initial velocity guess, a fast calculation is recommended. Setting `ttotal` to 100, for example, and a timestep of $1e-9$ with 31 cores will simulate a total time of 3.1 microseconds in less than 1 minute for a single species. Choosing in this case Trypheniline in N₂ at a gas pressure of 300K and a field of $1e6$ V/m has the following input file. We will save velocities, angular velocities and ion paths.

DSMCH2 VALUES CONFIG

Anallainb.xlsx Saveme.txt N2 He

interface 0 0 0

n 800

pr 101325

Te 300

ttotal 100

fromv 1

to v 1

Particlevguess 160.06

Enlargedomain 1.0

threadc 31

seed 129

enhance 1

field $1e6$

charge 1

mgas 28.013

mgas2 4.006

alpha_pol 1.7

alpha_pol2 0.2073

dgas 3.1

timestep $1e-9$

mixture 0

fraction 0

EHSS 0

draw 0

to_surface 1

maxvel 7000

velpotincrease 1.02

printvelocity 1

printangvelocity 1

printionpath 1

The output will look something like:

RESULTS FOR IMOS 2

The time is 05-Aug-2025 05:26:30

The file is Anallainb.xlsx and the molecule is 1

190.573991	-1.526189	4.269378	8849
------------	-----------	----------	------

155.115167	4.154406	-3.095655	8444
------------	----------	-----------	------

IMoS2 V0.9

185.107627	13.770833	-1.139785	8373
161.217658	1.452412	17.189610	8463
162.385899	4.241847	-15.835948	8617
164.502515	-19.870095	-0.672849	8424
169.325676	-1.169837	8.161886	8341
156.894030	17.112441	16.117222	8378
178.952604	22.676399	-14.917747	8477
166.161184	-7.978576	-0.126982	8599
154.033090	1.039505	26.076815	8587
170.696292	33.225930	-4.269161	8489
147.637017	-18.688950	29.944625	8514
143.310905	-7.290877	0.460451	8543
173.215844	-12.712486	-14.716226	8646
163.883023	27.191918	7.979629	8472
178.031680	0.155357	14.899301	8608
154.951744	-5.959551	5.374092	8544
178.225709	4.608416	25.339806	8629
159.301413	5.814083	6.695794	8484
193.033969	-5.504950	4.727544	8754
162.596309	-11.736201	-8.194190	8504
181.234412	7.703360	-19.639273	8474
168.585140	-17.388989	-6.581761	8611
181.917593	2.217654	-6.128920	8512
166.825496	-27.418514	12.421015	8606
175.587825	-6.936065	-3.086265	8526
157.293379	-0.388950	0.191185	8376
179.485166	-18.074013	-4.750643	8483
161.180478	-20.810473	-3.711770	8464
157.315238	-7.388638	-3.414925	8718

The total number of collisions is 264509

Average velocity x: 167.69607 m/s

Average velocity y: -1.46706 m/s

Average velocity z: 2.24407 m/s

This tells you that a good initial estimate for the velocity is 167m/s. We should also have a file labeled ionpath_1.txt which contains the data for the position of the ion as a function of the time step. We also have the ion velocity as a function of time. Calculating the 3D distribution and plot the result for both the ion path and the distribution, it will yield:

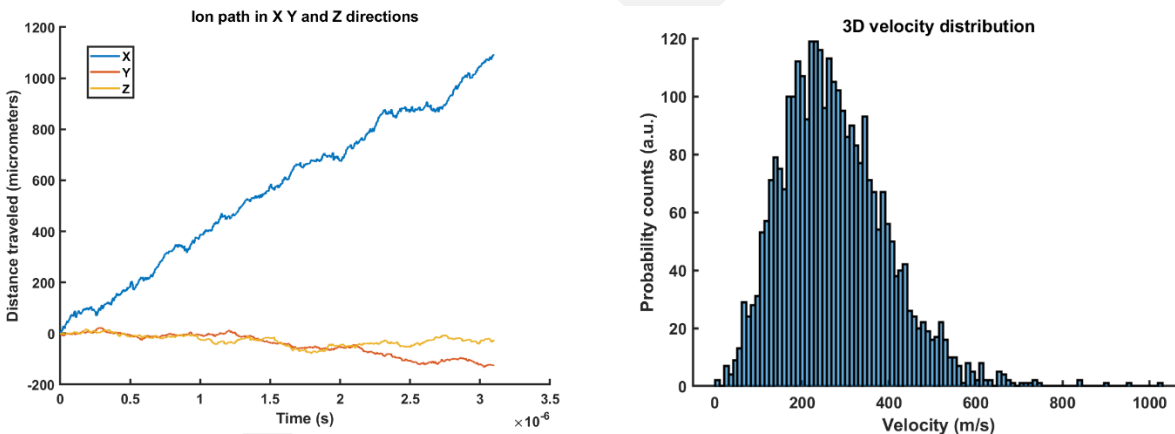


Figure 10.1 – Ion path and ion velocity distribution for a quick run

Note that the distribution will improve its statistics with more time (this was only a 1 minute run!).

10.2 RUNNING A SIMPLE CASE WITH MULTIPLE SPECIES

We would like to run all ions in the Analiain.xlsx file for 15.36ms total in a supercomputer with 128 cores with a constant field of 1e5 V/m and at 1 atmosphere and 300K. The gas is He. The results will be compared to those of IMoS. We will

record the ion velocity in the X, Y and Z directions. The total time is about 1 day. Note that the data recorded can exceed 1Gb.

1. The input file will look something like:

DSMCH2 VALUES CONFIG

Anallainb.xlsx Saveme.txt He N2

interface 0 0 0

n 800

pr 101325

Te 300

ttotal 120000

fromv 1

toV 16

Particlevguess 160.06

Enlargedomain 1.0

threadc 128

seed 129

enhance 0

field 1e5

mgas 4.006

alpha_pol 0.2073

timestep 1e-9

mixture 0

fraction 0.1

to_surface 1

maxvel 7000

velpotincrease 1.02

printvelocity 1

2. Run the program in the supercomputer.
3. Note that the program will take the LJtable.xlsx and use the He parameters chosen.
4. The output will look something like this (for example model 5).

You have selected Anallainb.xlsx as your file and Model 5 as your molecule. You can start a calculation process.

The pressure is 101325

number of particles is 800

The temperature is 300

ttotal is 200000

02-Aug-2025 19:54:33

45 56295353 49.4988512183 -0.3927002825 -0.6999829536

01 55969112 48.2510221002 -0.0793332204 0.0637785286

68 56183076 48.9913654957 -0.1076712599 0.0480139258

70 56203348 48.9860937718 -0.4064141337 0.4841120066

93 56266271 49.5509960672 0.1752979143 -0.0460749998

96 56258145 49.0467512841 0.6351284776 0.2265513933

23 56221840 48.9570329888 0.4347278373 -0.0326685428

102 56262743 48.1858116277 -0.5233858252 -0.1501837855

28 56253775 49.7599753609 -0.3046196865 0.2939691968

25 56429750 48.5029914074 0.0105564530 0.4365815499
127 56107160 50.3721381558 0.5969250017 -0.1011964692
56 56145475 49.2092981219 0.1301792940 -0.1010382503
121 56448629 48.6680446834 0.2603154038 -0.4708361476
124 56454580 49.7532362730 -0.4362742533 0.5750839188
29 56156091 48.7218232666 -0.4421110898 0.3965027479
71 56244878 49.1018383892 0.4104704366 0.2958144625
17 55908559 49.7000996146 -0.0154250197 -0.2032039593
39 55996636 49.4939593620 -0.4588145572 0.2671241809
123 56287120 48.4825246491 0.4034920474 -0.0234194975
44 56384979 48.5240543860 -0.4422231316 0.3778033443
84 56511745 48.6166455451 -0.5758945865 -0.2721869402
50 56094943 49.3715869546 -0.2896193534 -0.1749446521
99 56378085 49.4489451001 -0.8105760414 0.4055249531
117 56479636 49.4408574089 -0.1631242211 0.2086811663
126 56257412 49.8163554368 -0.0078082038 0.3160918617
87 56191510 49.4634641034 -0.3138692830 -0.3386864275
35 55885696 49.2891577722 0.0003310940 -0.5789336987
46 56458870 48.8456483777 0.0791977534 -0.0882586240
120 56458689 49.4746615374 0.3466457704 -0.8705155100
78 56658523 49.1566165238 0.2865249293 1.0916141312
69 56453086 49.3904105451 -0.6652091562 -0.2861105077
60 56066986 49.4623277124 0.0624492602 -0.4793336187
26 56675485 48.3724253384 0.1715299002 -0.1542800687
55 56193249 50.0391880092 -0.2106300219 -0.2880817265
24 56241377 48.6986239411 0.1208950724 -0.0991538349
89 56218503 49.1945227672 -0.5890827811 -0.6487179858
31 56469738 49.0563577630 -0.5406459604 -0.2896026084
57 56402011 49.8601157591 -0.0105615740 0.2839306515
107 56184572 49.5580145262 0.3705407670 -0.1898169781
110 56549760 49.0739851833 0.1918300224 -0.1496766606
11 55962889 50.2206601022 -0.4135900473 -0.1481340438
81 56189259 49.7190304540 0.8050145687 -0.4659213216
63 56206672 48.8471102575 0.1992038645 0.0988009384
125 56233282 49.7196401794 0.1660429067 -0.2203441965
49 56340653 49.6334524266 0.3520761255 0.0614954335
27 56114501 49.3911472873 0.0650554774 -0.7285217604
10 56212343 48.9453835734 -0.1558012478 -0.5913775294
41 56283533 50.0910363831 -0.1556047142 0.3138230231
95 56696406 49.4075290286 -0.1987639835 0.5941928185
76 56247297 49.5348056933 0.1499213211 -0.3062977174
88 56349485 49.3104590596 0.3265560774 0.0174584930
34 55940368 50.0145097256 0.3241848450 0.5396054065
54 56395544 49.2714237684 0.3591711585 0.3013031870
66 56308677 49.6268231560 -0.3461427641 -0.1766087764
61 56038590 50.3569286787 -0.2245406324 0.8459748929
106 56423804 48.4887060883 -0.5026360694 0.3358778581

94 56138366 48.9372976815 0.2130846080 0.3212378450
12 56270157 48.4560967563 0.0535709188 -0.8977224301
14 56354425 48.6874608801 -0.2008079724 -0.0265301783
83 56238821 49.8905702941 -0.6150554198 -0.2114372349
48 56542516 49.6419486499 -0.0174774239 -0.0693670329
3 56562482 48.5113714635 0.0344226050 -0.1539139714
52 56533039 49.1385639252 0.8585368769 0.0391745571
51 56383355 49.7259225304 0.4176514973 0.7250091094
47 56609899 49.6656308668 0.5458282910 -0.6388265447
30 56408622 49.6466990794 -0.0643719561 -0.5008149542
100 56176542 49.4790067394 -0.0084080319 -0.4045690407
19 56486824 48.5048695907 0.0123923091 -0.3889451061
79 56394672 49.1428828966 0.5651358452 -0.1441582191
108 56185392 49.4844507155 0.2676592605 0.3318278106
53 55959693 50.1844649067 -0.2556758629 -0.0731190499
20 56387745 48.8589815866 0.0631018218 0.2366347929
5 56203526 49.7854632256 -1.0005858825 0.4979125571
65 56438989 49.5452382756 0.2285456713 0.4572334680
72 56447926 49.3662410141 -0.2806785799 0.1547316958
40 56098676 50.1469784534 0.1473739518 -0.1370135623
92 55840466 50.8921617432 0.1375145999 -0.4743035718
33 56703056 49.4244912882 -0.1289262761 -0.6649007632
109 56382132 49.3447647007 0.5457332439 -0.0626027007
32 56225027 48.9696631879 -0.0099989101 -0.4661588495
104 55905437 49.9117529804 0.5276683209 -0.2306268760
2 56227334 49.3893970645 0.0313116555 -0.2817355213
98 56105162 48.5455652070 -0.7554474261 0.0384926917
16 56289713 49.7186375854 0.7372816014 0.5580653387
13 56335507 49.8130433810 -0.3045439561 0.0844493203
122 56215554 49.6751240449 0.7501091133 -0.0580992660
115 56229534 49.0976815082 -0.7054673480 -0.0540387914
80 56362381 49.9979174548 0.3755302257 -0.5696950606
91 56066981 49.6702273426 -0.7108851365 -0.1003529894
8 56588104 49.4766528300 -0.1765826944 0.6555978016
111 56578874 48.5477426982 -0.1285489768 0.0001599622
37 56504584 49.4450260135 0.3260658620 -0.9526066021
21 56725895 49.2386419247 0.2928373340 -0.2658384383
43 56277981 49.7318510578 0.4340242581 0.0385955340
119 56227411 49.9189400555 0.9289141721 -0.0847890661
62 56635243 49.5021504640 0.0498818804 0.0270637303
59 56085309 49.3665264732 0.1404046159 -0.4699567625
4 56209440 49.9562393638 -0.3011198207 0.2772481839
116 56149123 49.7269824048 0.3180486587 0.2913412023
75 56388828 49.5319176155 -0.0826195902 0.0811992408
86 56446187 49.4505105229 -0.0195613150 0.1445447431
112 56507856 48.5827386770 0.0236487169 -0.7604762966
67 56348900 49.2955436385 0.0669103172 0.0275091762

113 56523526 49.0477896508 0.1170243699 0.1245556888
42 56579477 49.1374470825 0.1537202665 0.2353835899
105 56752635 49.0519367897 0.1511125709 -0.6777826007
90 56331391 49.8257078914 -0.2175427948 -0.0083806887
82 56635554 48.8042421724 0.0282728433 -0.4910601910
77 56348624 50.0295006341 0.1484253000 -0.0401443552
64 56632664 49.0993872894 -0.5560625761 -0.3008294216
128 56326262 50.3590481038 0.0535989069 -0.4082615932
9 56174966 49.1278453066 0.8570002174 0.1243496556
38 56390619 49.5285719212 0.4066860238 -0.2270584707
18 56345393 49.8464986294 -0.1717984550 0.1605215296
15 56541914 49.0249046526 0.1475064547 -0.3534246174
103 56407942 49.2601192615 -0.1749153242 0.1996058193
22 56577884 49.4624823159 -0.1446910622 0.2580676411
36 56186010 50.1164586116 -0.6046215589 0.2970014689
73 56107140 49.6128080158 0.4788851422 0.1404846636
118 56095752 48.9754511936 -0.2374867799 0.2371944751
97 56347591 49.1289472148 -0.1590532821 0.5129160039
6 56461210 49.8732014693 -0.0594256342 0.3533969799
58 56549955 49.7577768162 -0.4595632496 -0.1735482697
114 56338803 49.6470068351 -0.4254290059 0.7392424786
7 56266415 49.6101480246 0.1128824956 -0.3486367501
1 56494843 49.3394355268 0.2209093601 0.5365198700
74 56105233 48.9512479704 -0.2272718706 0.5749264088
85 56359703 48.5206905409 0.0054765071 0.0036141988

The total number of collisions is 7208515891

Velocidad media x 49.3604 m/s

Velocidad media y 0.0032911 m/s

Velocidad media z -0.024846 m/s

Elapsed time is 217567.225315 seconds.

-----END of OUTPUT-----

To compare the results, we have to divide the drift velocity by the electric field to yield $4.94604 \text{ cm}^2/\text{Vs}$ for model 5. For model 3 and 4, the program gives: $4.89673 \text{ cm}^2/\text{Vs}$ and $8.71655 \text{ cm}^2/\text{Vs}$ respectively. And so forth.

The IMoS 1 program using the same LJ parameters can be compared to the results from IMoS 2 in the graph below.

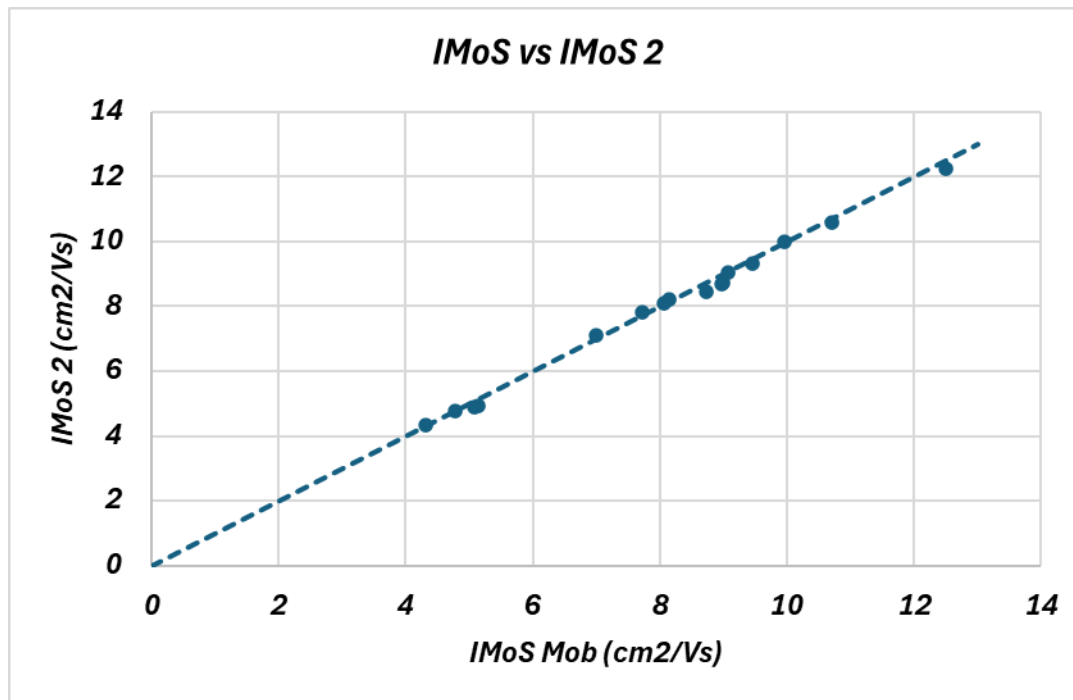


Figure 10.2 – IMoS vs IMoS 2 mobility results

10.3 RUNNING C60 FOR DIFFERENT TEMPERATURES AND COMPARISON TO IMOS 1 RESULTS.

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

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

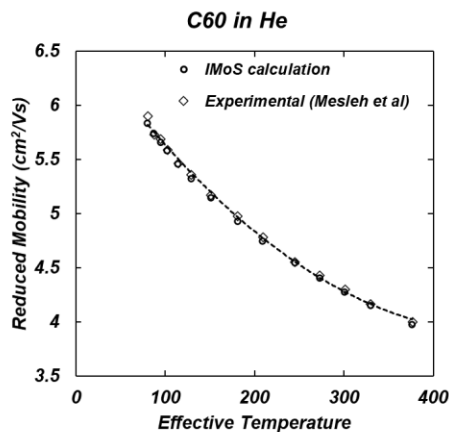


Figure 10.3 C60 at different temperature (experiment vs simulation) based on Mesleh's manuscript.

Now we would like to do the same thing with IMoS 2. The input will just choose C60 (sheet 10 of Anallainb.xlsx) and repeat the result for different temperatures. For N₂ at 1 atmosphere and at 200K, an input would look like:

```
DSMCH2 VALUES CONFIG
HalAniline.xlsx Saveme.txt N2 He
interface 0 0 0
n 800
pr 101325
Te 200
ttotal 120000
fromv 10
tov 10
Particlevguess 8.06
Enlargedomain 1.0
threadc 31
seed 126
enhance 1
field 1e5
charge 1
mgas 28.013
mgas2 4.006
alpha_pol 1.7
alpha_pol2 0.2073
dgas 3.1
timestep 1e-9
mixture 0
fraction 0
EHSS 0
draw 0
to_surface 1
maxvel 7000
velpotincrease 1.02
printvelocity 1
printangvelocity 1
printionpath 1
plotter 1
```

The results are plotted below in terms of reduced mobility for N₂ and He at different temperatures.

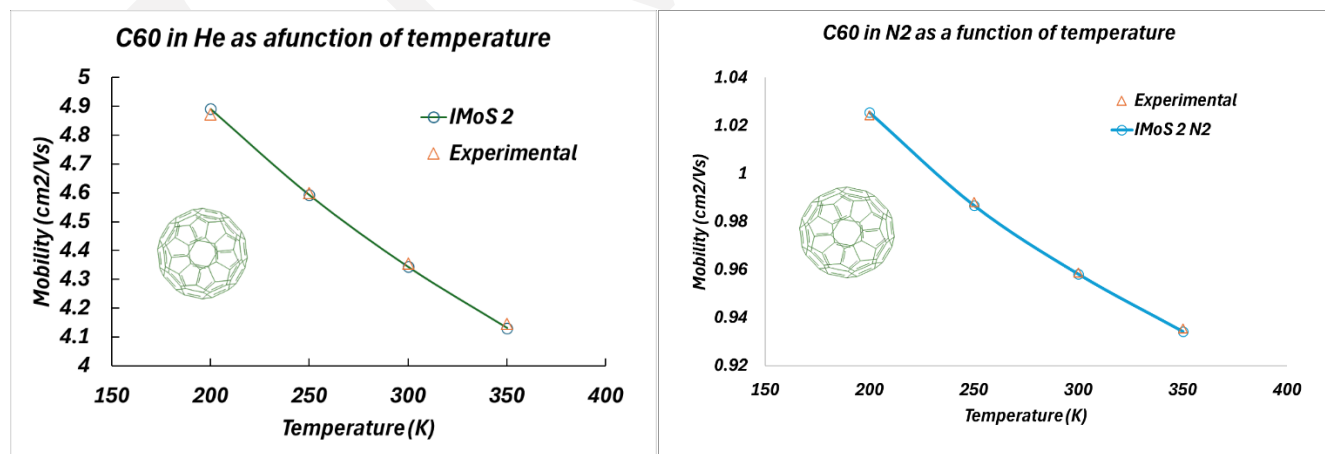


Figure 10.4 C60 at different temperature (experiment vs simulation) for IMoS 2 in He and N₂.

We now would like to use a time-varying field. The first thing we want to populate is the field matrix which in this case will look like:

[illegible]

Here the rows represent the field changing in time, while the columns represent the field changing in space. The total frequency will be 1e6 Hz (period of 1e-6 s). Note that the number of rows (5 positive and 15 negative) make it so that the total average field is 0. While the number of columns could be reduced to 1, it is kept in there so as to understand that field can also change in space with a total wavelength value established by the program (default is 8mm). In order to propagate the ion in a direction perpendicular to the field, we set a value to `vgas` of 200 m/s as these are pretty high fields. `Vgas` is only used to modify the position and does not affect the collisions in any way.

```

DSMCH2 VALUES CONFIG
Anallainb.xlsx Saveme.txt N2 He
interface 0 0 0
n 800
pr 101325
Te 300
total 1000
from mv 1
tov 1
Particlevguess 160.06
Enlargedomain 1.0
threadc 31
seed 126
enhance 1
field 1e6
charge 1
mgas 28.013
mgas2 4.006
alpha_pol 1.7
alpha_pol2 0.2073
dgas 3.1
timestep 1e-9
mixture 0
fraction 0
EHSS 0
draw 0
to_surface 1
maxvel 7000
velpotincrease 1.02
printvelocity 1
printangvelocity 1
printionpath 1
plotter 1
Twave 1
frequency 1e6
vgas 200

```

The frequency should always coincide with the ending one or several cycles. For example, here given a timestep of $1e-9$ and 1000 steps (ttotal 1000), will finish the run after one full cycle of FAIMS for each core. This should be done in the

same way for space variation, either before or in postprocessing so that different core results can be appended to each other. The results show the expected triangular shape for Tryphenylene.

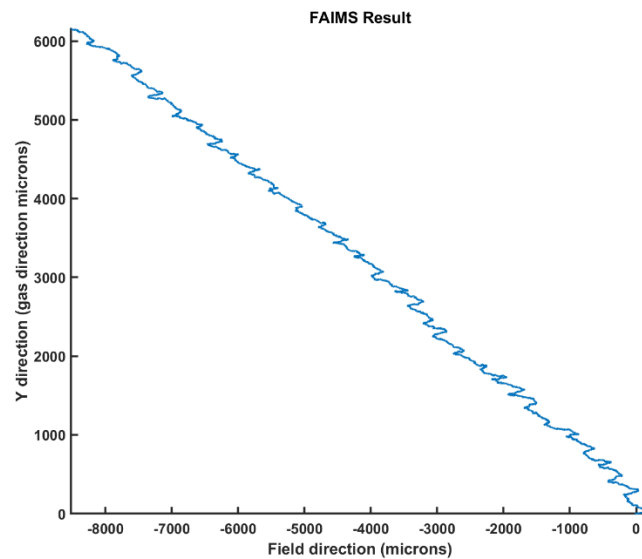


Figure 10.5 Ion path when FAIMS is used. A vgas is used to displace the ion in the y direction.

We can try to correct the displacement by adding a compensation field. The matrix will be shifted by a positive $E_{comp}=100000$ V/m and rerun. This will yield a new direction for the ion path that is meant to allow it to get to the detector as in any FAIMS. The result is provided below and compared to no compensation field

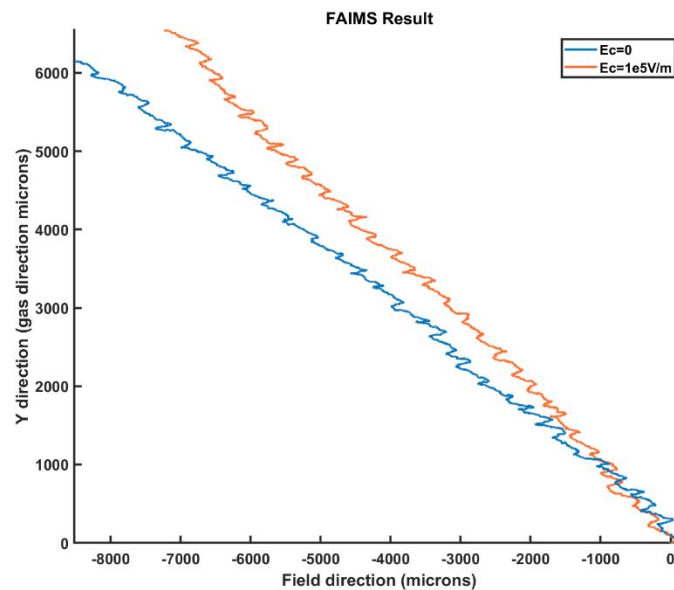


Figure 10.6 Ion path when FAIMS is used comparing a compensation field of 0 and $1e5$ V/m.

More examples will be added in future versions.

11 EXAMPLE OF A COMPLETE OUTPUT FILE

For completeness, a result file is printed here for comparison using Anallainb.xlsx

RESULTS FOR IMOS 2

The time is 04-Aug-2025 12:45:28

The file is Anallainb.xlsx and the molecule is 1

The fraction of gas number 2 is 0.10

191.660056	-4.737122	-12.302884	9767
196.990687	-21.216606	-3.153248	9637
182.068949	-5.953157	-6.328347	9466
193.062176	-12.290889	-0.127610	9897
203.512952	-6.306581	26.956548	9645
202.039694	-10.376807	-18.264163	9980
197.784353	15.582065	12.937693	9969
168.555532	3.874573	2.899819	9706
181.506886	-22.882378	3.111086	9654
186.599069	6.748587	7.383541	9840
193.476143	-14.074808	9.007362	9881
148.276741	11.109906	-20.291854	9513
171.219374	-2.863711	-1.515312	9984
173.280283	22.573325	-19.594842	9621
185.081119	-26.582735	6.255972	9682
177.805348	3.934838	0.413890	9953
180.028511	-15.447965	-12.419191	9678
218.209114	15.695575	-4.223348	9779
179.403127	-20.177396	-15.911094	9777
189.586582	-16.036689	31.145554	9920
172.915257	7.488750	-4.122131	9523
178.925515	-14.279899	0.707479	9693
177.337271	-6.761884	-9.779905	9662
192.698689	-6.688878	5.748912	9786
186.681277	-6.788601	3.325302	9598
179.930345	-29.966404	0.254383	9717
175.554686	29.254035	-25.128952	9633
192.910934	-5.150622	15.681880	9836
204.485970	-24.907765	25.410186	9756
183.508224	20.899027	-0.877139	9673
189.875798	9.023789	13.132071	9477

The total number of collisions is 301703

Average velocity x: 185.64421 m/s

Average velocity y: -4.10666 m/s

Average velocity z: 0.33328 m/s

The moment of Inertia is given by

1.62152e-44	-9.82814e-49	-0
-9.82814e-49	1.65973e-44	-0
-0	-0	3.28125e-44

Dipole moment value is given by 0.538562 Debyes

Dipole moment vector value is given by -0.538554 0.002961 0.000000 Debyes

INPUT FILE

DSMCH2 VALUES CONFIG

Anallainb.xlsx Saveme.txt N2 He

interface 0

n 800

pr 101325

Te 300

ttotal 100

fromv 1

to v 1

Particlevguess 160.06

Enlargedomain 1

threadc 31

seed 129

enhance 1

field 1e+06

charge 1

mgas 28.013

mgas2 4.006

alpha_pol 1.7

alpha_pol2 0.2073

dgas 3.1

timestep 1e-09

mixture 1

fraction 0.1

EHSS 0

draw 0

to_surface 1

maxvel 7000

velpotincrease 1.02

printvelocity 1

printangvelocity 1

printionpath 1

12 AUTHOR, ACKNOWLEDGEMENTS AND REFERENCES

12.1 AUTHOR

Carlos Larriba-Andaluz is the author and owner of the program IMoS 2. He can be contacted through email clarriba@purdue.edu or 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, 20]

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