

IMoS (Ion Mobility Software)

User Guide

Version 1.13

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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 is needed 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 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 (if it exists) 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 (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 interface and governing file IMoS.cla 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 program (application). IMoS v1.13 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 v1.13

- The User interface has been modified to allow calculation of High Field effects for Multistuctures.
- The system now allows Dispersion voltage versus compensation voltage to be obtained for high field and high field with multistucture.
- Intro has been created for the interface.
- The interface now has a config.txt file that allows the change of the default quantities that appear on it.
- Gas temperature calculations are now between ~10% and ~90% faster than the previous version.
- notsaved file (when you want to run and not save) is saved with a time stamp.
- Runs can be canceled when you chose the same name for the savefile.
- Small bugs

+IMoS v1.12

- The User interface has been modified to allow calculation of High Field effects up to the 4th approximation. A secondary option to calculate T-wave CCS using T-wave parameters is being tested.
- High field calculations are now ~20% faster than regular mobility calculations for the same method.
- An error where EHSS would not give the correct mobility in Helium has been corrected. The CCS has not been affected by this.
- The ability to do several files within a folder has been implemented for High Field calculations.
- The output file and input files have been modified to allow output for high fields. The new parameters appear in this guide.
- A new parameter allows the program to show the Drag Force tensor applied on the molecule for non-High Field calculations.
- A known error in the Mac version where EHSS can only be used with 30 atoms is being worked on.

+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 v.1.09

- 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
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 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: $T_{eff} = T + mv_d^2/3k_b$ (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.

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), the Trajectory Method (TM)[2, 4-8] as well as higher field effects. The degree of accuracy of the calculation is directly proportional to the computational time.

3.1 PROJECTION APPROXIMATION (PA)

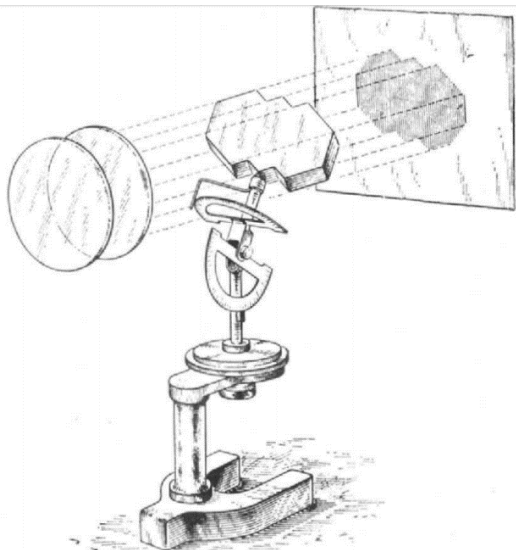


Fig. 5.

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

As the name suggests, CCS is directly related to area of interaction between gas and ion. In its simplest 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 CO₂ or N₂. The 40% value comes from the general assumption of diffuse reemission for heavy gases like N₂ and CO₂. 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, ξ , 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, Δp , 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 τ_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.

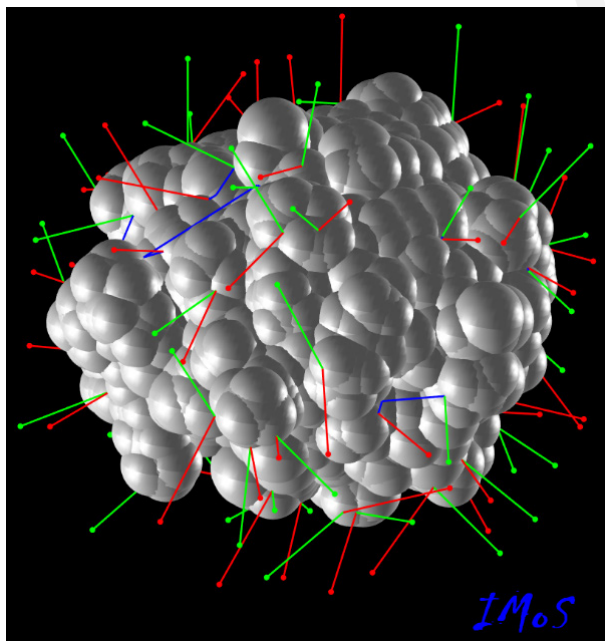


Figure 3.2 EHSS/DHSS of Cytochrome C ion. Red are incoming gas molecules; green are re-emitted gas molecules and blue are partially scattered molecules that collide more than once with the ion.

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. A 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 may be 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

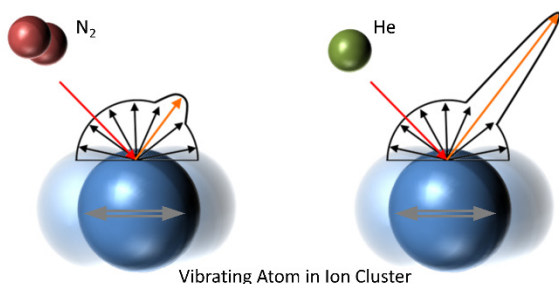


Figure 3.3 A cartoon of the expected reemission mechanisms for two different gases. On the left, for a diatomic gas molecule heavier than most organic atoms, a more diffuse collision is expected with a very small contribution of specular collisions. On the right, for a spherical light gas molecule like 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 0-300Å² range of CCS is to set the accommodation coefficient to 0.48 to yield a value close to the TMLJ.

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

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 a particular distribution. For example, if accommodation is chosen to be 0.91 with diffuse reemission and velocity from a Maxwell distribution at the surface temperature, the resulting value for a sphere would be expected to be the characteristic 1.3573 from the Millikan oil experiments[9, 10]. Due to scattering from 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% energy of that of Maxwell which more closely yields the 1.36 value for non-spherical ions. Figure 3.3 shows how two different gas molecules may have different types on interaction with an atom, where one can gas could have a more elastic re-emission while a heavier ion could have a more elastic one[2]. In all, EHSS should only be used for small ions in light gases, yielding similar results to PA, and DHSS should be used for singly charged large particles for which $\Omega \sim 1.36 \cdot PA$ is expected with

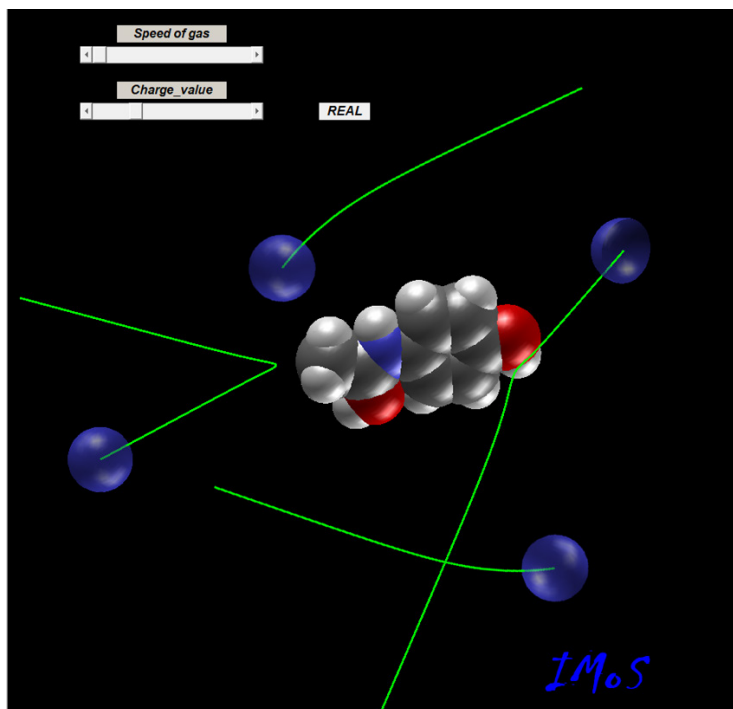


Figure 3.4 IMoS cartoon of the TMLJ 4-6-12 potential interaction.

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 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.

or N₂ 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 N₂ charges (where 2 is the center charge) and index i indicates the charges on the ion. The orientation of the N₂ 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 N₂ 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 N₂ molecule together with a 4-∞ potential and conserves not only linear momentum but also angular momentum of the gas molecule. Similar 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 HIGH FIELD CALCULATIONS USING MATRIX COLLISION INTEGRALS

This feature allows for the calculation of High Field effects using the two-temperature theory up to the 4th approximation. This method employs Collision Integrals to do the different approximation and hence its approach is different from that of the above methods. The end result at low fields should however be equivalent to those of the algorithms above under similar conditions while allowing the calculation to occur at high fields more accurately. The kinetic theory behind the calculation of high fields is complex and not the subject of this manual. Here, a concise explanation is made leaving the complete explanation to an accompanying article in the explanation folder of this software: [Gandhi2022FourthApproximationexplanation.pdf](#) and its supplementary information.

The theory is based on the approach by Kihara and later on by Viehland, Mason, McDaniel and Schamp. In the two-temperature theory, the first approximation to the mobility is given by (repeated here for convenience):

$$\langle K \rangle_I = \frac{3e}{16n} \sqrt{\frac{2\pi}{\mu k_b T_{eff}}} \frac{1}{\Omega_{(T_{eff})}^{(1,1)}}$$

For higher order approximations, the mobility is given by a series of corrections that depend on even powers of the field over the concentration $\left(\frac{E}{n}\right)$. For example, for the 4th approximation:

$$\langle K \rangle_{IV} = \langle K \rangle_I \left(1 + \alpha_0 + \alpha_1 \left(\frac{E}{n}\right)^2 + \alpha_2 \left(\frac{E}{n}\right)^4 + \alpha_3 \left(\frac{E}{n}\right)^6 \right)$$

Here, the α_i coefficients are quite complex functions of collision integrals of the type $\Omega_{(T_{eff})}^{(l,s)}$ and where each subsequent approximation order provides an additional power term. These coefficients are in general dependent on the field through the effective temperature T_{eff} . The algorithm allows the user to state the gas temperature as well as one or a range of effective temperatures. To relate the effective temperature of choice to the field over the concentration, the second moment of the Boltzmann's equation, related to the ion's energy, must be calculated. The second moment can be calculated with its own degree of approximation and in this algorithm, the degree of approximation is the same as that chosen for the mobility. In general, the second moment solution may be written generally as:

$$\frac{3}{2} k_b T_{eff} = \frac{3}{2} kT + \frac{1}{2} m v_d^2 (1 + \beta)$$

where β includes the higher order terms (whose values are shown in the accompanying manuscript). Given that $v_d = Kn \left(\frac{E}{n}\right)$, it is therefore clear that the equation establishes a relation between the field and the effective temperature of interest.

The effective temperature can be defined as the ion's translational temperature at a given field over concentration for a particular ion-gas system. That is, upon a collision, one can assume that the temperature of the gas is T and the temperature of the ion is T_{eff} . This occurs due to higher relative kinetic energy upon an ion-gas encounter.

While the two-temperature theory seems to be accurate for small ions in light gases, it is expected to contain errors at higher fields and polyatomic gases. The reason is that within the assumptions of the two-temperature theory, it was assumed that the collisions between ion and gas are elastic. However, due to the internal degrees of freedom of both ion and gas, this cannot be expected to happen for ion – gas collisions at high relative kinetic energies, where the collisions are bound to be inelastic. In particular, for polyatomic gases, there is an energy mode of escape through rotation and vibration into the internal degrees of freedom of the gas that cannot be recovered. This effect is being calculated currently and a correction is expected to be added in future versions. For the time being, one can assume that this effect is small for most ions at low to

mid fields. There are examples of High field calculations in the appropriate chapter below. The only possible methods that may be used with high fields are TMLJ for all gases and TMLJ/qp for Nitrogen.

3.5 CALCULATION METHODS TABLE

A table describing possible methods.

Method	Definition	Advantages	Disadvantages	Speed Comparison
PA	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.
EHSS /DHSS	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 ξ 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.
TDHSS	Trajectory Method with 4 – ∞ 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.
TMLJ	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.
TMLJ qp	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.
DTM	Diatomic trajectory method with 4 – ∞ 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.
High Field	Same as TMLJ and/or TMLJ qp	High field up to the 4 th approximation.	Needs one TMLJ calculation per effective temperature.	Slightly slower than TMLJ per each calculation.

3.6 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 5GHz computer using 12 physical cores. It compares version 1.12 and 1.13 for the TMLJ and TMLJqpol methods with an increase of more than 50% under most scenarios. For 20205 atoms (mAb protein) TMLJ takes only 34 minutes to complete. Use this result as an approximation as speed varies from computer to computer.

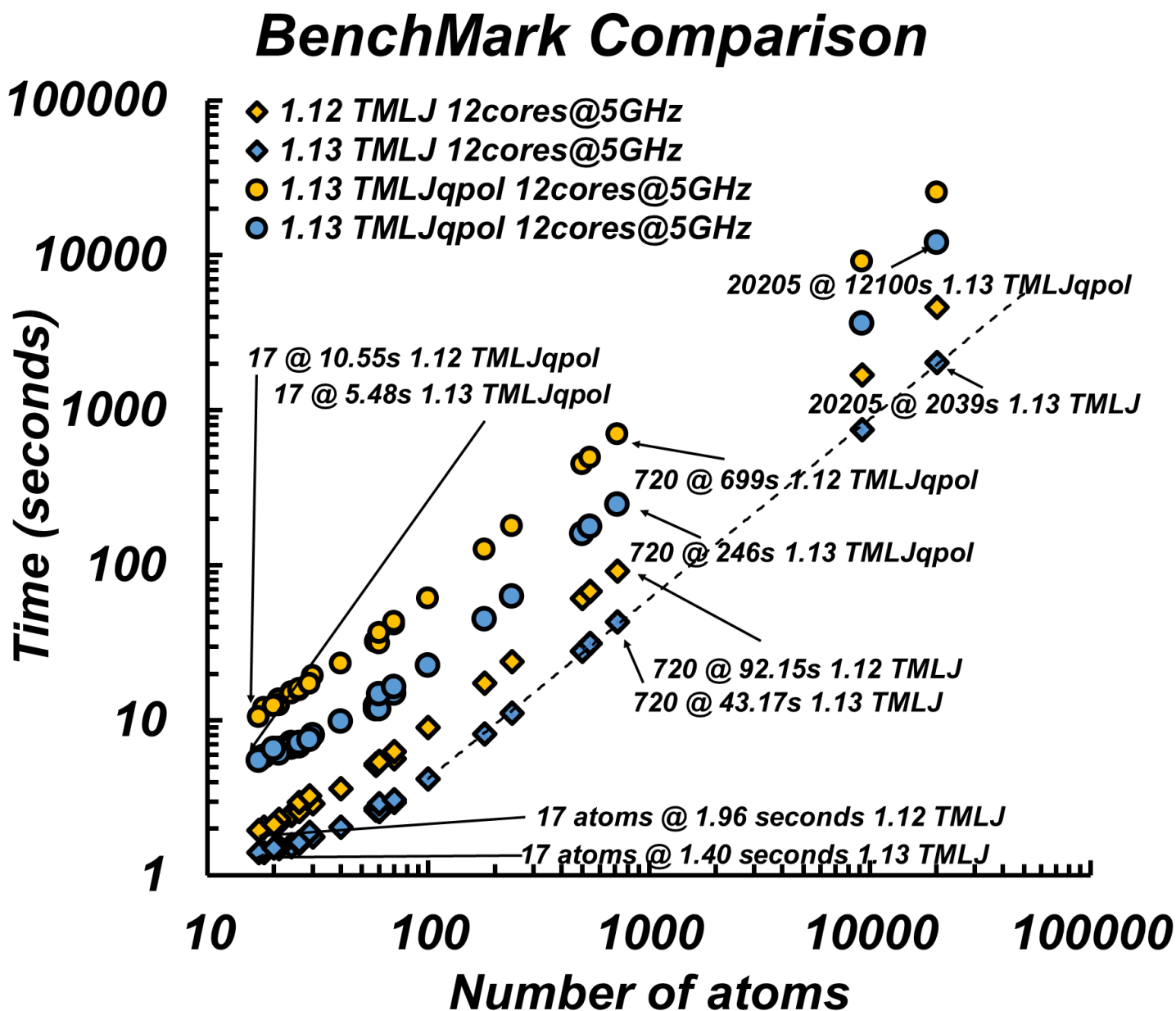


Figure 3.5 Benchmark comparison for the TMLJ method and TMLJqpol versions 1.12 and 1.13

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 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 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 “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.

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 foldernameandpath`”.
- 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
Root	
Readme.txt	"Readme" file detailing the installation process.
IMoSXXWin64.exe	IMoS V1.13 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. It might not appear in some versions
Icon.ico	Icon file.
Splash.png	Splash screen picture.
IMoS.cla	Master configuration / input file. Edit with a text editor to change inputs to IMoS.
IMoS2.cla	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.xml	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.
Config.txt	File that allows the interface default values to be changed. This file is created the first time that IMoS is started. Modifications to this file only alter the interface default values and do not affect the calculations (aside from altering the interface values).
Filefolder	
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-Ethylanilene_pop.mfj	Mobcal .mfj type file that can be run with IMoS.
pdb1y32mod12.pdb	Humanin molecule with different models.
xtal-fix-charge6-cytoc.pdb	Crystal structure of Cytochrome C directly taken from PDB database.
Sphertest.xlsx	Sphere to test Millikan and Epstein's 1.36 value.
Smallions.xlsx	DFT of small ions to test High Fields and Effective temperatures
	Alkylammonium salts for Multistructure high field calculations.
Explanations Folder	
IMoS_UserManual_113.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 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
savefolder	
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.
SPEED folder	
speed.exe	File used to transform Gaussian outputs into excel files to be used with IMoS.
Optimizer folder	
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.
Workhorse folder	
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.
Workmulecla folder	
Different IMoS.cla files	“interface 0 3” option or “interface 1 0” with appropriate checkbox will run all .cla files contained in this folder
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_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.

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 VdW's 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.

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 79-80 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. If no charges are placed on Column 79-80 or there are no partial charges present (see below), the program will not run for high-field calculations as they require charges.

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 to a pdb Model.

If a pdb file has different chains, the interface version 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 ENDMDL.

6.3 STRUCTURE FILE FOR MOBICAL

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 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 – Avogadro– and solver – Gaussian– 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....

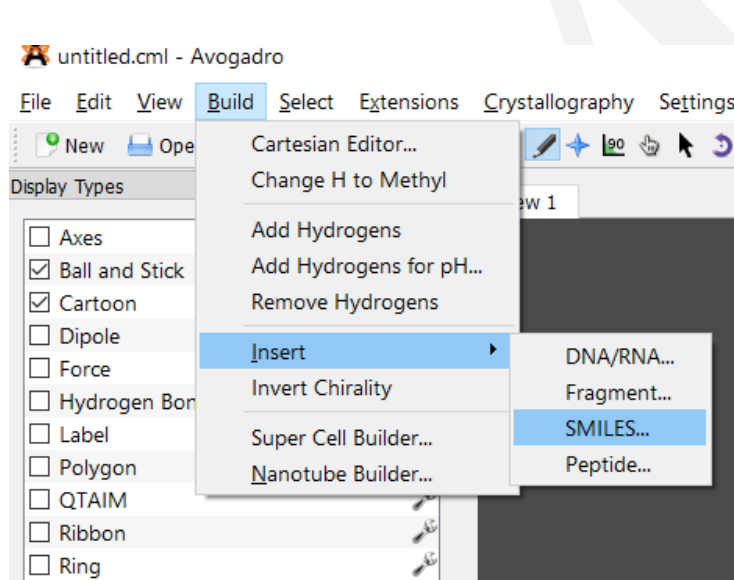


Figure 7.1 - Import molecular structure using SMILES

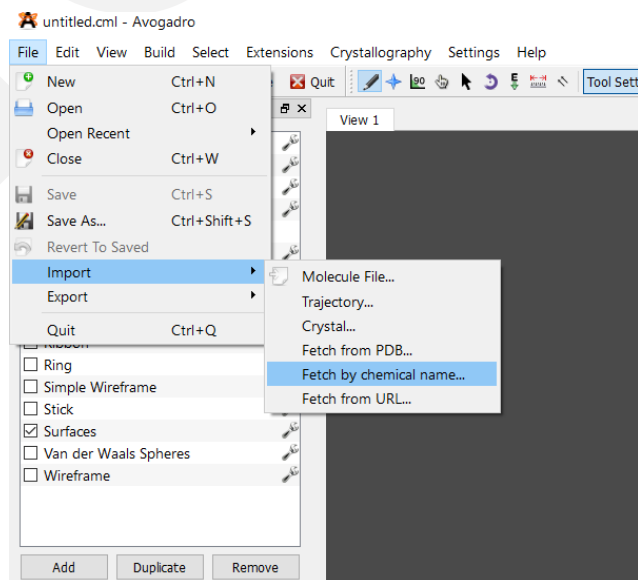


Figure 7.2 - Import molecular structure using name

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.

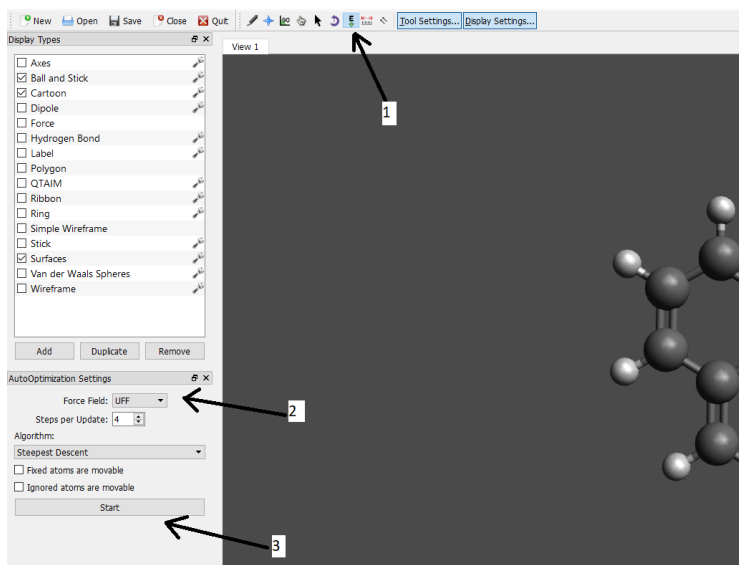


Figure 7.3 - Force Field Optimization

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.

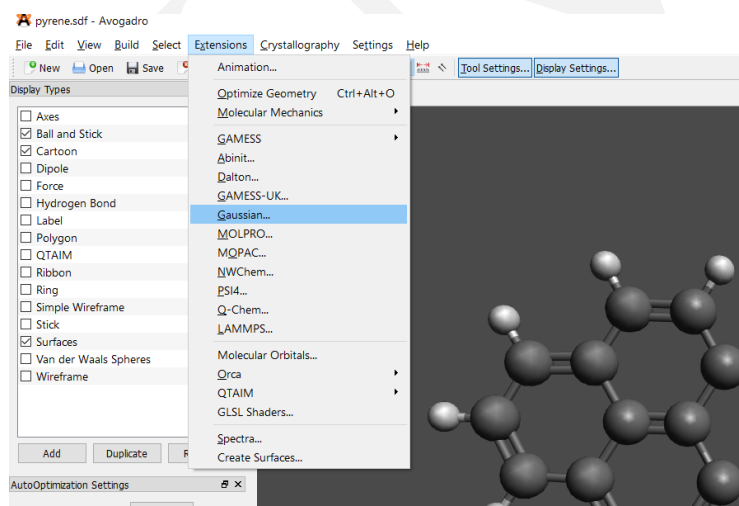


Figure 7.4 – Gaussian in Avogadro

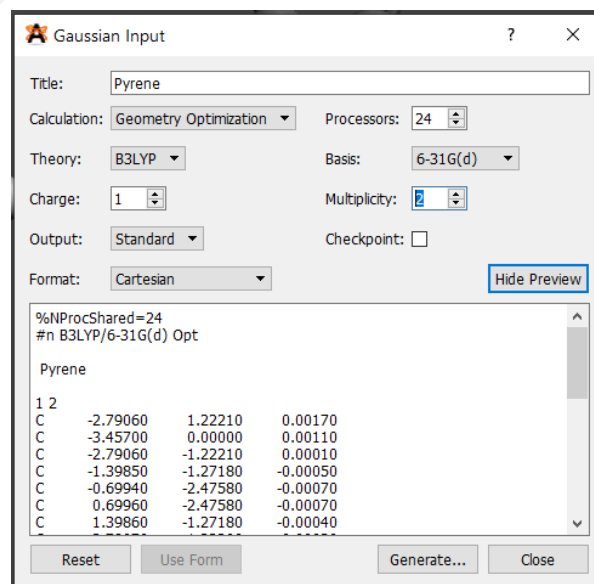


Figure 7.5 – Gaussian dialog box

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

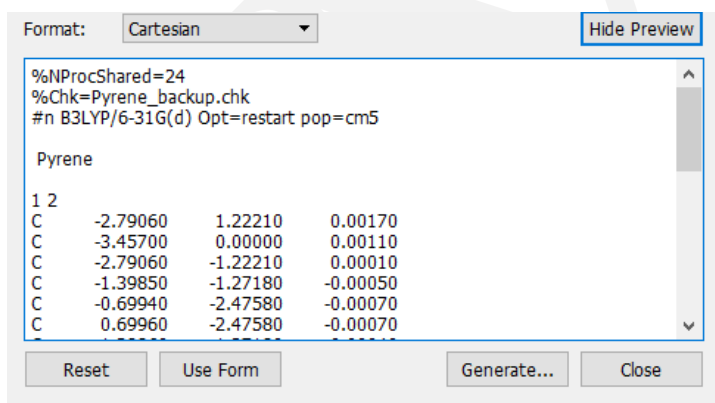


Figure 7.6 – Manually edited Gaussian file

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

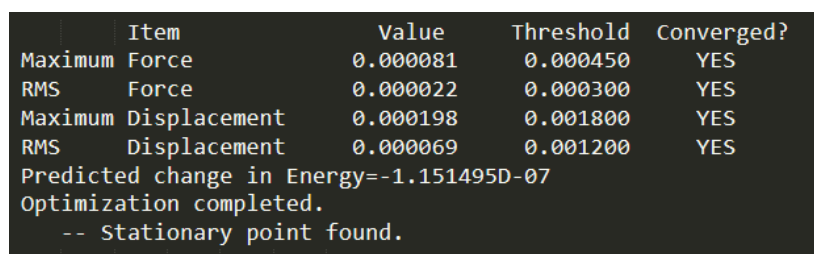
To run Gaussian on a Linux cluster, please load gaussian and then run Gaussian (e.g. Gaussian 16) from the command line by specifying the input molecule and output file. If Pyrene.com is the input file and Pyrene.txt is the output file.

```
>> 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.

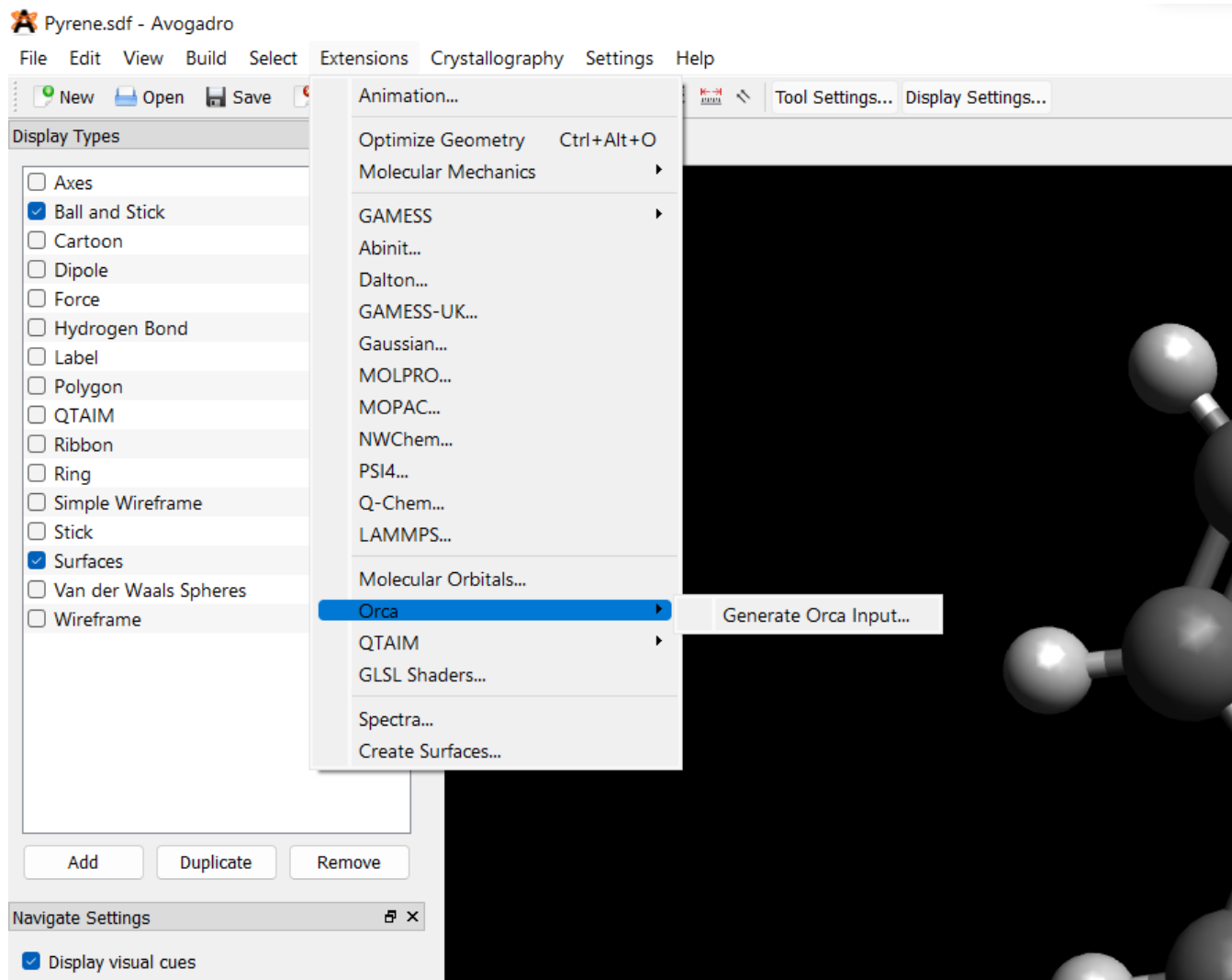


Figure 7.8 – ORCA in Avogadro

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).

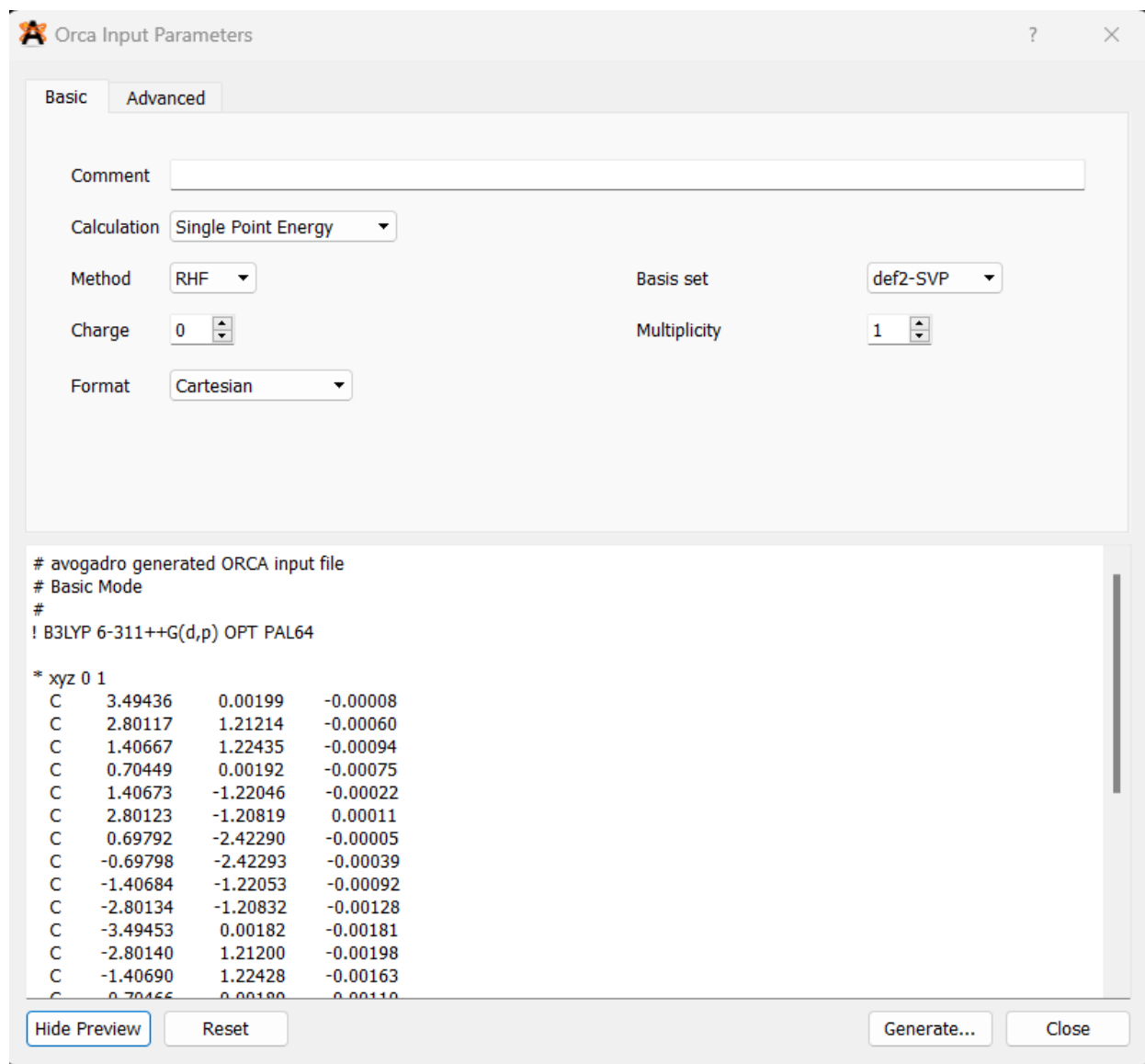


Figure 7.9 – Orca dialog box (functional and the basis set are edited manually)

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 and explains the basics of the program with and without the User Interface. From 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 with four sub-panels highlighted by red boxes and labels:

- File Window:** Contains a file list (e.g., Anallainb.xlsx, C60positions.xlsx), a Data Path field (C:\Users\CLA lab1\Documents\), and buttons for Load File and Plot Figure.
- Status Window:** Displays method information (TMLJ (parallel)), collision cross section (4567.9246 Å²), mobility (0.78207 cm²/Vs), and time taken (908.737 seconds). It also indicates "Calculations complete!".
- Calculation Parameters:** Shows parameters for N. Orientations (500, 3, 3), N. Total / Orient. (300000, 30000), Accommodation (0.0), Timestep (100), Diffuse? (1), Reemission vel (Elastic(mean)), Other(Specify) (m/s), and SASimplify? (Simplify, Connolv, Recolored).
- Calculation Method and Plotting Options:** Includes Gas and molecule parameters (Gas: N2, Red Coeff: 1, Charge: 25, Gas Radius: 1.5 Å, Mgas: 28.00 Da, Pressure: 101325 Pa, Mweight: 145745 Da, Temperature: 304 K, Polarization: 1.7 Å³), Calculation methods (Projected Area, Travelling-Salesman, PA-MonteCarlo, EHSS/DHSS, Trajectory Method, TDHSS, LenJon, QPol, TM Diatomic), Group Tasks (All structure files, All .cla files, Optimize LJ), High E/n Effects (Enable High Field, QPol for E/n, First/Second/Third/Fourth Approximation, Single T_eff: 420 K, T_eff range (in K) 420-690-34, Custom Range), DMS (Enable Dispersion Plot, ft val, time val, Multi structures), T-wave MS (Enable Calculator, Mobility: 307 cm²/Vs, Wave sp.: 630 m/s, Max Volt: 40 V, Wave len.: 12 mm), Parallel Options (Threads: 12, RS: 1, Seed: 13, DragT: 1), and Plotting: OFF. A large Calculate button is at the bottom.

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

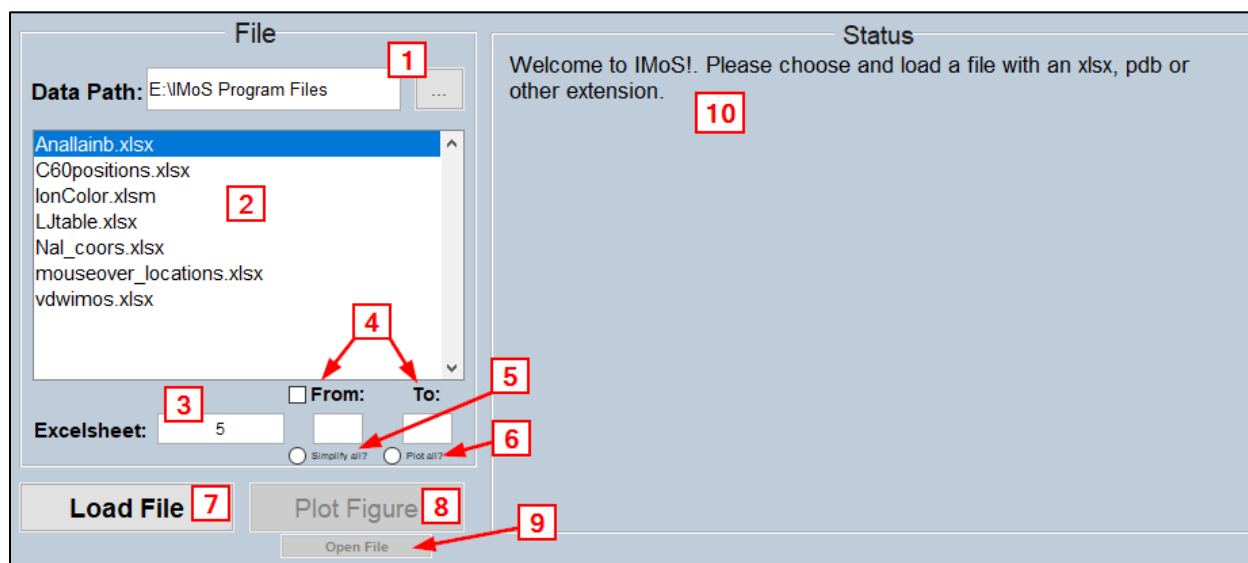


Figure 8.2 - File and Status Window

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 Panel). 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 options, each with a red box and a number indicating a specific parameter:

- 1**: N. Orientations: PA (500), EHSS/DHSS (3), TM/DTM (3)
- 2**: N. Total / Orient.: EHSS/DHSS (300000), TM/DTM (300000)
- 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 buttons

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 Coefficient

Only valid for EHSS/DHSS, TDHSS and DTM methods. Percentage of the number of accommodated gas molecules. 1 for full accommodation, and 0 for fully elastic. This parameter 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 $CCS=1.44PA$ 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.

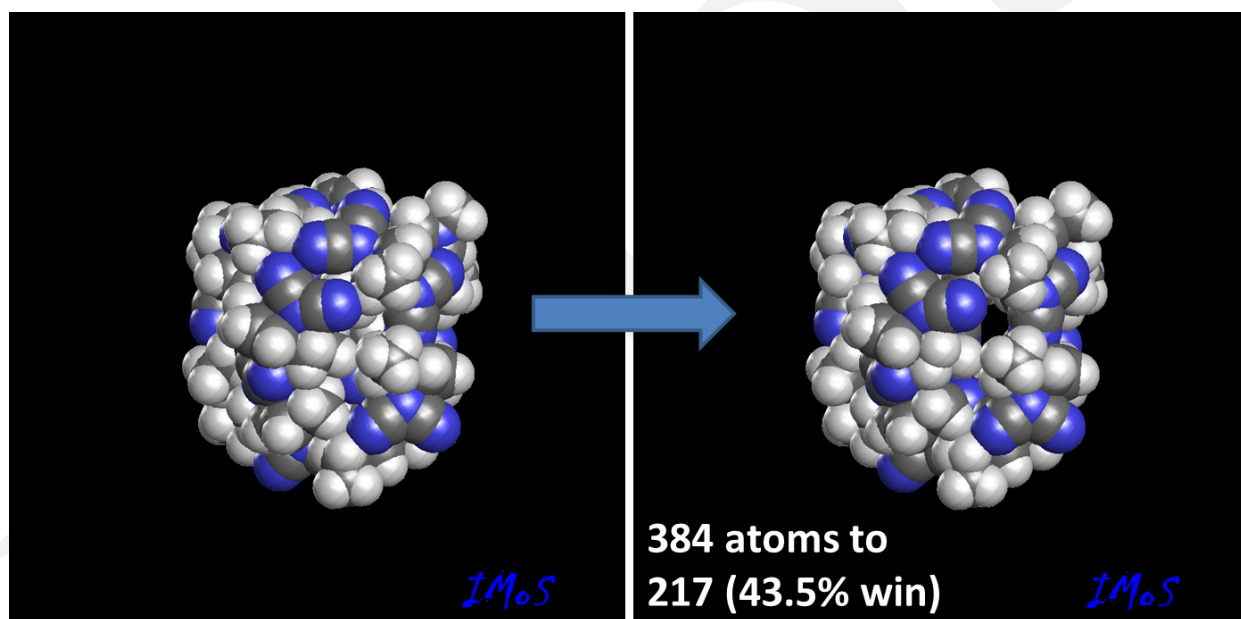


Figure 8.4 – Molecule reduced from 384 atoms to 217 through Solvent Accessible Surface simplify algorithm.

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 the 'Gas and molecule parameters' panel with the following parameters and values:

Parameter	Value	Unit
Gas	N2	
Red Coeff	1	
Charge	1	
LJ Table		
Gas Radius	1.5	Å
Mgas	28.00	Da
VdW Table		
Pressure	101325	Pa
Mweight	256000	Da
Color Table		
Temperature	304	K
Polarization	1.7	Å ³
ReloadColor		

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 (N₂ 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 according 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 4th data column is set to -1. The table also incorporates the atom labels used on the 7th 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.

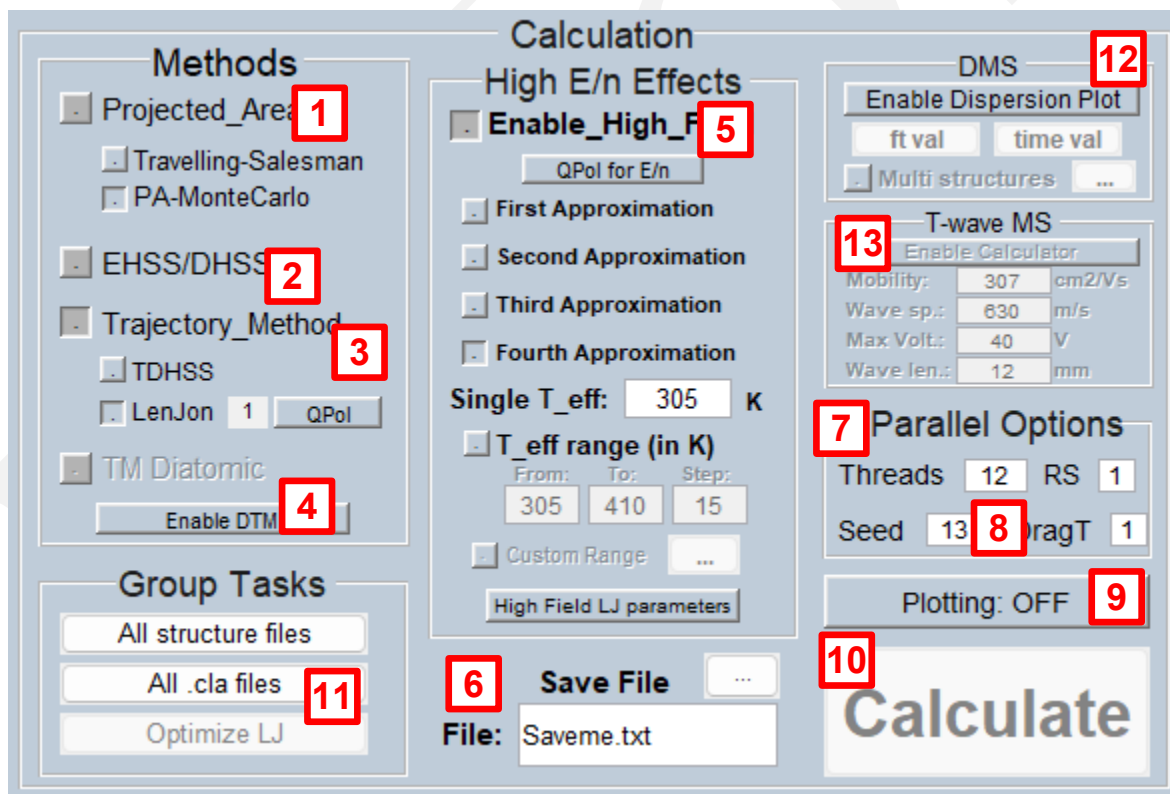


Figure 8.6 - Method and Plotting Parameters

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. Two options:

- Travelling Salesman Method: Inaccurate for point contact particles with point contact gas molecules. Used for Plotting. Not parallelized in v. 1.13.
- PA Monte Carlo: General Projected Area Method. Calculates the area from random shooting. Parallelized, and not available when using the plotting option.

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). See examples.

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 – High Field Calculations.

Once the enable effects box has been clicked, the program will now calculate high field approximations as a function of specified effective temperatures. First check the approximation one wishes to calculate (up to the fourth). Then choose whether you would like to calculate the mobility and CCS for a single effective temperature, a linearly spaced range of temperatures or a custom set of temperatures. There is an option to use quadrupole interaction for nitrogen gas as well as the possibility to use a different set of Lennard-Jones parameters (sheet in LJtable.xlsx labeled “High-field”). You can deselect all the other calculations when high field is selected as they will run separately and can be avoided. See examples.

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 – Parallel Options. 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) and DragRG

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).

DragRG allows the program to calculate the Drag tensor for the cases of EHSS as well as TMLJ. This tensor will appear in the output file.

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.

8.6.11 #11 – Group tasks

Group tasks allow the user to calculate several files from a folder (All structure files), or several configuration files (*.cla) from a folder and allows you to optimize the LJ parameters by choosing a range of values from sigma and epsilon for a particular element. See chapter 9 and examples to understand how they work.

8.6.12 #12 – DMS dispersion plot and Multistucture high-field calculations

This option allows the user to obtain a high-field dispersion plot based on the amplitude and time used for the dispersion voltage. The default is a bisinusoidal wave, but it can be altered by the user to choose a custom one. Since some ions might modify their structure as their effective temperature increases with the increasing field, a dispersion plot can be created using multiple structures at different temperatures. Please see the example of how this operates in Chapter 10.

8.6.13 #13 – T-wave Calculator

This option is disabled at this time.

8.7 CONFIG.TXT FILE

The default values that appear on the interface can be modified using the config.txt file. This file is created the first time that IMoS is open creating an initial configuration window with some of the basic parameters that can be changed. After this window is closed, the config.txt will be created. You can use it to set the default number of threads to be used, the pressure value or the seed number to be used. The file works as follows:

- All parameters that can be modified are initially written down in the file as shown in figure 8.7 below.
- The format of the config.txt file is *parameter = value* and the name of the *parameter* is very specific.
- It only modifies the default values that appear on the interface and it will not affect the runs aside from changing the interface default parameters. The Imos.cla file will not be modified by the config.txt.
- Setting the value *setup* to 0 will open the configuration window again and will rewrite the config.txt to its default state.
- Erasing the config.txt will also bring up the configuration window and recreate the config.txt.
- If a value is deleted in the config.txt file, a warning will appear in the command window and a default value will be used instead.


```

# This is the configuration file for the interface.
# Please check the imos.cla file for the configuration file for the runs.
# If you delete this file, it will get repopulated the next time
# you run the interface.
# To use it, always put an equal sign followed by the number/word/list
# of numbers desired with spaces in between
setup = 1
Gas Pressure = 101325
Gas Temperature = 304
Threads = 7
Seed = 13
RS = 1
DragT = 1
Number of Orientations for PA = 500
Number of Total Gas Molecules for EHSS = 300000
Number of Total Gas Molecules for TM = 300000
Accommodation = 0.0
Timestep = 100
Projected Area = 0
TrajectoryMethod = 1
LenjonMethod = 1
TDHSS = 0
qp01 = 1
EHSS/DHSS = 0
High_field = 0
TeffRangeenable = 0
TeffRangecustomenable = 0
DMSenable = 0
DMSMultistrenable = 0
Red coefficient of gas = 1
Gas Radius = 1.5
Number of Centered Charges = 1
Molecular Mass of the Gas Molecule = 28
Molecular Mass of the Ion = 256000
Gas polarizability = 1.7
Diffuse? = 1
Other Reemitted Velocity = 0
Velocity Option = Elastic(mean)
Gas = N2
qp01_EN = 1
HighFieldLJpage = 0
Teff = 305
Tefffrom = 305
Teffto = 410
Teffstep = 15
TeffRange = 305 307 309 314 320 330 350 380 420 470 530 600 680 770 870 980 1100
ftval = 0 33333333333333 0 288851170070000 0 903710000988118 0 903710000988118

```

Figure 8.7 A partial capture of config.txt. This file alters the default parameters that appear on the interface. It is not the IMoS.cla file and does not alter the runs.

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 Chapter 8 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 that can be added are explained. Note that the best way to create a file with the appropriate configuration is to

run a case in the interface with a very small number of collisions and check the output. The output should have the file to be generated and used without the interface.

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 know that a pdb file contains partial charges. If *partialc* is set to 1, IMoS looks for the variable *chargelines* which has two values. If *chargelines* 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 [chargelines]

Chargelines has two values (*chargelines* XX XX). They correspond to the first and last column that contain the partial charges in the pdb file. The parameter is only read if *partialc* is set to 1. Default is *chargelines* 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 mean more accurate (recommended is 100-450) but slower.

9.3.13 [HEN]

To enable high field calculations, you can use the parameter HEN. The number that follows the parameter can be any from 1 through 4 and establishes the approximation order. For example, HEN 4 will provide high field calculations to the 4th approximation.

9.3.14 [qpolen]

Allows for quadrupole ion potential to be used in high-field calculations with N₂ as a gas. It will not work with other gases. The excel table for the Lennard-Jones parameters is the same as that for the TM qpol method unless the high field LJ parameters are selected, in which case that table will be used.

9.3.15 [Teff]

Teff is the parameter used if a single effective temperature is to be calculated for high-field. This temperature has to be different and higher than the gas temperature. Cannot be used with [Tefffrom][Teffto][Teffstep] or [TeffRange].

9.3.16 [Tefffrom][Teffto][Teffstep]

These three parameters must always appear together on separate lines. They establish the range and step size to calculate mobility at high fields using a range of linearly spaced effective temperatures. Cannot be used in combination with [Teff] or [TeffRange].

9.3.17 [TeffRange]

Allows the user to select custom values of the effective temperature to be run at high field. Cannot be used with [Tefffrom][Teffto][Teffstep] or [Teff]. This parameter requires a second parameter to function properly called DNR CustomRange that will be explained below. To use [TeffRange] select the temperatures followed by spaces, e.g., to run five custom temperatures, write TeffRange 420 450 500 550 2000

9.3.18 [DNRCustomRange]

This parameter must be included in the imos.cla if TeffRange is used. It must be the first parameter (before *interface*) and it is followed by at least as many zeros (or more) than the number of temperatures used in the custom range. For the example above, DNRCustomRange 0 0 0 0 0 0 0 0 0 0 0 should appear before the *interface* parameter.

9.3.19 [HFLJ]

If set to 1 HFLJ will use the sheet Highfield in the LJTable.xlsx for high-field calculations. Default value is 0.

9.3.20 [DragRG]

Selecting DragRG to 1 will provide with the drag tensor calculation for the EHSS and TMLJ options. The tensor is given in units of force per velocity (N/(m/s)).

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.

IMoS V1.13

```

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 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 pair. 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 1st Temp 1st structure, 1st Temp 2nd structure 2nd Temp 1st structure, 2nd Temp 2nd 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 manually 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 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 IMoSXXXW64.exe (for Windows) or IMoSXXXL64.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 IMoSXXXW64.exe (for Windows) or IMoSXXXL64.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

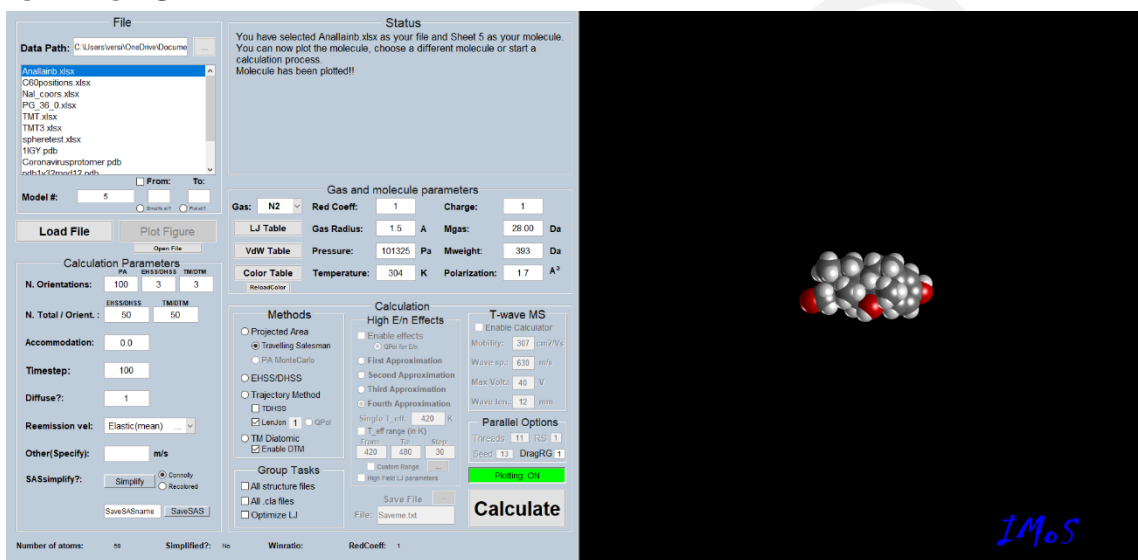


Figure 10.1 - Plotting Example (File Loaded)

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 run. 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.

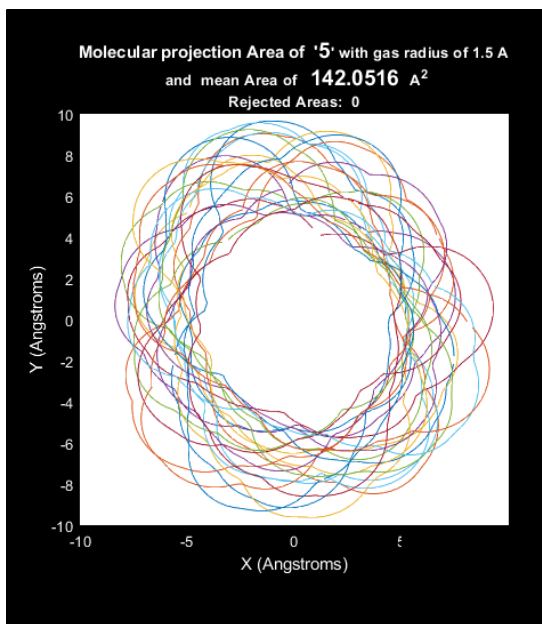


Figure 10.2 - Projected Area Plotting

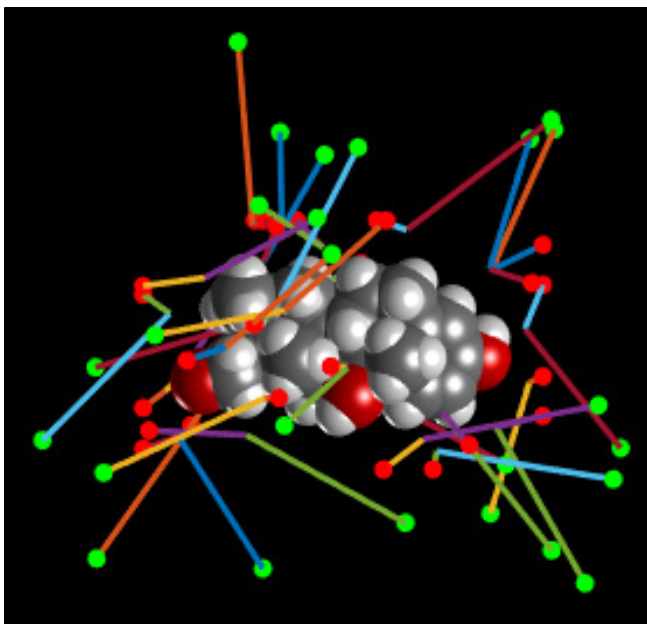


Figure 10.3 - EHSS/DHSS Plotting

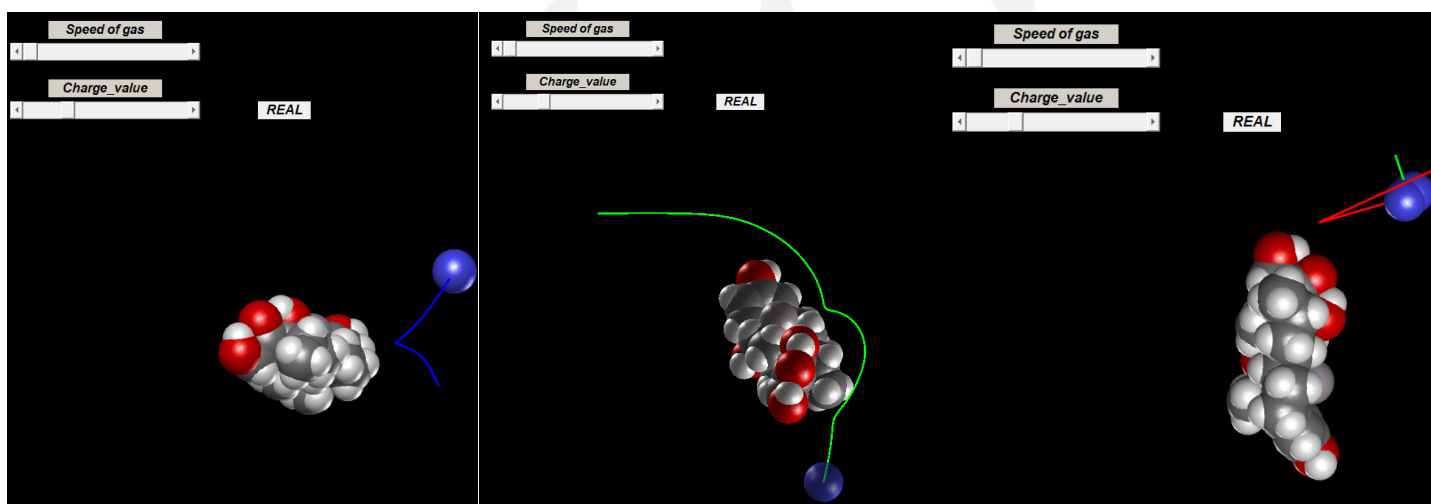


Figure 10.4 - Trajectory Method Plotting. Left TDHSS, middle LJTM, right DTM

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 \AA^2 .
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 equal to 1 \AA^2 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 A² and the Mobility is 223.3518 cm²/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 A² and the Mobility is 154.6756 cm²/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 A² and the Mobility is 160.4256 cm²/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 A² and the Mobility is 164.6316 cm²/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 A² and the Mobility is 164.0676 cm²/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 $\sqrt{128kT/9\pi m}$, 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 A² and the Mobility is 158.3608 cm²/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 A² and the Mobility is 164.241 cm²/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 A² and the Mobility is 167.9696 cm²/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 list 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 ²¹)	sigma (A)		
Gas: N2	H	0.4806000000	2.3000000000	COLLISION CROSS SECTION (A ²)	MOBILITY (cm ² /Vs)
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 A3	N	0.9291600000	4.2000000000		
Radius of gas: 1.50 A	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 A	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		

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
-1.241000	3.538000	0.000000	1.70000	0.0164670000		12
-1.236000	4.623000	0.000000	1.10000	0.1477940000	228	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
	(A ²)	(A ²)	(%)	Qpol CCS (A ²)	(%)
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%
Error Avg(%)			1.05%		1.14%

Figure 10.9 - IMoS Results Comparison

10.6 RUN IMoS AT DIFFERENT GAS 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 GROUP TASKS 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 structure 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 IMoS113(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 temperatures.

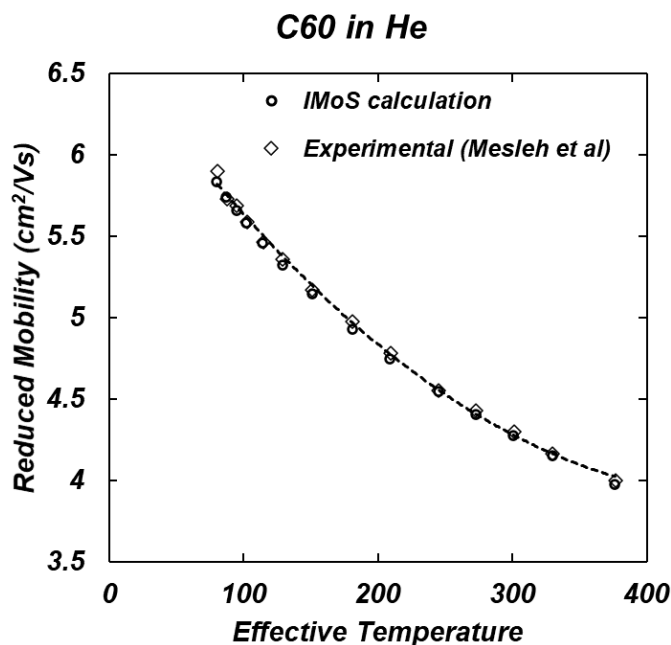


Figure 10.10 C60 at different temperature (experiment vs simulation) based on Mesleh's manuscript.

10.7 (DEPRECATED) USING IMoS AS AN APPROXIMATION FOR HIGHER FIELDS. EFFECTIVE TEMPERATURE.

This example is DEPRECATED but it is left here as a possible exercise. For calculations at higher fields, please follow the examples below. 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. 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[19].

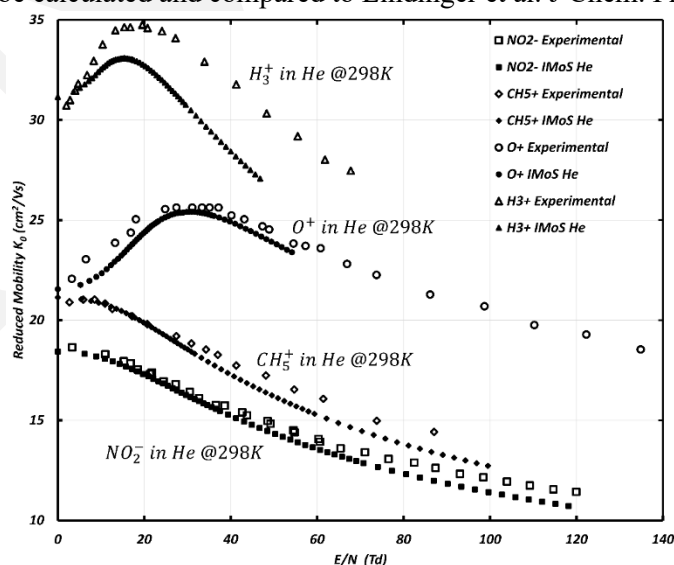


Figure 10.11 High Field Using IMoS and Effective Temperature

10.8 OPTIMIZING L-J PARAMETERS/VDW RADII AT CONSTANT TEMPERATURE.

To optimize L-J parameters, please follow reference [20]. 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 Analiainb.xlsx file. This can be done from the interface or directly from the IMoS.cla file.

1. Interface.

- Open interface. Load any molecule of the Analiainb.xlsx file.
- 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.
- Select only the Trajectory M. LenJon option in N2. **Only this one.**
- Make sure 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.
- In the GROUP TASKS group, check the Optimize LJ box.
- Open the *Optinput.txt* file in the Optimizer folder. These will be the parameters to set:

```

lfrom 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.**
- Press Calculate and wait for completion. Note that these calculations could take several hours if too many calculations are required.
- 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 ϵ and σ (like below).

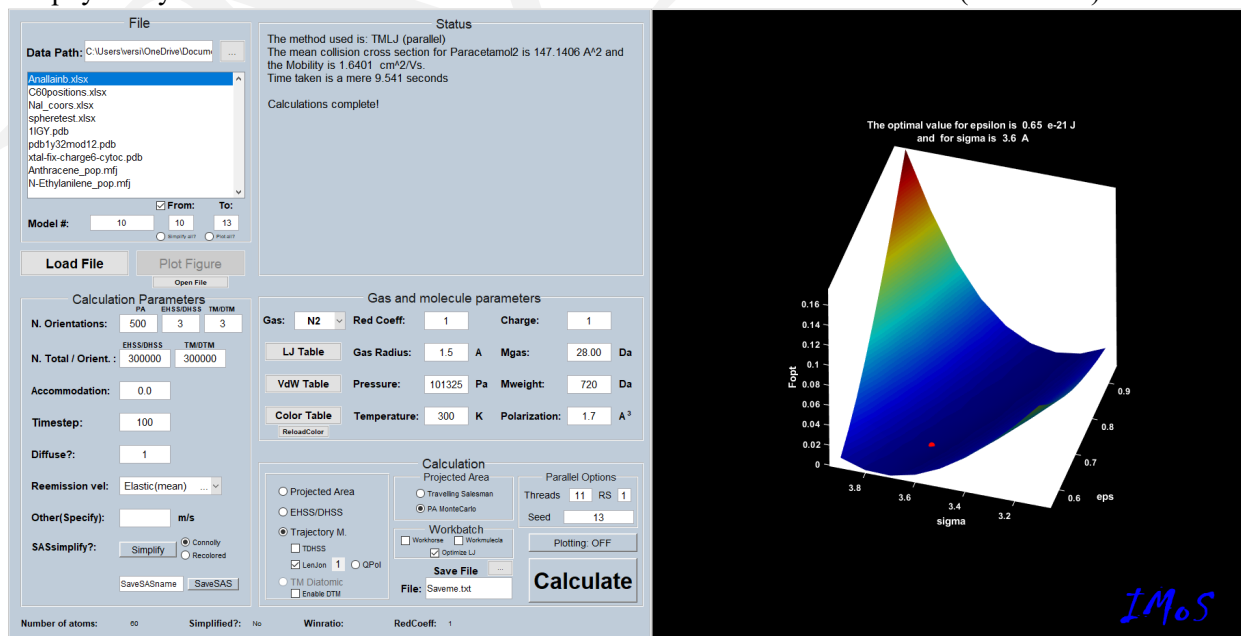


Figure 10.12 Optimization of Carbon L-J parameters using IMoS Optimizer

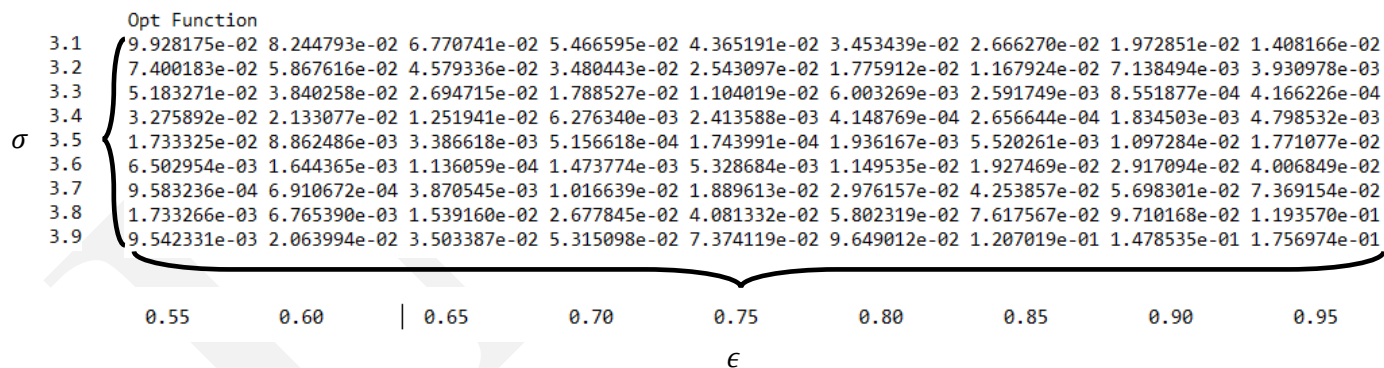
2. No Interface.

- 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 IMoS113(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 ϵ and σ (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:



- The optimization of the vdw radii is similar. Repeat the exercise with the following parameters:

```
efrom 0.55
eto 0.95
ejump 0.05
sfrom 3.1
sto 3.9
sjump 0.1
vdwfrom 0.5
vdwto 1.4
vdwjump 0.1
atom 1
structures 4
Temp 300
result 19
expected 108.0448 82.2882 146.3141 88.578
```

- j. When the value of `vdwfrom` differs from the `vdwto`, the program will attempt a `vdw` radii optimization and not a LJ optimization. Instead of the trajectory method, select either PA or EHSS or TDHSS as your method (only one of them).
- k. In this case we chose the first 4 structures of the of the `Analiainb.xlsx` file in N2. Check the From: To: box in the File parameters. In the From box, choose 1, in the To box choose 4. This will run molecules Triphenylene, Nethylaniline, Dexamethasone, Acetaminophen.
- l. We will optimize the value of the Hydrogen atom. Select for example PA as the method.
- m. Press Calculate.
- n. The results are given in `resultsopt19.txt` :

```

CCS calculated
100.464527 72.554166 133.104776 80.019220
100.464527 72.574887 133.114752 80.045015
100.658603 72.895470 133.373995 80.358029
101.452350 73.841226 134.190787 81.152516
102.884641 75.393718 135.634167 82.390431
104.895185 77.504474 137.693124 84.046161
107.371831 80.060750 140.344284 86.101370
110.233356 82.974989 143.536560 88.499532
113.412316 86.110448 147.110974 91.213929
116.873711 89.419670 150.998372 94.187970

Mobility calculated cm^2/Vs
2.338926 3.389066 1.724360 3.015761
2.338926 3.388099 1.724230 3.014789
2.334417 3.373198 1.720879 3.003045
2.316153 3.329995 1.710404 2.973645
2.283909 3.261424 1.692203 2.928966
2.240133 3.172602 1.666899 2.871265
2.188461 3.071304 1.635410 2.802729
2.131652 2.963434 1.599039 2.726781
2.071901 2.855529 1.560186 2.645635
2.010539 2.749852 1.520020 2.562098
CCS Expected
108.044800 82.288200 146.314100 88.578000

Opt Function
3.640205e-02 3.627404e-02 3.413577e-02 2.815311e-02 1.950847e-02 1.031857e-02 3.218027e-03 8.411183e-04 5.540741e-03 1.922426e-02

vdw
5.000000e-01
6.000000e-01
7.000000e-01
8.000000e-01
9.000000e-01
1.000000e+00
1.100000e+00
1.200000e+00
1.300000e+00
1.400000e+00

Temperatures
300.0000

Optimal for vdw radii is 1.200000 A

```

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.

- Open interface. Load any molecule from file: Anallainb.xlsx.
- 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.
- Select only the Trajectory M. LenJon option in He.
- 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.
- In the Workbatch group, check the Optimize LJ box.
- 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, ...)

- Copy LJTableHedefault.csv to LJTable.csv. If the LJ parameters for the other atoms are different from default, customize as appropriate.
- Press Calculate and wait for completion. Note that these calculations could take several hours if too many calculations are required.
- 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 ϵ and σ .

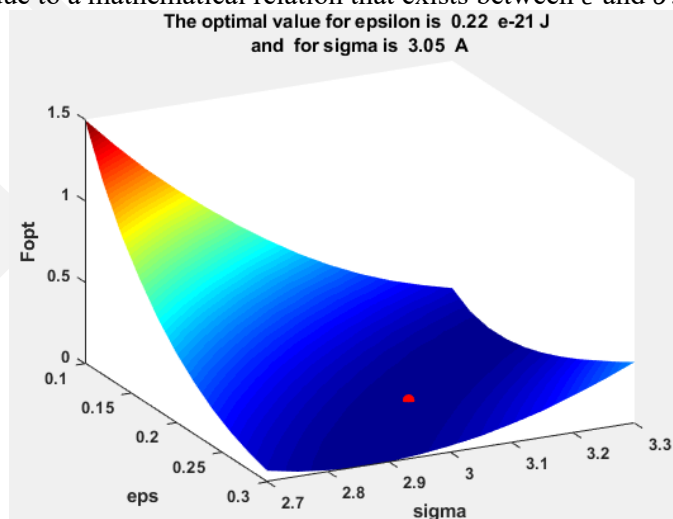


Figure 10.13 Optimization of Carbon L-J parameters using IMoS Optimizer (Temperature and LJ change)

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 (*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:

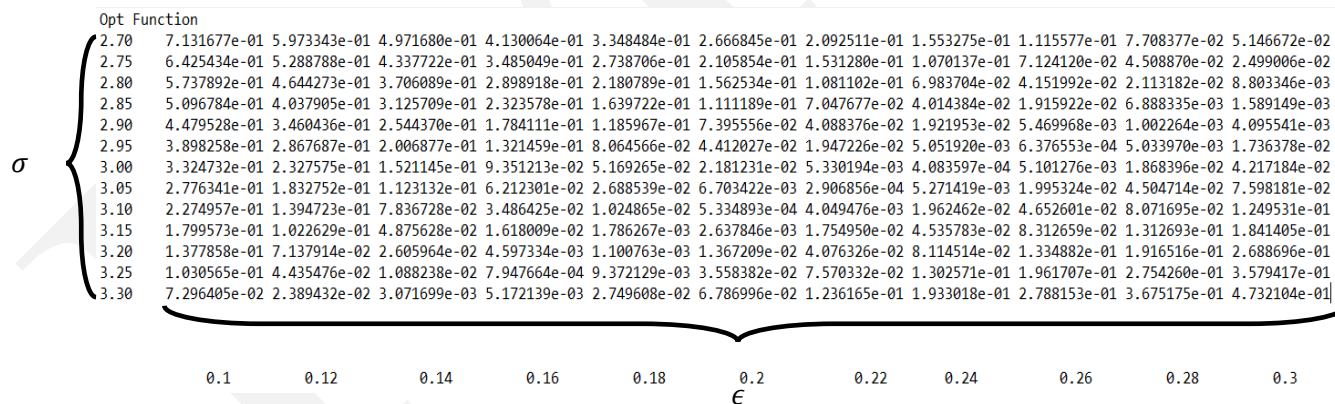
```

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 IMoS113(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 ϵ and σ .
- 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:



This example can also be done with vdw radii. However, the only method that changes with temperature is TDHSS so using it with PA or EHSS is unnecessary.

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.

1. Put files in the Workhorse folder.
 - a. Files in the folder could be: Anthracene_pop.mfj, NEthylanilene_pop.mfj, Anallainb.xlsx, C60positions.xlsx, ch3.xlsx, CH4.xlsx, pdb1y32mod12.pdb, and xtalfixcharge6cytoc.pdb, pdb1y32mod12twomodelsonly.pdb, Anthracene_pop2.mfj
 - b. .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 pdb1y32mod12twomodelsonly.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.
 - c. .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.
2. The Workhorse can be run with or without the interface:
 - a. No interface: Change IMoS.cla parameter *interface* to *interface 0 2*. Execute IMoS113(platform) executable. The parameters are selected from IMoS.cla.
 - b. 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.
3. 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 an appropriate folder name. Sequentially, IMoS will copy the content from each .cla file to ImoS.cla and calculate the CCS accordingly.

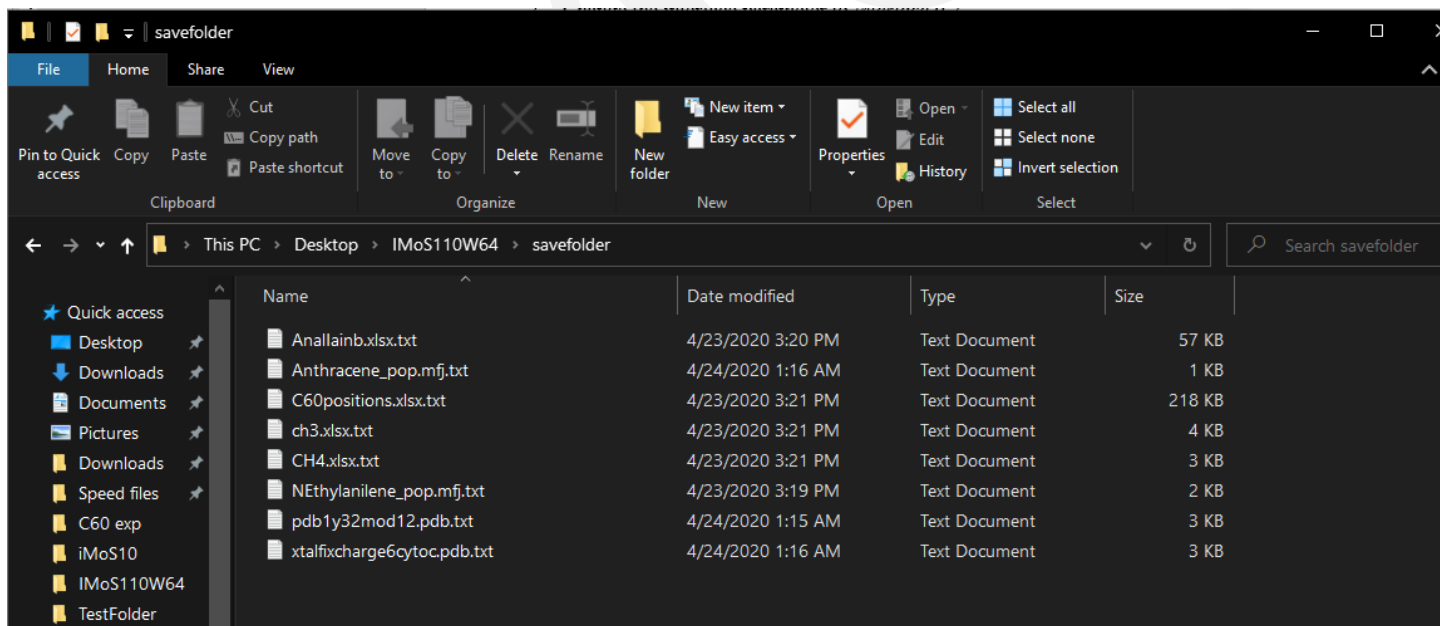


Figure 10.14 savefolder after analysis

10.11 USING IMoS TO RUN HIGH FIELDS UP TO THE FOURTH APPROXIMATION.

This example showcases the use of the high-field calculation subroutine for ImoS using a variety of different effective temperatures.

1. Interface

- a. Deselect all Methods from the Methods portion of the Calculations window.
- b. Check enable effects in the High E/N Effects window.
- c. Select your appropriate approximation. In this case, select the fourth.
- d. Choose whether you want to run one single effective temperature, a linear range or a custom range by selecting (or deselecting) T_eff range or Custom Range tick boxes.
- e. Select the gas and appropriate parameters. In this case, N2 is chosen as the gas.
- f. Choose the name of the save file you would like to use, the seed and the number of threads.
- g. Select your ion of interest, in this case Analianb.xlsx model 5 and press load file.
- h. The calculate button should now be enabled. Press calculate.
- i. If single T_eff is chosen to be 420K, the summary of the results in the output file will be:

Summary of all the calculations:

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
Betamethasone	420.00	183.2452	124.1042	121.7291	121.5919	121.5584	0.9641	0.9852	0.9865	0.9860

- j. If T_eff range is selected and the temperature variation is 420 to 480 K with a step of 30 K, the output file summary will be:

Summary of all the calculations:

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
Betamethasone	420.00	183.2452	124.1042	121.7291	121.5919	121.5584	0.9641	0.9852	0.9865	0.9860
Betamethasone	450.00	179.6217	141.2673	137.9687	137.7401	137.6800	0.9502	0.9759	0.9778	0.9772
Betamethasone	480.00	176.4711	157.3805	153.0902	152.7480	152.6523	0.9364	0.9664	0.9690	0.9683

- k. If the custom range checkbox is clicked after clicking Teff_Range. Click on the ... button for a popup to appear where a range of temperatures can be typed with each temperature followed by spaces. If the default values are chosen the following output summary is expected.

Summary of all the calculations:

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
Betamethasone	305.00	202.9267	10.8740	10.8715	10.8715	10.8715	1.0216	1.0218	1.0218	1.0218
Betamethasone	320.00	199.5785	43.8176	43.6876	43.6863	43.6861	1.0141	1.0173	1.0174	1.0174
Betamethasone	340.00	195.5795	66.3918	65.9605	65.9513	65.9498	1.0039	1.0111	1.0112	1.0112
Betamethasone	380.00	188.7716	98.4318	97.1395	97.0864	97.0752	0.9839	0.9984	0.9990	0.9987
Betamethasone	450.00	179.6217	141.2673	137.9687	137.7401	137.6800	0.9502	0.9759	0.9778	0.9772
Betamethasone	600.00	166.5854	215.4065	206.6302	205.6264	205.2958	0.8873	0.9312	0.9372	0.9363
Betamethasone	800.00	156.3634	302.2185	285.0331	282.4052	281.4061	0.8186	0.8774	0.8889	0.8887
Betamethasone	1200.00	145.4787	462.8543	427.7605	420.9698	418.0529	0.7184	0.7901	0.8094	0.8118
Betamethasone	1600.00	139.4494	616.1397	562.8449	551.4327	546.2681	0.6491	0.7247	0.7482	0.7529
Betamethasone	2000.00	135.4765	765.5827	694.1885	678.0349	670.5178	0.5976	0.6737	0.6995	0.7058
Betamethasone	5000.00	123.0419	1829.3729	1626.7705	1575.7628	1550.8750	0.4161	0.4815	0.5082	0.5178
Betamethasone	10000.00	116.0108	3505.0568	3095.7136	2989.7646	2937.2971	0.3121	0.3643	0.3870	0.3960

- l. The results of the reduced mobility can be plotted as a function of the field over concentration. Note that there are four different values regarding the four different approximations (for both mobility and field over concentration). Also, note that the high choice of Teff is not reasonable but the program will let you calculate the mobility.

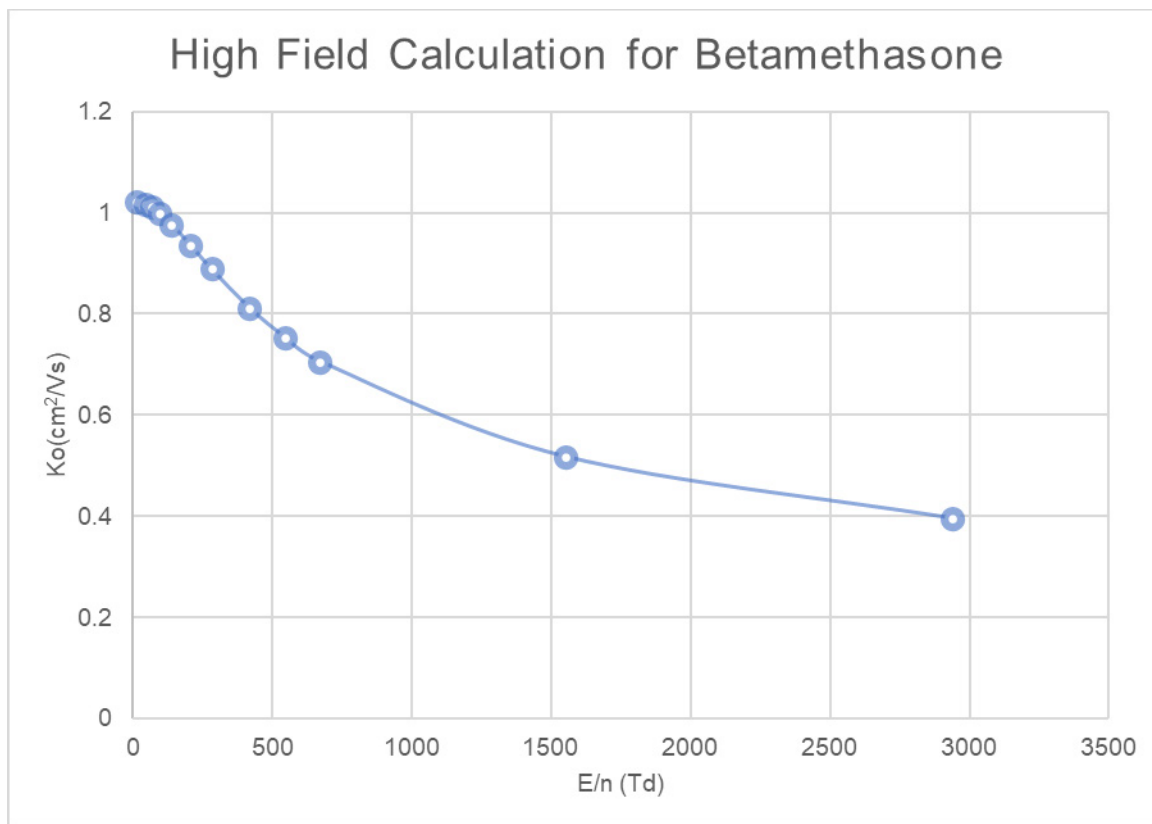


Figure 10.15 Reduced mobility of Betamethasone as a function of E/n.

2. No Interface

- a. On the imos.cla file make sure that the interface is set to 0 0.
- b. If a single temperature is used, the following variables should be added to the imos.cla file aside from the general ones.

```
HEN 4
Teff 420
```

- c. Run the imos executable. The output should be the same as with the interface, namely:

Summary of all the calculations:

Ion	Teff (K)	CCS (Å²)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm²/Vs)	<Ko2> (cm²/Vs)	<Ko3> (cm²/Vs)	<Ko4> (cm²/Vs)
Betamethasone	420.00	183.2452	124.1042	121.7291	121.5919	121.5584	0.9641	0.9852	0.9865	0.9860

- d. If a linear range is used, the following variables should be added (Teff must be removed).

```
HEN 4
Tefffrom 420
Teffto 480
Teffstep 30
```

The expected results are the same as those for case j. in the interface version.

- e. For the particular case where a custom range is to be employed, the first lines of the imos.cla file must be rewritten as:

10.12 USING IMoS TO RUN HIGH FIELDS UP TO THE FOURTH APPROXIMATION CHOOSING SEVERAL FILES FROM THE WORKFOLDER.

1. Interface
 - a. Deselect all Methods from the Methods portion of the Calculations window.
 - b. Select All structure files from the Group Tasks. This will calculate all the structure files in the workfolder (including excel with all its sheets, mfj mobcal files and pdb files). **NOTE:** The pdb files must contain at least one charge in the 79-80 column on one of the atoms or must have partial charges. If a pdb file is present without those, the program will stop calculating.
 - c. Make sure that the files Analiainc.xlsx, anthracene_pop.mfj and pdb1y32mod12twomodelonly.pdb are in the workhorse folder. Make sure that the .pdb file contains at least a charge on one atom of partial charges.
 - d. Check enable effects in the High E/N Effects window.
 - e. Select your appropriate approximation. In this case, select the fourth.
 - f. Choose whether you want to run one single effective temperature, a linear range or a custom range by selecting (or deselecting) T_eff range or Custom Range tick boxes.
 - g. Select the gas and appropriate parameters. In this case, the N2 is chosen as the gas.
 - h. Choose the name of the save file you would like to use, the seed and the number of threads.
 - i. Select an ion (not important which one it is) and press load file.
 - j. To speed up the calculation for testing only, you may want to reduce the number of total trajectories to 10000 instead of 300000 (on the N. Total / Orient.: TM/DTM box). Note that the high-field calculations will always use the TM/DTM box.
 - k. The calculate button should now be enabled. Press calculate.
 - l. If T_eff range is selected and the temperature variation is 420 to 480 K with a step of 30 K, the results will be shown for the individual molecules (with the name of the molecules) in the savefolder. Note that each file (e.g., Anallainc.txt) contains the calculations of all the molecules or models within the file.
 - m. A Summary.txt file will appear with the main results on the workhorse folder.
2. No interface
 - a. On the imos.cla file make sure that the interface parameter is set to 0 2. Follow closely example 10.10 as necessary as well as 10.11b for the appropriate values for the imos.cla concerning high fields.
 - b. Once the files have been chosen and the imos.cla file is appropriate. Run the imos executable.

OPTIMIZATION CANNOT BE USED WITH HIGH-FIELDS AT THIS TIME. USE THE EXAMPLES ABOVE FOR DIFFERENT TEMPERATURES INSTEAD.

10.13 USING IMoS TO CALCULATE MULTI STRUCTURE DISPERSION PLOT FOR SALT STRUCTURES

This example showcases the way we can use IMoS for multi structures calculation. Here, we will see the multi structure calculation for three structures for salt TDDA.

1. Interface

- Select the “TAA_multiTemperature_candidate2.xlsx” from the file window. Type in 1 and 3 into the From and To boxes to run calculations for the multi structure dispersion plot on three structures of salt TDDA. Be sure to check the *From: To:* checkbox to enable running multiple files. Click *Load File* to import the data into the program. A visualization of the structures is shown in the figure below. The structures have been obtained using MD at three different temperatures and we will assume that these structures are the structures that would be observed at the effective temperatures of 295K, 390K and 480K.

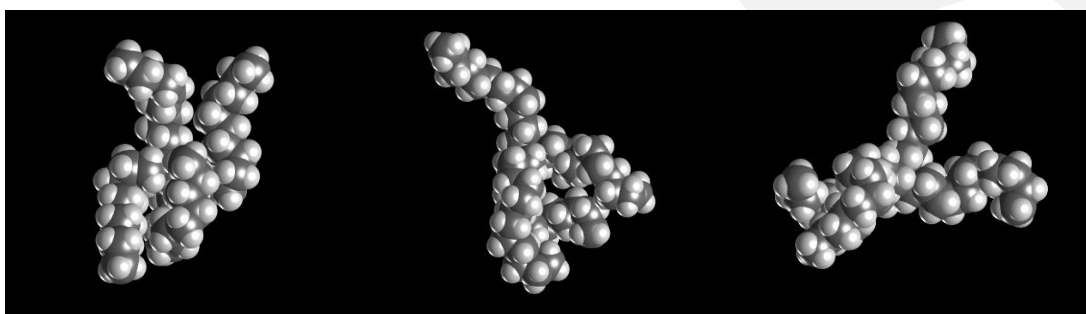


Figure 10.16. Three Structures of TDDA at different temperatures- TDDA at 295K (a), TDDA at 390K (b) and TDDA at 480K (c).

- For this example, select Nitrogen from the *Gas* list. Make sure that the gas temperature is smaller or equal to the smallest effective temperature of your structures. In this case, the gas temperature will be 295K.
- Deselect all calculations from the regular Methods section and check *Enable_High_Fields* checkbox. Select the *Fourth Approximation*.
- Select the *T_eff range (K)* from 295K to 665K with a step of 40K. You can also select the *custom range* and type the effective temperatures there. Note that the temperatures selected here do not necessarily agree with the temperatures at which you have calculated your structures. The program will automatically interpolate the results from the different structures at the different effective temperatures selected.
- Click *Enable Dispersion Plot* and click the *multi structures* check box as shown below.

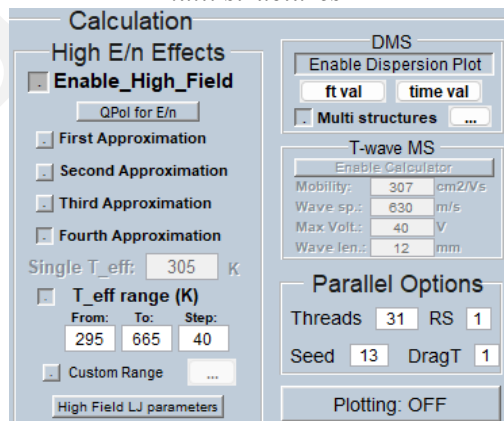


Figure 10.17. High Field and Multi Structure Options

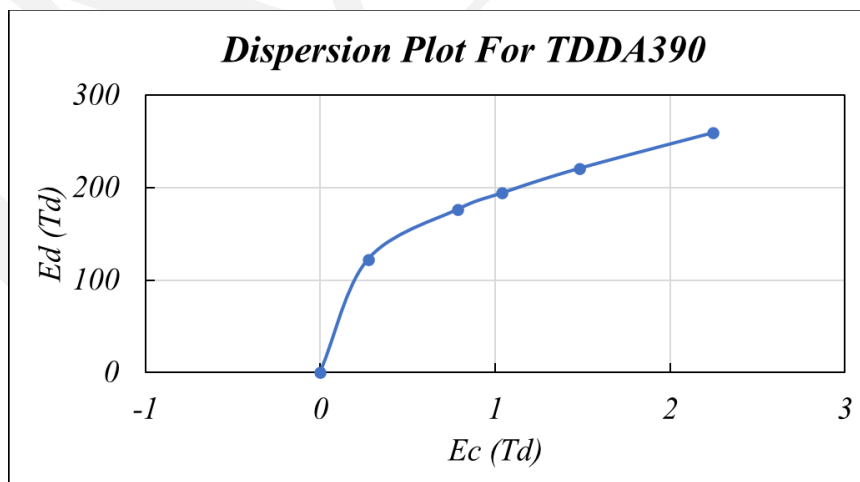
- f. Click the ... button to the right side of the *Multi structures* button to select the temperatures at which the structures were calculated. The number of temperatures must match the number of structures selected. Here, we are choosing 295K, 390K and 480K in the option dialog that appears. Make sure that the first temperature is the same or higher than the gas temperature. Click *Save and Close*.
- g. If desired, change the dispersion voltage wave and time in the *ft_val* and *time_val* buttons. The default is the bisinusoidal wave.
- h. If just testing, decrease the number of gas molecules per orientation (N. Total/ Orient) for TM/DTM to 3000 for a quicker calculation. Leave at 300000 for accurate calculations.
- i. Choose the name of the save file. Click the *Calculate* button.
- j. Once the calculation is performed, open the save file to view the results. This file includes the fourth approximation results and the dispersion plot for all the structures individually. An excerpt is shown below. One can use the results to plot independent Dispersion plots also shown below:

```
The TM Method used is High Field
Performing TMLJ calculations for: TAA_multiTemperature_candidate2.xlsx and molecule TDDA_390_25.txt.

Results
-----
Summary of ion calculations:
Ko represents reduced mobility!
Ion      Teff      CCS      E/n1      E/n2      E/n3      E/n4      <Ko1>      <Ko2>      <Ko3>      <Ko4>
      (K)      (A2)      (Td)      (Td)      (Td)      (Td)      (cm2/Vs)  (cm2/Vs)  (cm2/Vs)  (cm2/Vs)
-----
TDDA_390_25.txt 295.00    354.1648  0.0000    0.0000    0.0000    0.0000    0.5866    0.5866    0.5866    0.5866
TDDA_390_25.txt 335.00    343.7433  123.8779  122.4690  122.4173  122.4083  0.5672    0.5742    0.5744    0.5743
TDDA_390_25.txt 375.00    335.2650  180.7824  177.0524  176.8190  176.7657  0.5496    0.5623    0.5631    0.5628
TDDA_390_25.txt 390.00    332.6328  199.3272  194.6107  194.2786  194.1977  0.5432    0.5577    0.5588    0.5584
TDDA_390_25.txt 415.00    328.2378  228.0397  221.5611  221.0291  220.8879  0.5336    0.5510    0.5525    0.5521
TDDA_390_25.txt 455.00    321.8966  270.3892  260.8600  259.9241  259.6499  0.5197    0.5411    0.5435    0.5430

Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)
Ion      Ed      Ec      alpha      E/n
      (Td)  (Td)  (Td)      (Td)
-----
TDDA_390_25.txt 0.0000  0.0000  0.0000    0.0000
TDDA_390_25.txt 122.4083  0.2728  -0.0210   122.4083
TDDA_390_25.txt 176.7657  0.7866  -0.0406   176.7657
TDDA_390_25.txt 194.1977  1.0360  -0.0480   194.1977
TDDA_390_25.txt 220.8879  1.4797  -0.0588   220.8879
TDDA_390_25.txt 259.6499  2.2471  -0.0744   259.6499
```

(a)



(b)

Figure 10.18 (a) Results of the High Field and Dispersion Plot for TDDA390K from the save text file & (b) Dispersion Plot

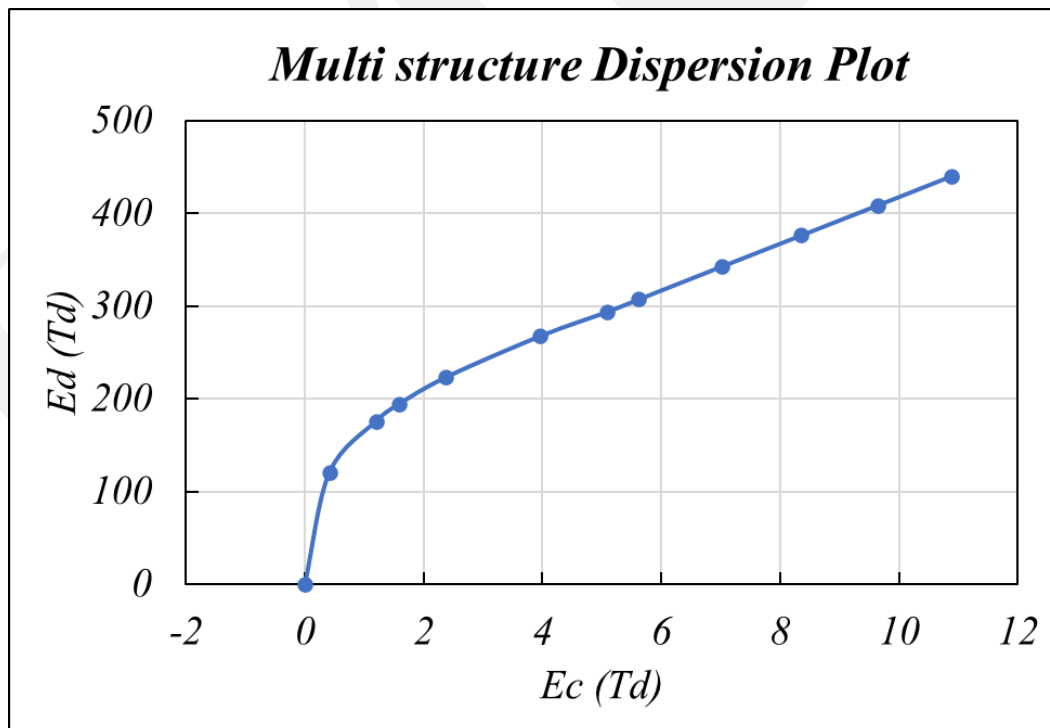
- k. At the end of all three structures, one can find the ‘MULTI STRUCTURE Dispersion plot’. This dispersion plot combines all three structures.

```

MULTI STRUCTURE Dispersion plot
alpha is obtained by dividing Mobility by zero field Mobility (not reduced)
Teff      Ed      Ec      alpha      Kho
          (Td)    (Td)    (Td)      (Td)
-----
295      0.0000    0.0000    0.0000    0.6007
335     120.7366    0.4134   -0.0306    0.5823
375     176.0853    1.1975   -0.0593    0.5650
390     194.1977    1.5758   -0.0703    0.5584
415     223.4554    2.3732   -0.0911    0.5460
455     267.5088    3.9492   -0.1222    0.5272
480     293.9303    5.0867   -0.1406    0.5162
495     307.5485    5.6216   -0.1455    0.5133
535     342.9243    7.0157   -0.1594    0.5049
575     376.6164    8.3559   -0.1721    0.4973
615     408.8633    9.6351   -0.1835    0.4904
655     440.3625   10.8782  -0.1948    0.4837

```

(a)



(b)

Figure 10.19 (a) Results of the High Field and Dispersion Plot data for multi structures from the save text file & (b)Dispersion Plot

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 TMLJ (no qpol) and a linear range of effective temperatures at high-fields using N₂. **Note the use of accommodation=0.48 to match TMLJ.**

IMoS v1.13 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 107.3718 A² and the Mobility is 2.203 cm²/Vs.
Time taken is 0.15279 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 126.0748 A² and the Mobility is 1.876 cm²/Vs.
Time taken is a mere 0.58103 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 145.3655 A² and the Mobility is 1.6272 cm²/Vs.
Time taken is a mere 5.1968 seconds
The drag tensor is given by:
7.721874e-16 8.323686e-18 -2.792726e-18
-2.979231e-18 7.858860e-16 7.372675e-19
6.419341e-18 -1.046522e-18 1.395772e-15
in units of kg/s (and includes reduced mass correction)

The TM Method used is TDHSS(4-inf with reemission choice)
Accommodation coefficient: 4.800000e-01
Diffuse Scattering?: 1
Reemission_vel(mean): 520.27 m/s 92% Maxwell Distributed
Timestep: 100
Reemvel(not used if LJ=1): 92% Maxwell Distributed
The average collision cross section for Tryphenylene is 144.7777 A² and the Mobility is 1.6338 cm²/Vs.
Time taken is a mere 4.5509 seconds

The TM Method used is High Field
Performing TMLJ calculations for: AnalIainb.xlsx and molecule Tryphenylene.

Results

Summary of ion calculations:

Ko represents reduced mobility!

Ion	Teff (K)	CCS (A2)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm2/Vs)	<Ko2> (cm2/Vs)	<Ko3> (cm2/Vs)	<Ko4> (cm2/Vs)
Tryphenylene	420.00	127.4914	84.3387	83.3786	83.3646	83.3582	1.4186	1.4374	1.4380	1.4376
Tryphenylene	450.00	124.2561	95.4537	94.0573	94.0227	94.0100	1.4062	1.4303	1.4313	1.4308
Tryphenylene	480.00	121.4560	105.8006	103.9169	103.8507	103.8281	1.3930	1.4223	1.4238	1.4231

LJTM calculation parameters:

Number of loops (itn) = 1
Number of velocity points (inp) = 5
Number of random rotations and impact parameters (imp) = 180000
Total Trajectories = 900000

Max time step = 1.00e-13 second
Min time step = 1.00e-16 second
Time step corrector = 100.00

IMoS V1.13

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
 Maximum value of [1-cosX] at b_max (cmin) = 0.000100
 Seed = 13
 Time taken is a mere 15.5136 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
 The average collision cross section for NEthylaniline is 80.0608 A² and the Mobility is 3.0917 cm²/Vs.
 Time taken is 0.10158 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 95.6617 A² and the Mobility is 2.5872 cm²/Vs.
 Time taken is a mere 0.86285 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 120.4957 A² and the Mobility is 2.0542 cm²/Vs.
 Time taken is a mere 4.1703 seconds
 The drag tensor is given by:
 6.509812e-16 1.454947e-17 -1.399524e-17
 2.138339e-18 8.368574e-16 -3.861352e-17
 2.789131e-18 -4.969763e-17 8.519931e-16
 in units of kg/s (and includes reduced mass correction)

The TM Method used is TDHSS(4-inf with reemission choice)
 Accommodation coefficient: 4.800000e-01
 Diffuse Scattering?: 1
 Reemission_vel(mean): 520.27 m/s 92% Maxwell Distributed
 Timestep: 100
 Reemvel(not used if LJ=1): 92% Maxwell Distributed
 The average collision cross section for NEthylaniline is 124.268 A² and the Mobility is 1.9919 cm²/Vs.
 Time taken is a mere 3.4612 seconds

The TM Method used is High Field
 Performing TMLJ calculations for: AnalIainb.xlsx and molecule NEthylaniline.

Results

Summary of ion calculations:
 Ko represents reduced mobility!

Ion	Teff (K)	CCS (A ²)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<Ko1> (cm ² /Vs)	<Ko2> (cm ² /Vs)	<Ko3> (cm ² /Vs)	<Ko4> (cm ² /Vs)
NEthylaniline 420.00	420.00	102.6095	64.8665	64.5733	64.5861	64.5851	1.8445	1.8557	1.8555	1.8553
NEthylaniline 450.00	450.00	99.4364	72.9974	72.5285	72.5416	72.5391	1.8388	1.8547	1.8547	1.8543
NEthylaniline 480.00	480.00	96.6701	80.4726	79.7933	79.8017	79.7962	1.8314	1.8523	1.8524	1.8519

LJTM calculation parameters:

Number of loops (itn) = 1
 Number of velocity points (inp) = 5
 Number of random rotations and impact parameters (imp) = 180000
 Total Trajectories = 900000

Max time step = 1.00e-13 second
 Min time step = 1.00e-16 second
 Time step corrector = 100.00

Ratio of potential energy to kinetic energy at the starting of Traj (sw1) = 0.001000
 Maximum value of [1-cosX] at b_max (cmin) = 0.000100
 Seed = 13
 Time taken is a mere 11.3743 seconds

PARAMETERS USED:

Gas: N2

IMoS V1.13

Reduction Coef: 1.000
Molecular mass of Gas: 28.00 Da
Alpha polarization: 1.70 A3
Radius of gas: 1.50 A
Temperature: 304 K
Pressure: 101325 Pa

Lennard Jones parameters for basic
Atom eps(J*10²¹) sigma(A)

Atom	eps(J*10 ²¹)	sigma(A)
H	0.4806000000	2.3000000000
C	0.7449300000	3.5000000000
O	0.6888600000	3.5000000000
N	0.9291600000	4.2000000000
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 OF REGULAR CALCULATIONS

For High Field calculations, check full results or summary results below

COLLISION CROSS SECTION (A ²)	MOBILITY (cm ² /Vs)
107.371831	2.203003
126.074797	1.875984
145.365517	1.627212
144.777653	1.633819
80.060750	3.091711
95.661652	2.587216
120.495651	2.054221
124.267955	1.991863

SUMMARY OF HIGH FIELD CALCULATIONS

Ion	Teff (K)	CCS (A ²)	E/n1 (Td)	E/n2 (Td)	E/n3 (Td)	E/n4 (Td)	<K01> (cm ² /Vs)	<K02> (cm ² /Vs)	<K03> (cm ² /Vs)	<K04> (cm ² /Vs)
Tryphenylene 420.00	127.4914	84.3387	83.3786	83.3646	83.3582	83.3522	1.4186	1.4374	1.4380	1.4376
Tryphenylene 450.00	124.2561	95.4537	94.0573	94.0227	94.0100	94.0100	1.4062	1.4303	1.4313	1.4308
Tryphenylene 480.00	121.4560	105.8006	103.9169	103.8507	103.8281	103.8281	1.3930	1.4223	1.4238	1.4231
NEthylaniline 420.00	102.6095	64.8665	64.5733	64.5861	64.5851	64.5851	1.8445	1.8557	1.8555	1.8553
NEthylaniline 450.00	99.4364	72.9974	72.5285	72.5416	72.5391	72.5391	1.8388	1.8547	1.8547	1.8543
NEthylaniline 480.00	96.6701	80.4726	79.7933	79.8017	79.7962	79.7962	1.8314	1.8523	1.8524	1.8519

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

IMoS V1.13

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
-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

```
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excelfile      Savefile      Gas
/filefolder/AnalIainb.xlsx /savefolder/Ex11.txt  N2

interface 0 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 100
Boxdomain 16
Diffuse? 1
reemvel 6
Other 0
Simplify 0
PA 1
PATSA 0
EHSS/DHSS 1
TM 1
TDHSS 1
qp01 0
LennardJones 1
DTM 0
HEN 4
Tefffrom 420
Teffto 480
Teffstep 30
seed 13
Numthreads 11
Repeatseed 1
DragRG 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 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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