DASSAULT SYSTEMES

BIOVIA

USER MANUAL

BIOVIA TmoleX 2025

A Graphical User Interface to the TURBOMOLE Quantum Chemistry Program Package

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Acknowledgments and References

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1. Installation

1.1. Windows

Prerequisites: Windows 10 or Windows 11 in 64bit mode, the 32bit version is deprecated
TmoleX2024 uses Java version 11 and recent OpenGL routines.
If you are not able to visualize molecules, please consider to update your graphics card driver.

The Windows version of TmoleX is distributed as a single executable file, called TmoleX_windows-x64_2025_0.exe. To install TmoleX, simply double-click this file and follow the installation instructions.

After installation, TmoleX is available in your Windows Start Menu or as an icon on your desktop.

Please Note :

TURBOMOLE 7.9 for Windows is included in the TmoleX package. You will not have to install it additionally. Some features of TURBOMOLE that are based on classical Unix scripts are not yet ported to Windows:

- Numerical second derivatives (script NumForce)
- automatic BSSE calculations (program jobbsse)

The TURBOMOLE version for Windows(64bit) includes serial and parallel 64-bit executables.

Known Limitations:

- Installation path and user names must not contain the @ character, i.e. installation paths like C:\Program Files\TMoleX@local\ will cause TmoleX not to function correctly. TmoleX by default stores user configuration files in the user's home folder, by default C:\Users\<user-name>, and if the user name itself contains an @, TmoleX will not work properly either.

1.2. Linux

Prerequisites: Linux distribution based on a) Kernel 4.x and newer and b) GLIBC 2.15 or newer

The Linux version of TmoleX is distributed as a single file called TmoleX_unix_2025_0.bin Please make sure that the file has execute permissions (chmod a+rx TmoleX_unix_2025_0.bin) before starting it, then follow the instructions on screen.

The full version of TURBOMOLE 7.9 is included in the TmoleX package.

Features that are not supported by TmoleX can be used by the command line version. After the installation of TmoleX, TURBOMOLE can be used from the command line as usual. Just set `$TURBODIR` to the TURBOMOLE directory of the TmoleX installation, and extend the PATH to `$TURBODIR/scripts` and `$TURBODIR/bin/`sysname`` (the binary directory).
Or, alternatively, a shell can be started by TmoleX with the correct settings by using the right-mouse menu in the project list (see below).

1.3. Mac OS

Prerequisites: Mac OS X 10.8 to 11.5 on Intel based systems

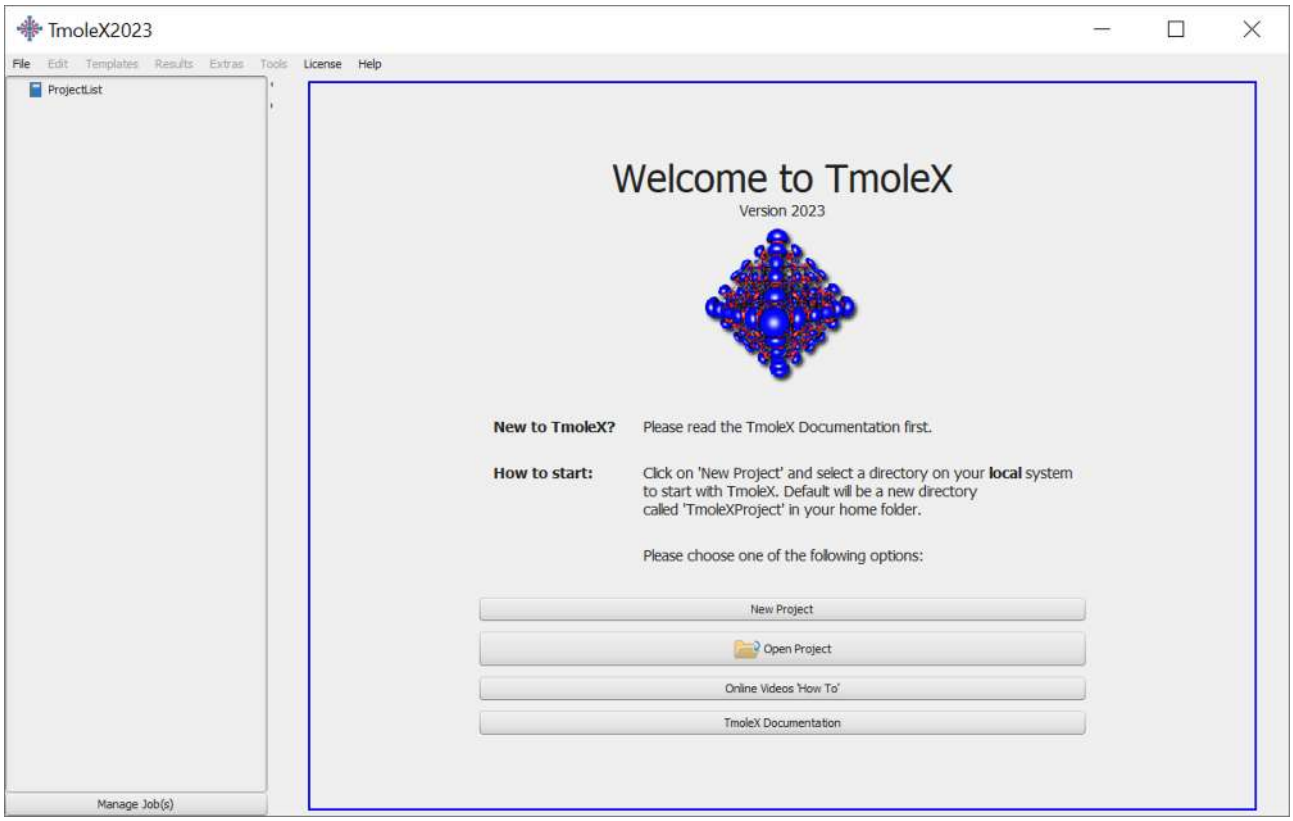
The Mac OS version of TmoleX is distributed as a single file called TmoleX_macos_2025_0.dmg. To install TmoleX, simply double-click this file and follow the installation instructions.

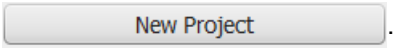
After installation, TmoleX is available in the chosen folder (by default in /Application/BIOVIA/TmoleX2025). Features that are not supported by TmoleX can be used by the command line version. After the installation of TmoleX, TURBOMOLE can be used from the command line as usual. Just set `$TURBODIR` to the TURBOMOLE directory of the TmoleX installation, and extend the PATH to `$TURBODIR/scripts` and `$TURBODIR/bin/`sysname`` (the binary directory).

2. A quick tour

2.1. Starting the program

Starting TmoleX for the first time, you will get into the Welcome panel:



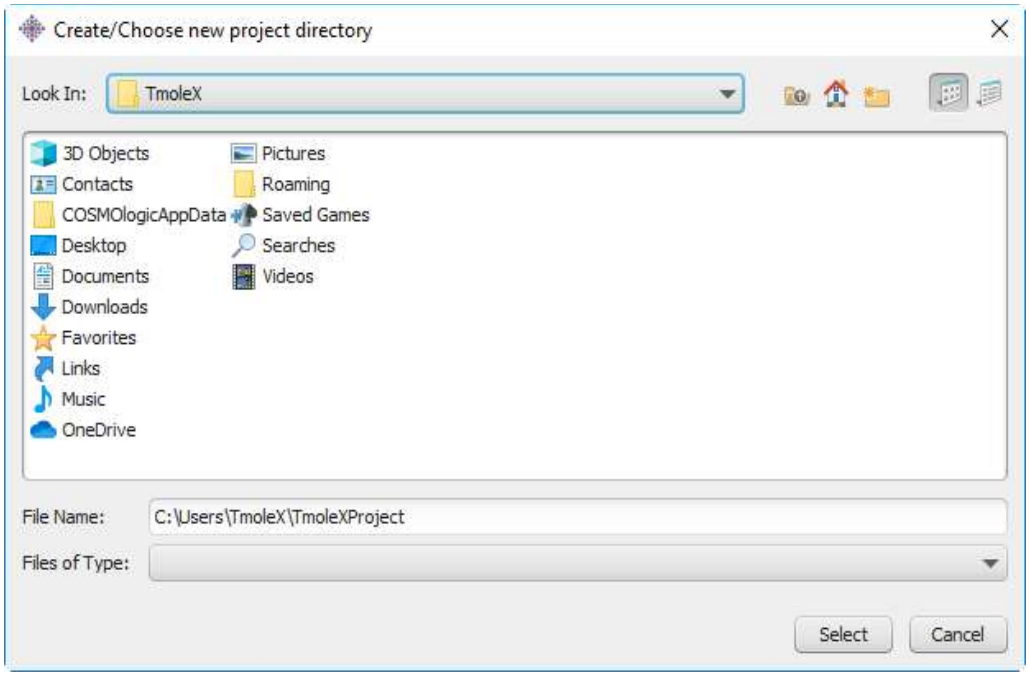
To start with TmoleX, create a new project by klicking on 

.

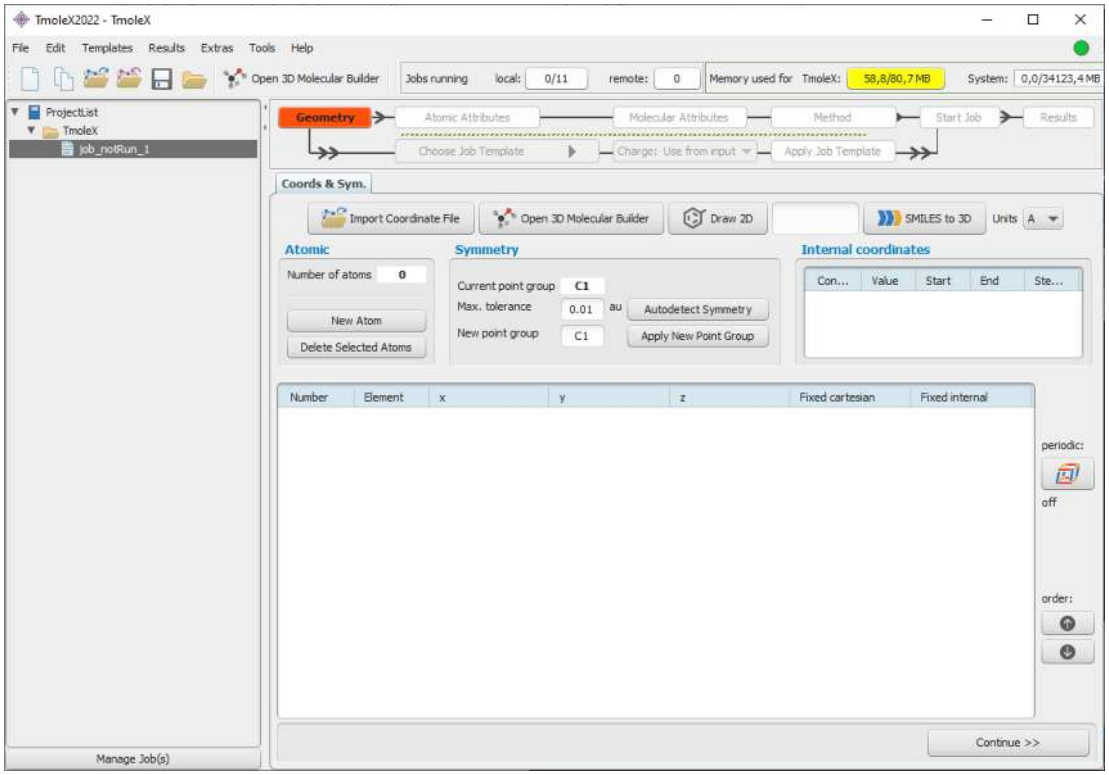
Alternatively open an existing project (from former TmoleX versions) or watch the introductive online videos first.

2. A quick tour

All projects will require a new directory on your hard disk – where this directory shall be located and which name it shall have is asked in the window that pops up:



The default directory is called TmoleXProject in your home folder. Just click on Select to accept the default or generate a new directory and choose this one. You are now ready to perform your first Turbomole job:



2.2. An illustrative example: Part 1

This section will guide you through the process of performing a DFT energy calculation and a ground state geometry optimization of a molecule, for which input coordinates exist, e.g. benzene.

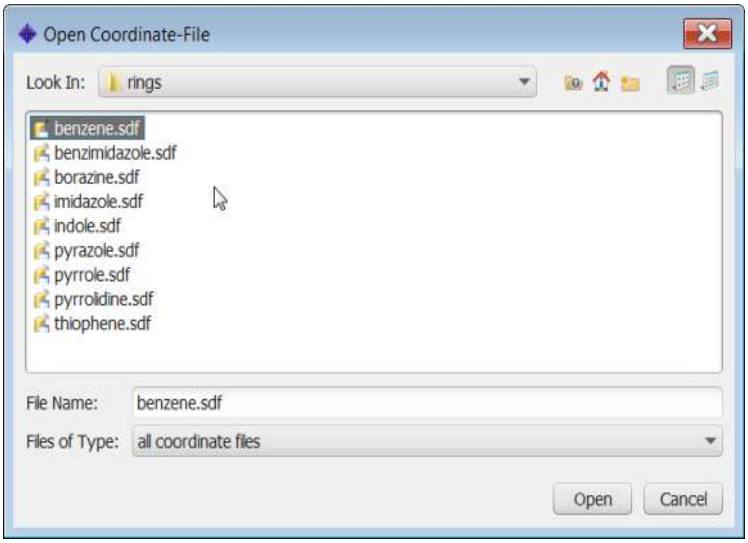
Option 1: Read in a coordinate containing file. The buttons



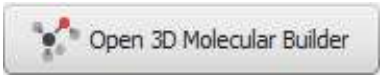


◄— or —►

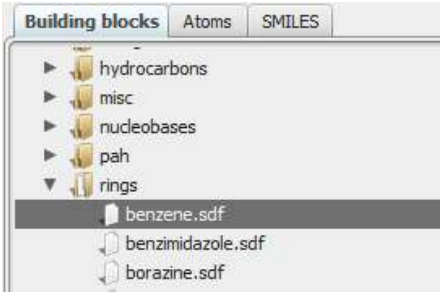
in the tool bar and the main window or the menu 'Import Coordinate File' in the pull-down menu 'File' will open a file browser. Select the coordinate file and load the molecular structure of benzene into TmoleX (first change to your home directory and from there to BIOVIA_COSMO-RS_TURBOMOLE/TmoleX2023_1/building_blocks/rings/).



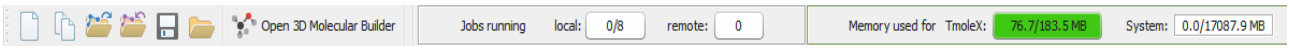
Option 2: click on 'Open 3D Molecular Builder'



and double-click on the benzene entry on the right side which is also located in the rings section.



2.3. The tool bar



The tools in the tool bar act only on the job that you are currently working on, i.e. which is opened in the project list.



Create new job within the current project.



Create new batch job within the current project.



Read or import coordinates (besides TURBOMOLE also many different formats).



Save/Export current coordinates in various formats.



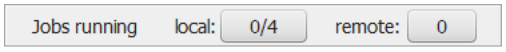
Save current job to disk.



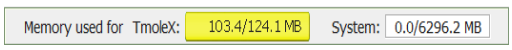
Open the directory of the current job in the default file browser of your OS.



Open molecular viewer. Can also be used to build new molecules.



TmoleX can run jobs on your local machine as well as on remote systems. It also includes a simple queuing-system. By clicking on either the local or the remote button a list of running jobs will open.

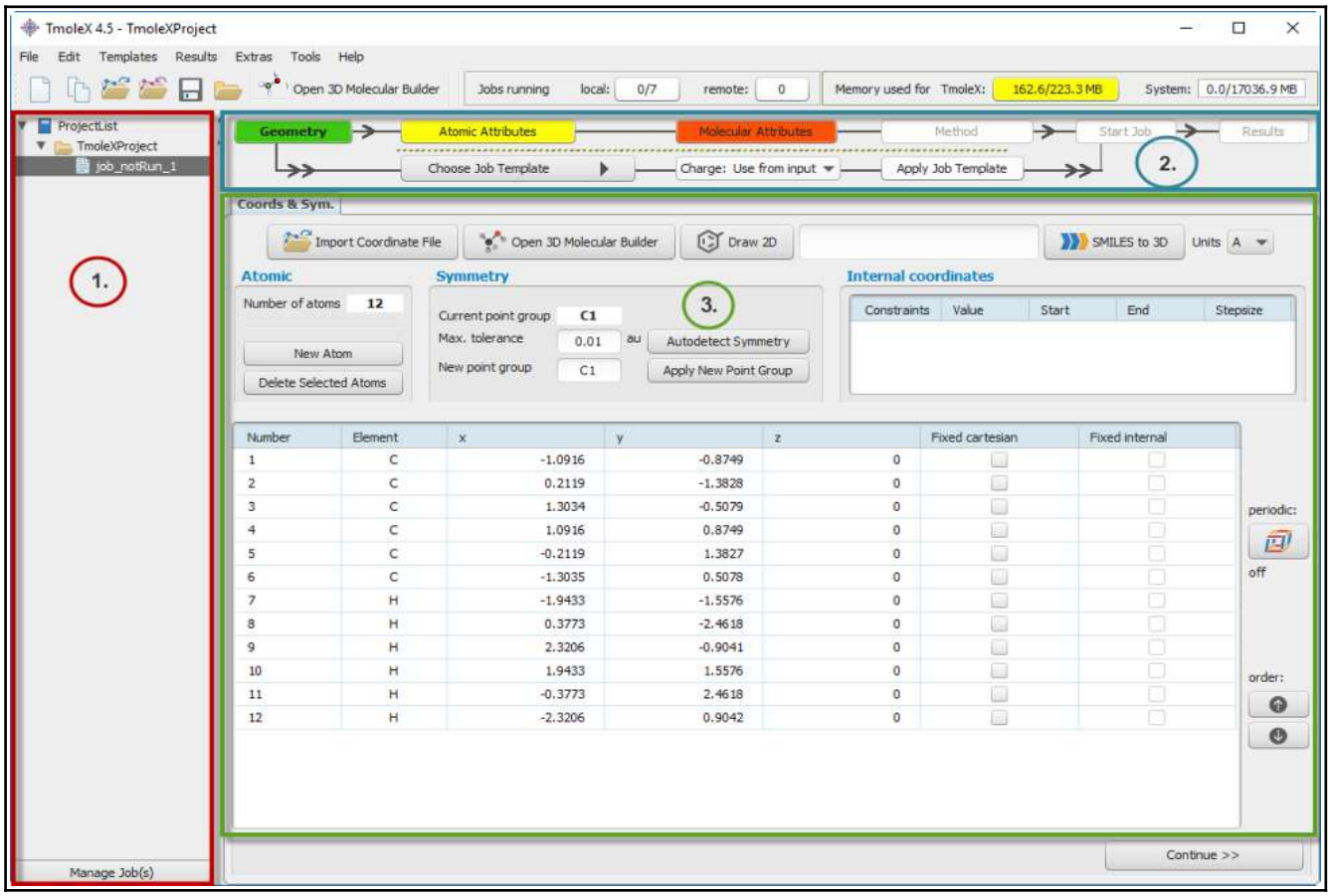


The memory usage of TmoleX itself and the jobs that are running on your local system is displayed here – click on the TmoleX button (the yellow one in this example) to free unused memory (starts Java garbage collector)

2.4. The sections

TmoleX is structured as an interactive TURBOMOLE input program, similar to the 'define' program, which generates the input on the command line.

1. On the left you will find a list of open projects and jobs of each project,
2. on the top the general task menu (Geometry, Atomic Attributes, Molecular Attributes, etc.)
3. in the main frame the data assigned to the chosen task.

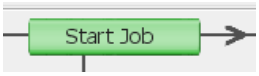


2. A quick tour

The input is divided into four different sections:



The kind of job or property that shall be calculated can be set in the Start Job panel:



Results after a successful run can be viewed and further investigated in the Results panel:



You should follow the menu structure in the main frame from left to right. The traffic light colors are indicating which steps have been accomplished and for which steps input is needed.

Color code

Red: No valid data is available. User action required.

Yellow: Default settings available – unchecked by user so far.

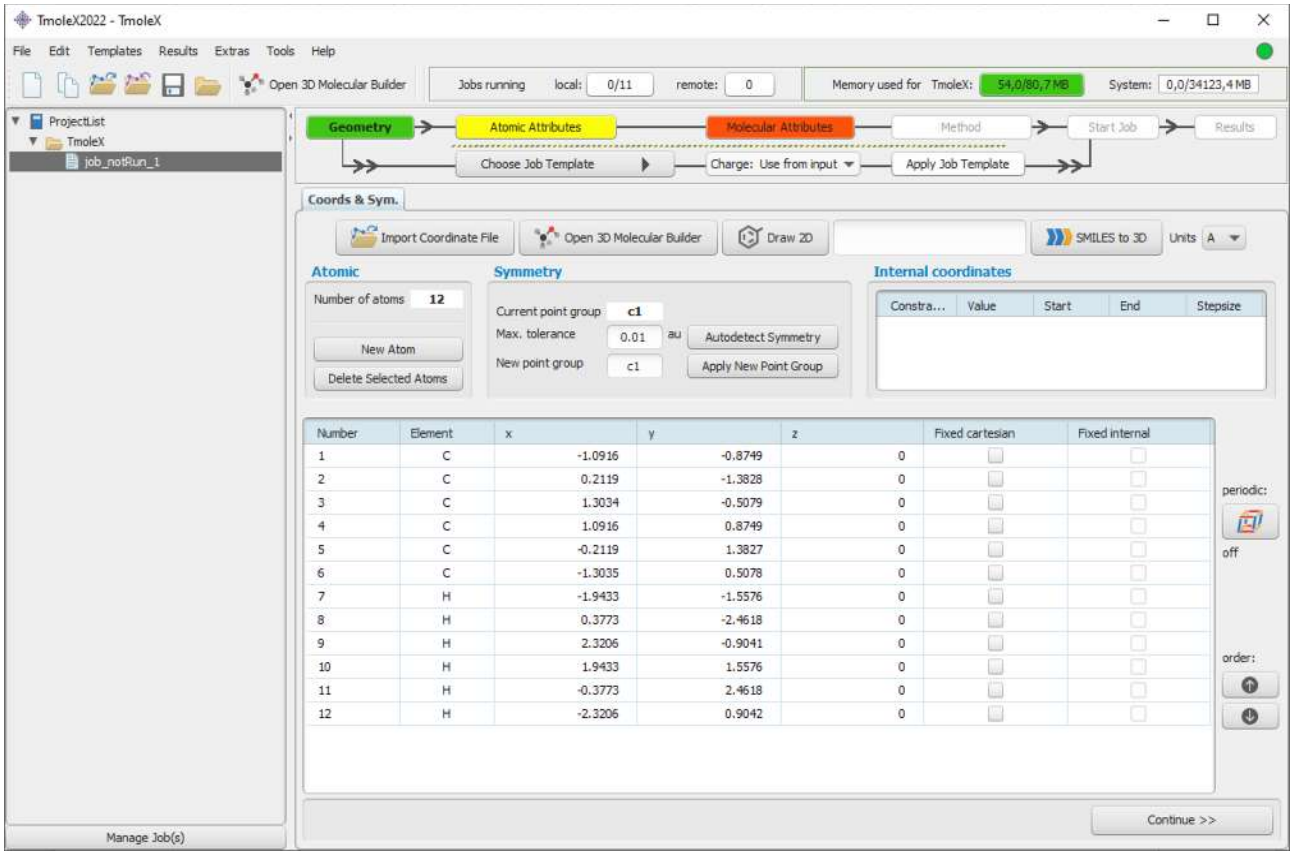
Green: The data is correct or user did already visit this section.

Grey: Section is currently not available (like Results for a job which did not run yet)

2.5. An illustrative example: Part 2

2.5.1 Geometry panel

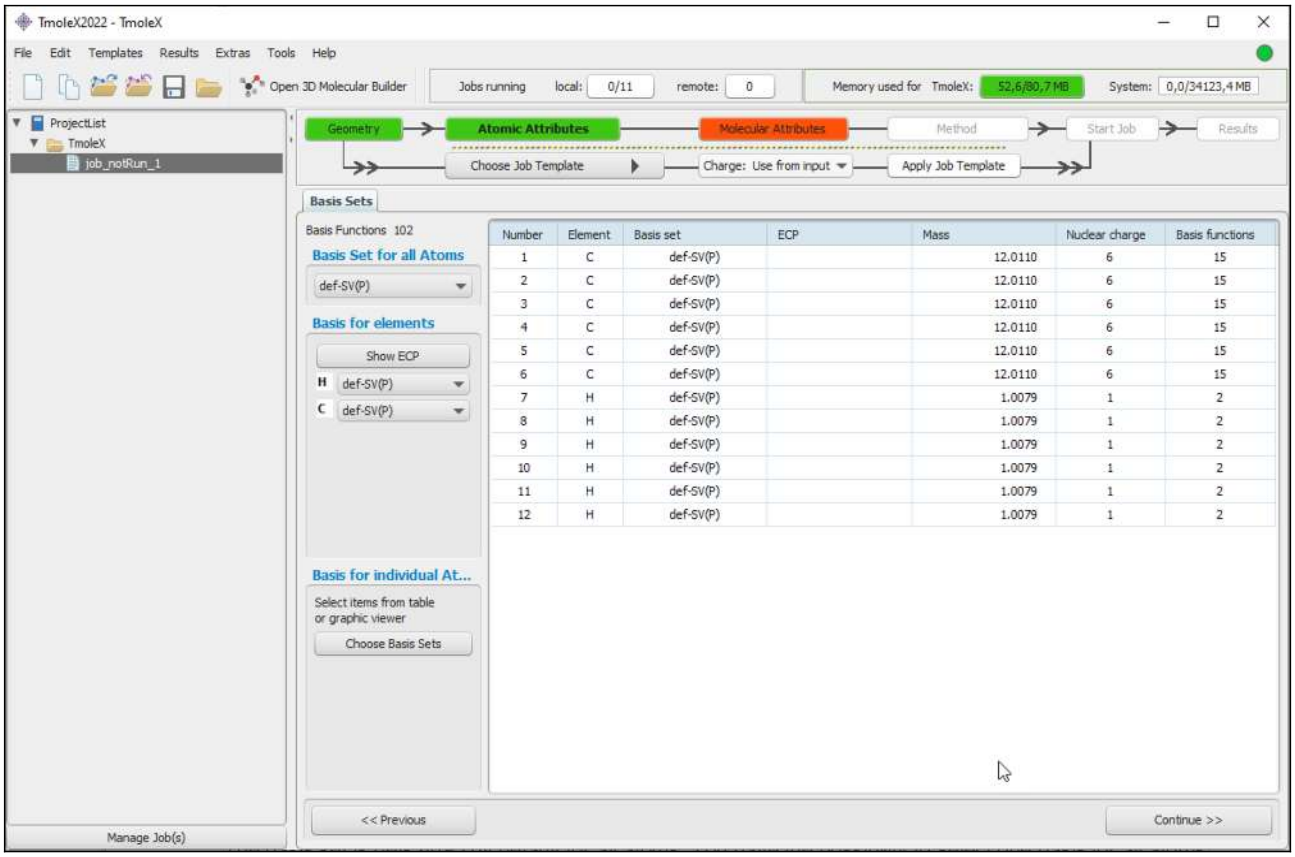
After reading in the coordinates, you are in the Geometry section. Here, you can choose the symmetry, create internal coordinates, add atoms, or modify the structure.



2.5.2 Basis set panel

The basis set is being defined in the 

panel:



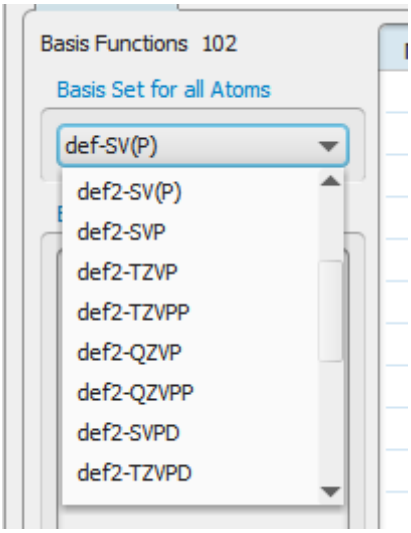
The basis set is def-SV(P) by default for all atoms. You have the possibility to select one basis for all atoms, basis sets for given elements, or basis sets for individual selected atoms.

Hint:

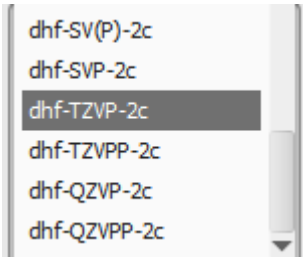
If you are not familiar with the modern Karlsruhe/Ahlrichs type basis sets but with old Pople type basis sets only:

6-31G*	is of similar quality than	def-SV(P),
6-31G**	--	def-SVP, and
6-311G**	--	def-TZVP.

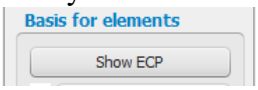
The drop-down selection 'Basis Set for all Atoms' contains just the Karlsruhe family of basis sets since those are available throughout the periodic table.

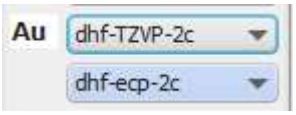


For heavy elements a basis set which is optimized for two-component ECPs and two-component calculations:



check the automatically loaded ECPs by clicking on





Selecting one of those will enable the relativistic 'Two component treatment' options in the Method section later on.

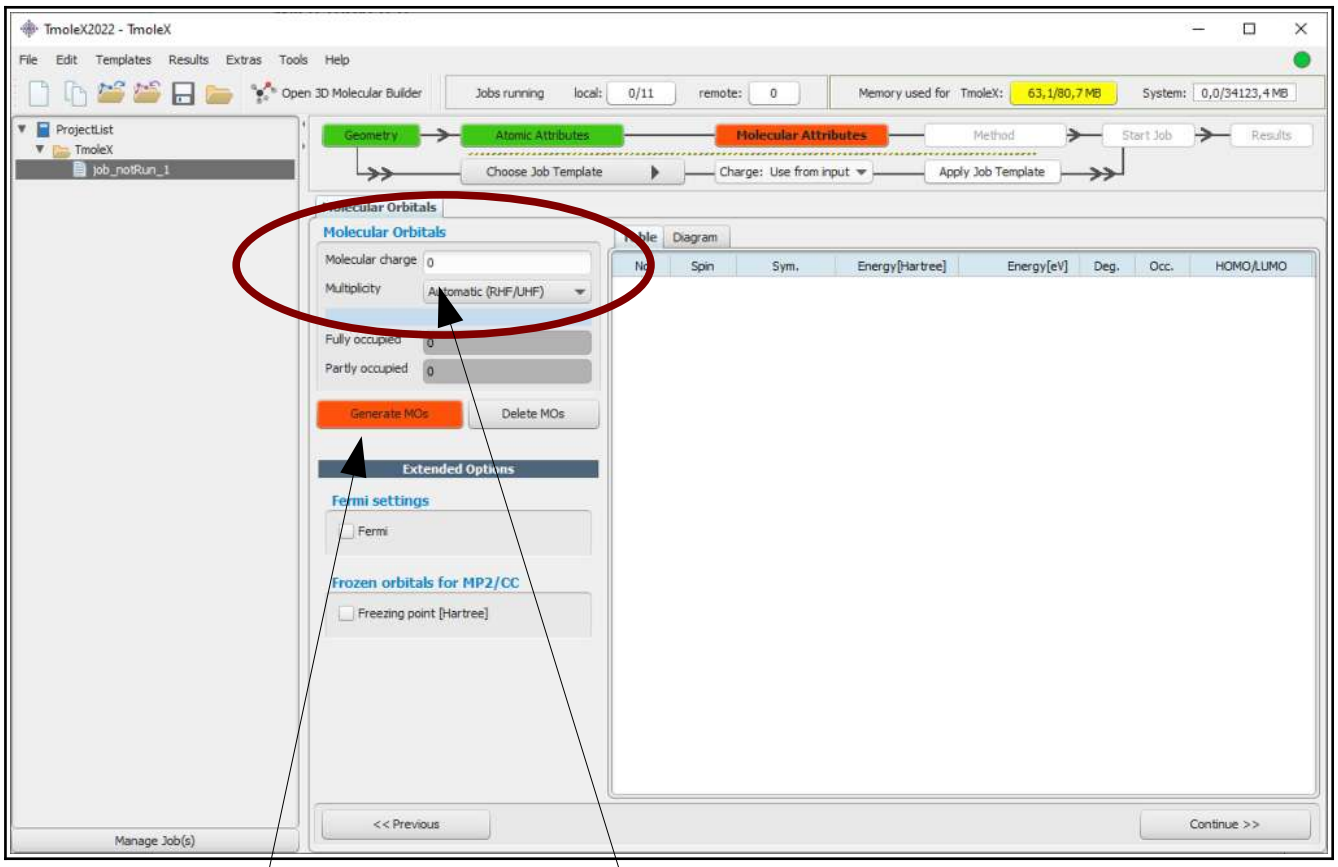
NOTES:

Standard basis sets which require an ECP will read in and use those ECPs automatically, e.g. all def- and def2- basis sets for elements beyond Kr. If you use a basis set from the extended list of the ‘Basis for elements’ section, make sure that ECPs are correctly assigned in case they are needed.

If you miss some basis sets which are present in the basis set library or if you have added own basis sets to the basis set library, add them to the file *basis_set_names.txt* which can be found in the TmoleX directory (<Install-path>/BIOVIA/TmoleX2025/TmoleX/).

2.5.3 Molecular start orbitals panel

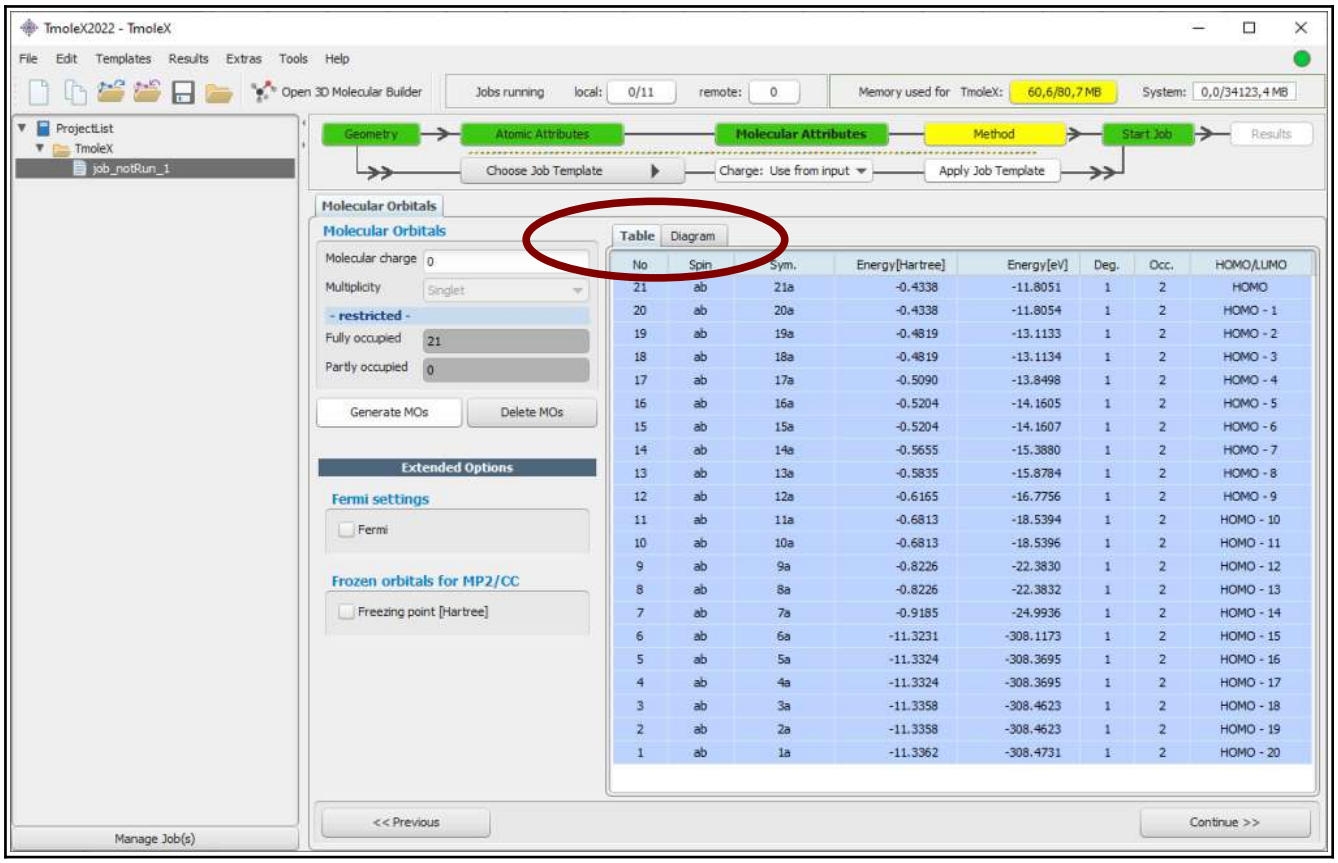
For any TURBOMOLE calculation an initial set of molecular orbitals is required. This is done with an extended Hückel calculation in the 'Molecular Attributes' panel. If you do not (yet) have valid start orbitals, the button will remain red.



Click on 'Generate MOs'

Do not forget to set the molecular total charge before generating orbitals for IONS!!

The generation takes only a (very) short time to compute and the initial molecular orbital are displayed.



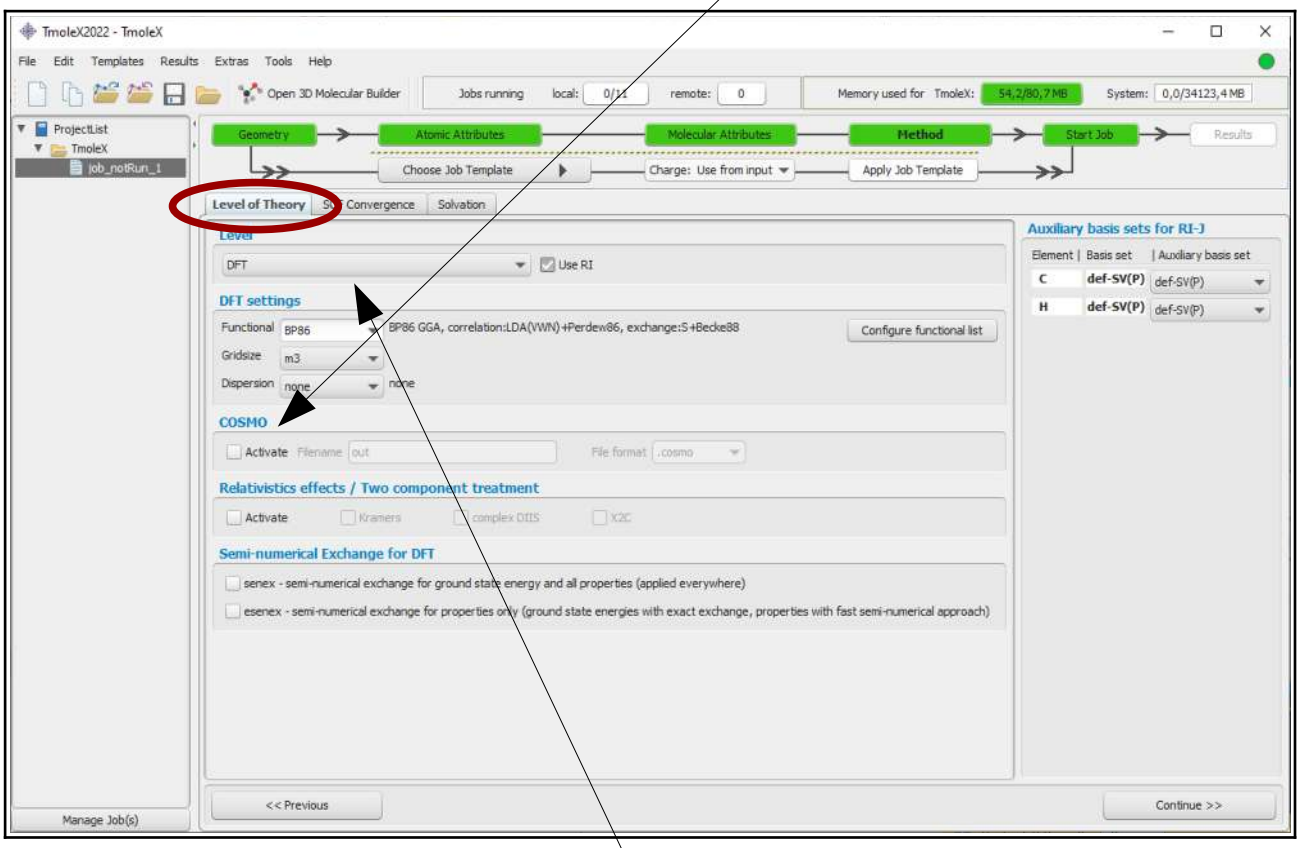
The default for the multiplicity is *automatic* – TmoleX will generate molecular orbitals by doing an Extended Hückel Guess and fills in the electrons according to the orbital energies. It will recognize closed and open shell cases and switches to restricted (RHF) or unrestricted (UHF) settings.

Note that you have to generate new orbitals if you change the multiplicity. In this case, i.e. multiplicity *not* set to automatic, will always result in unrestricted calculations!

In this panel you can also freeze core orbitals for correlated calculations or switch on Fermi smearing.
Switch from Table to Diagram to see the orbital occupation graphics. Use the left mouse button to set a freezing point for frozen core approximation settings, and the right mouse button to zoom in (or click once to zoom out).

2.5.4 Level of theory: Select method

In the Method panel you can choose the level of theory, activate COSMO, select auxiliary basis sets, and advanced SCF settings can be changed.

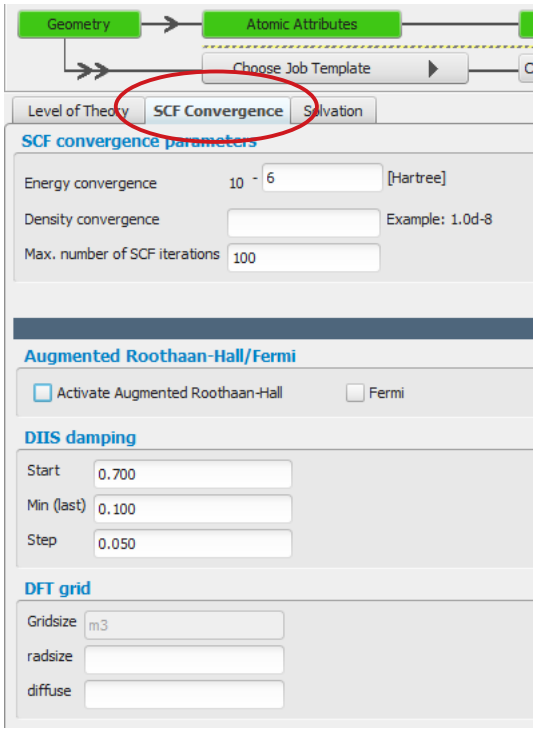


The level of theory for your calculation can be set here. Currently ten different methods are available within TmoleX:

- Semi-empirical xtb (GFN1 or GFN2) or MOPAC (AM1, PM3, MNDO)
- Hartree-Fock
- DFT (with or without RI-J), RI-DFT is the default if you start a new session of TmoleX, DFT+Dispersion can be chosen as option within this level
- DFT periodic boundary conditions 1D, 2D, 3D periodic RI-DFT calculations
- RI-RPA post-DFT RPA method
- MP2 RI-MP2 or low-scaling PNO-MP2
- CC2
- ADC(2) (MP2)
- CCSD RI-CCSD or low-scaling PNO-CCSD
- CCSD(T) RI-CCSD(T) or low-scaling PNO-CCSD(T0) or PNO-CCSD(T)

Spin-scaled (SCS, SOS) MP2 or CC2 calculation can also be used as sub-options to the MP2 and CC2 level.

Settings for SCF convergence and special COSMO selections (recommended only for expert users) can also be found in the method section.



Energy and/or density convergence criteria can be entered in this panel. A density convergence criteria is useful for properties and methods that need a very accurate density like post-Hatree-Fock methods or TDDFT.

Note that the format of the parameters is different: The exponent has to be entered for the energy convergence while the density convergence threshold is a total number like 1d-8 (use `d` instead of `e` like `1e-8`, because TURBOMOLE reads them in as double precision number). This difference is due to the fact that the two corresponding TURBOMOLE keywords, `$scfconv` and `$denconv` in the control file are have to be given exactly like this – so TmoleX here tries to help to understand the default TURBOMOLE input.

The augmented Roothaan-Hall method or Fermi smearing to resolve convergence issues can be applied here.

Changing the default DIIS damping settings might be needed for complicated electronic structures like transition metal compounds. If the energy does not converge within many SCF iterations, the DIIS damping factors should be increased. See the TURBOMOLE manual for details about DIIS.

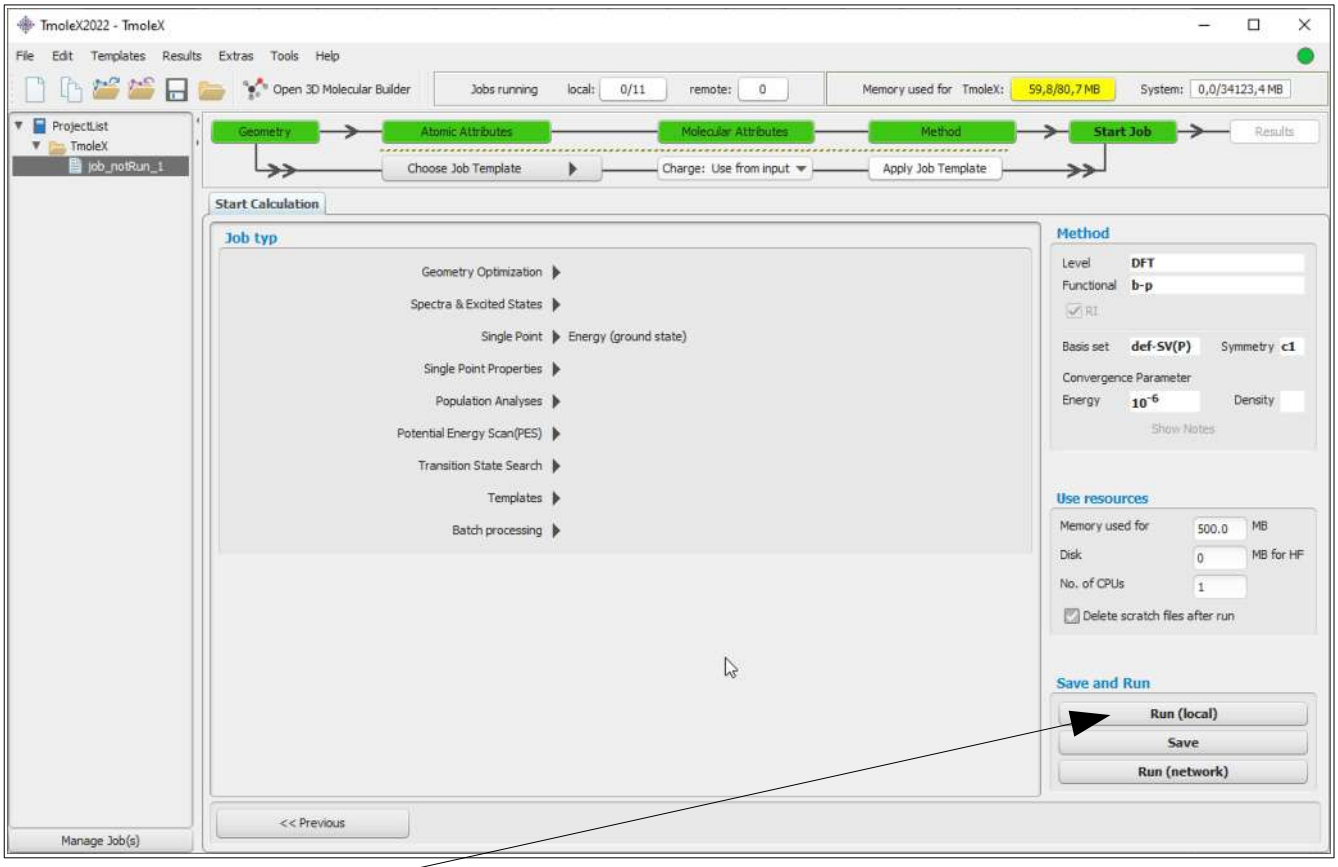
DFT grid settings are needed in very special cases like the usage of the SCAN functional.
Please check the TURBOMOLE documentation to get more information about different DFT grid sizes and when to use those.

The semi-numerical exchange for DFT (senex) can be activated by setting either or both of the options given in the panel (senex and esenex). If the first option is activated (senex), semi-numerical exchange will be used for all DFT functionals that include either exact or range-separated Hatree-Fock exchange (hybrid functionals and local hybrid functionals).
Senex for ground state energy calculations and geometry optimizations speeds up the calculation only for large systems, but it has a much more significant impact on the total computational time if higher derivatives like TDDFT (UV/Vis, CD spectra) or vibrational frequencies (and IR or Raman) are calculated.

The savings in time do, however, imply a numerical deviation from the analytical, exact, calculation of the exchange, but it has been shown that for properties this error is small in general if the default integration grids are used. Thus, TmoleX does not offer a possibility to set non-default grid sizes as it can be done from the command line version of TURBOMOLE.

2.5.5 Start Job: Select kind of job and start it

In the Start Job panel, a **single point energy** calculation can be started.



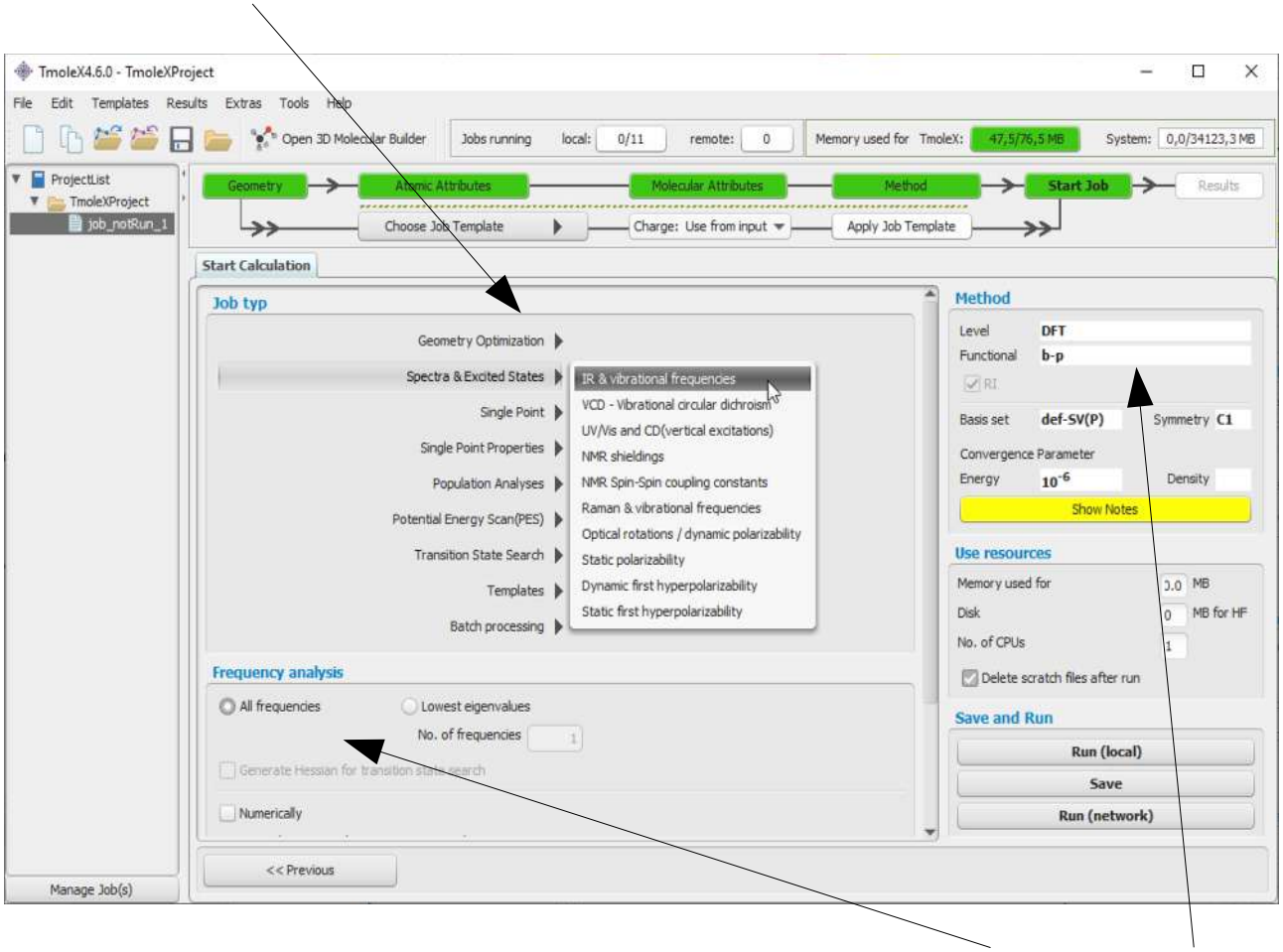
'Run (local)' will start the calculation in a subfolder of your project directory.

'Save' writes the complete input to disk for further use on the command line or later usage if needed. Saving the job to a directory will also add a script call *start-job* to the selected directory which can be used to start the job on the command line.

'Run (network)' starts the calculation on a remote Linux/Unix computer, see chapter 9.

2. A quick tour

Click through the Job type options to see what kind of jobs are supported by TmoleX.



Depending on the job type, different options for the chosen job are displayed in the Options section. The Method section briefly summarizes the settings done in the four menus before (method, symmetry, basis set, etc.).

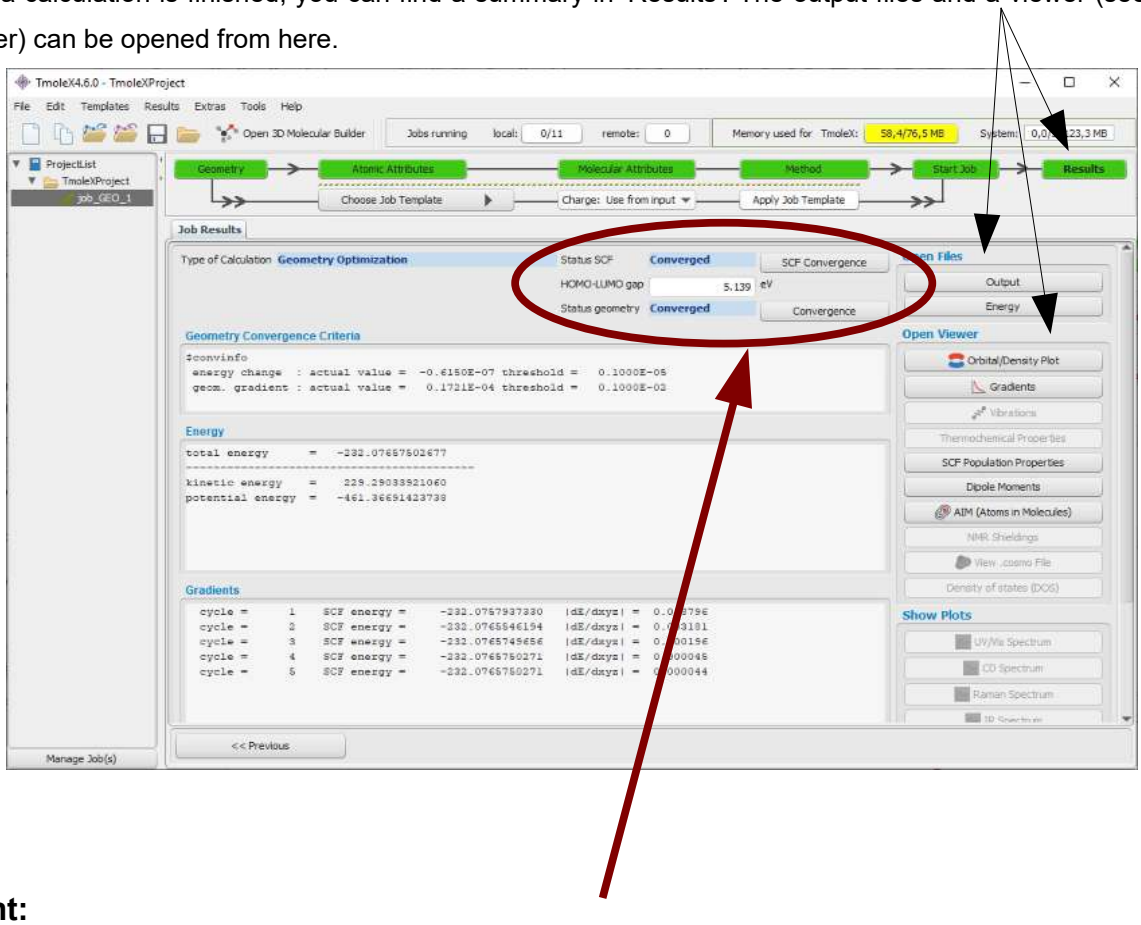
The Show Notes button shows up in yellow if TmoleX detects a combination of basis set, job type and method which might require different defaults. Please click on this button to see the hint!

Finally, the 'Use resources' part can be used to set (maximum) amount of memory (RAM) and disk space for the calculation. If and how important those settings are depends on the method and job type. For ground state single-point energies and geometry optimizations at Hartree-Fock or DFT level, neither more memory nor more disk space will speed up the calculation significantly. For vibrational frequencies (IR and Raman spectra), post-Hartree-Fock methods or excited state calculations, more memory can improve efficiency a lot.

Please note that the given memory value is *not* the total amount of RAM the program will use, just the parts that can be adjusted. Hence, do not enter more than roughly 80% of your total memory here to avoid huge performance problems!

2.5.6 Results

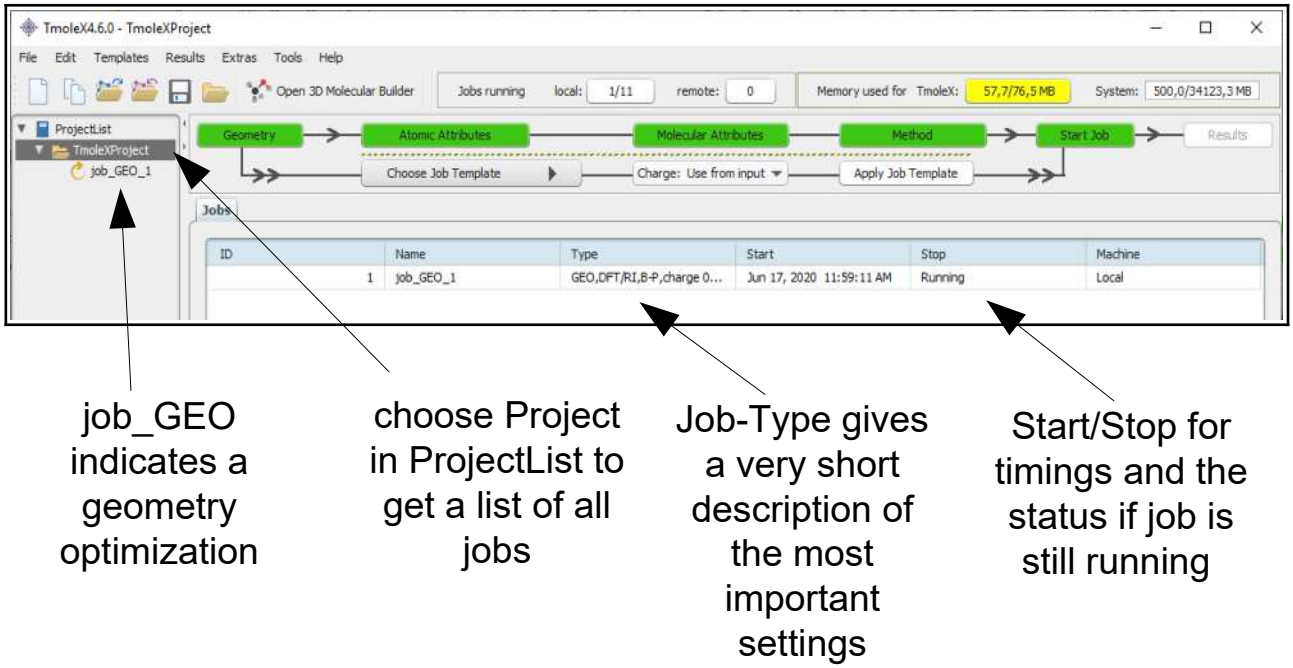
Whenever a calculation is finished, you can find a summary in 'Results'. The output files and a viewer (see. next chapter) can be opened from here.



Important:

- Check the Status of the molecular orbitals and the status of the geometry optimization!
- In case that the orbitals (MOs) are not converged, restart the job – perhaps more SCF iterations or higher DIIS damping is required (see Method section)
- If the geometry is not converged, restart the optimization allowing more geometry cycles.
- Also make sure that the HOMO-LUMO gap is positive. Otherwise you have a hole in the occupation (which might be what you want, but usually this should not be the case), and you did not get the proper ground state of the electronic structure.

2.6. Job Administration



job_GEO indicates a geometry optimization

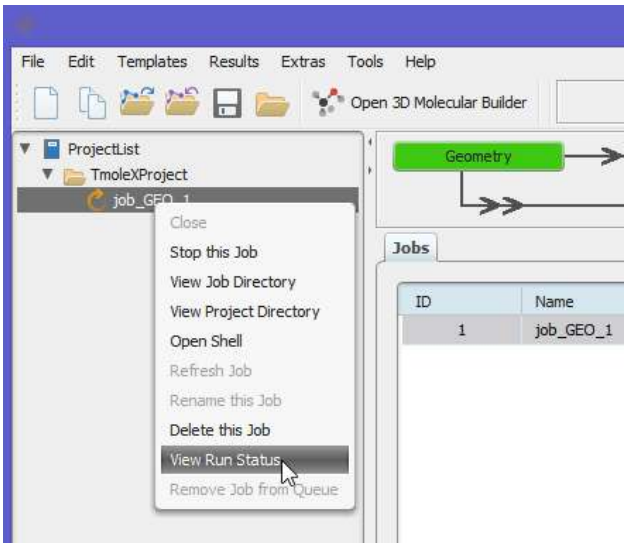
choose Project in ProjectList to get a list of all jobs

Job-Type gives a very short description of the most important settings

Start/Stop for timings and the status if job is still running

While the job is running and if you select the project itself in the project list on the left, the lower part of the TmoleX window will show the current status of the selected job (there is just one job on the example above).

Click on the name of the Project in the ProjectList and use the right mouse menu in the 'Jobs' section to close (remove just from the list, let all files on disk), stop (stop running jobs, let files on disk), delete (delete job from the list and delete the files from disk) jobs. 'View Job directory' will open the default file browser on your system with the directory where the selected job is running or was running. 'View run status' can be chosen for running jobs.



The progress and status of all calculation belonging to your project, which are currently running or ran before, can be accessed via the “Job-Administration” by clicking on the project name *itself* instead of a job within the project. After starting a first job, you can instantly set up and even launch a new one. For performance considerations you will however prefer running only one job at a time in most cases.

Note: TmoleX does not yet cover all possible kinds of calculations and input options that TURBOMOLE offers. If you need additional options but want to use TmoleX, you can manually edit the control file. Please refer to the TURBOMOLE manual for further information.

Internal simple queuing system

Set the number of cores of your machine in the Extras → Settings menu. Then, TmoleX will take care of the number of jobs you are starting:



The green section is related to the memory usage. First by TmoleX itself (click on the button to start Java's garbage collector to give free unused memory) and then by the jobs which are running (estimated from your memory settings when starting those jobs).

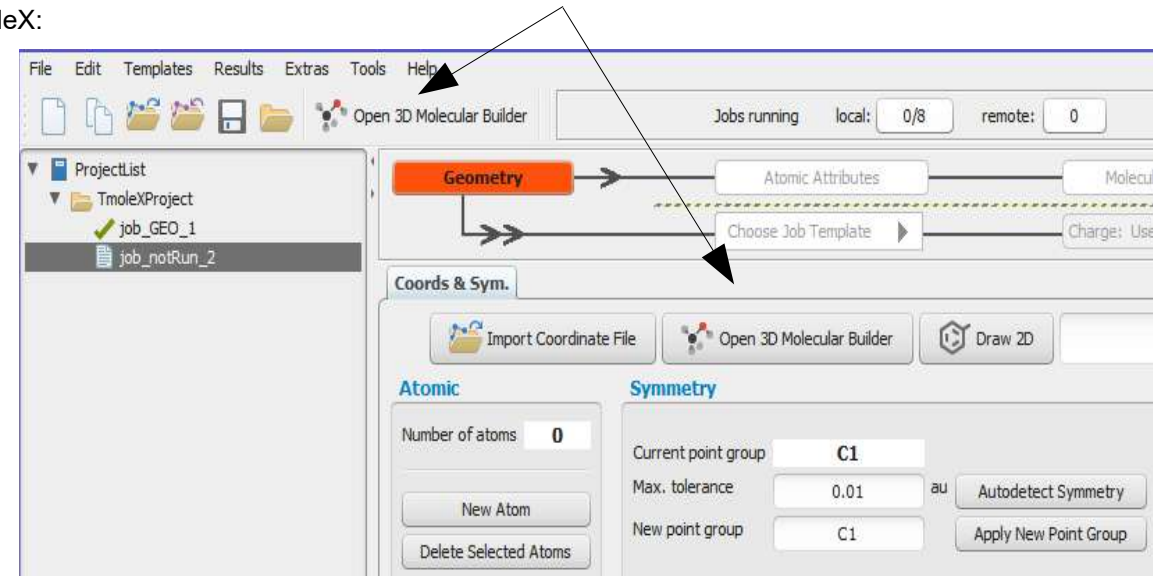
The grey section shows the number of local and remote jobs. Note that only jobs from open projects are shown – closing a project with running jobs will is not recommended as TmoleX will loose the connection and might not be able to correctly reopen them!

Whenever the number of running local jobs is exceeded, TmoleX will start the next job only after another one has finished. Several jobs can be started that way without blocking your system. The jobs that are scheduled for running are shown with an own icon in the job list.

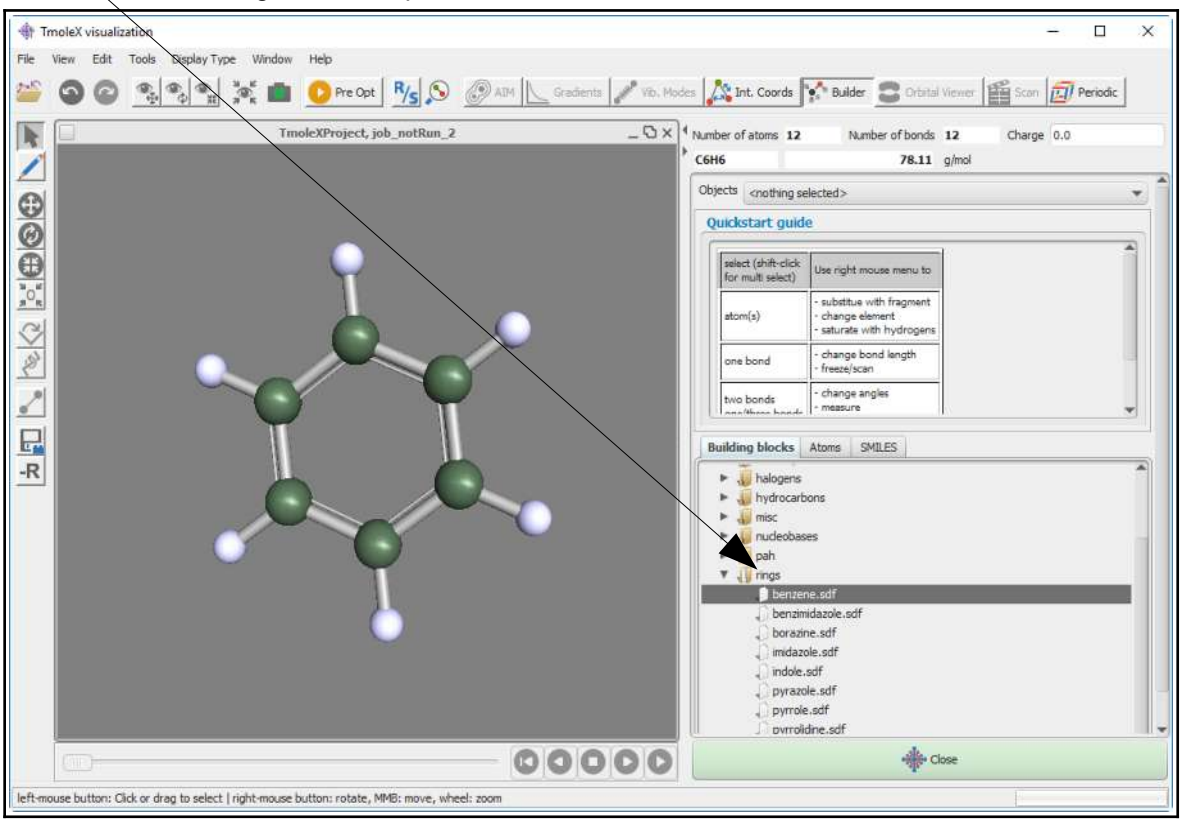
3. The 3D visualization

3.1. The 3D builder

To open the molecular builder click on either the button in the tool bar or the button in the Geometry panel of TmoleX:



The molecule builder can be used most conveniently by starting from building blocks and modifying these. Double-click on a building block to import it in the builder.



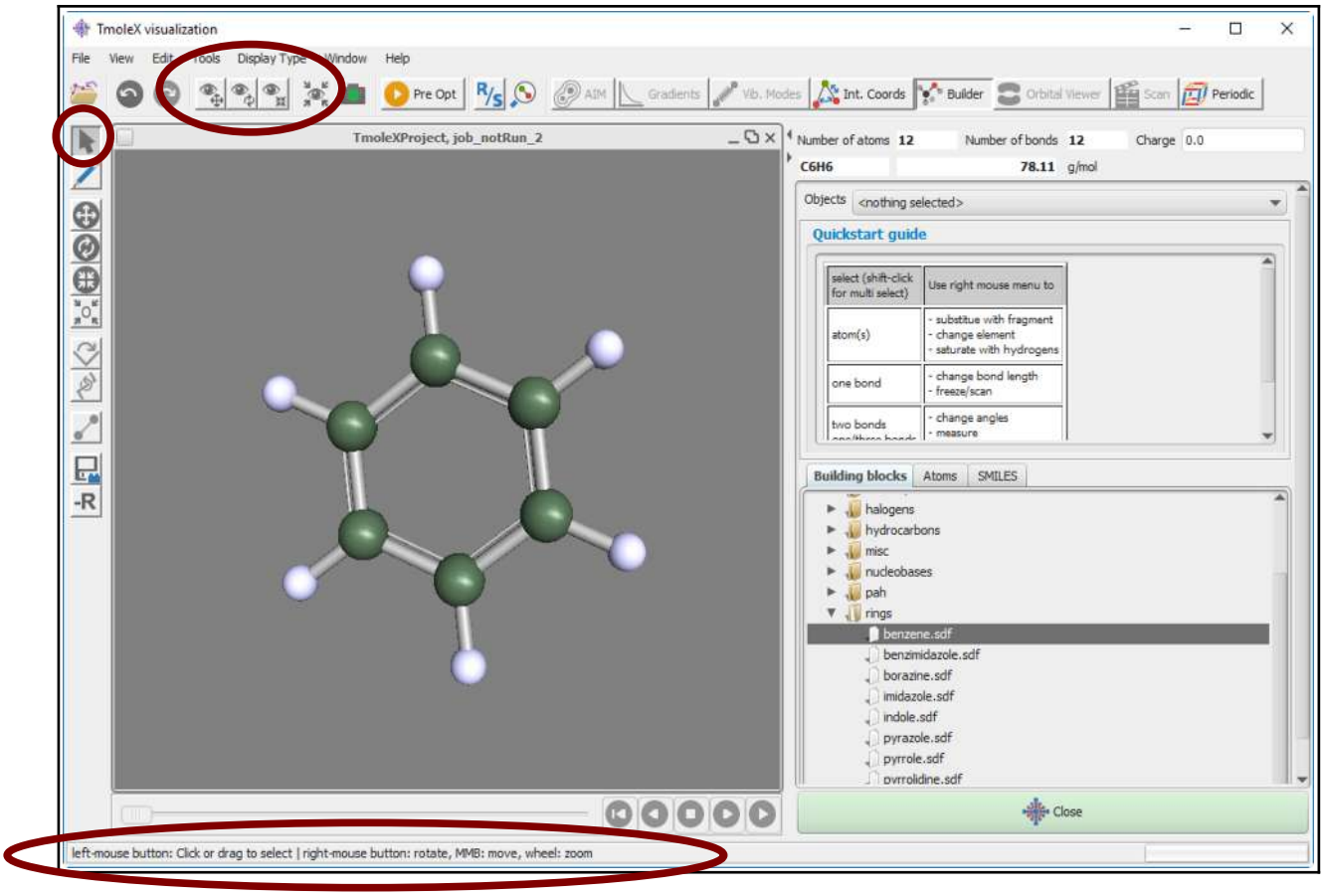
3.2. Navigation

Left mouse button or  or q on the keyboard: *Select*

Right mouse button or  : *Rotate view*

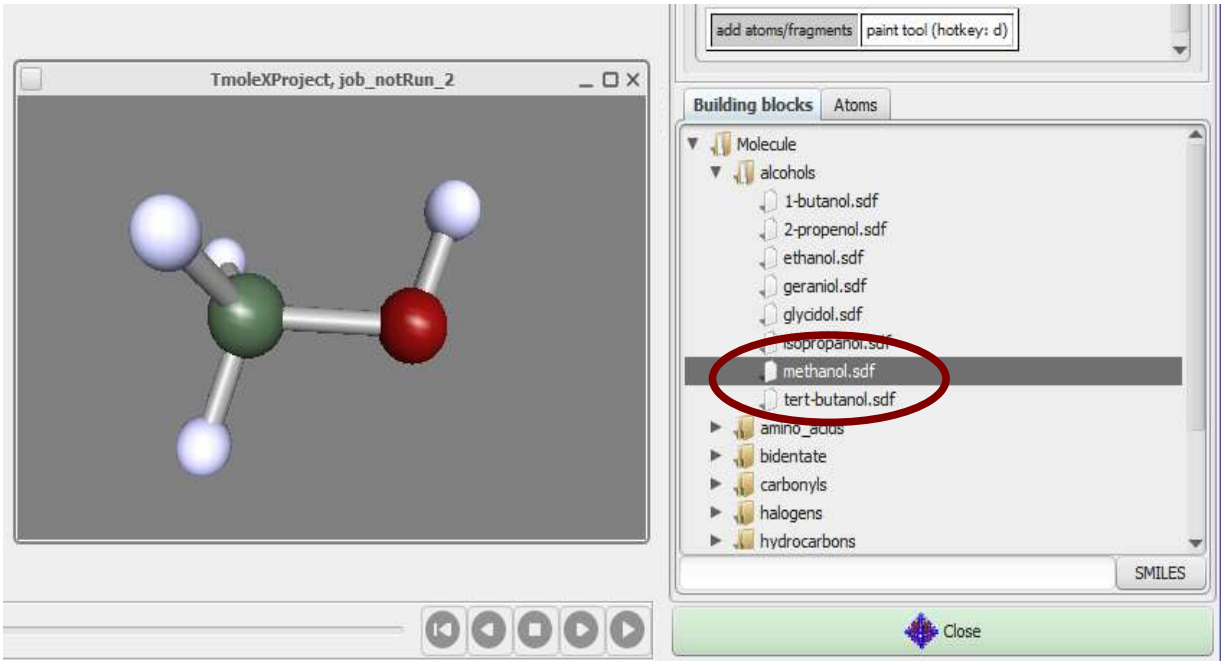
Middle mouse button or  : *Move*

Scroll wheel or  : *Zoom*

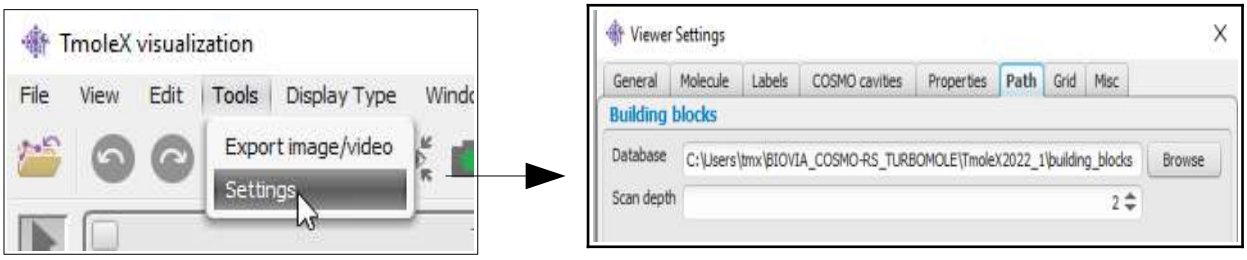


3.3. Building blocks: Pre-stored structures

There are different ways to add molecules and fragments which build up a structure.
Double-click or drag-and-drop molecules from the Molecules section on the right to the window:



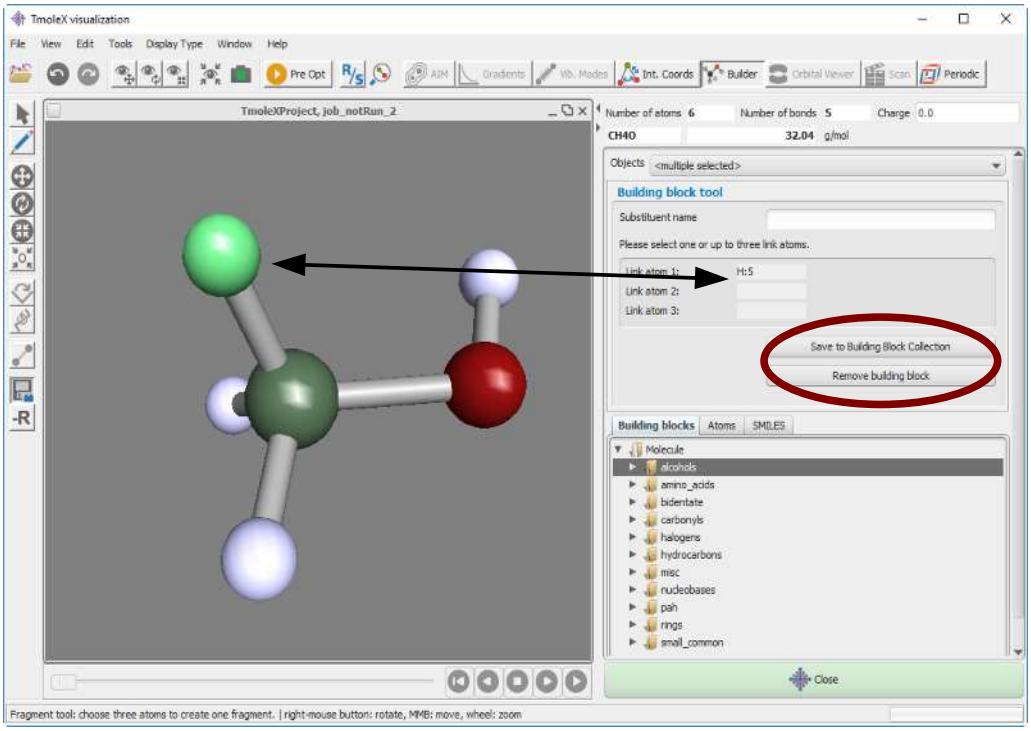
The molecules in the right part of the window are by default taken from the *building_blocks* directory of the TmoleX installation. This can be changed to a user-defined directory in the Tools → Visual settings menu:



The files are stored in standard sdf format, and a second file with the same name but *.sdf.fr* ending is being generated which contains the connecting atom number(s) and the substitutive name.

3.3.1 Generate and store your own building blocks

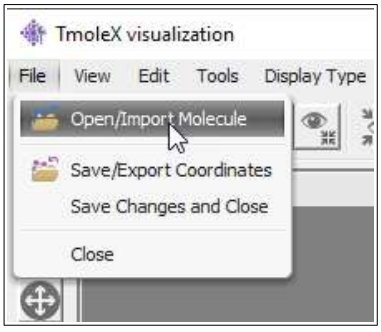
To save your own building blocks to the list, just use the 'Add to building block library' icon: 
The right side of the TmoleX builder will change accordingly.



A substitutive name (the molecule you want to store without the link atoms(s)) can be entered. To select one or several link atoms, please just click on them to add to the link atom list or re-select them to remove them from the list. The 'Save to Building Block Collection' button will then open a default file saving window where you can store the file and possibly generate new directories in the building block section.

3.4. Import structure

Instead of building a molecule from scratch, an existing molecule in different formats (sdf, ml2, xyz, cosmo, …) can be imported using the File/Open menu entry within the visualizer.

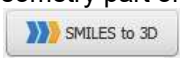


This structure can then be used for modification or being saved in the user data base as described above.

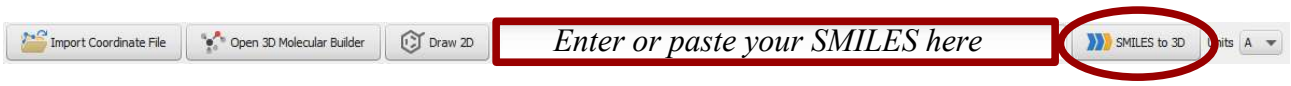
3.5. Use SMILES code

Most organic compounds can be described with the SMILES notation
(see https://en.wikipedia.org/wiki/Simplified_molecular-input_line-entry_system)
and there are several web sites which provide SMILES code for a large number of structures like
ChemSpider (http://www.chemspider.com/).

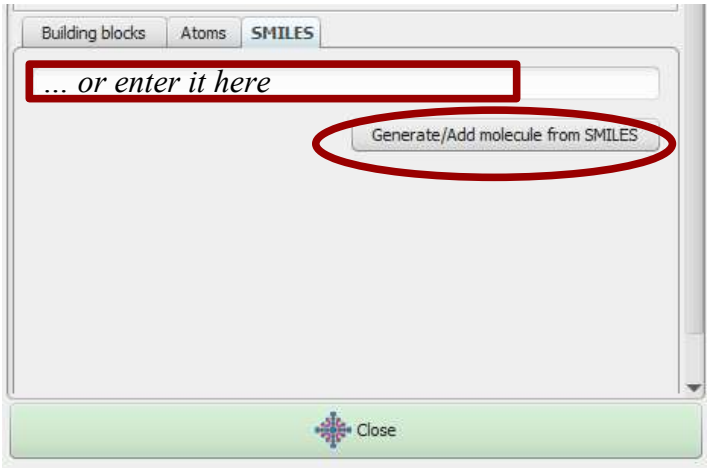
If you have a SMILES code, there are two ways to add it to the 3D builder:

1. directly in TmoleX in the geometry part of the input generation, just add the SMILES code to the field shown below and click on 

:



2. or in the Builder switch to the SMILES panel, add it to the input field and click on the button:



The difference is that clicking on the 

in TmoleX will replace whatever you already had as structure in the Builder, while adding SMILES to the Builder itself will act as adding one of the fragments or structures of the fragment library.

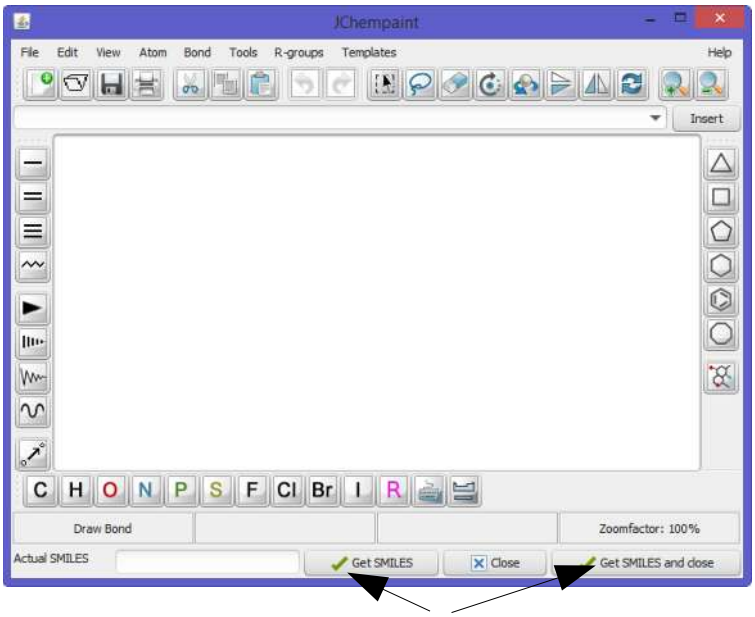
The SMILES to 3D conversion is done using RDKit (http://www.rdkit.org/).

SMILES can also be processed in a list, see chapter 8.1.

3.6. The 2D Builder

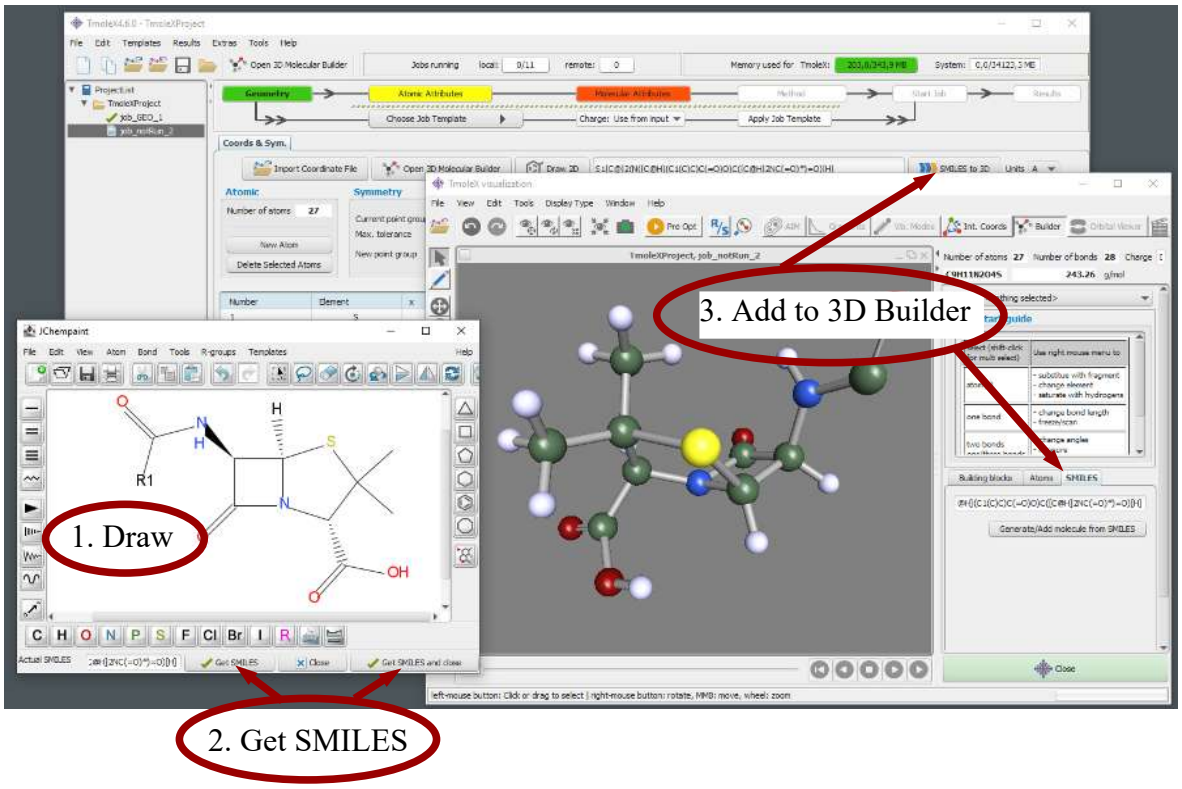
If you start the 2D builder, click on 

to open a new window of JChemPaint



Draw your structure in JChemPaint and click on 'Get SMILES' or 'Get SMILES and close' to copy and paste the resulting SMILES of your painting into TmoleX and the 3D builder (if open).

Detailed information about JChemPaint can be found on https://jchempaint.github.io/



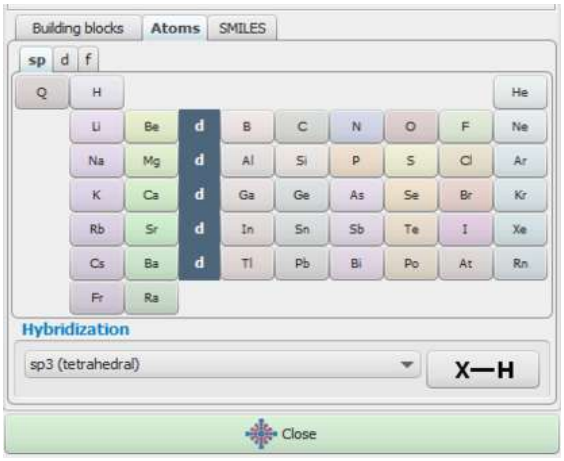
3.7. Easy building: Paint tool

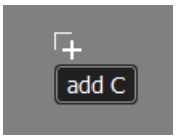
A quite handy way to build is the paint tool

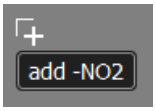


which can be chosen by clicking on the  button or hitting the D key on the keyboard.

In the paint modus, select an atom or a molecule from the Molecules/Atoms section in the builder:

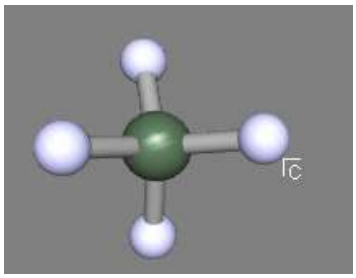


This will change your cursor to the element symbol: 

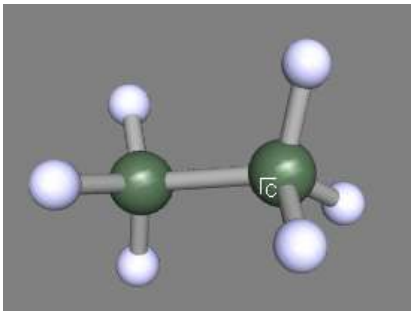
to add a C or 

to add a nitro group, resp.

Click on the background to add the atom or molecule or click on an existing atom to replace it with the selected atom/fragment.

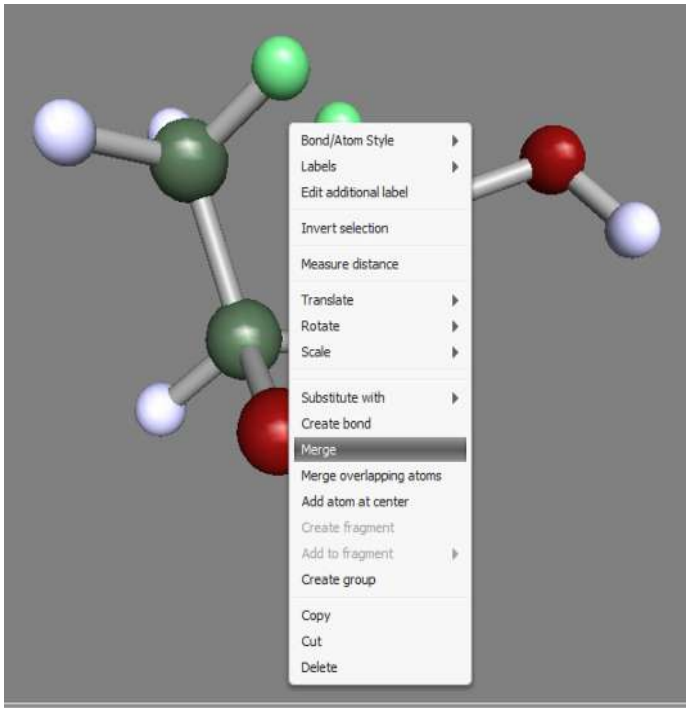


Click on the hydrogen

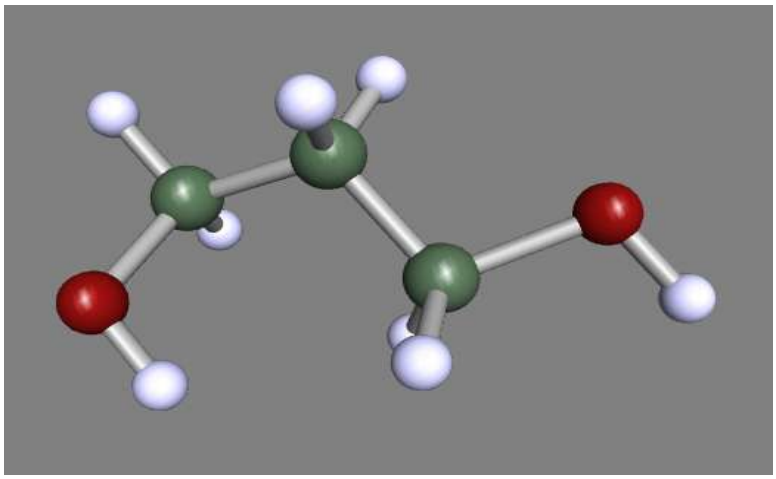


3.8. Build complex molecules by merging fragments

a) Load two molecules, select one atom from each of two different fragments:

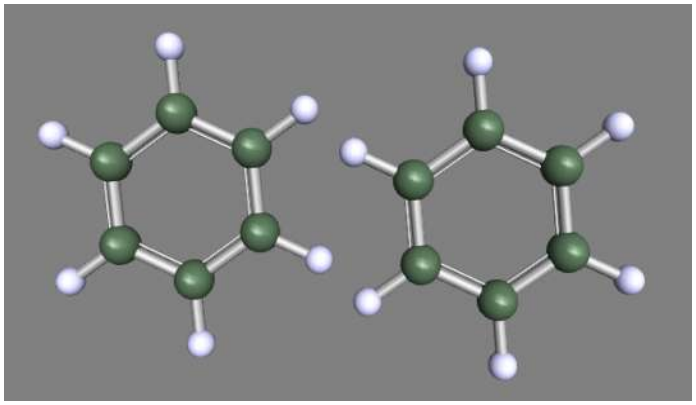


b). Use the right mouse button and select the *Merge* option. TmoleX will join the two fragments and re-arrange the resulting structure such that the overlap of the atoms is minimal:



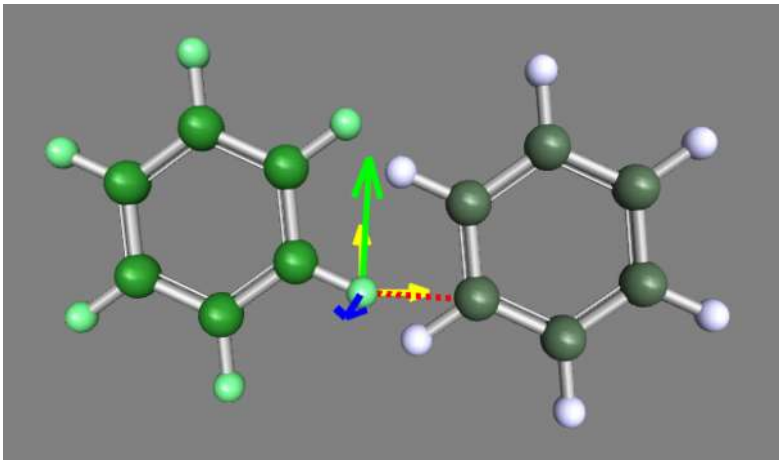
To merge two fragments which are not just connected by one bond, a more powerful option is to merge overlapping atoms.

a) read in two benzene

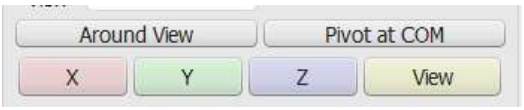


b) move one fragment close to the second one. This can be done in two ways:

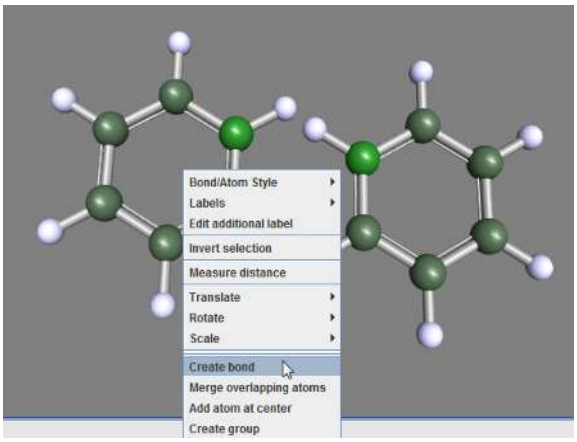
i) select one of the two benzene by **double-clicking on one atom** and then select the translate tool (or hit w on the keyboard)

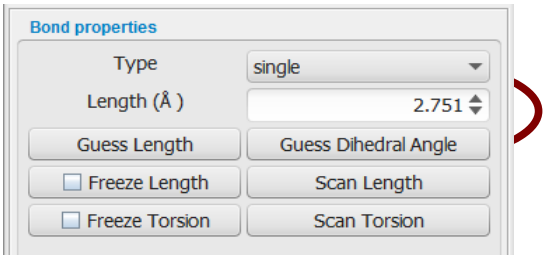


Hold left mouse button and move the fragments such that they overlap (switch to another direction and/or use the 'along view' button to move in the direction of the monitor system of coordinates).



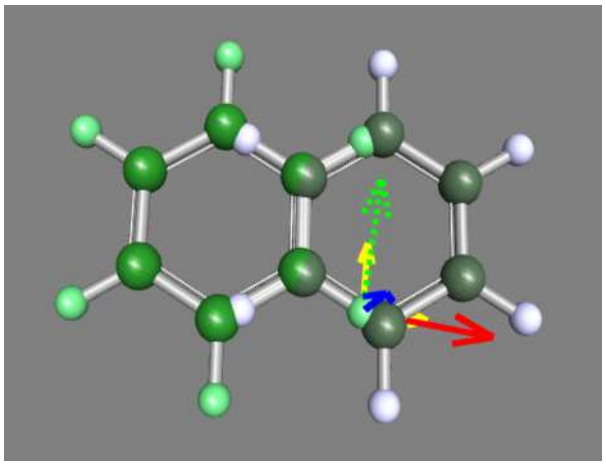
ii) create a bond between two atoms, select it and change its length to zero



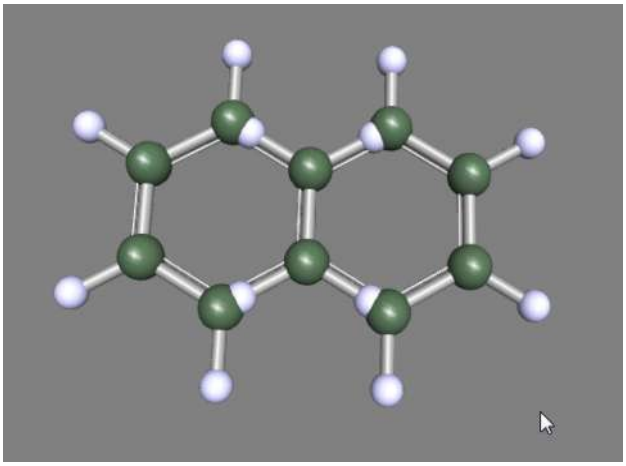


iii) and even easier: Select two **bonds** of the two benzene rings and select 'Merge bonds'

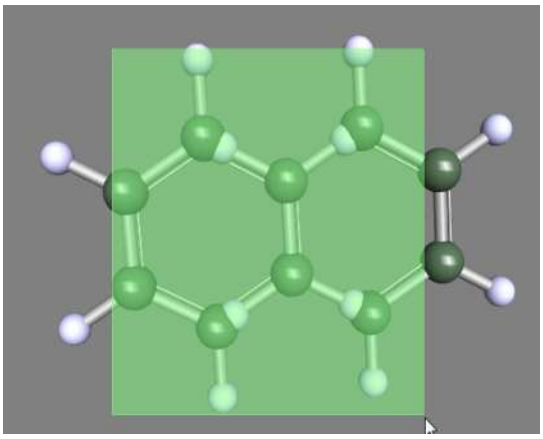
The moved fragment should look like this:

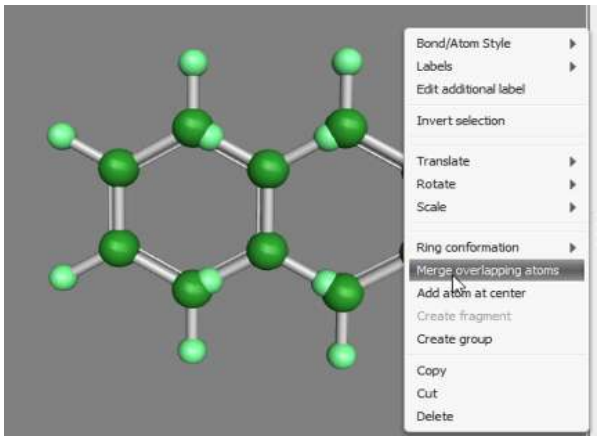


The zero-bond length method leads to:

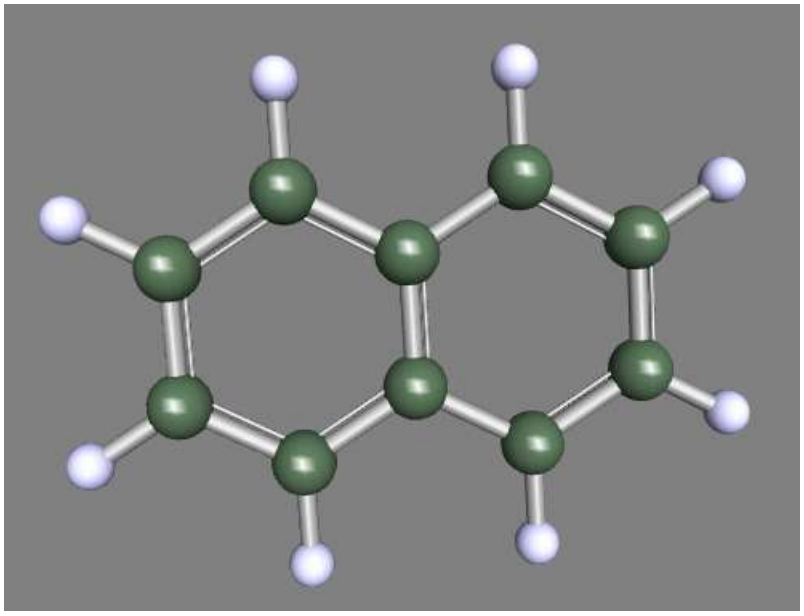


Double-click on the background (or hit the Esc key or use the left mouse button) to get to selection mode. Draw a box around the overlapping part and select 'Merge overlapping atoms' from the right-mouse button menu:





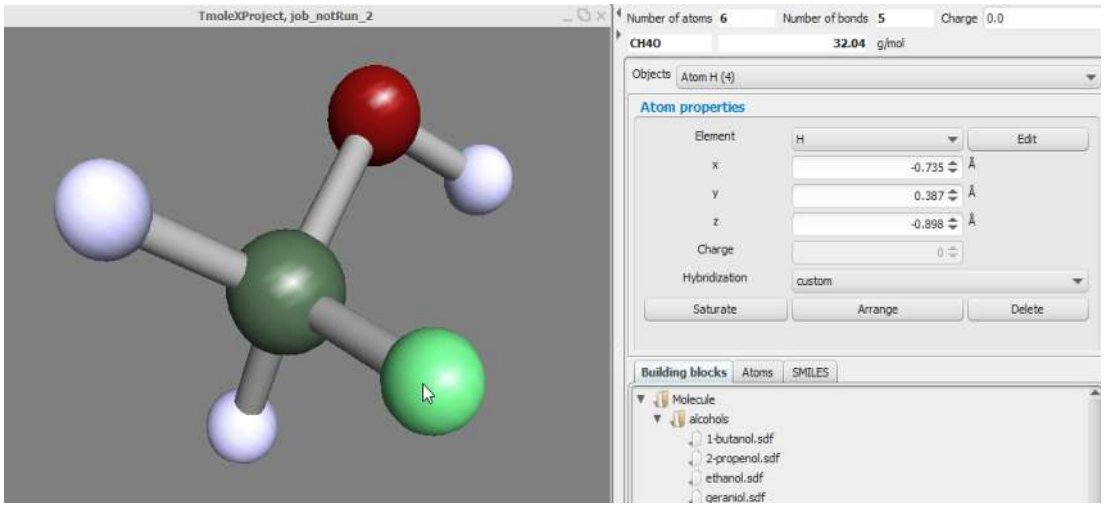
All atoms which have a (little bit) of overlap will be joined in a way that the lighter atoms is being deleted.



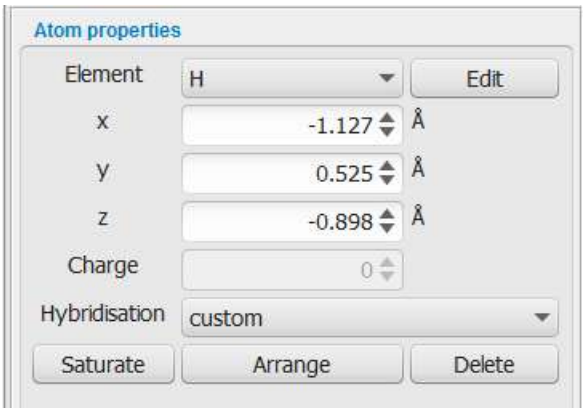
The trick to set a bond length to zero works only in cases where the selected bond is not part of a ring!

3.8.1 Building step by step 1

Change to selection mode (q or ESC key or arrow button on the left side) if you are not already in this mode.
Select an atom:



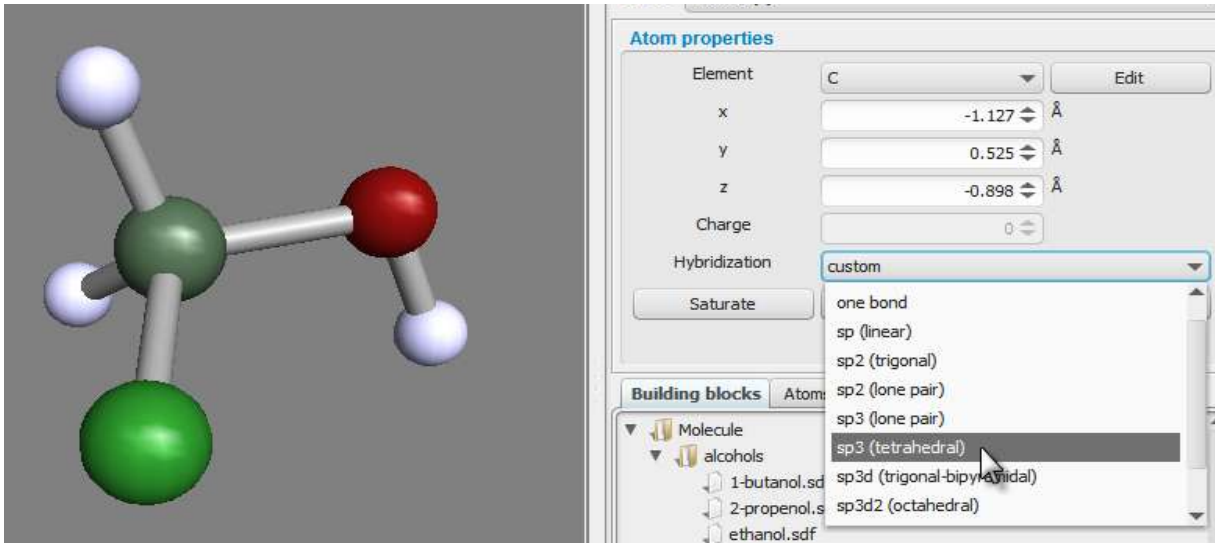
On the right side the properties of the selected item (atom, bond, measure, etc.) are shown.
For objects which are hard to select with the mouse, the Objects chooser can help since it contains all displayed objects, including measurements and constraints.



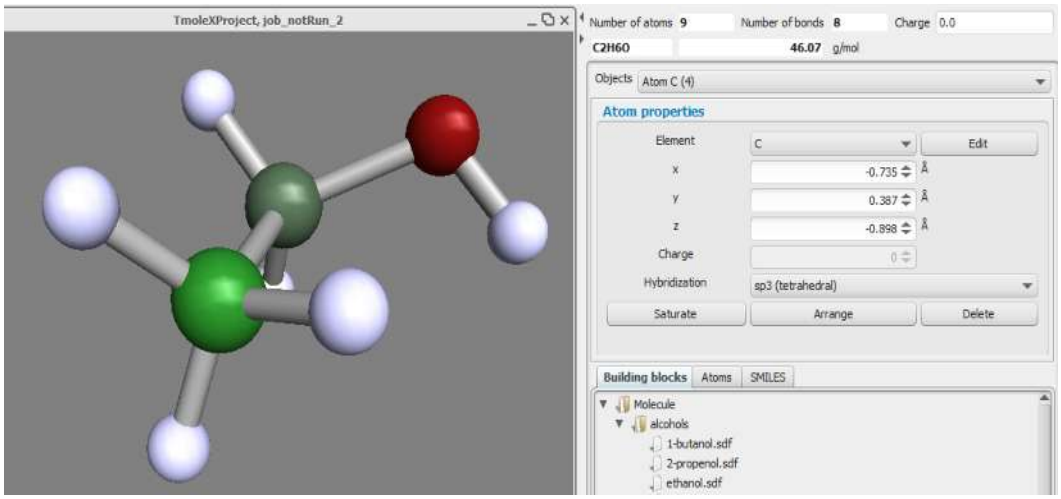
Most entries can be changed in the fields.

3. The 3D visualization

Change the Element from H to C and also the Hybridisation to sp3(tetrahedral):

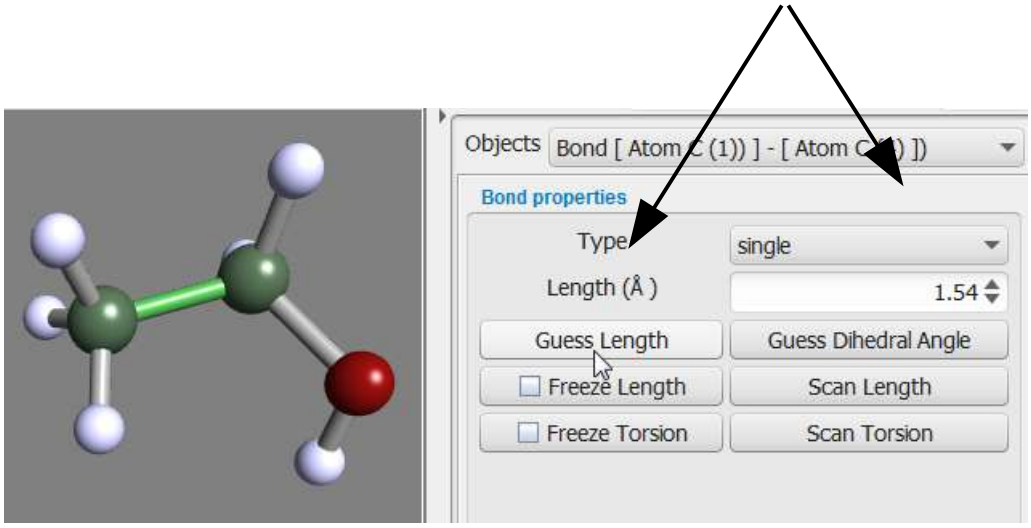


Next, click on Saturate to add missing hydrogens to the selected atom according to the given hybridisation.
NOTE: The saturate button does just add hydrogens to atoms with user-defined hybridisation settings. It does not place them in a chemical correct way. Use the 'Arrange' button next to 'Saturate' to let TmoleX guess a more reasonable arrangement of the added hydrogens.

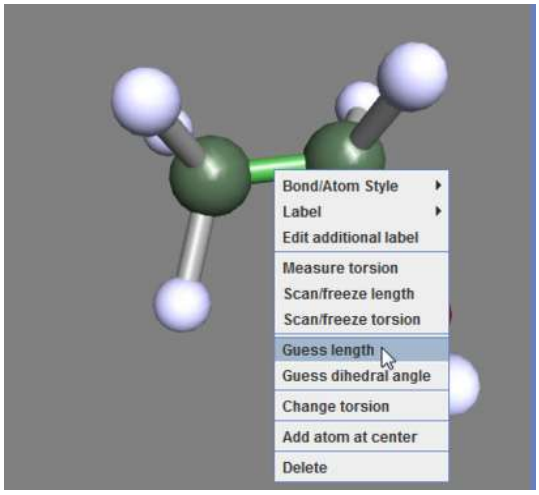


3.8.2 Change bond length

Now the bond length to the newly created methyl group is set to a default single-bonded C-C length, but can be changed by selecting the bond. Either enter a new value or let TmoleX guess the length according to vdW radii:

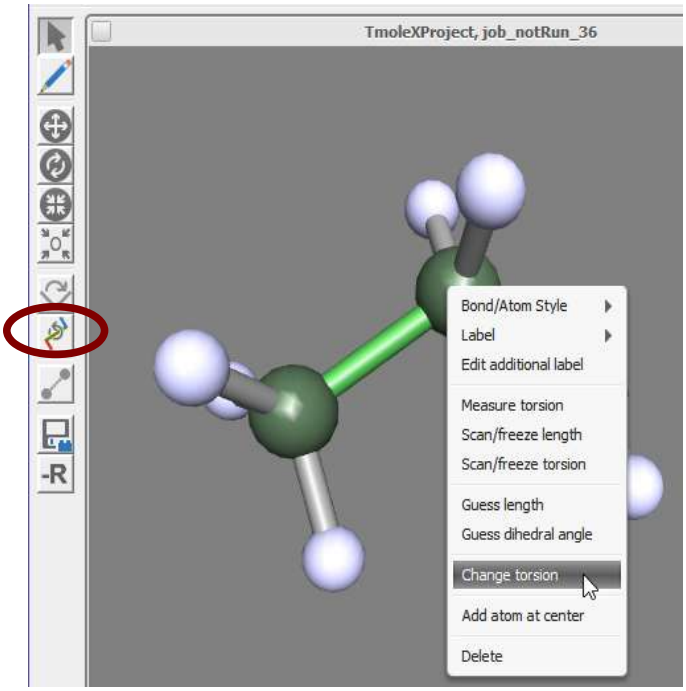


The length and also many other things can be done by using the context menu of the right mouse button:
Hint: If you want to change a bond length (or an angle or torsion) and there are no bonds to select, simply add a new bond between two selected atoms using the right mouse menu.

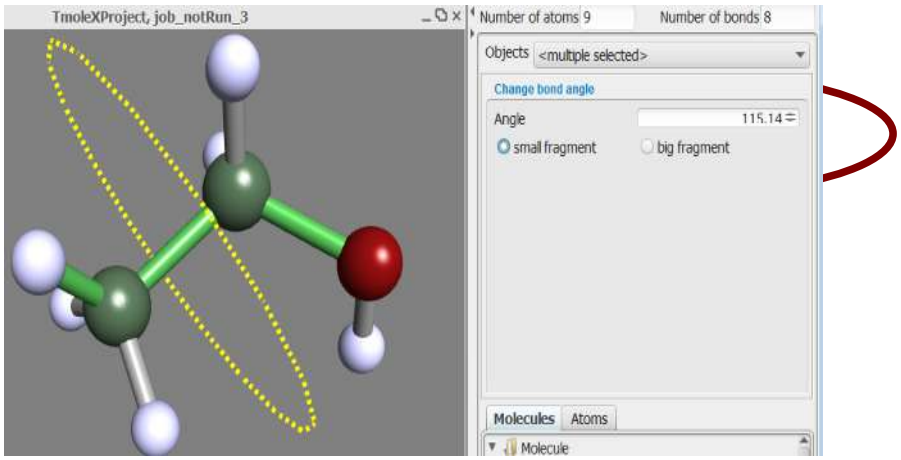


3.8.3 Change torsion

To **change the dihedral angle**, click on the middle bond or select three bonds (holding shift key will add selections) which define the angle and then either use the button on the left that will show up or again the right mouse menu:

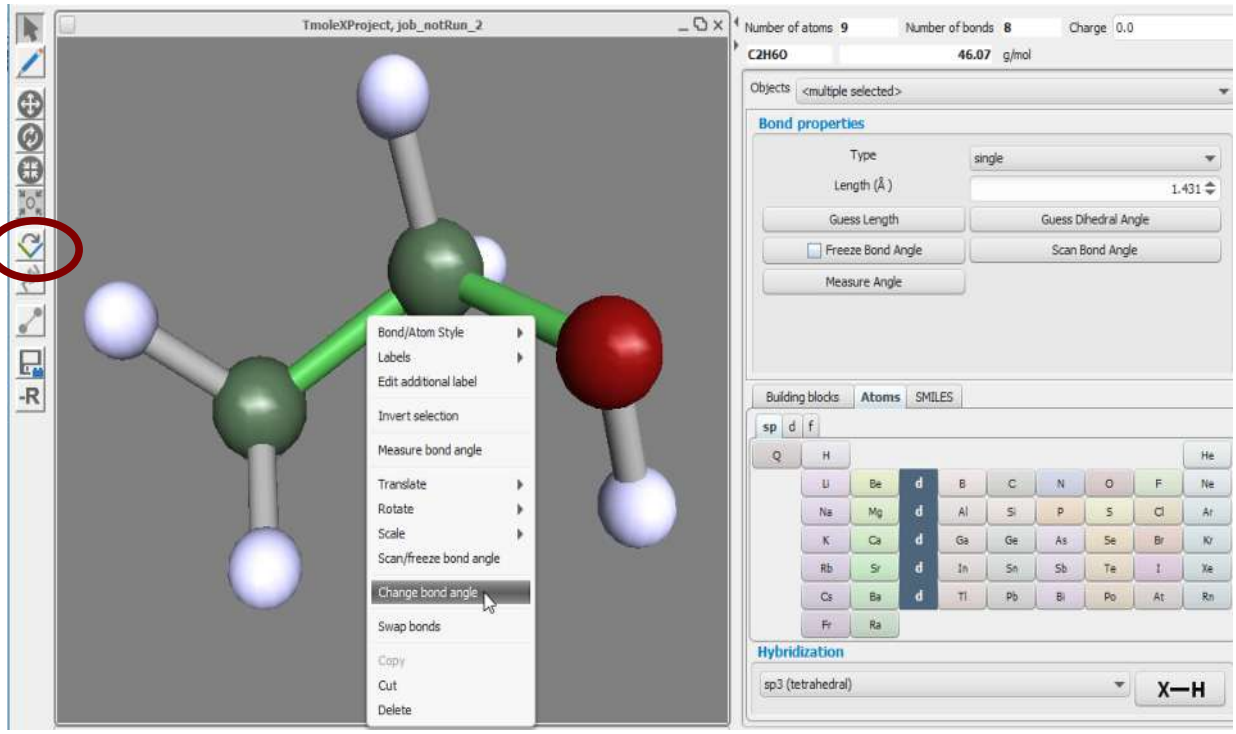


The torsion around which the molecule will be rotated is being shown. Use the left mouse button to change the angle – moving to right or up will increase the value, moving the mouse to the left or down will decrease the angle. The value of the angle can be entered directly on the right side, and one can also choose if the smaller or the bigger fragment is being moved.

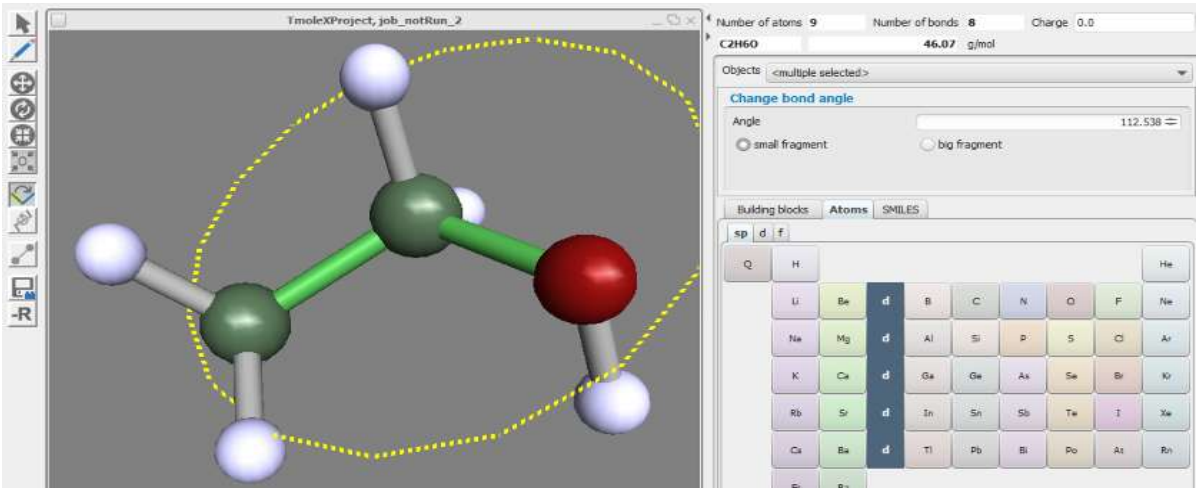


3.8.4 Change bond angle

To **change a bond angle**, select two adjacent bonds (shift-click for the second one) and either click on the button on the left side or use the right mouse button to change the value:

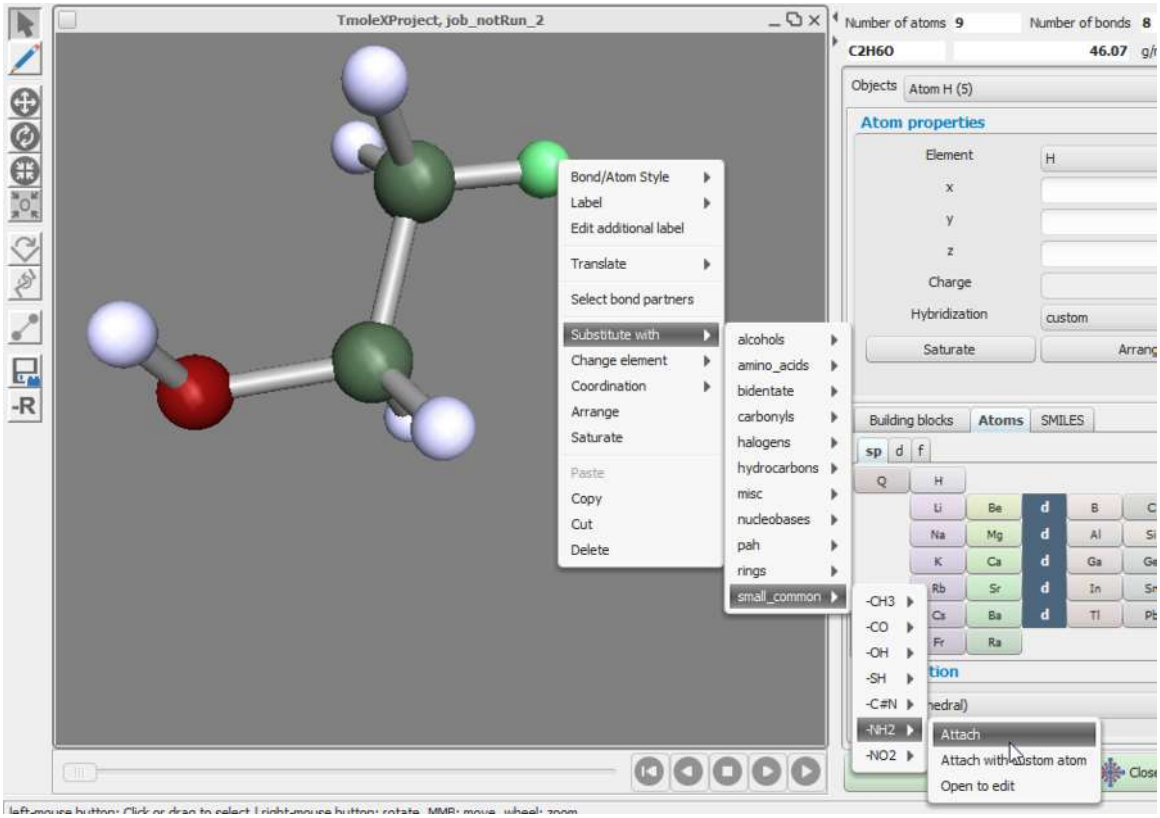


The properties of the angle are shown and can either be changed by clicking on the left mouse button and dragging the mouse or by editing the field:
Like for torsional angles, the small and big fragment option decides which part of the molecule is being moved.



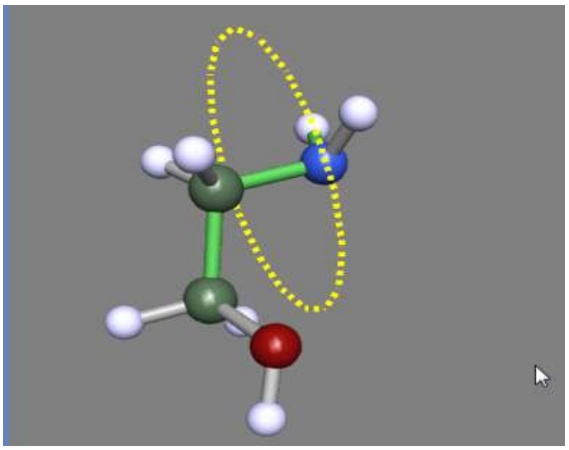
3.8.5 Building step by step 2

Instead of changing an atom to a different element, to change hybridisation and use the saturate option, an atom can also be replaced by a pre-stored fragment.



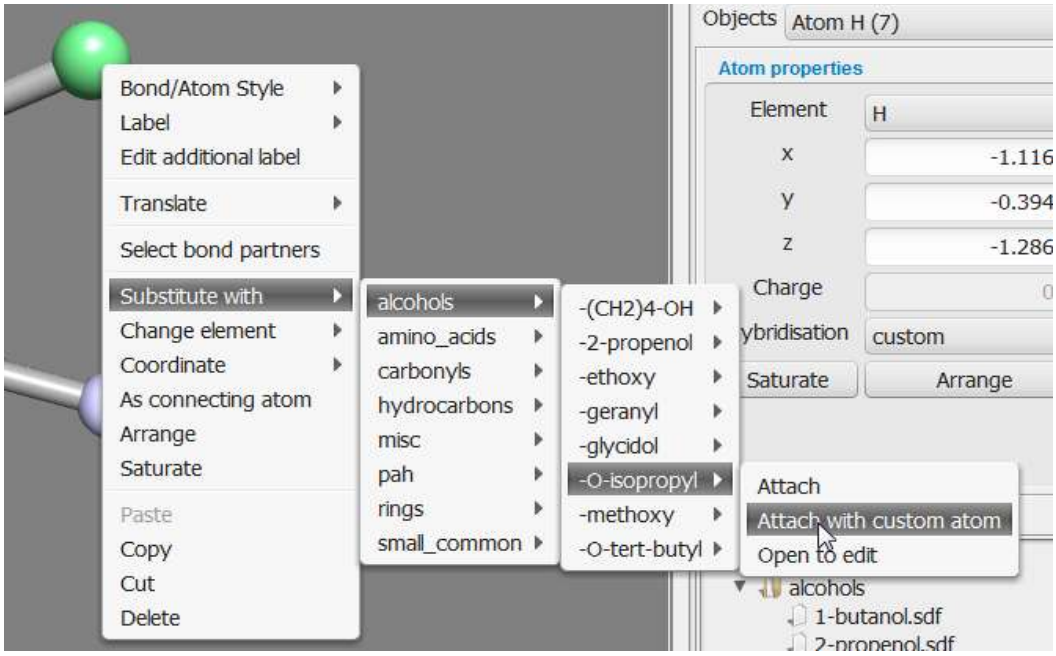
Select an atom, use the right mouse button and click on 'Substitute with'.

Note: The fragments that are shown are the molecules of the user data base (or the default pre-stored molecules after installation as shown here). When choosing *Attach,* the connecting atom – which was marked as such when saving the structure to your fragment data base – will directly be substituted.

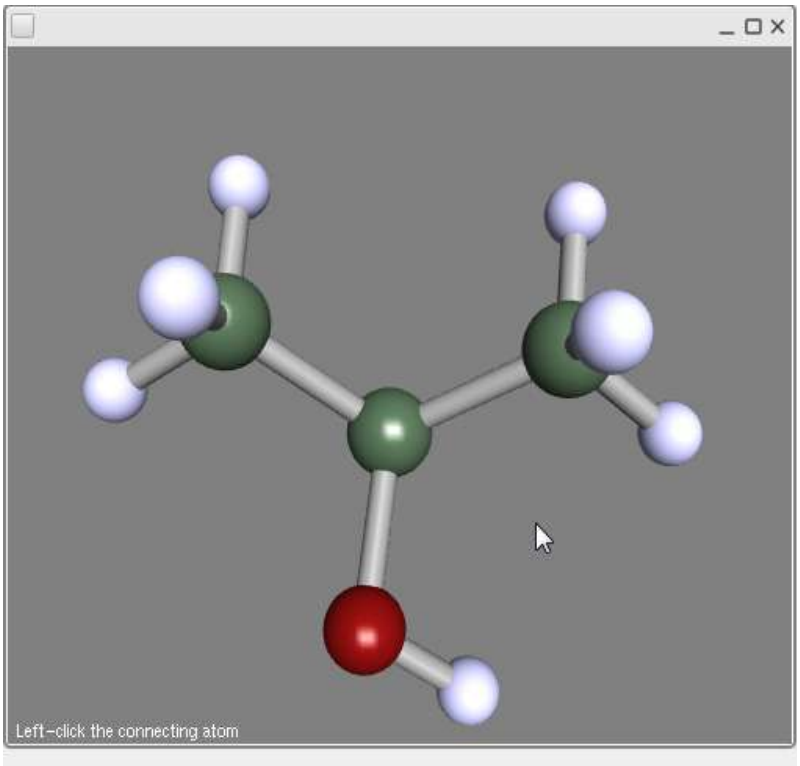


The builder will automatically switch to the dihedral mode. Use the left mouse button to rotate around the new bond. To get back to the selection mode, double-click on the background, hit the Esc key or use the button.

Alternatively any other atom can be used as connecting atom:



Choosing 'Attach with custom atom' will open the structure of the fragment in an own window.

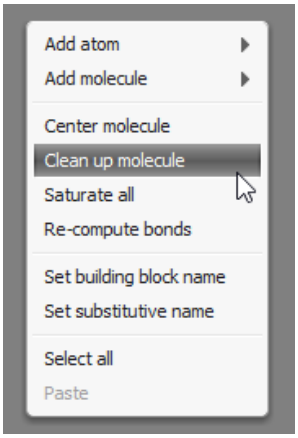


Just click with the left mouse button on the atom (one of the hydrogens in this case) to select the connecting atom.

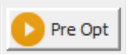
3.9. Pre-optimization

There are different options to pre-optimize a guess structure:

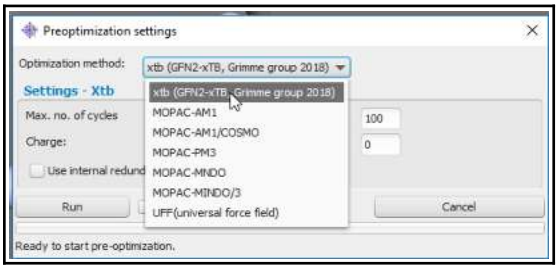
- Unselect all objects by clicking on the background
  Use the right mouse button and select:



  A very simple rearrangement which minimizes the overlap of the van-der-Waals radii of all atoms

- By clicking on the 

button, different methods for geometry optimizations at semi-empirical or force-field level are available:

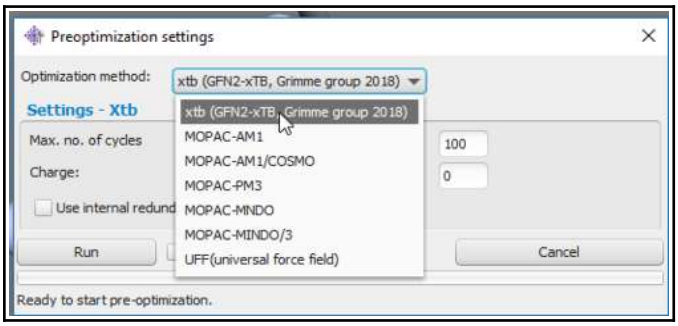


- Default is to use the xtb module (extended tight-binding semi-empirical program) from the Grimme group in its TURBOMOLE implementation.
  Details about the method can be found here: http://dx.doi.org/10.1021/acs.jctc.8b01176

- Another option is to use MOPAC7, which is included in the default installation of TmoleX. Available methods are AM1, PM3 and MNDO.

- UFF – a universal force field as implemented in TURBOMOLE

The window opened by the Pre-Opt button provides several options.



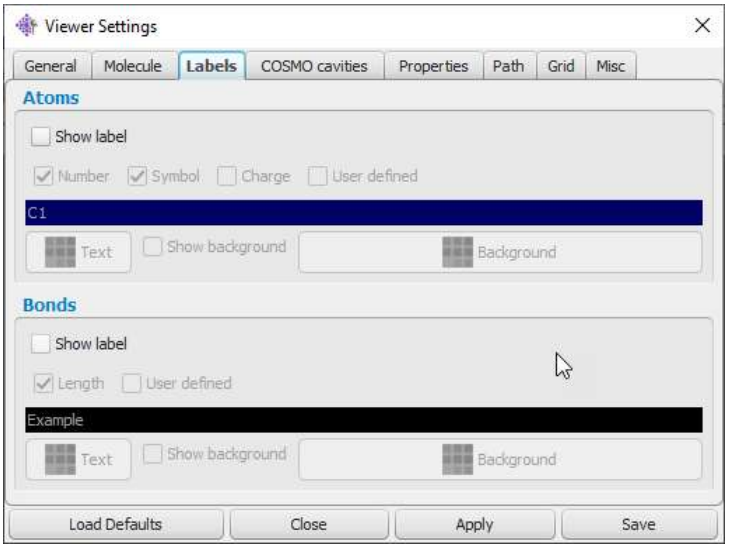
GFN2-xTB is the default as it offers geometry optimization of molecules and cluster containing elements from H to Rn. AM1, PM3, MNDO, MNDO/3 are the available methods provided by MOPAC (they all are parametrized for a certain number of elements). AM1/COSMO is the default setting for COSMOtherm input files at BP-SVP level (first do a geometry optimization at this level and then a single-point DFT calculation with COSMO and SVP basis set). Unrestricted calculations can be done with UHF for MOPAC jobs, guess structures for transition states can also be searched. A molecular charge has to be entered to calculate ions.

3.10. Labels and Measurements

Labels for atoms and bonds as well as measures of lengths and angles can be switched on or off for the complete structure or individually for each object.

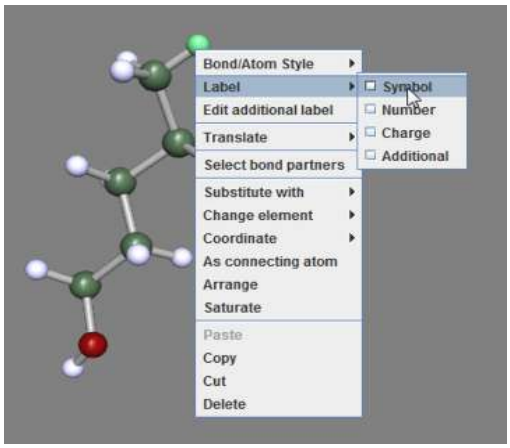
- Display labels for all atoms or bonds

  In the 3D viewer select Tools → Settings and switch to the Labels section:



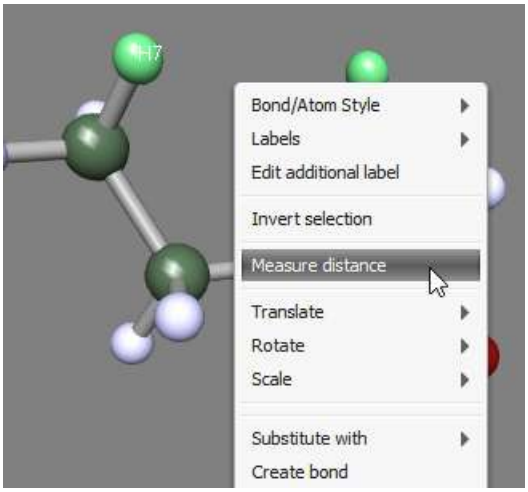
  For atoms the atom number, the element symbol, the charge and additional text (which can be entered by the user with the right mouse button menu within the viewer window) can be displayed. Depending on the background colour and the colour of bonds and atoms the labels can be hard to read. The background settings here refer to the background of the text field only.

- To display labels of one or several atoms/bonds only, use the right mouse menu:

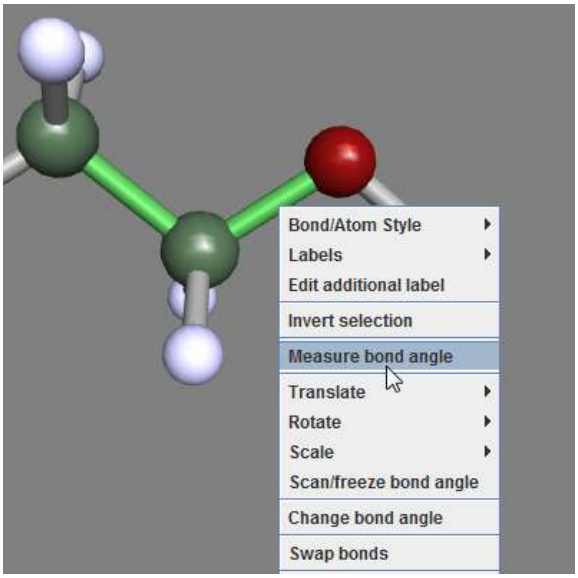


  Own text can be entered in the second item of the right mouse menu. To add or remove labels for several atoms or bonds, just select several items and then use the right mouse button for the selection.

- Measures can be added with the right mouse menu, what is measured depends on what you have selected:
  - select two atoms: measure distance



  - select two bonds: measure angle



  - select three bonds: measure torsion...

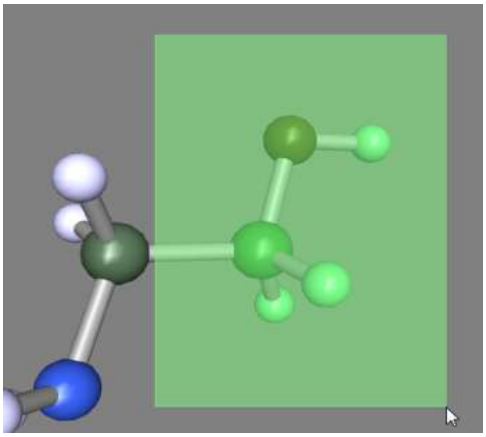
Measures can be selected and deleted with the Measures pull down list:



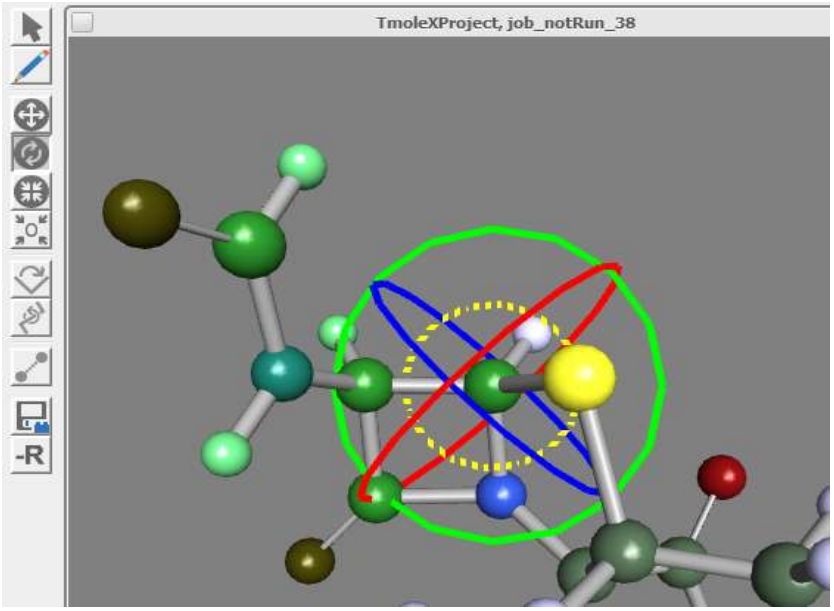
3.11. Moving, Rotating, Scaling

It is often helpful to move or rotate parts of the molecule to a new position. This can be done within TmoleX with several powerful possibilities, but the usage is not self-explaining. So here are the options:

- Select several atoms,



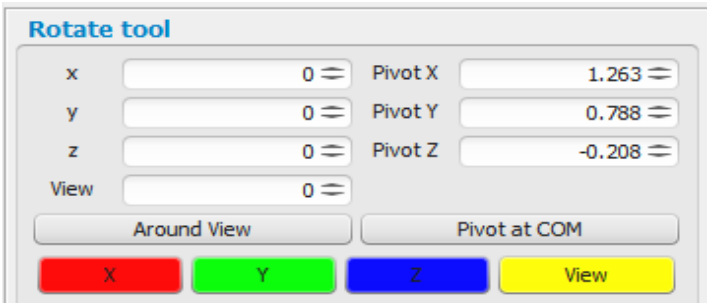
hold shift key and select the atom around which the rotation shall be done. **The last atom that is selected will be by default the centre of the rotation!** Use the right mouse menu or the button  or the key 'e' to switch to rotation mode.



Rotation of the selected atoms can be done using x,y,z axis as rotation axis. In addition to that, the yellow circle indicates the rotation around the axis that is perpendicular to your screen – at the

moment you activate the rotation mode. Use the right mouse button to rotate the view, the middle mouse button to move the camera and the scroll wheel for zoom. Those mouse movements will not change the coordinates, just the view.

To rotate around x,y, z, or the initial view direction, use the left mouse button and drag the mouse.



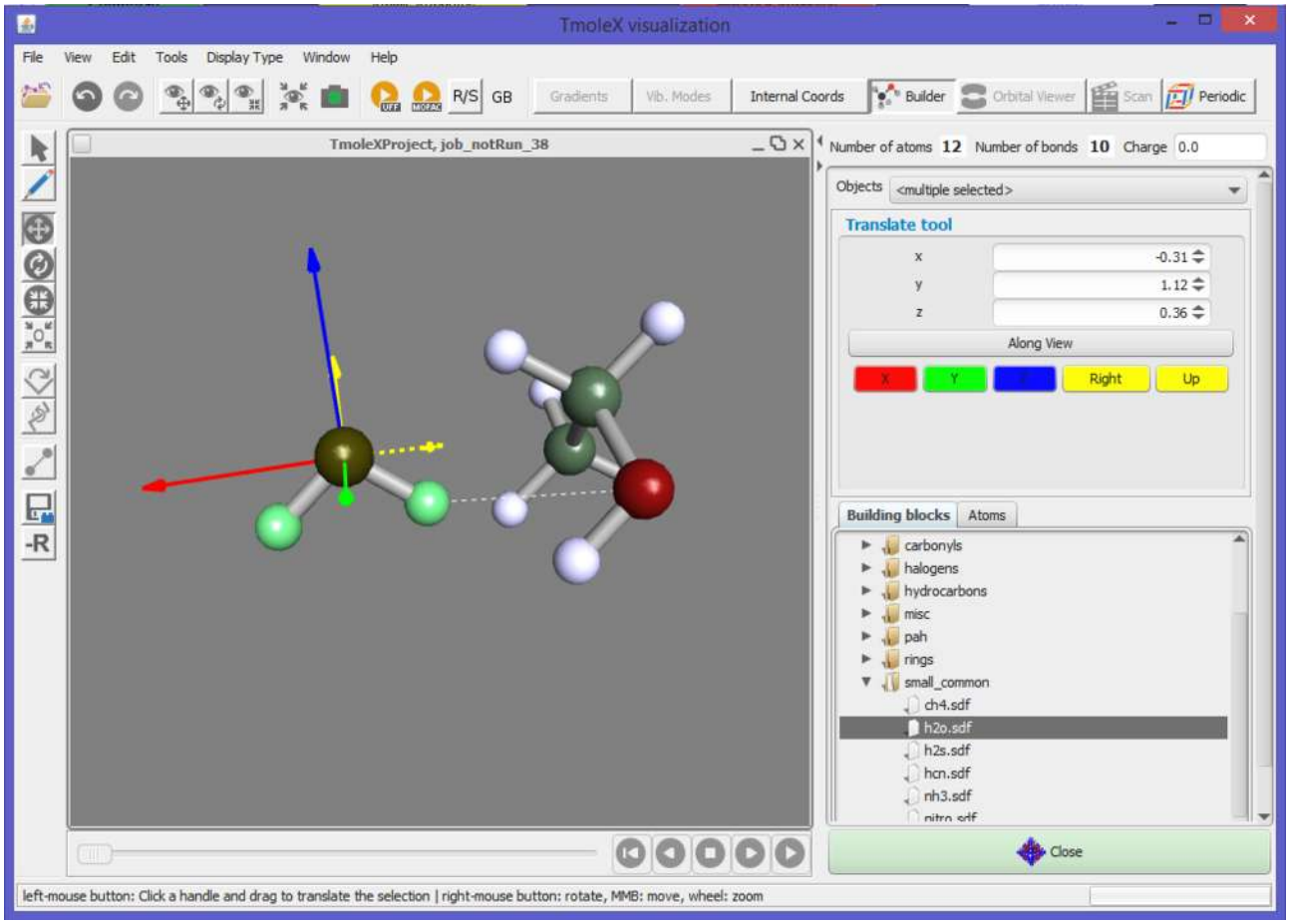
Use the coloured buttons on the right side of the window to switch the rotation axis, or click directly on the coloured circles.
The 'around view' button will reset the yellow 'view' rotation axis to your current viewing direction. Note that rotating the view with the right mouse button does not change the rotation axis!
The 'Pivot at COM' changes the centre of the rotation to the centre of mass of the selected atoms.
Rotation angles can be entered (in degrees) to the corresponding X,Z,Y, View fields. The center of rotation, i.e. the pivot, can also be entered manually if needed.

Note that the selected atoms which will be rotated do not have to be connected.

- Moving atoms or fragments is very similar to the rotation procedure described above. Select the atoms that shall be moved and use the right mouse menu (Translate), or the button , or press the key 'w'.

  Hints:

  - Double-click on an atom to select the whole fragment (all atoms that are connected by bonds).
  - There is an option 'Select bond partners' in the right mouse menu which extends the selection around each already selected atom to its next (bonded) neighbours.



Again, change the direction of movement either by clicking on the coloured buttons on the right side, or by clicking on the coloured arrows.

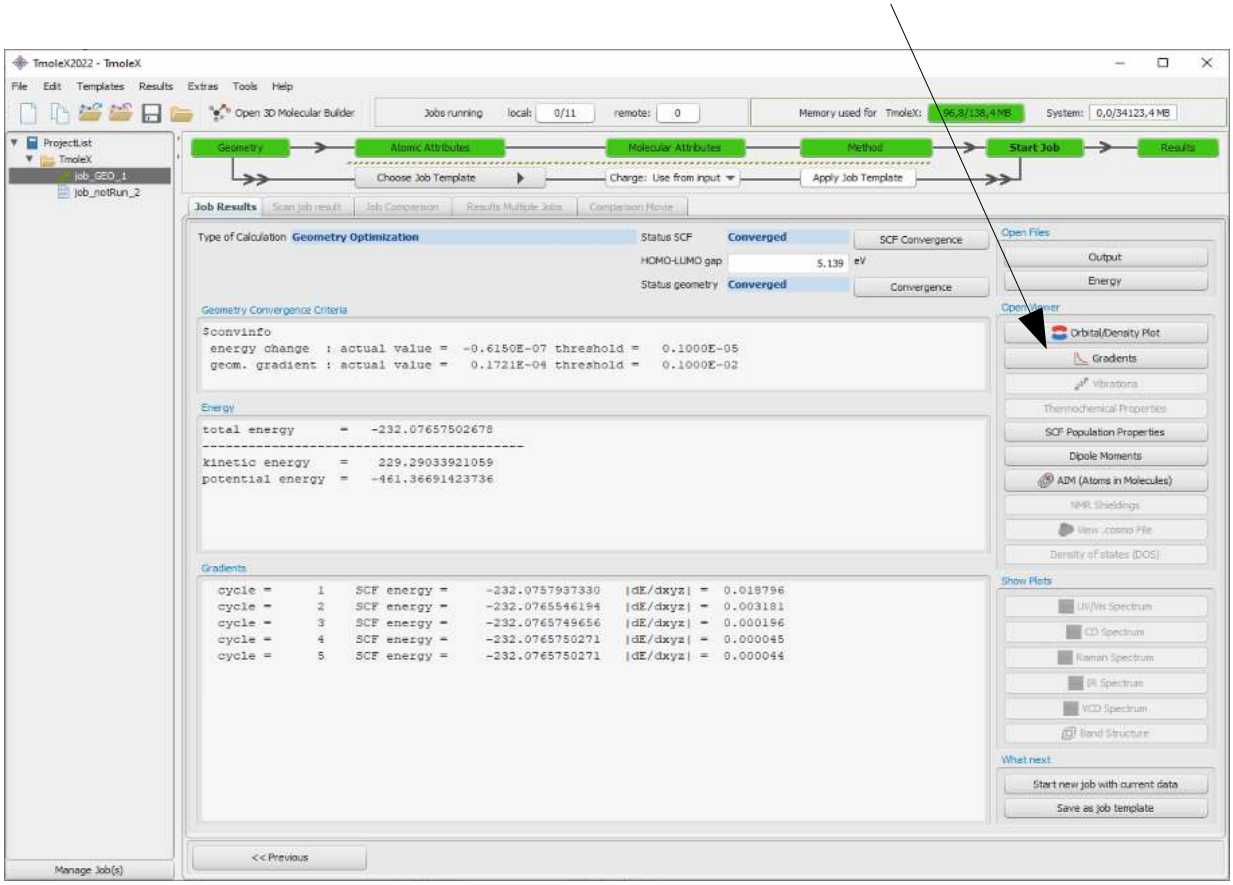
Note:

- Holding the left mouse button and moving the mouse to the *right or up* will move along the *positive direction* (plus x,y,z values), and moving the mouse *down or to the left* will *decrease* the coordinates – no matter from which direction you are looking at the structure! This can sometimes lead to the fact that moving, for example, the mouse to the left will move the fragment to the right (because you are looking at the structure from 'behind').
- Again, in addition to the absolute directions x,y,z, you can move the selected atoms along the direction that corresponds to the 2D coordinates of your screen: Right/Left and Up/Down. Click on 'along view' to reset the Right and Up direction to your current view on the structure.

- Finally, the scale tool  (key 'r') scales or resizes relative distances between atoms. Add a benzene ring, select it, and use this tool to see what it does.

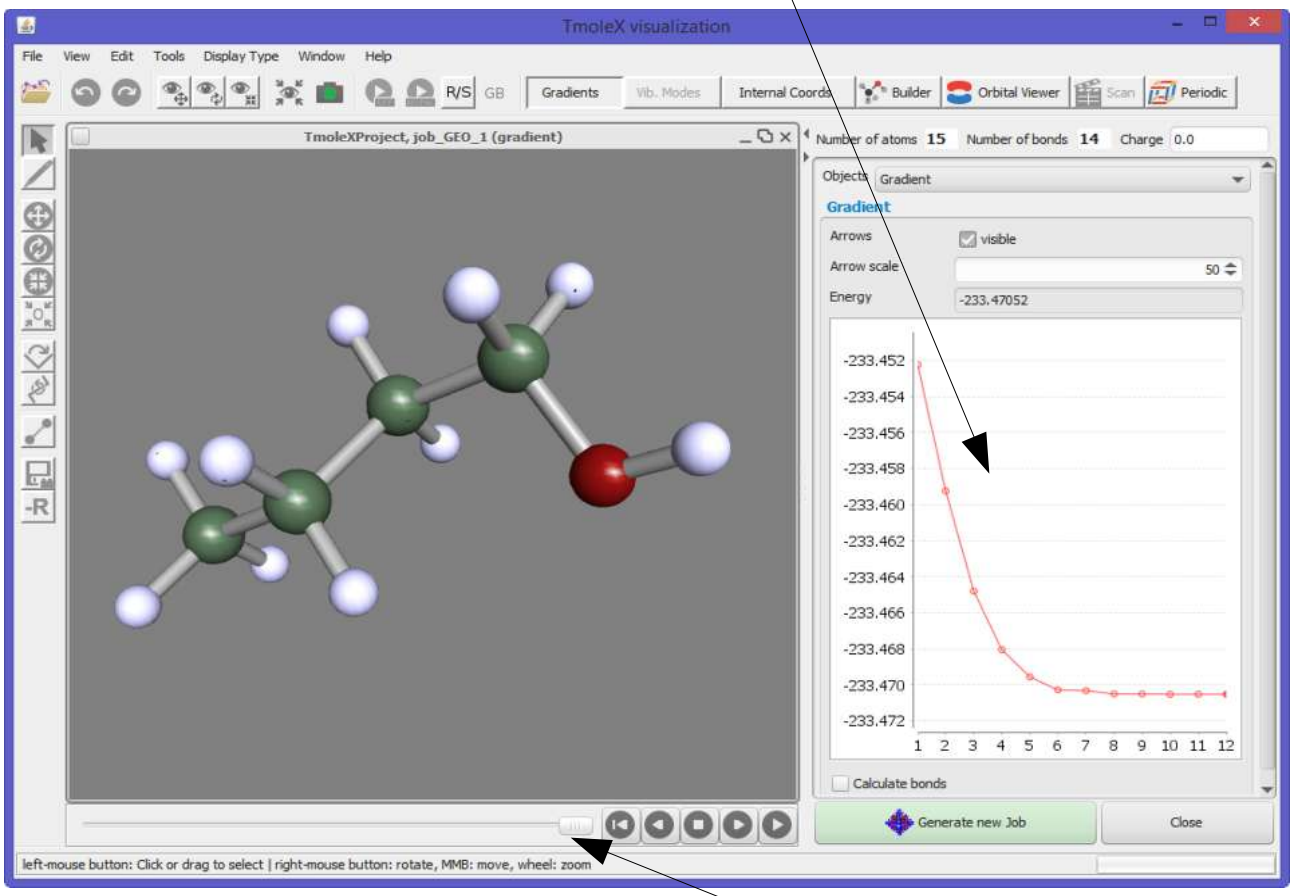
3.12. The gradient viewer

Once you have completed a geometry optimization, you can open the gradient viewer from the results panel.



3. The 3D visualization

The total energies for the optimization steps can be viewed here. Click on a circle to visualize that step.

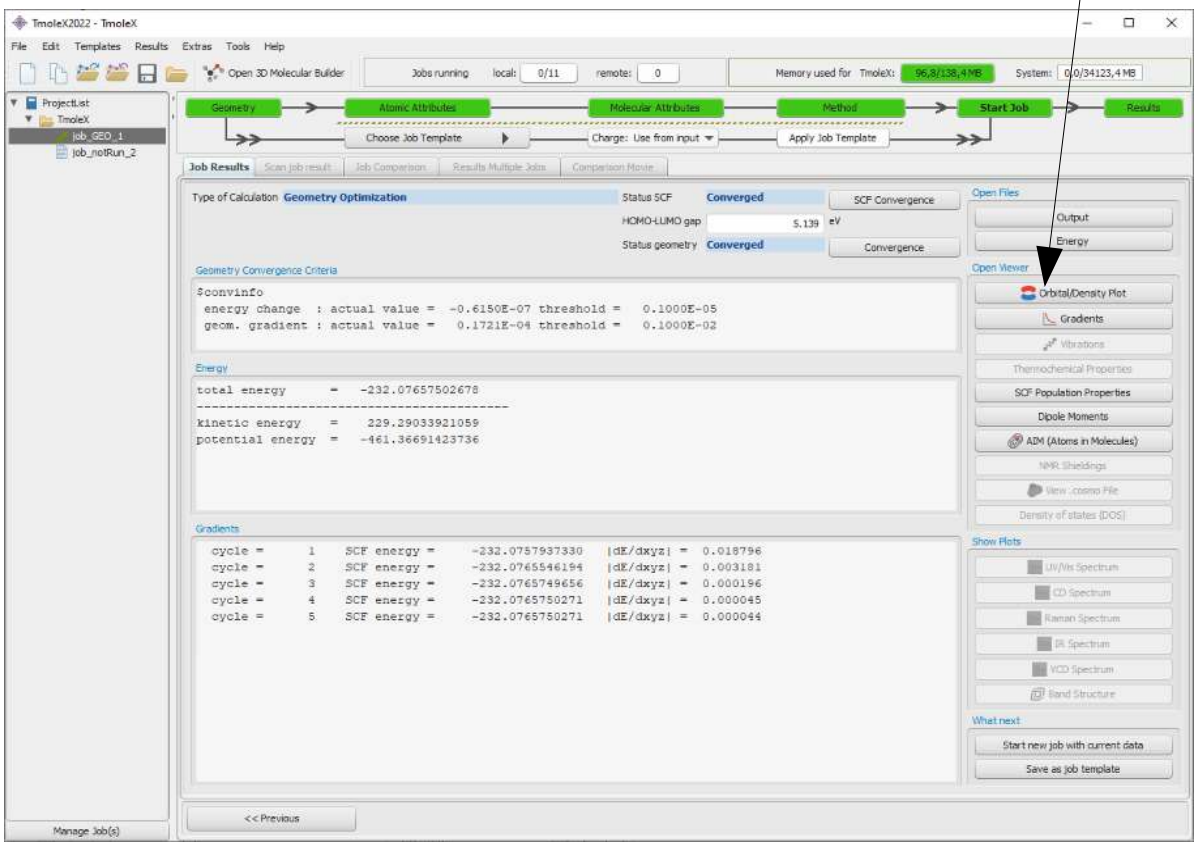


The different geometry can also be viewed as a movie by using the play buttons or moving the slider. The smaller < and > go stepwise back and forth. It is also possible to click on one of the circle in the graphics on the right which plots the total energy vs the geometry cycle.

The 'Calculate bonds' check can be set to re-check the bonds with respect to the atom distances in each step.

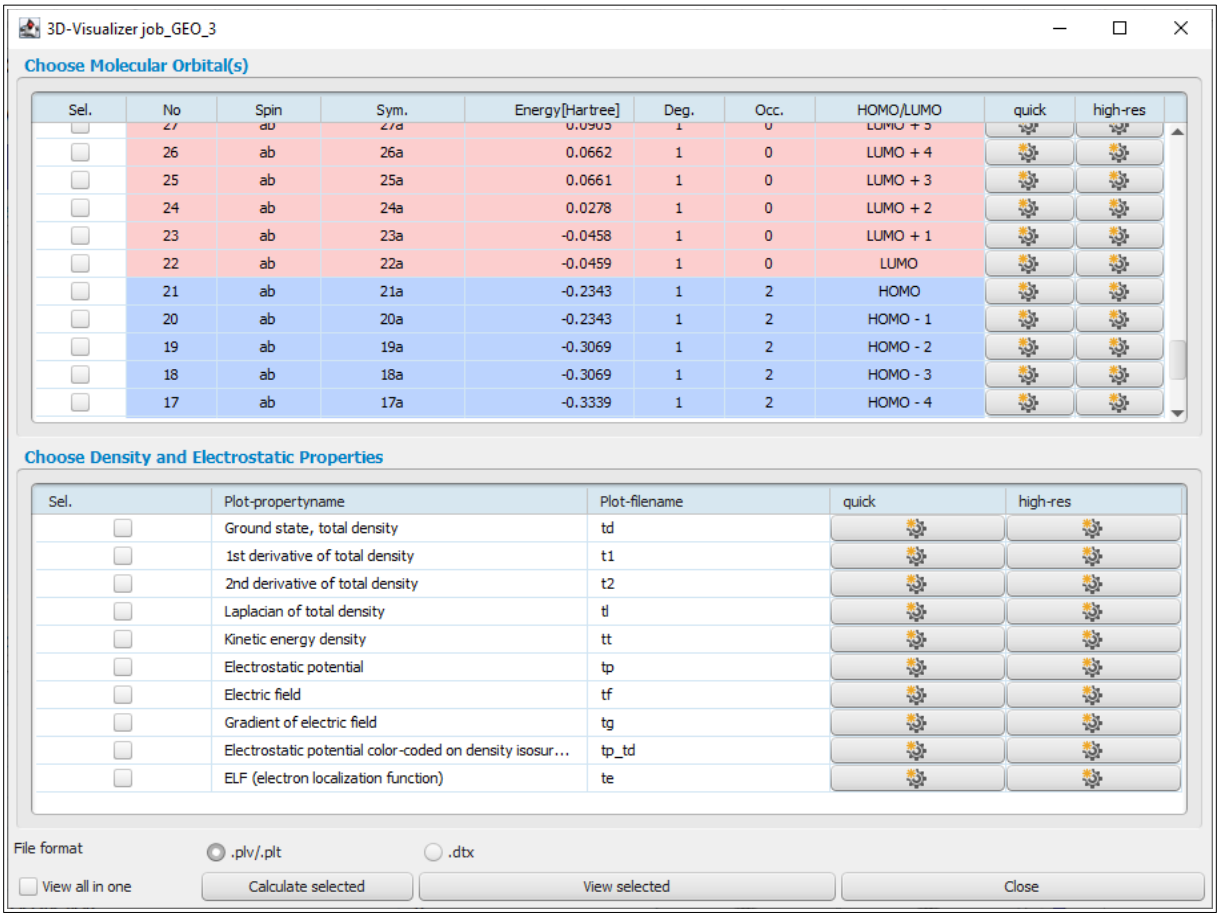
3.13. Surface plots of Orbitals, densities, fields

Once you have converged molecular orbitals, TURBOMOLE offers the possibility to write different properties on a grid for a visual post-processing. This is reproduced in TmoleX interactively starting from 'Orbital/Density Plot'.



3. The 3D visualization

The new window which opens allows you to generate 3D data for visualization as well as to start the 3D viewer with previously or newly generated data:



The upper section is the list of molecular orbitals, the lower section is for electrostatic and density derived properties.

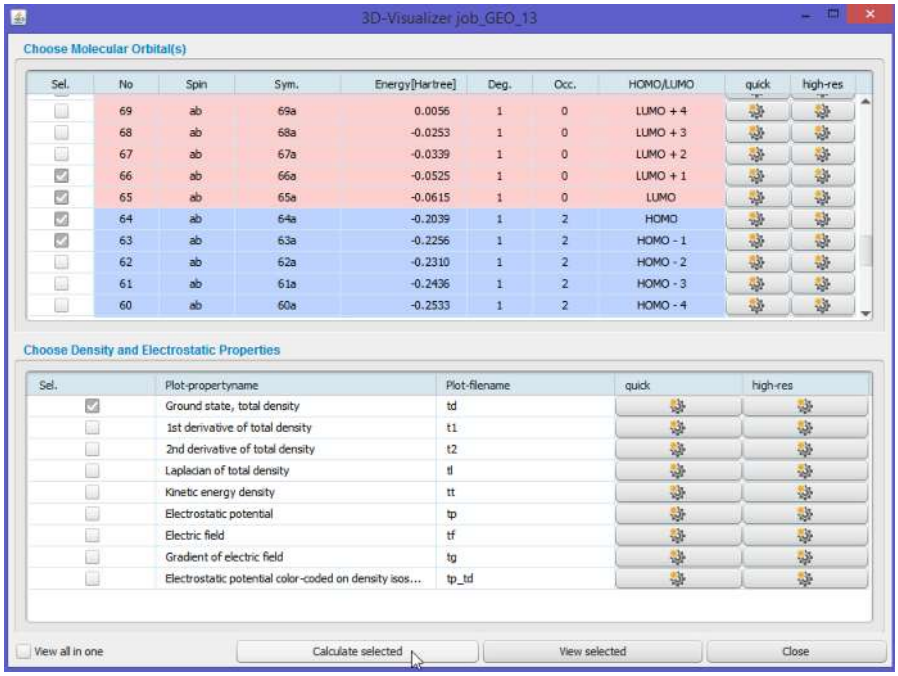
For each of the properties there are two options: 'quick' and a 'high-res'. The first one is to generate the data on a coarse grid to keep the time for generating the 3D files low. This is useful to quickly check the shape and position of orbitals, densities, etc. The second option generates the data on a finer grid, generating smoother surfaces, but can require significantly more CPU time to generate the data. This is recommended for graphics aimed for publication.

There are three possibilities to generate 3D data:

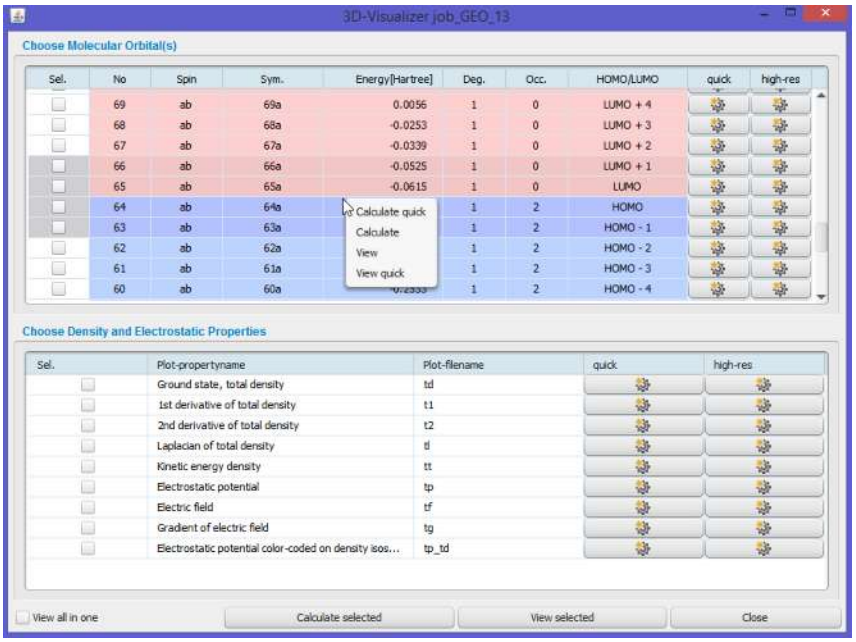
1. directly click on one of the buttons  and TmoleX will directly start to generate the data.

2. set checks in the first column for each orbital and property you want to visualize and then click on 

.



3. as usual, a right mouse menu is available. Simply select one or several lines in the tables and click on the right mouse button.

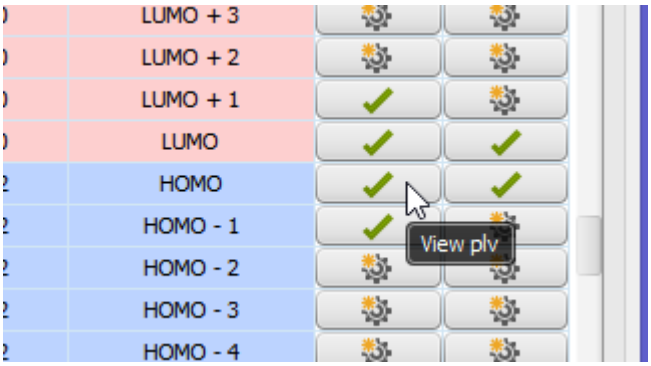


3. The 3D visualization

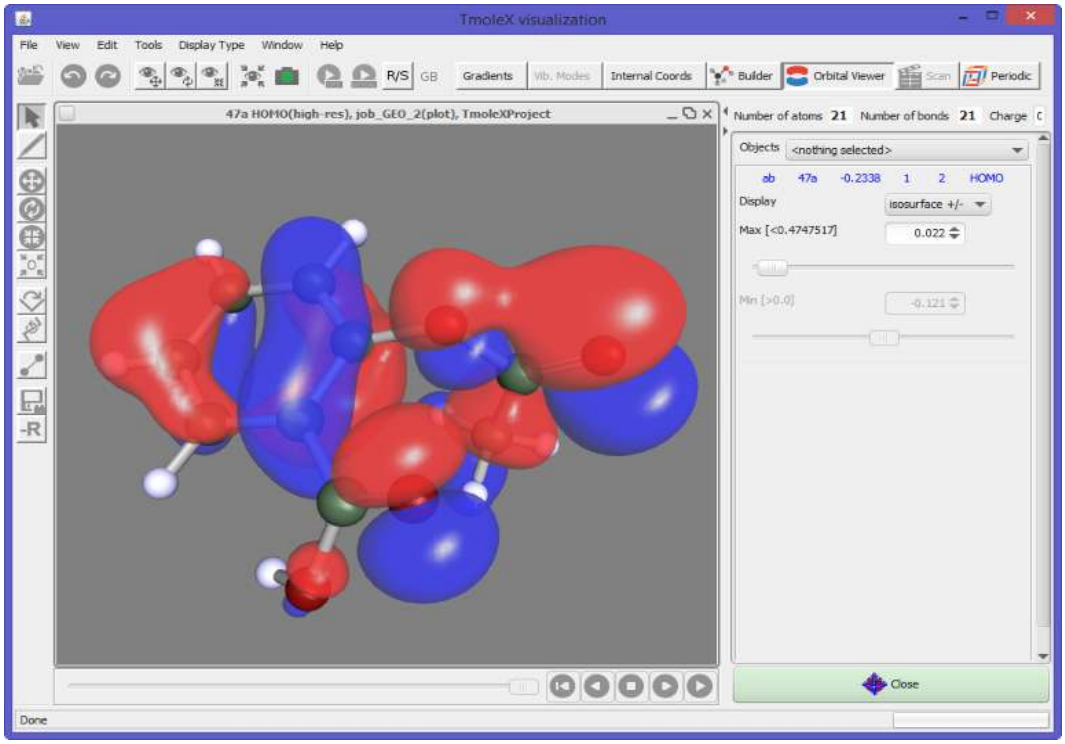
If you choose several options like orbitals, densities, electrostatic potential, etc., each property will have its own progress bar. All properties which require solving integrals like electrostatic properties, densities and their derivatives are quite expensive. Especially for larger molecules, generating 3D plot files can take (much) longer than the single-point calculation or a geometry optimization!

When the calculation is finished, the orbitals or properties can be selected for visualization. Several properties can be displayed in the same window. Check the memory usage of TmoleX from time to time when using this option!

Just click directly on the buttons which have now a green check to show that 3D data is already available for visualization:



Alternatively, use the right mouse button or the selection column and the 'View selected' button.



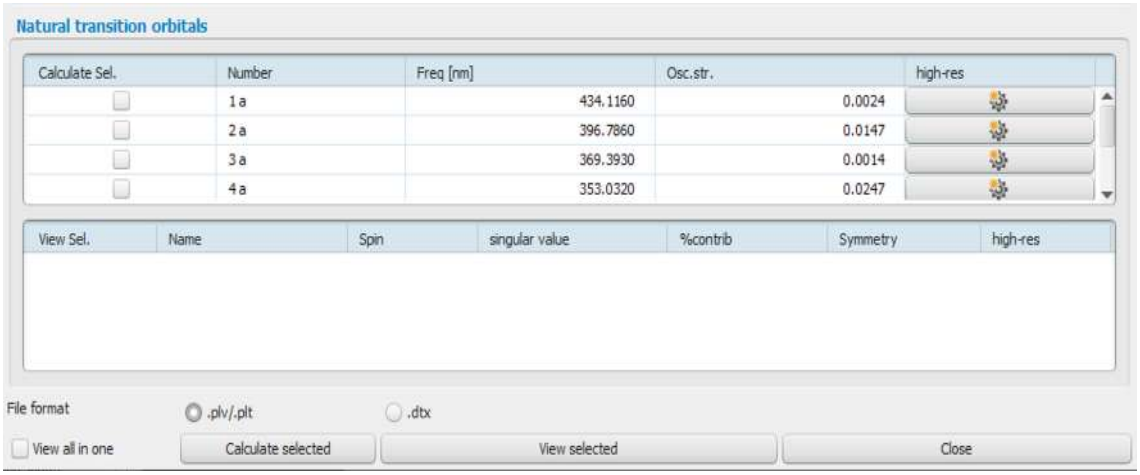
There are a lot of options and possibilities when visualizing 3D surfaces. The most important things are:

- while it can be annoying that the full 3D grid is being calculated, which can be very time consuming, TmoleX can now use this data to generate the 2D surface for a given iso-value on-the-fly.
  Use the slider or the field for the iso-value to change the threshold.

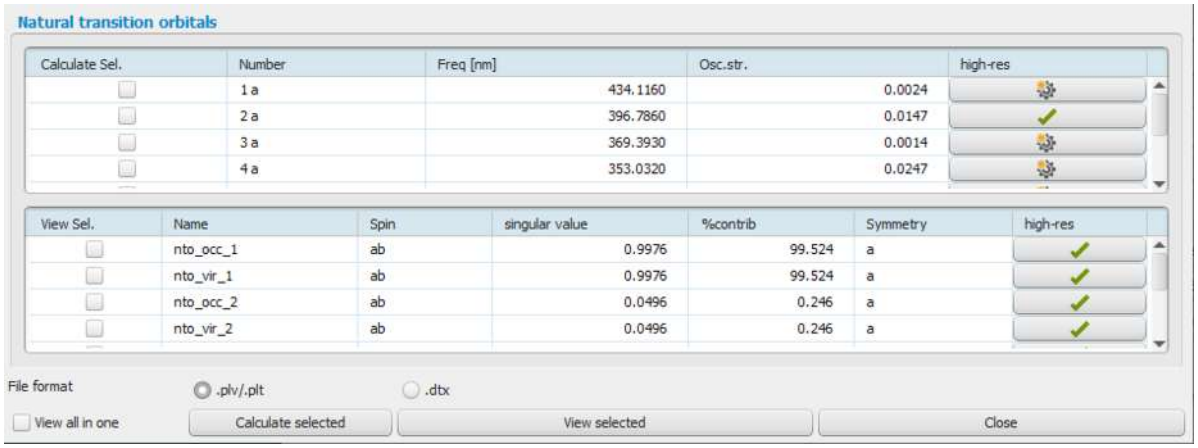
- The 'Display' options are:
  - isosurface – use one iso-value to plot the surface at this value
  - cloud – plot each point of the 3D grid which is within the Min and Max value. The colours of the points depend on the Min-Max range.
  - Isoplot – plot a plane (or an arbitrary surface which can be given as implicit equation like x^2+y^2+z^2-4. Avoid blanks and let the mouse pointer rest over the field to get some help) coloured with the value of the chosen property. Colour depends on the Min-Max range. If you see nothing, not enough, or not enough colours, change Min and/or Max value.
  - Isoplot again – click 'on isosurface' and a file chooser will open. Click on e.g. td.plt (total density) and set an iso-value below. This will result in a 2D surface which represents the iso-value of the density and the colour on the surface is given by the value of the chosen property at that points. Typical example: open electrostatic potential, use the isoplot option, choose td.plt for the total density and set an iso-value. This will give a typical picture of a electrostatic potential on an density-isosurface.
  - Isosurface +/- – plots two iso-densities: one at the positive value and one at the negative value. A typical molecular orbital picture.

3.14. Plotting Natural transition orbitals

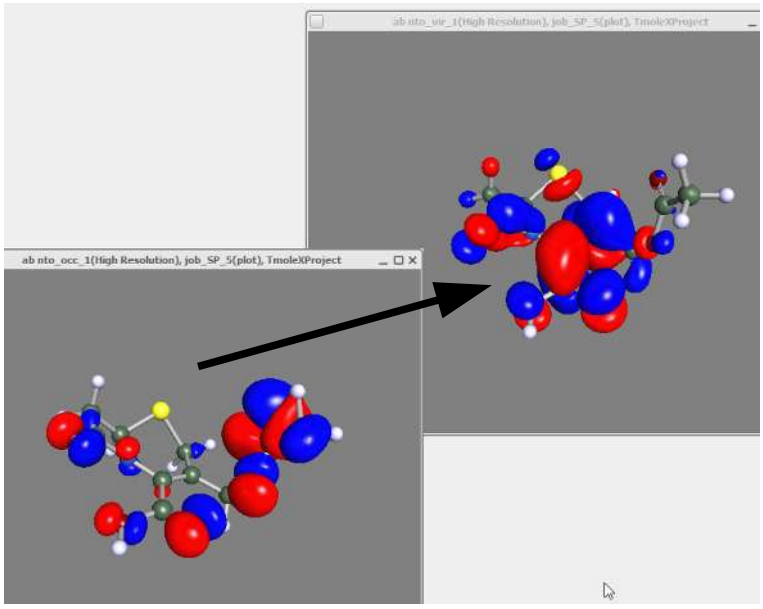
TDDFT natural transition orbitals can be generated for job types which calculate excited states using TDDFT (full RPA or within the Tamm-Dancoff approximation TDA), e.g. after a “UV/Vis and CD (vertical excitations)” job. The 3D orbital plot window will contain a list of excited states and offers the possibility to generate natural transition orbitals for one of those states.



3D plot data (plt files) for NTOs can be generated as usual by clicking on the button of the excited state. The lower part of the table will be filled with the occupied and virtual natural transition orbitals:



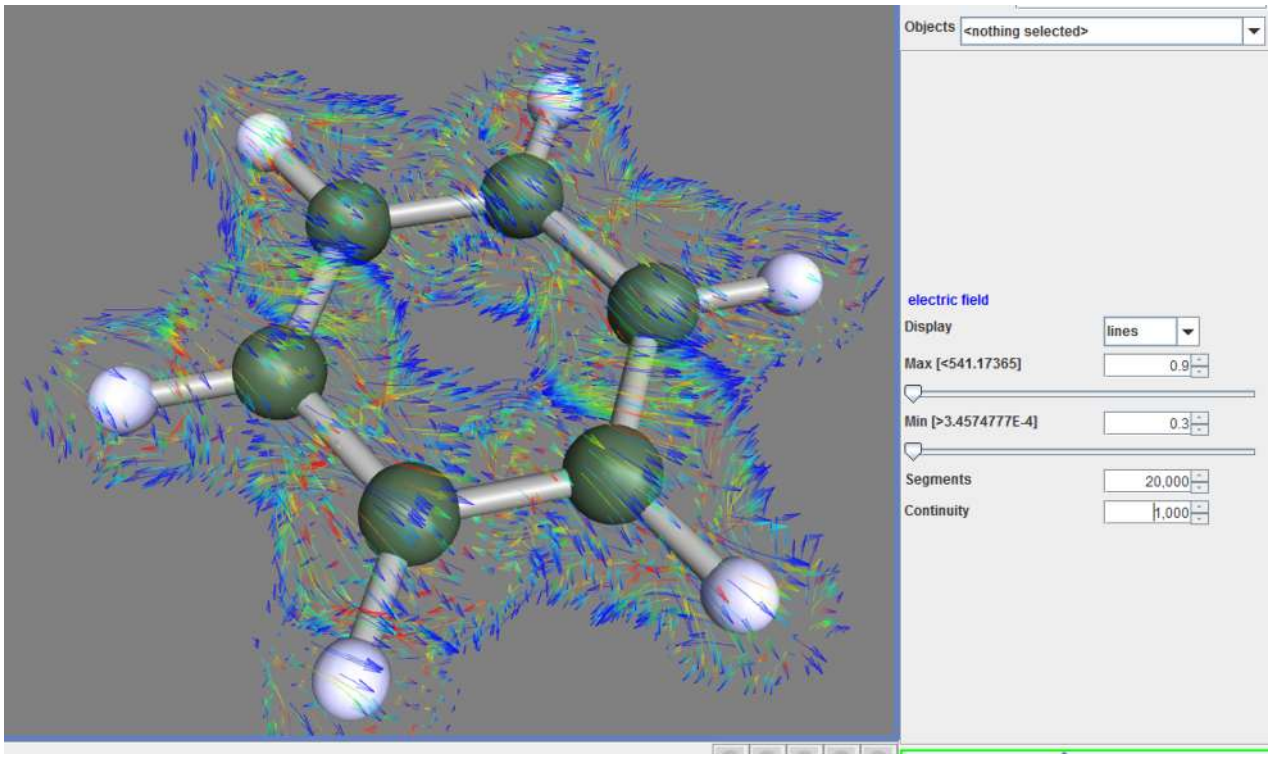
In the example shown above, the 2nd excited state at 396.8 nm has been selected, resulting in several natural transition orbitals. The “%contrib” column shows the percentage of the orbitals contributing to the excited states. The occupied NTOs are named ‘nto_occ_<number>’ and the virtual ones ‘nto_vir_<number’. To visualize the transition (from ‘occ’ to ‘virt’ using the same NTO number), the first two entries can be selected and visualized.



Visualization of natural transition orbitals from a TDDFT excited state calculation. Transition from the nto_occ_1 NTO to the nto_vir_1 orbital.

3.15. Vector plots

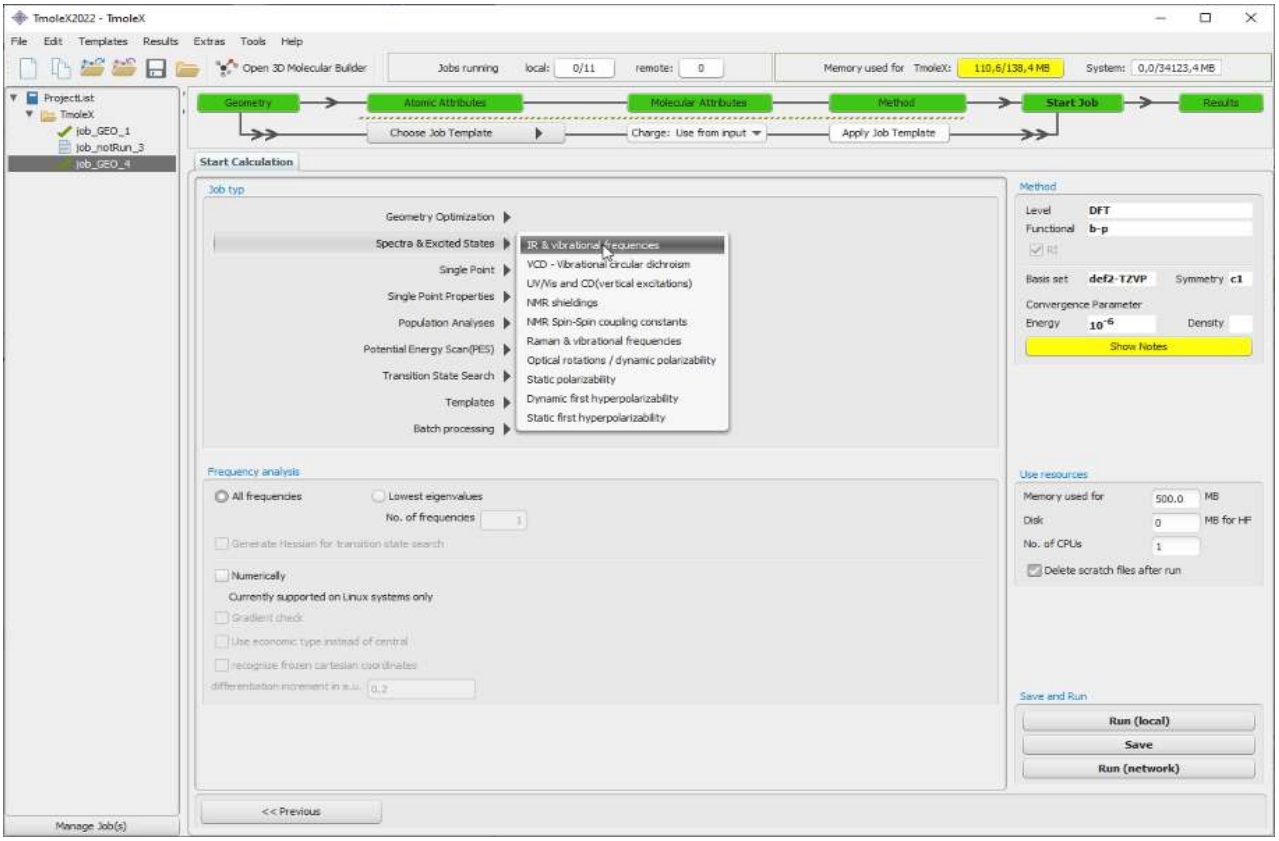
Vector fields can be visualized too, the best way to get an idea of the field depends on the property. Most options are similar to those described above.



4. Properties

4.1. Vibrational frequencies

If you have an optimized geometry, you might want to follow it up by a frequency calculation, either in order to check, if you are in minimum, or because you are interested in the IR spectrum.

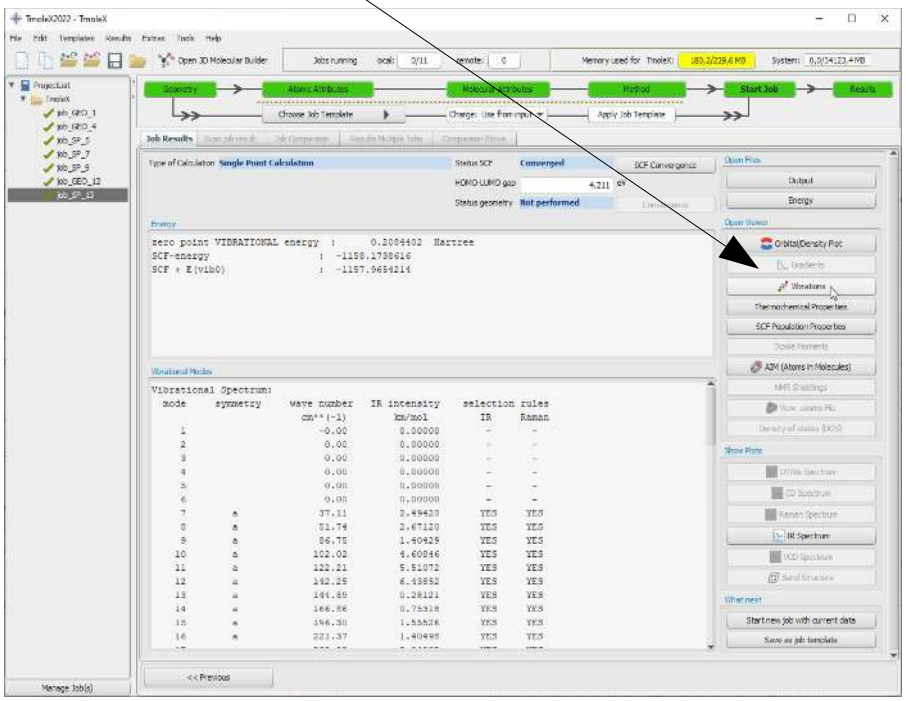


Choose 'IR & vibrational frequencies' in the 'Start Job' panel and click on Run.

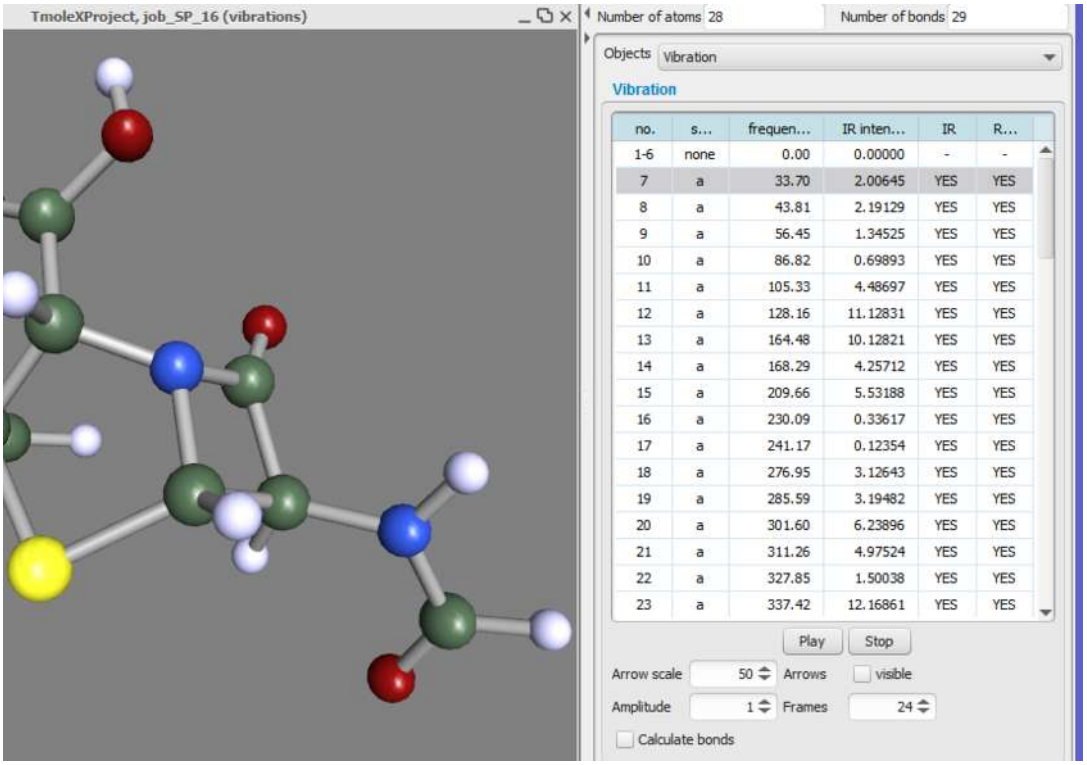
In addition to analytic 2nd derivatives, TURBOMOLE is also able to perform 2nd numerical derivatives for all properties which have an analytic gradient implemented. For post-Hartree-Fock calculations, the numerical option is chosen by default.

NOTE: 2nd numerical derivatives can not be performed with the Windows version of TmoleX. Please submit such jobs to (remote) Linux systems.

To visualize the vibrational frequencies and/or to distort the structure along a vibrational mode, start the 3D Viewer by clicking on the 'Vibrations' button.



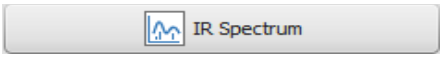
Select a specific mode and click 'play'.



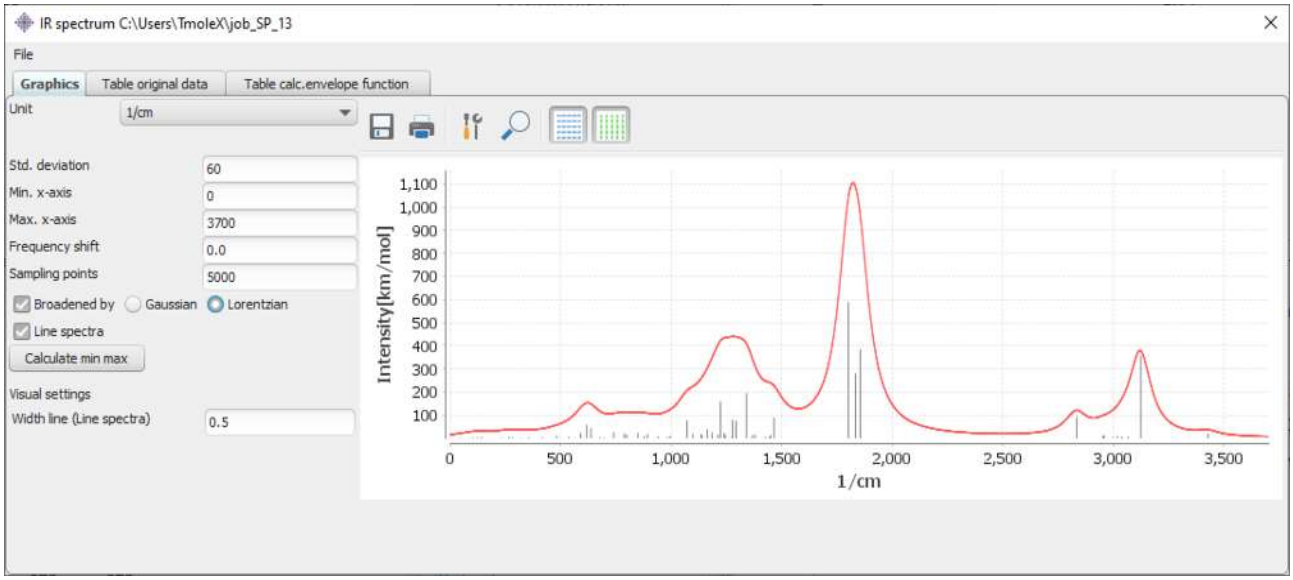
no.	s...	frequen...	IR inten...	IR	R...
1-6	none	0.00	0.00000	-	-
7	a	33.70	2.00645	YES	YES
8	a	43.81	2.19129	YES	YES
9	a	56.45	1.34525	YES	YES
10	a	86.82	0.69893	YES	YES
11	a	105.33	4.48697	YES	YES
12	a	128.16	11.12831	YES	YES
13	a	164.48	10.12821	YES	YES
14	a	168.29	4.25712	YES	YES
15	a	209.66	5.53188	YES	YES
16	a	230.09	0.33617	YES	YES
17	a	241.17	0.12354	YES	YES
18	a	276.95	3.12643	YES	YES
19	a	285.59	3.19482	YES	YES
20	a	301.60	6.23896	YES	YES
21	a	311.26	4.97524	YES	YES
22	a	327.85	1.50038	YES	YES
23	a	337.42	12.16861	YES	YES

Select one or several modes first. Use the play buttons and/or the slider to see the vibration.

4.2. IR spectrum

Use the 

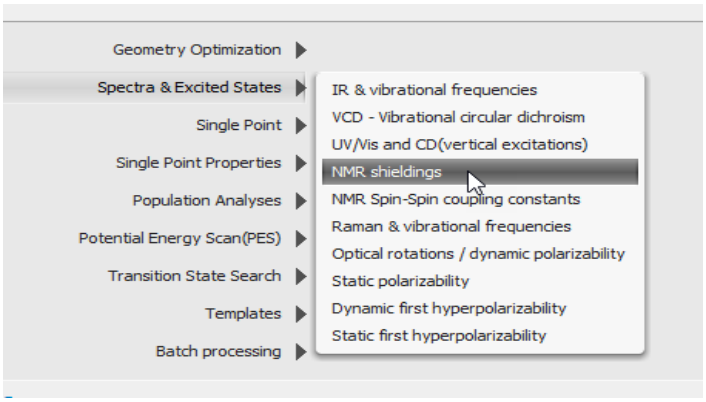
to open the IR spectrum:



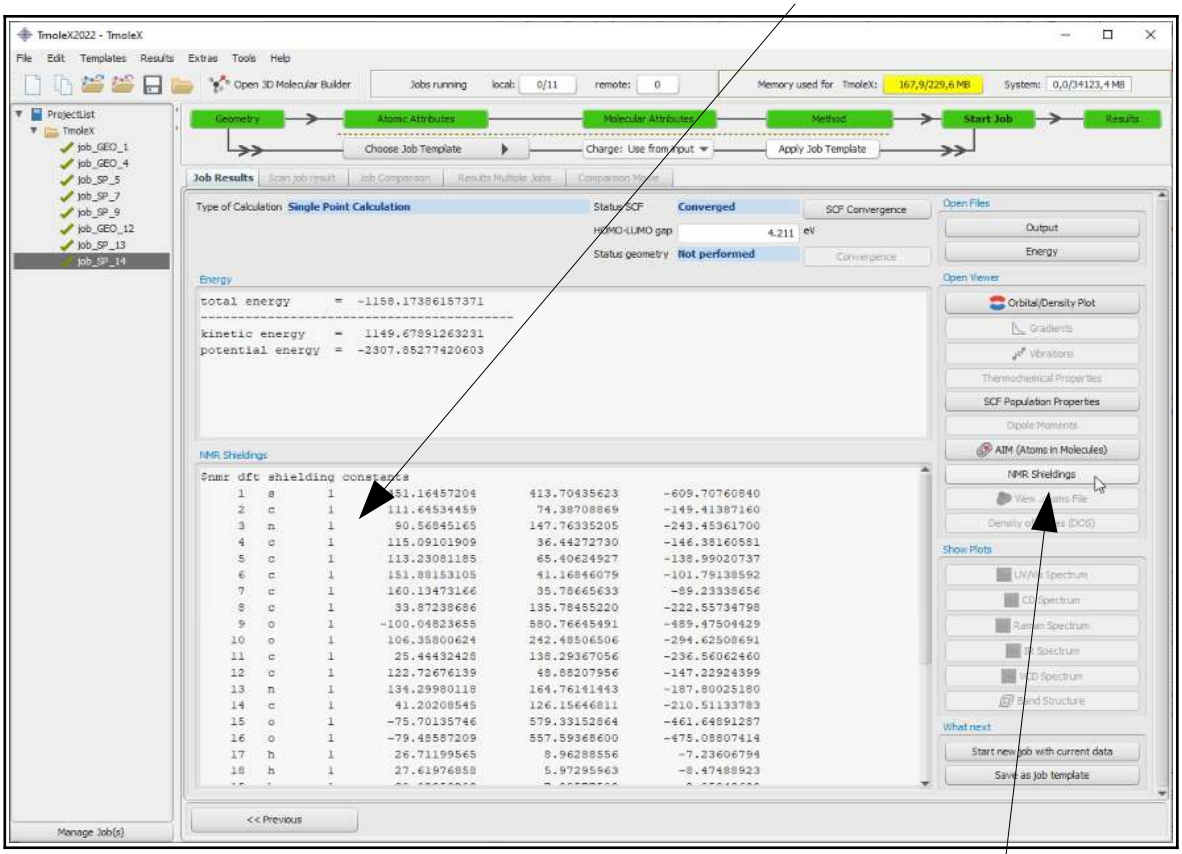
Standard deviation for the broadening Gaussians or Lorentzians, a frequency shift, number of sampling points, etc. can be entered. The tables with the original data (line spectrum) and calculated data (points that define the broadened lines) can be used to copy and paste the data to a spread sheet or a statistics program.

4.3. Nuclear magnetic shielding

For the calculation of nuclear shieldings choose this job type and simply run it.



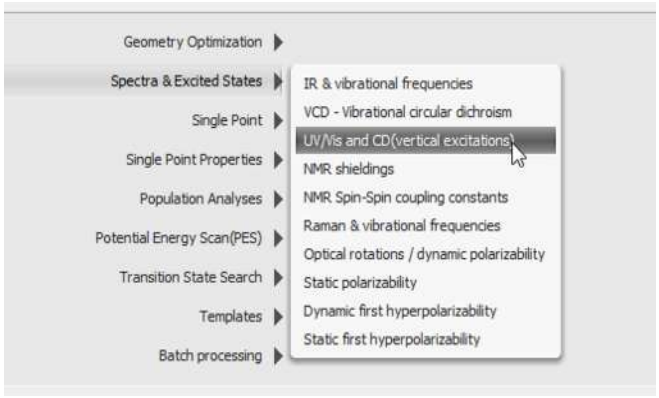
In the 'Results' panel you can see the shielding constants in a text window.



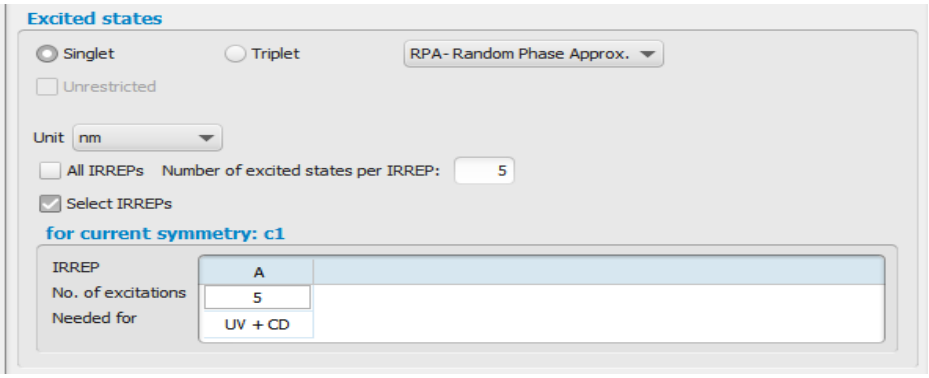
Copy and paste the values to a spread sheet for further usage. Note that to get the NMR shifts, you have to do a calculation also on the reference molecule (like TMS for carbon) with the same method and basis set. The NMR shieldings can also be displayed as labels in the viewer, click on 'NMR Shieldings' to open this view.

4.4. UV/Vis and CD spectra (TD-DFT)

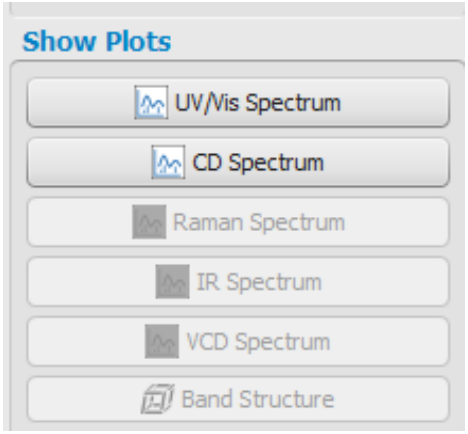
A TD-DFT calculation is set up like a normal DFT calculation. Then choose 'Excited States' in the job selection



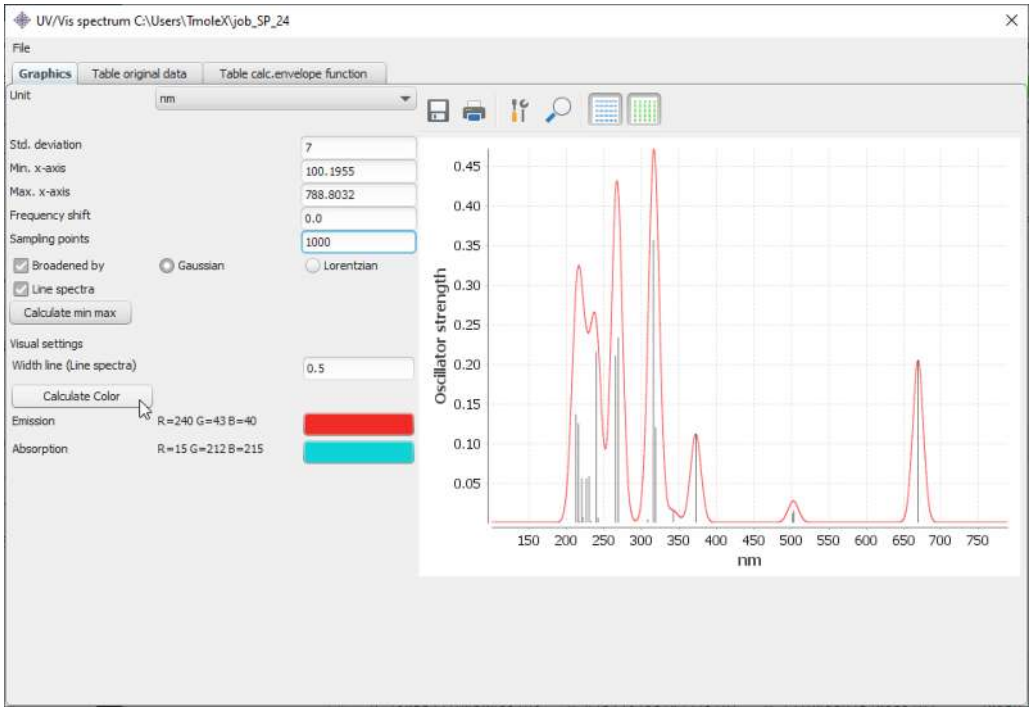
This opens a new option section for the job. Select singlet or triplet, either full (RPA) TDDFT or using the Tamm-Dancoff (TDA) approximation, the number of excitations, and run it.



The spectra can be opened with the CD or UV/Vis Spectrum button.



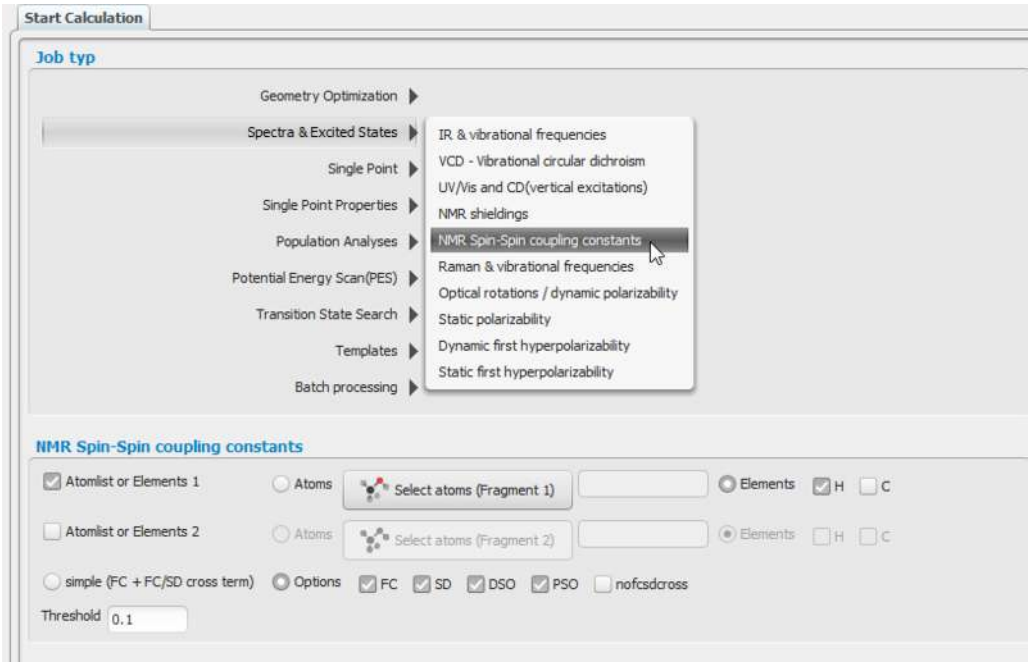
The UV/Vis spectra can be visualized in a similar way to those of IR as described above.



In addition to the spectrum, the colour prediction tool of TURBOMOLE can be used to predict the emission and absorption spectrum. In the example shown here, indigo in water has been calculated, using PBE0 functional. If the number of excited states is chosen such that the whole visible spectrum is calculated, TmoleX will show the predicted colours. Otherweise, TmoleX will print a message that the spectrum is either not complete, i.e. the number of computed excited states was too low, or the prediction is colourless (transparent).

4.5. NMR Spin-Spin coupling constants

Spin-Spin coupling constants at HF and DFT level can be calculated in the Start Job panel by selecting the appropriate entry.



The calculation of all coupling constants between all atoms using the full theory including all terms can be quite time demanding, while usually only a subset of this data is needed to compare with experiment. Hence, it is recommended to select only those atoms or elements, coupling constants are of interest.

- Atomlist or Elements 1
  Select either a list of atoms (using the 3D Builder, 

) or one or several elements (by setting checks in the Elements section).
  Only those atoms/elements will be considered for the spin-spin coupling constants calculation, all possible pairs from the selection are generated.

- Atomlist or Elements 2
  To further reduce the computational effort, this list of atoms or elements defines the nuclei to calculate right-hand side integrals for.

- All four terms to calculate spin-spin coupling constants according to Ramsey can be switched on or off individually:
  - Fermi-contact (FC)
  - spin–dipole (SD)
  - paramagnetic spin–orbit contributions (PSO)
  - diamagnetic spin–orbit contributions (DSO)

  In addition the FC/SD cross contributions are included in the full tensor unless the ‘nofcsdcross’ option is activated.

- Only coupling constants larger than the selected threshold (default is 0.1 Hz) are printed.

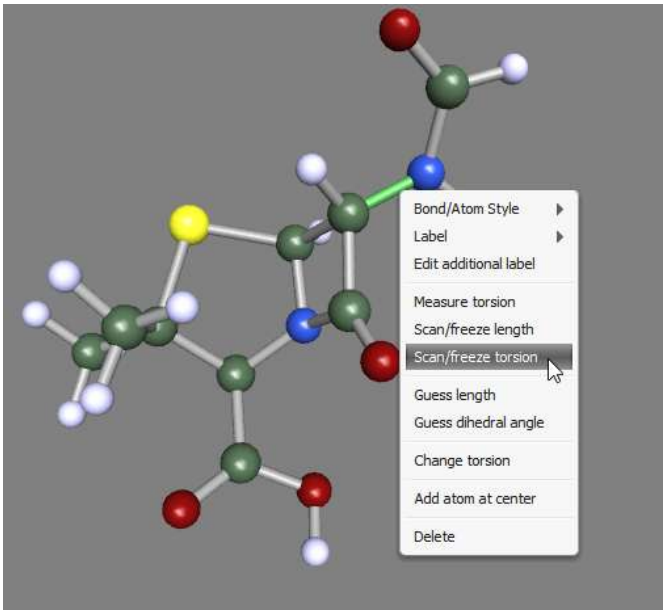
5. Constrained optimization and Scan jobs

5.1. Defining fixed internal coordinates

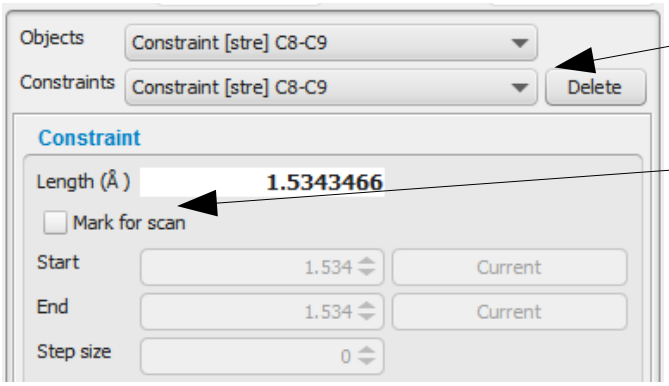
TmoleX allows to define internal coordinates. Bonds, bond angles and torsions can be fixed within the builder.

To define a constraint, select one, two or three bonds:

- select one bond, click on the right mouse and choose Scan/freeze length:



On the right the options for freezing a bond length are show:

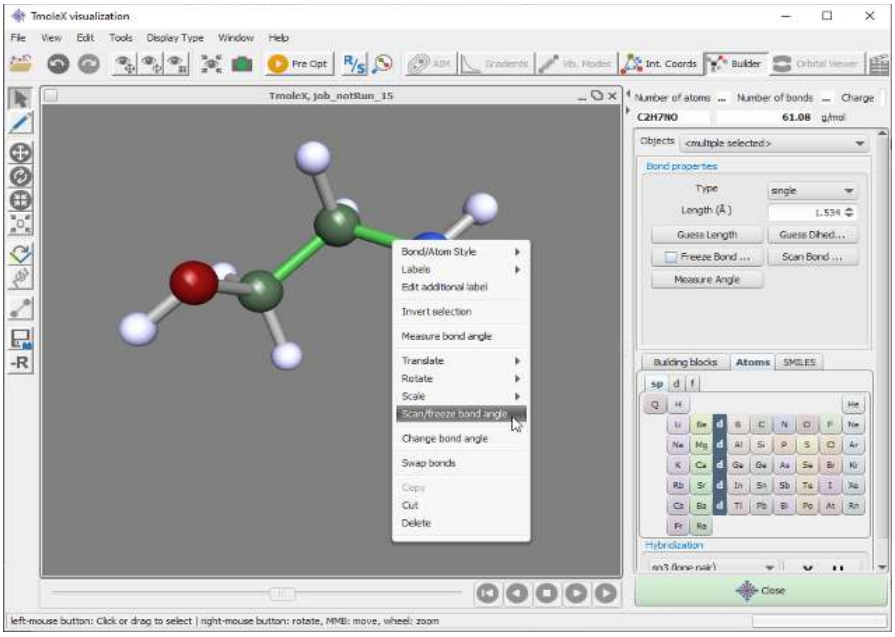


To delete constraints, select here and delete.

To scan along the coordinate, activate the check box and set minimum, maximum

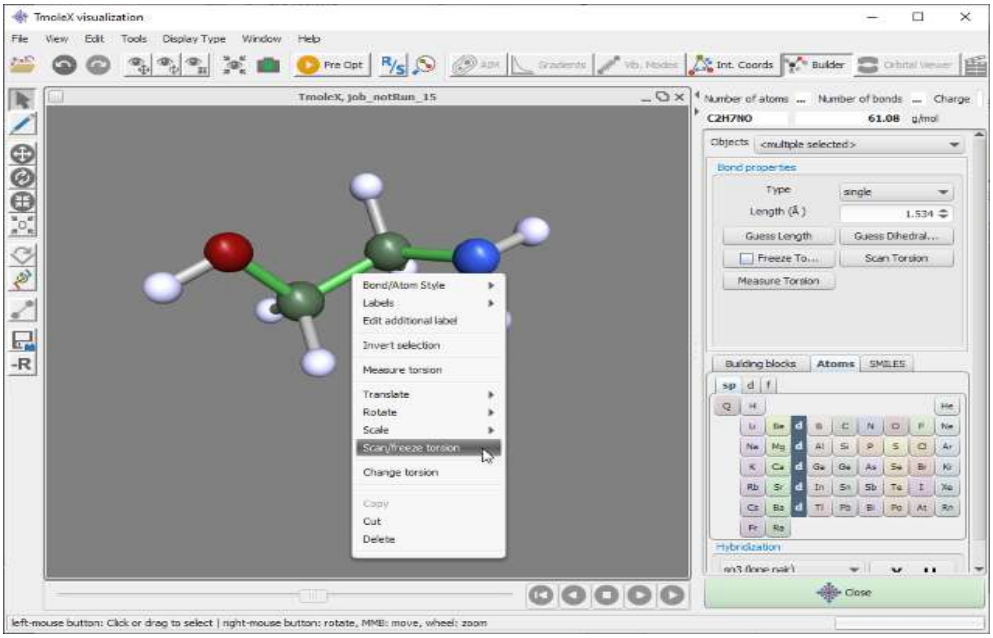
the step *width* (not the number of steps!)

- Select two adjacent bonds, click on the right mouse button and use the Scan/freeze bond angle option:



Again, on the right side you will get the same options for scan jobs as shown above.

- Select *one or three* bonds to freeze a torsion. If you just select one, TmoleX will take just one of the possible torsional angles. If you use the 'Change torsion' or the corresponding button on the left side of the window, the value of the internal coordinate is shown and can be changed as usual with dragging the mouse while keeping the left mouse button pressed.



5.2. Use internal coordinates

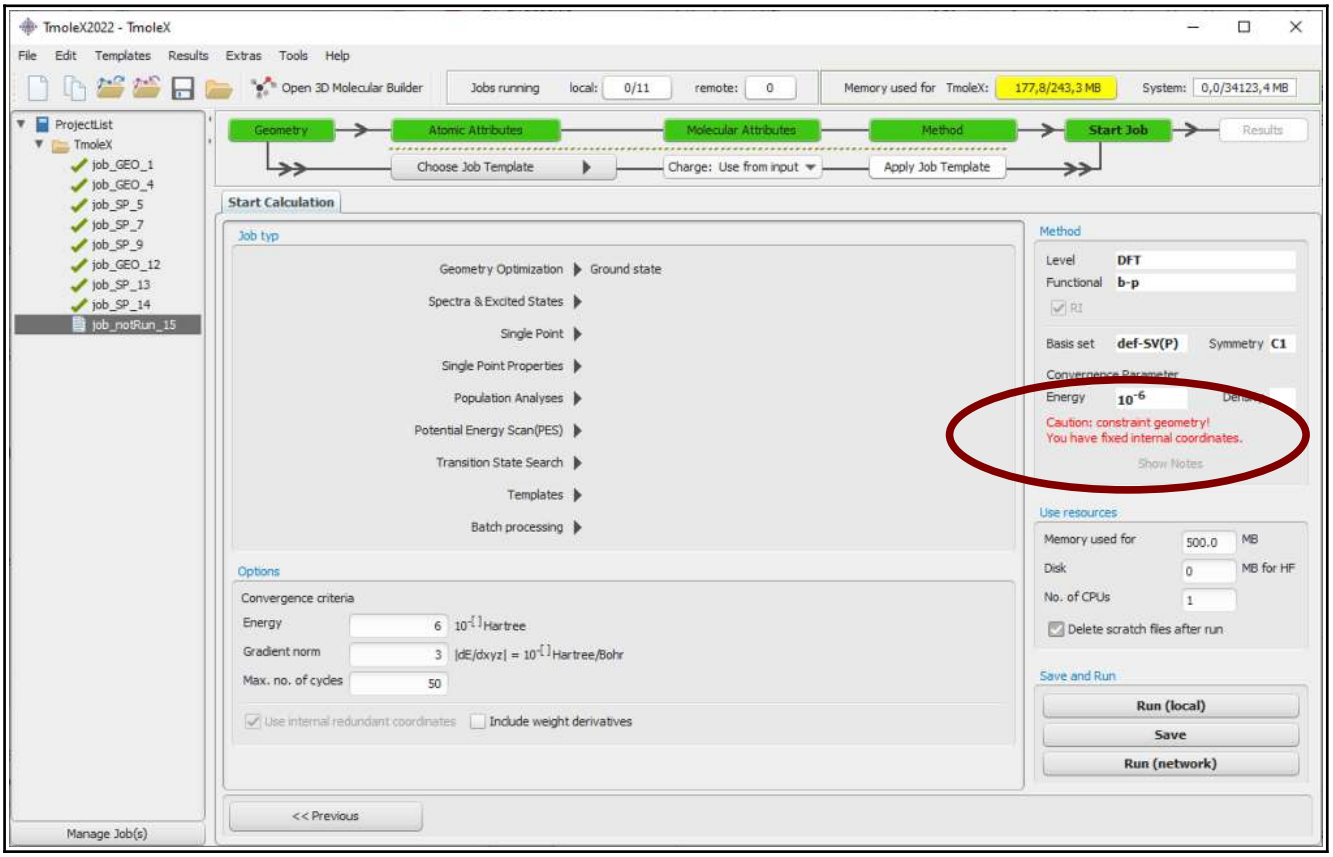
TmoleX will automatically generate a list of internal redundant coordinates if you accept that when being asked for. If you use constraints or scan jobs, internal redundant coordinate usage must be activated when starting a geometry optimization!

Be careful with linear combinations (several lines of definitions for one internal coordinate) – while they can be fixed, this is usually not what one really wants!

There is a possibility to visualize the set of internal redundant from within the Geometry panel.

5.3. Start constrained optimization

A constrained search is automatically done if a usual geometry optimization job is started while having internal (or Cartesian) coordinates fixed. TmoleX will show a message in the panel whenever such jobs are started:

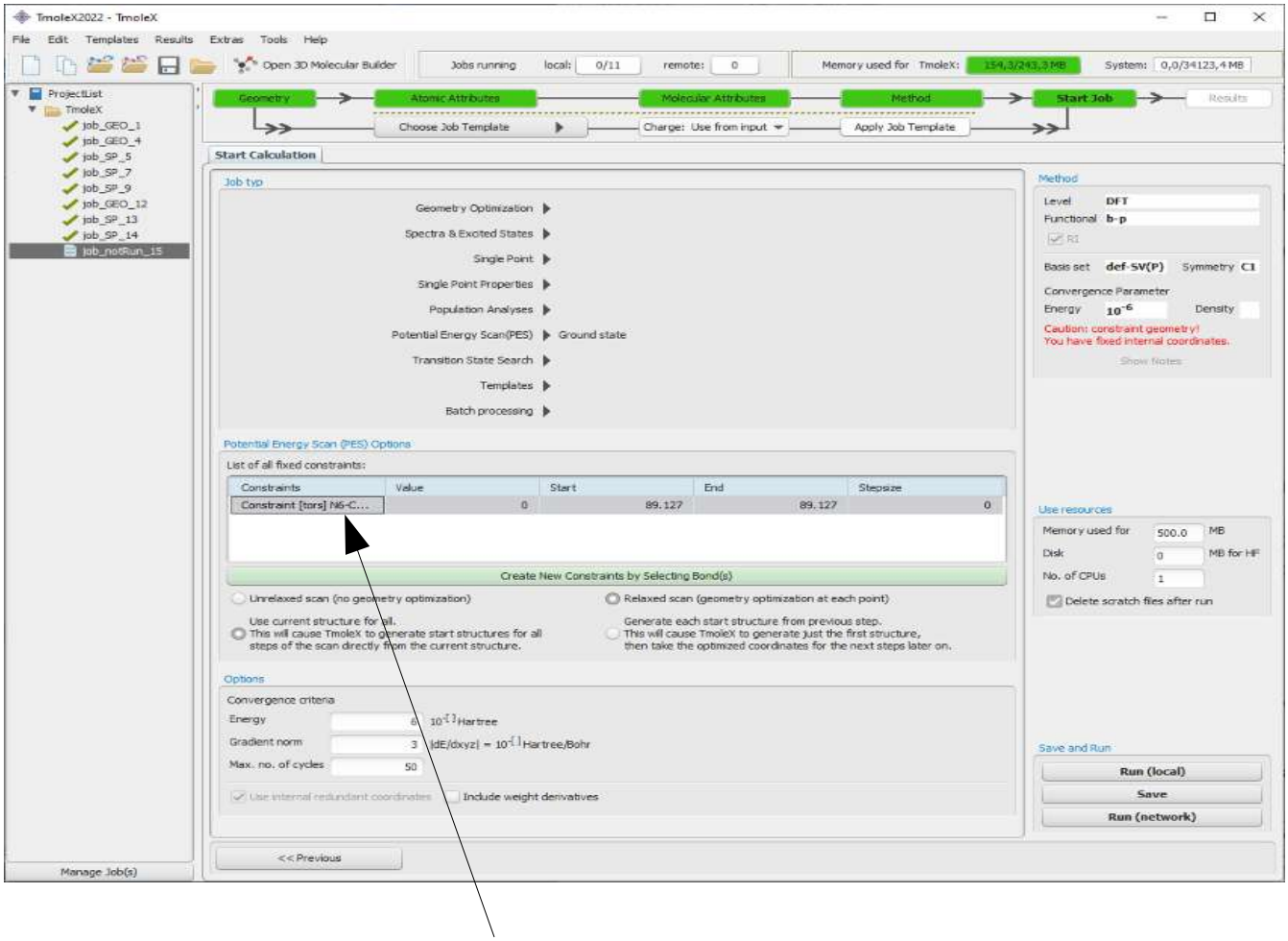


If you have frozen bonds, angles or torsions, make sure to use internal redundant coordinates, otherwise your settings will be ignored! As long as you have constraints defined it is not possible to run an optimization without internal coordinates.
Constrains are always applied in this section, no matter if ground or excited states calculations are done, minimum search (geometry optimization), potential energy scans, or transition state searches are started.

5.4. Scan along an internal coordinate

The potential energy scan (PES) method can be applied if internal coordinates are defined, and at least one of them is defined as fixed. Scan will run a couple of geometry optimizations for a range of values of an internal coordinate.

Note that **all** fixed internal coordinates will be kept fixed, not just the one that you have defined to be scanned along! For a one-dimensional scan job, only one internal coordinate should be defined as fixed.

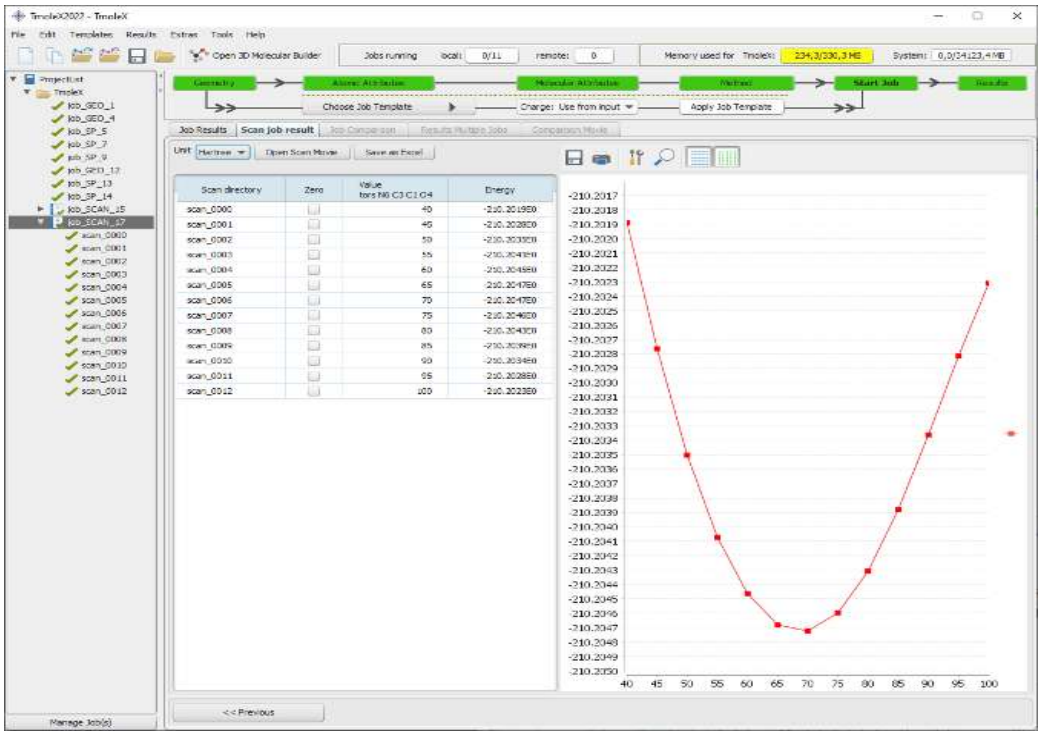


The list of fixed internal coordinates is shown in the PES scan Options section. To define a new fixed internal coordinates, use the Create New Constraints by Selecting Bond(s) button. This is not needed if you did that in the builder already.

The different options how the start geometries are generated are described in the panel itself. Unrelaxed scans and relaxed scans are possible (single-point or geometry optimization calculations will be done).

We recommend to use the 'Use current structure for all' option, because if one of the steps fail, the remaining jobs will have problems too otherwise.

The job can then be started as usual, also as a remote calculation. A typical result is shown here:



The final optimized structures are stored for each of the scan points in a multi-coord file – similar to the gradient view. This can be viewed like a movie with the button Open Scan Movie.

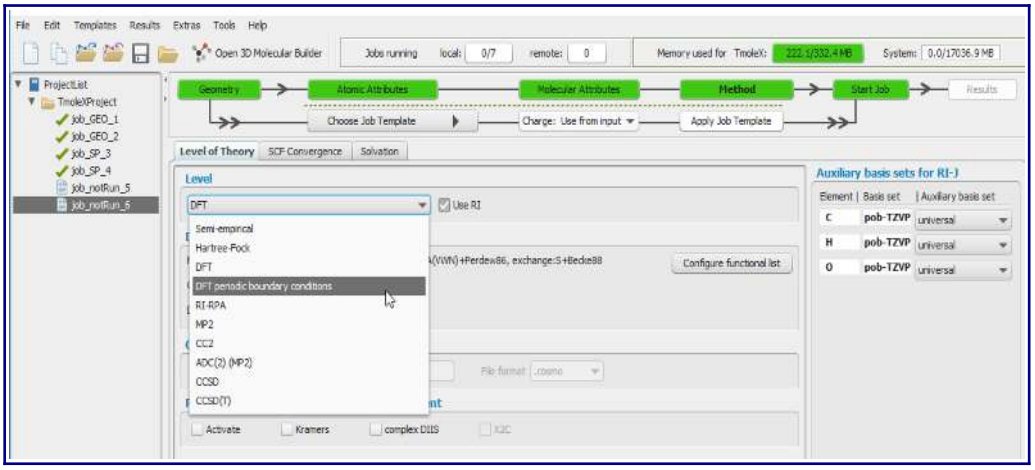
5.5. Scan along several internal coordinates

The number of internal coordinates which can be used for scans is only limited by technical issues. If, for example, the number of constraints is – relative to the number of degrees of freedom – very high, TmoleX might not be able to generate all intermediate structures of all combinations due to steric reasons.

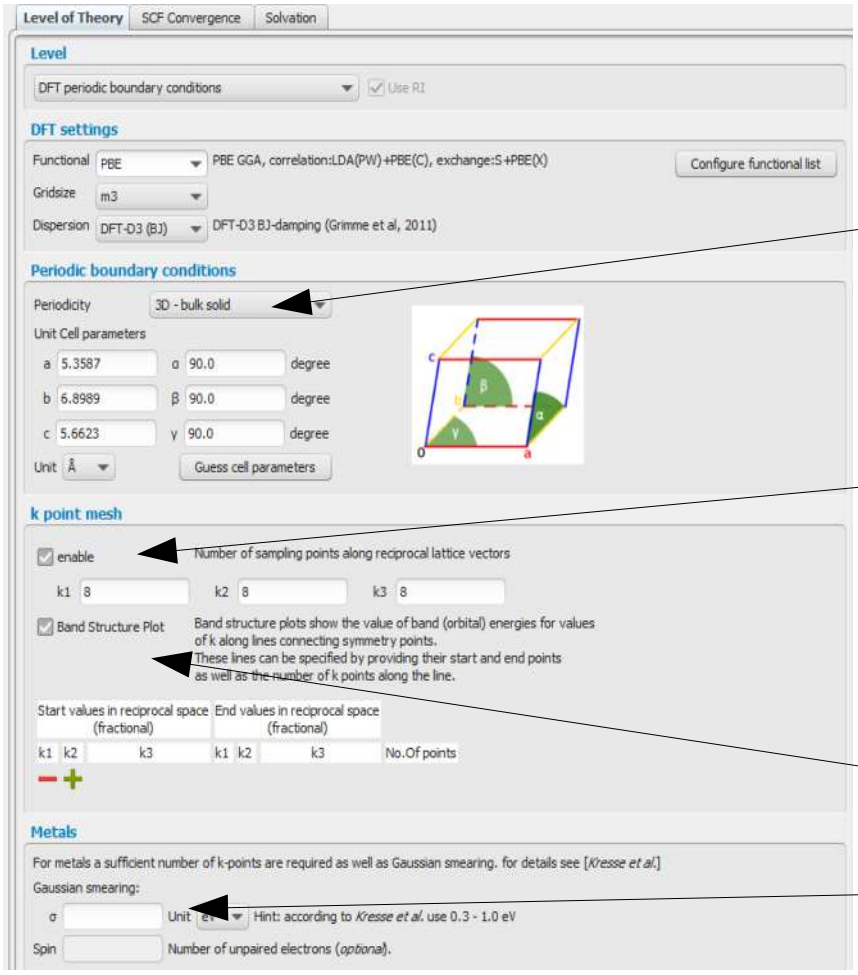
It is also possible to combine constraints (like fixing an angle to a certain value) with scans. If the number of internal scan-coordinates is larger than one, TmoleX will not show a graph of the result but just the table with the values of each internal coordinate and the total energy in the last column. This table can be exported to a spread sheet program or other data analysis tools.

6. Periodic boundary conditions

To enable periodic boundary conditions, just choose the appropriate level from the Method panel:



This opens a bunch of options.



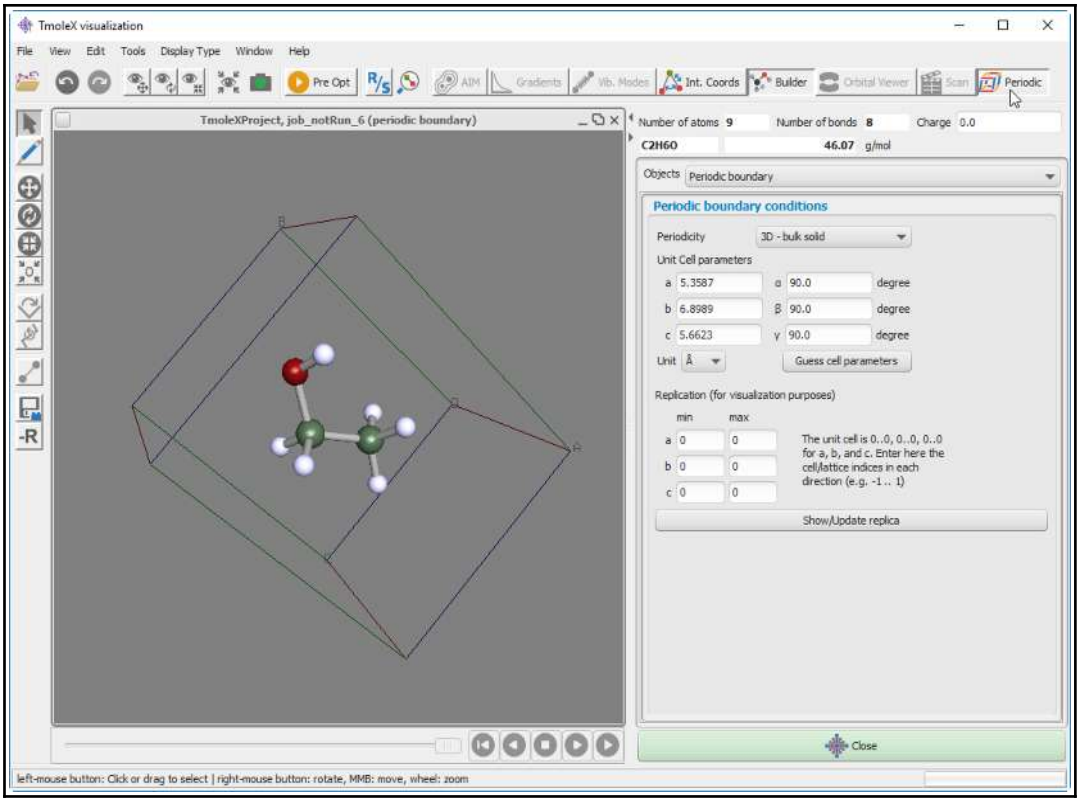
Select periodicity: 1D, 2D or 3D

To use k-points, just enable the check and tell TmoleX how many k-points you want in each direction in k space.

For a later band structure plot, enable the check here and set the path in reciprocal space (from → to) Check your text book for location of symmetry points like L, K, ...

Metals need fractional occupation numbers. Gaussian smearing is being used, set the width of the smearing here.

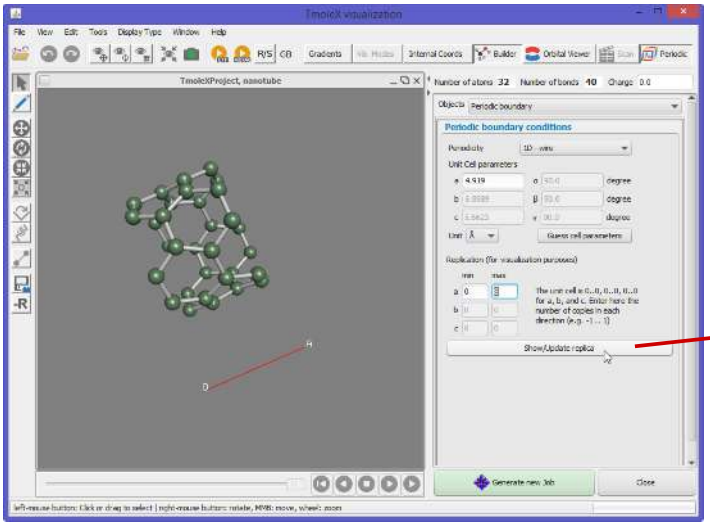
Alternatively, the cell parameters can also be modified in the Builder by clicking on the 'Periodic' button.

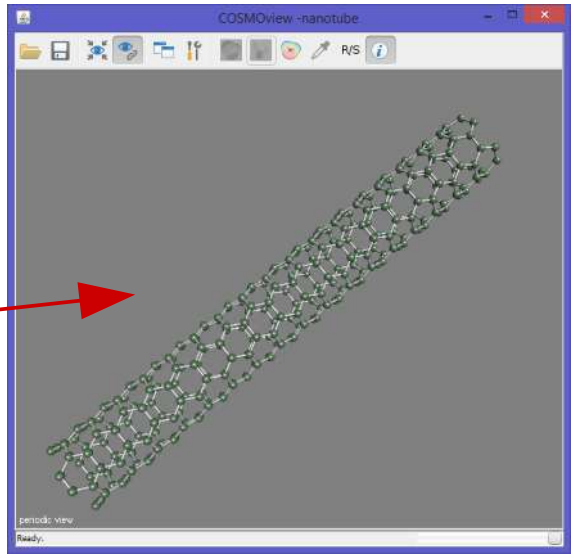


This will add the unit cell within the Builder.

Hint: click on the 'Center molecule' button  to centre the molecule in the middle of the unit cell.

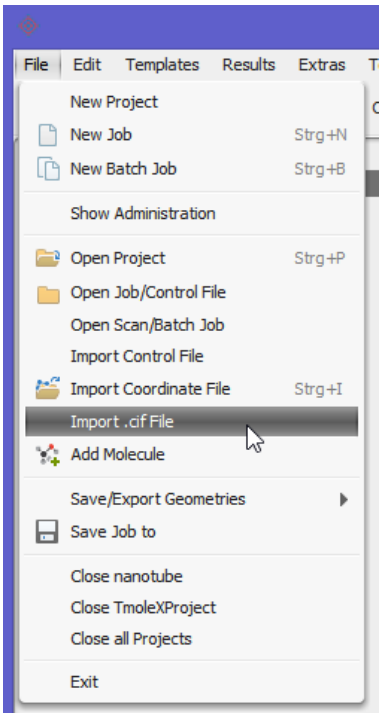
Set the cell parameters and select the number of replications in each direction. TmoleX will open a new viewer with the number of replications of the unit cell. This structure can be exported as picture or coordinate file.





6.1. Import of cif files

TmoleX can import cif files (Crystallographic Information File) using the File menu:



The coordinates and the cell parameters are imported and the builder is opened to visually check the settings. Note that the cif file format is very versatile and TmoleX supports only a limited number of known keywords.

One of the following keywords *must* be present in the cif file:

symmetry_equiv_pos_as_xyz

or

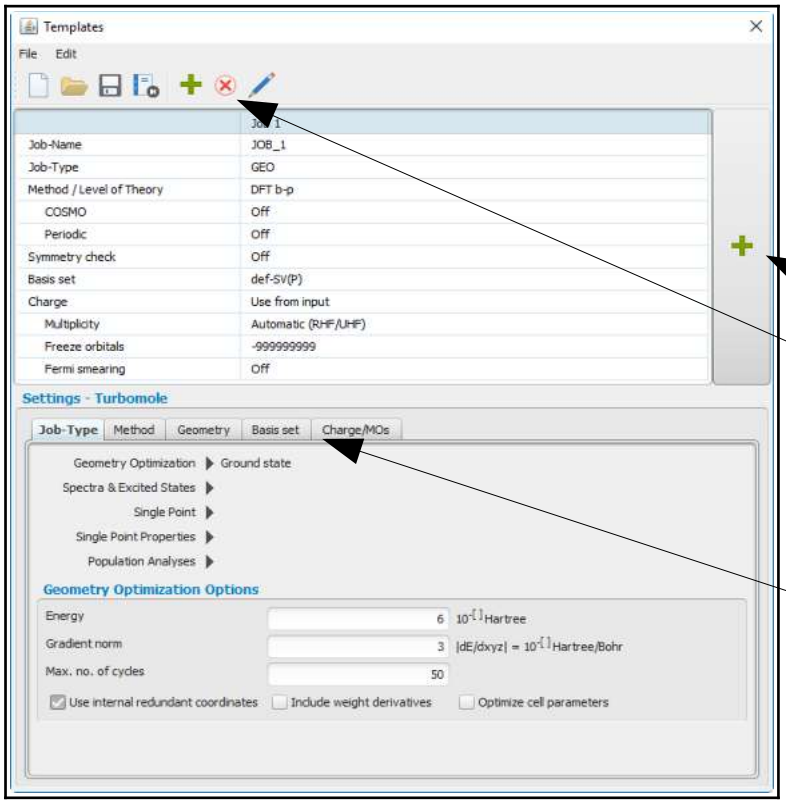
space_group_symop_operation_xyz

7. Job Templates

7.1. Define job templates

TmoleX offers the possibility to save the most important settings of your jobs like basis set, method or job type to a template. This helps to reduce the time needed for an input preparation if the same kind of job has to be performed for a set of molecules.

To read, modify or create a job template, choose 'Templates' from the TmoleX menu:



Use File menu or the open button to read in existing template to modify or apply.

Create new job template.

Change the Job name using

Click on to add a job to the workflow.

Click on to remove a job from the workflow.

The settings here are the same as in the different TmoleX panels.

Save the template or

apply it without saving.

At this point, *TmoleX does not check for consistency* of different settings. So please do first a usual job, run it, and check if the combinations are possible.

Defining multiple jobs in one job template will tell TmoleX to run them one after the other, using the coordinates of the preceding step.

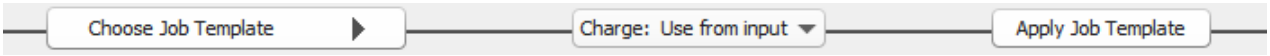
job 1 —*Use final coordinates of job 1*→ job 2 —*Use final coordinates of job 2*→ job 3 —*Use final coordinates of job 3*→ ....

A typical work flow would be:

RI-DFT geometry optimization with small basis set → frequency analysis → geometry optimization with larger basis set → CD + UV/Vis spectra at DFT level→ single point energy calculation with post-Hartree-Fock method.
The template will have to be named when saving and can be found in the pull-down menu afterwards.

7.2. Apply job templates

To use a template, just choose a saved template from either the template tool bar



or from the menu 'Templates'. TmoleX will alter the settings accordingly, generate start orbitals, and brings you directly to the start-job panel.

The molecular **charge** can be either those of the template (if the Charge pull-down menu is let empty) or whatever the user chooses in the tool bar.

Generate a new job, read in or build a molecule. Then select a template (set the charge or use the default) and click on Apply Job Template. TmoleX will prepare the input and jump to the start job panel:



	job 1	job 2
OPT+FREQ.xml		
Job-Name	Job1	Job2
Symmetry check	on	on
Basis functions	def-SV(P)	def-SV(P)
Charge	used from input	used from input
Multiplicity	Automatic (RHF/UHF)	Automatic (RHF/UHF)
Freeze	off	off
Level of theory	DFT+Disp DFT-D3 BJ-damping (Grimme et al, 2011) b-p	DFT+Disp DFT-D3 BJ-damping (G...
Cosmo	off	off
Job-Type	GEO	FREQ

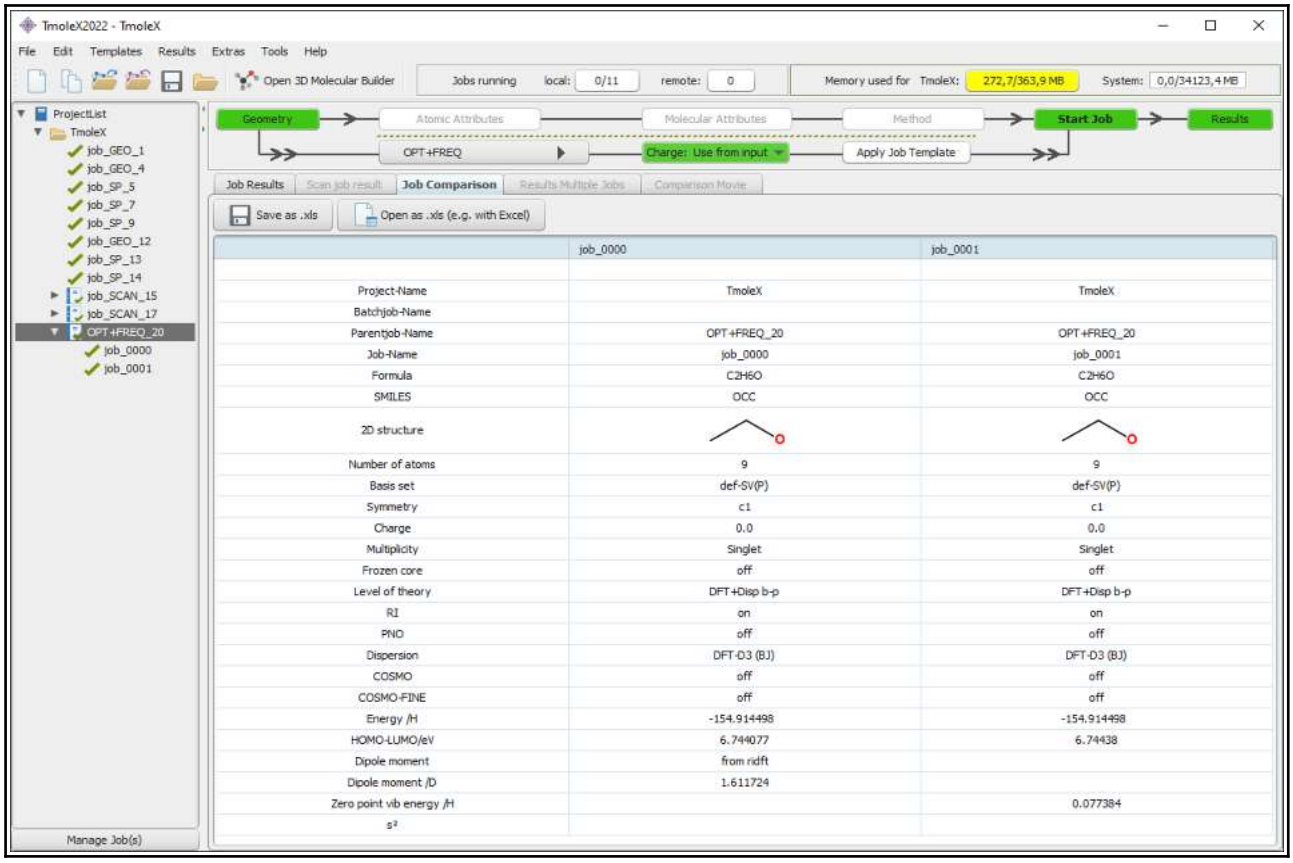
The job can either be started on the local system or submitted to a remote machine using the Run(network) button.

While the job is running, the icons in the job tree will change. The job status during the run can also be displayed and visualized:

Here the first job, a geometry optimization, is running. The status of this job is therefore printed as Energy vs. the geometry cycle.

7.3. Results of job templates

Multi-template jobs will create sub-directories for each individual job. Selecting an individual job will present the results of this step as for a usual non-template job. Selecting the template itself in the job tree will give a summary as table:



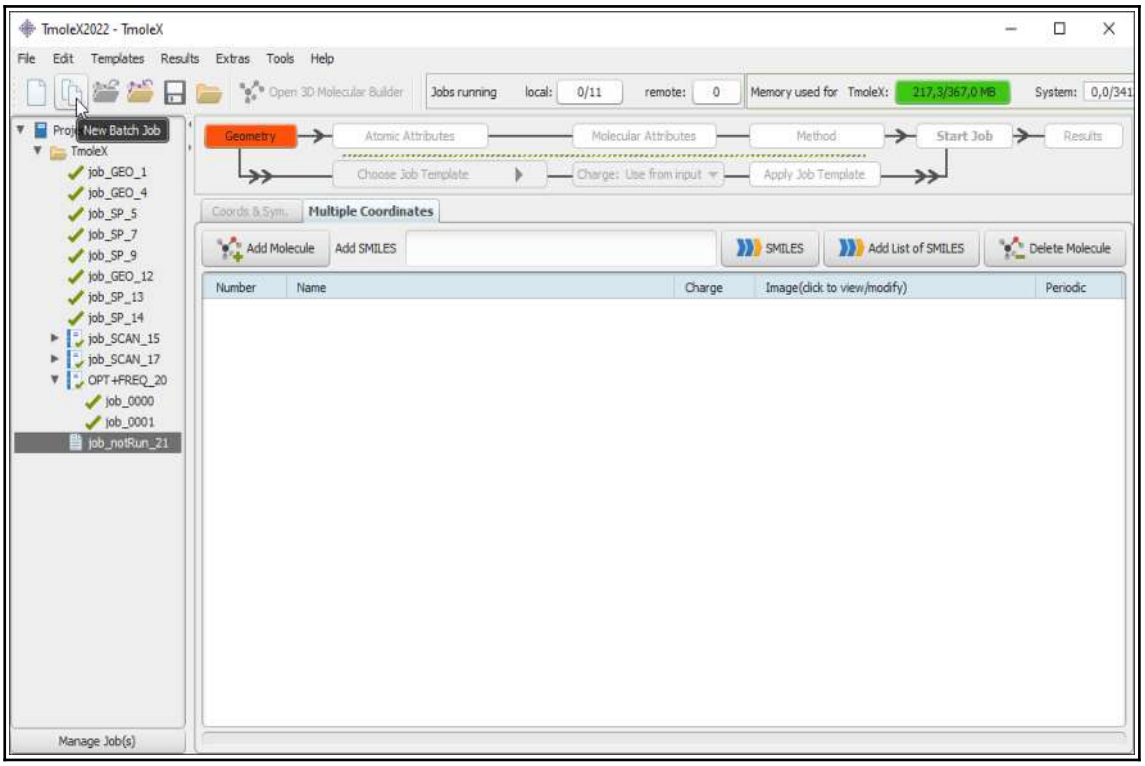
	job_0000	job_0001
Project-Name	TmoleX	TmoleX
Batchjob-Name		
Parentjob-Name	OPT+FREQ_20	OPT+FREQ_20
Job-Name	job_0000	job_0001
Formula	C2H6O	C2H6O
SMILES	OCC	OCC
2D structure		
Number of atoms	9	9
Basis set	def-SV(P)	def-SV(P)
Symmetry	c1	c1
Charge	0.0	0.0
Multiplicity	Singlet	Singlet
Frozen core	off	off
Level of theory	DFT+Disp b-p	DFT+Disp b-p
RI	on	on
PNO	off	off
Dispersion	DFT-D3 (BJ)	DFT-D3 (BJ)
COSMO	off	off
COSMO-FINE	off	off
Energy /H	-154.914498	-154.914498
HOMO-LUMO/eV	6.744077	6.74438
Dipole moment	from ridft	
Dipole moment /D	1.611724	
Zero point vib energy /H		0.077384
s^2		

This example is ethanol, the job template was OPT+FREQ from the predefined list of job templates.

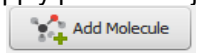
8. Batch processing

The job templates described in the previous chapter can easily be applied to any kind of structure, the user does not have to take care of anything else but to read in the coordinates or build a molecule, set the charge or accept the defaults, apply the template and start the job.

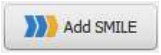
To open a new batch job, just use the File → New Batch Job entry in the menu or click on the  button in the tool bar. TmoleX will generate a new job, the geometry menu of this job is shown:



8.1. Read in and use several molecules

Batch jobs apply predefined job templates to a list of molecules. The molecules have to be read in from file by using the 

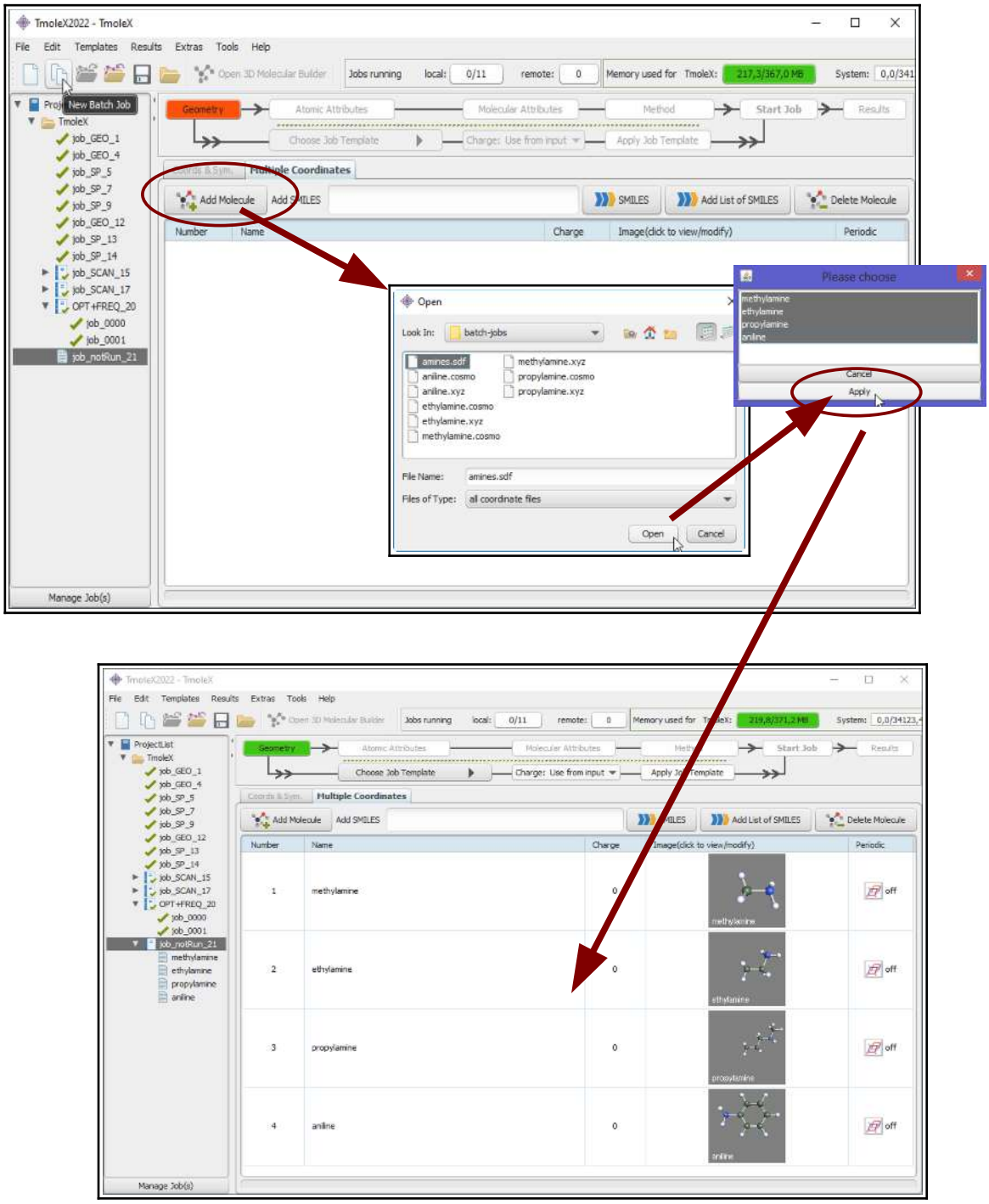
button. This opens a file browser which also allows to read in file formats which contain multiple structures like sdf. Multiple selections within the file browser are of course also possible.

Alternatively, SMILES can be entered in the 'Add SMILES' text field and added by 

or by hitting the <Enter> key.

To import or use a list of SMILES, please use the 

button to open a simple text editor where you can either enter or copy&paste your SMILES codes and the name of the molecules (lines that start with # are remarks and will be ignored). The first column is the SMILES code and the second one the name of the molecule.



The charge may or may not be imported correctly, so check and eventually change the charges in the table!

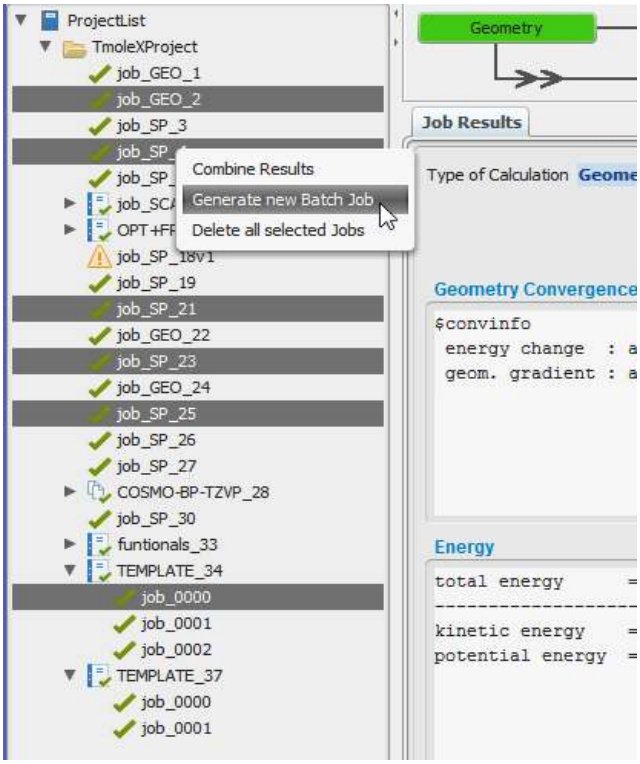
The multiplicity can also be changed, but it is recommended not to do that since TmoleX will use the TURBOMOLE default it determines from a Hückel calculation.

Ions are shown in different background colours, a quick look on the table should to sufficient to identify non-neutral compounds.

Double-click on a graphical representation of the molecules to open the builder.

Generate batch jobs from existing jobs

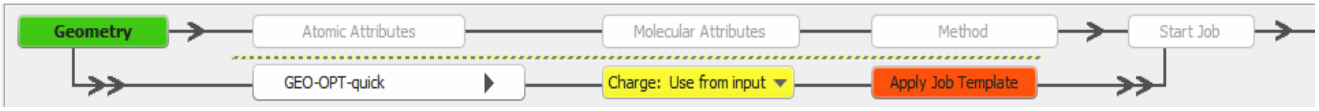
Another possibility to generate a new batch job and to read in structures is to select a list of finished jobs in your project and job tree and click on the right mouse button.



8.2. Apply templates for batch jobs

Once you have a complete list of molecules to perform calculations on, select a job template from the tool bar.

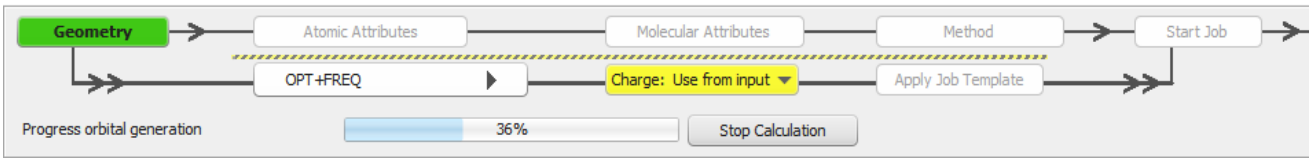
Important: The charge field can either have numeric entries which will assign the given charge to *all* molecules, or it can be set to 'Use from input' – in this case the charges that are displayed in the table will be used. The default, which applies when no charge is imported from the coordinate files and you did not set a charge by hand, is zero.



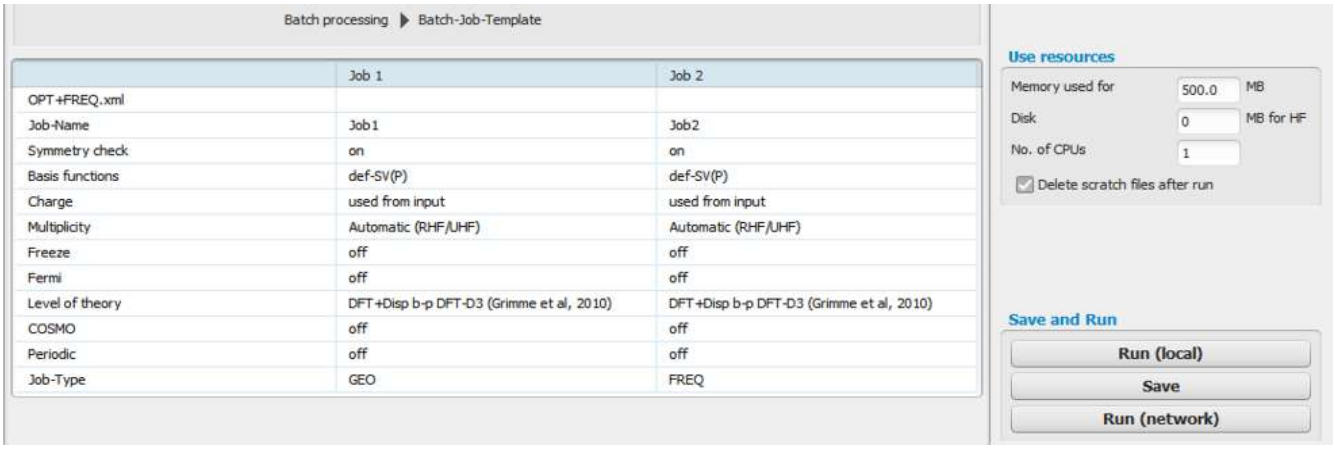
All settings for basis set, method, job type, etc. can not be changed in batch jobs since they are defined in the job template. In this example the charge field is a yellow default, so TmoleX will use the charges printed in the table. Otherwise they are overwritten.

Before starting a batch job, you have to click on 

to assign all settings of the template to your individual jobs. Possible errors or problems can thus be detected before the whole batch is started or sent to a remote system. This process can take some time, depending on the number and size of the molecules as well as the number of steps defined in your template.



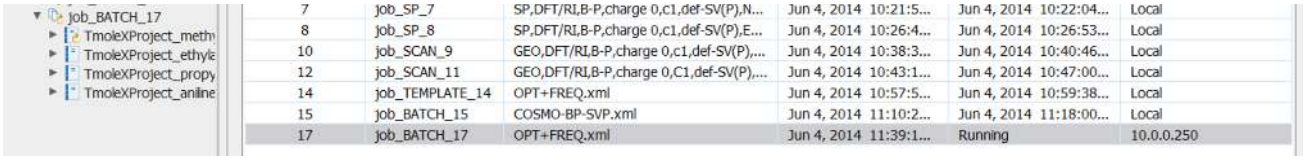
After applying the job template, a short overview is printed in the Start Job section:



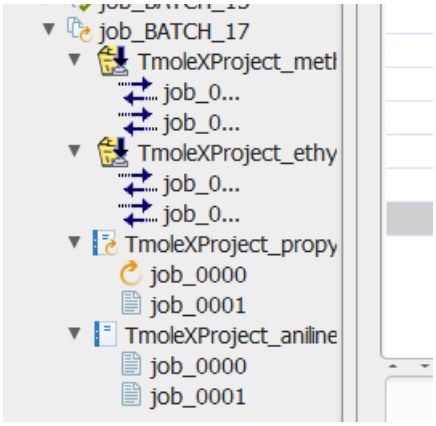
8.3. Run local or remote batch jobs

After a job template has been applied and TmoleX has finished to generate the input files of all steps and for all molecules in the list, the complete set of calculations can be simply started as you would start a usual job. So either use the **Run (local)** button to use the system TmoleX is running on, or the **Run (network)** button to submit everything to a remote system.

While the job is running the icons in the job list on the left side of your TmoleX window will show their current status.



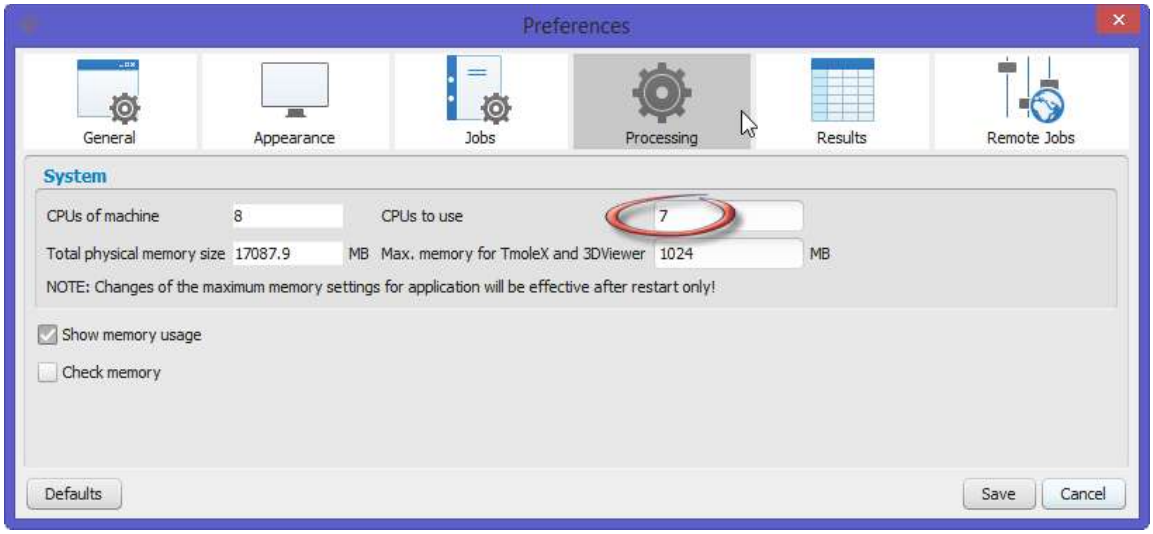
On remote systems the resulting files will only be copied back after all steps have finished to avoid too much traffic on the network. TmoleX, however, checks from time to time which job is currently running and whether or not the whole batch is complete. For single jobs which are finished but not yet transferred back to your local desktop machine, the icon switches to .



Using many cores or CPUs on your local system

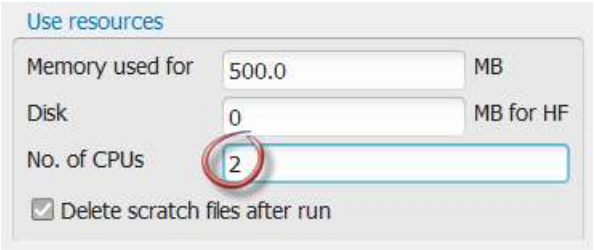
As you can see in the screen shot printed above, several different jobs can run at the same time when a batch job is being used. To be able to use several CPUs on your system, you have to tell TmoleX how many of them you allow the program to use on your local machine.

To do that, just select the Extra → Preferences entry in the menu and you will get a new window:



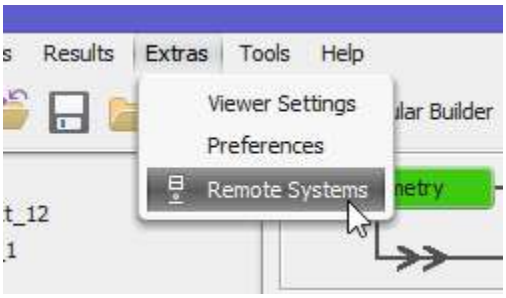
Set the number of available processes here, but it is recommended not to use all available cores to let at least one of them free for being utilized by TmoleX and your operating system.

When starting the job, just set the number of CPUs in the Start job panel directly:

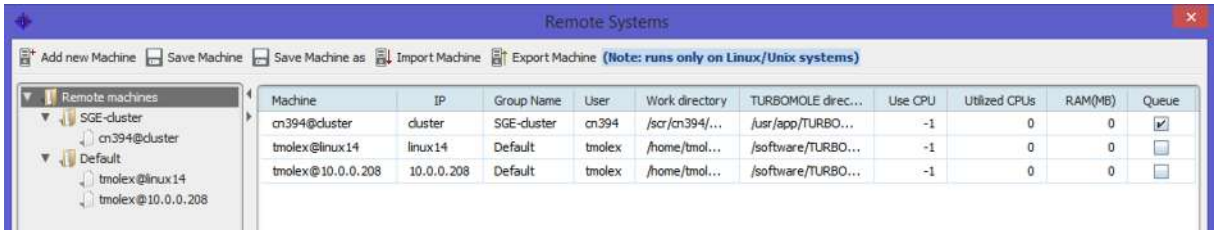


Using many cores or CPUs on remote systems

Similar to the local system settings, you can also set the number of CPUs on remote systems using the Extra menu:

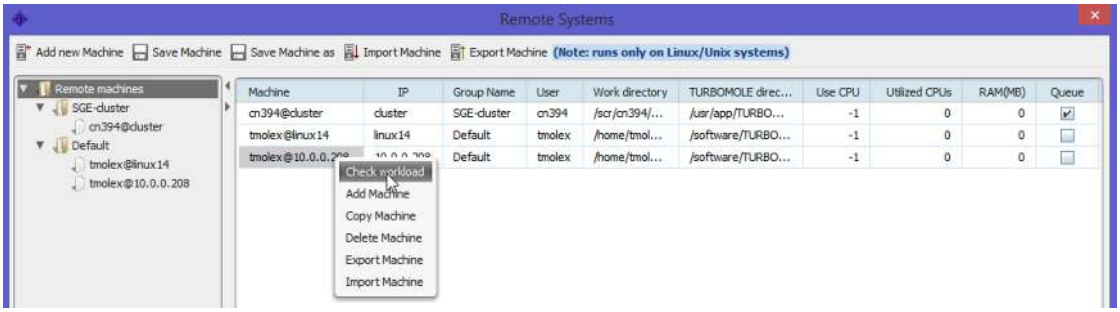


this will open:

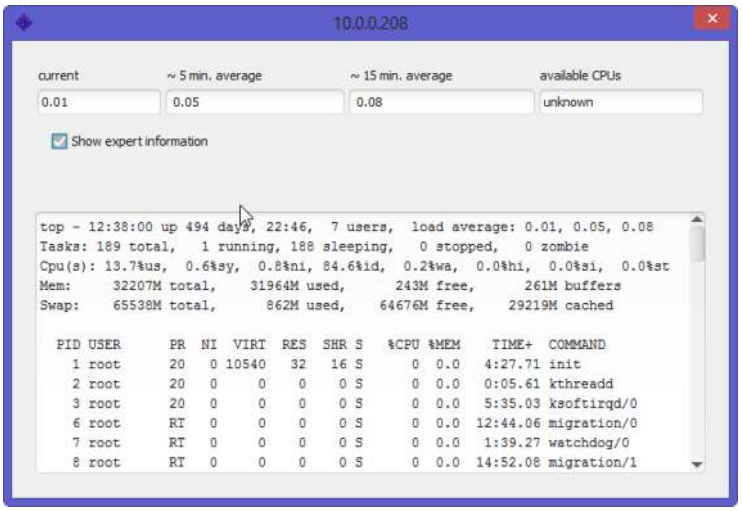


There is the entry:

- Use CPU – the total number of CPUs TmoleX is allowed to run on that system (for all jobs). The default is -1 which is equivalent to *unlimited*.



To see how many jobs are already running on the remote system, use the right mouse button menu and click on 'Check workload'. This will call 'top' on the remote system and show the results:



In the first line, the load, i.e. the number of running (time consuming) processes is shown. If you did set the number of total CPUs on the remote system as described on the last page, it is also shown here as 'available CPUs'.

The three entires are:

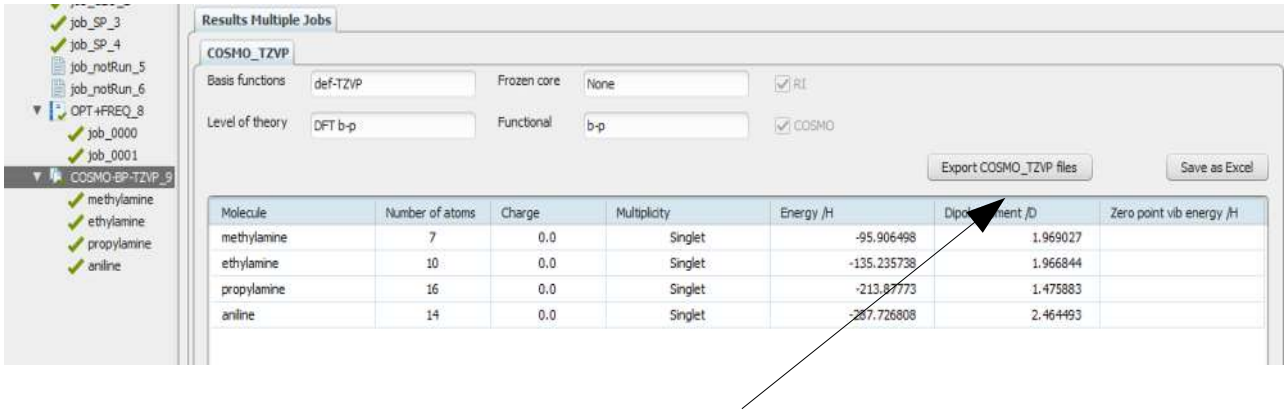
- current – number of CPUs in use right now
- ~ 5 min. ago – number of CPUs in use approximately 5 minutes ago
- ~15 min. ago – number of CPUs in use approximately 15 minutes ago

This gives quite a helpful hint how occupied the system already is and whether or not some new jobs have been started recently or how many old jobs stopped in the last 15 minutes.

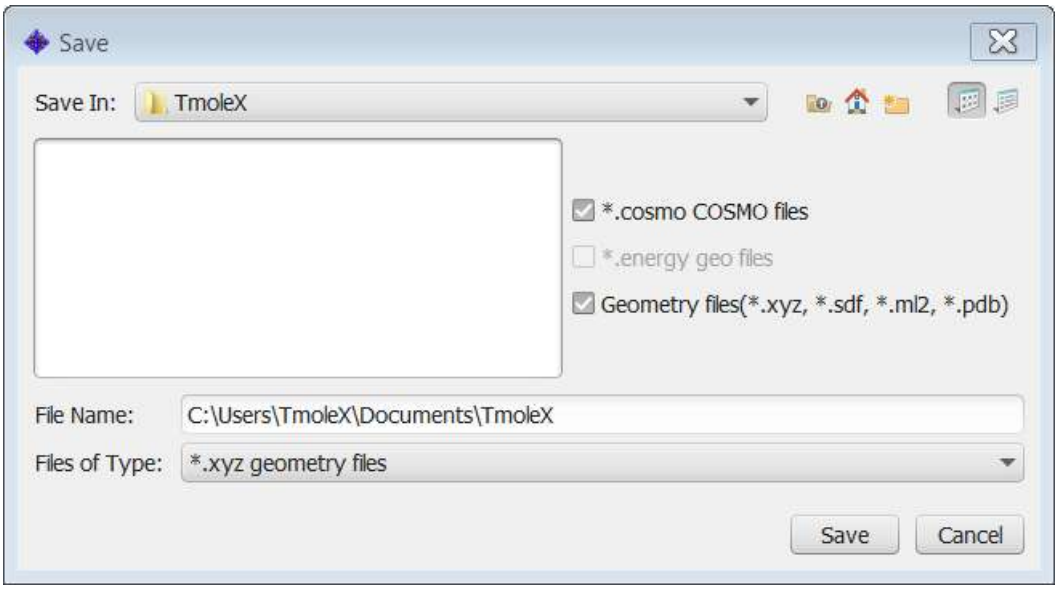
If you activate the 'Show expert information' check box, you will see the detailed output of 'top' – which users run which jobs on the machine, how much CPU time and how much memory they use. In the example given here, only the user tmolex is running jobs (entries with significant %CPU values).

8.4. Visualize and export results of batch jobs

The results of finished batch jobs are given as tables in the Results section. Each sub-job has an own tab in the table.



The resulting table can be saved as spread sheet. The Export Files button allows to save COSMO, energy or coordinates files of different format:



COSMO and energy files are usually only needed for the COSMO*therm* program. TmoleX will save all files of the given type to the chosen directory.

9. Remote jobs

TmoleX as well as the Demo version of TmoleX, which is freely available from the BIOVIA website, is able to start jobs on remote Linux/Unix machines using a secure shell.

9.1. Security information

To determine if you do want to use this feature and worry about security, here is a short outline of the procedure used by TmoleX to access to remote systems.

- ssh and scp are used to start jobs and to copy the files from one system to another.

  As the password is set in TmoleX and then used in the execution of ssh and scp, this can be seen as potential security risk. It thus recommended to enable passwordless ssh and to enable this feature in the expert settings of the TmoleX remote execution window.

  We use a locally modified version of PuTTY (http://www.chiark.greenend.org.uk/~sgtatham/putty/)

  PuTTY is copyright 1997-2009 Simon Tatham.

  Portions copyright Robert de Bath, Joris van Rantwijk, Delian Delchev, Andreas Schultz, Jeroen Massar, Wez Furlong, Nicolas Barry, Justin Bradford, Ben Harris, Malcolm Smith, Ahmad Khalifa, Markus Kuhn, Colin Watson, and CORE SDI S.A.

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- PuTTY uses its own repository for public ssh keys, so ssh connections that do not require a password on your local machine at the command line might not work if OpenSSH or any other ssh program is used. Run ssh from the TmoleX directory to check that manually.

- jobs can be killed while they run on a remote system. For that purpose, a kill-job script is being stored in the directory where the job is running. This script does kill all processes that are running in the directory the script itself is located – but this will only work on systems where a /proc directory is present (usually all Linux systems and most Unix systems either).

- Passwords entered in the password field **will not be saved** to disk. Hence, they have to be entered each time TmoleX has been started, but kept in memory as long as TmoleX runs.

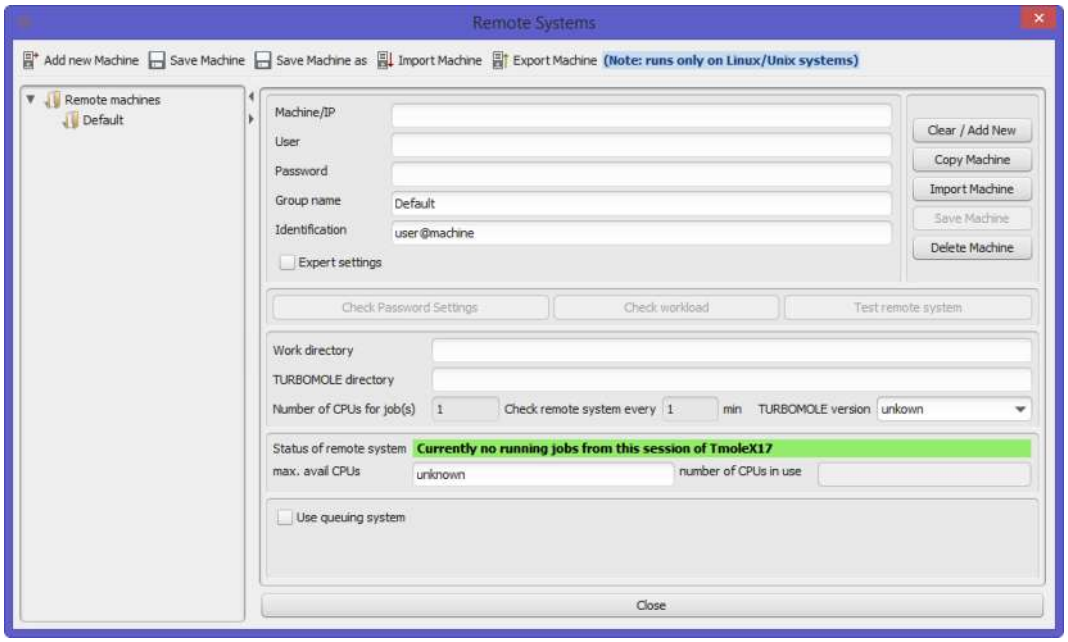
9.2. Add new remote machine

When starting a remote job for the first time, or when you want to add several external machines, several things have to be set, TmoleX needs to know in order to be able to run TURBOMOLE there.

To start a job on a remote machine, or to set or change settings, click on Run (network) in the 'Start Job' panel.



TmoleX will first save the input file to a local disk under the usual naming scheme, and then open a new window that looks like this one:



General informations about a remote system are:

1. The name or the IP address of a remote machine (Machine/IP field)

2. User name on that machine

3. Password to log in
   Please note that if your password contains characters like " you might need to type \" instead.

Those three fields have to be filled in first. To check if the settings are correct, and if a connection can be established, click on Check Password Settings. TmoleX will try to log in and determine the home directory of the user which has been given in the User field.

If the connection has been successful, the home directory will be added to the 'Work Directory' field.

4. Work directory tells TmoleX in which path on the remote machine the job shall run – a fast local disk should be chosen here.

5. TURBOMOLE directory has to be set to the TURBOMOLE installation directory on the target system.

   The default behaviour of ssh when starting remote jobs without an explicit shell or terminal is such that not all settings on the remote system are sourced. So it is very likely that your TURBOMOLE settings (like $TURBODIR, $PATH, etc) are not available in such a case.

   It is therefore unavoidable to set the PATH to the TURBOMOLE directory on the remote system by hand.

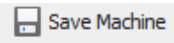
6. The number of CPUs can be left unchanged.

   Note that this field is not to tell TmoleX how many CPUs or cores are available in general, but how many CPUs shall be used for the calculation of each job!

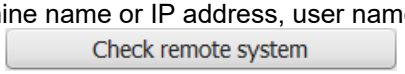
7. Note that all jobs are started on the remote system with `nohup`. TmoleX does not get a notice when the job has finished, so it has to check actively whether the job is still running or not. The frequency for those checks can be given in minutes.

8. The TURBOMOLE version on the remote machine is needed to determine which program is used for post-Hartree-Fock calculations. Since version 7.0 CCSD and CCSD(T) jobs are done by the program `ccsdf12` and not by `ricc2` any more as it was in previous versions. Some methods like DFT-D4 or PNO-CCSD(T) are only available in newer versions (at least 7.3).

9. The queueing system option can be used to submit remote jobs to a queue which is accessible on the remote machine.

After settings 1-5 are complete, click on 

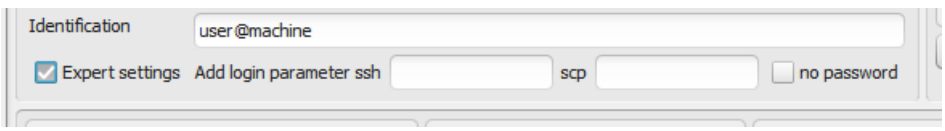
. The 'Identification' is used as name in the list of known remote systems given in the tree on the left side of the window.

Configuring a remote system such that number crunching programs like TURBOMOLE can utilize the hardware resources correctly is not a trivial task. Most Linux/Unix systems restrict the permissions for memory or disk space for each individual user for security reasons. TmoleX is able to submit a script which checks for the most important settings to a remote system. If machine name or IP address, user name, password and TURBOMOLE installation directory are set, the button 

can start this process. TmoleX will show the results in an own output window. Search for ERROR messages in case a remote system is not able to run serial or parallel TURBOMOLE jobs. The TURBOMOLE manual contains a section which helps to install the command line version on Linux/Unix machines.

If you are not able to figure out what to change in order to use a remote system, please contact the Support Team.

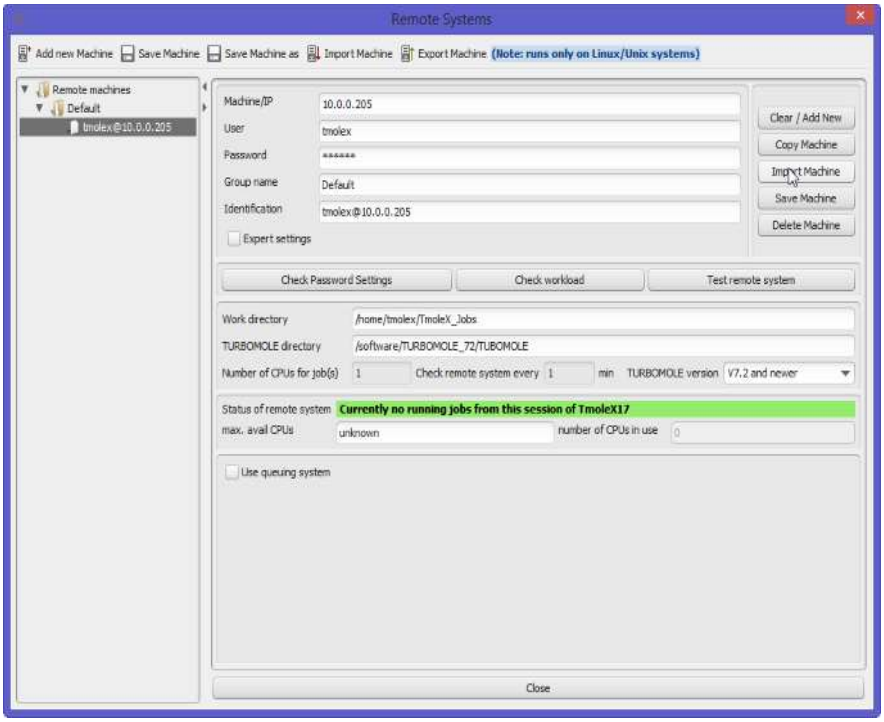
Expert settings:



You can add individual options to the ssh and scp commands and/or use passwordless ssh (if it is enabled with putty – otherwise you could copy your own ssh and scp binaries to the TmoleX/extapps/putty directory).

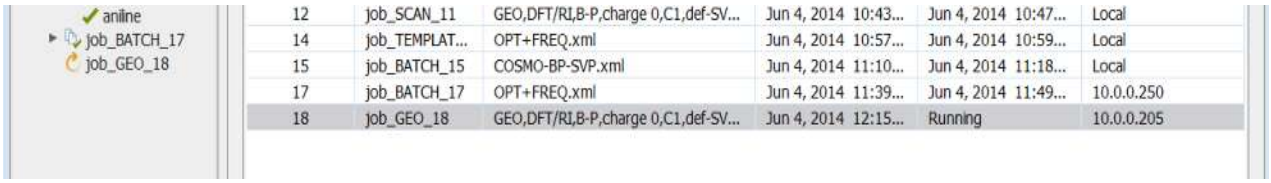
9.3. Start a remote job

Starting jobs can be done by choosing a machine in the list of saved systems:



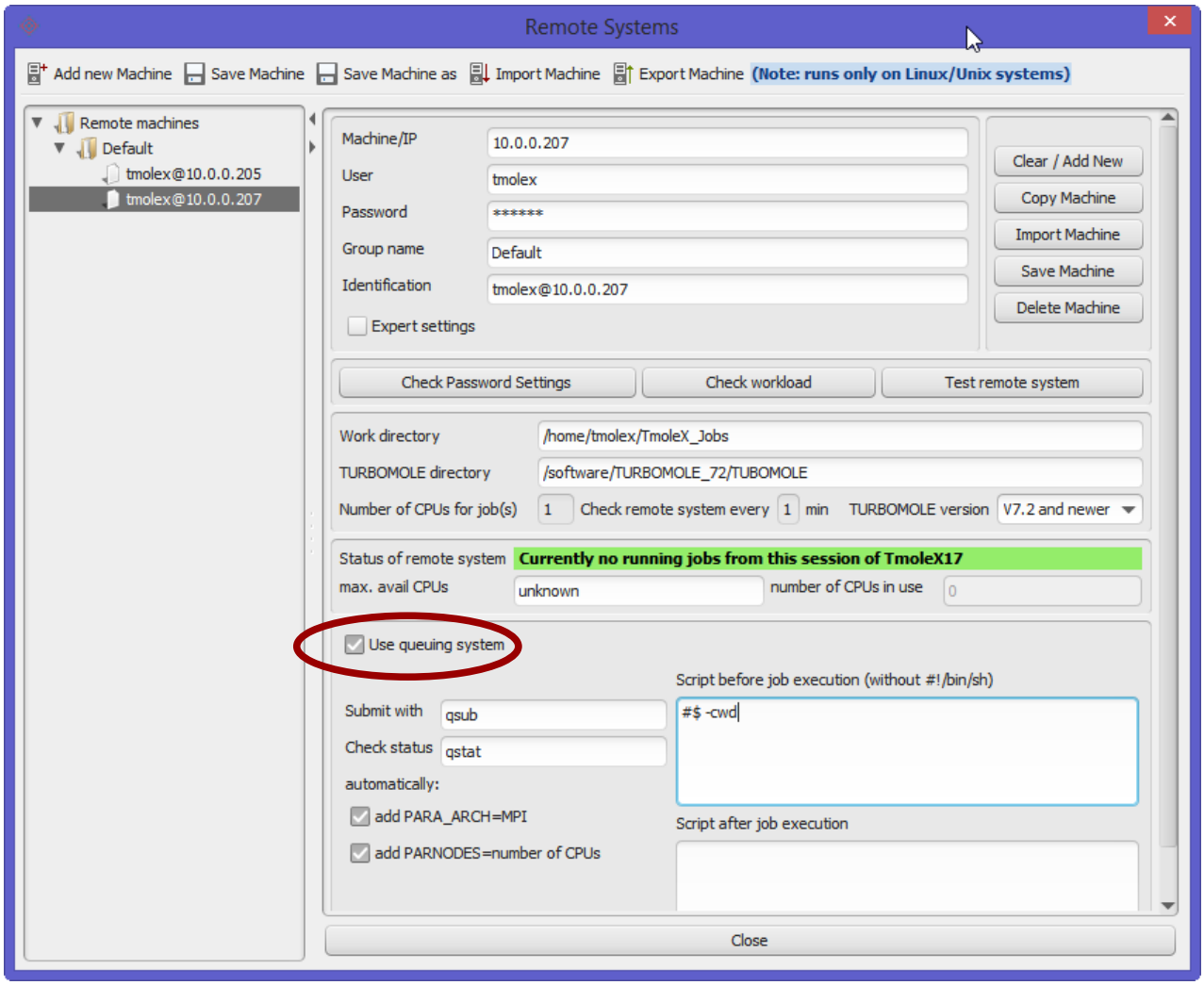
A simple click on 'Start' will start the job on the chosen system.

The job list shows on which machine a calculation has been started or is still running. The right mouse button menu in this list allows to kill a job also on a remote machine.



Note that the Stop time is not the end of the job itself, but the time when TmoleX noticed that the job has finished!

9.4. Using a queuing-system on a remote cluster



Currently PBS, LSF and SGE are successfully tested. Activate the queue option in the remote job start panel:

To be able to support as many queuing systems as possible, the number of options is kept very small.

1. Submit with – this is the command that is used on the given remote system to submit a job to the queue. Here you can give just the name but also options.

   For PBS and SGE like queuing systems

   ```
   qsub
   ```

   is the default. For LSF it should be:

   ```
   bsub <
   ```

For unsupported queuing systems it is possible to write a script on the remote cluster that sets the number of CPUs and the list of nodes that shall be used for the job and submits the start script to the queue. The name (and probably the path) to this self-written script can then be entered in this field.

2. Check status – this is the command that is called on the remote system if the 'View run status' option from the right-mouse menu of the Job administration is chosen.

   The output of the status command is shown directly underneath the job list.

3. Script before job execution (without #!/bin/sh)

   This is the field where a usual script that is used to submit jobs to a queue can be entered.

Example for PBS:

```
#PBS -S /bin/bash
#Name of your run :
#PBS -N TmoleX-job
#Number of nodes to run on:
#PBS -l nodes=1
#
# Export environment:
#PBS -V

cd $PBS_O_WORKDIR
```

Example for SGE/Univa Grid Engine:

```
#$ -S /bin/bash
#$ -N TmoleX-job
# Export environment:
#$ -V
# make sure to be in the right
# directory:
#$ -cwd
```

This is a PBS/SGE example for a serial run.

There are several things one has to take care of. TmoleX will use the given entry and include it in its own settings:

1. do not give a `#!/bin/...` line here, TmoleX adds its own commands in sh format, so TmoleX will add a first line containing `#!/bin/sh` to the final script.

2. Make sure to change the directory to where the input files are copied:

   PBS:
   `cd $PBS_O_WORKDIR`

   SGE:
   `#$ -cwd`

   LSF:

   `cd $LS_SUBCWD`

   must be somewhere in your own script.

3. Ask your queuing system for the right number of CPUs – this has to match the 'Number of CPUs' field of the TmoleX setting. Depending on the queuing-system, it will not allow a different number than what the script will start.

   $PARNODES is set by TmoleX, so if you set it in this field, it will be overwritten.

4. $TURBODIR is being set by TmoleX, so you do not have to enter it again here.

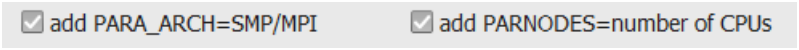
5. The commands to start the TURBOMOLE jobs are of course added by TmoleX automatically.

4. Parallel settings

TURBOMOLE contains two different parallelization schemes. SMP runs almost all jobs in parallel on a multi-core, multi-CPU or NUMA system. MPI on the other hand is able to utilize several different nodes for one job, but the number of parallelized modules is smaller than in the SMP version.

TmoleX by default sets SMP for parallel remote jobs which are submitted to a remote system *without* using the queuing system option, and MPI whenever the queuing system option is activated. The number of (total) CPUs is also set automatically.

In some cases a queuing system requires different settings than TmoleX applies by default. The two options



help to overwrite those defaults. If you uncheck one of the two or both options, make sure to add the environment variables PARA_ARCH and PARNODES by hand if needed.

Note that you have to tell your queuing system about the number of CPUs you want to use.

PBS:
```
#PBS -l select=4:ncpus=8
```

SGE:
```
#$ -pe mpi 32
```

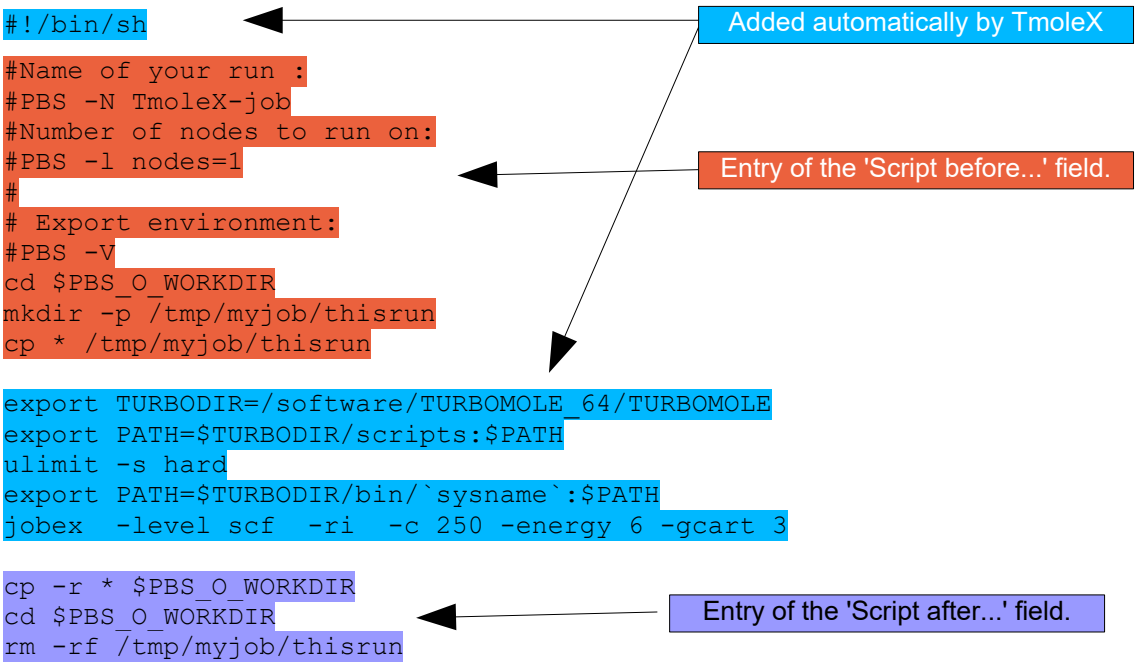
The default in PBS is to set the number of nodes with 'select=' and the number of CPUs per node by 'ncpus='. In this example, 4 nodes with a total number of 32 CPUs will be used. So set PARNODES to 32.

For SGE like queuing systems one has to tell SGE which parallel environment (-pe) one wants to use. The name for the PE depends on your local SGE installation, so please check existing SGE submit scripts or ask you system administrator.

5. Script after job execution

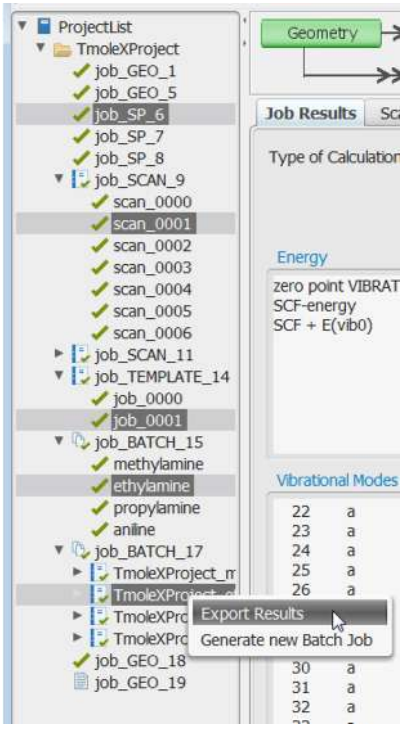
The script that is being submitted to the queue can be extended with the entries in this field. Useful if you want to do some post-processing on the remote machine.

Say you are running a geometry optimization and submit the following script to the queue:

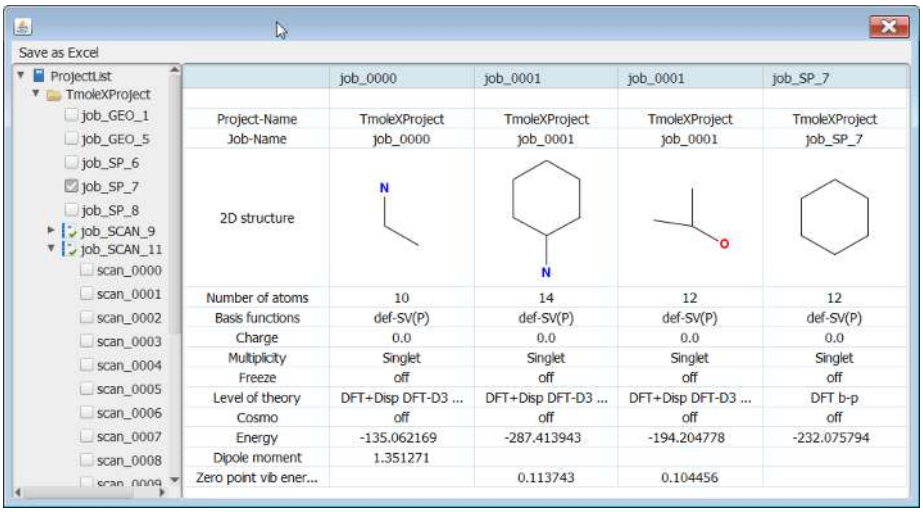


10. Combine Results

To combine and collect results from different jobs, select different jobs from the job tree by holding <Shift> or <Control> key and clicking on the jobs, then use the right mouse button and select 'export results':



TmoleX will generate a table with the most important data.



	job_0000	job_0001	job_0001	job_SP_7
Project-Name	TmoleXProject	TmoleXProject	TmoleXProject	TmoleXProject
Job-Name	job_0000	job_0001	job_0001	job_SP_7
2D structure				
Number of atoms	10	14	12	12
Basis functions	def-SV(P)	def-SV(P)	def-SV(P)	def-SV(P)
Charge	0.0	0.0	0.0	0.0
Multiplicity	Singlet	Singlet	Singlet	Singlet
Freeze	off	off	off	off
Level of theory	DFT+Disp DFT-D3 ...	DFT+Disp DFT-D3 ...	DFT+Disp DFT-D3 ...	DFT b-p
Cosmo	off	off	off	off
Energy	-135.062169	-287.413943	-194.204778	-232.075794
Dipole moment	1.351271			
Zero point vib ener...		0.113743	0.104456	

Additional results can be added to the table by selecting the jobs on the left side in the project list.

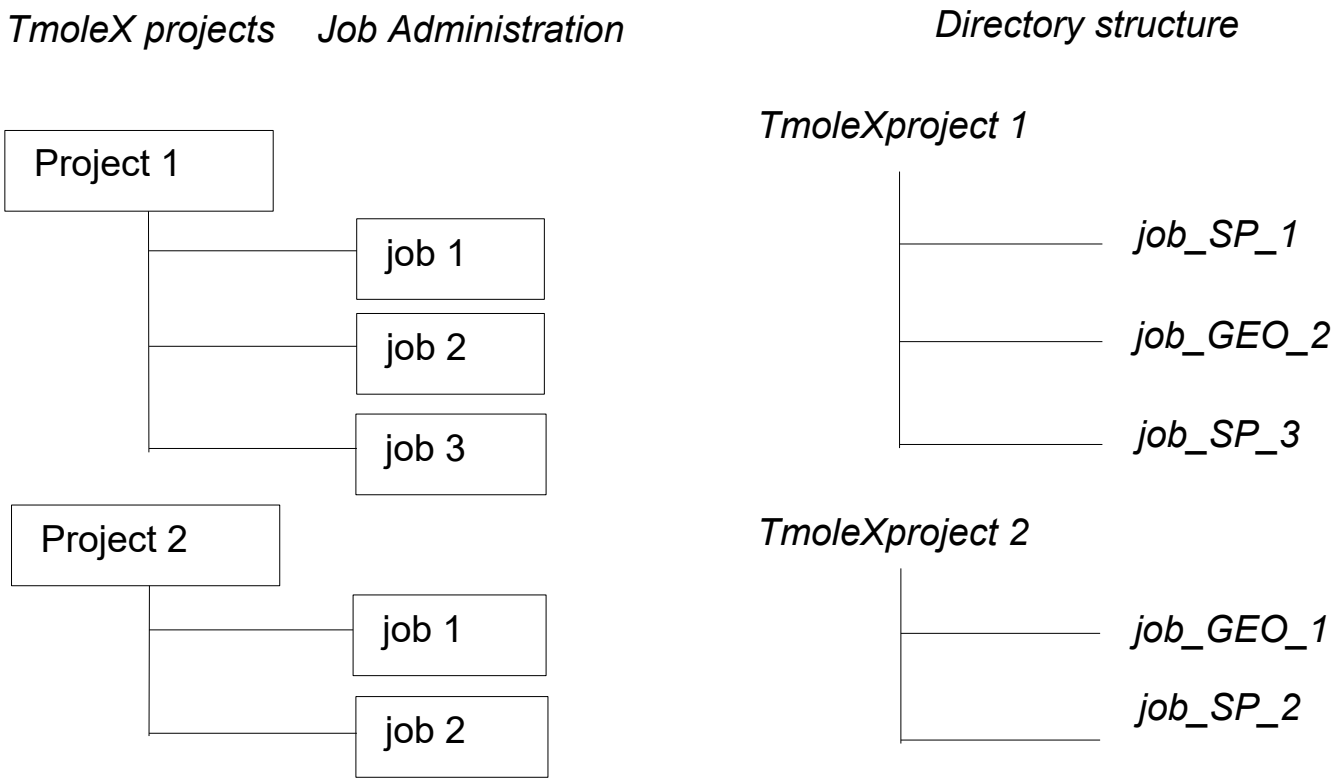
11. Project and Job management

Individual Turbomole jobs are collected in TmoleX projects which contain information about the job types, start- and end times of finished jobs, and the machine where the jobs have been running (either the local machine or the name or IP address of the remote system).

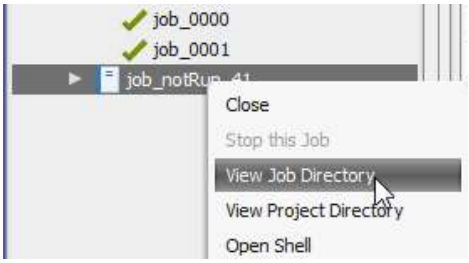
A job must always run within a given project since the project directory is the location where the job is being created as sub-directory.

11.1 Location on disk

Each project has its own project file (project-name.xml) and its own directory structure:

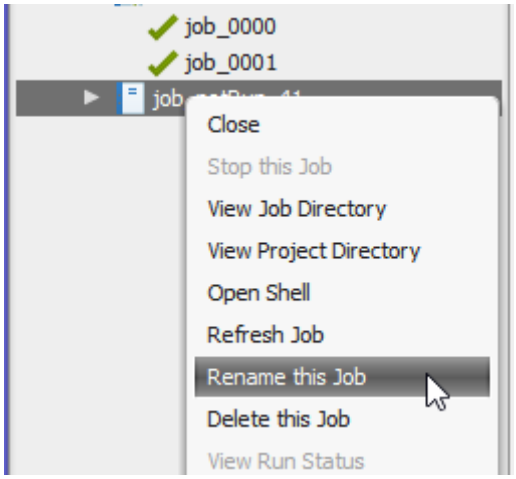


To open the system-own file explorer at the location on your disc where the project or the jobs are stored, just right-click on the name of the job or project and select 'View job directory':



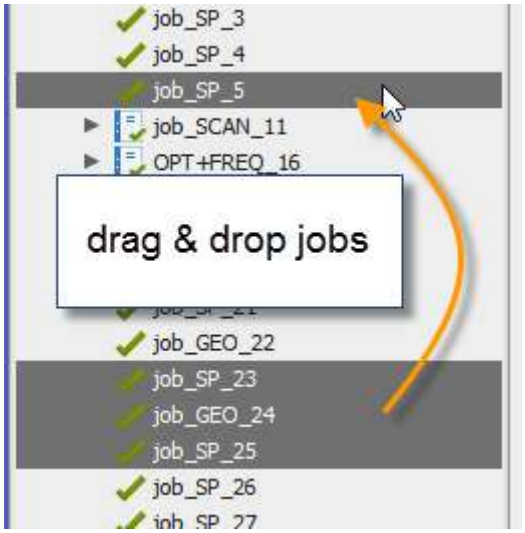
11.2 Renaming Jobs

When starting a job, it can be given an individual name when TmoleX asks you where to save the job (default is the project directory). But it is also possible to rename the job after it has finished. To do that, just use (again) the right-mouse menu of a job:



11.3 Order Jobs and Projects

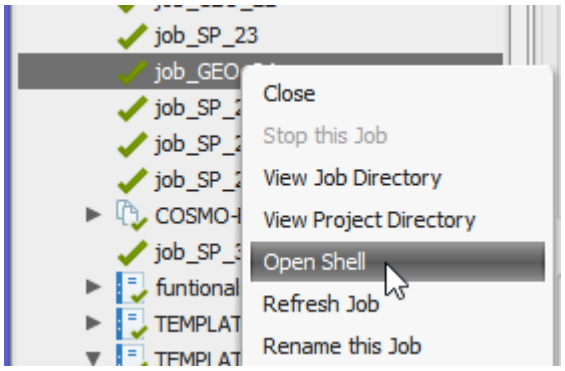
To change the order of the jobs (and projects), just drag-and-drop a job to a new position. Multiple selections are allowed:



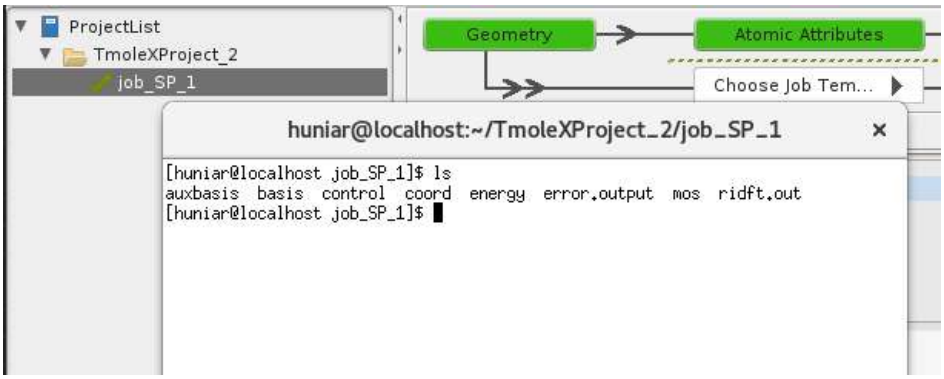
Explore the other right-mouse menu entries to more or to make a copy of jobs - to the same project or to an existing and opened project or to a new project which will be generated.

11.4 Use command line

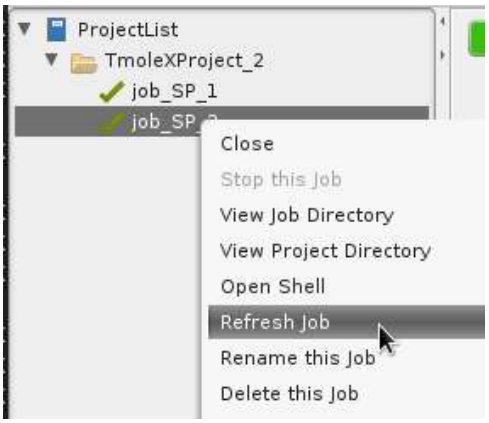
Once you have created a complete input for Turbomole, or if you have a finished job, it is possible to open a shell (xterm under Linux, terminal under MacOS, cmd.exe under Windows):



It will open a shell in the directory of that job and with the Turbomole settings:



$TURBODIR and the $PATH (or %PATH% under Windows) are already set, so any Turbomole module can be called from this shell. If whatever you do does produce new results and data, the files can be re-read by selecting:



Switch to the Results panel to visualize and use the new data.