Quantemol

UCL

Quantemol-N

A 15-minute introduction to the programme

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Quantemol-N

Quantemol-N 3.8 can calculate:

- Elastic cross sections
- Electronic excitation cross sections (extended to high energies)
- Super-Elastic cross-sections between excited states
- Electron impact dissociation
- Scattering reaction rate
- Resonance parameters
- Dissociative electron attachment
- Now works for atoms!

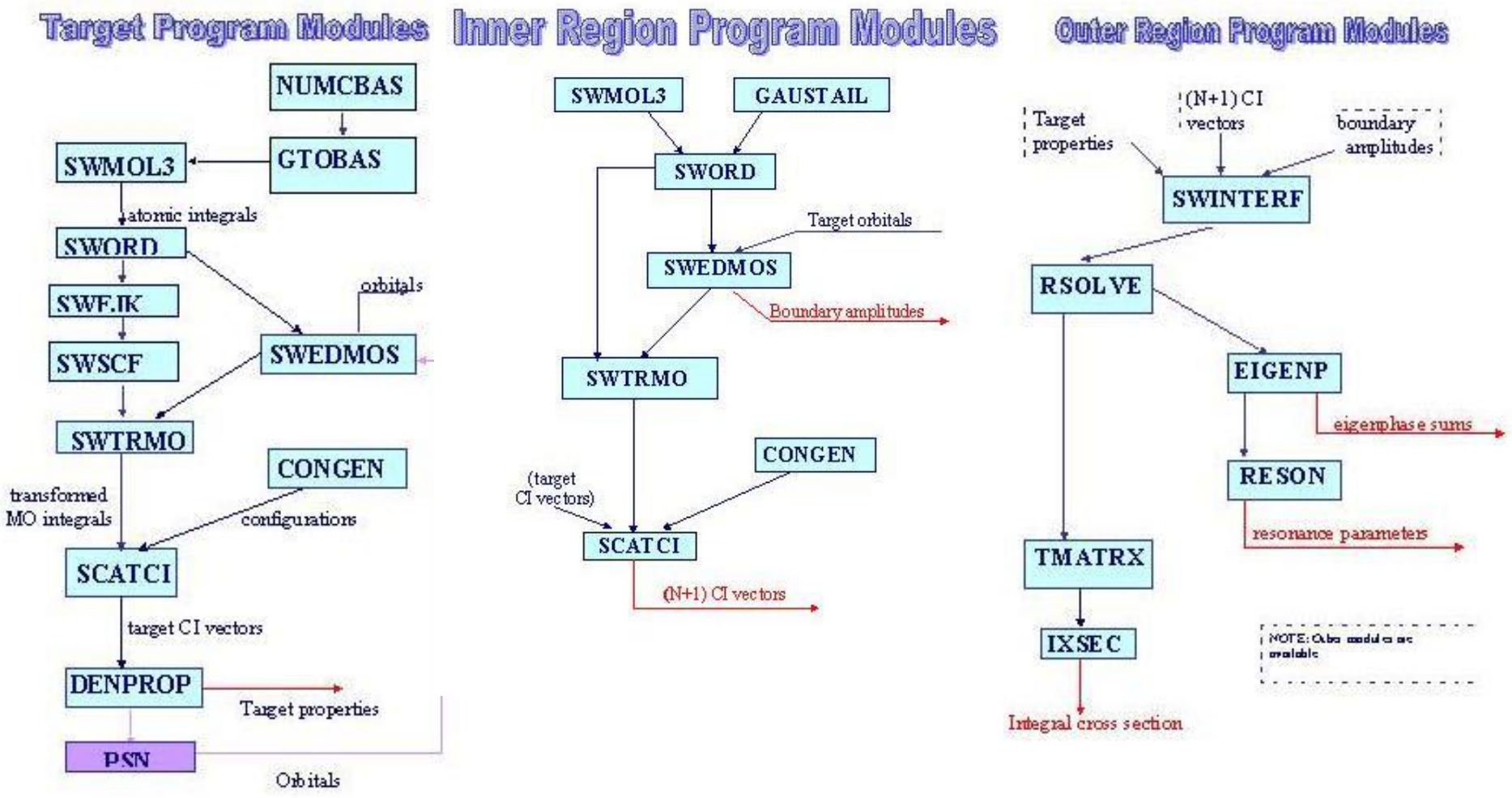
Quantemol -N3.9 (to be released shortly):

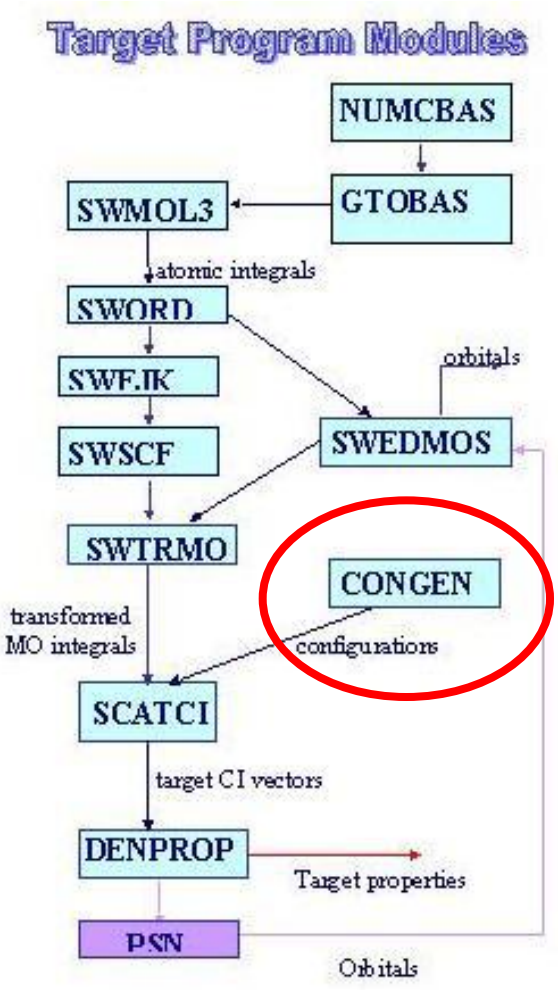
- Differential cross sections
- Momentum transfer cross sections
- Parallel computing version

Quantemol experts can help you calculate:

- Vibrational excitation cross sections

The UK Molecular R-Matrix Codes





An example….

```
cat > congen.data << EOF
&STATE
sname="2b1 Congen Calculation",
iscat=1,
megul=71,
symtyp=2,
qntot=2,1,0,
nelect=25,
nob=10,3,3,0,
nob0=10,3,3,0,
nrefo=4,
reforb=0,1,15,0,0, 0,9,1,1,0, 1,1,5,0,0, 2,1,4,0,0,
confpf=0,
lndo=8000000,
&END
&WFNGRP
gname="Configurations",
nelecg=25,
nrefog=4,
reforg=0,1,15,0,0, 0,9,1,1,0, 1,1,5,0,0, 2,1,4,0,0,
ndprod=2,
nelecp=8,17,
nshlp=1,3,
pqn=0,1,4, 0,5,10, 0,1,3, 0,1,3,
mshl=0, 0, 1, 2,
npcupf=1,
&END
EOF
```

Note: This is just the congen input for 1 state. This had to be repeated 8 times in total to get all the correct target states (all with slightly different inputs)

So how effective is Q-N at simplifying the process of setting up a calculation?

So less lines than the input for 1 repeat of 1 module in 1 region if it were done manually!

This job file gets created by following the step by step wizard.

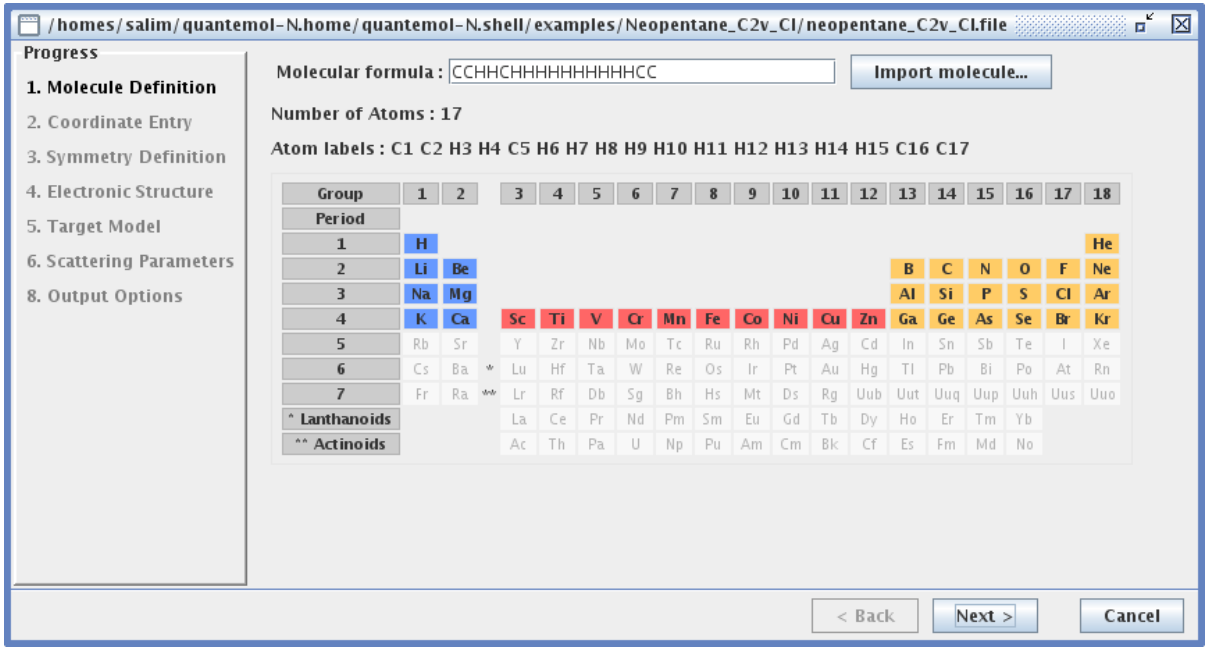
```
molecule=C3N
C1=[0.0, 0.0, -1.9604410372164502]
C2=[0.0, 0.0, -0.74884103721645]
C3=[0.0, 0.0, 0.6257589627835498]
N4=[0.0, 0.0, 1.7866589627835499]
pointGroup=C2v
symEquivAtoms=[C1, C2, C3, N4]
optimise=false
singleOccup=[1, 0, 0, 0]
doubleOccup=[8, 2, 2, 0]
model=CIHF
basis=DZP
basisNAtomSym_C=1
basisNAtomSym_N=1
basis_C=
basis_N=
stepEnergy=0.02
rmatRadius=12
minEnergy=0.02
maxEnergy=10.0
cutOff=10.0
targetStates=2
casLimit=1
attachCalc=false
affinity=1.262118
dissEnergy=0.0
vibEnergy=1000.0
fragments=[C2N, C-]
```

Quantemol-N can be applied to:

- •Closed shell molecules.
- •Open shell molecules, radicals.
- •Neutral and positively charged species.
- •Molecules with up to 17 atoms tested.

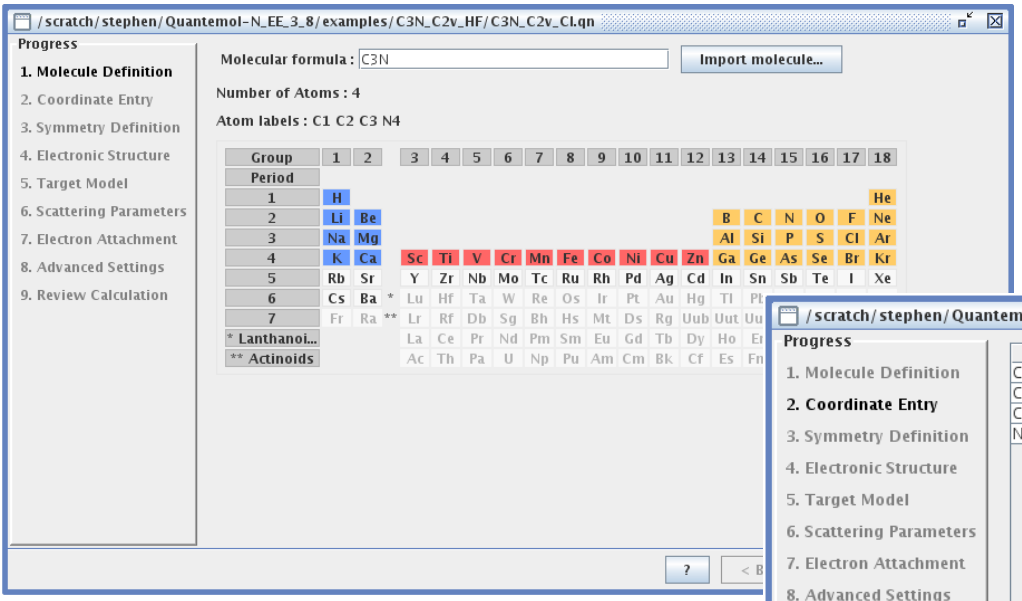
Advantages of using Quantemol-N, user friendly interface; full tutorial system; 40+ example library; easy to use results format; and 24/7 service support from Quantemol team

Inputs:
Screen 1

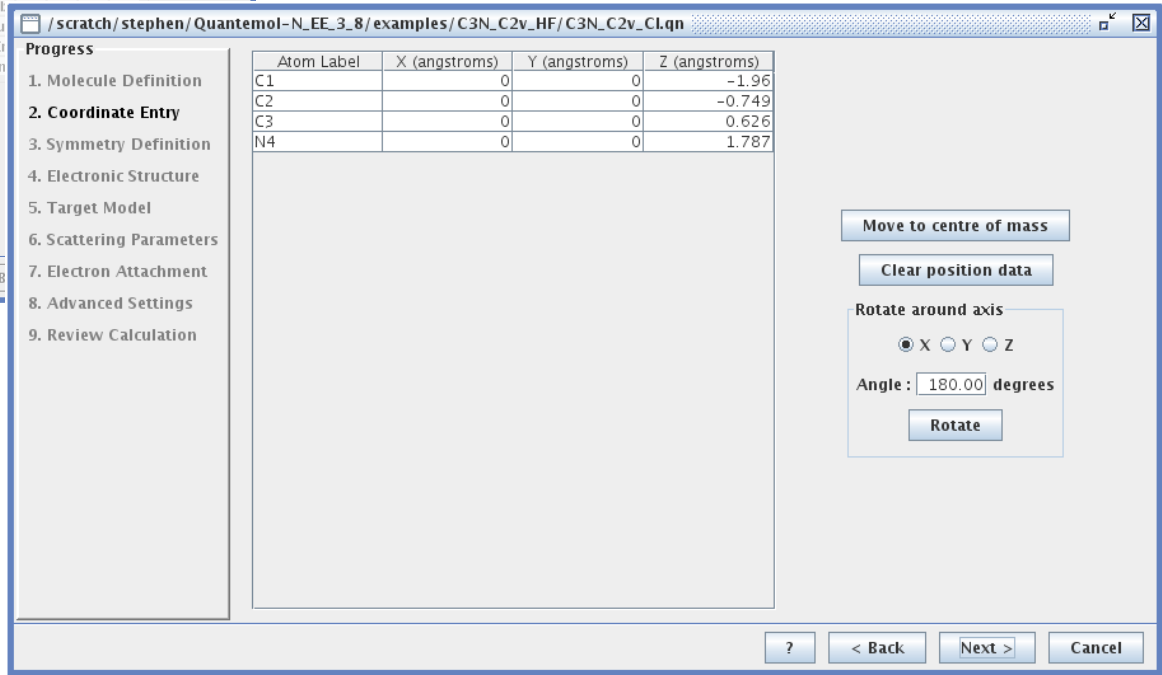


Input Screens

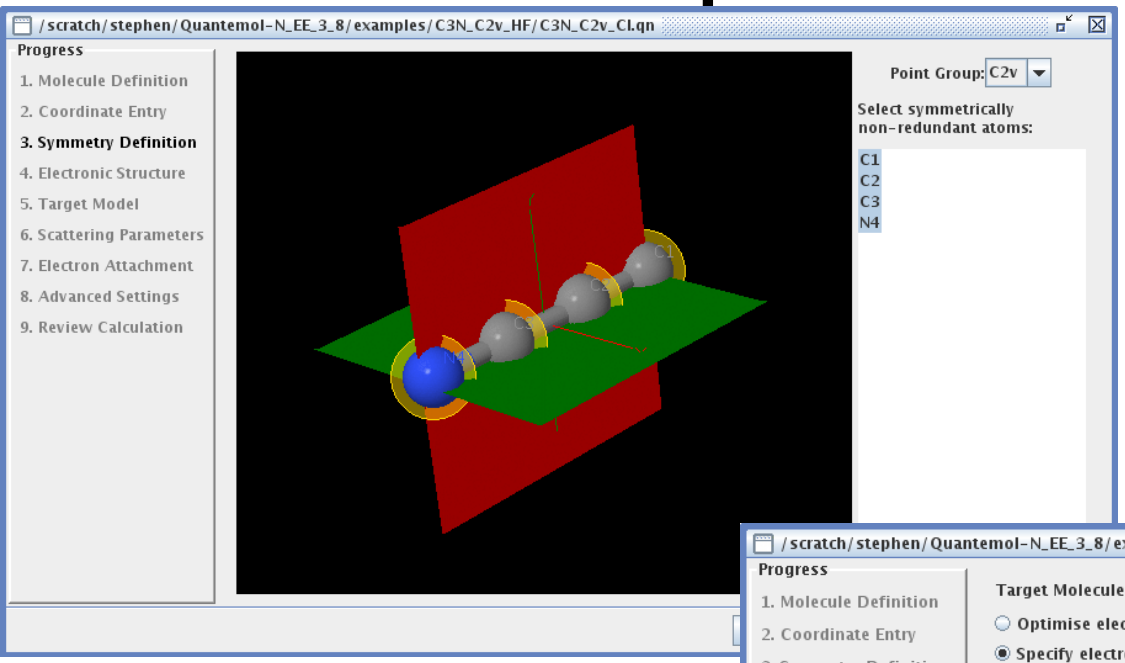
1. The first screen gives you a choice of atoms to define your molecule. Obviously the larger the number of electrons the longer the calculation will take. Some molecules from the grey area can be calculated but with supervision of the team, we will be glad to hear a request from you.



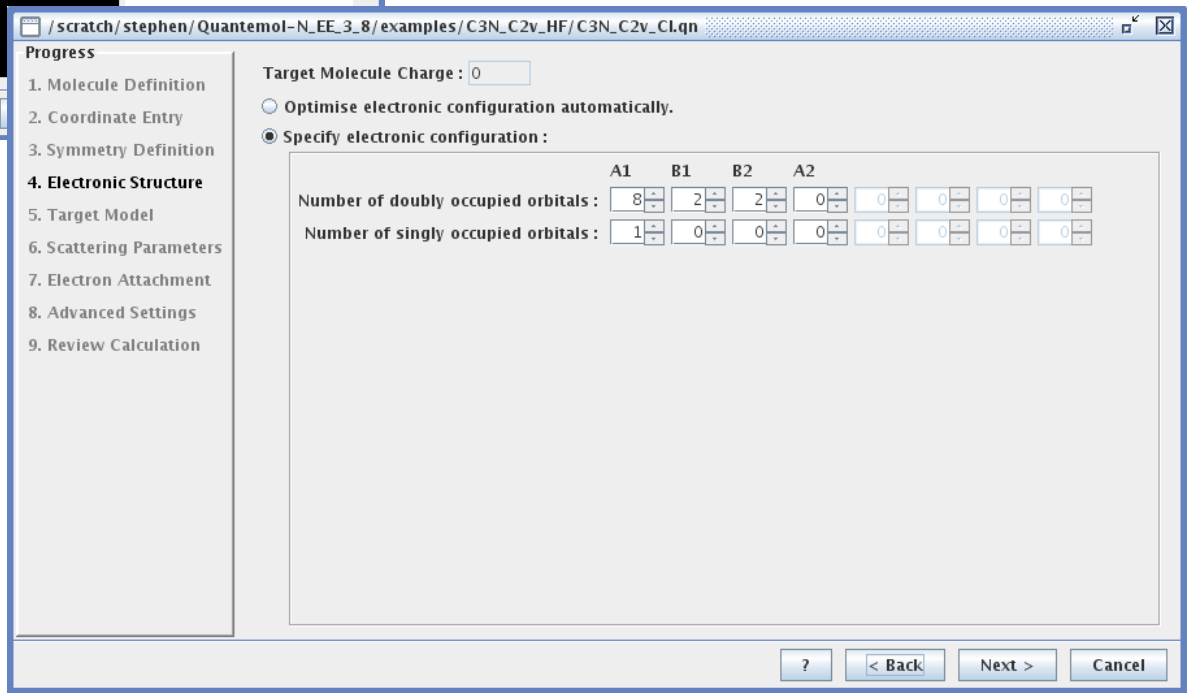
2. The second screen asks you to define the molecule's geometry



Input Screens

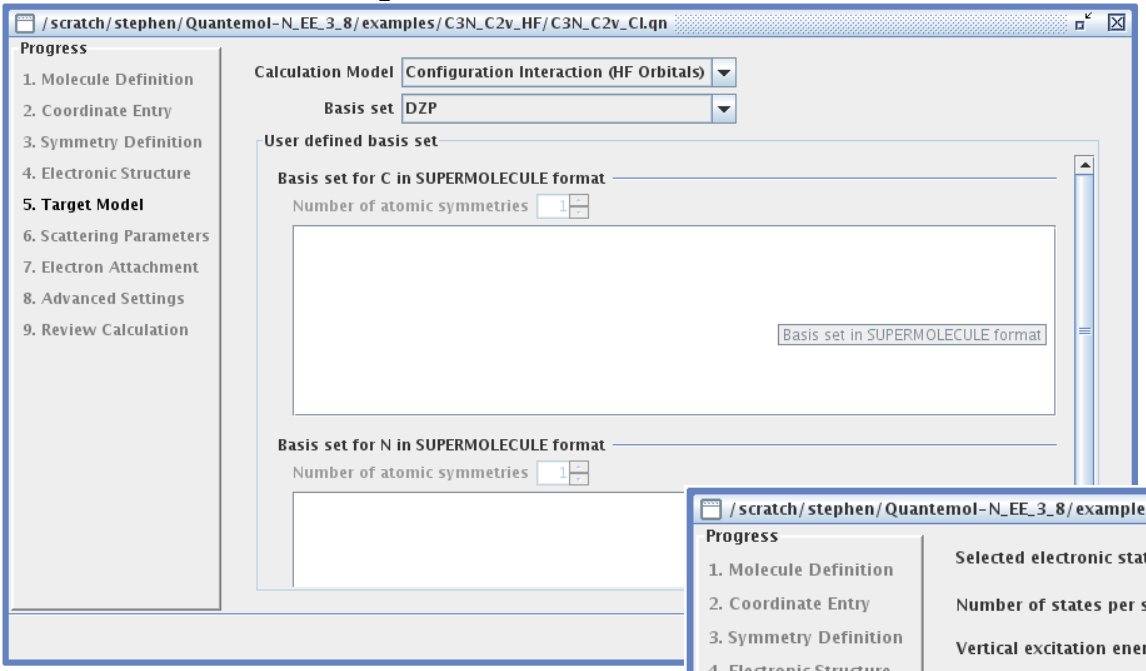


3. Screen three suggests you to choose non-symmetrical atoms, which can help us to make calculation quicker as symmetry will be taken into account.

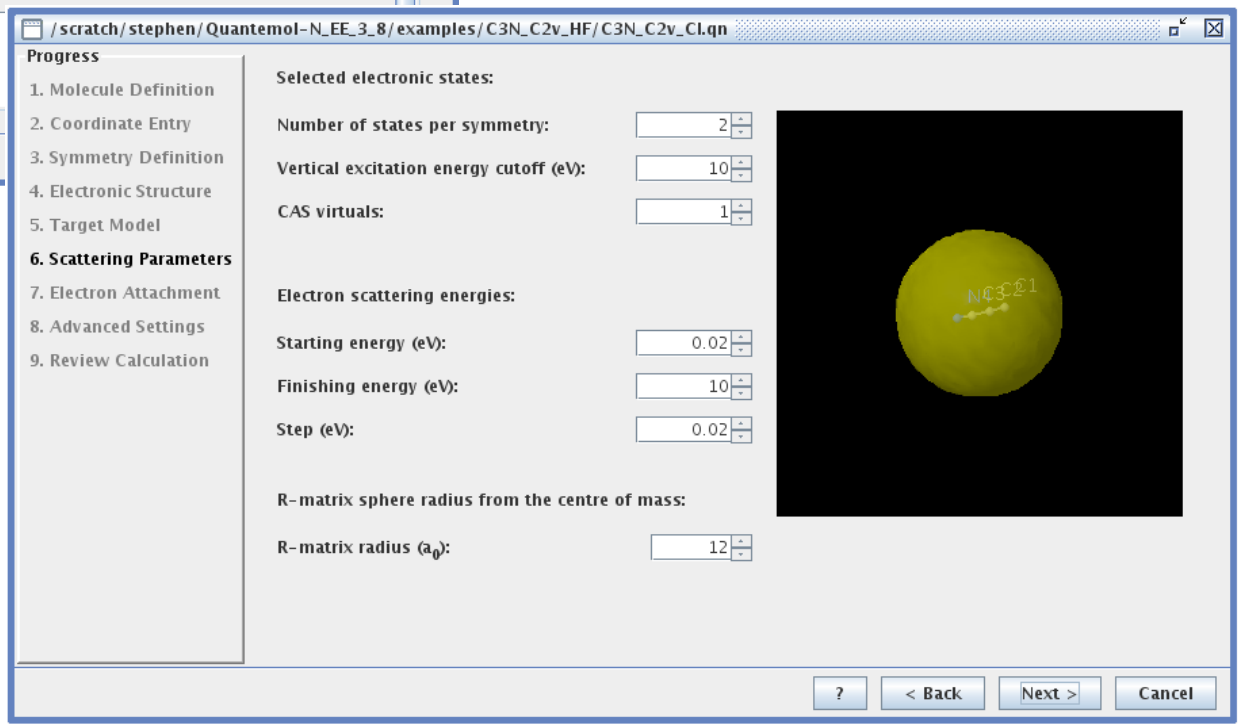


4. Screen four allows the definition of electron occupation for the states attributed to the symmetry chosen. It also allows positive ions to be defined if required,

Input Screens and outputs

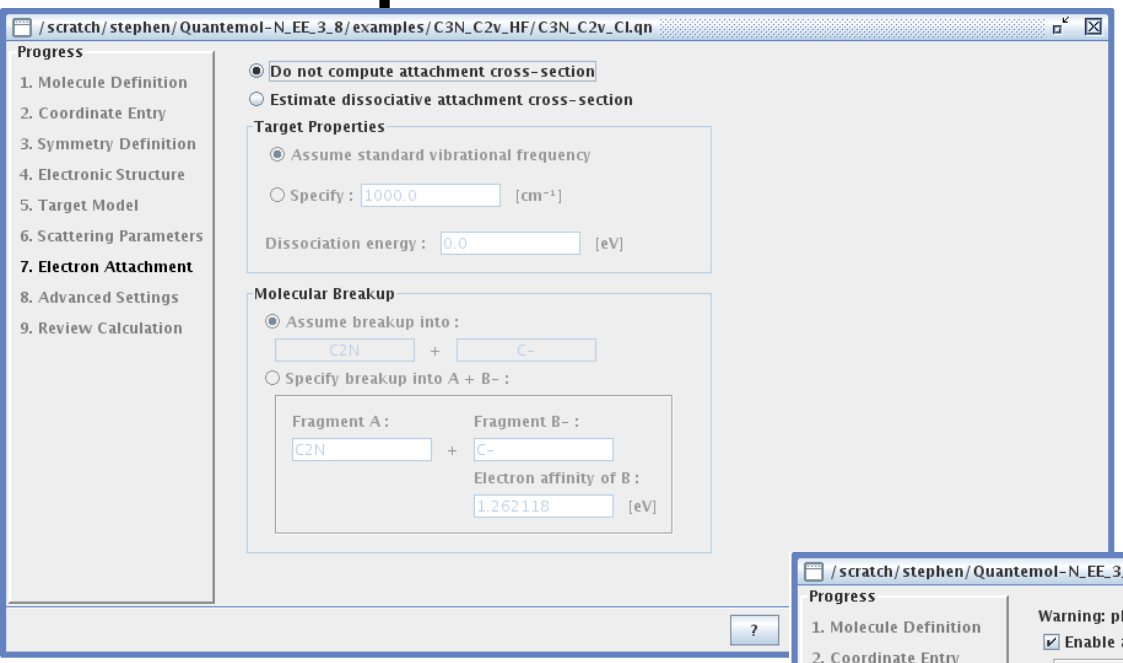


5. Screen five is where you select a basis set to use for the calculation, either from the basis set library contained in QN, or a custom basis set on each atom (which can be obtained online in SuperMolecule format).

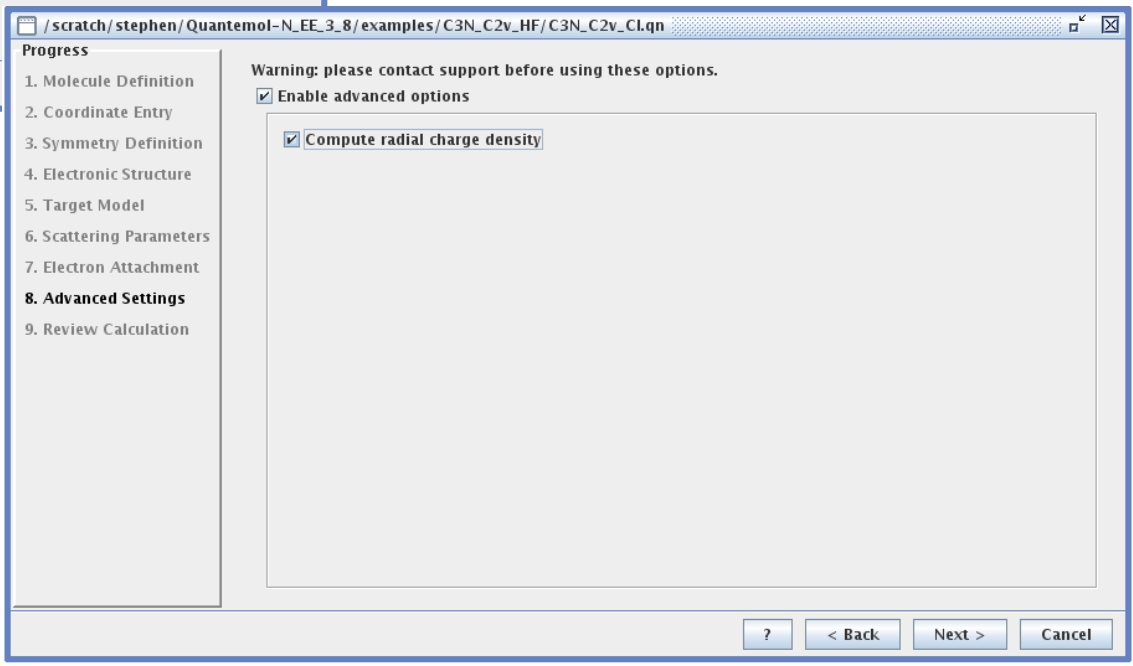


6. Screen fix shows you scattering parameters. The R-matrix radius can be specified. It is 10a by default which will often surfice. If you are using a particularly diffuse basis set, this may need to be increased.

Input Screens and outputs



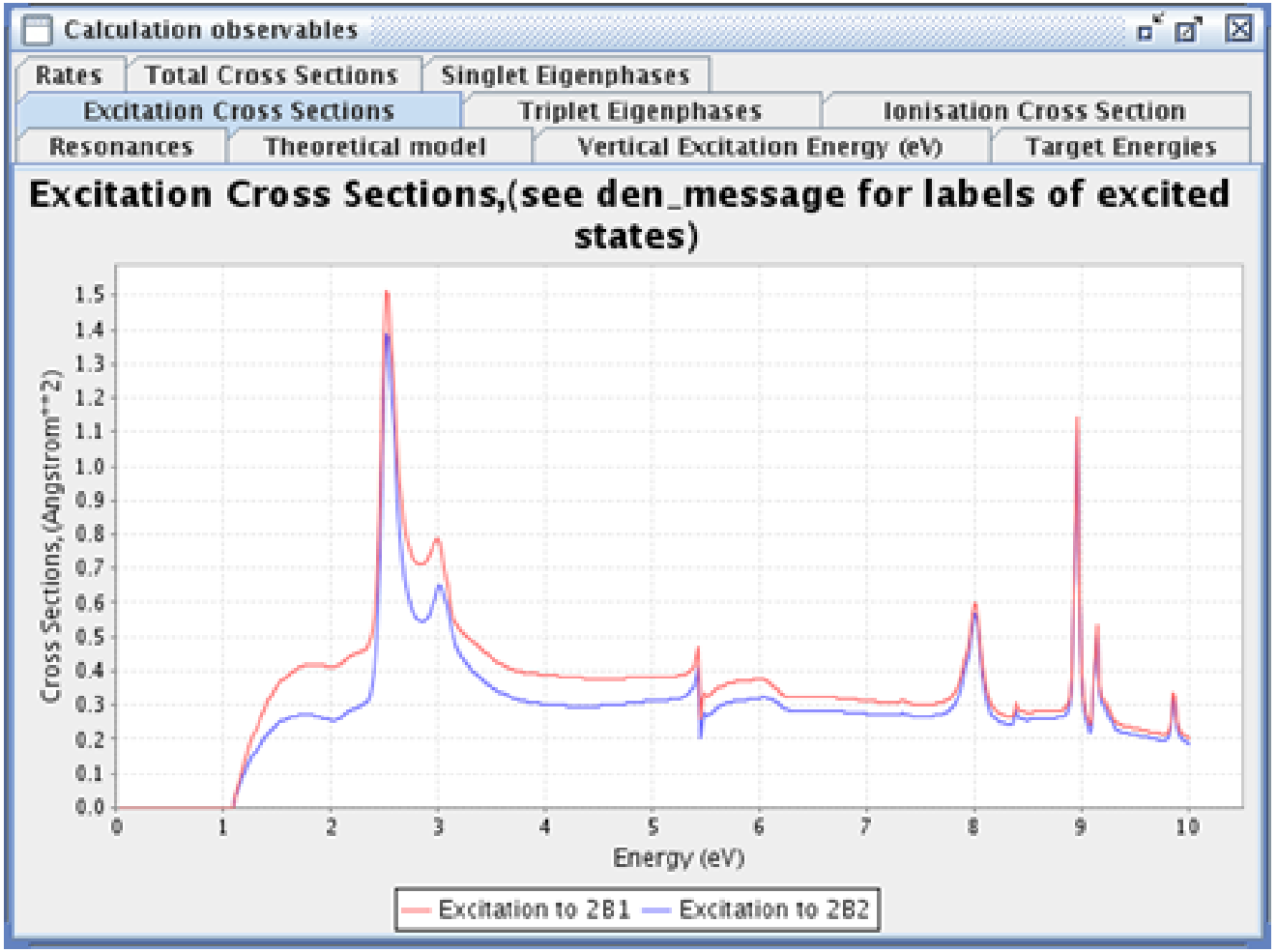
7. Seventh screen offers to calculate dissociative attachment, parameters of which can be specified



8. Advanced settings on the eighth screen allow you to specify in more detail your calculation settings, but should be used only with supervision of Quantemol team for validated results. This panel allows to turn on the option for calculating the radial charge density (note-This significantly increases the calculation time)

Results

Results are automatically plotted and presented in a tabbed results window. These can be quickly called up again at a later date in the exact same format. The data is also available as text files for post analysis and use in models



DEMO SESSION

Some useful websites:
http://cccbdb.nist.gov/ - Good for geometries, data comparisons
https://bse.pnl.gov/bse/portal - Basis set database

I'll now hand over to Sergio for the introduction to Quantemol-D, if you'd like to try Q-N please grab me during the software hands-on!