

# 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:

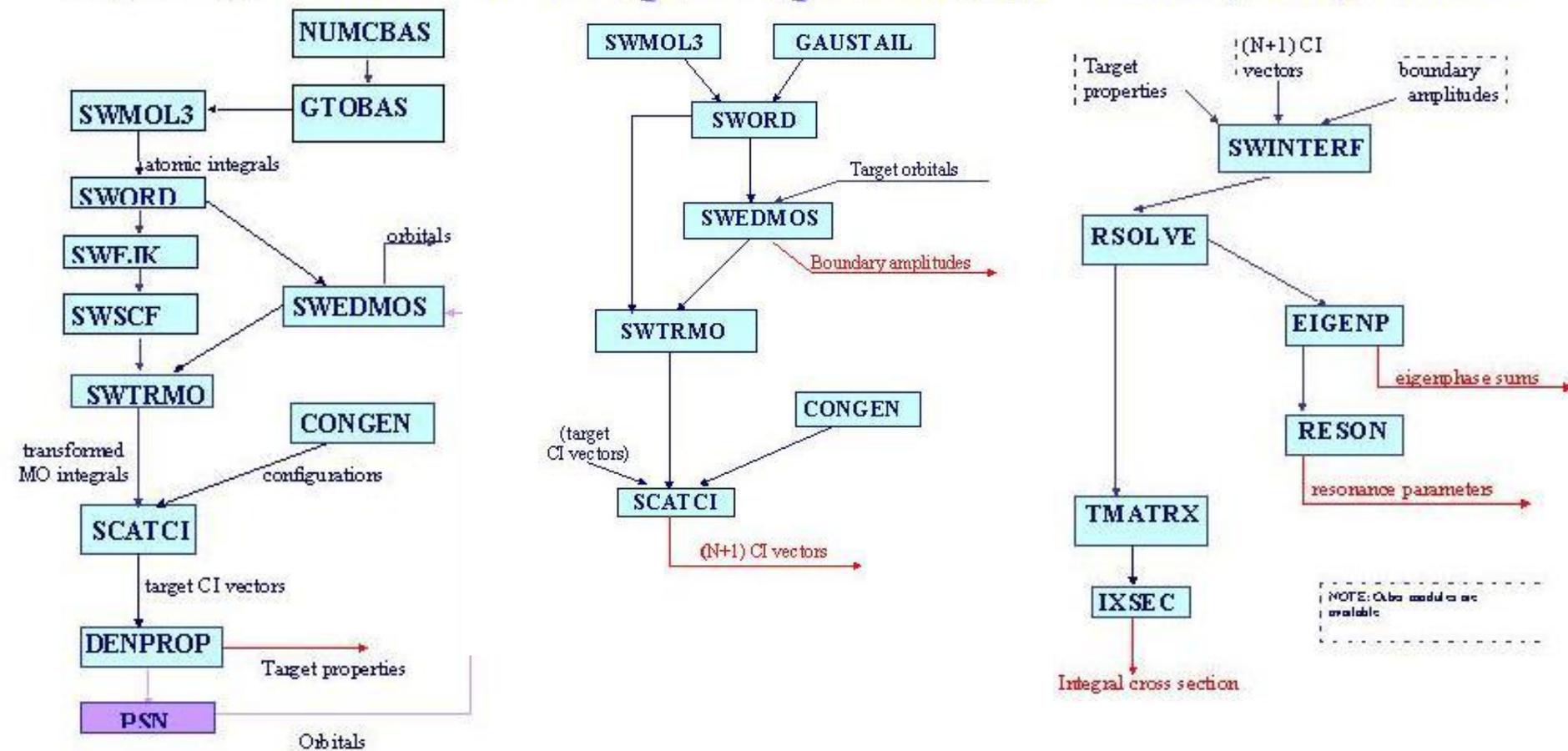
- Vibrational excitation cross sections

# The UK Molecular R-Matrix Codes

## Target Program Modules

## Inner Region Program Modules

## Outer Region Program Modules



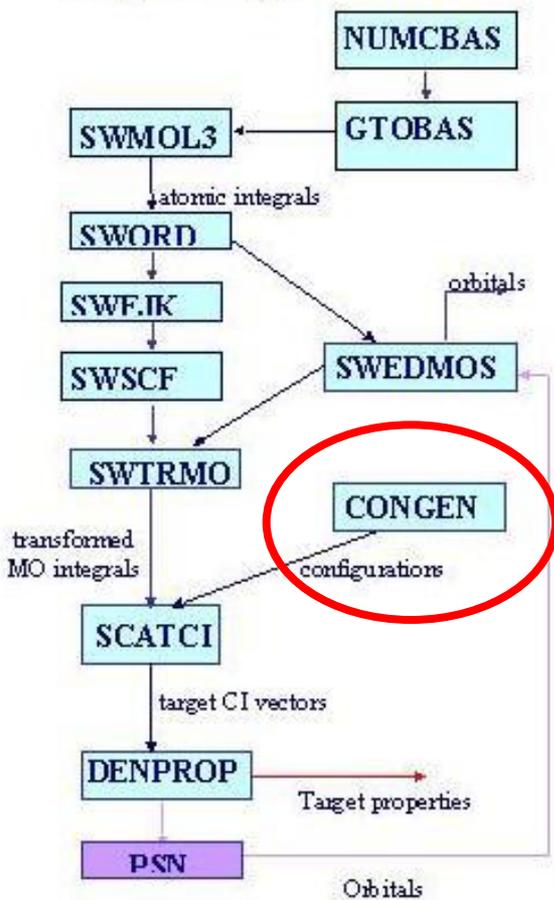
## An example....

```

cat > congen.data << EOF
&STATE
sname="2b1 Congen Calculation",
iscat=1,
megul=71,
syntyp=2,
qntot=2,1,0,
nselect=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)

### Target Program Modules



## 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.*

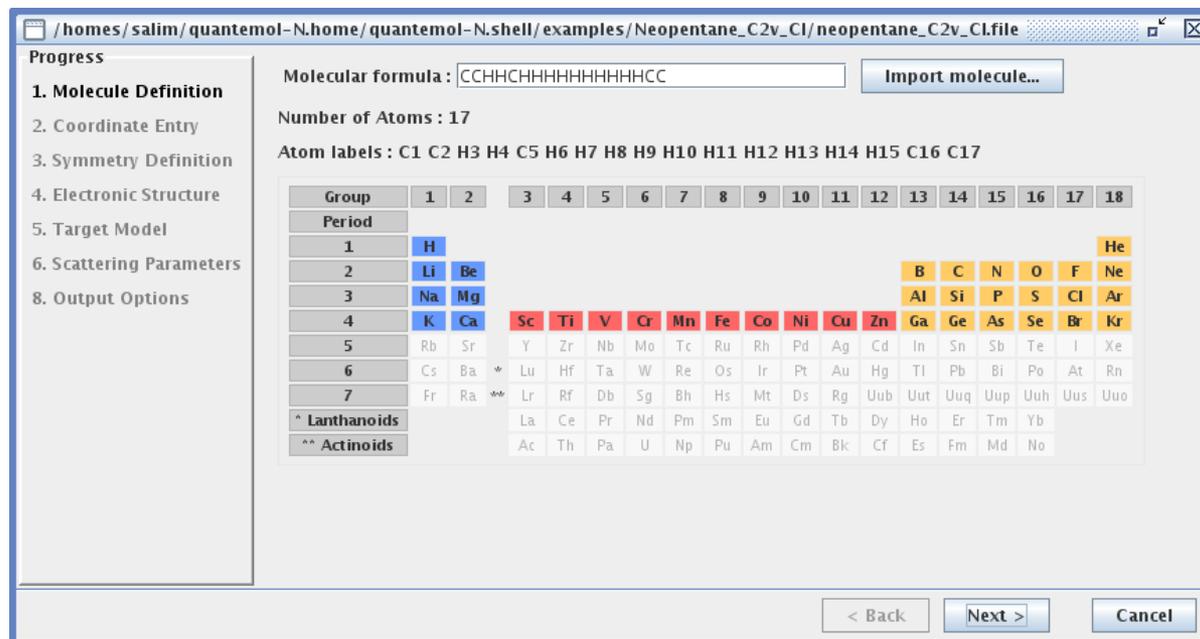
```
molecule=C3N
C1=[0.0, 0.0, -1.9604410372164502]
C2=[0.0, 0.0, -0.74884103721645]
C3=[0.0, 0.0, 0.6257589627835498]
N4=[0.0, 0.0, 1.7866589627835499]
pointGroup=C2v
symEquivAtoms=[C1, C2, C3, N4]
optimise=false
singleOccup=[1, 0, 0, 0]
doubleOccup=[8, 2, 2, 0]
model=CIHF
basis=DZP
basisNAtomSym_C=1
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



Progress

1. Molecule Definition
2. Coordinate Entry
3. Symmetry Definition
4. Electronic Structure
5. Target Model
6. Scattering Parameters
8. Output Options

Molecular formula :

Number of Atoms : 17

Atom labels : C1 C2 H3 H4 C5 H6 H7 H8 H9 H10 H11 H12 H13 H14 H15 C16 C17

Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period 1	H																	He
Period 2	Li	Be											B	C	N	O	F	Ne
Period 3	Na	Mg											Al	Si	P	S	Cl	Ar
Period 4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Period 5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Period 6	Cs	Ba	* Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Period 7	Fr	Ra	** Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo
* Lanthanoids			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb		
** Actinoids			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No		

< Back

# 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.

The screenshot shows the 'Molecule Definition' screen in Quantemol. The window title is '/scratch/stephen/Quantemol-N\_EE\_3\_8/examples/C3N\_C2v\_HF/C3N\_C2v\_CI.qn'. The 'Progress' sidebar on the left lists steps 1 through 9, with '1. Molecule Definition' selected. The main area contains a text box for 'Molecular formula' with 'C3N' entered, an 'Import molecule...' button, and a 'Number of Atoms : 4' label. Below this, 'Atom labels : C1 C2 C3 N4' are listed. A periodic table is displayed with elements highlighted in various colors (blue, yellow, red, grey) to indicate their availability for selection.

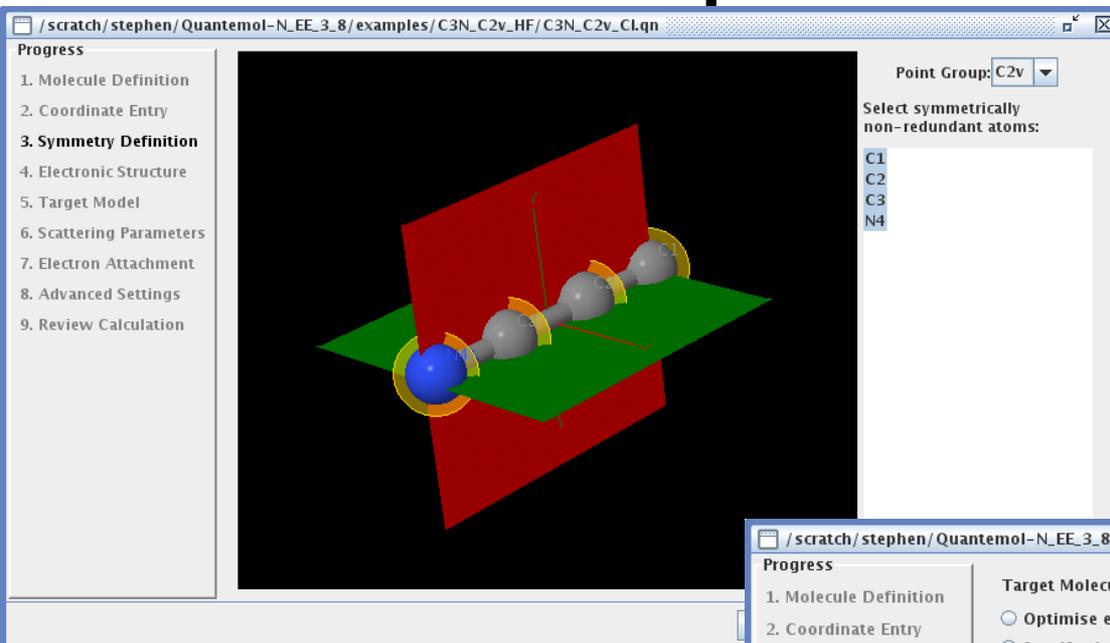
2. The second screen asks you to define the molecule's geometry

The screenshot shows the 'Coordinate Entry' screen in Quantemol. The window title is '/scratch/stephen/Quantemol-N\_EE\_3\_8/examples/C3N\_C2v\_HF/C3N\_C2v\_CI.qn'. The 'Progress' sidebar on the left lists steps 1 through 9, with '2. Coordinate Entry' selected. The main area features a table for entering atomic coordinates:

Atom Label	X (angstroms)	Y (angstroms)	Z (angstroms)
C1	0	0	-1.96
C2	0	0	-0.749
C3	0	0	0.626
N4	0	0	1.787

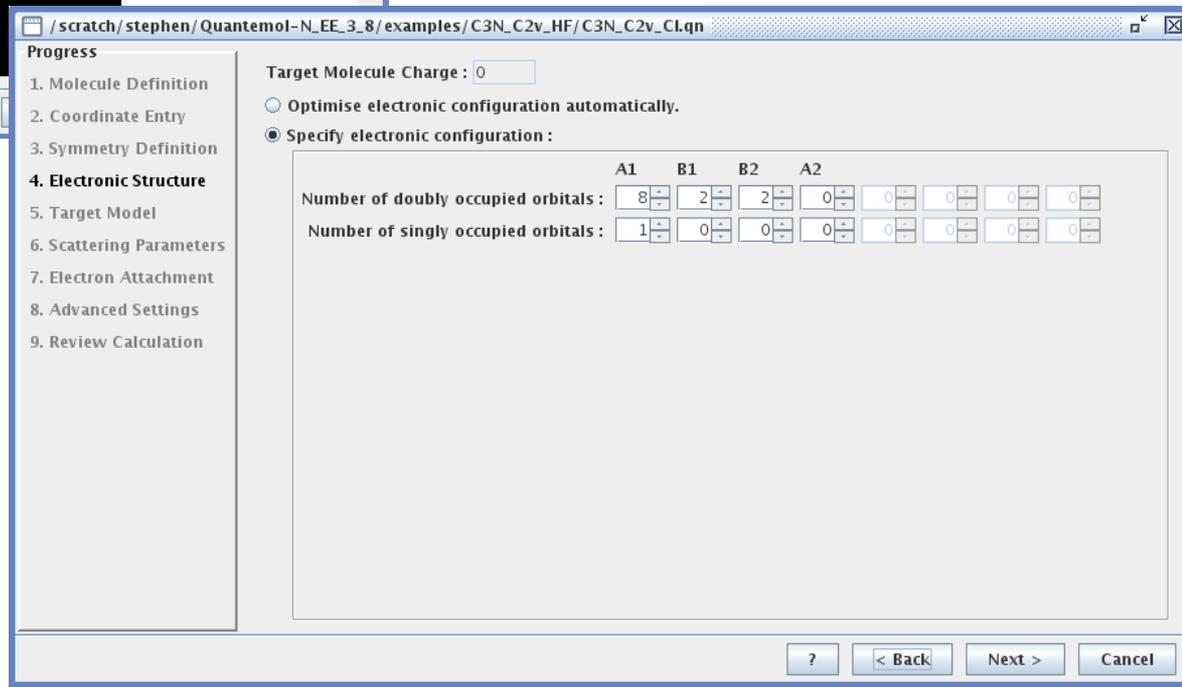
Below the table, there are several control buttons: 'Move to centre of mass', 'Clear position data', 'Rotate around axis' (with radio buttons for X, Y, and Z, where X is selected), 'Angle : 180.00 degrees', and 'Rotate'. At the bottom of the window, there are navigation buttons: '?', '< Back', 'Next >', and 'Cancel'.

# Input Screens

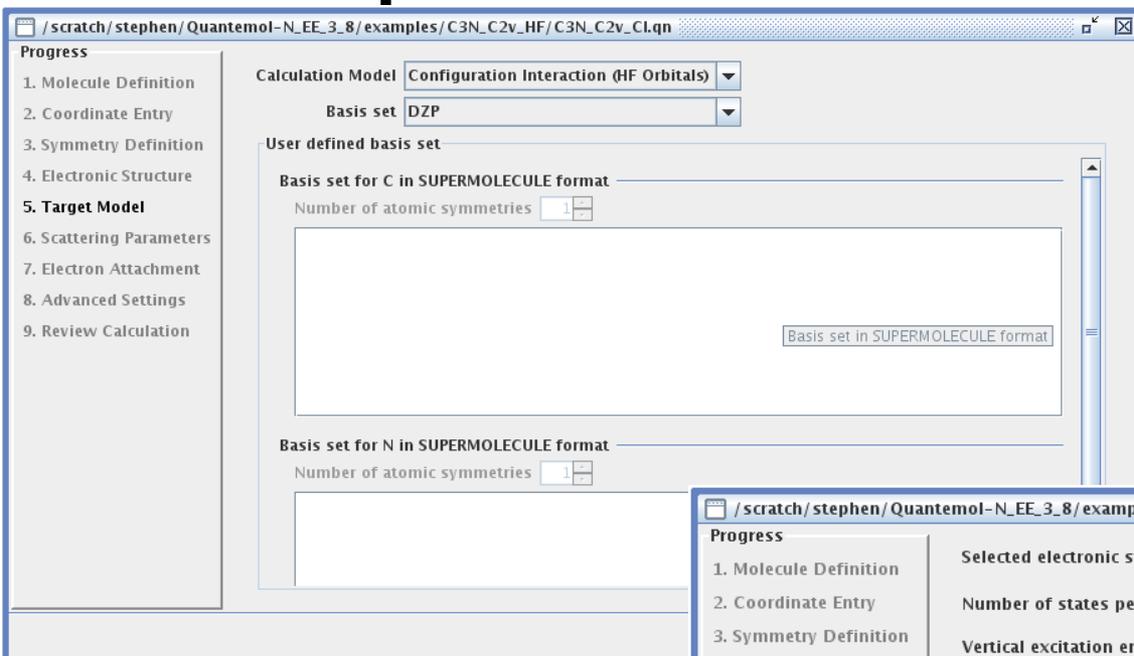


3. Screen three suggests you to choose non-symmetrical atoms, which can help us to make calculation quicker as symmetry will be taken into account.

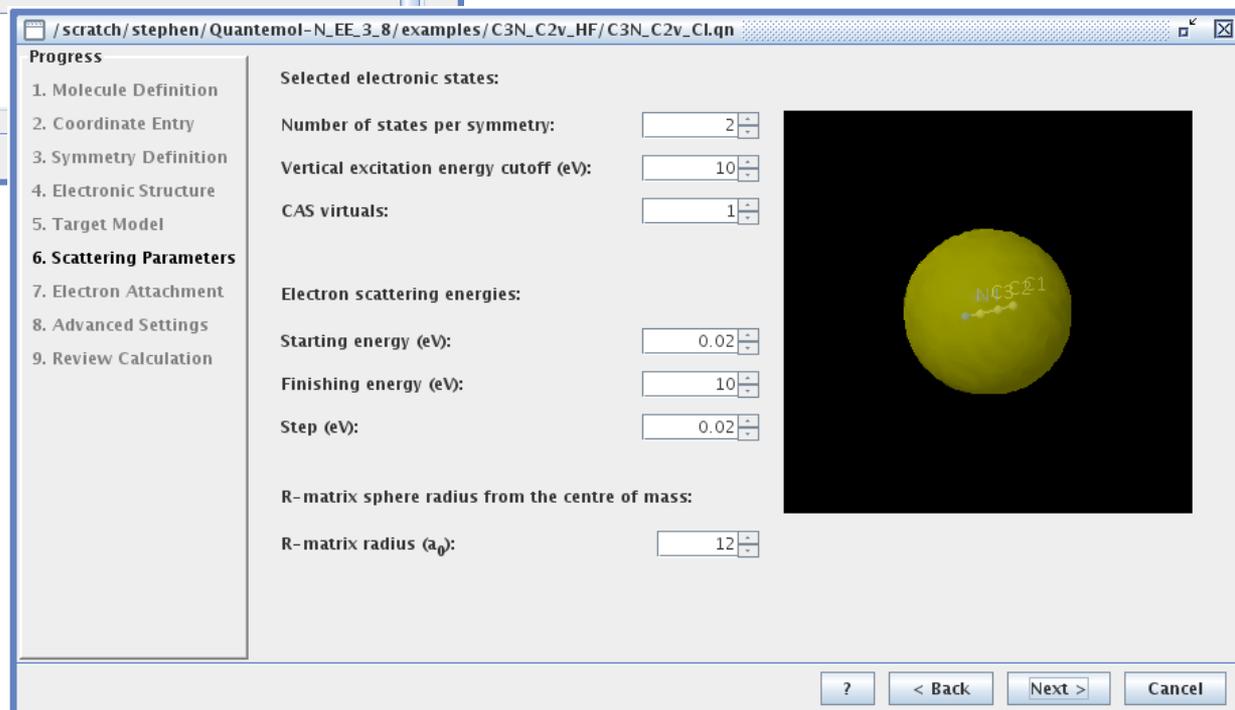
4. Screen four allows the definition of electron occupation for the states attributed to the symmetry chosen. It also allows positive ions to be defined if required,



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

# Input Screens and outputs

Progress

1. Molecule Definition
2. Coordinate Entry
3. Symmetry Definition
4. Electronic Structure
5. Target Model
6. Scattering Parameters
7. **Electron Attachment**
8. Advanced Settings
9. Review Calculation

Do not compute attachment cross-section  
 Estimate dissociative attachment cross-section

Target Properties

Assume standard vibrational frequency  
 Specify : 1000.0 [cm<sup>-1</sup>]  
Dissociation energy : 0.0 [eV]

Molecular Breakup

Assume breakup into :  
C2N + C-  
 Specify breakup into A + B - :  
Fragment A : C2N + Fragment B - : C-  
Electron affinity of B : 1.262118 [eV]

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

Progress

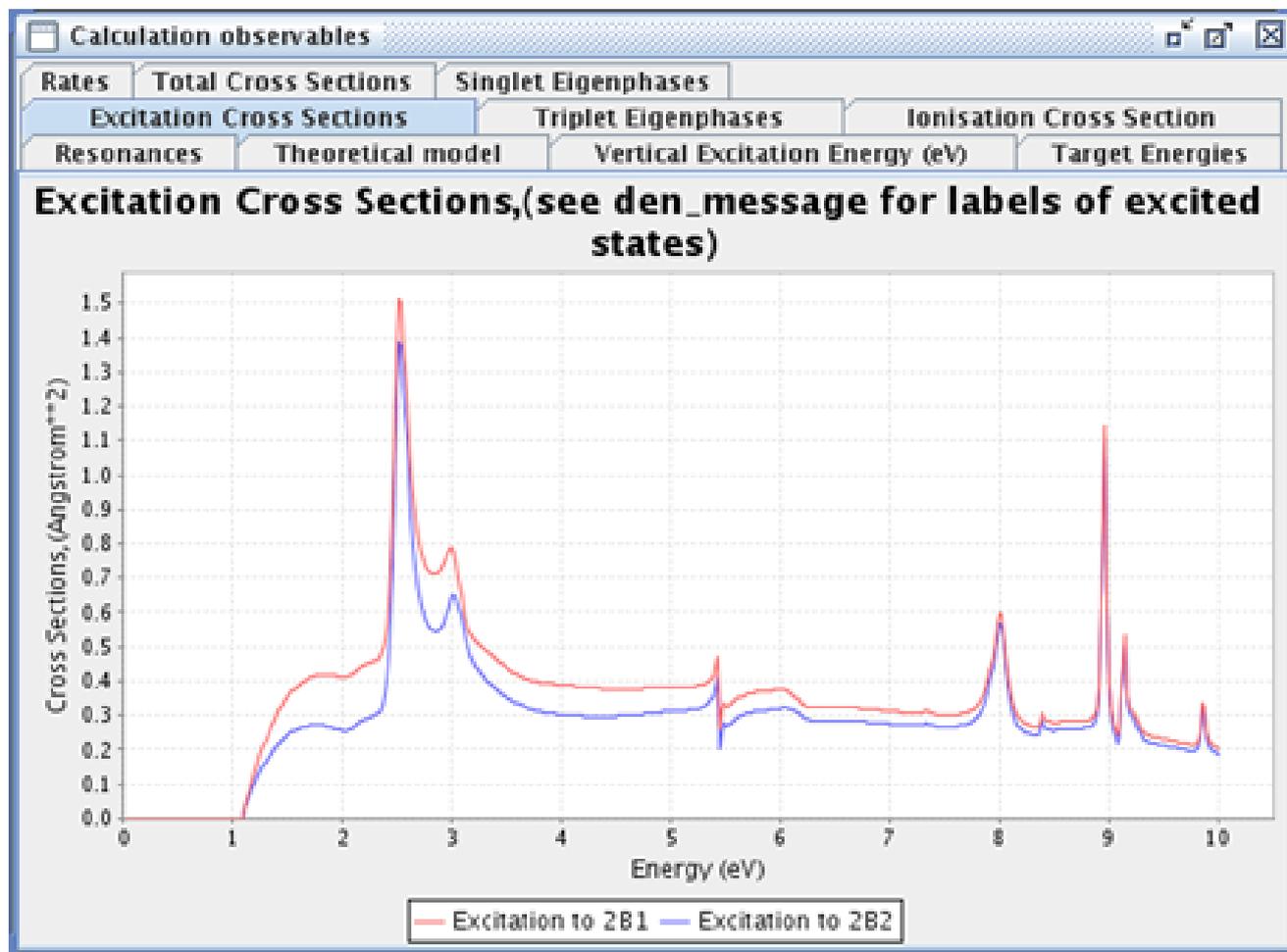
1. Molecule Definition
2. Coordinate Entry
3. Symmetry Definition
4. Electronic Structure
5. Target Model
6. Scattering Parameters
7. Electron Attachment
8. **Advanced Settings**
9. Review Calculation

Warning: please contact support before using these options.  
 Enable advanced options  
 Compute radial charge density

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!***