

Quantemol 

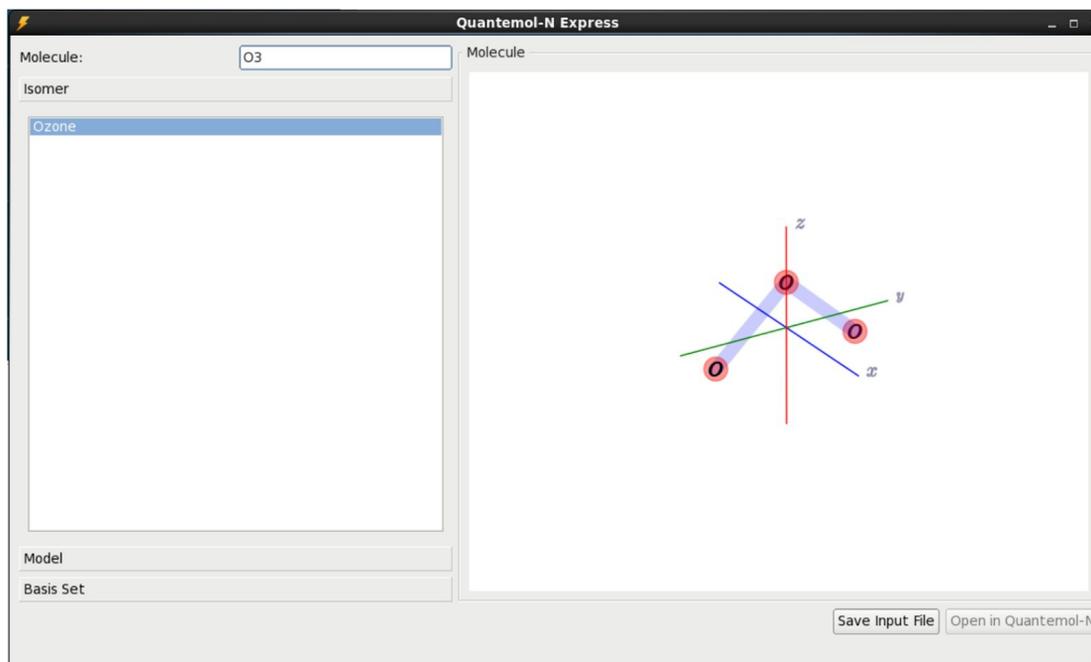
QW
Electron Scattering
Walkthrough


Q-workshop

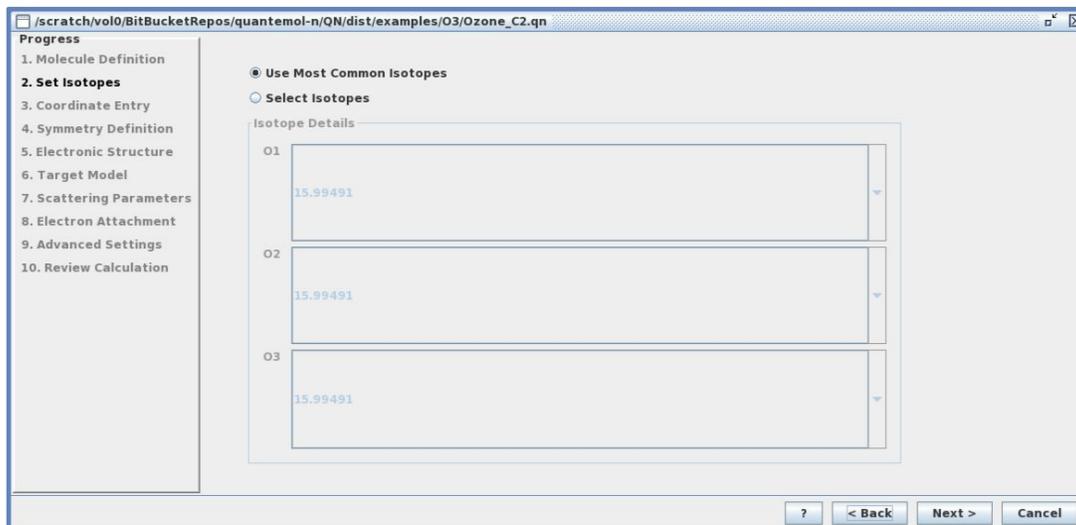
1. To start Quantemol-N please double click on the Express icon:



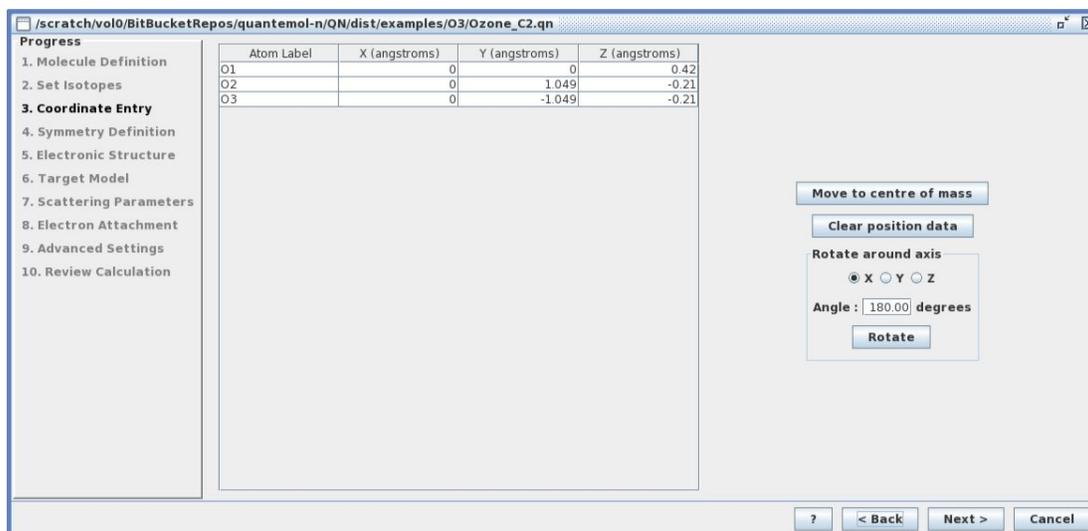
And choose “Run In Terminal”



2. The QN Express will open up. Enter a molecular formula, e.g. O3, or the name of a molecule, e.g. Ozone, into the “Molecule:” field and click enter. The geometry of the molecule will be downloaded from the NIST website.
3. Click “Save Input File” in the lower right hand corner of the Express. You can just save the molecule in the first screen that opens, saving the molecule here will create the .qn input file to be used in QN.
4. Identifying symmetries will speed up our calculation. We can see from the name of the .qn file that a C2 symmetry/point group has already been selected for the molecule, in the case of O3 either the C2 or C2v point group can be used.
5. Try Entering other molecules in the “Molecule:” field and see what point groups are chosen, for example:
CO2 has D2h
CH4 has D2

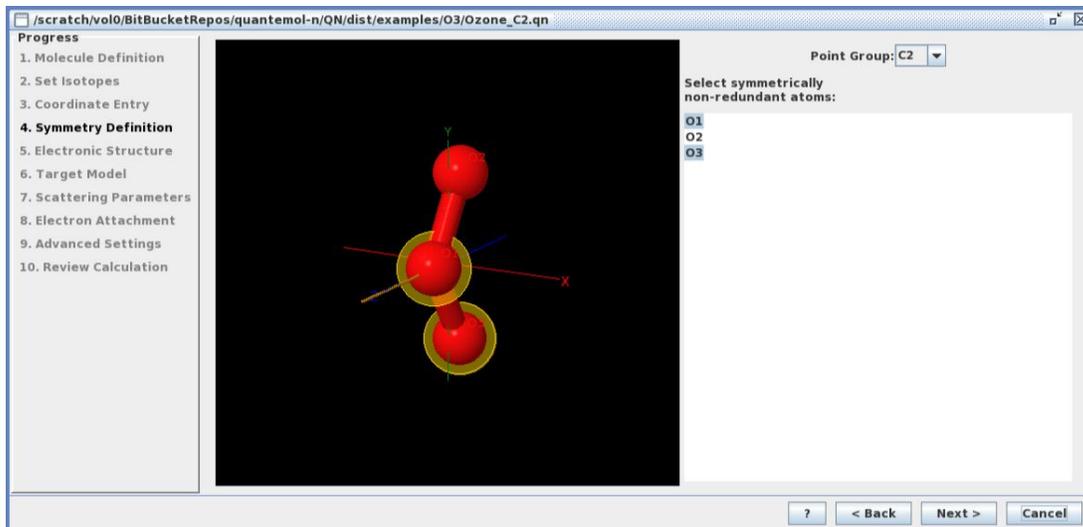


10. The next screen is the “Coordinate Entry” screen. We can see that the molecule's geometry has been imported from the NIST database by the Express. If we click the “Move to the centre of mass” button we can see the geometries given are in the centre of mass frame.



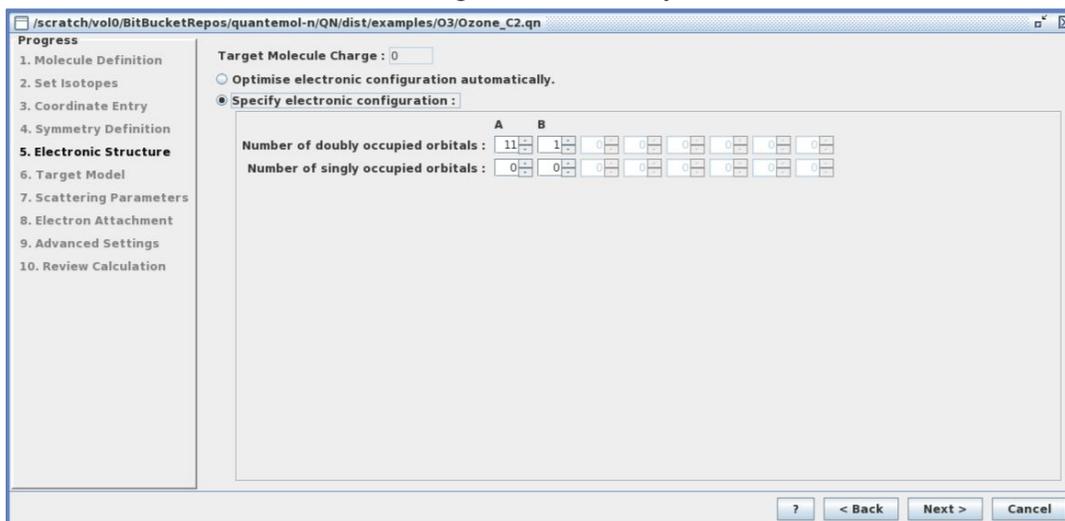
Click “Next”.

11. The fourth screen is the “Symmetry Definition” screen. We can see on this screen that a point group has been chosen and the appropriate atoms selected for this point group calculation.

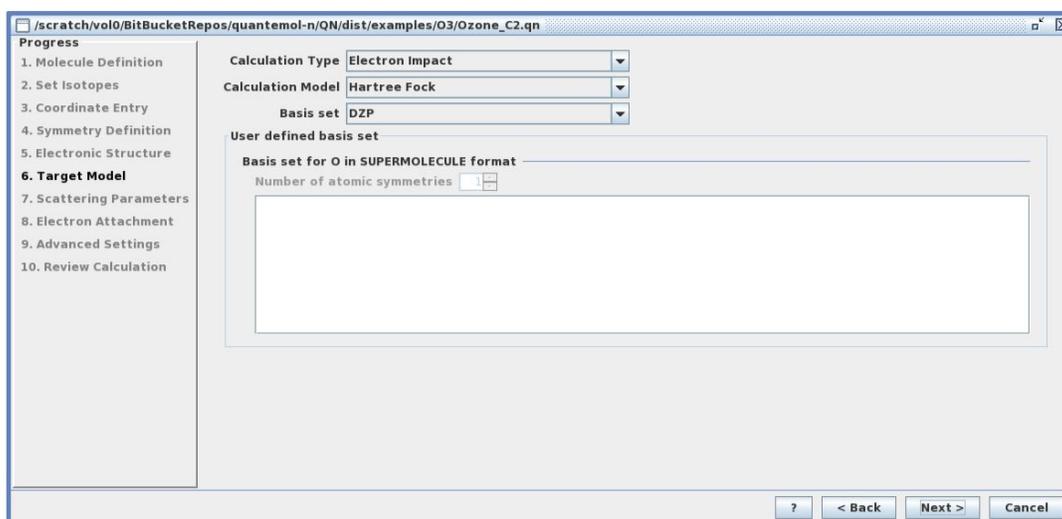


Click “Next”.

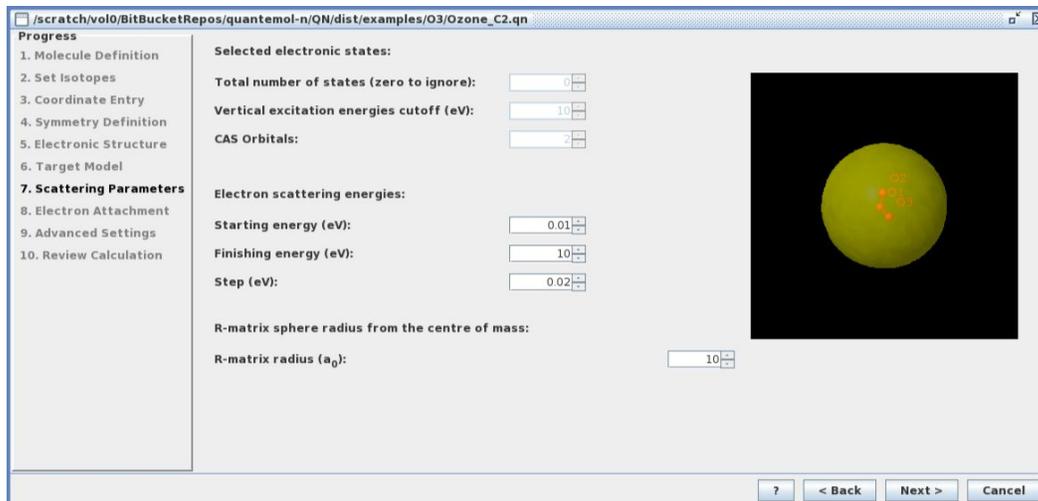
12. The fifth screen is the “Electronic Structure” screen. This screen allows the user to define the ground state electron configuration of the molecule. For the time being we will leave the “Optimise electronic configuration automatically” radio button selected and we will see if this calculates the electron configuration correctly.



13. In some cases this does not find the correct configuration and this has to be done manually, quantemol support will be happy to go through this with you. Click “Next”.
14. The sixth screen is the “Target Model” screen. This screen allows the user to choose the type of scattering they would like to model, either electron scattering or photon scattering, by selecting from the “Calculation Type” dropdown. For the time being please choose “Electron Impact”.



15. This screen also allows the user to set up their calculation. The user can calculate the scattering using either the Hartree Fock (HF) model, also known as the static exchange model, or the Configuration Interaction (CI) model. For the time being select the Hartree Fock model, this will give us quick qualitative results and we can then go back and run a CI calculation if we want better results.
16. The “Target Model” screen also allows the user the choose a “Basis set” for the molecule. Basis sets are sets of functions used to calculate the molecular orbitals. A selection of basis sets are provided for the molecule chosen of varying size, size being the number of functions in the set. Choosing a basis set is really a matter of the user’s judgement but certain basis sets are likely to produce good results. We will select one of these now: DZP. The user can also import a different basis set for their molecule but we will not do than now. Quantemol is always happy to help advise users on selecting basis sets. Please click next.
17. The seventh screen is the “Scattering Parameters” screen. Because we have chosen to do a HF calculation some of the fields are greyed out. We will leave these for now. You can choose the energy range you would like for the incident electrons, for example 0.01 - 10 eV and the size of the increments.



18. The field “R-Matrix Radius” is the one field in the whole program that relates to the R-Matrix theory. Because we have chosen a small size molecule and a medium size basis set write 10 in this field for the time being. Please click next.
19. We will skip over the eighth and the ninth screens for now.
20. The tenth screen is the “Review Calculation” screen. Click the “Save” button. We have to save another .qn file with the changes that have been made since we saved in the Express. You can either save over your original file or save another .qn file.
21. Click the “Run” button and say “Yes” you are sure you want to run.
22. This calculation will take a couple of minutes. Certain details of the calculation will be printed to the screen some of which may be of interest for example electron configuration:

```

Calculation Output
*****
Running SCF calculation for the ground state
*****
Optimising ground state.
SCF complete now
ORBITAL ENERGIES ARE:
SYM 1 ORB 1 -566.18 EV 2.000 OCC
SYM 2 ORB 1 -563.23 EV 2.000 OCC
SYM 1 ORB 2 -563.23 EV 2.000 OCC
SYM 1 ORB 3 -48.07 EV 2.000 OCC
SYM 2 ORB 2 -39.44 EV 2.000 OCC
SYM 1 ORB 4 -28.34 EV 2.000 OCC
SYM 2 ORB 3 -23.34 EV 2.000 OCC
SYM 1 ORB 5 -21.61 EV 2.000 OCC
SYM 2 ORB 4 -21.16 EV 2.000 OCC
SYM 1 ORB 6 -16.44 EV 2.000 OCC
SYM 2 ORB 5 -13.05 EV 2.000 OCC
SYM 2 ORB 6 -11.95 EV 2.000 OCC
SYM 1 ORB 7 -2.85 EV 0.000 OCC
SYM 1 ORB 8 9.73 EV 0.000 OCC
SYM 2 ORB 7 11.92 EV 0.000 OCC
SYM 1 ORB 9 19.33 EV 0.000 OCC
SYM 2 ORB 8 20.21 EV 0.000 OCC
SYM 2 ORB 9 20.70 EV 0.000 OCC
SYM 1 ORB 10 22.17 EV 0.000 OCC
SYM 2 ORB 10 23.34 EV 0.000 OCC
SYM 1 ORB 11 23.88 EV 0.000 OCC
SYM 1 ORB 12 24.02 EV 0.000 OCC
SYM 2 ORB 11 24.46 EV 0.000 OCC
SYM 2 ORB 12 26.38 EV 0.000 OCC
SYM 1 ORB 13 30.68 EV 0.000 OCC

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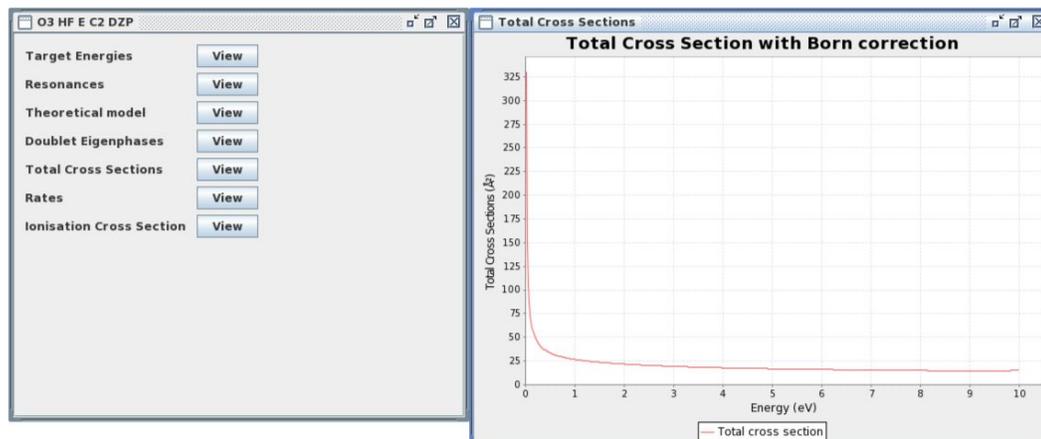
Or for a configuration interaction calculation excited states:

```

Calculation Output
*****
Vertical excitation energies in eV:
*****
Singlet A 0.0
Triplet B 1.0122119999995745
Triplet B 1.3224059999998181
Singlet B 1.583621999999828
Triplet A 1.869327000000187
Singlet A 2.0298660000001028
Triplet B 3.357714000000102
Singlet A 3.5100899999997464
Triplet A 7.417445999999534
Singlet B 8.481357000000005
Singlet A 8.48951999999955
Triplet B 9.78199499999992
Singlet B 9.795599999999599
Singlet A 10.369731000000098
Triplet A 10.494896999999613
Singlet B 11.245892999999795
Triplet B 11.47173599999956
Triplet A 11.550644999999857
Singlet A 12.149264999999623
Triplet B 12.483947999999906
Singlet A 12.641765999999732
Triplet B 13.292084999999666
Triplet A 13.349226000000016
Singlet A 13.474391999999531
Triplet A 13.57778999999987

```

23. When the calculation finishes a window will open saying “Do you wish to save?”, click “Cancel”.
24. A small results screen will appear which will allow you to look some results of the calculation. Please take a look at these results but bear in mind that the calculation just run was a Hartree Fock calculation so the results will not be exact.



25. The results shown in this window are just a small selection of the results produced by QN. Open a terminal and type:

```
j$ cd ~/Desktop/QNEE4.9.4/workspace/project/Ozone_C2
```
26. You can find in this folder all the data produced from the calculation, for example in the output files directory contains the file born.out which contains a selection of constants calculated for the molecule. Please ask an instructor if there are specific data you are looking for and they will help you navigate to it.
27. You will also find in this results directory (Depending on the calculation type and model)
 - Elastic cross-sections
 - Electronic excitation cross-sections*
 - Super-Elastic cross-sections between excited states*
 - Electron impact dissociation*
 - Ionisation cross-sections
 - Scattering reaction rate
 - Resonance parameters
 - Dissociative electron attachment**
 - Differential cross-sections
 - Momentum transfer cross-sections
 - Photoionisation cross-sections***

*Only produced in configuration interaction calculations

**Only produced if dissociative attachment calculation has been set up

***Only produced for photoionisation calculation type

