CalcALC User Manual

CalcALC is a Windows PC tool developed by Francis Pratt at ISIS for simulating and interpreting muon avoided level crossing (ALC) spectra of muoniated molecular radicals in both solid and liquid/gas phases using density functional theory (DFT).

It has two ways of working. It can either set up and automate Gaussian DFT calculations using the STFC SCARF compute cluster or it can take the output of previous independently made Gaussian or CASTEP magres calculations as the starting point for spectral simulation.

For the automatic mode, the starting point is a molecular structure defined in a file in pdb format. From this the user selects muon addition and substitution sites and a set of Gaussian jobs are prepared and submitted to the remote SCARF compute cluster which is operated by STFC Scientific Computing. Progress of the calculations is monitored and the completed DFT output files are returned to the host computer as the starting point for the spectral simulations.

From the single molecule Gaussian output files the program extracts muon and nuclear hyperfine parameters. It can also extract hyperfine parameters from CASTEP magres output files that may correspond to a periodic structure crystal calculation, such calculations have to be made independently before using CalcALC.

The radicals and strongly coupled nuclei contributing to the ALC spectrum are selected and used to build up the simulated spectrum using the Quantumtools python library developed by James Lord at ISIS.

The overall spectrum and its constituent components are finally plotted out using the GLE graphics layout engine.

Besides simulating the ALC spectra of open shell muon systems with finite hyperfine coupling, the program can also calculate electric field gradient tensors in closed shell diamagnetic muon systems and thus predict quadrupolar level crossing resonance (QLCR) spectra. Version 1.32 also now allows calculation of ZF/LF relaxation functions to be made in diamagnetic mode.

The CalcALC webpage is at: https://shadow.nd.rl.ac.uk/calcalc/

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What is needed to install and run CalcALC?

Windows

A windows machine or virtual machine is needed to run the software.

Python

A Python installation with the numpy module installed.

The windows path must include the location of python.exe and for python files which have the .py extension the default windows application must be set to python.exe.

Putty

For communicating with SCARF a full installation of **putty** is needed, giving the command line programs: putty.exe, plink.exe and pscp.exe. The windows path variable must include the location of these executables.

SCARF account

A SCARF account is needed for automatic calculation of hyperfine parameters of muon radical states using Gaussian DFT. Before using the CalcALC program test the SCARF account by using putty to log on to scarf.rl.ac.uk, saving the security key when prompted.

GLE4

The graphics package GLE4 is used to plot the polarisation spectra. This will be present on any system where the Wimda muon data analysis software has been fully installed or can be installed independently.

After these prerequisites have been checked and installed if necessary, the CalALC program can be installed.

CalcALC

The CalcALC installer program is CalcALCinstall.exe. After installation the PYTHONPATH environment variable should have been set to point to the location of the CalcALC installation folder.

Viewers for the pdb files are useful. Recommended are Jmol.jar as a simple java-based viewer and the CCDC viewer Mercury as a good full-featured option.

Running CalcALC

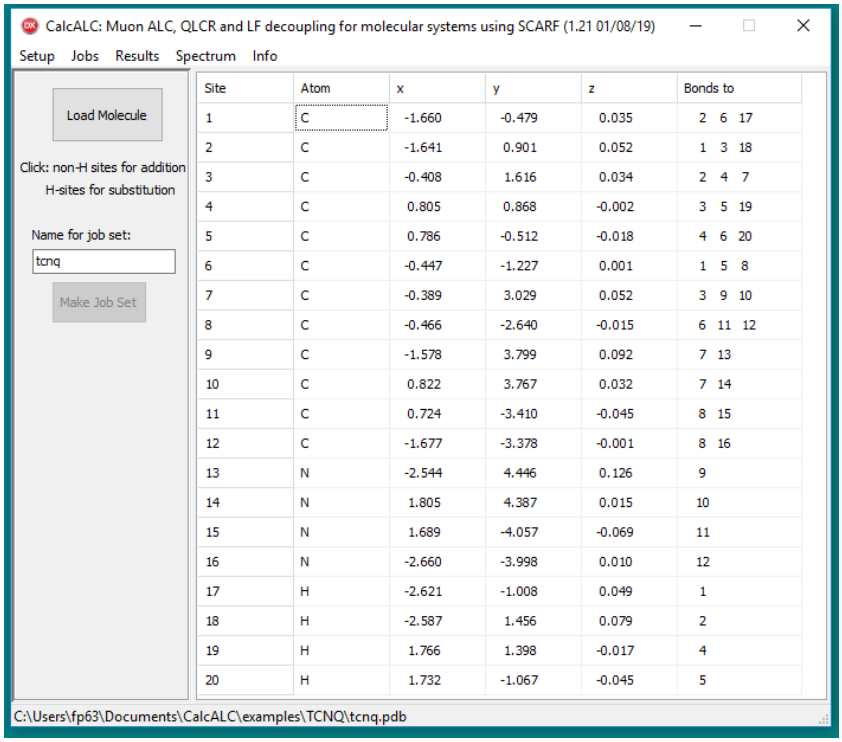
Step by step:

Step 1: Prepare the bare molecular structure in the form of pdb format file using suitable software (e.g. Mercury, Materials Studio, Crystalmaker etc.). A useful piece of software that allows conversion between structure formats is openbabel.

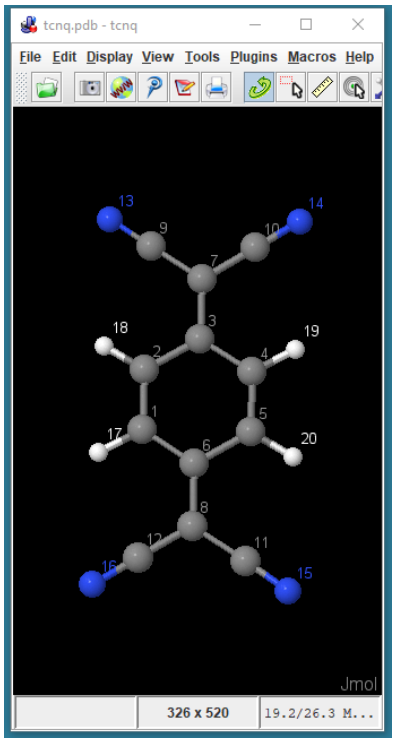
e.g. TCNQ

```
HETATM    1  C            1       -1.660  -0.479   0.035
HETATM    2  C            2       -1.641   0.901   0.052
HETATM    3  C            3       -0.408   1.616   0.034
HETATM    4  C            4        0.805   0.868  -0.002
HETATM    5  C            5        0.786  -0.512  -0.018
HETATM    6  C            6       -0.447  -1.227   0.001
HETATM    7  C            7       -0.389   3.029   0.052
HETATM    8  C            8       -0.466  -2.640  -0.015
HETATM    9  C            9       -1.578   3.799   0.092
HETATM   10  C           10        0.822   3.767   0.032
HETATM   11  C           11        0.724  -3.410  -0.045
HETATM   12  C           12       -1.677  -3.378  -0.001
HETATM   13  N           13       -2.544   4.446   0.126
HETATM   14  N           14        1.805   4.387   0.015
HETATM   15  N           15        1.689  -4.057  -0.069
HETATM   16  N           16       -2.660  -3.998   0.010
HETATM   17  H           17       -2.621  -1.008   0.049
HETATM   18  H           18       -2.587   1.456   0.079
HETATM   19  H           19        1.766   1.398  -0.017
HETATM   20  H           20        1.732  -1.067  -0.045
CONECT    1    2    6   17
CONECT    2    1    3   18
CONECT    3    2    4    7
CONECT    4    3    5   19
CONECT    5    4    6   20
CONECT    6    1    5    8
CONECT    7    3    9   10
CONECT    8    6   11   12
CONECT    9    7   13
CONECT   10    7   14
CONECT   11    8   15
CONECT   12    8   16
CONECT   13    9
CONECT   14   10
CONECT   15   11
CONECT   16   12
CONECT   17    1
CONECT   18    2
CONECT   19    4
CONECT   20    5
END
```

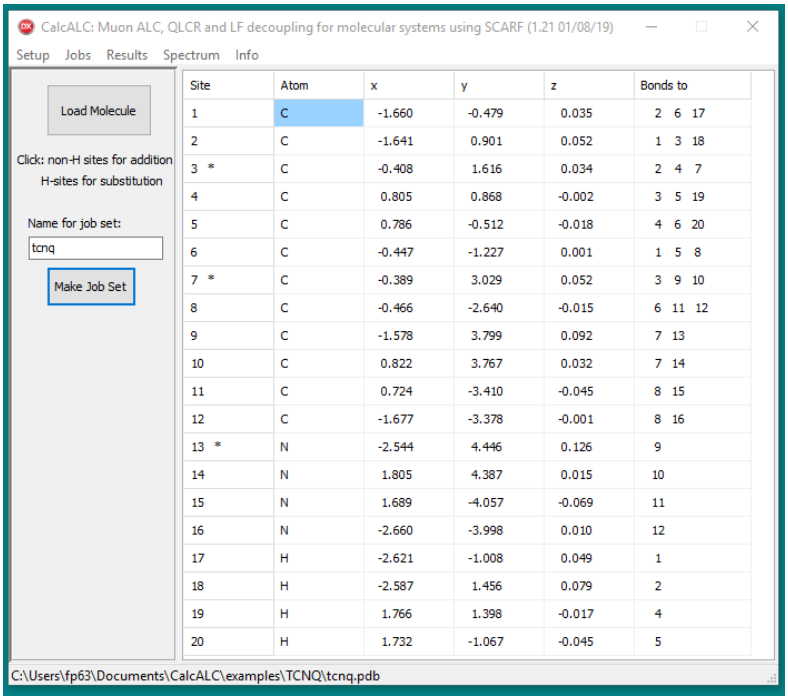
Step 2: Use the 'Load Molecule' button in the main CalcALC window to load in the pdb file. A viewer such as Jmol.jar or Mercury can be used to view the site numbering.



Site	Atom	x	y	z	Bonds to
1	C	-1.660	-0.479	0.035	2 6 17
2	C	-1.641	0.901	0.052	1 3 18
3	C	-0.408	1.616	0.034	2 4 7
4	C	0.805	0.868	-0.002	3 5 19
5	C	0.786	-0.512	-0.018	4 6 20
6	C	-0.447	-1.227	0.001	1 5 8
7	C	-0.389	3.029	0.052	3 9 10
8	C	-0.466	-2.640	-0.015	6 11 12
9	C	-1.578	3.799	0.092	7 13
10	C	0.822	3.767	0.032	7 14
11	C	0.724	-3.410	-0.045	8 15
12	C	-1.677	-3.378	-0.001	8 16
13	N	-2.544	4.446	0.126	9
14	N	1.805	4.387	0.015	10
15	N	1.689	-4.057	-0.069	11
16	N	-2.660	-3.998	0.010	12
17	H	-2.621	-1.008	0.049	1
18	H	-2.587	1.456	0.079	2
19	H	1.766	1.398	-0.017	4
20	H	1.732	-1.067	-0.045	5



Click on the addition sites to include, each one selected will be marked by a *



Site	Atom	x	y	z	Bonds to
1	C	-1.660	-0.479	0.035	2 6 17
2	C	-1.641	0.901	0.052	1 3 18
3 *	C	-0.408	1.616	0.034	2 4 7
4	C	0.805	0.868	-0.002	3 5 19
5	C	0.786	-0.512	-0.018	4 6 20
6	C	-0.447	-1.227	0.001	1 5 8
7 *	C	-0.389	3.029	0.052	3 9 10
8	C	-0.466	-2.640	-0.015	6 11 12
9	C	-1.578	3.799	0.092	7 13
10	C	0.822	3.767	0.032	7 14
11	C	0.724	-3.410	-0.045	8 15
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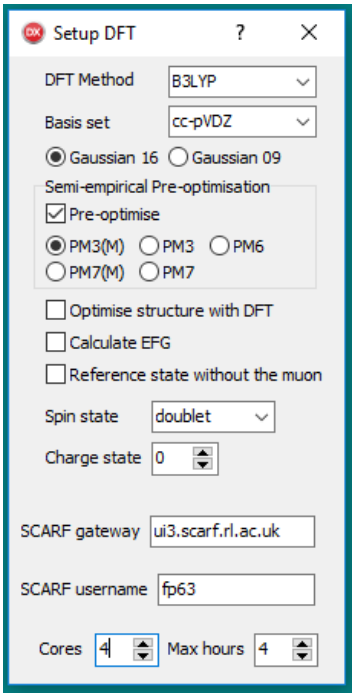
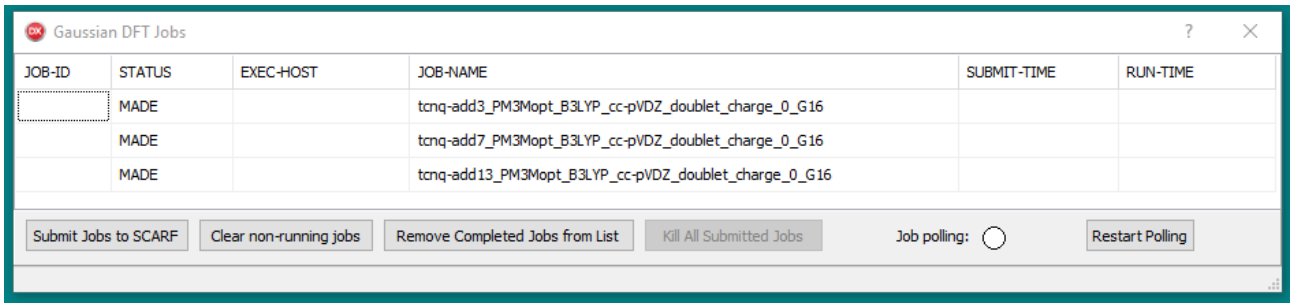
17	H	-2.621	-1.008	0.049	1
18	H	-2.587	1.456	0.079	2
19	H	1.766	1.398	-0.017	4
20	H	1.732	-1.067	-0.045	5

Clicking on an H site marks it as a muon site (substitution site). This also provides a way of marking the muon site if a muon has already been included in the molecular structure file.

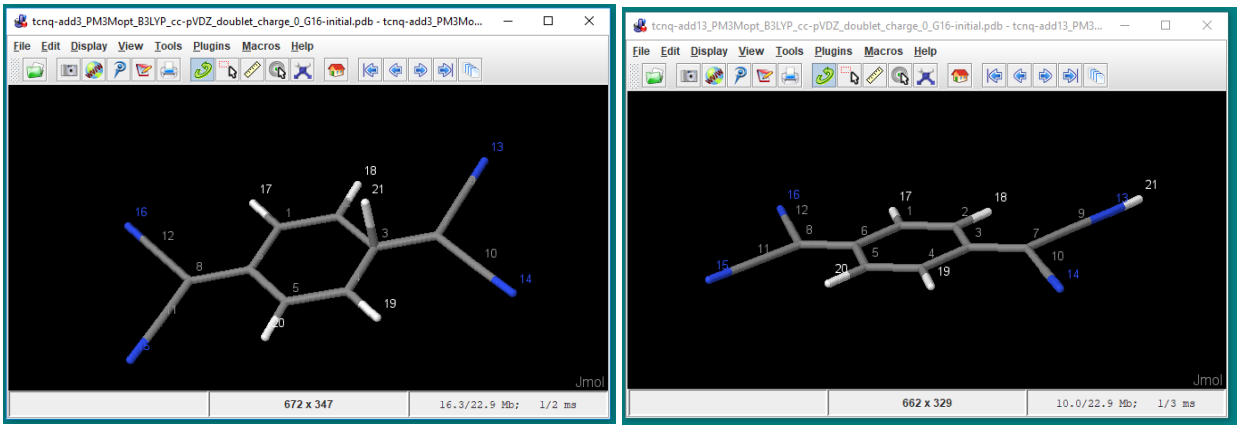
Step 3: Use the setup window to define the type of calculation. Pre-optimisation of the structure with semi-empirical methods before a single point DFT calculation provides an efficient and acceptably accurate calculation method. Full structural optimisation with DFT is also available as a much slower option.



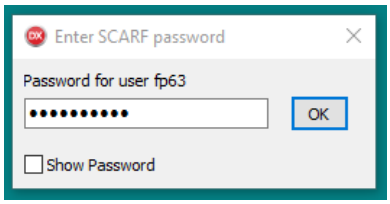
When ready click the 'Make Job Set' button in the main CalcALC window which will insert entries in the jobs list window.



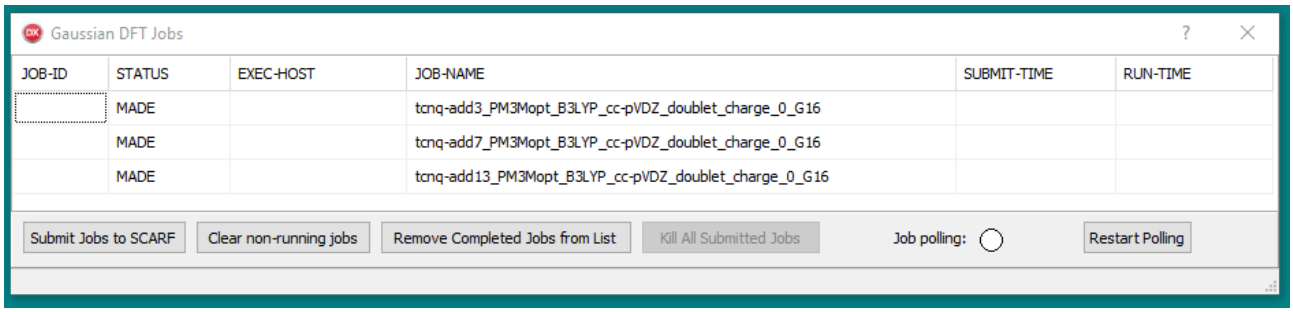
A viewer such as jmol.jar can be used to view and check the initial structure used for the radical.

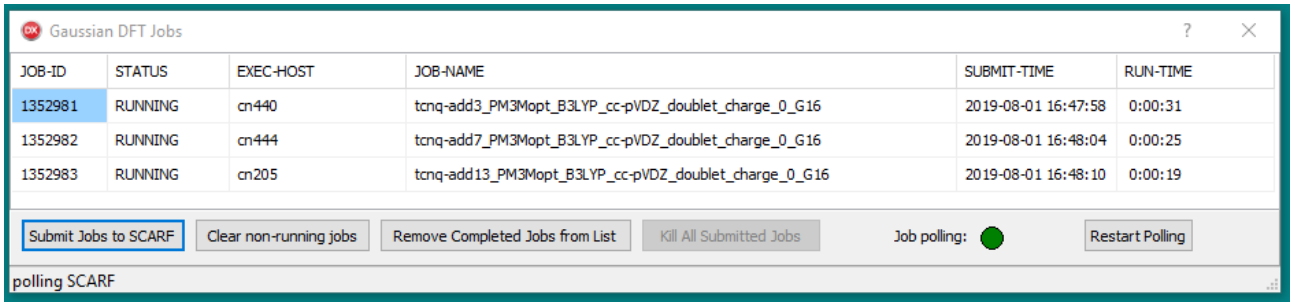


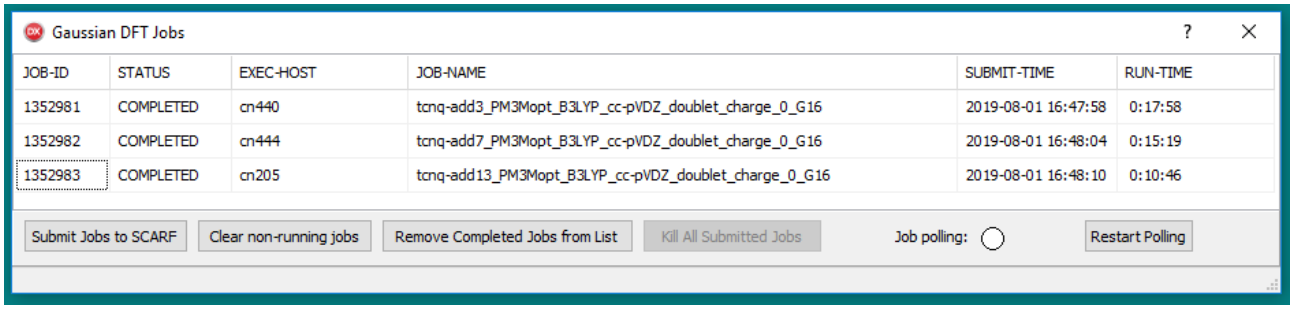
Step 4: The job set is submitted to SCARF from the Jobs window. A password will need to be supplied once within a session.



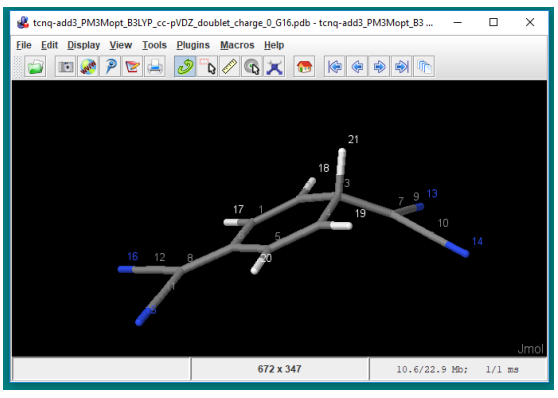
The set of jobs will be sent to SCARF and submitted to the queue and will start to run. The status of the jobs will be polled as they run.

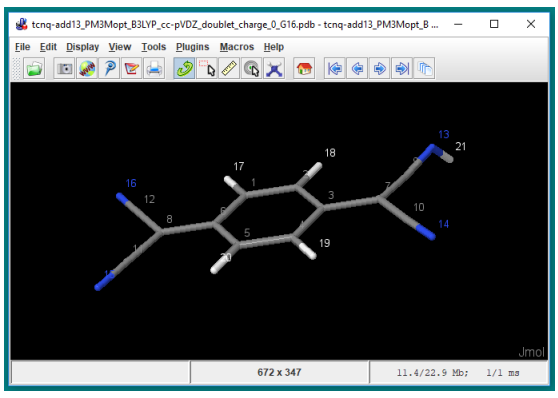




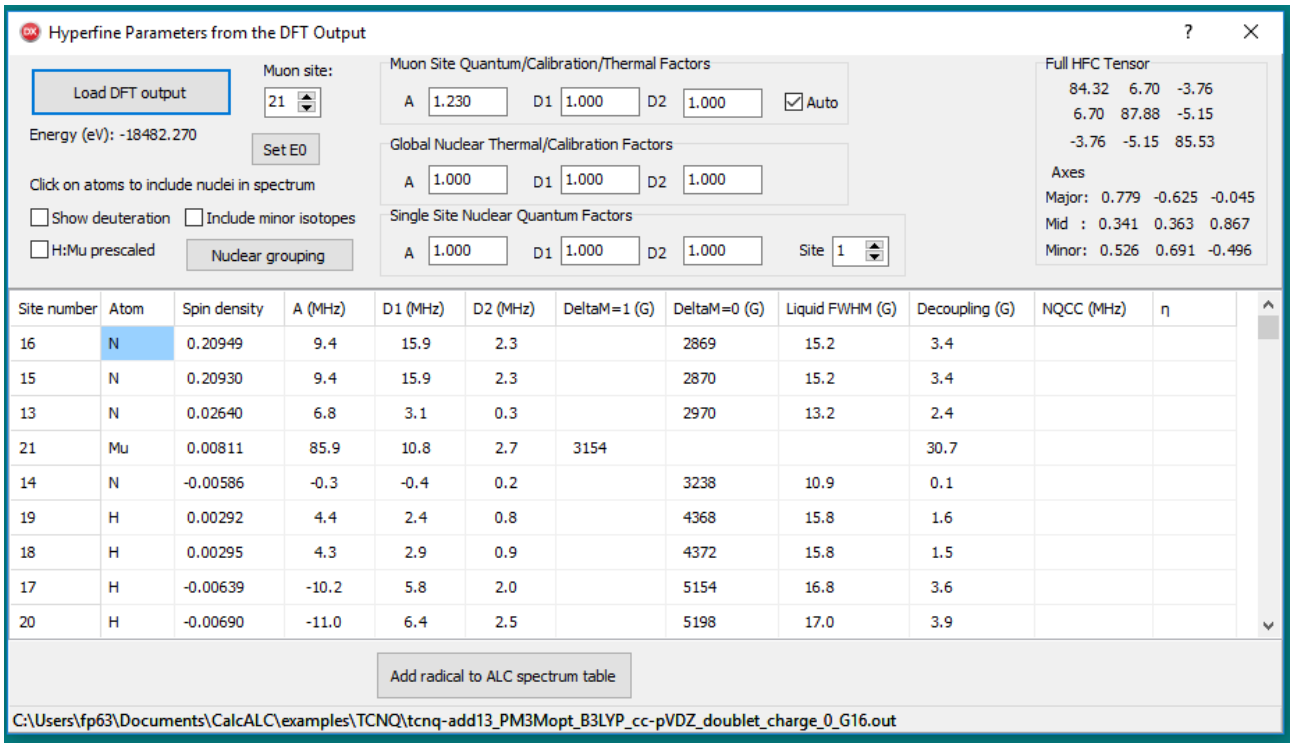


When each job is completed the results file JOB-NAME.out will be copied back to the working directory on the user pc. After a certain time, all of the jobs will have finished (or failed). If a job fails, an editor such as Notepad++ can be used to explore the output file and determine the problem. The final structures of the successful jobs JOB-NAME.pdb can again be viewed with jmol.jar.

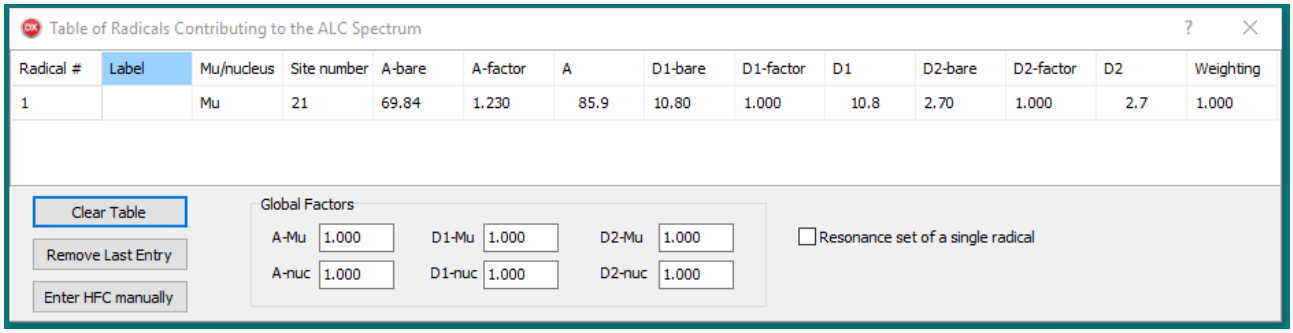




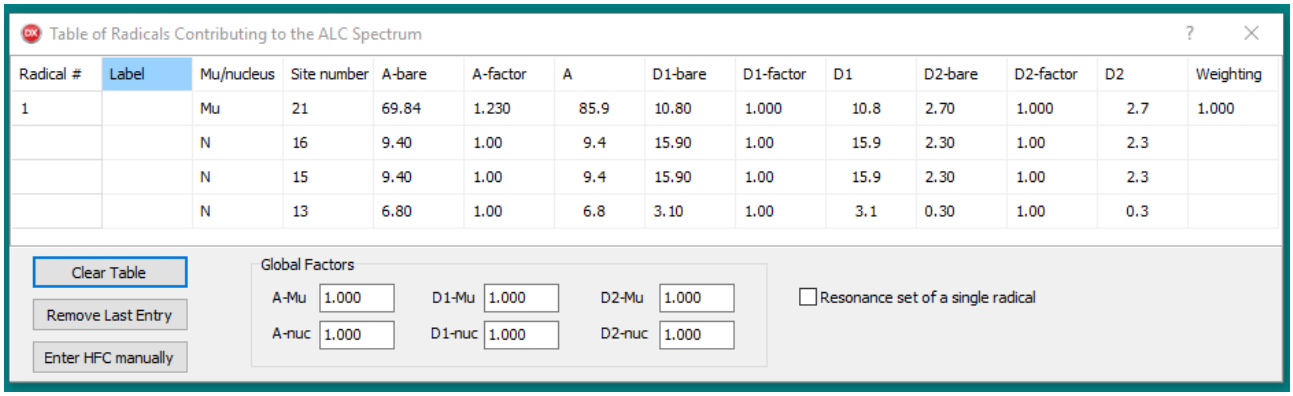
Step 5: The hyperfine parameters from the completed jobs are loaded into the results window and contributions to the ALC spectrum are selected and sent to the spectrum table to build up the spectrum. The muon and nuclei with spin are listed in the window.



Clicking 'Add radical to ALC Spectrum Table' adds the muon on its own to the spectrum producing a Δ_1 resonance.

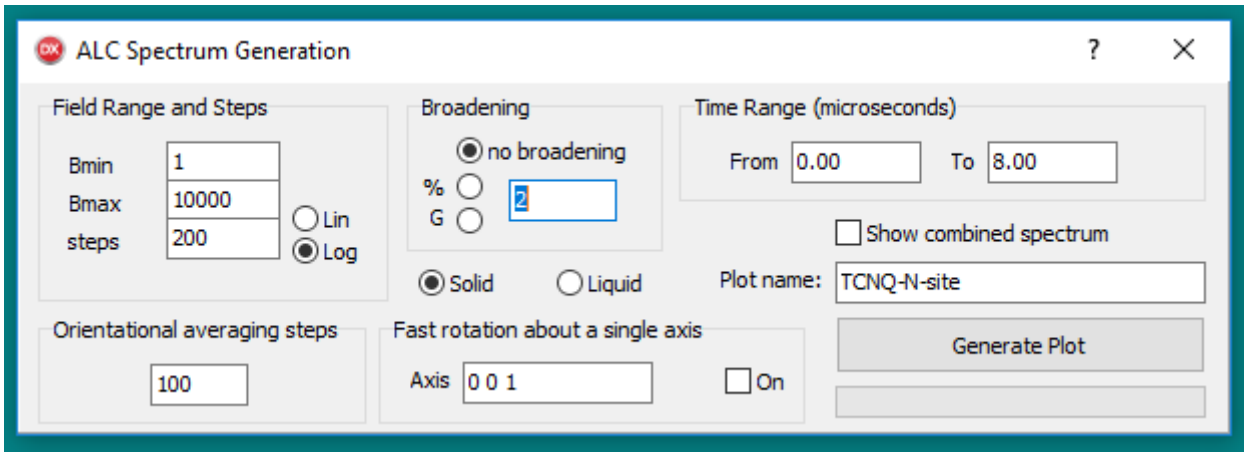


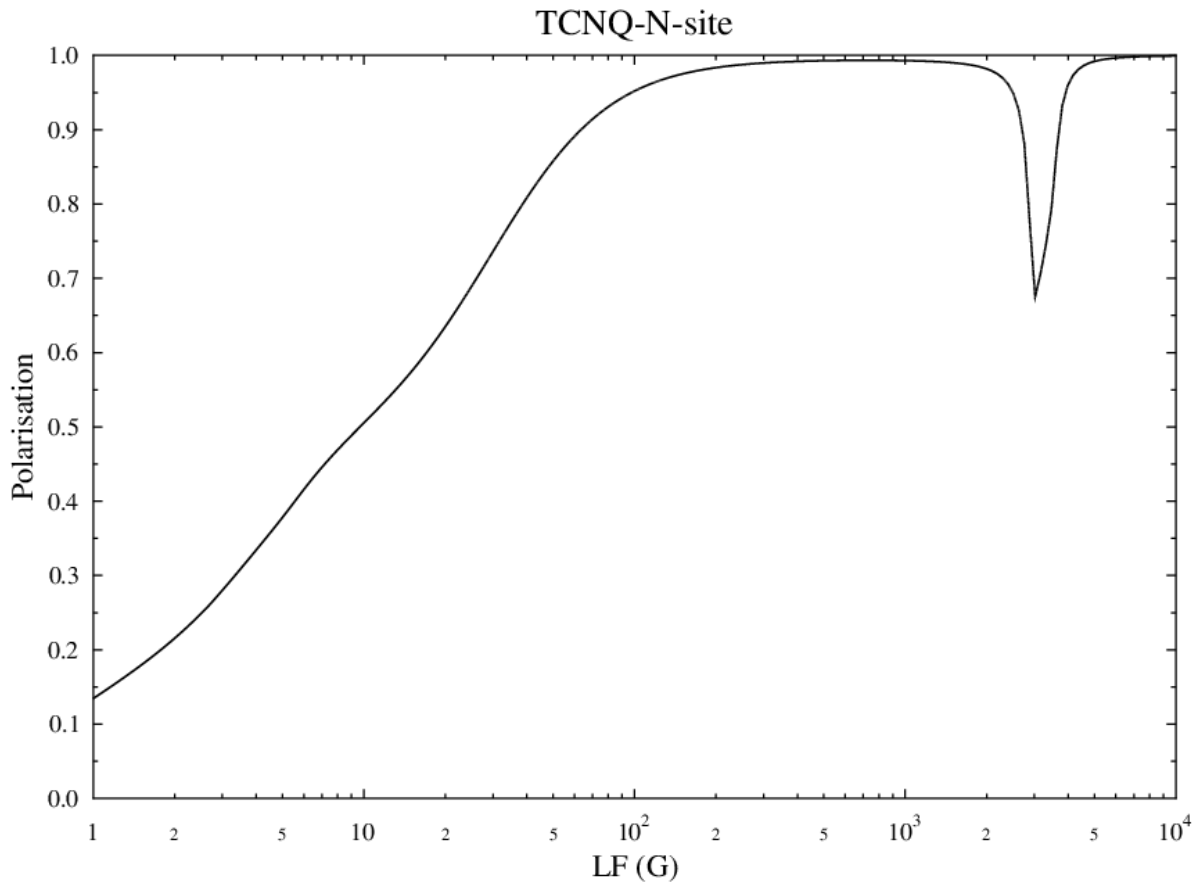
If one or more nuclei are clicked before adding the radical then the multispin system will show Δ_0 resonances as well.



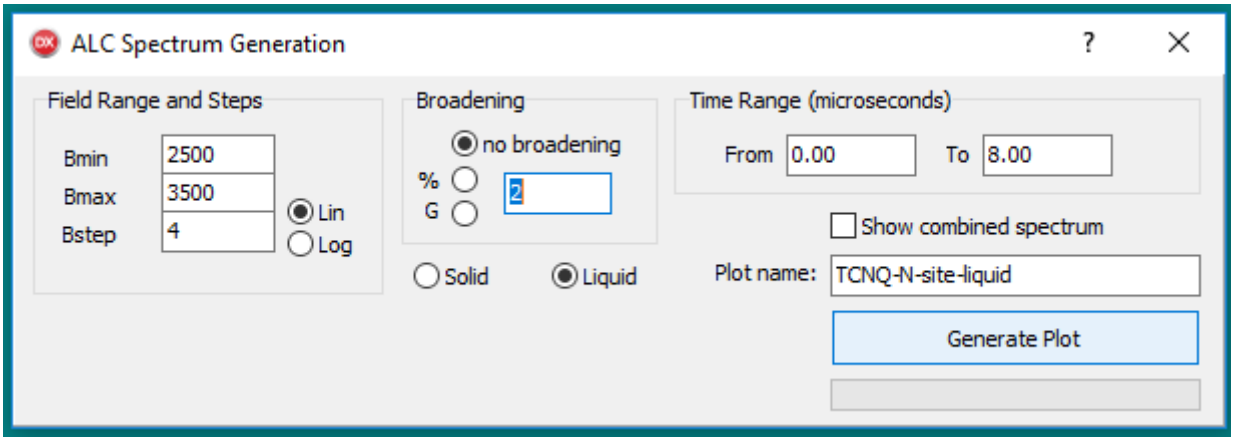
Step 6: Parameters are set up for calculating and plotting the spectrum and the plot is generated

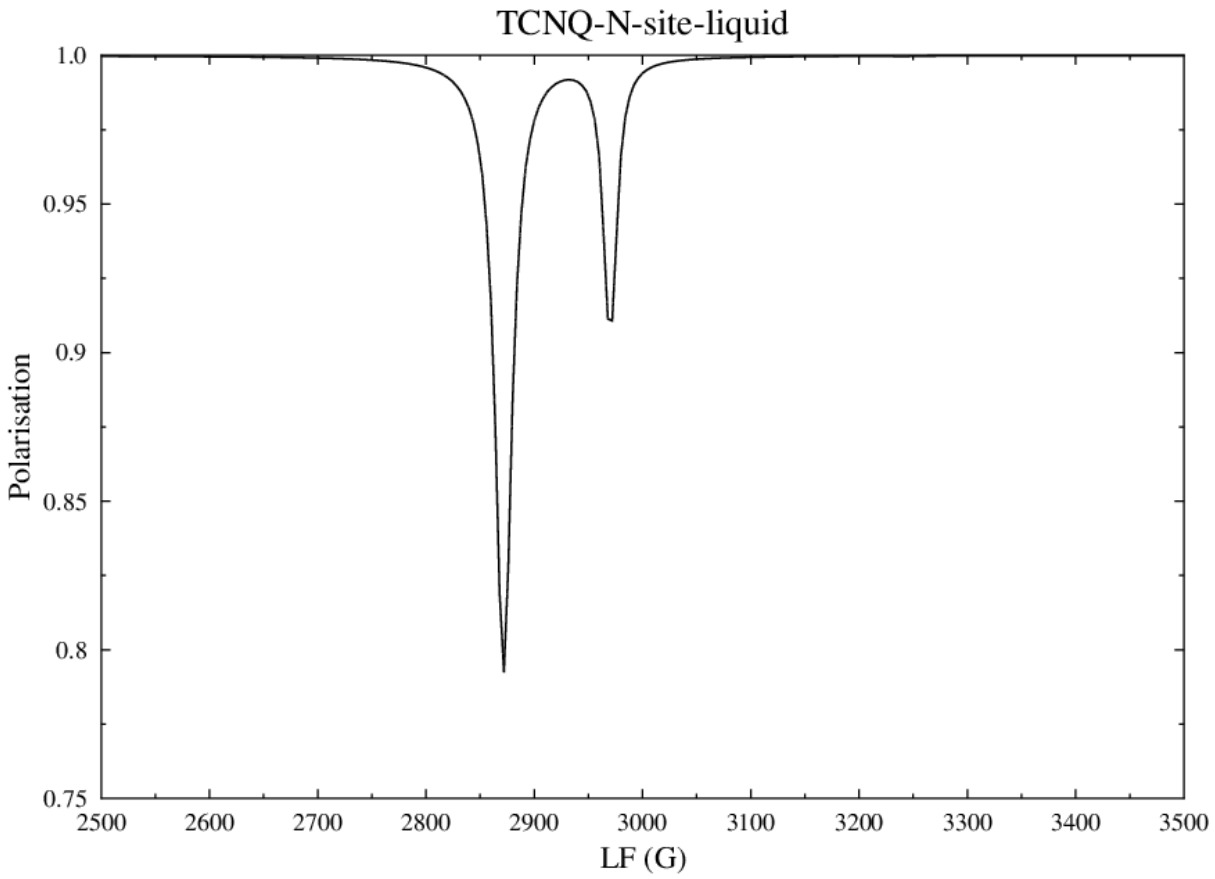
Solid state:



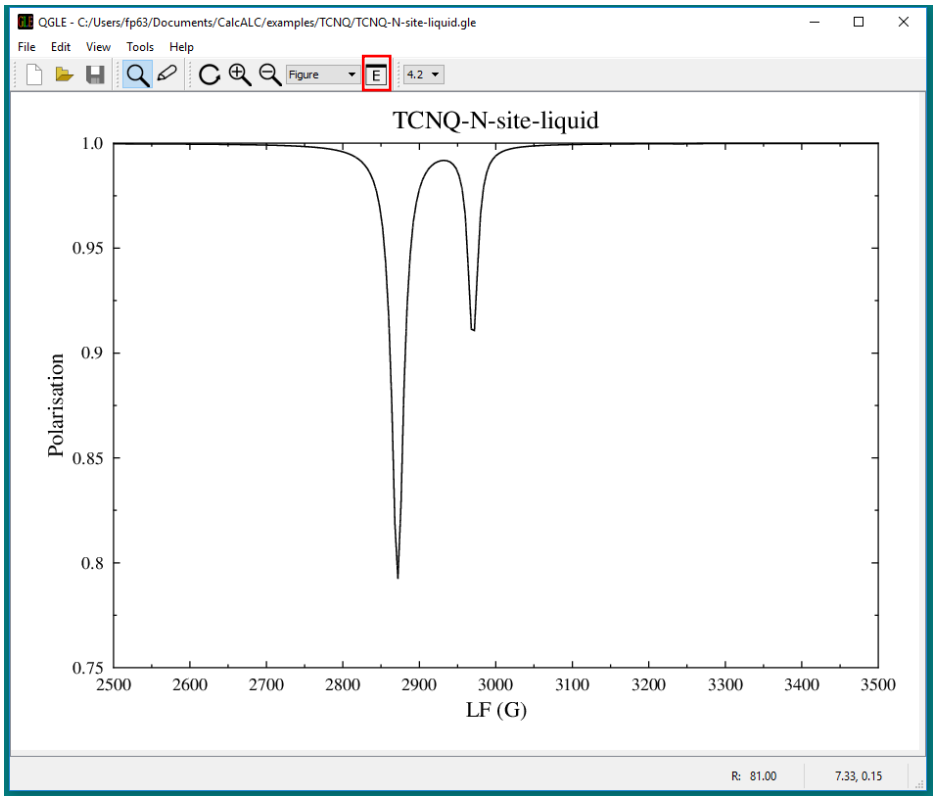


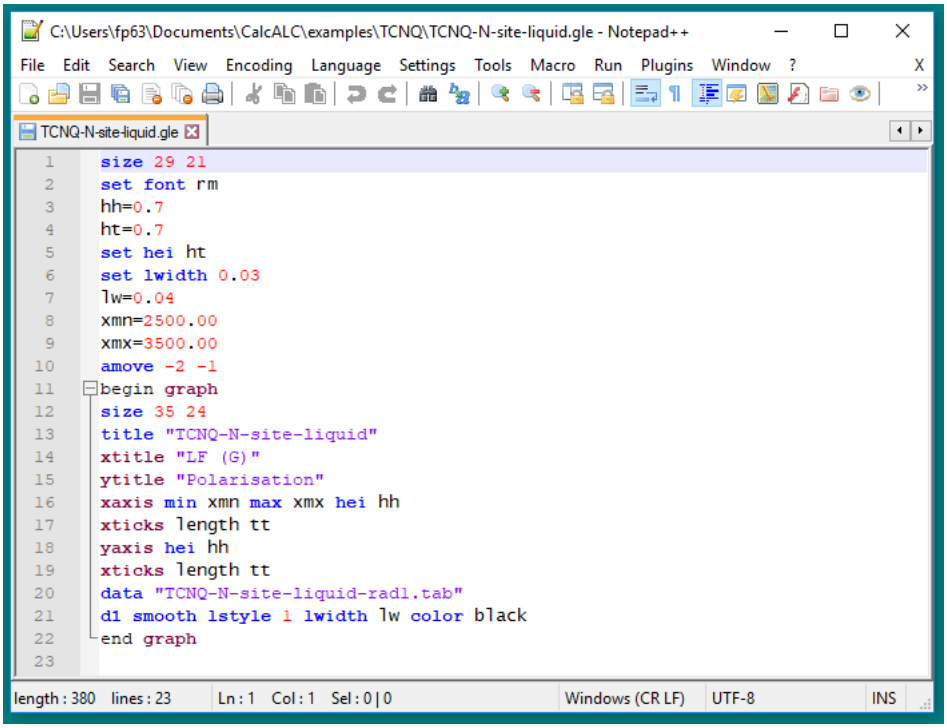
Liquid state just including Δ_0 resonances with the nitrogens:





Step 7: Fine tuning of the plot by editing the gle plot definition file. The gle file can be edited in a text editor such as notepad++ to alter titles, axis labels, axis scaling etc. The E button on the top of the QGLE window can be set up to link directly to the editor for convenience.





This provides a quick guide to the basic operation of CalcALC. Some additional features of CalcALC are introduced in the various examples provided in the \examples folder.