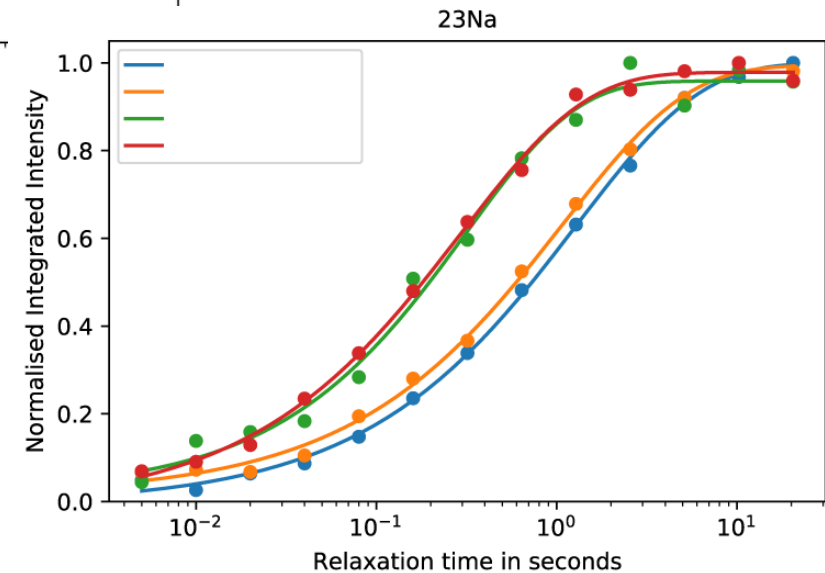
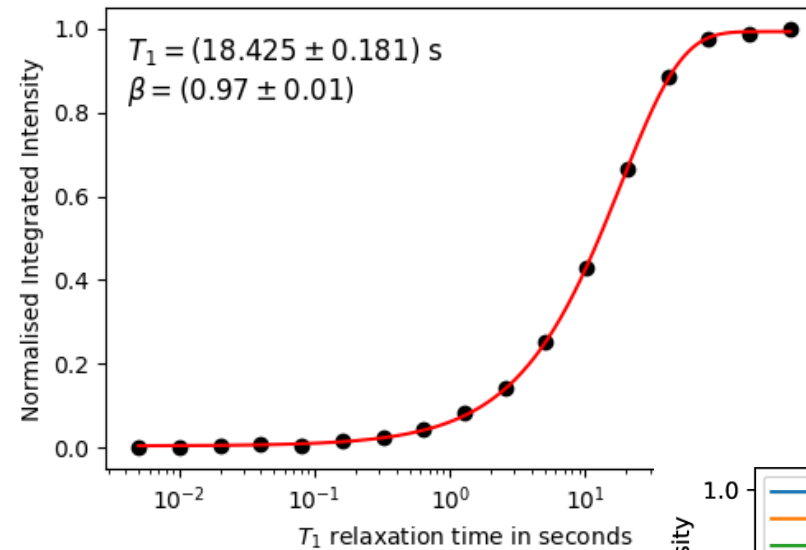
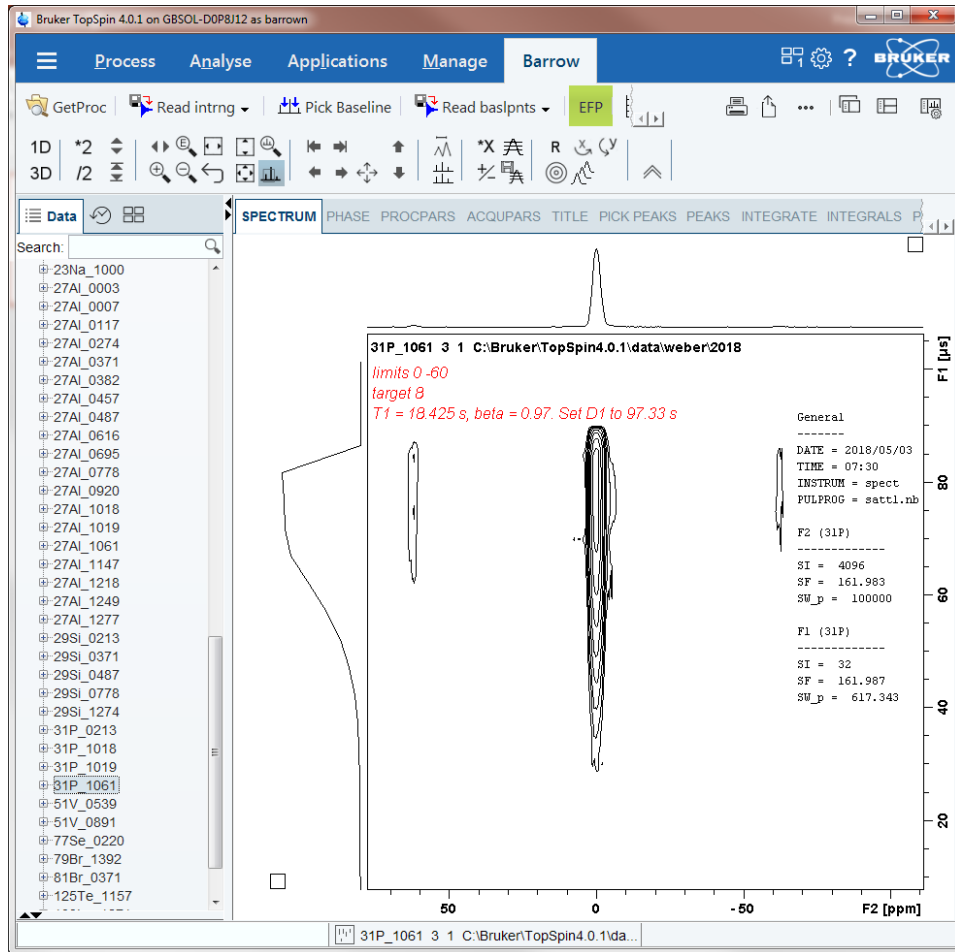


Automation using Python

Nathan Barrow

Johnson Matthey

T1 measurements, fitting & plotting



```
showt1.py (C:\Bruker\TopSpin4.0.1\exp\stan\nmr\py\user)
File Edit Search
Execute ☒ Warn on Execute

1 import subprocess
2 import os
3
4 #Get path info for current data set and format into path, append location of file.
5 curdat = CURDATA()
6 path = os.path.normpath("%s/%s/%s/pdata/1/t1plot.png" % (curdat[3], curdat[0], curdat[1]))
7
8 #open it up
9 if os.path.exists(path):
10     subprocess.call(["explorer", path])
11 else:
12     MSG("Figure cannot be found.")
```



nmrglue

a module for working with NMR data in Python

What is nmrglue?

Nmrglue is a module for working with NMR data. nmrglue provides a robust environment for rapid data processing. Nmrglue also provides a framework for connecting to various NMR data sources.

[Documentation](#)

[Install Guide](#)

What can nmrglue do?

```
T1Fit.py (C:\Bruker\TopSpin4.0.1\exp\stan\nmr\py\user)
File Edit Search
Execute ☒ Warn on Execute

1 #Processes satt1 spectrum, calls external script to integrate data, fit to stretched exponential and edit D1 of next EXPNO
2 #JPB, October 2016
3
4 import subprocess
5
6 #Process satt1 spectrum with SI = 4096, SI of 16k causes nmrglue some trouble. Sometimes.
7 #For ABS2 command, check ABSF1 and ABSF2 parameters in ProcPars are appropriate.
8 XCMD('SI 4096')
9 XCMD('XF2')
10 XCMD('ABS2')
11
12 #Get path info for current data set and format into path.
13 curdat = CURDATA()
14 path = ("%s/%s/%s" % (curdat[3], curdat[0], curdat[1]))
15
16 #Call the external T1 fitting script, passing the data path as an argument to be picked up by sys.argv.
17 #Waits for the external script to complete before finishing this Jython script.
18 subprocess.call(["C:\\Users\\SpectNO1\\AppData\\Local\\Continuum\\Miniconda3\\python", "C:\\Users\\SpectNO1\\T1Fit-o-matic.py", path])
19
20 #Re-loads experiment so that the updated title (containing the result) is visible
21 XCMD("re %s" % curdat[1])
```

1 : 1

Static PDF report

SSNMR EFAI Report № 20181249

Table 1. ^{27}Al quantification. Total integral from 80 ppm to -30 ppm and AlO_6 integral from 15 ppm to -30 ppm.

Sample	Total Relative Intensity ($\pm 3\%$)	AlO_6 Intensity ($\pm 3\%$)
[REDACTED]	100%	-2%
	85%	9%
	88%	11%
	67%	38%

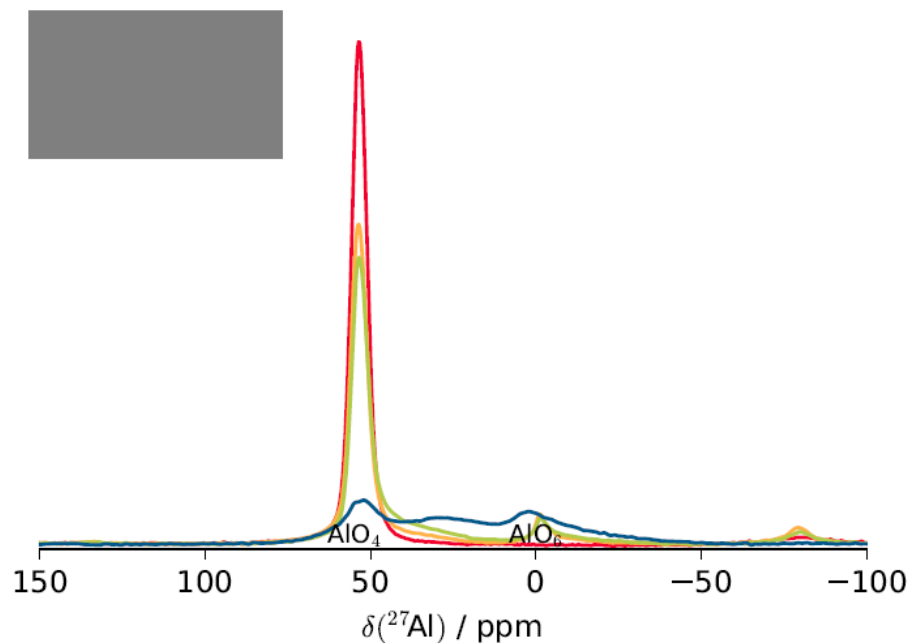
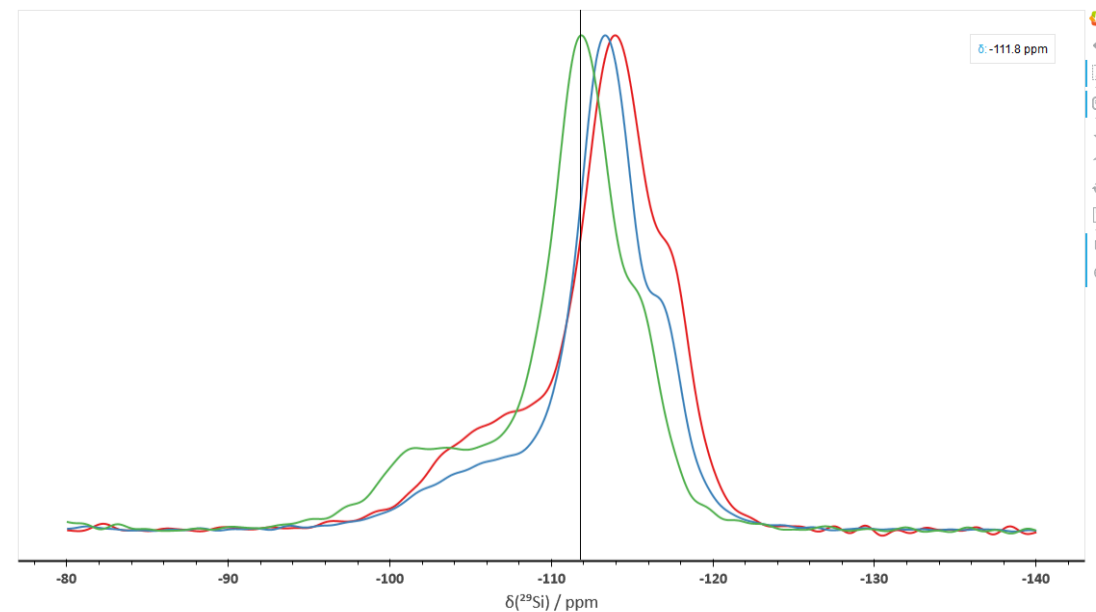


Figure 1. Normalised ^{27}Al solid-state MAS NMR spectra.

Dynamic HTML page



Click and drag or scroll to zoom. Click titles to show/hide. Click save to create a file for Word, PowerPoint, etc.