

Instructions for generating calculated Raman and absorption spectra

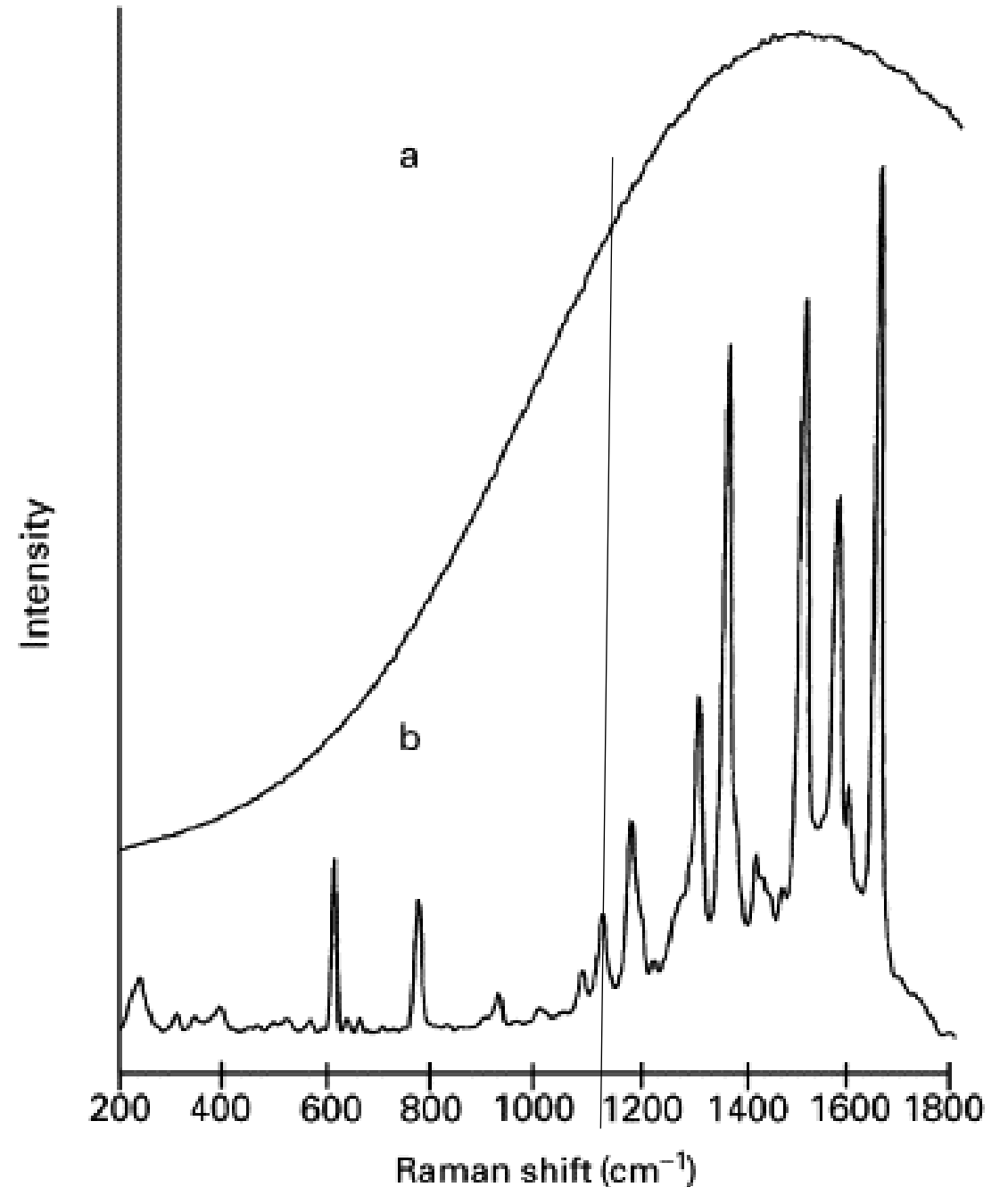
Procedure for obtaining Franck-Condon active modes:

Obtain relative intensities of Raman bands and make list

Rhodamine 6G Raman

We can use relative Raman cross sections to determine the displacement of modes in the excited state. All the modes in the Raman spectrum are Franck-Condon active. This means that they arise from vertical transitions. To a first approximation their intensity is proportional to $S e^{-S}$, where S is known as the electron-phonon coupling constant. These data are obtained using 514.5 nm excitation.

Source: Handai Biophotonics (2007)
Hiroshi Masuhara & Fumio Tokunaga, Eds.



Relative intensities of Raman bands

1662.0, 1.0
1595.0, 0.67
1491.0, 0.82
1354.0, 0.78
1296.0, 0.37
1178.0, 0.26
1124.0, 0.15

These are the entries in a file I called rhod6G.inp. This is used by the program `raman_spec`, which requests the input file, number of data points (here 7), output file name and Lorentzian width (use 10 cm^{-1}).

To run the program type at the command line
[Account] \$ `raman_spec`

Calculate an absorption spectrum

7

1662.0, 0.050, 298
1595.0, 0.034, 298
1491.0, 0.041, 298
1354.0, 0.039, 298
1296.0, 0.018, 298
1178.0, 0.013, 298
1124.0, 0.007, 298

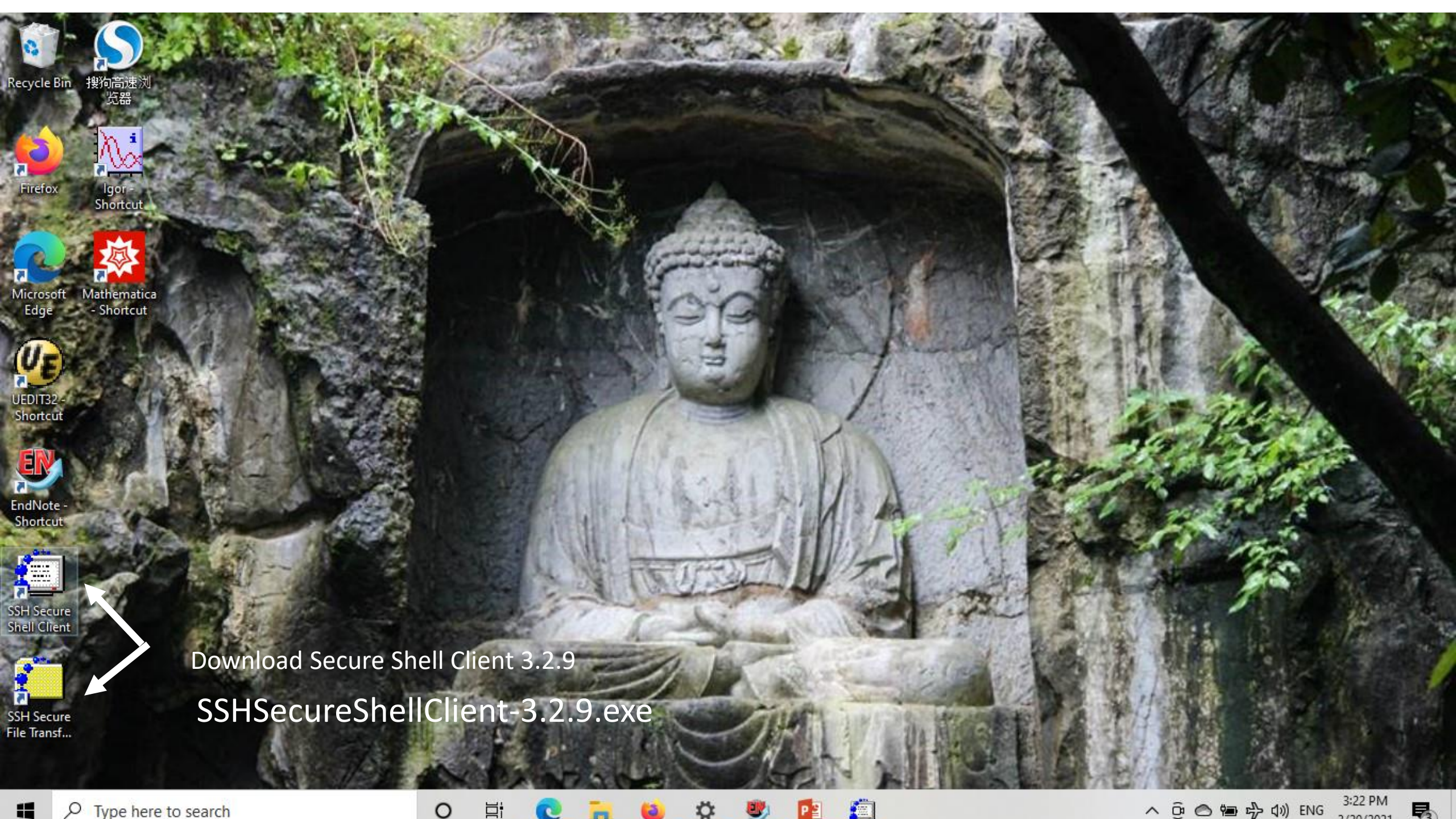
These are the entries in a file I called rhod6G.input. This is used by the program **timetherm**, which can be executed using a redirect (<) as shown below. If you just take the 7 most intense modes you can scale them to give an appropriate shape.

To run the program type at the command line

```
[Account] $ timetherm < rhod6G.input
```

Justification for scaling method

It is possible to measure absolute resonance Raman cross sections. In some cases, these can be obtained using an internal standard, such as sodium sulfate in the case of proteins. In the absence of a standard we can set S from the Franck-Condon factor equal to the relative intensities of normal high frequency modes. I did this first using 0.1 as the most intense mode. The calculated absorption spectrum had too much asymmetry. I divided the relative intensities by a factor of two and then reran **timetherm**. The result was a reasonable spectrum, but perhaps not the final result you will want to use to calculate the spectral overlap.

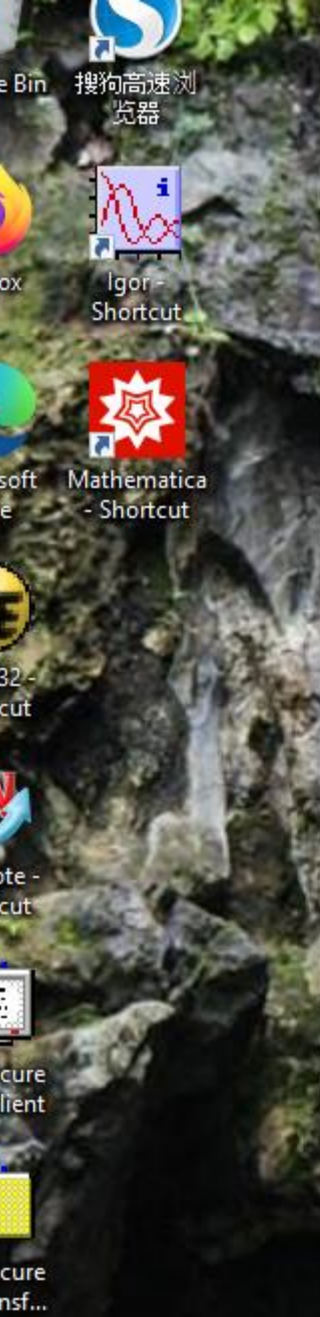


- Recycle Bin
- 搜狗高速浏览器
- Firefox
- Igor - Shortcut
- Microsoft Edge
- Mathematica - Shortcut
- UE
- UEDIT32 - Shortcut
- EN
- EndNote - Shortcut
- SSH Secure Shell Client
- SSH Secure File Transf...

Download Secure Shell Client 3.2.9
SSHSecureShellClient-3.2.9.exe

Use Secure Shell Client to connect to NCSU mainframe

Under File > Profiles you need to add and then edit a profile



- default - SSH Secure Shell

File Edit View Window Help

- Save Settings
- Save Layout
- Quick Connect...
- Profiles
- Print...
- Print Preview...
- Page Setup...
- Log Session...
- Connect...
- Disconnect
- Exit

files

(Build 283)
SSH Communications Security Corp - <http://www.ssh.com/>

SSH Secure Shell is a non-commercial version.
It does not include PKI and PKCS #11 functionality.

80x24



- default - SSH Secure Shell

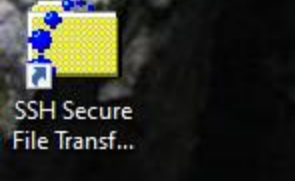
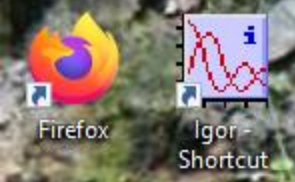
File Edit View Window Help

- Save Settings
- Save Layout
- Quick Connect...
- Profiles**
 - Edit Profiles...
 - Add Profile...**
 - defaultsftp
 - digital_ocean
 - hpc
- Print...
- Print Preview...
- Page Setup...
- Log Session...
- Connect...
- Disconnect
- Exit

files

```
ssh://[redacted]@[redacted]:22 [redacted]
[redacted] Security Corp - http://www.ssh.com/
[redacted] commercial version.
[redacted] ES #11 functionality.
```

Add current connection to profiles | 80x24



- default - SSH Secure Shell

File Edit View Window Help

Quick Connect Profiles

SSH Secure Shell 3.2.9 (Build 283)
Copyright (c) 2000-2003 SSH Communications Security Corp - http://www.ssh.com/

This copy of SSH Secure Shell is a non-commercial version.
This version does not include PKI and PKCS #11 functionality.

Add Profile

ncsu [Add to Profiles](#)

Not connected - press Enter or Space to connect 80x24

File Edit View Window Help

Save Settings

Save Layout

Quick Connect...

Profiles

Print...

Print Preview...

Page Setup...

Log Session...

Connect...

Disconnect

Exit



files

Edit Profiles...

Add Profile...

defaultsfpt

digital_ocean

hpc

ncsu

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

[franzen@login04 ~/CH452_ET]\$

Use Secure Shell Client to connect to NCSU mainframe

Under File > Profiles you need to add and then edit a profile.

Once you have input your password and used your two-factor login you should have a LINUX prompt \$.

A tar file is a way to package files for transport to other accounts. I will call this one ET.tar. Once you have ET.tar in The LINUX account type \$ tar -xvf ET.tar. This will unpack it.

I have provided word documents with all text that is in the files on the LINUX tar file.

Basic LINUX Commands

To see which files are in your directory type \$ ls (ls = list)

To edit files (not required) you type \$ vi [file]
(file must be ASCII)

To run programs just type the program name

\$ raman_spec some LINUX shells require \$./raman_spec

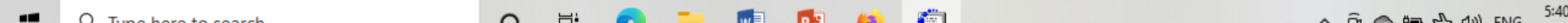
\$ timetherm some LINUX shells require \$./timetherm



Quick Connect Profiles

```
1296.0, 0.37
1178.0, 0.26
1124.0, 0.15
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
```

```
[franzen@login04 ~/CH452_ET]$ ls
params1.input raman_spec.f rhod6G.input timetherm
raman_spec rhod6G.inp rhod6G.out ttcalc
[franzen@login04 ~/CH452_ET]$ raman_spec
Enter Input Filename:
rhod6G.inp
Enter Number of Frequencies:
7
1662.000000000000000 1.0000000000000000000
1595.000000000000000 0.6700000000000000004
1491.000000000000000 0.8199999999999999995
1354.000000000000000 0.7800000000000000003
1296.000000000000000 0.3700000000000000000
1178.000000000000000 0.2600000000000000001
1124.000000000000000 0.1499999999999999999
Enter Output Filename:
tmp.out
Enter Lorentzian Width:
10
[franzen@login04 ~/CH452_ET]$
```





```
7
1662.0, 0.050, 298
1595.0, 0.034, 298
1491.0, 0.041, 298
1354.0, 0.039, 298
1296.0, 0.018, 298
1178.0, 0.013, 298
1124.0, 0.007, 298
7
0,1
0,1
0,1
0,1
0,1
0,1
0,1
0,1
1e-5
10
1.3
501
0.5
18000
400
4000
1
600
0
0
'abs'
1
'absr'
'absi'
'absm'
'repl'
1
'replr'
'repli'
'replm'
[franz@login04 ~/CH452_ET]$ vi params1.input
```

Basic LINUX Commands

To see which files are in your directory type `$ ls` (ls = list)

To edit files (not required) you type `$ vi [file]`
(file must be ASCII)

To run programs just type the program name

`$ raman_spec` some LINUX shells require `$./raman_spec`

`$ timetherm` some LINUX shells require `$./timetherm`

You can upload and download using the SSH format



defaultsftp - SSH Secure File Transfer

File Edit View Operation Window Help

Quick Connect Profiles

Local Name	Size	Type	Remote Name	Size	Type
OneDrive		System			
Stefan Franzen		System			
This PC		System			
Libraries		System			
Network		System			
Control Panel		System			
Recycle Bin		System			
Control Panel		System			
Firefox	993	Shortcut			
Microsoft Edge	2,259	Shortcut			
SSH Secure File Transfer Cl...	2,363	Shortcut			
SSH Secure Shell Client	1,405	Shortcut			
???????	993	Shortcut			
EndNote - Shortcut	1,510	Shortcut			

Transfer | Queue |

Source File	Source Directory	Destination Dire...	Size	Status	Speed	Time
-------------	------------------	---------------------	------	--------	-------	------

Not connected - press Enter or Space

Clipboard

- Paste
- Cut
- Copy
- Format Painter

15

Basic UNIX Commands

To view which files are in your directory type <code>ls</code>. To view the files you are permitted to read (<code>r</code>), write (<code>w</code>), or execute (<code>x</code>):

To view the permissions for a specific program enter:

<code>ls -l filename</code>

<code>ls -l filename</code>

<code>ls -l filename</code>

16

Basic UNIX Commands

To view which files are in your directory type <code>ls</code>. To view the files you are permitted to read (<code>r</code>), write (<code>w</code>), or execute (<code>x</code>):

To view the permissions for a specific program enter:

<code>ls -l filename</code>

<code>ls -l filename</code>

<code>ls -l filename</code>

17

Basic UNIX Commands

To view which files are in your directory type <code>ls</code>. To view the files you are permitted to read (<code>r</code>), write (<code>w</code>), or execute (<code>x</code>):

To view the permissions for a specific program enter:

<code>ls -l filename</code>

<code>ls -l filename</code>

<code>ls -l filename</code>

18

Basic UNIX Commands

To view which files are in your directory type <code>ls</code>. To view the files you are permitted to read (<code>r</code>), write (<code>w</code>), or execute (<code>x</code>):

To view the permissions for a specific program enter:

<code>ls -l filename</code>

<code>ls -l filename</code>

<code>ls -l filename</code>

19

Basic UNIX Commands

To view which files are in your directory type <code>ls</code>. To view the files you are permitted to read (<code>r</code>), write (<code>w</code>), or execute (<code>x</code>):

To view the permissions for a specific program enter:

<code>ls -l filename</code>

<code>ls -l filename</code>

<code>ls -l filename</code>

20

Basic UNIX Commands

To view which files are in your directory type <code>ls</code>. To view the files you are permitted to read (<code>r</code>), write (<code>w</code>), or execute (<code>x</code>):

To view the permissions for a specific program enter:

<code>ls -l filename</code>

<code>ls -l filename</code>

<code>ls -l filename</code>

defaultsftp - SSH Secure File Transfer

File Edit View Operation Window Help

- Save Settings Ctrl+S
- Save Layout
- Quick Connect...
- Profiles
 - Edit Profiles...
 - Add Profile...
 - defaultsftp
 - digital_ocean
 - hpc
 - ncsu
- Connect...
- Disconnect
- Exit
- Network
- Control Panel
- Recycle Bin
- Control Panel
- Firefox 993 Shortc...
- Microsoft Edge 2,259 Shortc...
- SSH Secure File Transfer Cl... 2,363 Shortc...
- SSH Secure Shell Client 1,405 Shortc...
- ???????? 993 Shortc...
- EndNote - Shortcut 1,510 Shortc...

Transfer	Queue					
Source File	Source Directory	Destination Dire...	Size	Status	Speed	Time

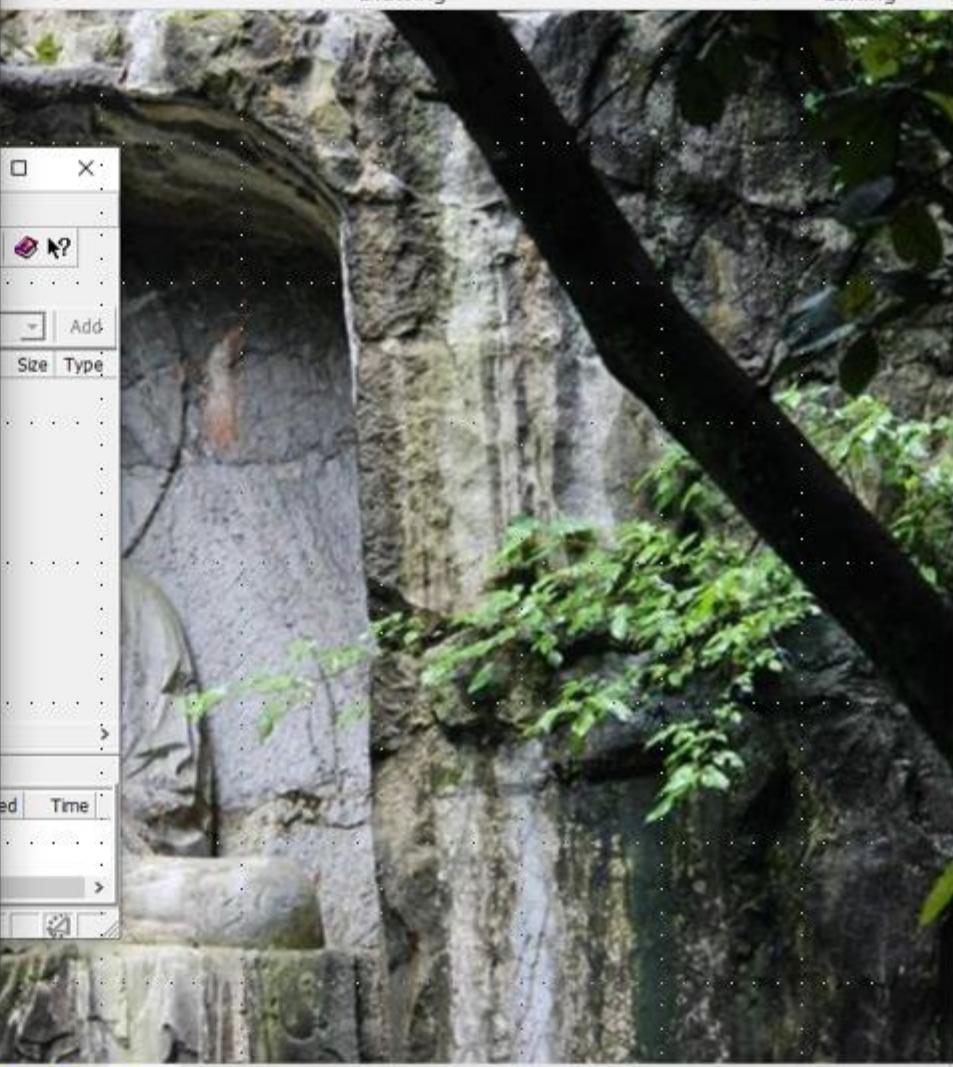
Art

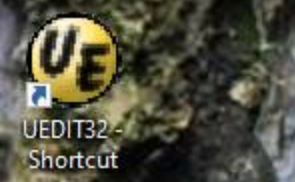
Drawing

- Shape Fill
- Shape Outline
- Shape Effects
- Arrange
- Quick Styles

Editing

- Find
- Replace
- Select





2:login.hpc.ncsu.edu - hpc - SSH Secure File Transfer

File Edit View Operation Window Help

Quick Connect Profiles

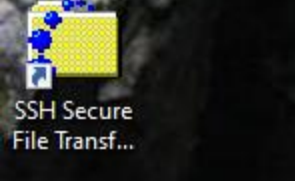
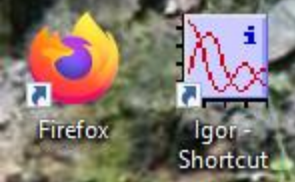
/franzen

Local Name	Size	Type	Remote Name	Size	Type
OneDrive		System	bck		Fold
Stefan Franzen		System	beowulf		Fold
This PC		System	bin		Fold
Libraries		System	BTL		Fold
Network		System	build		Fold
Control Panel		System	c		Fold
Recycle Bin		System	calcs		Fold
Control Panel		System	carma		Fold
Firefox	993	Shortc	carma_old		Fold
Microsoft Edge	2,259	Shortc	CH452_ET		Fold
SSH Secure File Transfer Cl...	2,363	Shortc	ch736		Fold
SSH Secure Shell Client	1,405	Shortc	CH736		Fold

Transfer | Queue |

Source File	Source Directory	Destination Dire...	Size	Status	Speed	Time

Connected to login.hpc.ncsu.edu - / SSH2 - aes128-cbc - hmac-sha1 - nc 44 items (8.6 KB)



2:login.hpc.ncsu.edu - hpc - SSH Secure File Transfer

File Edit View Operation Window Help

Quick Connect Profiles

rs\franz\ /franzen

Local Name	Size	Type	Remote Name	Size	Type
3D Objects		File fo	bck		Fold
Contacts		File fo	beowulf		Fold
Desktop		File fo	bin		Fold
Documents		File fo	BTL		Fold
Downloads		File fo	build		Fold
Favorites		File fo	c		Fold
Links		File fo	calcs		Fold
Music		File fo	carma		Fold
OneDrive		File fo	carma_old		Fold
Pictures		File fo	CH452_ET		Fold
Saved Games		File fo	ch736		Fold
Searches		File fo	CH736		Fold

Transfer | Queue |

Source File	Source Directory	Destination Dire...	Size	Status	Speed	Time

Connected to login.hpc.ncsu.edu - / SSH2 - aes128-cbc - hmac-sha1 - nc 44 items (8.6 KB)

Recycle Bin 搜狗高速浏览器

Firefox Igor - Shortcut

Microsoft Edge Mathematica - Shortcut

UEDIT32 - Shortcut

EndNote - Shortcut

SSH Secure Shell Client

SSH Secure File Transf...

2:login.hpc.ncsu.edu - hpc - SSH Secure File Transfer

File Edit View Operation Window Help

Quick Connect Profiles

s\Ufunzi\ Add /franzen Add

Local Name	Size	Type	Remote Name	Size	Type
CH452		File folder	bck		Fold
CH452_Web_Course		File folder	beowulf		Fold
			bin		Fold
			BTL		Fold
			build		Fold
			c		Fold
			calcs		Fold
			carma		Fold
			carma_old		Fold
			CH452_ET		Fold
			ch736		Fold
			CH736		Fold

Transfer | Queue |

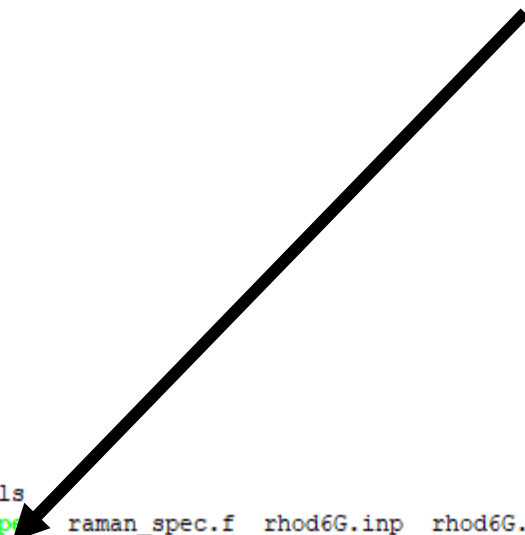
Source File	Source Directory	Destination Dire...	Size	Status	Speed	Time
-------------	------------------	---------------------	------	--------	-------	------

Connected to login.hpc.ncsu.edu - / SSH2 - aes128-cbc - hmac-sha1 - nc 44 items (8.6 KB)



```
ttcalc/absi
ttcalc/absm
ttcalc/repl
ttcalc/replr
ttcalc/repli
ttcalc/replm
ttcalc/rep2
ttcalc/rep2r
ttcalc/rep2i
ttcalc/rep2m
ttcalc/rep3
ttcalc/rep3r
ttcalc/rep3i
ttcalc/rep3m
ttcalc/rep4
ttcalc/rep4r
ttcalc/rep4i
ttcalc/rep4m
ttcalc/rep5
ttcalc/rep5r
ttcalc/rep5i
ttcalc/rep5m
ttcalc/rep6
ttcalc/rep6r
ttcalc/rep6i
ttcalc/rep6m
ttcalc/rep7
ttcalc/rep7r
ttcalc/rep7i
ttcalc/rep7m
ttcalc/rhod_800.txt
ttcalc/rhod_200.txt
ttcalc/rhod_600.txt
ttcalc/rhod_1000.txt
ttcalc/params1.input
ttcalc/rhod_1_600.txt
[franz@login04 ~/CH452_ET]$ ls
ET.tar  params1.input  raman_spec.f  rhod6G.inp  rhod6G.input  rhod6G.out  timetherm  tmp.out  ttcalc
[franz@login04 ~/CH452_ET]$ tar cvf ET.tar *
```

This slide is showing how the “tar file” was created. The LINUX tar command is widely used to bundle and send files. It is the precursor of zipping and compression software.





2:login.hpc.ncsu.edu - hpc - SSH Secure File Transfer

File Edit View Operation Window Help

Quick Connect Profiles

ig 2021\ Add 1452_ET Add

Local Name	Size	Type	Remote Name	Size	Type
computation		File folder	ttcalc		Folder
ppts		File folder	ET.tar	3,522,560	TAR File
refs		File folder	params1.input	1,761,280	INPUT F
ET.tar	3,522,560	TAR File	raman_spec	13,528	File
Fluorophor Spectra	1,487,331	Microsof.	raman_spec.f	1,984	F File
Instructions for raman_sp...	12,597,984	Microsof.	rhod6G.inp	90	INP File
			rhod6G.input	482	INPUT F
			rhod6G.out	560,000	OUT Fil
			timetherm	60,033	File
			tmp.out	560,000	OUT Fil

Transfer | Queue |

/	Source File	Source Directory	Destination Dire...	Size	Status	Speed	Time
↓	ET.tar	/home/franzen/...	C:\Users\franz\D...	3,522,...	Complete	1695.2 k...	00:00...
↓	timetherm	/home/franzen/...	C:\Users\franz\D...	60,033	Complete	321.0 kB/s	00:00...
↓	params1.in...	/home/franzen/...	C:\Users\franz\D...	1,761,...	Complete	1326.3 k...	00:00...

Connected to login.hpc.ncsu.edu - / SSH2 - aes128-cbc - hmac-sha1 - nc 10 items (6.5 MB)

Download the tar file from the website

Then download Secure Shell Client 3.2.9 and install it. Transfer the ET.tar file to your account. Untar it (see above). All the files will be ready for use. You can see how rhodamine 6G was treated. We also rhodamine 123 and rhodamine B. This analysis has not been carried out for fluorescein. This will be necessary in order to analyze the energy transfer efficiency.

Keep in mind that we also have coumarin and model of that molecule may lead to interesting possibilities.