

Running *ab initio* quantum chemistry calculations in Gaussian

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Accessing Gaussian at Princeton

The easiest way to use Gaussian is to get an account on Adroit following instructions [here](#). You will need to

1. Submit a request form
2. Fill out the confidentiality agreement
3. Email Doug Rosso (drosso@princeton.edu) to get approval

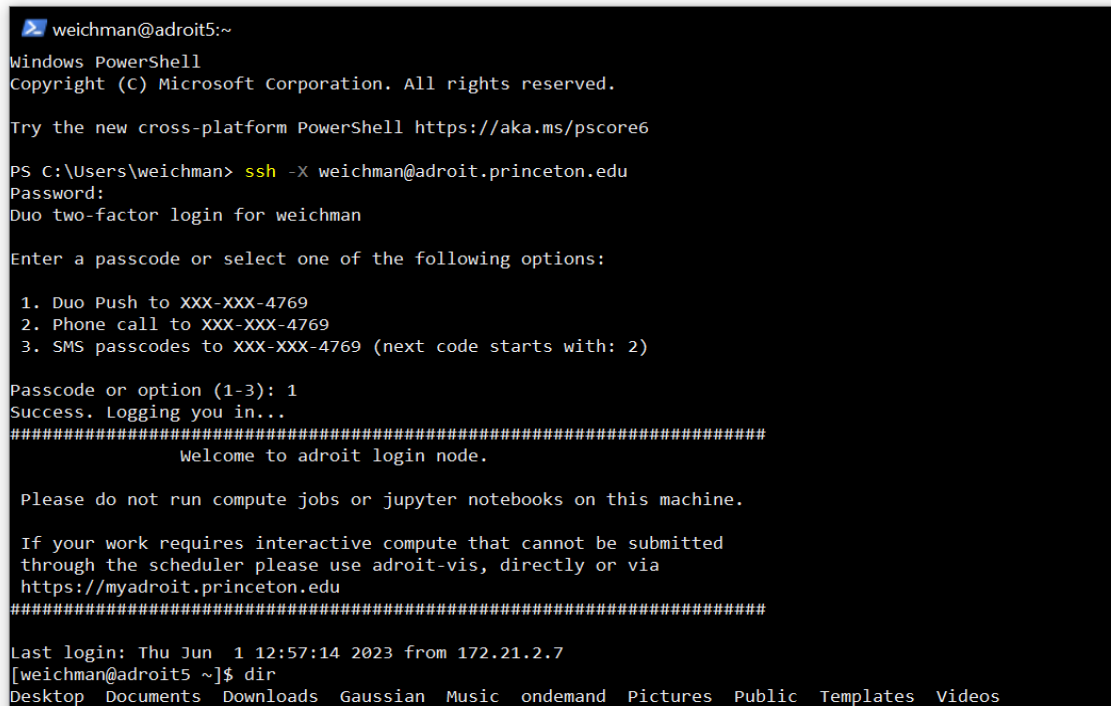
It then takes about a day for everything to get processed.

For calculations, it is simplest to log into Adroit via SSH and use the command line. You will need to be on campus or on the Princeton VPN for this to work.

On Windows, you can use PowerShell; on a Mac you should be able to use the normal terminal

```
ssh <YourNetID>@adroit.princeton.edu
```

You will be asked to enter your Princeton netID password and login with Duo.



```
weichman@adroit5:~
Windows PowerShell
Copyright (C) Microsoft Corporation. All rights reserved.

Try the new cross-platform PowerShell https://aka.ms/pscore6

PS C:\Users\weichman> ssh -X weichman@adroit.princeton.edu
Password:
Duo two-factor login for weichman

Enter a passcode or select one of the following options:

 1. Duo Push to XXX-XXX-4769
 2. Phone call to XXX-XXX-4769
 3. SMS passcodes to XXX-XXX-4769 (next code starts with: 2)

Passcode or option (1-3): 1
Success. Logging you in..
#####
      welcome to adroit login node.

Please do not run compute jobs or jupyter notebooks on this machine.

If your work requires interactive compute that cannot be submitted
through the scheduler please use adroit-vis, directly or via
https://myadroit.princeton.edu
#####

Last login: Thu Jun  1 12:57:14 2023 from 172.21.2.7
[weichman@adroit5 ~]$ dir
Desktop Documents Downloads Gaussian Music ondemand Pictures Public Templates Videos
```

If you're not familiar with working in a Unix command line, here are a couple of nice resources to get started with basic navigation:

- <https://mally.stanford.edu/~sr/computing/basic-unix.html>
- You can use [vim](#) or [emacs](#) to edit files from the command line. Both take a bit of time to learn, but are very useful. There is a [huge controversy](#) over which is better, but I am partial to vim myself.

If you hate using the command line, you can also access your Adroit account and view, edit, and download files through the web interface at <https://myadroit.princeton.edu>. This web portal also lets you use Visualization Mode to launch a desktop GUI interface on Adroit.

Running Gaussian jobs with slurm

All Gaussian calculations on Adroit and Della must be submitted through the job scheduler. Below is a sample script for running a Gaussian calculation for the pyrene molecule. You can more or less use this as-is to start with, just swap in your own email address and input and output file names.

"c16h10.slurm"

```
#!/bin/bash
#SBATCH --job-name=gaussianC16H10      # create a short name for your job
#SBATCH --nodes=1                      # node count
#SBATCH --ntasks=8                    # total number of tasks across all
nodes
#SBATCH --cpus-per-task=1              # cpu-cores per task (>1 if multi-
threaded tasks)
#SBATCH --mem=40G                      # total memory per node (4G per cpu-
core is default)
#SBATCH --time=08:00:00                # total run time limit (HH:MM:SS)
#SBATCH --mail-type=begin              # send email when job begins
#SBATCH --mail-type=end                # send email when job ends
#SBATCH --mail-user=[name]@[domain].edu
```

```
module purge
module load gaussian/g16
```

```
g16 c16h10_b3lyp_6-31g_d2h.com c16h12_b3lyp_6-31g_d2h.out
```

More information about what the settings for the job scheduler mean can be found [here](#).

You can run your slurm script with the command
sbatch c16h10.slurm

You can also look at running jobs using
squeue

to cancel a job you have started using
scancel [jobid]

Preparing Gaussian .com input files

If you're not yet familiar with preparing Gaussian input files, there are lots of useful resources on the internet

- <http://signe.teokem.lu.se/ulf/Methods/gaussian.html>
- <https://www.cup.uni-muenchen.de/ch/compchem/basic/g03input.html>

Here's an example of a typical geometry optimization & harmonic frequency calculation, for the pyrene molecule:

```
"c16h10_b3lyp_6-31g_d2h.com"
```

```
%chk=c16h10_b3lyp_6-31g_d2h           !checkpoint file name
#T B3LYP/6-31g opt freq(hpmodes, Raman)
    ! exclamation points designate comments
    ! #T specifies terse output
    ! B3LYP functional (basic, fine option for organic systems)
    ! 6-31g Pople-style basis set (pretty minimal)
    ! "opt" keyword specifies geometry optimization to find a stationary
point
    ! "freq" keywords specifies a calculation of harmonic frequencies once
opt is finished
    ! additional freq options:
    ! "Raman" computes Raman intensities in addition to IR intensities
    ! "Hpmodes" specifies high precision values for the normal mode
displacements
    ! you can add "iop(7/33=1)" to request that the dipole derivatives be
printed for vibrational normal modes, but it only works with freq, not opt
calculations

D2H symmetrized guess coordinates
    ! the line above just provides a descriptive label for the calculation

0 1    ! specifies a neutral, singlet molecule
C      -0.000    0.714    -0.000
C      -0.000   -0.714    -0.000
```

C	-0.000	1.431	1.239
C	-0.000	-1.431	1.239
C	-0.000	1.431	-1.239
C	-0.000	-1.431	-1.239
C	-0.000	0.682	2.470
C	-0.000	-0.682	2.470
C	-0.000	0.682	-2.470
C	-0.000	-0.682	-2.470
C	-0.000	2.839	1.213
C	-0.000	-2.839	1.213
C	-0.000	2.839	-1.213
C	-0.000	-2.839	-1.213
C	-0.000	3.531	-0.000
C	-0.000	-3.531	-0.000
H	-0.000	1.232	3.405
H	-0.000	-1.232	3.405
H	-0.000	1.232	-3.405
H	-0.000	-1.232	-3.405
H	-0.000	3.386	2.151
H	-0.000	-3.386	2.151
H	-0.000	3.386	-2.151
H	-0.000	-3.386	-2.151
H	-0.000	4.616	0.000
H	-0.000	-4.616	0.000

Some general tips:

- You can start with a guess geometry you build in a molecule editor like [Avogadro](#), or find a decent starting geometry from the literature (the latter is usually faster).
- Include a blank line at the end of the input file or you may encounter weird runtime errors.
- Always be thoughtful about then symmetry of your starting geometry - the opt calculation will preserve the starting symmetry. If you start with too high asymmetry, you may not find a stable structure. If you start with too low a symmetry, the calculation might optimize to an undesired distorted structure, or will take much longer to run because lower-symmetry species have many more nuclear degrees of freedom. After starting a calculation, check your output file right away to confirm that it has your desired point group correct.
- After running a freq calculation, inspect the vibrational frequencies in your output file to check for imaginary/negative values, which indicate you have not found a true minimum energy structure

More information

- [DFT functionals available in Gaussian 16](#) (click the "Keywords: Hybrid Functionals" tab). B3LYP is a safe option for organic systems; the long-range-corrected functional wb97XD is also a great choice.
- [Basis sets available in Gaussian 16](#)
- There are tons of things you can do in Gaussian beyond simple opt/freq calculations. Flipping through their [documentation](#) is the best way to get a sense of this.
- Here's [one tutorial](#) for how to do anharmonic rovibrational calculations in Gaussian.

Looking at Gaussian output files

GaussView is great for opening Gaussian output files if you can get your hands on it, but it doesn't look like this is widely available through Princeton anymore. [Avogadro](#) is freely available and serviceable in the absence of GaussView.

It's generally best to learn how to look through the output files directly.

- Search the output file for the word "termination" which for an opt/freq calculation appears midway, at the end of the opt calc.

```
687,1.2137693497\C,0.,2.8395700687,-1.2137693497\C,0.,-2.8395700687,-1
.2137693497\C,0.,3.5319371474,0.\C,0.,-3.5319371474,0.\H,0.,1.23294620
86,3.4059722749\H,0.,-1.2329462086,3.4059722749\H,0.,1.2329462086,-3.4
059722749\H,0.,-1.2329462086,-3.4059722749\H,0.,3.3858815925,2.1525344
757\H,0.,-3.3858815925,2.1525344757\H,0.,3.3858815925,-2.1525344757\H,
0.,-3.3858815925,-2.1525344757\H,0.,4.6173055238,0.\H,0.,-4.6173055238
,0.\Version=ES64L-G16RevA.03\State=1-AG\HF=-615.6347772\RMSD=7.222e-0
9\RMSF=4.565e-05\Dipole=0.,0.,0.\Quadrupole=-8.7766011,4.4589908,4.317
6103,0.,0.,0.\PG=D02H [C2"(H1C1C1.C1C1H1),SG(C12H8)]\ \@

In the race for quality, there is no finish line.
-- David T. Kearns
Job cpu time:      0 days  0 hours  0 minutes 23.6 seconds.
Elapsed time:     0 days  0 hours  0 minutes 23.6 seconds.
File lengths (MBytes):  RWF=      16 Int=      0 D2E=      0 Chk=      11 Scr=      1
Normal termination of Gaussian 16 at Fri May 26 18:09:36 2023.
Link1: Proceeding to internal job step number  2.

-----
#T Geom=AllCheck Guess=TCheck SCRF=Check GenChk RB3LYP/6-31G Freq
-----
Structure from the checkpoint file: "c16h10_b3lyp_6-31g_freq.chk"
-----
symmetrized coords from first run
-----
Charge = 0 Multiplicity = 1
Redundant internal coordinates found in file. (old form).
C,0,0,0,0.714801982,0.
C,0,0,0,-0.714801982,0.
C,0,0,0,1.432216949,1.2391970617
C,0,0,0,-1.432216949,1.2391970617
C,0,0,0,1.432216949,-1.2391970617
C,0,0,0,-1.432216949,-1.2391970617
C,0,0,0,0.6827039791,2.4694139052
C,0,0,0,-0.6827039791,2.4694139052
C,0,0,0,0.6827039791,-2.4694139052
C,0,0,0,-0.6827039791,-2.4694139052
C,0,0,0,2.8395700687,1.2137693497
C,0,0,0,-2.8395700687,1.2137693497
```

- From here you can scroll up a bit to find the optimized geometry and rotational constants

```

Framework group D2H["C2"(HCC.CCH),SG(C12H8)]
Deg. of freedom 13
Standard orientation:
-----
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
-----
1 6 0 -0.000000 0.000000 0.714802
2 6 0 0.000000 -0.000000 -0.714802
3 6 0 0.000000 1.239197 1.432217
4 6 0 0.000000 1.239197 -1.432217
5 6 0 -0.000000 -1.239197 1.432217
6 6 0 -0.000000 -1.239197 -1.432217
7 6 0 0.000000 2.469414 0.682704
8 6 0 0.000000 2.469414 -0.682704
9 6 0 -0.000000 -2.469414 0.682704
10 6 0 -0.000000 -2.469414 -0.682704
11 6 0 0.000000 1.213769 2.839570
12 6 0 0.000000 1.213769 -2.839570
13 6 0 -0.000000 -1.213769 2.839570
14 6 0 -0.000000 -1.213769 -2.839570
15 6 0 -0.000000 0.000000 3.531937
16 6 0 0.000000 -0.000000 -3.531937
17 1 0 0.000000 3.405972 1.232946
18 1 0 0.000000 3.405972 -1.232946
19 1 0 -0.000000 -3.405972 1.232946
20 1 0 -0.000000 -3.405972 -1.232946
21 1 0 0.000000 2.152534 3.385882
22 1 0 0.000000 2.152534 -3.385882
23 1 0 -0.000000 -2.152534 3.385882
24 1 0 -0.000000 -2.152534 -3.385882
25 1 0 -0.000000 0.000000 4.617306
26 1 0 0.000000 -0.000000 -4.617306
-----
Rotational constants (GHZ): 1.0055830 0.5524279 0.3565521
*****

```

- You can find the optimized energy by searching the file for the phrase "SCF Done" and finding the *last* value, which should be the smallest converged value:

```

Initial guess orbital symmetries:
Occupied (AG) (B1U) (B3G) (B2U) (AG) (B1U) (AG) (B2U) (B3G)
(B1U) (B1U) (AG) (B3G) (B2U) (B1U) (AG) (AG) (B1U)
(B2U) (AG) (B3G) (AG) (B1U) (B2U) (AG) (B3G) (B1U)
(B2U) (B1U) (AG) (B3G) (B2U) (AG) (B1U) (AG) (B2U)
(B3G) (AG) (B3U) (B1U) (B2U) (B3G) (B1U) (B2U)
(B2G) (B1G) (AG) (B3G) (B3U) (AU) (B3U) (B2G)
(B1G)
Virtual (AU) (B3U) (B2G) (B1G) (B2G) (AG) (B1U) (AU) (B2U)
(AG) (B3G) (B3U) (B1U) (B2U) (AG) (B1U) (B3G)
(B2G) (AG) (B2U) (B1U) (B3G) (B2U) (AG) (B1U)
(B3G) (B2U) (AG) (B1U) (B1U) (B3G) (B2U) (B3G)
(B3U) (B1U) (AG) (B2G) (B1G) (AG) (B2U) (B3U)
(B3G) (AU) (AG) (AG) (B1U) (B2G) (B2U) (B3U) (B2U)
(B1U) (B3G) (B1G) (AG) (B2U) (B1U) (AG) (B1U)
(B3U) (B2G) (B3G) (B1G) (AU) (B2G) (AU) (B3U)
(B3G) (B1U) (AG) (B1U) (B2U) (B3G) (AG) (B1U)
(B2U) (AG) (B3G) (B2G) (B2U) (B1U) (AG) (B2U)
(B1U) (AG) (B3G) (B3G) (AG) (B1U) (B3G) (B1U)
(B2U) (B2U) (AG) (B1U) (B3G) (AG) (B2U) (B1U)
(B3G) (B2U) (AG) (B3G) (B1U) (AG) (B2U) (B1U)
(B3G) (B1U) (AG) (B1U) (B3G)
SCF Done: E(RB3LYP) = -615.634777247 A.U. after 8 cycles
NFOck= 8 Conv=0.72D-08 -V/T= 2.0055
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=1 I1Cent= 0 IopCLX= 0 NMat=1 NMatS=1 NMatT=0.

```

Note that this value is given in Hartrees. The absolute value of this energy doesn't mean much; it's more useful when considering energy differences between states or molecular isomers.

- Going to the very end of the file for an opt/freq calculation, you can scroll up to find the harmonic vibrational frequencies, and their infrared intensities, and normal mode atomic displacements

	70	71	72
	AG	B1U	AG
Frequencies --	3206.6530	3216.5226	3217.1302
Red. masses --	1.0970	1.0975	1.0972
Frc consts --	6.6459	6.6899	6.6908
IR Inten --	0.0000	90.3023	0.0000
Raman Activ --	317.0461	0.0000	755.3283
Depolar (P) --	0.3087	0.7499	0.1495
Depolar (U) --	0.4718	0.8571	0.2602

Atom	AN	X	Y	Z	X	Y	Z	X	Y	Z
1	6	0.00	0.00	0.00	0.00	0.00	0.00	-0.00	-0.00	0.00
2	6	-0.00	0.00	-0.00	0.00	-0.00	0.00	0.00	-0.00	-0.00
3	6	0.00	0.00	-0.00	-0.00	-0.00	0.00	0.00	-0.00	0.00
4	6	-0.00	0.00	0.00	-0.00	0.00	0.00	-0.00	-0.00	-0.00
5	6	-0.00	-0.00	-0.00	0.00	0.00	0.00	-0.00	0.00	0.00
6	6	0.00	-0.00	0.00	0.00	-0.00	0.00	0.00	0.00	-0.00
7	6	-0.00	-0.04	-0.02	0.00	-0.00	-0.00	-0.00	-0.01	-0.00
8	6	0.00	-0.04	0.02	0.00	0.00	-0.00	0.00	-0.01	0.00
9	6	0.00	0.04	-0.02	-0.00	0.00	-0.00	0.00	0.01	-0.00
10	6	-0.00	0.04	0.02	-0.00	-0.00	-0.00	-0.00	0.01	0.00
11	6	-0.00	0.00	0.00	0.00	-0.02	-0.01	-0.00	-0.02	-0.01
12	6	0.00	0.00	-0.00	0.00	0.02	-0.01	0.00	-0.02	0.01
13	6	0.00	-0.00	0.00	0.00	0.02	-0.01	0.00	0.02	-0.01
14	6	-0.00	-0.00	-0.00	0.00	-0.02	-0.01	-0.00	0.02	0.01
15	6	-0.00	0.00	0.01	0.00	0.00	-0.05	-0.00	-0.00	-0.05
16	6	0.00	0.00	-0.01	0.00	-0.00	-0.05	0.00	-0.00	0.05
17	1	0.00	0.42	0.25	0.00	0.02	0.01	0.00	0.07	0.04
18	1	-0.00	0.42	-0.25	0.00	-0.02	0.01	-0.00	0.07	-0.04
19	1	-0.00	-0.42	0.25	0.00	-0.02	0.01	-0.00	-0.07	0.04
20	1	0.00	-0.42	-0.25	0.00	0.02	0.01	0.00	-0.07	-0.04
21	1	0.00	-0.01	-0.01	-0.00	0.26	0.15	0.00	0.26	0.15
22	1	-0.00	-0.01	0.01	-0.00	-0.26	0.15	-0.00	0.26	-0.15
23	1	-0.00	0.01	-0.01	0.00	-0.26	0.15	-0.00	-0.26	0.15
24	1	0.00	0.01	0.01	-0.00	0.26	0.15	0.00	-0.26	-0.15
25	1	0.00	-0.00	-0.12	-0.00	-0.00	0.57	0.00	0.00	0.55
26	1	-0.00	-0.00	0.12	-0.00	0.00	0.57	-0.00	0.00	-0.55

It can be helpful to write little command line bash scripts to extract useful numbers from the output files. Here's one I use to extract vibrational frequencies and IR intensities from the output file

"freq.bash"

```
#!/bin/bash
```

```
cat $1 | grep "Frequencies -- " | awk -F" " '{print $3 "\n" $4 "\n" $5 }' > tmp
cat $1 | grep "IR Inten " | awk -F" " '{print $4 "\n" $5 "\n" $6 }' > tmp2
paste tmp tmp2 | column -s $'\t' -t
rm tmp tmp2
```

Run this script from the Adroit unix command line using

```
bash freq.bash c16h10_b3lyp_6-31g_d2h.out > c16h10_freq_list.dat
```