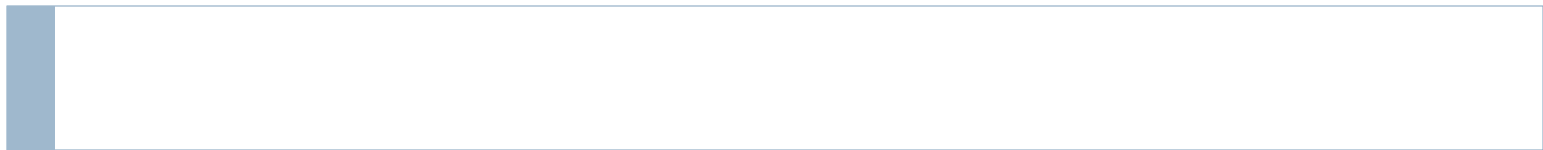


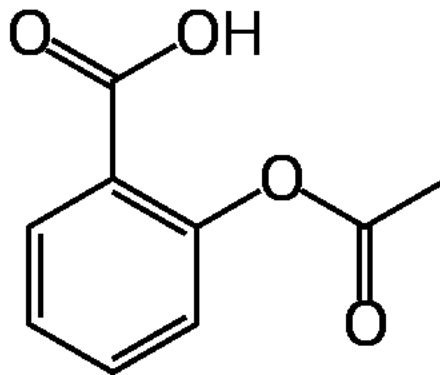
Gaussian tutorial

-Infrared spectra calculation



In this tutorial

- ▶ **Gaussian 03** program was used to perform the calculation.
- ▶ **GaussView 5.0** was used to prepare the input file for Gaussian.
- ▶ Exemplified compound: **Aspirin**



Drawing the compound by GaussView

The image displays the GaussView 5.0.8 software interface. The main window is titled "GaussView 5.0.8" and contains a menu bar (File, Edit, View, Calculate, Results, Windows, Help) and a toolbar. The current fragment is labeled "Carbon Tetrahedral". Below the toolbar, there is a "Builder Fragment:" section with a button labeled "Carbon Tetrahedral". The main view area shows a 3D ball-and-stick model of a carbon tetrahedron, with a central cyan carbon atom and four white hydrogen atoms. To the right, a separate window titled "G1:M1:V1 - New" is open, showing a solid blue background. The text "View window" is overlaid in red on this window. At the bottom of the View window, the status bar reads "0 atoms, 0 electrons, neutral, singlet" and "Build Select Placement".

Builder window

View window

0 atoms, 0 electrons, neutral, singlet Build Select Placement

Drawing the compound by GaussView

The image displays the GaussView 5.0.8 software interface. The main window shows the 'benzene' molecule being constructed. The 'Builder Fragment' dropdown menu is set to 'benzene'. The 'Ring Fragments' panel is open, showing a grid of various ring structures, with the benzene ring selected. The 'G1:M1:V1 - New' window shows a 3D ball-and-stick model of the benzene molecule. The status bar at the bottom of the 3D window indicates '12 atoms, 42 electrons, neutral, singlet' and 'Build Select Placement'.

GaussView 5.0.8

File Edit View Calculate Results Windows Help

benzene

Builder Fragment: benzene

Ring Fragments

G1:M1:V1 - New

12 atoms, 42 electrons, neutral, singlet

Build Select Placement

Drawing the compound by GaussView

The image displays the GaussView 5.0.8 software interface. The main window shows a menu bar (File, Edit, View, Calculate, Results, Windows, Help) and a toolbar. A red box highlights the 'Build' icon in the toolbar. Below the toolbar, the 'Builder Fragment' dropdown menu is set to 'Carbon Trivalent (S-S-D)', also highlighted with a red box. The 'Element Fragments' window is open, showing a periodic table with 'C' (Carbon) selected. Below the periodic table, the 'Select Carbon Fragment' section shows several options, with the 'Carbon Trivalent (S-S-D)' fragment highlighted in blue. To the right, a 3D ball-and-stick model of a molecule is displayed in a window titled 'G1:M1:V1 - New'. The molecule consists of 14 atoms and 48 electrons, and is neutral with a doublet. The status bar at the bottom of the window reads '14 atoms, 48 electrons, neutral, doublet' and 'Build Select Placement'.

GaussView 5.0.8

File Edit View Calculate Results Windows Help

Carbon Trivalent (S-S-D)

Builder Fragment: Carbon Trivalent (S-S-D)

Element Fragments

Select Carbon Fragment:

Atom

G1:M1:V1 - New

14 atoms, 48 electrons, neutral, doublet

Build Select Placement

Drawing the compound by GaussView

The image shows the GaussView 5.0.8 software interface. The main window displays a 3D ball-and-stick model of a molecule, which is a benzene ring with a carbonyl group attached to one of the carbons. The model is rendered in a ball-and-stick style with a blue background. The text at the bottom of the main window reads "14 atoms, 56 electrons, neutral, singlet".

The interface includes a menu bar (File, Edit, View, Calculate, Results, Windows, Help) and a toolbar. A red box highlights the "Build" icon in the toolbar. Below the toolbar, the "Builder Fragment" dropdown menu is set to "Oxygen Trivalent (D-LP-LP)", also highlighted with a red box. The "Element Fragments" window is open, showing a periodic table of elements. The "O" element is highlighted in blue. Below the periodic table, the "Select Oxygen Fragment" section shows three options: "Atom", a double-bonded oxygen fragment (highlighted in blue), and a single-bonded oxygen fragment.

Drawing the compound by GaussView

The screenshot displays the GaussView 5.0.8 software interface. The main window shows a 3D ball-and-stick model of a molecule, which is a substituted benzene ring with a carboxyl group (-COOH) attached. The interface includes a menu bar (File, Edit, View, Calculate, Results, Windows, Help) and a toolbar with various construction tools. A red box highlights the 'Build' button in the toolbar. Below the toolbar, the 'Builder Fragment' dropdown menu is set to 'Oxygen Tetravalent (S-S-LP-LP)'. An 'Element Fragments' window is open, showing a periodic table with the element Oxygen (O) highlighted in blue. Below the periodic table, there are three options for oxygen fragments: a single oxygen atom, a carbonyl group (C=O), and a carboxyl group (C(=O)OH). The status bar at the bottom indicates '15 atoms, 64 electrons, neutral, singlet' and provides buttons for 'Build' and 'Select Placement'.

GaussView 5.0.8

File Edit View Calculate Results Windows Help

Oxygen Tetravalent (S-S-LP-LP)

Builder Fragment: Oxygen Tetravalent (S-S-LP-LP)

Element Fragments

H X Bq He

Li	Be	B	C	N	O	F	Ne										
Na	Mg	Al	Si	P	S	Cl	Ar										
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt									
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		

Select Oxygen Fragment:

Atom

15 atoms, 64 electrons, neutral, singlet

Build Select Placement

Drawing the compound by GaussView

The screenshot displays the GaussView 5.0.8 software interface. The main window shows a 3D ball-and-stick model of a molecule, which is a benzene ring with two hydroxyl groups attached, representing a dihydroxybenzene derivative. The interface includes a menu bar (File, Edit, View, Calculate, Results, Windows, Help) and a toolbar with various construction tools. A red box highlights the 'Build' button in the toolbar. Below the toolbar, the 'Builder Fragment' dropdown menu is set to 'Oxygen Tetravalent (S-S-LP-LP)'. An 'Element Fragments' window is open, showing a periodic table with the element Oxygen (O) highlighted in blue. Below the periodic table, the 'Select Oxygen Fragment' section shows three options: a single oxygen atom, a carbonyl group (C=O), and a hydroxyl group (O-H). The status bar at the bottom indicates '16 atoms, 72 electrons, neutral, singlet' and provides buttons for 'Build' and 'Select Placement'.

GaussView 5.0.8

File Edit View Calculate Results Windows Help

Oxygen Tetravalent (S-S-LP-LP)

Builder Fragment: Oxygen Tetravalent (S-S-LP-LP)

Element Fragments

Select Oxygen Fragment:

Atom

16 atoms, 72 electrons, neutral, singlet

Build Select Placement

Drawing the compound by GaussView

The image displays the GaussView 5.0.8 software interface. The main window shows a 3D ball-and-stick model of a molecule, which appears to be a substituted benzene ring. The interface includes a menu bar (File, Edit, View, Calculate, Results, Windows, Help), a toolbar with various drawing tools, and a 'Builder Fragment' dropdown menu set to 'Carbon Trivalent (S-S-D)'. A red box highlights the 'Carbon Trivalent (S-S-D)' option in the dropdown menu. Below the main window is the 'Element Fragments' panel, which contains a periodic table of elements. The 'C' element is highlighted in blue. Below the periodic table is a 'Select Carbon Fragment' section with several icons representing different carbon bonding environments: a single-bonded carbon atom, a carbon atom with a triple bond, a carbon atom with a double bond, a carbon atom with a single bond and a lone pair, and a carbon atom with a single bond and a radical. The main window also displays the text 'G1:M1:V1 - New' and '18 atoms, 78 electrons, neutral, doublet' at the bottom. The status bar at the bottom right contains the text 'Build Select Placement'.

Drawing the compound by GaussView

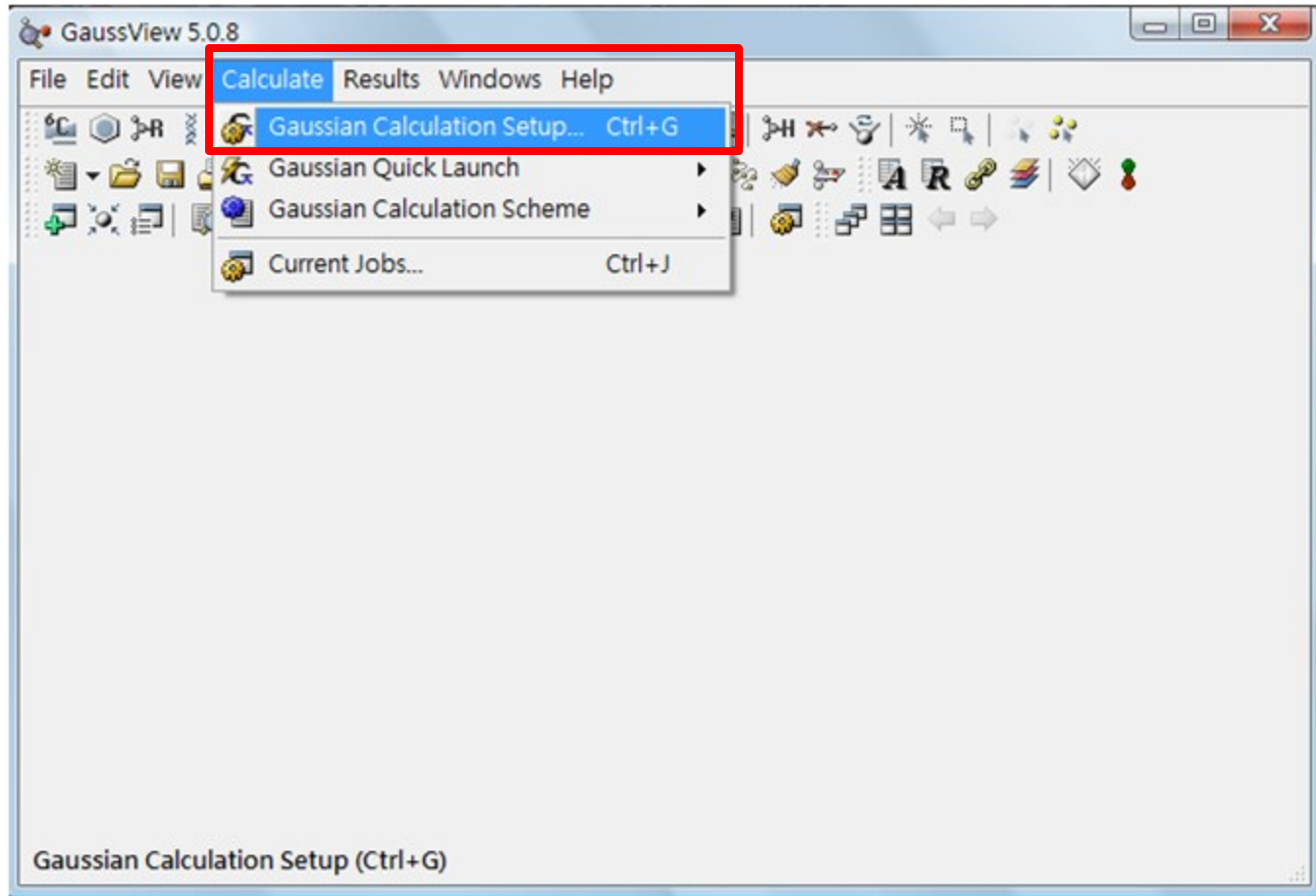
The image displays the GaussView 5.0.8 software interface. The main window shows a menu bar (File, Edit, View, Calculate, Results, Windows, Help) and a toolbar. A red box highlights the 'Build' icon in the toolbar. Below the toolbar, the 'Builder Fragment' dropdown menu is set to 'Oxygen Trivalent (D-LP-LP)', also highlighted with a red box. The 'Element Fragments' window is open, showing a periodic table with the element Oxygen (O) selected. Below the periodic table, the 'Select Oxygen Fragment' section shows three options: 'Atom', a double-bonded oxygen fragment, and a single-bonded oxygen fragment with two lone pairs. The main 3D view window, titled 'G1:M1:V1 - New', displays a ball-and-stick model of a complex organic molecule with a central ring system and several oxygen atoms. The status bar at the bottom of the 3D window shows 'Atom 18(O)' and 'Build Select Placement'.

Drawing the compound by GaussView

The screenshot displays the GaussView 5.0.8 interface. The main window shows a 3D ball-and-stick model of a molecule with 21 atoms (94 electrons, neutral, singlet). The molecule consists of a benzene ring with a carboxylic acid group (-COOH) and a hydroxyl group (-OH) attached to adjacent carbons. The interface includes a menu bar (File, Edit, View, Calculate, Results, Windows, Help), a toolbar with various construction tools, and a 'Builder Fragment' dropdown menu set to 'Carbon Tetrahedral'. A separate 'Element Fragments' window is open, showing a periodic table with Carbon (C) selected. Below the periodic table, there are options to select a carbon fragment: 'Atom', 'C≡', 'C=C', 'C=C', and 'C' (tetrahedral).

► File → Save → aspirin.pdb

Calculation setup



Calculation setup

G1:M1:V1 - Gaussian Calculation Setup

Title: **Aspirin.pdb**
Keywords: **# opt freq b3lyp/6-31+g geom=connectivity**
Charge/Mult: **0 1**

Job Type Method Title Link 0 General Guess NBO PBC Solvation Add. Inp.

Opt+Freq

Optimize to a Minimum Use RFO step Use Quadratic Macrostep
Calculate Force Constants Never Use tight convergence criteria
Compute Raman Default Compute VCD Save Normal Modes
Compute ROA No Read Incident Light Freqs Default Skip diag. of full matrix

Select Normal Modes Modes: Atoms: Anharmonic Corrections Specify Anharmonic Modes: 1

Additional Keywords: Update

Scheme: (Unnamed Scheme)

Submit... Quick Launch Cancel Edit... Retain Defaults Help

Calculation setup

G1:M1:V1 - Gaussian Calculation Setup

Title:

Keywords: **# opt freq hf/6-31+g geom=connectivity**

Charge/Mult: **0 1**

Job Type **Method** Title Link 0 General Guess NBO PBC Solvation Add. Inp.


Multilayer ONIOM Model

Method: Ground State ▾ Hartree-Fock ▾ Default Spin ▾

Basis Set: 6-31G ▾ + ▾ (▾ ▾ , ▾ ▾)

Charge: 0 Spin: Singlet ▾

Additional Keywords:

Scheme: (Unnamed Scheme) ▾ 

Calculation setup

- ▶ Save → aspirin.gjf (Gaussian input file)

```
%chk=D:\GaussianTutorial_IR\aspirin.chk
# opt freq hf/6-31+g geom=connectivity      Route section

Aspirin.pdb      Title section

0 1              Molecular specification
C               -1.07170000    0.20620000    0.00000000
C               -1.78620000   -0.20620000    0.00000000
C               -1.78620000   -1.03130000    0.00000000
C               -1.07170000   -1.44380000    0.00000000
C               -0.35720000   -1.03130000    0.00000000
C               -0.35720000   -0.20620000    0.00000000
C               -1.07170000    1.03130000    0.00000000
O                0.35720000    0.20620000    0.00000000
O               -1.78620000    1.44380000    0.00000000
O               -0.35720000    1.44380000    0.00000000
C                1.07170000   -0.20620000    0.00000000
O                1.07170000   -1.03130000    0.00000000
C                1.78620000    0.20630000    0.00000000
H               -2.71281439    0.32885679    0.00000000
H               -2.71284247   -1.56630815    0.00000000
H               -1.07170000   -2.51380000    0.00000000
H                0.56944247   -1.56630815    0.00000000
H               -0.53260360    2.38763981    0.00000000
H                1.59069807    1.25828812    0.00000000
H                2.34727926   -0.05220221    0.87365134
H                2.34727926   -0.05220221   -0.87365134
```

```
1 2 2.0 6 1.0 7 1.0
2 3 1.0 14 1.0
3 4 2.0 15 1.0
4 5 1.0 16 1.0
5 6 2.0 17 1.0
6 8 1.0
7 9 2.0 10 1.0
8 11 1.0
9
10 18 1.0
11 12 2.0 13 1.0
12
13 19 1.0 20 1.0 21 1.0
14
15
16
17
18
19
20
21
```

- ▶ Submit job

Job processing window

The screenshot shows the Gaussian 09 Revision-A.01 Job processing window. The window title is "Gaussian 09 Revision-A.01". The menu bar includes "File", "Process", "Utilities", "View", and "Help". The toolbar contains icons for job control (start, pause, stop, refresh) and editing (find, print). The "Batch Data" field is empty. The "Active Job" field shows "C:\Jobs\methylpropene.gjf". The "Output File" field shows "methylpropene.out". The "Run Progress" bar indicates "C:\G09W\J502.exe is processing...". The main area displays Gaussian output text, including parameters like HarFok, ScadFX, FoFCou, and convergence information. The status line at the bottom reads "Iteratively Solving the Self-Consistent Field Equations".

Labels pointing to the window components:

- Menu bar
- Job control icons
- Current batch job
- Output filename
- Editing icons
- Toolbar
- Batch control file
- Input filename
- Job progress display
- Gaussian output area
- Status line

```
HarFok: IExCor= 402 AccDes= 0.000+00 IRadAn= 1 IDoU= 1
ScadFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: PMM=F IPFlag= 0 PMFlag= 100000 PMFlg1= 0
MFxFlg= 0 DoJE=I BraDBF=F KetDBF=I PulRan=I
Omega= 0.000000 0.000000 1.000000 0.000000 0.000000 ICntrl=
NMat0= 1 NMatS0= 1 NMatI0= 0 NMatD0= 1 NMatDS0= 0 N
IICent= 4 NGrid= 0.
Petite list used in FoFCou.
Initial guess orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
The electronic state of the initial guess is 1-A.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
```

Iteratively Solving the Self-Consistent Field Equations

Job edit window

Menu bar — File Edit Check-Route Set-Start

Current input file — C:\Jobs\methylpropene.gjf

Link 0 section — % Section

Route section — Route Section #T B3LYP/6-31 G(d)

Title section — Title Section 2-MethylPropene

Charge & spin multiplicity — Charge, Multipl. 0 1

Molecular structure —

Appears only when editing an existing input file —

Create/edit additional job steps —

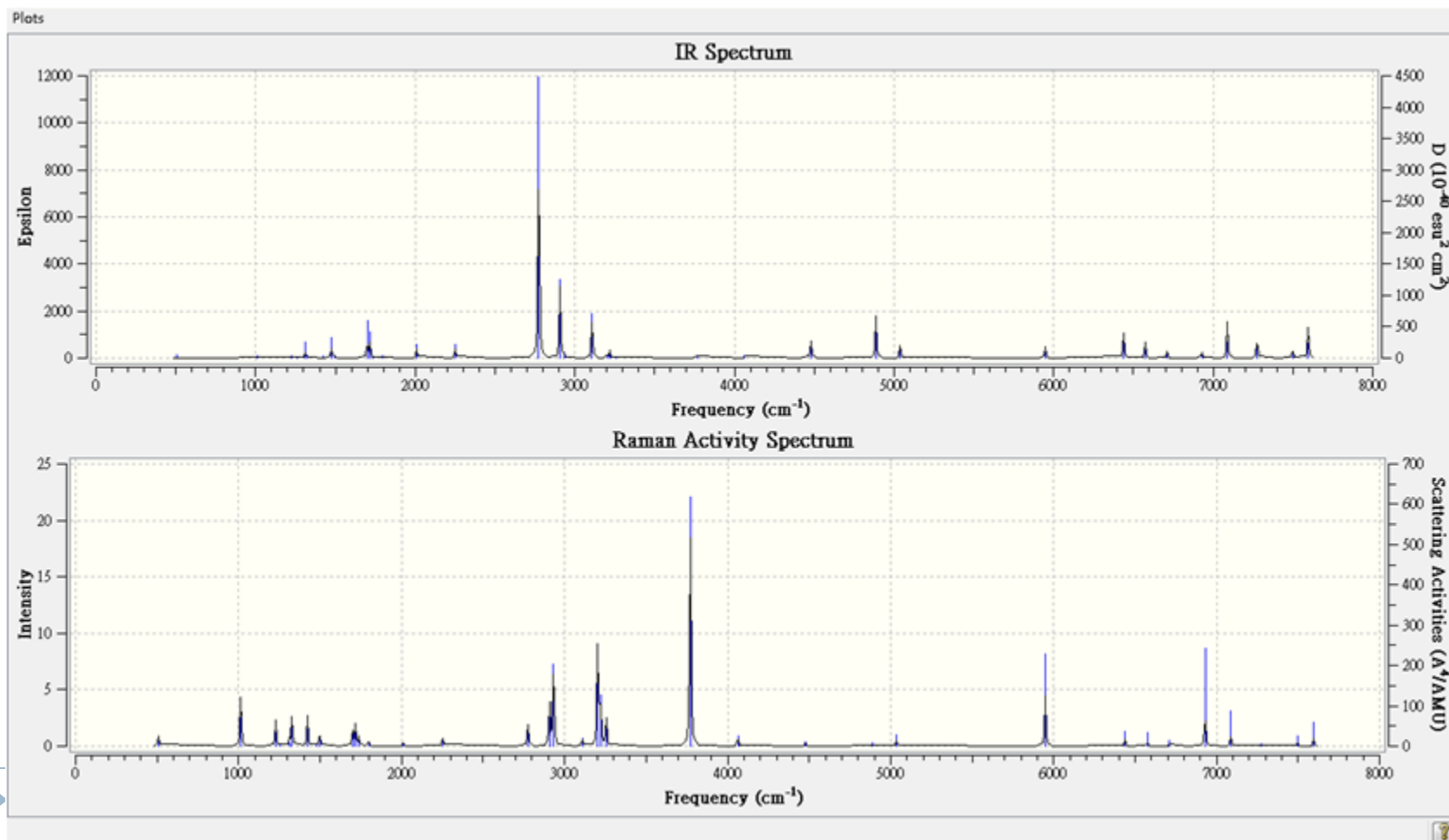
Task icons —

Number of addl. job steps — Additional Steps 0

Molecule Specification			
C-CM	-2.53	0.19	0.00
H-HA	-2.00	-0.73	0.00
H-HA	-3.60	0.19	0.00
C-CM	-1.86	1.37	0.00
C-CT	-2.63	2.70	0.00
H-HC	-1.93	3.51	0.07
H-HC	-3.24	2.76	-0.88

Viewing vibrational frequencies in GaussView

- ▶ File → Open → aspirin.out
- ▶ Results → Vibrations



Viewing vibrational frequencies in GaussView

