

Molecule Name: Formaldehyde  
 frequencies (in wavenumbers,  $\text{cm}^{-1}$ , report to 1 decimal place)

Description	HF/3-21G	B3LYP/6-31G(d,p)	Experiment
CH <sub>2</sub> symmetric stretch (Mode 1, B1)	1377.2	1198.7	1249.1
CO stretching (Mode 2, B2)	1378.4	1274.1	1167.3
CH <sub>2</sub> scissoring (Mode 3, A1)	1692.6	1553.9	2782.5
CH <sub>2</sub> asymmetric stretch (Mode 4, A1)	1915.4	1845.6	1746.1
CH <sub>2</sub> rocking (Mode 5, A1)	3162.8	2903.6	1500.1
CH <sub>2</sub> wagging (Mode 6, B2)	3234.0	2961.7	2903.6

Describe the trend of differences between theory and experiment here.

The theoretical vibrational frequencies calculated using HF/3-21G and B3LYP/6-31G(d,p) methods tend to be higher than the experimental values from the NIST WebBook. The differences are more significant for lower-frequency modes, such as the CH<sub>2</sub> symmetric stretch and wagging modes, where the computed values are notably larger than experimental data. For higher-frequency modes, the calculated values are still higher but the discrepancy is smaller. The trend suggests that while B3LYP/6-31G(d,p) provides results closer to the experimental frequencies, both methods tend to overestimate the vibrational frequencies due to limitations in the computational models, which do not fully account for real-world factors like anharmonicity, temperature, thermal effects.

Thermochemical corrections at B3LYP/6-31G(d,p) (kcal/mol, 1 decimal place)

Molecule	Zero point energy	Thermal correction to the enthalpy	Thermal correction to the free energy
CH <sub>2</sub> O	0.3	0.5	0.1
CHClO	16.8	19.2	3.6
CCl <sub>2</sub> O	20.5	23.0	4.0
CF <sub>2</sub> O	22.0	24.5	4.5

Append the archive entries here.

## formaldehyde\_B3LYP.log

Activities Terminal Thu 15:39

hd8136@warrior:~

File Edit View Search Terminal Help

1\GINC-WARRIOR\Freq\R3LYP\6-31G(d,p)\C1H2O1\HD8136\27-Feb-2025\0\#

N Geom=AllCheck Guess=TCheck SCRF=Check GenChk R3LYP\6-31G(d,p) Freq\

\Formaldehyde B3LYP\6-31G(d,p) calculation\0,1,C\_0.3121022655\_0.30965

67713,0.2046525317\H\_0.7548819474,-0.628538124,0.0067383899\H,-0.7765

938275\_0.4544696333\_0.0067385104\_0.06899314748\_1,2985290497\_0.6871894

45\Version\ES64L-G16Rev.01\State=1-41\HF=-114.5031984\RMSD=5.727e-09

\RMSE=2.666e-04\ZeroPoint=.0276405\Thermal=0,\0.296874\|Pole=-0.467627

1,-0.6613872,-0.2865797\|DipoleDerivs=0.8721664,0.0188776,0.1467129,0.01

80776,0.8849481,0.2874779,0.1467129,0.2874779,0.2694703,0.0631269,0.1

175293,0.0875558,-0.1184031,-0.2035324,-0.0553409,0.0054971,-0.053885,0

0.8516497,-0.2595629,0.0405975,-0.0546947,0.0488084,-0.0078976,-0.01132

19,-0.0526359,-0.0127777,0.0516497,-0.594766,-0.1765648,-0.099574,0

1765648,-0.6743169,0.1488153,-0.099574,-0.1488153,-0.3727697\Polar=1.5

2457499,1.3945823,16.2317961,2.0925035,2.9591696,8.2573155\Quadrupole

=-0.0099763,-0.1066337,-0.116601,-0.1358564,-0.074286,-0.1650536\PG=C2V

[C2(C101),(SGVH2)]\NIMag=0\|0.69679755,0.15977535,0.80976683,0.152926

51.0,2.262509,-0.2678778,-0.12048875,0.08944589,0.01313193,0.10524082,

0.09415696,0.21335877,-0.02556736,-0.09013156,0.25434900,0.01449294,

0.02652976,-0.029848184,-0.00895098,0.04945434,0.03198045,-0.26673858,0

0.04457501,-0.02848261,-0.00883123,0.00335081,-0.00482586,0.29443153,0

0.0396395,-0.07310877,-0.00385915,0.02530741,0.00129996,-0.00009648,0

2324785,0.06515830,-0.02984334,0.04842156,-0.06298183,0.00151755,-0.00

458208,0.0185156,-0.04946254,0.00840112,0.03198044,-0.31557040,-0.2937

92351,-0.02113675,0.31635312,-0.29379626,-0.52329928,-0.19455688,-0.02

462172,-0.04229612,-0.0282889,-0.02467717,0.00665057,-0.00870059,0.34

309515,0.55893883,-0.13757612,-0.19455688,-0.14191510,-0.06614040,-0.0

1930490,0.01248575,-0.01615434,-0.01222378,0.01248576,0.15987085,0.226

08556,0.11694359\|-0.00837229,-0.00052648,-0.00022815,0.00054339,0.000

39151,0.000012422,0.00035099,0.00018177,0.00012422,-0.00003309,-0.00004

680,-0.00002028\\\@

... UNTIL SCIENCE IS MIXED WITH EMOTION AND APPEALS TO THE HEART AND IMAGINATION , IT IS LIKE DEAD INORGANIC MATTER; AND WHEN IT IS SO MIXED AND SO TRANSFORMED IT IS LITERATURE.

-- JOHN BURROUGHS

AD\hd8136@VDCCHM744005:~

File Edit View Search Terminal Help

Gau-4673.rwf Gau-4673.s

benzene.fchk benzene.chk

benzene.fchk benzene.log

benzene\_esp.cube formaldehyde

de\_HF.gjf methane\_20250129.png

methane\_gs\_optfreq\_20250129.gjf ondemand styrene.chk

styrene.fchk styrene.gj

styrene.fchk styrene.log

styrene\_esp.cube styrene\_ho

mo.cube styrene\_lumo.cube

test test\_gauss

ian\_input.gjf

sftp> exit

AD\hd8136@VDCCHM744005:~\$ /usr/local/bin/gv/gvleve.exe

AD\hd8136@VDCCHM744005:~\$

## formaldehyde\_HF.log

The figure shows a dual-monitor Linux desktop environment. The left monitor displays a terminal window titled 'hd8136@warrior:~' with a yellow icon. It contains the output of a Gaussian QM9 calculation for benzene, showing various energy terms and final coordinates. The right monitor displays another terminal window titled 'AD/hd8136@VDCCHM744005:~' with a blue icon. This window shows a Gaussian job submission script for methane, including sections for file inclusion, calculation control, and visualization.

```
File Edit View Search Terminal Help
1|1|GINC-WARRIOR\Freq\1.RHF|3-21G\1\H2101\HD8136\27-Feb-2025\0\\#N Geom-A
llCheck Guess-TCheck SCRF-check Genchk RHF\3-21G Freq\|Formaldehyde HF
/3-21G calculation|0\|C_0.3099957325_0.3654050038_0.202817014\H_0.73
7791027_0.610182869_0.00854966\H_0.7535938261_0.4444132359_0.008549
1774_0.0.9660288816_1.2944242713_0.6054106255\|Version=ES64L_G10rev8
1|1|A1|H=F|-13.22182|RMSD=2.196e-10|RMSF=3.875e-05|ZeroPoint=0.0
289792\|Thermal\0.0318326\|Dipole=-0.5692639,-0.8050395,0.3488666\|Dipol
eDeriv=0.856321,-0.0536241,0.1211325,-0.0536241,0.8124662,0.1713028,-0
.1211325,0.1713028,-0.557677,-0.0629332,0.0978116,-0.036851,0.1137474
,-0.1353081,-0.6842421,0.00899186,-0.0460976,0.088299,-0.1937429,0.0675
027,-0.039163,-0.051567,-0.0044940,-0.0177541,-0.0437677,-0.014498,-0.0
80299,-0.5936451,-0.1116901,-0.6726157,-0.110786
5,-0.0782834,-0.1107065,-0.4163658\Polar=12.5119615,2.0017682,13.92725
31,2.1535154,3.0452191,6.1215695\ParamDeriv=3.3248808,-2.8679524,-1.88
78052,-0.2176362,-0.0136042,-0.1059229,1.6991907,5.1173482,0.333087,-0
.6136044,-0.2171124,-0.1497933,-1.8305945,-1.1302432,1.0314556,-1.54715
13,-2.1879442,-0.2462629,-0.921491,-2.5512883,-1.571819,-0.6137099,0.19
74567,-0.2210694,-1.3148583,-2.7650593,-7.4000359,-0.2856389,-1.003503,-0
.5048681,-0.4249344,-2.7965031,-0.8739014,1.0879381,-1.0888937,-0.602478
5,-0.9443242,-0.9173002,-0.3399803,-1.122011,0.1094765,-0.5496828,-0.211
6961,-1.8970315,-0.175897,-0.0212943,-0.585201,-0.0401505,-1.010875,-0.09
9487,-0.2924592,-0.0689707,-0.4228046,-0.6024699,-3.7979508,-4.5019406,-0
.6556959,-1.5088947,-0.3066769,-0.4354563,-0.5924286,-4.258323,-6.891051,-0
.3066711,-1.7258164,-0.0145109,-0.3902853,-0.7427914,-0.1349057,-2.5272899,
3.5748332,-3.2512696\HyperPolar=-41.83265,-7.2959654,8.0158367,-48.52
35948,-0.5333197,-0.489107,-7.8301006,-3.6492772,-5.1667234,-5.595763
Quadrupole=0.0466117,-0.132941,-0.0923294,-0.24546,-0.0931383,-0.131714
\PGe=C2V [C2(C101)_SGV(H2)]\NI[Mag=0]\o.78735318,0.16698465,0.985362323,
0.16526406,0.23371253,0.31568416,-0.13515887,0.10604128,0.01779243,0.1
2354687,0.18466226,-0.26239427,-0.03366115,-0.10495977,-0.38427708,0.81
722689,-0.03325686,-0.07838308,-0.01086219,0.05942237,-0.05948180,-0.1
48412,-0.04072693,-0.03766668,-0.01124911,0.00891761,-0.00701429,-0.38
16687,-0.8427195,-0.08326963,-0.0855541,-0.0316893,-0.00627829,-0.00649
039,-0.02484412,-0.07765789,-0.03709495,-0.0051512,-0.07838307,-0.01875
59,-0.00677664,-0.02280995,-0.05937823,-0.01031926,-0.03948187,-0.33791019
,-0.13168286,-0.14538798,-0.02286111,-0.00002010,-0.00014422,-0.0246328
4,-0.04956121,-0.02415887,-0.33968192,-0.31368286,-0.05969992,-0.2056066
79,-0.03277089,-0.04216109,-0.02567511,-0.01681042,-0.00533286,-0.00869
374,-0.36326418,-0.59652816,-0.14538978,-0.20560679,-0.15891801,-0.00960
583,-0.01898457,-0.01609170,-0.01469726,-0.0153842,-0.01609170,0.169692
87,-0.2397564,-0.12673461,-0.00006052,-0.00008559,-0.00003709,-0.00006
359,-0.00008357,-0.00009054,-0.00003473,-0.0000847,-0.0000954,-0.00002938,
0.00004155,-0.00001801||@
```

## Vibrational frequency and thermochemistry screenshots:

Activities Terminal Thu 15:14

```
hd8136@warrior:~
```

File Edit View Search Terminal Help

```
Low frequencies --- -18.8812 -3.2435 -0.0015 -0.0013 -0.0009 5.8423
Low frequencies --- 1337.1541 1378.4097 1692.5805
Diagonal vibrational polarizability:
  0.0740205  0.5943699  0.7161962
Diagonal vibrational hyperpolarizability:
  0.0000000 -0.0000000 -7.5816390
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering
activities (A**4/AMU), depolarization ratios for plane and unpolarized
incident light, reduced masses (AMU), force constants (mdyne/A),
and normal coordinates:
```

	1	2	3
B1	B2	A1	
Frequencies	-- 1337.1541	1378.4097	1692.5805
Red. masses	-- 1.3646	1.3405	1.2184
Frc consts	-- 1.4376	1.5007	2.0566
IR Inten	-- 4.9179	20.0986	15.8908
Raman Activ	-- 0.1418	5.2227	16.7600
Depolar (P)	-- 0.7500	0.7500	0.6148
Depolar (U)	-- 0.8571	0.8571	0.7615
Atom AN	X Y Z X Y Z X Y Z		
1 6	-0.17 0.00 -0.00	0.00 -0.15 -0.00	0.00 -0.00 0.05
2 1	0.76 -0.00 0.00	-0.00 0.27 0.64	-0.00 0.33 0.62
3 1	0.76 -0.00 -0.00	0.00 0.27 -0.64	-0.00 -0.33 0.62
4 8	0.64 0.00 0.00	-0.00 0.08 0.00	-0.00 0.00 -0.11
	4	5	6
	A1	A1	B2
Frequencies	-- 1915.4226	3162.8465	3233.9935
Red. masses	-- 4.4262	1.0522	1.1151
Frc consts	-- 9.5678	6.2016	6.8717
IR Inten	-- 69.3661	21.6044	120.3612
Raman Activ	-- 4.7461	120.6421	49.2829
Depolar (P)	-- 0.1991	0.1828	0.7500
Depolar (U)	-- 0.3321	0.3090	0.8571
Atom AN	X Y Z X Y Z X Y Z		
1 6	-0.00 0.00 0.44	-0.00 0.00 0.06	-0.00 -0.10 0.00
2 1	0.00 -0.49 -0.35	0.00 0.61 -0.36	0.00 0.59 -0.38
3 1	0.00 0.49 -0.35	0.00 -0.61 -0.36	0.00 0.59 0.38
4 8	0.00 0.00 -0.29	0.00 -0.00 -0.00	0.00 -0.00 -0.00

:

```
AD\hd8136@VDCCHM744005: ~
```

File Edit View Search Terminal Help

```
Gau-19193.inp Gau-4673.d
2e Gau-4673.int
Gau-4673.rwf Gau-4673.s
kr benzene.chk
benzene.fchk benzene.gj
f benzene.log
benzene_esp.cube formaldehy
de_HF.gjf methane_20250129.png
methane_gs_optfreq_20250129.gjf ondemand
styrene.chk
styrene.fchk styrene.gj
styrene.log
styrene_esp.cube styrene.ho
mo(cube) styrene_lumo.cube
test test_gauss
ian_input.gjf sftp> []
```

Activities Terminal Thu 15:13

```
hd8136@warrior:~
```

File Edit View Search Terminal Help

```
incident light, reduced masses (AMU), force constants (mdyne/A),
and normal coordinates:
```

	1	2	3
B1	B2	A1	
Frequencies	-- 1198.7178	1274.1402	1553.9337
Red. masses	-- 1.3696	1.3429	1.1284
Frc consts	-- 1.1595	1.2845	1.5940
IR Inten	-- 1.5871	12.6212	6.7947
Atom AN	X Y Z X Y Z X Y Z		
1 6	-0.17 0.00 0.00	-0.00 -0.15 -0.00	-0.00 -0.00 0.01
2 1	0.76 -0.00 -0.00	0.00 0.25 0.65	0.00 0.35 0.61
3 1	0.76 0.00 0.00	0.00 0.25 -0.65	0.00 -0.35 0.61
4 8	0.64 -0.00 -0.00	0.00 0.08 0.00	0.00 0.00 -0.09
	4	5	6
	A1	A1	B2
Frequencies	-- 1845.5890	2903.6390	2961.6985
Red. masses	-- 6.7712	1.0451	1.1210
Frc consts	-- 13.5890	5.1916	5.7935
IR Inten	-- 96.3981	54.2739	158.2541
Atom AN	X Y Z X Y Z X Y Z		
1 6	0.00 -0.00 0.56	-0.00 0.00 0.06	0.00 -0.10 0.00
2 1	-0.00 -0.46 -0.24	0.00 0.61 -0.36	-0.00 0.60 -0.37
3 1	-0.00 0.46 -0.24	0.00 -0.61 -0.36	-0.00 0.60 0.37
4 8	-0.00 0.00 -0.39	0.00 -0.00 0.00	-0.00 0.00 -0.00

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 6 and mass 12.00000  
 Atom 2 has atomic number 1 and mass 1.00783  
 Atom 3 has atomic number 1 and mass 1.00783  
 Atom 4 has atomic number 8 and mass 15.99491  
 Molecular mass: 30.01056 amu.

Principal axes and moments of inertia in atomic units:

	1	2	3
Eigenvalues	-- 6.33100 46.70489 53.03589		
X	0.00000 0.00000 1.00000		

:

```
AD\hd8136@VDCCHM744005: ~
```

File Edit View Search Terminal Help

```
Gau-19193.inp Gau-4673.d
2e Gau-4673.int
Gau-4673.rwf Gau-4673.s
kr benzene.chk
benzene.fchk benzene.gj
f benzene.log
benzene_esp.cube formaldehy
de_HF.gjf methane_20250129.png
methane_gs_optfreq_20250129.gjf ondemand
styrene.chk
styrene.fchk styrene.gj
styrene.log
styrene_esp.cube styrene.ho
mo(cube) styrene_lumo.cube
test test_gauss
ian_input.gjf sftp> []
```

## Thermochemistry screenshots:

The screenshot shows a Safari browser window on a Mac OS X desktop. The address bar says "webbook.nist.gov". The main content area displays the NIST Thermochemistry tables for formaldehyde. At the top, there's a navigation bar with links to "Topic: Lecture 10: The uncertainty principle...", "Neil Turck - Wikipedia", and "Assignment #2 - Frequency Calculations a...". Below that is a note about NIST subscription sites. The main section is titled "Vibrational and/or electronic energy levels" and includes a note about symmetry: "Symmetry:  $C_{2v}$  Symmetry Number  $\sigma = 2$ ". It lists vibrational modes with their wavenumbers and intensities. A note at the bottom credits "Source: Shimanouchi, 1972".

The screenshot shows a terminal window on a Linux desktop. The title bar says "Activities Terminal" and the prompt is "hd8136@warrior:~". The terminal window displays Gaussian output for benzene and styrene. The benzene output includes rotational constants, zero-point vibrational energy, and vibrational temperatures. The styrene output shows various energy components like thermal, electronic, and rotational energies, along with Log10(Q) and Ln(Q) values. The background shows a red and orange abstract wallpaper.