



Computational Spectroscopy

II. *ab initio* Methods

from part (g) Advanced Methods for Thermochemistry
Chemistry 713

Updated: February 28, 2008



Advanced Methods for Thermochemistry

1. Thermodynamics from Gaussian data
2. Rate constants from Gaussian data
3. “High accuracy” extrapolation methods
 - G1, G2, G3, CBS-4M, CBS-Q, CBS-QB3
4. Condensed phase methods
 - treatments of solvation

Thermodynamic quantities available from a Gaussian FREQ calculation

A portion of the G03 output ".log" file.

```
# freq hf/3-21+g geom=connectivity
```

```
...
Vinyl fluoride frequency
```

```
...
```

```
-----
- Thermochemistry -
-----
```

```
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
```

```
...
```

```
This molecule is an asymmetric top.
```

```
Rotational symmetry number 1.
```

```
Rotational temperatures (Kelvin) 3.05888 .50432 .43294
```

```
Rotational constants (GHZ): 63.73686 10.50837 9.02106
```

```
Zero-point vibrational energy 124526.4 (Joules/Mol)
29.76253 (Kcal/Mol)
```

```
Warning -- explicit consideration of 1 degrees of freedom as
vibrations may cause significant error
```

```
Vibrational temperatures: 739.91 1123.38 1431.13 1558.02 1624.71
(Kelvin) 1789.79 2083.59 2245.96 2657.35 4809.88
4928.00 4962.46
```

```
Zero-point correction= .047430 (Hartree/Particle)
```

```
Thermal correction to Energy= .050672
```

```
Thermal correction to Enthalpy= .051616
```

```
Thermal correction to Gibbs Free Energy= .023092
```

```
Sum of electronic and zero-point Energies= -175.909354
```

```
Sum of electronic and thermal Energies= -175.906112
```

```
Sum of electronic and thermal Enthalpies= -175.905167
```

```
Sum of electronic and thermal Free Energies= -175.933691
```

(cont'd)....

	E (Thermal)		S
	KCal/Mol	Cal/Mol-Kelvin	
Total	31.797	9.146	60.033
Electronic	.000	.000	.000
Translational	.889	2.981	37.405
Rotational	.889	2.981	21.503
Vibrational	30.019	3.185	1.126
Vibration 1	.868	1.218	.623
	Q	Log10(Q)	Ln(Q)
Total Bot	.238974E-10	-10.621649	-24.457250
Total V=0	.156464E+12	11.194414	25.776090
Vib (Bot)	.174410E-21	-21.758428	-50.100631
Vib (Bot) 1	.315520E+00	-.500974	-1.153534
Vib (V=0)	.114192E+01	.057635	.132710
Vib (V=0) 1	.109123E+01	.037916	.087305
Electronic	.100000E+01	.000000	.000000
Translational	.122716E+08	7.088902	16.322799
Rotational	.111655E+05	4.047877	9.320581