Formaldehyde

PC Spartan '04

		Term cm-1	ZPE kJ/mol	Enthalpy kJ/mol	Entropy J/mol.K	Cv J/mol.K	% in Ground	IR Int.
1	B2	1337.320	7.9989	0.0252	0.0977	0.5471	99.84	4.91
2	B1	1378.502	8.2453	0.0213	0.0822	0.4763	99.87	20.12
3	A1	1692.671	10.1244	0.0057	0.0216	0.1574	99.97	15.89
4	A1	1915.649	11.4581	0.0022	0.0082	0.0687	99.99	69.43
5	A1	3162.230	18.9143	0.0000	0.0000	0.0005	100.00	21.63
6	B1	3233.279	19.3393	0.0000	0.0000	0.0003	100.00	120.49
Total	Vibrations		76.0804	0.0545	0.2099	1.2502		

ZPE: Zero-point vibrational energy = $\frac{1}{2}N_A h\nu_o$ for each vibration

Vibrational Enthalpy: = $\frac{Nh\nu_o e^{-h\nu_o/kT}}{1-e^{-h\nu_o/kT}}$ for each vibration

Total Vibrational Enthalpy = $U-U(0)_{vib} + E_{zero\ point}$

Vibrational Entropy: $=-R \ln(1-e^{-h\nu_o/kT}) + \frac{U - U(0)_{vib}}{T}$

$=-R \ln(1-e^{-h\nu_o/kT}) + \frac{Nh\nu_o}{T}\frac{e^{-h\nu_o/kT}}{(1-e^{-h\nu_o/kT})}$ for each vibration

Ideal Gas	2.4789 kJ/mol		

add RT = 2.4789 kJ/mol, to give ΔH.

Translation	3.7184	151.1685	12.4716

Translational Enthalpy: 3.7184 kJ/mol **= 3/2 RT**

Translational Entropy: 151.1685 kJ/mol.K

$= R \ln\left(\frac{(2\pi mkT)^{3/2} e^{5/2} V}{N_A h^3}\right)$ Sackur-Tetrode Equation

Rotation	3.7184	66.7678	12.4716

Rotational Enthalpy: 3.7184 kJ/mol **= RT or 3/2RT**

Rotational Entropy: 66.7678 J/mol.K

$= R \ln\left(\frac{kT}{\sigma\tilde{B}hc}\right) + R$ diatomic or

$=R \ln \frac{\pi^{1/2}}{\sigma}\left(\frac{kT}{\tilde{A}hc}\right)^{1/2}\left(\frac{kT}{\tilde{B}hc}\right)^{1/2}\left(\frac{kT}{\tilde{C}hc}\right)^{1/2} + \frac{3}{2}R$ for nonlinear

Totals	86.0507	218.1462	26.1935	kJ/mol
Gibb's Free Energy (H - TS)	21.0104	kJ/mol		