Formaldehyde

PC Spartan '04

		Term	ZPE	Enthalpy	Entropy	Cv	% in	
		cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground	IR Int.
1	В2	1337.320	7.9989	0.0252	0.0977	0.5471	99.84	4.91
2	В1	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	В1	3233.279	19.3393	0.0000	0.0000	0.0003	100.00	120.49
Т	otal'	Vibrations	76.0804	0.0545	0.2099	1.2502		
	3 4 5 6	2 B1 3 A1 4 A1 5 A1 6 B1	cm-1 1 B2 1337.320 2 B1 1378.502 3 A1 1692.671 4 A1 1915.649 5 A1 3162.230	cm-1 kJ/mol 1 B2 1337.320 7.9989 2 B1 1378.502 8.2453 3 A1 1692.671 10.1244 4 A1 1915.649 11.4581 5 A1 3162.230 18.9143 6 B1 3233.279 19.3393	cm-1 kJ/mol kJ/mol B2 1337.320 7.9989 0.0252 B1 1378.502 8.2453 0.0213 A1 1692.671 10.1244 0.0057 A1 1915.649 11.4581 0.0022 A1 3162.230 18.9143 0.0000 B1 3233.279 19.3393 0.0000	cm-1 kJ/mol kJ/mol J/mol.K 1 B2 1337.320 7.9989 0.0252 0.0977 2 B1 1378.502 8.2453 0.0213 0.0822 3 A1 1692.671 10.1244 0.0057 0.0216 4 A1 1915.649 11.4581 0.0022 0.0082 5 A1 3162.230 18.9143 0.0000 0.0000 6 B1 3233.279 19.3393 0.0000 0.0000	cm-1 kJ/mol kJ/mol J/mol.K J/mol.K B2 1337.320 7.9989 0.0252 0.0977 0.5471 B1 1378.502 8.2453 0.0213 0.0822 0.4763 A1 1692.671 10.1244 0.0057 0.0216 0.1574 A1 1915.649 11.4581 0.0022 0.0082 0.0687 A1 3162.230 18.9143 0.0000 0.0000 0.0005 B1 3233.279 19.3393 0.0000 0.0000 0.0003	cm-1 kJ/mol kJ/mol J/mol.K J/mol.K Ground 1 B2 1337.320 7.9989 0.0252 0.0977 0.5471 99.84 2 B1 1378.502 8.2453 0.0213 0.0822 0.4763 99.87 3 A1 1692.671 10.1244 0.0057 0.0216 0.1574 99.97 4 A1 1915.649 11.4581 0.0022 0.0082 0.0687 99.99 5 A1 3162.230 18.9143 0.0000 0.0000 0.0005 100.00 6 B1 3233.279 19.3393 0.0000 0.0000 0.0003 100.00

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

Vibrational Enthalpy: =
$$\frac{\text{Nhv}_0 \text{ e}^{-\text{hv}_0/\text{kT}}}{1 - \text{e}^{-\text{hv}_0/\text{kT}}}$$

for each vibration

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

Vibrational Entropy: =-R $ln(1-e^{-h\nu_0/kT}) + \frac{U - U(0)_{vib}}{T}$

=-R
$$ln(1-e^{-h\nu_{o}/kT}) + \frac{Nh\nu_{o} e^{-h\nu_{o}/kT}}{T (1-e^{-h\nu_{o}/kT})}$$

for each vibration

Ideal Gas

2.4789 kJ/mol

add RT = 2.4789 kJ/mol, to give Δ H.

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

12.4716

Rotation

3.7184 66.7678

Rotational Enthalpy: $3.7184 \text{ kJ/mol} = \mathbf{RT or 3/2RT}$

Rotational Entropy: 66.7678 J/mol.K

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

$$= R \ln \frac{\pi^{1/2}}{\sigma} \left(\frac{kT}{\tilde{A}hc}\right)^{1/2} \left(\frac{kT}{\tilde{B}hc}\right)^{1/2} \left(\frac{kT}{\tilde{C}hc}\right)^{1/2} + \frac{3}{2}R \qquad \text{for nonlinear}$$
Totals 86.0507 218.1462 26.1935 kJ/mol

Gibb's Free Energy (H - TS) 21.0104 kJ/mol