

Formaldehyde HF/3-21G(*)

SCF total energy: -113.2218201 hartrees $2\text{H}^+ + \text{C}^{6+} + \text{O}^{8+} + 16\text{e}^- \rightarrow \text{H}_2\text{C}=\text{O}$

PC Spartan '04

	Term	ZPE	Enthalpy	Entropy	Cv	% in	
	cm-1	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground	IR Int.
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1	B2	1337.320	7.9989	0.0252	0.0977	99.84	4.91
2	B1	1378.502	8.2453	0.0213	0.0822	99.87	20.12
3	A1	1692.671	10.1244	0.0057	0.0216	99.97	15.89
4	A1	1915.649	11.4581	0.0022	0.0082	99.99	69.43
5	A1	3162.230	18.9143	0.0000	0.0000	100.00	21.63
6	B1	3233.279	19.3393	0.0000	0.0000	100.00	120.49
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Total Vibrations		76.0804	0.0545	0.2099	1.2502		
Ideal Gas			2.4789				
Translation			3.7184	151.1685	12.4716		
Rotation			3.7184	66.7678	12.4716		
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Totals			86.0507	218.1462	26.1935		
Gibb's Free Energy (H - TS)			21.0104				

Atomic Energies in Hartrees (au)

Atom	HF/3-21G(*)	B3LYP/6-311G*	B3LYP/6-311+G**
H	-0.496199	-0.5021559	-0.5021559
C	-37.4810698	-37.8559888	-37.8572669
N	-54.1053904	-54.5985435	-54.6007232
O	-74.3936572	-75.0853748	-75.0898713

Use $\text{H}_2\text{C}=\text{O} \rightarrow 2\text{H} + \text{C} + \text{O}$ to get D_e and the spectroscopic D_0 after ZPE correction

For $2\text{H} + \text{C} + \text{O} \rightarrow \text{H}_2\text{C}=\text{O}$ get $-D_e$ and then $-D_0 = \Delta_r G^\ominus(0)$ after ZPE correction:

SCF energy = $-113.2218201 - 2*(-0.496199) + -37.4810698 + -74.3936572 = -0.3546951$ H = -931.252 kJ/mol
 $= -D_e$

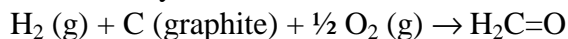
$\Delta_r G^\ominus(0) = -931.252 \text{ kJ/mol} + 76.0804 \text{ kJ/mol} = -855.17 \text{ kJ/mol}$ zero point energy correction

$\Delta_r G^\ominus(298.15\text{K}) = -931.252 \text{ kJ/mol} + 21.0104 \text{ kJ/mol} = -910.24 \text{ kJ/mol}$ (i.e. 35% error)

Literature value from experimental thermodynamics tables: $\Delta_r G^\ominus = -1412.02 \text{ kJ/mol}$

(Incidentally $\Delta_r G^\ominus$ at B3LYP/6-311+G** = -1528.84 kJ/mol or 8% error)

To get the thermodynamic $\Delta_r H^\ominus$ and $\Delta_r G^\ominus$:



you need to do calculations at the same level for H_2 and O_2 . However, accurate values for C (graphite) can't be determined from MO calculations, so comparable values aren't available. The corresponding value for C (graphite) can only be approximated from experimental values. Then you would combine



with $\text{H}_2(\text{g}) + \text{C}(\text{graphite}) + \frac{1}{2}\text{O}_2(\text{g}) \rightarrow 2\text{H} + \text{C} + \text{O}$