Example: Find Heat of Reaction at a Different Temperature

C_p approach

Wanted: Heat of Rxn at 1200 C T= 1200 C

CO + 1/2 O2 ==> CO2

DelH_c= -282.99 kJ/gmol at 25 C

Heat capacities

	a	b	c	d	T	form	DelH_f	Stoich Coeff
CO	2.90E-02	4.11E-06	3.55E-09	-2.22E-12	C	1	-110.52	-1
O2	2.91E-02	1.16E-05	-6.08E-09	1.31E-12	C	1	0	-0.5
CO2	3.61E-02	4.23E-05	-2.89E-08	7.46E-12	C	1	-393.5	1

Basis: 1 gmol of CO

Integrate heat capacities for reactants $\int_{1200}^{25} C_p dT$			**moles**	**n_i * Int Cp**
CO	-3.79E+01	kJ/mol	1	-3.79E+01
O2	-3.97E+01	kJ/mol	0.5	-1.99E+01

Integrate heat capacities for products $\int_{25}^{1200} C_p dT$				
CO2	6.01E+01	kJ/mol	1	6.01E+01

$$\Delta H_{rxn} = \left(\sum n_i \int_{1200}^{25} C_p dT\right)_{reactants} + \Delta H_{rxn,25\,C} + \left(\sum n_i \int_{25}^{1200} C_p dT\right)_{prod}$$

Delta H = -2.81E+02

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Heat capacities

	a	b	c	d	T	form	DelH_f	Stoich Coe	Moles
CO	2.90E-02	4.11E-06	3.55E-09	-2.22E-12	C	1	-110.52	-1	-1
O2	2.91E-02	1.16E-05	-6.08E-09	1.31E-12	C	1	0	-0.5	-0.5
CO2	3.61E-02	4.23E-05	-2.89E-08	7.46E-12	C	1	-393.5	1	1

DelH at 1200 C

Alternate Approach:

Calculate H of products vs. H of reactants

	H at 1200 C	
CO	-72.65	kJ/gmol
O2	39.71	kJ/gmol
CO2	-333.37	kJ/gmol

$$\hat{H}_i = \Delta\hat{H}_{i,f}^{\square\,o} + \int_{T_{ref}}^{T} \hat{C}_p dT$$

$$\Delta\hat{H}_{rxn}^{\square\,\square} = \sum n\hat{H}_i$$

DelH_r at 1200 C = -280.566 kJ/gmol

Example: Find Heat of Reaction at a Different Temperature

ΔC_p approach

Wanted: Heat of Rxn at 1200 C

CO + 1/2 O2 ==> CO2

DelH_c=	-282.99	kJ/gmol	at	25	C						
Heat capacities											
	a	b	c	d	T	form	DelH_f	Stoich Coeff			
CO	2.90E-02	4.11E-06	3.55E-09	-2.22E-12	C	1	-110.52	-1			
O2	2.91E-02	1.16E-05	-6.08E-09	1.31E-12	C	1	0	-0.5			
CO2	3.61E-02	4.23E-05	-2.89E-08	7.46E-12	C	1	-393.5	1			

$$\Delta C_p = a' + b'T + c'T^2 + d'T^3$$

$$a' = \sum \nu_i a_i,\ b' = \sum \nu_i b_i,\quad \text{etc.}$$

Del Cp =	**sum(vi*ai)**	**sum(vi*bi)**	**etc.**								
	a'	**b'**	**c'**	**d'**							
Del Cp =	-7.39E-03	3.24E-05	-2.94E-08	9.03E-12							
DelHr at 25 C=		-282.98									
Basis: 1 gmol of CO											
DelH at	1200	C	-280.57	kJ/gmol							
			exothermic								

$$\Delta H_T = \Delta H_{r,25\,C} + \int_{25\,C}^{T} \Delta C_p dT$$

$$= \Delta H_{r,25\,C} + a'(T-25) + \frac{b'}{2}(T^2 - 25^2) + \frac{c'}{3}(T^3 - 25^3) + \frac{d'}{4}(T^4 - 25^4)$$