Example: Find Heat of Reaction at a Different Temperature

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
Del Cp =	-7.39E-03	3.24E-05	-2.94E-08	9.03E-12				

$$\nabla C_p = a'T + b'T^2 + c'T^3 + d'T^4 \qquad a' = \sum \nu_i a_i,\ b' = \sum \nu_i b_i,\ \text{etc.}$$

Basis: 1 gmol of CO

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

DelH at 1200 C -280.58 kJ/gmol

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

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

DelH_r at 1200 C = -280.57 kJ/gmol

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