

Example: Find Heat of Reaction at a Different Temperature

Wanted: Heat of Rxn at 1200 C



DelH_c= -282.99 kJ/gmol at 25 C

Heat capacities

	a	b	c	d	T	form	DelH _f	Stoich Coef
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

$$\nabla C_p = a'T + b'T^2 + c'T^3 + d'T^4$$

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

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

Basis: 1 gmol of CO

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

DelH at 1200 C -280.58 kJ/gmol

ff

25⁴)

Example: Find Heat of Reaction at a Different Temperature

Wanted: Heat of Rxn at 1200 C
 $\text{CO} + 1/2 \text{O}_2 \Rightarrow \text{CO}_2$

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 = $\sum(v_i \cdot a_i) + \sum(v_i \cdot b_i) \cdot T$ etc.

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

Basis: 1 gmol of CO

DelH = DelH_r (at 25 C) + Integral (Del Cp dT)

DelH = DelH_r(at 25 C) + a*DelT + b*(T²-T¹²) + etc.

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

$$\Delta \hat{H}_{rxn} = \sum v_i \hat{H}_i$$