Temperature Dependence of Reacton Enthalpy, $\Delta_r H$

$$\begin{array}{llcl}
T_1: & R & \xrightarrow{\Delta_r H_{T_1}} & P \\
 & \uparrow & & | \\
 & C_p^{re}(T_1 - T_2) & & C_p^{pr}(T_2 - T_1) \\
 & | & & \downarrow \\
T_2: & R & \xrightarrow{\Delta_r H_{T_2}} & P
\end{array}$$

it doesn't matter how you get there!

$$\Delta_r H_{T_2} = C_p^{re}(T_1 - T_2) + \Delta_r H_{T_1} + C_p^{pr}(T_2 - T_1)$$

$$\Delta_r H_{T_2} = \Delta_r H_{T_1} + (C_p^{pr} - C_p^{re})(T_2 - T_1)$$

$$\Delta_r H_{T_2} - \Delta_r H_{T_1} = \Delta_r C_p \, \Delta T \qquad \Delta_r C_p = C_p^{pr} - C_p^{re}$$

$d\Delta_r H = \Delta_r C_p \, dT$ Kirchhoff's Law 1858

In general $A + B \rightarrow C + D$ $\quad \Delta_r H = H_C + H_D - H_A - H_B$

$$\left(\frac{\partial \Delta_r H}{\partial T}\right)_P = \left(\frac{\partial H_C}{\partial T}\right)_P + \left(\frac{\partial H_D}{\partial T}\right)_P - \left(\frac{\partial H_A}{\partial T}\right)_P - \left(\frac{\partial H_B}{\partial T}\right)_P$$

$$\left(\frac{\partial \Delta_r H}{\partial T}\right)_P = C_p(C) + C_p(D) - C_p(A) - C_p(B) = \Delta_r C_p$$

$C_p(A) = a(A) + b(A)T + c(A)T^2 \qquad C_p(B) = a(B) + b(B)T + c(B)T^2$

for the reaction:

$$\Delta_r C_p = (a(C)+a(D) - a(A) - a(B)) + (b(C) + b(D) - b(A) - b(B))T + (c(C) + c(D) - c(A) - c(B))T^2$$

set $\Delta a = a(C)+a(D) - a(A) - a(B)$ etc.

$$\Delta_r C_P = \Delta a + \Delta b T + \Delta c T^2$$

$$d\Delta_r H = \Delta_r C_p dT = (\Delta a + \Delta b T + \Delta c T^2) dT$$

$$\Delta_r H_{T_2} - \Delta_r H_{T_1} = \int_{T_1}^{T_2} (\Delta a + \Delta b T + \Delta b T^2)\, dT$$

$$\Delta_r H_{T_2} = \Delta_r H_{T_1} + \Delta a(T_2 - T_1) + \frac{\Delta b}{2}(T_2^2 - T_1^2) + \frac{\Delta c}{3}(T_2^3 - T_1^3)$$

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or let $T_1 \rightarrow 0$ and set $T_2 = T$: $\qquad \Delta_r H_T = \Delta_r H_o + \Delta a T + \dfrac{\Delta b}{2} T^2 + \dfrac{\Delta c}{3} T^3$

C_p(rxn)	C_p (NH3)	C_p (H2)	C_p(N2)	
-31.205	25.89	29.07	26.98	T
0.0308795	3.26E-02	-8.37E-04	5.91E-03	$T^2/2$
-5.8952E-06	-3.05E-06	2.01E-06	-3.38E-07	$T^3/3$

H_f^0(298) -4.61E+04 0.00E+00 0.00E+00 Joules

I(Cp(T)dT	H(NH3)	H(H2)	H(N2)
1000	4.117E+04	2.932E+04	2.982E+04
350	1.101E+04	1.015E+04	9.800E+03
298	9.135E+03	8.643E+03	8.300E+03
Delta(1000-298)	3.203E+04	2.068E+04	2.152E+04

	∫(Cp)dt	H_{rxn}
$N_2+3H_2=2NH_3$	-1.950E+04	-1.117E+05
per mole of NH_3	-9.748E+03	-5.586E+04

C_p Correction

Textbook= -9.753 -5.59E+04

-21905.91 14068.6384 -1912.87264

-9750.1442

H_{rxn} -5.59E+04 Joules

-55.86 kJ