

CADET \_\_\_\_\_ SECTION \_\_\_\_\_ TIME OF DEPARTURE \_\_\_\_\_

## DEPARTMENT OF CHEMISTRY &amp; LIFE SCIENCE

CH365 2022-2023

WRITTEN PARTIAL REVIEW II

12 October 2022, A-Hour

TEXT: Smith, Van Ness, Abbott &amp; Swihart

SCOPE: Lessons 10-20

TIME: 55 Minutes

References Permitted: Open notes, book, internet, CHEMCAD, Mathematica, Excel.

**INSTRUCTIONS**

1. Do not mark this exam or open it until “begin work” is given.
2. You have 55 minutes to complete the exam.
3. Solve the problems in the space provided. Show all work to receive full credit.
4. There are 3 problems on 4 pages in this exam (not including the cover page). Write your name on the top of each sheet.
5. Save CHEMCAD and Mathematica files on your desktop and re-save frequently.
6. Upload all CHEMCAD and Mathematica files to your SharePoint directory.
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(TOTAL WEIGHT: 200 POINTS)

DO NOT WRITE IN THIS SPACE

PROBLEM	VALUE	CUT
A	80	
B	70	
C	50	
TOTAL CUT		
TOTAL GRADE	200	

Problem:    Weight:  
A                      80

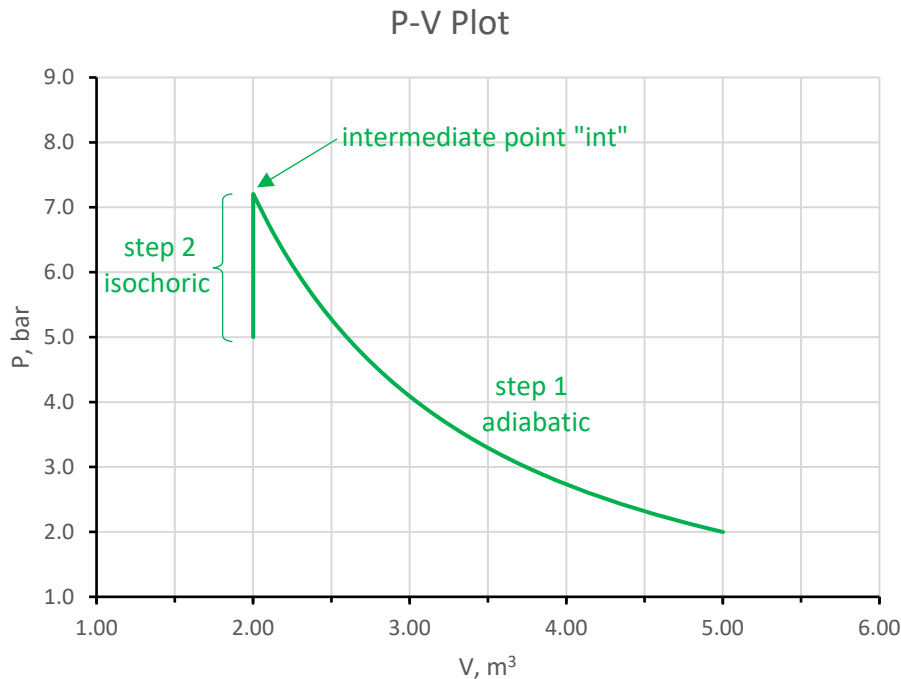
0.200 kmol of an ideal gas in a closed system is changed from an initial state of 5.0 m<sup>3</sup>, 2.0 bar and 721.7 K to a final state of 2.0 m<sup>3</sup>, 5.0 bar, and 721.7 K by a two-step process consisting of an adiabatic compression followed by cooling at constant volume. (a) Sketch the process path in the PV axes below. (b) Calculate Q, W, ΔU and ΔH for the overall process in units of kJ. (c) Calculate the intermediate temperature after step 1.

$$R = 8.314 \text{ J/(mol} \cdot \text{K)} = 0.08314 \text{ (bar} \cdot \text{m}^3\text{)/(kmol} \cdot \text{K)}$$

$$C_P = (7/2) \cdot R, \text{ and}$$

$$C_V = (5/2) \cdot R$$

**Solution, part (a):**



**Solution, part (b):**

The overall process is isothermal ( $T_2=T_1$ ), so  $\Delta H_{\text{Overall}} = \Delta U_{\text{Overall}} = 0 \text{ kJ}$   
ANS

Equation 3.23c gives the P-V relation for an adiabatic process. Let the intermediate state be denoted with subscript “int” with  $V_{\text{int}} = V_2$  since the second step is at constant volume.

Also  $\gamma = C_P/C_V = (7R/2)/(5R/2) = 1.4$  from equation 3.24:

Solve for intermediate pressure,  $P_{\text{int}}$ :

$$P_{\text{int}} = P_1 \left( \frac{V_1}{V_{\text{int}}} \right)^\gamma = 2.0 \text{ bar} \cdot \left( \frac{5.0 \text{ m}^3}{2.0 \text{ m}^3} \right)^{1.4} = 7.213 \text{ bar}$$

Once  $P_{\text{int}}$  is known, the adiabatic work for step 1 is given by equation 3.26:

$$W_{\text{Step1}} = \frac{P_{\text{int}} \cdot V_{\text{int}} - P_1 \cdot V_1}{\gamma - 1} = \frac{7.213 \text{ bar} \cdot 2.0 \text{ m}^3 - 2.0 \text{ bar} \cdot 5.0 \text{ m}^3}{1.4 - 1} = 11.067 \text{ bar} \cdot \text{m}^3$$

Step 2 is at constant volume, so work is zero since  $\Delta V = 0$ :

$$W_{\text{Step2}} = -P \cdot \Delta V = 0.$$

The total overall work is the sum of the work of each step:

$$W_{\text{Overall}} = W_{\text{Step1}} + W_{\text{Step2}} = 11.067 \text{ bar} \cdot \text{m}^3 + 0 \text{ bar} \cdot \text{m}^3 = 11.067 \text{ bar} \cdot \text{m}^3$$

Now convert the units to kJ:

$$W_{\text{Overall}} = 11.067 \text{ bar} \cdot \text{m}^3 \left( \frac{1 \text{ J}}{10^{-5} \text{ bar} \cdot \text{m}^3} \right) \cdot \left( \frac{1 \text{ kJ}}{1000 \text{ J}} \right) = \underline{\underline{1106.7 \text{ kJ}}}_{\text{ANS}}$$

Finally, for Q:

$$\Delta U_{\text{Overall}} = Q_{\text{Overall}} + W_{\text{Overall}} = 0 \Rightarrow Q_{\text{Overall}} = -W_{\text{Overall}} = \underline{\underline{-1106.7 \text{ kJ}}}_{\text{ANS}}$$

**Solution, part (c):**

Let “int” designate the intermediate state, so  $P_{\text{int}} = 7.213 \text{ bar}$  and  $V_{\text{int}} = V_2 = 2 \text{ m}^3$ :

$$PV = nRT \Rightarrow T_{\text{int}} = \frac{P_{\text{int}} \cdot V_3}{n \cdot R} = \frac{7.213 \text{ bar} \cdot 2.0 \text{ m}^3}{0.200 \text{ kmol} \cdot \left( 0.08314 \frac{\text{bar} \cdot \text{m}^3}{\text{kmol} \cdot \text{K}} \right)} = \underline{\underline{867.6 \text{ K}}}_{\text{ANS}}$$

Problem:    Weight:  
B                      70

An engineering plan for a vinyl chloride plant includes a pipeline carrying chlorine (Cl<sub>2</sub>) at a volumetric flow rate of 3.402 MMSCFD (million standard cubic feet per day). Standard conditions are 60°F and 1.00 atm.

Use the Peng-Robinson (PR) equation of state, Table 3.1, and gas constant  $R = 10.73 \text{ ft}^3 \cdot \text{psia}/(\text{lbmol} \cdot \text{R})$  to determine the molar flow rate of Cl<sub>2</sub> in lbmol/d.

**Solution:**

```

In[2]:= P = 14.696; (*psia*)
T = 60 + 459.67; (*convert degrees F to 519.67 Rankine*)
R = 10.73; (* ft^3*psia / (lbmol*R), given*)
ω = 0.069; (*App. B, p.665*)
Tc = 417.2 * 1.8; (*p.665, convert K to R*)
Pc = 77.10 * 14.5038; (*p. 665 convert bar to psia, App A*)
Tr1 = T / Tc; (*reduced temperature*)

In[9]:= σ = 1 + √2; (*Table 3.1, p.100*)
ε = 1 - √2;
Ω = 0.07780;
ϖ = 0.45724;
α = (1 + (0.37464 + 1.54226 * ω - 0.26992 * ω^2) * (1 - √Tr1))^2;
a = ϖ * (α * R^2 * Tc^2) / Pc; (*eq.3.45, p.98*)
b = Ω * (R * Tc) / Pc; (*eq.3.44, p.98*)

In[16]:= eq1 = P == (R * T) / (V - b) - (a) / ((V + ε * b) * (V + σ * b)); (*eq.3.41 p.97*)

In[17]:= ans = Quiet[Solve[eq1, V]]
Out[17]= {{V → 0.762119123451}, {V → 3.72668886255}, {V → 374.377576912}}

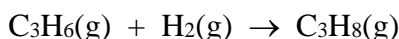
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Use V and molar flow rate to solve for volumetric flow rate (V<sup>t</sup>):

$$\frac{3.402 \times 10^6 \text{ ft}^3}{\text{day}} \cdot \frac{1 \text{ lbmol}}{374.378 \text{ ft}^3} = \underline{\underline{9,087 \frac{\text{lbmol}}{\text{day}}}} \quad \text{ANS}$$

Problem: Weight:  
C 50

Hydrogenation refers to the treatment of substances with hydrogen, H<sub>2</sub>. Hydrogenation is important in the petrochemical and food processing industries. For example, hydrogenation of polyunsaturated fatty acids in vegetable oils reduces most of the carbon-carbon double bonds, making the oil safer and healthier for consumption. Hydrogenation reactions of hydrocarbons typically involve the reaction of alkenes with hydrogen to form alkanes at high temperatures and pressures, usually over a supported metal catalyst such as Raney nickel. Steam is often used as a diluent to control the temperature in the reactor. In this problem, you will consider the hydrogenation of propylene to form propane:



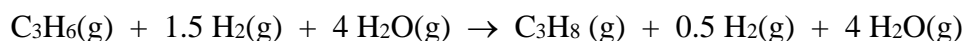
Calculate the standard gas-phase heat of hydrogenation of propylene at 435 °C and 1.00 bar in 50% excess hydrogen, with 4.00 moles of steam added per mole of propylene as a diluent to control the reactor temperature. The process is isothermal with reactants and products at 435 °C.

The following table contains ideal gas heat capacity polynomial coefficients and standard heats of formation at 298 K from Appendix C:

species	a	b×10 <sup>3</sup>	c×10 <sup>6</sup>	d×10 <sup>-5</sup>	ΔH <sub>f,298</sub> <sup>0</sup> , J/mol
C <sub>3</sub> H <sub>6</sub>	1.637	22.706	-6.915	0.000	19,710
H <sub>2</sub>	3.249	0.422	0.000	0.083	0
H <sub>2</sub> O	3.470	1.450	0.000	0.121	-241,818
C <sub>3</sub> H <sub>8</sub>	1.213	28.785	-8.824	0.000	-104,680

**Solution:**

Balanced Reaction:



Solution in Mathematica is shown on the following page.

Mathematica Solution:

```

In[1]:= (*Stoichiometric coefficients*)
(*Propylene, hydrogen, water, ethane, hydrogen, water*)
v = {-1, -1.5, -4, 1, .5, 4};

In[2]:= (*Standard Heats of Formation*)
ΔHf298 = {19 710, 0, -241 818, -104 680, 0, -241 818};

In[3]:= (*Heat of Reaction at 298 K*)
ΔH298 = Plus @@ (v * ΔHf298) (*J/mol*)

Out[3]= -124 390.

In[4]:= (*Heat Capacity polynomial coefficients, Table C.1:*)
a = {1.637, 3.249, 3.470, 1.213, 3.249, 3.470};
b = {22.706, 0.422, 1.450, 28.785, 0.422, 1.450} * 10-3;
c = {-6.915, 0.000, 0.000, -8.824, 0.000, 0.000} * 10-6;
d = {0.000, 0.083, 0.121, 0.000, 0.083, 0.121} * 105;

In[8]:= Δa = Plus @@ (v * a);
Δb = Plus @@ (v * b);
Δc = Plus @@ (v * c);
Δd = Plus @@ (v * d);

In[12]:= (*Temperatures, K*)
T = 435 + 273.15; (*708.15 K*)
T0 = 298.15;

In[14]:= (*Gas constant*)
R = 8.314; (* $\frac{\text{J}}{\text{mol}\cdot\text{K}}$ *)

In[15]:= (*Equation 4.21 for MCPH*)
MDCPH = Δa +  $\frac{\Delta b}{2} * (T + T0) + \frac{\Delta c}{3} * (T^2 + T0^2 + T * T0) + \frac{\Delta d}{T * T0}$ 

Out[15]= -1.3760160059

In[16]:= (*Equation 4.22 for corrected heat of reaction*)
(*Gives molar heat of reaction in J/mol*)
ΔH708 = ΔH298 + MDCPH * R * (T - T0)

Out[16]= -129 080.4808
          ANS

```

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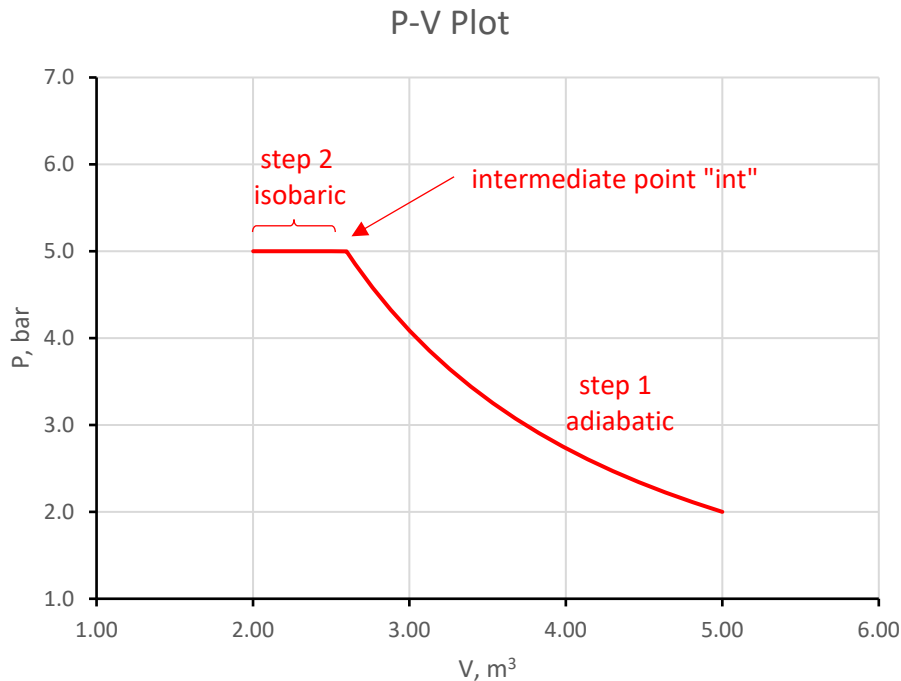
0.400 kmol of an ideal gas in a closed system is changed from an initial state of 5.0 m<sup>3</sup>, 2.0 bar and 300.7 K to a final state of 2.0 m<sup>3</sup>, 5.0 bar, and 300.7 K by a two-step process consisting of an adiabatic compression followed by cooling at constant pressure. (a) Sketch the process path in the PV axes below. (b) Calculate Q, W, ΔU and ΔH for the overall process in units of kJ. (c) Calculate the intermediate temperature after step 1.

$$R = 8.314 \text{ J/(mol} \cdot \text{K)} = 0.08314 \text{ (bar} \cdot \text{m}^3\text{)/(kmol} \cdot \text{K)}$$

$$C_P = (7/2) \cdot R, \text{ and}$$

$$C_V = (5/2) \cdot R$$

**Solution, part (a):**



**Solution, part (b):**

The overall process is isothermal ( $T_2 = T_1$ ), so  $\Delta H_{\text{Overall}} = \Delta U_{\text{Overall}} = 0 \text{ kJ}$   
ANS

Equation 3.23c gives the P-V relation for an adiabatic process. Let the intermediate state be denoted with subscript “int” with  $P_{\text{int}} = P_2$  since the second step is at constant pressure.

Also  $\gamma = C_P/C_V = (7R/2)/(5R/2) = 1.4$  from equation 3.24:



Solve for intermediate volume,  $V_{\text{int}}$ :

$$PV^\gamma = \text{constant} \Rightarrow P_1 V_1^\gamma = P_{\text{int}} V_{\text{int}}^\gamma \Rightarrow V_{\text{int}} = V_1 \left( \frac{P_1}{P_{\text{int}}} \right)^{-1/\gamma} = 8.0 \text{ m}^3 \cdot \left( \frac{5.0 \text{ bar}}{2.0 \text{ bar}} \right)^{-1/1.4} = 2.599 \text{ m}^3$$

Once  $V_{\text{int}}$  is known, adiabatic work for step 1 is given by equation 3.26:

$$W_{\text{Step1}} = \frac{P_{\text{int}} V_{\text{int}} - P_1 V_1}{\gamma - 1} = \frac{2.0 \text{ bar} \cdot 2.599 \text{ m}^3 - 2.0 \text{ bar} \cdot 5.0 \text{ m}^3}{1.4 - 1} = 7.482 \text{ bar} \cdot \text{m}^3$$

Since step 2 is at constant pressure,  $W_{\text{Step2}} = -P\Delta V$ :

$$W_{\text{Step2}} = -P\Delta V = -5.0 \text{ bar} \cdot (2.0 \text{ m}^3 - 2.599 \text{ m}^3) = 2.993 \text{ bar} \cdot \text{m}^3.$$

The total overall work is the sum of the work of each step:

$$W_{\text{Overall}} = W_{\text{Step1}} + W_{\text{Step2}} = 7.482 \text{ bar} \cdot \text{m}^3 + 2.993 \text{ bar} \cdot \text{m}^3 = 10.474 \text{ bar} \cdot \text{m}^3$$

Now convert the units to kJ:

$$W_{\text{Overall}} = 10.474 \text{ bar} \cdot \text{m}^3 \left( \frac{1 \text{ J}}{10^{-5} \text{ bar} \cdot \text{m}^3} \right) \cdot \left( \frac{1 \text{ kJ}}{1000 \text{ J}} \right) = \underline{\underline{1047.4 \text{ kJ}}}_{\text{ANS}}$$

Finally, for Q:

$$\Delta U_{\text{Overall}} = Q_{\text{Overall}} + W_{\text{Overall}} = 0 \Rightarrow Q_{\text{Overall}} = -W_{\text{Overall}} = \underline{\underline{-1047.4 \text{ kJ}}}_{\text{ANS}}$$

**Solution, part (c):**

$$PV = nRT \Rightarrow T_{\text{int}} = \frac{P_{\text{int}} \cdot V_{\text{int}}}{n \cdot R} = \frac{5.0 \text{ bar} \cdot 2.599 \text{ m}^3}{0.400 \text{ kmol} \cdot \left( 0.08314 \frac{\text{bar} \cdot \text{m}^3}{\text{kmol} \cdot \text{K}} \right)} = \underline{\underline{390.8 \text{ K}}}_{\text{ANS}}$$

Problem:    Weight:  
B                      70

An engineering plan for a vinyl chloride plant includes a pipeline carrying ethylene (C<sub>2</sub>H<sub>4</sub>) at a volumetric flow rate of 7.530 MMSCFD (million standard cubic feet per day). Standard conditions are 60°F and 1.00 atm.

Use the Peng-Robinson (PR) equation of state, Table 3.1, and gas constant R = 10.73 ft<sup>3</sup>·psia/(lbmol·R) to determine the molar flow rate of C<sub>2</sub>H<sub>4</sub> in lbmol/d.

**Solution:**

```
In[1]:= P = 14.696; (*psia*)
      T = 60 + 459.67; (*convert degrees F to 519.67 Rankine*)
      R = 10.73; (* ft^3*psia / (lbmol*R), given*)
      ω = 0.087; (*App. B, p.665*)
      Tc = 282.3 * 1.8; (*p.665, convert K to R*)
      Pc = 50.40 * 14.5038; (*p. 665 convert bar to psia, App A*)
      Tr1 = T / Tc; (*reduced temperature*)
```

```
In[8]:= σ = 1 + √2; (*Table 3.1, p.100*)
      ε = 1 - √2;
      Ω = 0.07780;
      Ξ = 0.45724;
      α = (1 + (.37464 + 1.54226 * ω - .26992 * ω^2) * (1 - Tr1^(1/2)));
      a = Ξ * (α * R^2 * Tc^2) / Pc; (*eq.3.45, p.98*)
      b = Ω * (R * Tc) / Pc; (*eq.3.44, p.98*)
```

```
In[15]:= eq1 = P == (R * T) / (V - b) - a / ((V + ε * b) * (V + σ * b)); (*eq.3.41, p.97*)
```

```
In[16]:= ans = Quiet[Solve[eq1, V, Reals]]
```

```
Out[16]= {{V -> 376.68277418}}
```

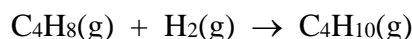
Use V and molar flow rate to solve for volumetric flow rate (V<sup>l</sup>):

$$\frac{7.530 \times 10^6 \text{ ft}^3}{\text{day}} \cdot \frac{1 \text{ lbmol}}{376.683 \text{ ft}^3} = 19,990.3 \frac{\text{lbmol}}{\text{day}}$$

ANS

Problem: Weight:  
C 50

Hydrogenation refers to the treatment of substances with hydrogen, H<sub>2</sub>. Hydrogenation is important in the petrochemical and food processing industries. For example, hydrogenation of polyunsaturated fatty acids in vegetable oils reduces most of the carbon-carbon double bonds, making the oil safer and healthier for consumption. Hydrogenation reactions of hydrocarbons typically involve the reaction of alkenes with hydrogen to form alkanes at high temperatures and pressures, usually over a supported metal catalyst such as Raney nickel. Steam is often used as a diluent to control the temperature in the reactor. In this problem, you will consider the hydrogenation of 1-butene to form n-butane:



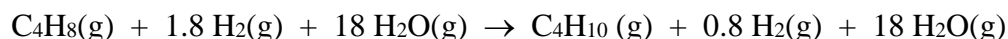
Calculate the standard gas-phase heat of hydrogenation of 1-butene at 575 °C and 12.00 bar in 80% excess hydrogen, with 18.00 moles of steam added per mole of propylene as a diluent to control the reactor temperature. The process is isothermal with reactants and products at 575 °C.

The following table contains ideal gas heat capacity polynomial coefficients and standard heats of formation at 298 K from Appendix C:

species	a	b×10 <sup>3</sup>	c×10 <sup>6</sup>	d×10 <sup>-5</sup>	ΔH <sub>f,298</sub> <sup>0</sup> , J/mol
C <sub>4</sub> H <sub>8</sub>	1.967	31.630	-9.873	0.000	-540
H <sub>2</sub>	3.249	0.422	0.000	0.083	0
H <sub>2</sub> O	3.470	1.450	0.000	0.121	-241,818
C <sub>4</sub> H <sub>10</sub>	1.935	36.915	-11.402	0.000	-125,790

**Solution:**

Balanced Reaction:



Solution in Mathematica is shown on the following page.

Mathematica Solution:

```

(*Stoichiometric coefficients*)
(*1-butene, hydrogen, water, butane, hydrogen, water*)
v = {-1, -1.8, -18, 1, .8, 18};

In[ ]:= (*Standard Heats of Formation*)
ΔHf298 = {-540, 0, -241818, -125790, 0, -241818};

In[ ]:= (*Heat of Reaction at 298 K*)
ΔH298 = Plus @@ (v * ΔHf298) (*J/mol*)

Out[ ]:= -125250.

In[ ]:= (*Heat Capacity polynomial coefficients, Table C.1:*)
a = {1.967, 3.249, 3.470, 1.935, 3.249, 3.470};
b = {31.630, 0.422, 1.450, 36.915, 0.422, 1.450} * 10-3;
c = {-9.873, 0.000, 0.000, -11.402, 0.000, 0.000} * 10-6;
d = {0.000, 0.083, 0.121, 0.000, 0.083, 0.121} * 105;

In[ ]:= Δa = Plus @@ (v * a);
Δb = Plus @@ (v * b);
Δc = Plus @@ (v * c);
Δd = Plus @@ (v * d);

In[ ]:= (*Temperatures, K*)
T = 575 + 273.15;
T0 = 298.15;

In[ ]:= (*Gas constant*)
R = 8.314; (*  $\frac{\text{J}}{\text{mol}\cdot\text{K}}$  *)

In[ ]:= (*Equation 4.21 for MCPH*)
MDCPH = Δa +  $\frac{\Delta b}{2} * (T + T0) + \frac{\Delta c}{3} * (T^2 + T0^2 + T * T0) + \frac{\Delta d}{T * T0}$ 

Out[ ]:= -1.06741542321

In[ ]:= (*Equation 4.22 for corrected heat of reaction*)
(*Gives molar heat of reaction in J/mol*)
ΔH848 = ΔH298 + MDCPH * R * (T - T0)

Out[ ]:= -130130.970506
          ANS

```