

Clase 48 18 Noviembre 2020

Título de la nota

18/11/2020

$$M_M = \sum_{i=1}^n M_i y_i$$

$$\overline{C_{PM}} = \sum_{i=1}^n \overline{C_{Pi}} y_i$$

$$\overline{C_{VM}} = \sum_{i=1}^n \overline{C_{Vi}} y_i$$

y_{H_2}	y_{O_2}	(J)	(J)	(J/K)	(J)	(J)	(J)
		ΔU_M	ΔH_M	ΔS_M	q_M	w_M	ΔG_M
0	1	0	0				
0.3	0.7	0	0				
0.5	0.5	0	0				
0.7	0.3	0	0				
1.0	0	0	0				

1 mol de mezcla

$$y_{O_2} = 0.1 \quad y_{H_2} = 0.9$$

$$\Delta G_M = (1 \text{ mol}) (8.314 \text{ J/mol}\cdot\text{K}) (298.15 \text{ K}) (0.1 \ln 0.1 + 0.9 \ln 0.9)$$
$$= (1 \text{ mol}) (8.314 \text{ J/mol}\cdot\text{K}) (298.15 \text{ K}) (-0.23025 - 0.09482)$$

$$\Delta G_M = -805.79 \text{ J}$$

$$\Delta S_M = \frac{-\Delta G_M}{T} = -\left(\frac{-805.79 \text{ J}}{298.15 \text{ K}}\right) = 2.7026 \text{ J/K}$$

$$y_{O_2} = 0.3 \quad y_{H_2} = 0.7$$

$$\Delta G_M = \left[(1 \text{ mol}) (8.314 \text{ J/molK}) (298.15 \text{ K}) (0.3 \ln 0.3 + 0.7 \ln 0.7) \right]$$
$$= \left[(1 \text{ mol}) (8.314 \text{ J/molK}) (298.15 \text{ K}) (-0.3611 - 0.2496) \right]$$

$$\Delta G_M = -1514.04 \text{ J}$$

$$\Delta S_M = \frac{-\Delta G_M}{T} = -\left(\frac{-1514.04 \text{ J}}{298.15 \text{ K}} \right) = 5.07 \text{ J/K}$$

$$y_{O_2} = 0.5 \quad y_{H_2} = 0.5$$

$$\Delta G_M = (1 \text{ mol}) (8.314 \text{ J/mol}\cdot\text{K}) (298.15 \text{ K}) (0.5 \ln 0.5 + 0.5 \ln 0.5)$$
$$= (1 \text{ mol}) (8.314 \text{ J/mol}\cdot\text{K}) (298.15 \text{ K}) (-0.3465 - 0.3465)$$

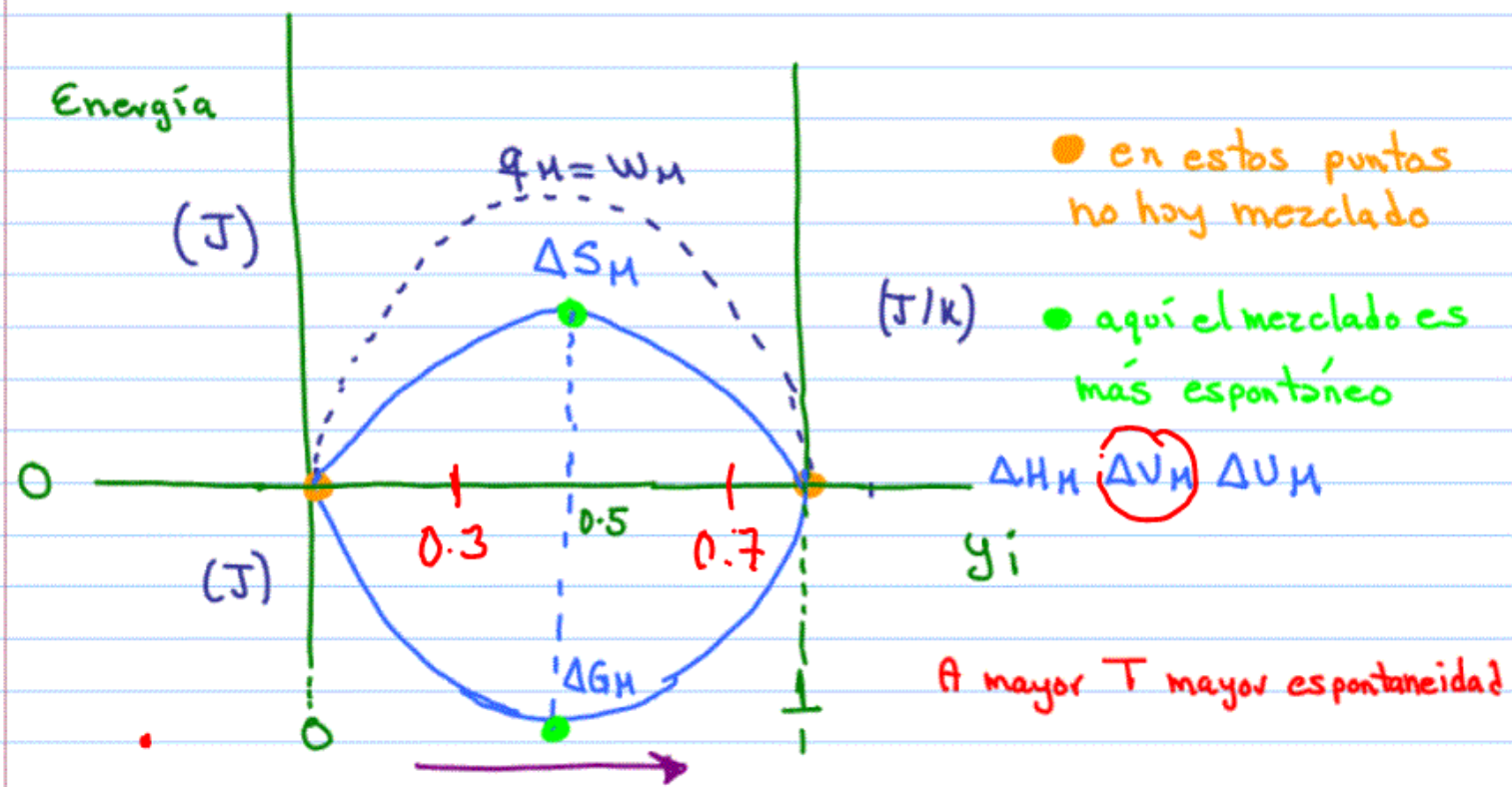
$$\Delta G_M = -1718.18 \text{ J}$$

$$\Delta S_M = \frac{-\Delta G_M}{T} = -\left(\frac{-1718.18 \text{ J}}{298.15 \text{ K}}\right) = 5.76 \text{ J/K}$$

25°C isotérmico (Mezcla de O_2 e H_2) (1 mol total); obtener una gráfica de energía como f(y)

y_{O_2}	y_{H_2}	$\Delta G_M (J)$	$\Delta S_M (J/K)$	
0	1.0	0	0	→ aquí se debe a que no existe mezclado
0.1	0.9	-805.79	2.70	
0.3	0.7	-1514.04	5.07	
0.5	0.5	-1718.18	5.72	→ aquí se espera que sea máximo el valor
0.7	0.3	-1514.04	5.07	
0.9	0.1	-805.79	2.70	
1.0	0.0	0	0	→ aquí se debe a que no existe mezclado

Si se grafica energía vs y_i



$$\Delta V_M = V_{total} - \sum_{i=1}^n V_i$$

$$V_{total} = V_{exp} = 0$$

ideal.

predicciones

Mezclado (I)

$$\Delta H_M = \Delta U_M = 0$$

$$q_M = w_M \quad \Delta S_M = + \quad \Delta G_M = -$$

Comp. Isot. Rev (II)

$$\Delta H_{II} = \Delta U_{II} = 0$$

$$q_{II} = w_{II} = - \quad \Delta S_{II} = - \quad \Delta G_{II} = +$$



$$n_{\text{CH}_4} = \frac{2500 \text{ g}}{16 \text{ g/mol}} = 156.25$$

$$n_{\text{CH}_3\text{CH}_3} = \frac{1500 \text{ g}}{30 \text{ g/mol}} = 50.00$$

$$\underline{206.25}$$

n_{total}

$$y_{\text{CH}_4} = \frac{156.25}{206.25} = 0.7576$$

$$y_{\text{CH}_3\text{CH}_3} = \frac{50}{206.25} = 0.2424$$

$$\begin{aligned}
 V_{\text{total}} &= \frac{n_{\text{total}} R T_{\text{eq}}}{p_{\text{total}}} \\
 &= \frac{(206.25 \text{ mol}) \left(\frac{0.082 \text{ atm L}}{\text{mol K}} \right) (303.15 \text{ K})}{2 \text{ atm}} \\
 &= 2563.51 \text{ L}
 \end{aligned}$$

$$V_{\text{CH}_4} = V_{\text{Total}} y_{\text{CH}_4} = (2563.51 \text{ L})(0.7576) = 1942.05 \text{ L}$$

$$V_{\text{CH}_3\text{CH}_3} = V_{\text{total}} y_{\text{CH}_3\text{CH}_3} = (2563.51 \text{ L})(0.2424) = 621.47 \text{ L}$$



Amagat 2563.51 L

$$p_{\text{CH}_4} = p_{\text{total}} y_{\text{CH}_4} = (2 \text{ atm})(0.7576) = 1.5152 \text{ atm}$$

$$p_{\text{CH}_3\text{CH}_3} = p_{\text{total}} y_{\text{CH}_3\text{CH}_3} = (2 \text{ atm})(0.2424) = 0.4848 \text{ atm}$$

Dalton 2 atm ✓

$$M_M = \sum_{i=1}^n M_i y_i$$

$$= (16 \text{ g/mol})(0.7576) + (30 \text{ g/mol})(0.2424)$$

$$= 19.3939 \text{ g/mol}$$

$$\overline{C_{pH}} = \sum_{i=1}^n \overline{C_{pi}} y_i$$

$$= \overline{C_{pCH_4}} y_{CH_4} + \overline{C_{pCH_3CH_3}} y_{CH_3CH_3}$$

$$= \left(\frac{8.5379 \text{ cal}}{\text{mol K}} \right) (0.7576) + \left(\frac{12.539 \text{ cal}}{\text{mol K}} \right) (0.2424)$$

$$= \frac{9.5079 \text{ cal}}{\text{mol K}}$$

$$C_{VM} = \overline{C_{PM}} - R$$

$$= \frac{9.5079 \text{ cal}}{\text{mol K}} - \frac{1.9886 \text{ cal}}{\text{mol K}}$$

$$= \frac{7.5193 \text{ cal}}{\text{mol K}}$$

$$\Delta H_M = \Delta U_M = 0$$

$$\Delta S_M = - \left[n_{\text{total}} R \sum_{i=1}^n y_i \ln y_i \right]$$

$$= - \left[(206.25 \text{ mol}) \left(\frac{1.9886 \text{ cal}}{\text{mol K}} \right) \left(0.7576 \ln 0.7576 + 0.2424 \ln 0.2424 \right) \right]$$

$$= 227.1529 \frac{\text{cal}}{\text{K}}$$

$$\Delta G_M = \Delta H_M - T\Delta S_M$$

$$= 0 - T\Delta S_M$$

$$= - (303.15\text{K}) \left(227.1529 \frac{\text{cal}}{\text{K}} \right)$$

$$= - 68864.7456 \text{ cal}$$

$$q_M = W_M$$

$$q_M = T \Delta S_M$$

$$= (303.15 \text{ K}) \left(227.1529 \frac{\text{cal}}{\text{K}} \right)$$

$$= 68864.845 \text{ cal.}$$



MEZCLADO DE GASES
Modelo perfecto e ideal

Insertar en las celdas de color amarillo los valores correspondientes Los resultados en las celdas de color verde

Constantes de Cp como función de T (cal/molK)

Gases	a	b	c	d	e	mi (g)	ni (mol)	yi	Mi (g/mol)	pi (atm)	Vi (L)
Metano	8.5379e+0	0.0000e+0	0.0000e+0	0.0000e+00	0.0000e+000	2500.0000	156.2500	0.7576	16.0000	1.5152	1942.0530
Etano	1.2539e+1	0.0000e+0	0.0000e+0	0.0000e+00	0.0000e+000	1500.0000	50.0000	0.2424	30.0000	0.4848	621.4570
	0.0000e+0			0.0000e+00	0.0000e+000	0.0000	0.0000	0.0000	20.1700	0.0000	0.0000
	0.0000e+0			0.0000e+00	0.0000e+000	0.0000	0.0000	0.0000	39.9400	0.0000	0.0000
	0.0000e+0	0.0000e+0	0.0000e+0	0.0000e+00	0.0000e+000	0.0000	0.0000	0.0000	44.0000	0.0000	0.0000
							ntotal				
							206.2500	1.0000			

CpM como función de T (cal/molK)

a	b	c	d	e	R (cal/molK)	T (K)	P total (atm)	V total (L)
9.5079	0.00e+0	0.00e+0	0	0	1.9886	303.15	2.0000	2563.51

CvM como función de T (cal/molK)

a	b	c	d	e
7.5193	0.00e+0	0.00e+0	0	0

P total (atm) 2.0000
V total (L) 2563.51



M _M (g/mol)	19.3939	ΔH _M (cal)	0	ΔU _M (cal)	0	ΔS _M (cal/K)	227.1643	ΔG _M (cal)	-68864.8456
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q _M (cal)	68864.8456	w _M (cal)	68864.8456
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Dr. Juan Carlos Vázquez Lira 2020

Con apoyo del programa DGAPA-UNAM-PAPIME PE-200419

II Comp. Isot. Rev.

$$\Delta U_{II} = \Delta H_{II} = 0$$

$$V_2 = \frac{1}{2} V_1$$

$$q_{II} = w_{II} = nRT \ln \frac{V_2}{V_1}$$

$$= (206.75 \text{ mol}) \left(\frac{1.9886 \text{ cal}}{\text{mol K}} \right) (303.15 \text{ K}) \ln 0.5$$

$$= -86183.55 \text{ cal}$$

$$\Delta S_{II} = \frac{q_{II}}{T} = \frac{-86183.55 \text{ cal}}{303.15 \text{ K}}$$

$$= -284.29 \text{ cal/K}$$

$$\Delta G_{II} = -T\Delta S$$
$$= 86153.55 \text{ cal}$$

No Favorable no espontáneo

$$\begin{aligned}\Delta G_M + \Delta G_{II} &= \Delta G_{total} \\ &= -68864.8456 \text{ cal} + 86183.5593 \\ &= 17318.71 \text{ cal}\end{aligned}$$