Molar heat capacity & frozen mode

Thursday, November 16, 2017 1:22 PM

- C_{vm} (we put V in subscript to emphsize that we get this heat capacity with fixed volume)

$\Delta E_{th} = Q$ (when : $\begin{cases} \Delta E_{bond} = 0 \\ W = 0 \end{cases}$)

$Q = \#\text{ moles} \times C_{vm} \times \Delta T$

The unit of C_{vm} : [Energy] / {[Tempature] × [moles]}

We also know: $\Delta E_{th} = \frac{1}{2} \#\text{ modes in total} \times k_B \times \Delta T$

total # of modes = # modes per molecule × # molecules

= # modes per molecule × N_A × # moles

Put it back :

$\Delta E_{th} = \frac{1}{2} \#\text{ modes per molecule} \times \#\text{ moles} \times N_A k_B \times \Delta T$ ($N_A k_B \to R$)

$= Q = \#\text{ moles} \times C_{vm} \times \Delta T$

So: $C_{vm} = \frac{1}{2} \#\text{ modes per molecule} \times R$

- Answer for Act. 3.15 4) :

The meaning of slope : heat capacity C

$Q = \Delta E_{th} = C \Delta T$

Therefore : $C = \#\text{ moles} \times C_{vm}$

$C_{vm} = C / \#\text{ moles}$

We know from Act. 3.13 that we have 50 atomes for these slopes.

$50 = \#\text{ moles} \times N_A$

$\# \text{ moles} = 50 / N_A$

For $C_1 = 2.1 \times 10^{-21}\ J \cdot K^{-1}$

$C_{vm1} = 2.1 \times 10^{-21} / 50 \times N_A\ J \cdot K^{-1} \cdot mol^{-1}$

$= \frac{2.1 \times 10^{-21} \times 6.02 \times 10^{23}}{50}\ J \cdot K^{-1} \cdot mol^{-1}$

$\doteq 25.3\ J \cdot K^{-1} \cdot mol^{-1} \doteq 3R$

$C_2 = 1 \times 10^{-21}\ J \cdot K^{-1} \doteq$

$C_{vm2} \doteq \frac{1 \times 10^{-21} \times 6.02 \times 10^{23}}{50}\ J \cdot K \cdot mol^{-1}$

$\doteq 12\ J \cdot K \cdot mol^{-1} \doteq 1.4 R$

$(R = N_A k_B = 8.31)$

Due to the defination of C_{vm}:

1 : # modes per molecule $= 3 \times 2 = 6$

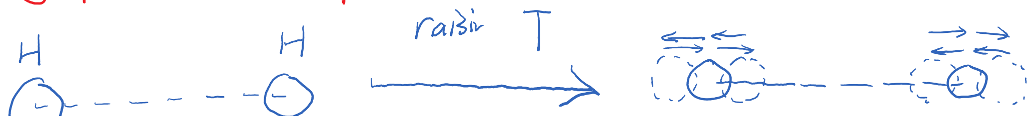
2 : # modes per molecule $= 1.4 \times 2 \approx 3$

It is consistent with our predictions.

- The meaning of frozen modes

When temperature is low (maybe room temperature), some modes are not activiated due to insufficient thermal energy.

If the temperature is raising, the system has enough energy to activiate new modes (to get over the energy gap), then frozen modes will be defroze.



T is low
No vibration

T is high
Energy of vibration = PE + KE
each of them owns 1 mode
total modes for vibration are 2