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Optimization of Molar Thermal Capacity for Graphite and N_2

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Abstract: When teaching *Physical Chemistry* by Atkins et al., the author realized that the empirical formula for the molar thermal capacity at constant pressure $C_{p,m} = a + bT + \frac{C}{T^2}$ has optimum $C_{p,m}$ for an obtained temperature. The optimum is obtained by taking the derivative $\frac{dC_{p,m}}{dT} = 0$.

Key words: The mole capacity at constant pressure and mole, optimization of the mole capacity and temperature.

1. Introduction

Recently during past two to three decades optimization work has been done for various equations including the figure of merits in chromatography [1].

In present work the empirical equation for thermal capacity [2], has been used to obtain the T_{opt}, $C_{p,m_{opt}}$ where $\frac{dC_{p,m}}{dT} = 0$ the result is obtained for the optimum temperature and optimum thermal capacity.

2. Theory

$$C_{p,m} = a + bT + \frac{C}{T^2}$$

In *Physical Chemistry* by Atkins et al. [2]:

$$\frac{dC_{p,m}}{dT} = b - 2CT^{-3} = 0$$

$$b = 2CT^{-3}$$

$$T = \sqrt[\frac{-1}{3}]{\frac{b}{2C}}$$

$$T_{opt} = \sqrt[\frac{-1}{3}]{\frac{4.77 \times 10^{-3}}{2 \times 8.54 \times 10^5}}$$

For the graphite, *b*, *c* are obtained from the table as given in Ref. [2].

$$T_{opt} = \sqrt[\frac{1}{3}]{\frac{17.08}{4.77} \times 10^8 \times 10^1 \times 10^1} =$$

$$\sqrt[\frac{1}{3}]{\frac{17.08}{4.77} \times 10^3} = 717$$

$$C_{p,m_{opt}}(712) = 16.86 + 4.77 \times 10^{-3}$$

$$\times 717 + \frac{8.54 \times 10^5}{(712)^2}$$

$$= 16.86 + 3.4 + 1.68 = 21.94$$

By similar procedure, $C_{p,m_{opt}}$ and T_{opt} are obtained for CO_2 and N_2. The curves T, $C_{p,m}$ obtained for CO_2 and N_2 and graphite (Figs. 1-3). The $C_{p,m_{opt}}$ and T_{opt} are graphed in Fig. 4.

3. Conclusion

To our knowledge the formula for the thermal capacity has not been optimized. In present work this is done.

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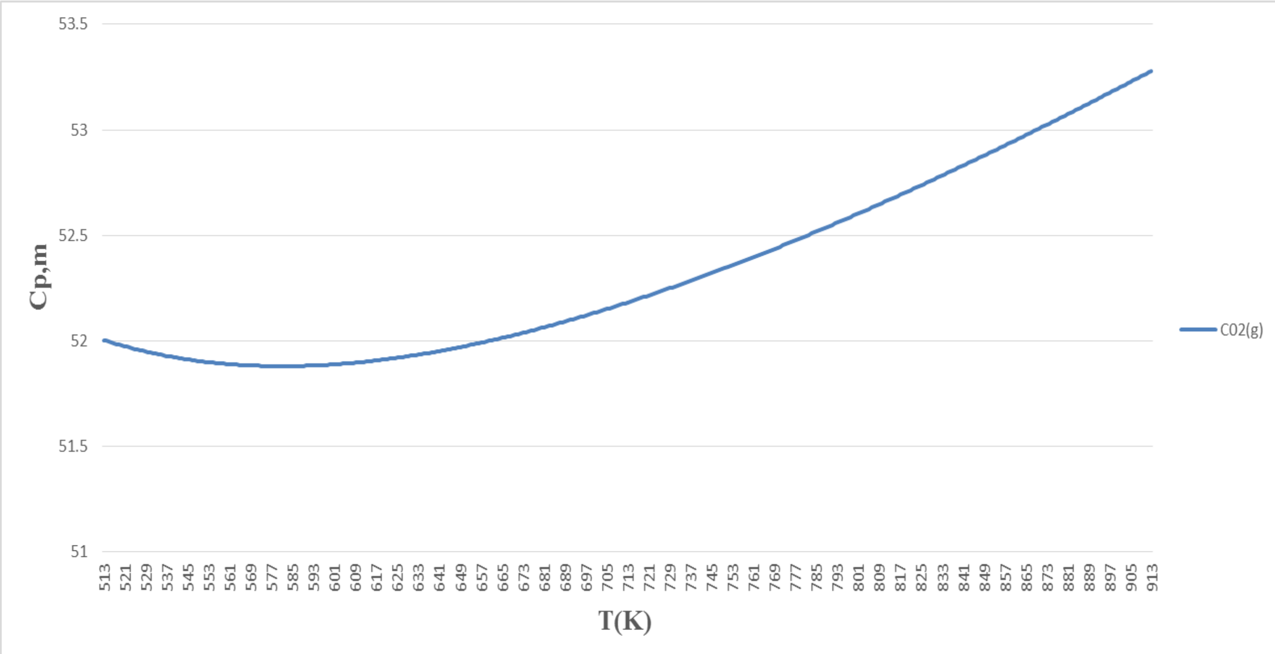

Fig. 1 Thermal capacity versus temperature for carbon dioxide.

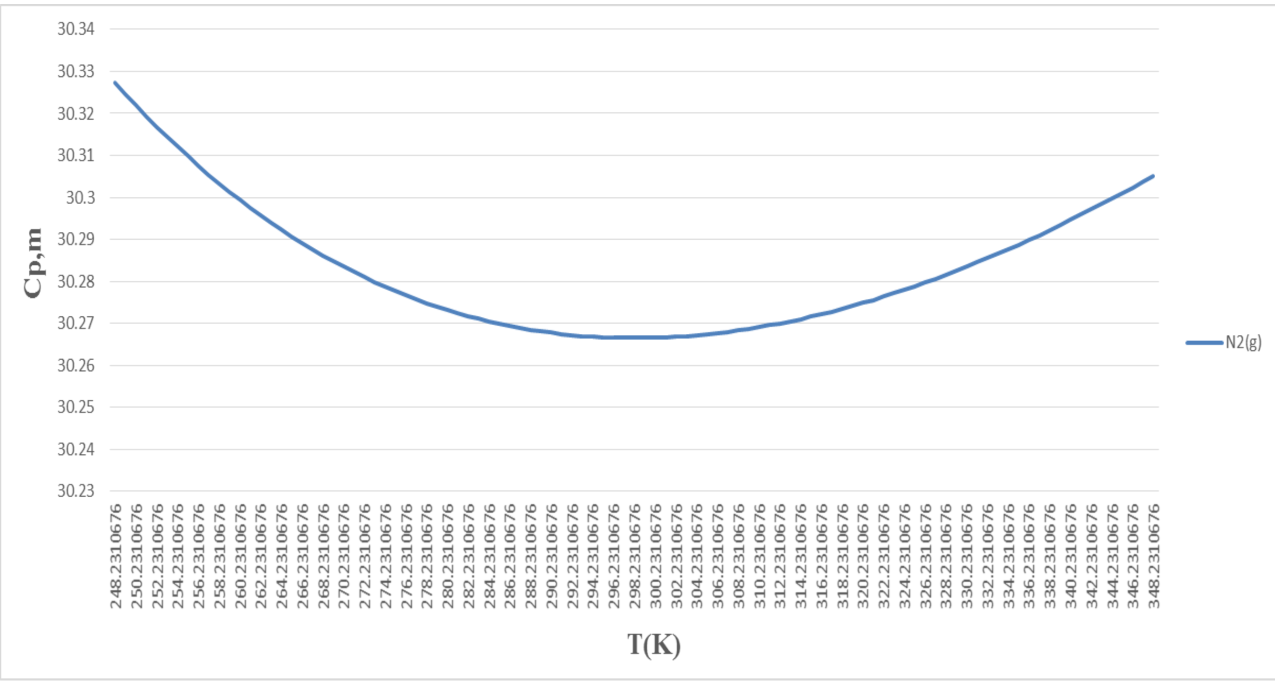

Fig. 2 Thermal capacity versus temperature for nitrogen.

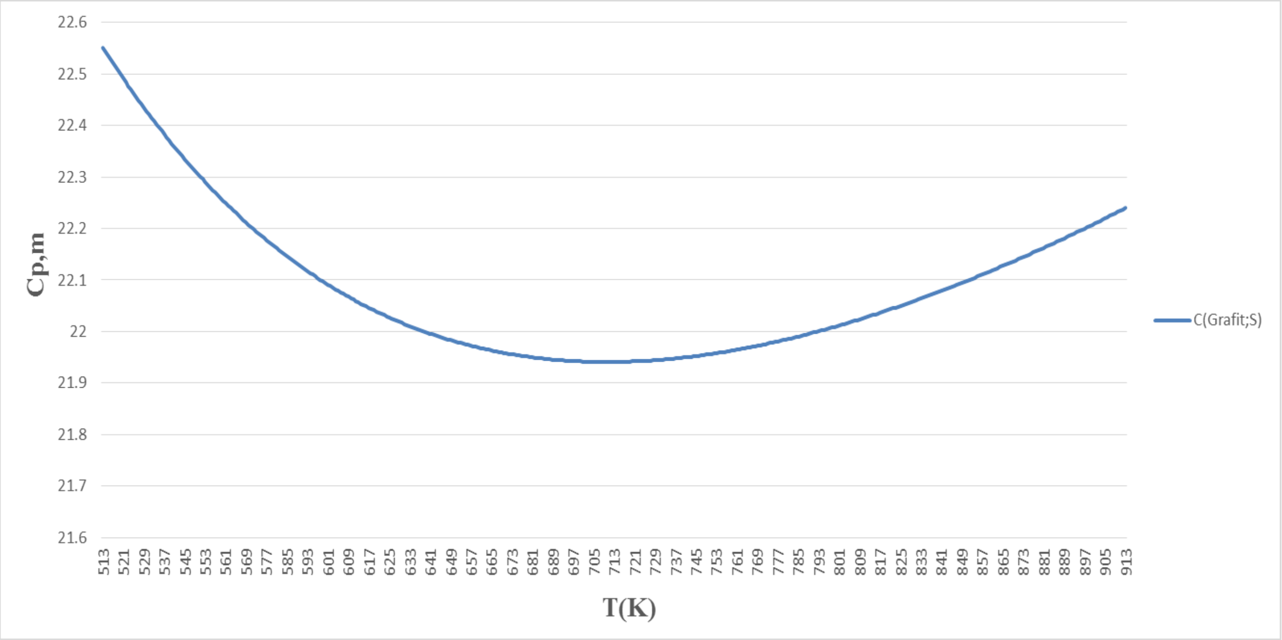

Fig. 3 Thermal capacity versus temperature for graphite.

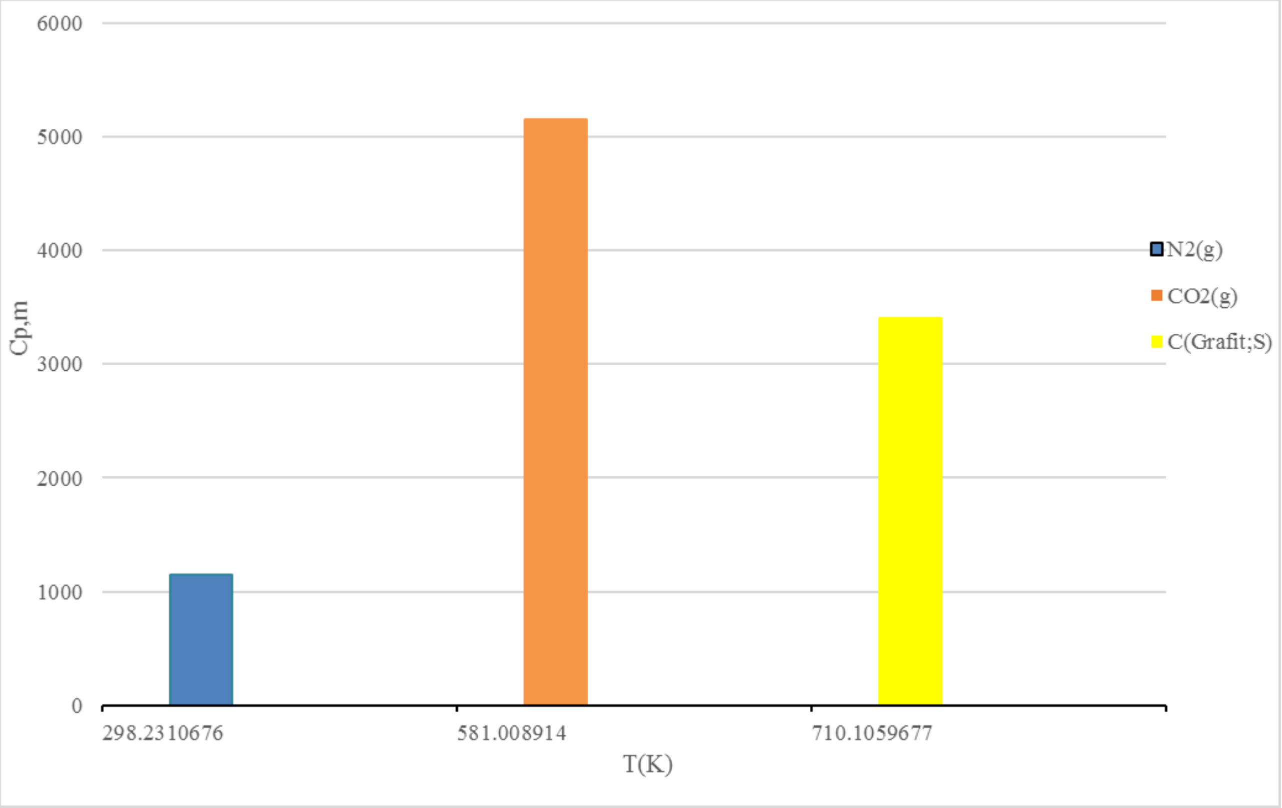

Fig. 4 Thermal capacity versus temperature optimization for three maters (nitrogen, carbon dioxide and graphite).

References

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