cheg231 homework 4 question 2

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date: 9/23/2024

Calculate the heat energy required to heat one mole of nitrogen from 298 to 600 K at 1 bar

Energy balance gave us

$$Q = N(\underbar{H}_f - \underbar{H}_i)$$

another way to represent $\underbar{H}_f - \underbar{H}_i$ is

$$= \int_{T_i}^{T_f} \frac{d\underbar{H}}{dT}$$

We know that

$$C_p = \frac{d\underbar{H}}{dT}$$

So the heat required to heat a mole of nitrogen from 298 to 600 is

$$Q = N \int_{298}^{600} C_p(T)\, dT$$

and the $C_p(T)$ comes from the stanley sandler appendix data. also N = 1

In [1]:
```
import numpy as np
from scipy.integrate import simpson

def nitrogen_cp(T):
    return 28.883 - (0.157e-2 * T) + (0.808e-5 * T**2) - (2.871e-9 * T**3)

temperatures = np.linspace(298, 600, 300)

heat_integrated = simpson(nitrogen_cp(temperatures), temperatures)
print(f'calculated heat (integrated): {heat_integrated:.2f} J')
```

```
calculated heat (integrated): 8932.90 J
```

this can also quick be compared to the heat if C_p is assumed constant and not a function of temperature

$$NC_p \int_{298}^{600} dT = NC_p(T_f - T_i)$$

or if nitrogen has the

In [2]:
```
cp_roomtemp = nitrogen_cp(298)
heat = 1 * cp_roomtemp * (600-298)

print(f'calculated heat (const. Cp): {heat:.2f} J')
print(f'error: {abs(heat - heat_integrated) / heat * 100:.2f}%')
```

```
calculated heat (const. Cp): 8775.12 J
error: 1.80%
```

Next calculate the heat energy required to heat one mole of ethane from 298 to 600 K at 1 bar

similar buildup as the last part and also calculating if the C_p is assumed constant

In [3]:
```
def ethane_cp(T):
    return 6.895 + (17.255e-2 * T) - (6.402e-5 * T**2) + (7.280e-9 * T**3)

temperatures = np.linspace(298, 600, 100)

heat_integrated = simpson(ethane_cp(temperatures), temperatures)
print(f'calculated heat (integrated): {heat_integrated:.2f} J')

cp_roomtemp = ethane_cp(298)
print(f'cp room temp: {cp_roomtemp:.2f}')
```

```python
heat1 = 1 * cp_roomtemp * (600-298)
print(f'calculated heat (const cp = cp(298K)): {heat1:.2f} J')

# ethane has 3 + 3 = 6 degrees of freedom, so ideal gas C_v is (6/2) * R
# so the ideal gas C_p will be (6/2) * R + R = 4*R
heat2 = (4 * 8.31415) * (600-298)
print(f'calculated heat (ideal gas): {heat2:.2f} J')

print('\n-----------------------------\n')

print(f'error (const cp = cp @ room temp): {abs(heat1 - heat_integrated) / heat_integrated * 100:.2f}%')
print(f'error (ideal gas): {abs(heat2 - heat_integrated) / heat_integrated * 100:.2f}%')
```

```
calculated heat (integrated): 21656.54 J
cp room temp: 52.82
calculated heat (const cp = cp(298K)): 15952.34 J
calculated heat (ideal gas): 10043.49 J

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error (const cp = cp @ room temp): 26.34%
error (ideal gas): 53.62%
```

Should you assume a constant value of the heat capacity for ethane?

No, the C_p cannot be assumed constant since the difference in calculated heat is ~26% if assumed constant and over 50% error if assumed to be the predicted ideal gas C_p! this is because the temperature dependence of ethane is much greater than for nitrogen on this temperature range. Looking back at the graph made for question 1 the nitrogen looks super flat, but the ethane increased quite a lot--almost 3x (started around 50 and ended close to 150)