CHEG231 HW5 Q1

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The molar entropy can be calculated using this equation

$$\underbar S = Cp^* \ln(T)$$

Where Cp^* is the molar heat capacity, and T is the temperature.

In [12]:

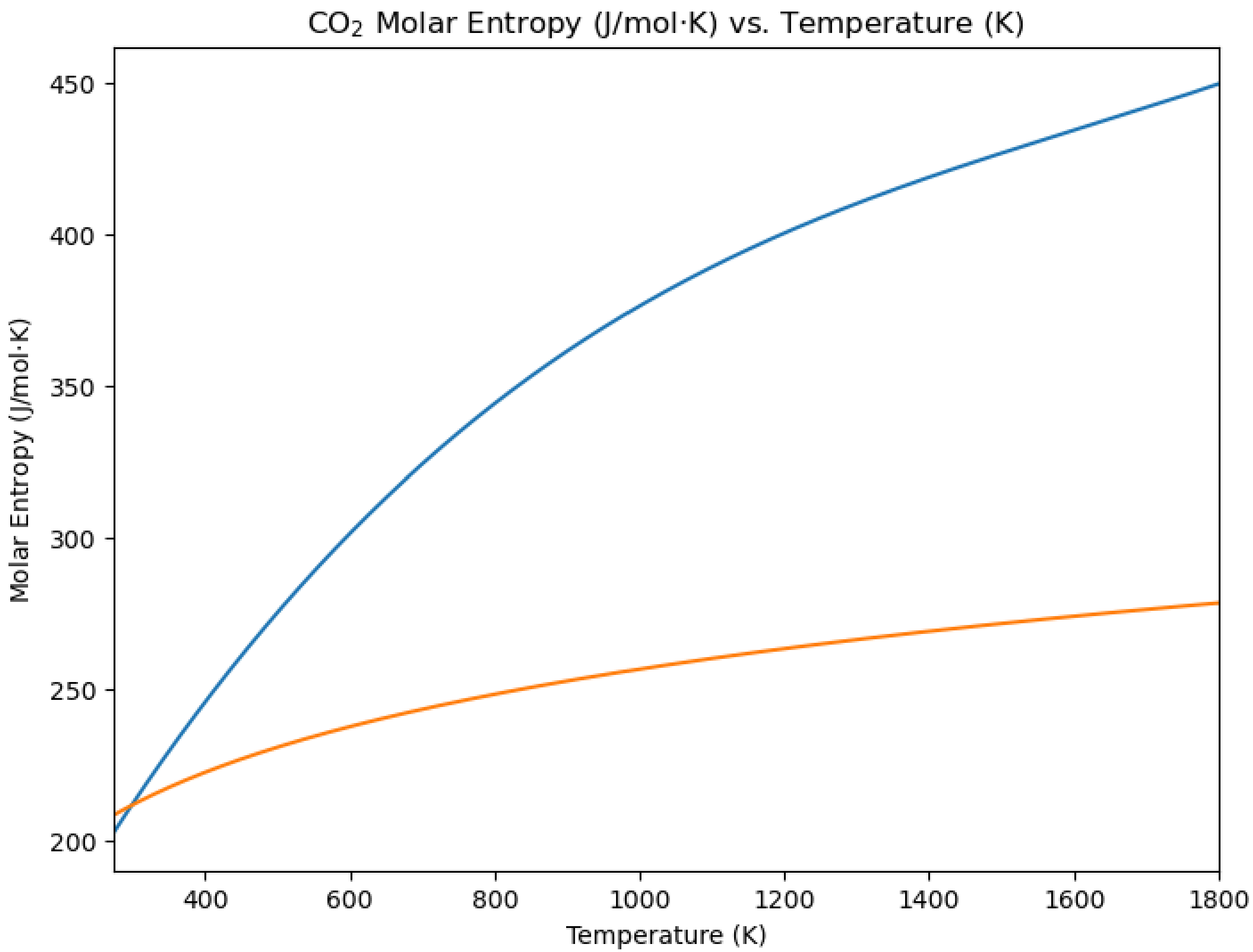
```
import numpy as np
import matplotlib.pyplot as plt

def co2_cp(T):
    return 22.243 + (5.977e-2 * T) - (3.499e-5 * T**2) + (7.464e-9 * T**3)

x = np.arange(273, 1800)
y = co2_cp(x) * np.log(x)
y_ideal = 37.15 * np.log(x)

fig,ax = plt.subplots(figsize=(8,6), dpi=100)

ax.plot(x,y, label='Using Appendix II')
ax.plot(x,y_ideal, label='Using predicted Cp')
ax.set_xlabel('Temperature (K)')
ax.set_ylabel('Molar Entropy (J/mol$\cdot$K)')
ax.set_xlim(273,1800)
ax.set_title('CO$_2$ Molar Entropy (J/mol$\cdot$K) vs. Temperature (K)');
```



Clearly the constant value of Cp predicts fairly different molar entropy values, especially as the temperature increases. This is because as the temperature gets larger the higher order terms in the Cp polynomial start to influence the Cp more and cause this big of a difference between the first-principles predicted and the experimental