# Thermochemistry

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# Chapter 1

# Theory

## 1.1 Electronic Partition Function

a

$$U_e = 0 \tag{1.1}$$

a

$$S_e = Nk_B ln(2S + 1) \tag{1.2}$$

a

## 1.2 Translational Partition Function

The translational partition function is calculated as

$$q_t = \left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} V \tag{1.3}$$

Since the translational partition function depends on temperature and volume, the ideal gas equation is used to replace the volume for pressue.

$$PV = NRT \tag{1.4}$$

$$PV = \left(\frac{n}{N_A}\right) N_A k_B T \tag{1.5}$$

$$V = \frac{k_B T}{P} \tag{1.6}$$

$$q_t = \left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} \frac{k_B T}{P} \tag{1.7}$$

## 1.3 Molecular Rotational Partition Function

Linear Molecule

a

Non-Liner Molecule

a

## 1.4 Molecular Vibrational Partition Function

ada

# Chapter 2

# aa

H 1.00783 a.u.
O 15.99491 a.u.
N 14.00307 a.u.
C 12.0000 a.u.
Cu 62.92960 a.u.
Ni 57.93535 a.u.
Co 58.93320 a.u.
Pd 105.90320 a.u.
Rh 102.9048 a.u.
Ti 47.94795 a.u.