

# Useful Conversion Factors

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## 1 Energy Conversion Factors

$$\begin{aligned} 1 \text{ kcal/mol} &= 0.04336 \text{ eV} \\ &0.00159 \text{ h} \\ &349.75 \text{ cm}^{-1} \\ &6.948 \times 10^{-14} \text{ erg} \\ &4.184 \text{ kJ/mol} \end{aligned}$$

$$\begin{aligned} 1 \text{ eV} &= 23.06 \text{ kcal/mol} \\ &0.03675 \text{ h} \\ &8065.6 \text{ cm}^{-1} \\ &1.602 \times 10^{-12} \text{ erg} \end{aligned}$$

$$\begin{aligned} 1 \text{ h} &= 627.51 \text{ kcal/mol} \\ &27.212 \text{ eV} \\ &219,474.6 \text{ cm}^{-1} \\ &4.36 \times 10^{-11} \text{ erg} \\ &2 \text{ Ry} \end{aligned}$$

$$\begin{aligned} 1 \text{ erg} &= 1.439 \times 10^{13} \text{ kcal/mol} \\ &6.2415 \times 10^{11} \text{ eV} \\ &2.2937 \times 10^{10} \text{ h} \\ &5.034 \times 10^{15} \text{ cm}^{-1} \end{aligned}$$

## 2 Colors of Light

Table 1: Visible light

Color	nm	eV	cm <sup>-1</sup>
Red	700	1.77	14,300
Orange	620	2.00	16,100
Yellow	580	2.14	17,300
Green	530	2.34	18,900
Blue	470	2.64	21,300
Violet	420	2.95	23,800

Table 2: All light

Color	nm	eV	cm <sup>-1</sup>
Radio	$3 \times 10^{12} - 3 \times 10^8$	$4 \times 10^{-10} - 4 \times 10^{-6}$	$3 \times 10^{-6} - 3 \times 10^{-2}$
Microwaves	$3 \times 10^8 - 3 \times 10^6$	$4 \times 10^{-6} - 4 \times 10^{-4}$	$3 \times 10^{-2} - 3$
Far IR	$3 \times 10^6 - 3 \times 10^4$	$4 \times 10^{-4} - 4 \times 10^{-2}$	3 - 300
Near IR	$3 \times 10^4 - 700$	$4 \times 10^{-2} - 2$	300 - 15,000
Visible	700 - 420	2 - 3	15,000 - 24,000
Near UV	420 - 300	3 - 4	24,000 - 30,000
Vac UV	300 - 3	4 - 400	30,000 - $3 \times 10^6$
X-rays	3 - 0.003	400 - $4 \times 10^5$	$3 \times 10^6 - 3 \times 10^9$

## 3 Free Energies

$$\Delta(G) = RT \ln(K)$$

$$\Delta(G_1) - \Delta(G_2) = RT \ln \left( \frac{K_1}{K_2} \right)$$

$$\Delta\Delta(G) = 1 \text{ kcal/mol} \iff \frac{K_1}{K_2} = 5.4$$

$$\frac{K_1}{K_2} = 10^1 \iff \Delta\Delta G = 1.36$$

$$\frac{K_1}{K_2} = 10^2 \iff \Delta\Delta G = 2.76$$

$$\frac{K_1}{K_2} = 10^4 \iff \Delta\Delta G = 5.53$$

$$\frac{K_1}{K_2} = 10^6 \iff \Delta\Delta G = 8.29$$

$$\Delta G = 1.36 (pK_{a1} - pK_{a2})$$

## 4 Atomic Units

Length	Bohr radius, $a_0$	0.52918 Å
Force Constant	1 au	$1.5569 \times 10^6$ dyn/cm
Mass	au, $m_e$	$9.1095 \times 10^{-31}$ kg
		$5.5 \times 10^{-4}$ amu
	amu, $m(^{12}\text{C})/12$	$1.66 \times 10^{-27}$ kg
		1822 au
Time	au	$2.4189 \times 10^{-17}$ s
Dipole Moment	au	2.54 D
		$8.478 \times 10^{-30}$ C-m

## 5 Miscellaneous

### 5.1 Force Constants

$$1 \text{ dyn/cm} = 1.44 \times 10^{-3} \frac{\text{kcal/mol}}{\text{Å}^2}$$

$$1 \text{ Mdyn/cm} = 1440 \frac{\text{kcal/mol}}{\text{Å}^2}$$

## 5.2 Thermal

$$k_B T(298 \text{ K}) = 9.4366 \times 10^{-4} \text{ h}$$

$$RT(298 \text{ K}) = 2.4789 \text{ kJ/mol} = 0.5925 \text{ kcal/mol}$$

$$e^2 = 14.3998 \text{ eV-Å} = 332.059 \text{ (kcal/mol)-Å}$$